



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:23 AM GMT

PDB ID : 3OFL
Title : Crystal structure of Humanpapillomavirus18 (HPV18) capsid L1 pentamers bound to heparin oligosaccharides
Authors : Chen, X.S.; Dasgupta, J.
Deposited on : 2010-08-15
Resolution : 3.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

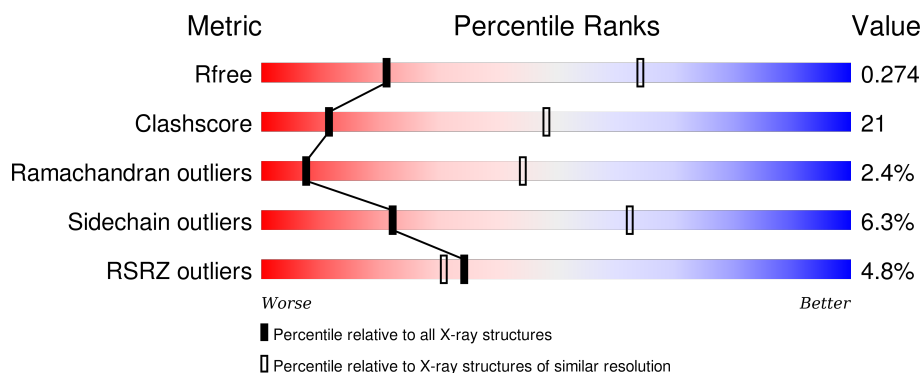
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	427	<div> <div>4%</div> <div>57%</div> <div>38%</div> <div>..</div> </div>
1	B	427	<div> <div>6%</div> <div>61%</div> <div>35%</div> <div>..</div> </div>
1	C	427	<div> <div>4%</div> <div>60%</div> <div>35%</div> <div>..</div> </div>
1	D	427	<div> <div>3%</div> <div>62%</div> <div>35%</div> <div>..</div> </div>
1	E	427	<div> <div>4%</div> <div>57%</div> <div>38%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	427	
1	G	427	
1	H	427	
1	I	427	
1	J	427	
1	K	427	
1	L	427	
1	M	427	
1	N	427	
1	O	427	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	JHM	E	501	-	-	X	-
3	IDS	E	502	-	-	X	-
3	JHM	E	505	-	-	X	-
4	IDS	D	504	-	-	X	-
4	JHM	D	509	-	-	-	X
4	JHM	N	601	-	-	-	X
5	JHM	A	517	-	-	-	X
5	IDS	A	518	X	-	-	X
5	JHM	A	519	-	-	-	X
5	JHM	B	527	-	-	-	X
5	IDS	B	528	-	-	-	X
5	JHM	B	529	-	-	X	X
5	IDS	B	530	-	-	X	-
5	JHM	C	571	-	-	-	X
5	IDS	C	572	X	-	-	-
5	JHM	E	511	-	-	-	X
5	JHM	F	591	-	-	-	X
5	IDS	F	592	-	-	-	X
5	IDS	F	594	-	-	-	X
5	JHM	N	607	-	-	X	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	IDS	N	608	X	-	X	X
5	JHM	N	609	-	-	X	X
6	IDS	B	534	X	-	-	-
6	IDS	B	538	X	-	-	-
6	IDS	F	584	-	-	X	X
6	IDS	F	590	-	-	-	X
7	JHM	E	547	-	-	-	X
7	IDS	E	548	X	-	-	X
7	IDS	E	550	X	-	-	-
7	JHM	F	567	-	-	X	X
7	IDS	F	570	-	-	X	X
7	JHM	H	575	-	-	-	X
7	JHM	H	577	-	-	-	X
7	IDS	H	578	-	-	X	X
7	IDS	H	580	X	-	-	-
7	IDS	J	554	X	-	X	X
7	JHM	J	555	-	-	X	X
7	IDS	J	556	X	-	-	-
7	JHM	J	561	-	-	X	-
7	IDS	J	564	X	-	X	-
7	IDS	J	596	-	-	-	X
7	JHM	J	597	-	-	-	X
7	IDS	J	598	X	-	-	X
7	IDS	J	600	X	-	-	-
7	JHM	L	613	-	-	-	X
7	IDS	L	614	X	-	-	-
7	JHM	L	615	-	-	-	X
7	IDS	L	616	X	-	-	X
7	IDS	L	618	X	-	-	-
7	JHM	L	619	-	-	X	-
7	IDS	L	620	X	-	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 51547 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	422	Total	C	N	O	S	0	0	0
			3315	2092	561	642	20			
1	B	422	Total	C	N	O	S	0	0	0
			3315	2092	561	642	20			
1	C	422	Total	C	N	O	S	0	0	0
			3315	2092	561	642	20			
1	D	422	Total	C	N	O	S	0	0	0
			3315	2092	561	642	20			
1	E	422	Total	C	N	O	S	0	0	0
			3315	2092	561	642	20			
1	F	422	Total	C	N	O	S	0	0	0
			3315	2092	561	642	20			
1	G	422	Total	C	N	O	S	0	0	0
			3315	2092	561	642	20			
1	H	422	Total	C	N	O	S	0	0	0
			3315	2092	561	642	20			
1	I	422	Total	C	N	O	S	0	0	0
			3315	2092	561	642	20			
1	J	422	Total	C	N	O	S	0	0	0
			3315	2092	561	642	20			
1	K	422	Total	C	N	O	S	0	0	0
			3315	2092	561	642	20			
1	L	422	Total	C	N	O	S	0	0	0
			3315	2092	561	642	20			
1	M	422	Total	C	N	O	S	0	0	0
			3315	2092	561	642	20			
1	N	422	Total	C	N	O	S	0	0	0
			3315	2092	561	642	20			
1	O	421	Total	C	N	O	S	0	0	0
			3307	2088	559	640	20			

There are 135 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	ALA	-	EXPRESSION TAG	UNP Q80B70
A	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
A	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
A	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70
A	433	GLY	-	LINKER	UNP Q80B70
A	434	GLY	-	LINKER	UNP Q80B70
A	435	SER	-	LINKER	UNP Q80B70
A	436	GLY	-	LINKER	UNP Q80B70
A	437	GLY	-	LINKER	UNP Q80B70
B	20	ALA	-	EXPRESSION TAG	UNP Q80B70
B	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
B	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
B	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70
B	433	GLY	-	LINKER	UNP Q80B70
B	434	GLY	-	LINKER	UNP Q80B70
B	435	SER	-	LINKER	UNP Q80B70
B	436	GLY	-	LINKER	UNP Q80B70
B	437	GLY	-	LINKER	UNP Q80B70
C	20	ALA	-	EXPRESSION TAG	UNP Q80B70
C	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
C	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
C	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70
C	433	GLY	-	LINKER	UNP Q80B70
C	434	GLY	-	LINKER	UNP Q80B70
C	435	SER	-	LINKER	UNP Q80B70
C	436	GLY	-	LINKER	UNP Q80B70
C	437	GLY	-	LINKER	UNP Q80B70
D	20	ALA	-	EXPRESSION TAG	UNP Q80B70
D	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
D	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
D	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70
D	433	GLY	-	LINKER	UNP Q80B70
D	434	GLY	-	LINKER	UNP Q80B70
D	435	SER	-	LINKER	UNP Q80B70
D	436	GLY	-	LINKER	UNP Q80B70
D	437	GLY	-	LINKER	UNP Q80B70
E	20	ALA	-	EXPRESSION TAG	UNP Q80B70
E	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
E	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
E	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70
E	433	GLY	-	LINKER	UNP Q80B70
E	434	GLY	-	LINKER	UNP Q80B70
E	435	SER	-	LINKER	UNP Q80B70

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Chain	Residue	Modelled	Actual	Comment	Reference
E	436	GLY	-	LINKER	UNP Q80B70
E	437	GLY	-	LINKER	UNP Q80B70
F	20	ALA	-	EXPRESSION TAG	UNP Q80B70
F	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
F	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
F	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70
F	433	GLY	-	LINKER	UNP Q80B70
F	434	GLY	-	LINKER	UNP Q80B70
F	435	SER	-	LINKER	UNP Q80B70
F	436	GLY	-	LINKER	UNP Q80B70
F	437	GLY	-	LINKER	UNP Q80B70
G	20	ALA	-	EXPRESSION TAG	UNP Q80B70
G	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
G	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
G	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70
G	433	GLY	-	LINKER	UNP Q80B70
G	434	GLY	-	LINKER	UNP Q80B70
G	435	SER	-	LINKER	UNP Q80B70
G	436	GLY	-	LINKER	UNP Q80B70
G	437	GLY	-	LINKER	UNP Q80B70
H	20	ALA	-	EXPRESSION TAG	UNP Q80B70
H	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
H	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
H	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70
H	433	GLY	-	LINKER	UNP Q80B70
H	434	GLY	-	LINKER	UNP Q80B70
H	435	SER	-	LINKER	UNP Q80B70
H	436	GLY	-	LINKER	UNP Q80B70
H	437	GLY	-	LINKER	UNP Q80B70
I	20	ALA	-	EXPRESSION TAG	UNP Q80B70
I	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
I	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
I	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70
I	433	GLY	-	LINKER	UNP Q80B70
I	434	GLY	-	LINKER	UNP Q80B70
I	435	SER	-	LINKER	UNP Q80B70
I	436	GLY	-	LINKER	UNP Q80B70
I	437	GLY	-	LINKER	UNP Q80B70
J	20	ALA	-	EXPRESSION TAG	UNP Q80B70
J	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
J	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
J	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70

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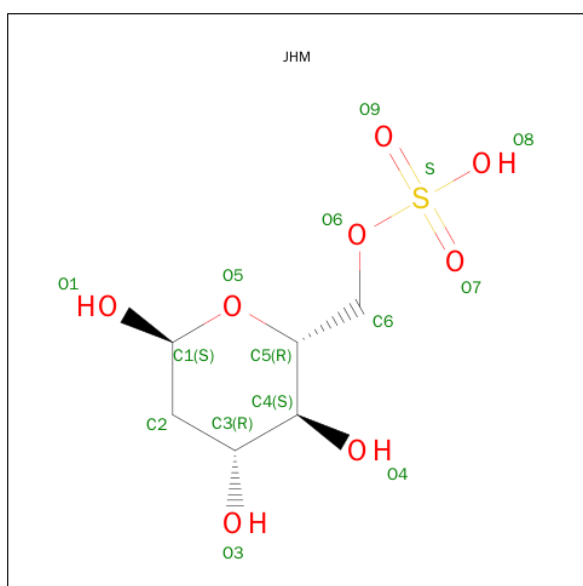
Chain	Residue	Modelled	Actual	Comment	Reference
J	433	GLY	-	LINKER	UNP Q80B70
J	434	GLY	-	LINKER	UNP Q80B70
J	435	SER	-	LINKER	UNP Q80B70
J	436	GLY	-	LINKER	UNP Q80B70
J	437	GLY	-	LINKER	UNP Q80B70
K	20	ALA	-	EXPRESSION TAG	UNP Q80B70
K	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
K	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
K	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70
K	433	GLY	-	LINKER	UNP Q80B70
K	434	GLY	-	LINKER	UNP Q80B70
K	435	SER	-	LINKER	UNP Q80B70
K	436	GLY	-	LINKER	UNP Q80B70
K	437	GLY	-	LINKER	UNP Q80B70
L	20	ALA	-	EXPRESSION TAG	UNP Q80B70
L	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
L	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
L	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70
L	433	GLY	-	LINKER	UNP Q80B70
L	434	GLY	-	LINKER	UNP Q80B70
L	435	SER	-	LINKER	UNP Q80B70
L	436	GLY	-	LINKER	UNP Q80B70
L	437	GLY	-	LINKER	UNP Q80B70
M	20	ALA	-	EXPRESSION TAG	UNP Q80B70
M	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
M	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
M	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70
M	433	GLY	-	LINKER	UNP Q80B70
M	434	GLY	-	LINKER	UNP Q80B70
M	435	SER	-	LINKER	UNP Q80B70
M	436	GLY	-	LINKER	UNP Q80B70
M	437	GLY	-	EXPRESSION TAG	UNP Q80B70
N	20	ALA	-	LINKER	UNP Q80B70
N	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
N	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
N	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70
N	433	GLY	-	LINKER	UNP Q80B70
N	434	GLY	-	LINKER	UNP Q80B70
N	435	SER	-	LINKER	UNP Q80B70
N	436	GLY	-	LINKER	UNP Q80B70
N	437	GLY	-	LINKER	UNP Q80B70
O	20	ALA	-	EXPRESSION TAG	UNP Q80B70

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Chain	Residue	Modelled	Actual	Comment	Reference
O	47	ASP	ASN	ENGINEERED MUTATION	UNP Q80B70
O	175	SER	CYS	ENGINEERED MUTATION	UNP Q80B70
O	393	GLN	HIS	ENGINEERED MUTATION	UNP Q80B70
O	433	GLY	-	LINKER	UNP Q80B70
O	434	GLY	-	LINKER	UNP Q80B70
O	435	SER	-	LINKER	UNP Q80B70
O	436	GLY	-	LINKER	UNP Q80B70
O	437	GLY	-	EXPRESSION TAG	UNP Q80B70

- Molecule 2 is 2-DEOXY-6-O-SULFO-ALPHA-D-ARABINO-HEXOPYRANOSE (three-letter code: JHM) (formula: C₆H₁₂O₈S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	E	1	Total	C	O	S	0	0
			15	6	8	1		

- Molecule 3 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	E	3	Total	C	O	S	0	0
			45	18	24	3		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	2	Total	C	O	S	0	0
			30	12	16	2		
4	D	2	Total	C	O	S	0	0
			30	12	16	2		
4	D	2	Total	C	O	S	0	0
			30	12	16	2		
4	E	2	Total	C	O	S	0	0
			30	12	16	2		
4	D	2	Total	C	O	S	0	0
			30	12	16	2		
4	C	2	Total	C	O	S	0	0
			30	12	16	2		
4	N	2	Total	C	O	S	0	0
			30	12	16	2		

- Molecule 5 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	E	4	Total	C	O	S	0	0
			60	24	32	4		
5	A	4	Total	C	O	S	0	0
			60	24	32	4		
5	D	4	Total	C	O	S	0	0
			60	24	32	4		
5	B	4	Total	C	O	S	0	0
			60	24	32	4		
5	A	4	Total	C	O	S	0	0
			60	24	32	4		
5	C	4	Total	C	O	S	0	0
			60	24	32	4		
5	F	4	Total	C	O	S	0	0
			60	24	32	4		
5	O	4	Total	C	O	S	0	0
			60	24	32	4		
5	N	4	Total	C	O	S	0	0
			60	24	32	4		

- Molecule 6 is a polymer of unknown type called SUGAR (10-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	10	Total	C	O	S	0	0
			150	60	80	10		
6	F	10	Total	C	O	S	0	0
			150	60	80	10		

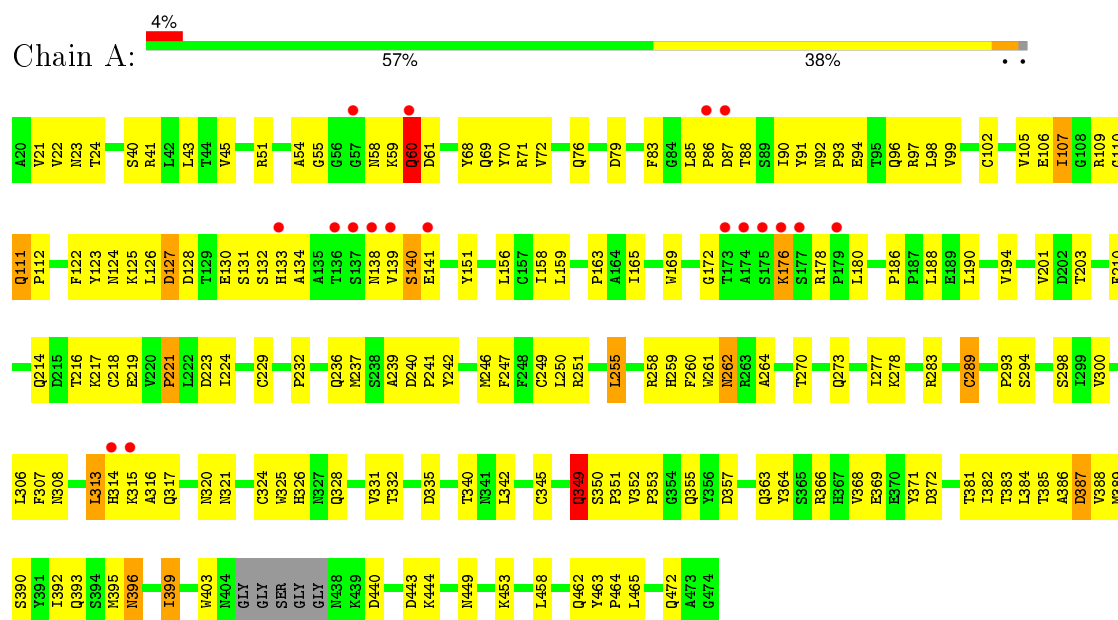
- Molecule 7 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	E	6	Total	C	O	S	0	0
			90	36	48	6		
7	J	6	Total	C	O	S	0	0
			90	36	48	6		
7	J	6	Total	C	O	S	0	0
			90	36	48	6		
7	F	6	Total	C	O	S	0	0
			90	36	48	6		
7	H	6	Total	C	O	S	0	0
			90	36	48	6		
7	J	6	Total	C	O	S	0	0
			90	36	48	6		
7	L	6	Total	C	O	S	0	0
			90	36	48	6		
7	L	6	Total	C	O	S	0	0
			90	36	48	6		

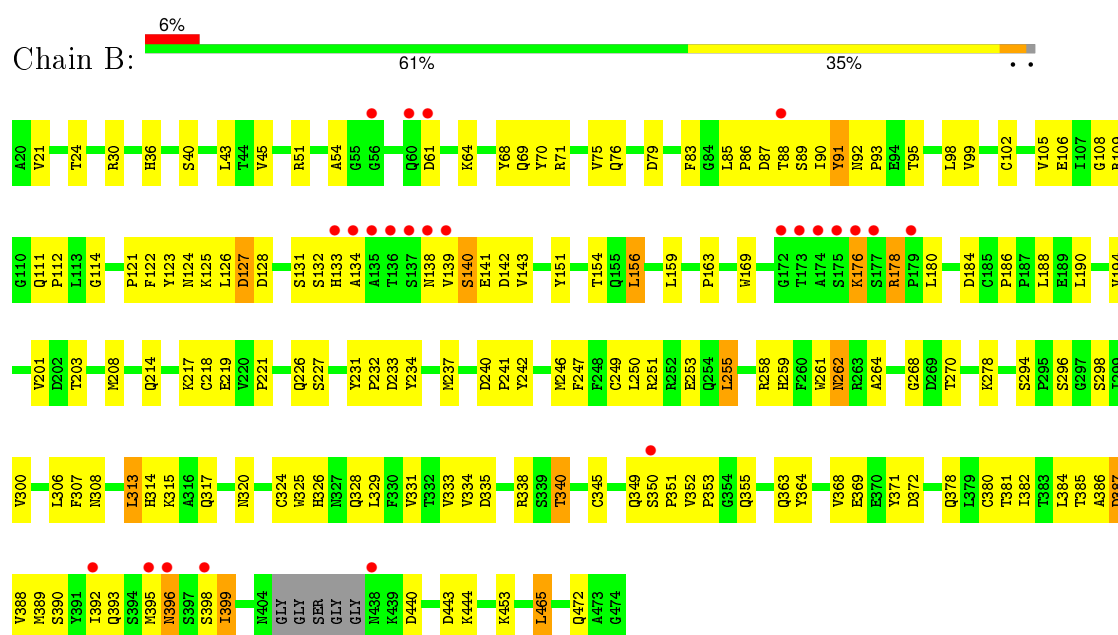
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: L1

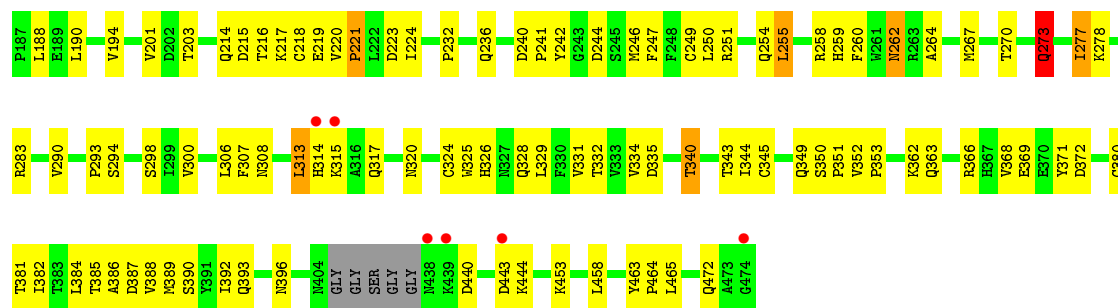


• Molecule 1: L1

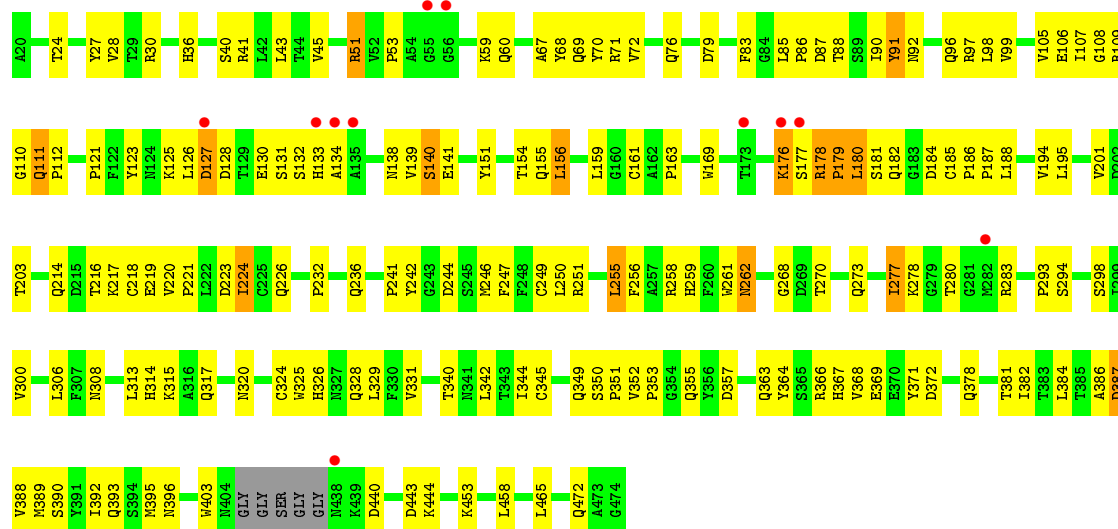


Chain E:

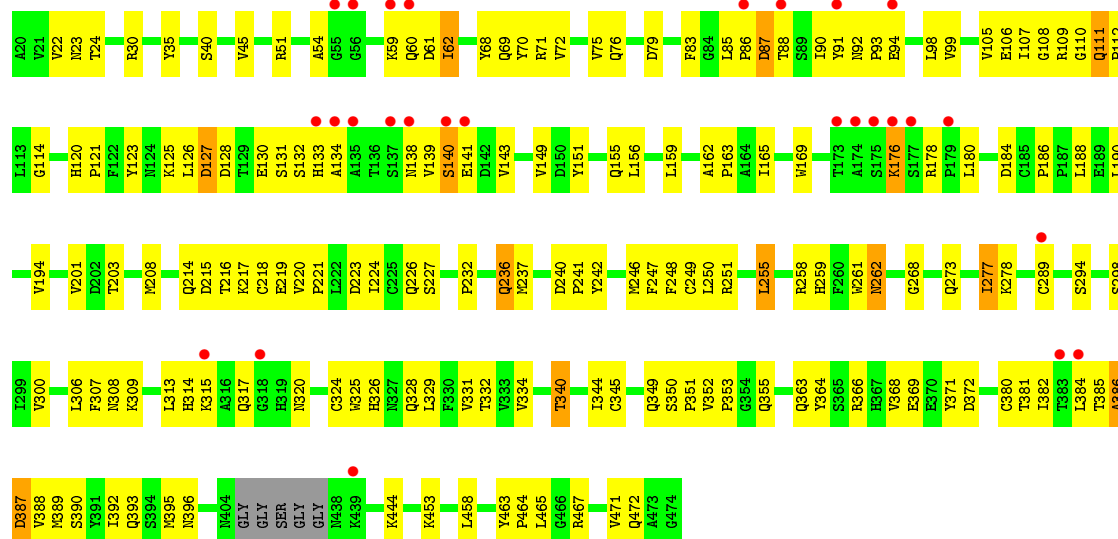
Sample	Category
A20	Green
V21	Green
V22	Green
N23	Green
T24	Green
R30	Green
H36	Green
S40	Green
R41	Green
V45	Green
R51	Green
A54	Green
G55	Green
G56	Green
G57	Green
D61	Green
Y68	Green
Q69	Green
Y70	Green
R71	Green
V72	Green
F73	Green
R74	Green
V75	Green
Q76	Green
L77	Green
P78	Green
D79	Green
P80	Green
N81	Green
K82	Green
F83	Green
G84	Green
L85	Green
P86	Green
D87	Green
T88	Green
S89	Green
I90	Green
Y91	Green
N92	Green
P93	Green
L98	Green
V99	Green
C102	Green
V105	Green
E106	Green
I107	Green
C108	Green
R109	Yellow
G110	Yellow
Q111	Yellow
P112	Yellow
L113	Yellow
G114	Yellow
L117	Yellow
P121	Yellow
F122	Yellow
Y123	Yellow
M124	Yellow
K125	Yellow
L126	Yellow
D127	Yellow
D128	Yellow
S131	Yellow
S132	Yellow
H133	Yellow
H133	Yellow
A134	Yellow
A135	Yellow
M138	Yellow
V139	Yellow
S140	Yellow
E141	Yellow
D142	Yellow
V149	Yellow
D150	Yellow
Y151	Yellow
Q155	Yellow
L156	Yellow
C157	Yellow
I158	Yellow
L159	Yellow
G160	Yellow
C161	Yellow
A162	Yellow
P163	Yellow
W169	Yellow
T173	Yellow
A174	Yellow
S175	Yellow
K176	Yellow
S177	Yellow
R178	Yellow
P179	Yellow
L180	Yellow
S181	Yellow
Q182	Yellow
G183	Yellow
D184	Yellow
C185	Yellow
C186	Yellow



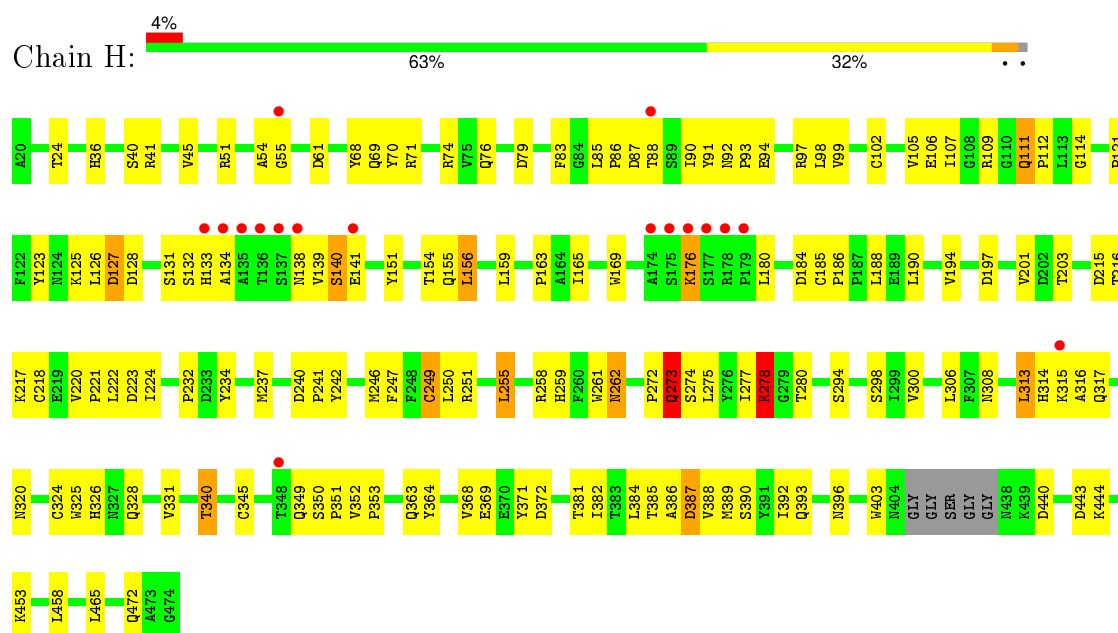
• Molecule 1: L1



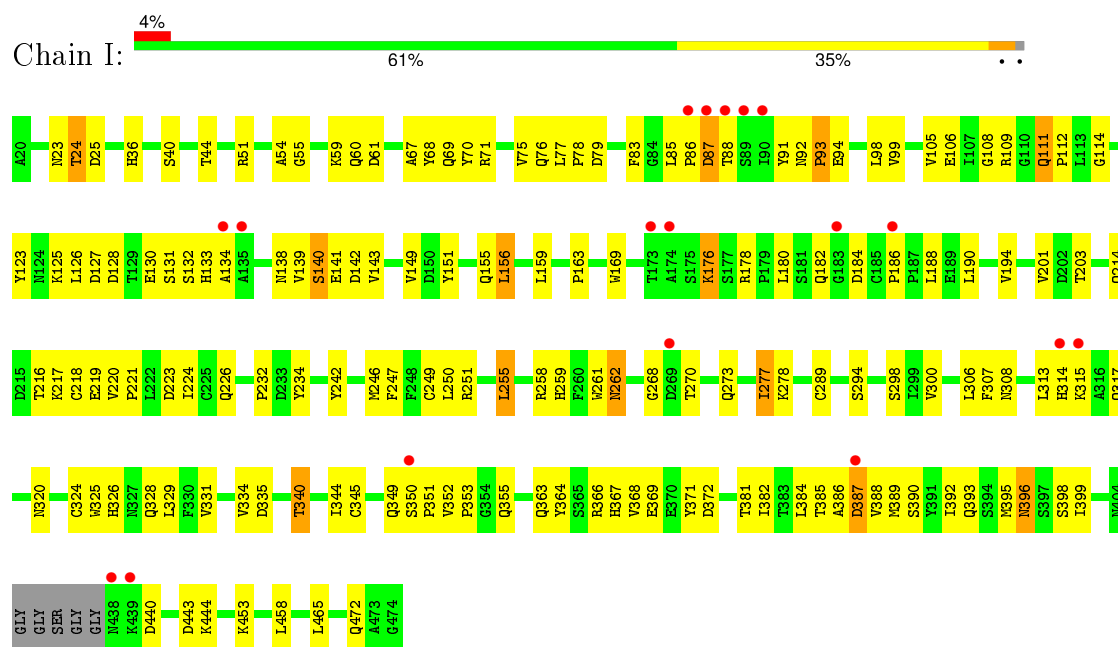
• Molecule 1: L1



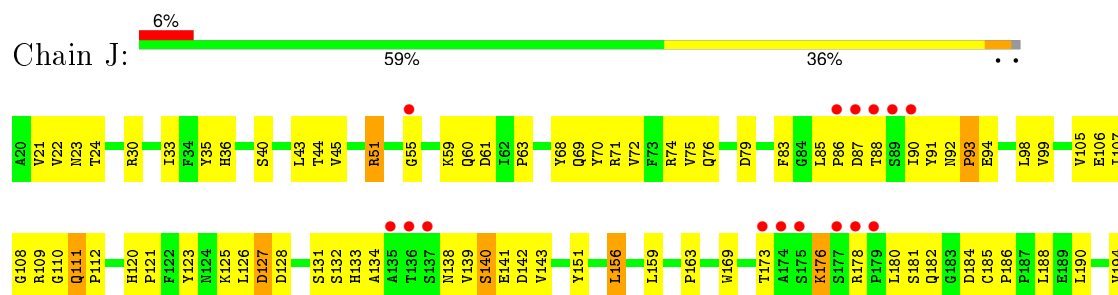
• Molecule 1: L1

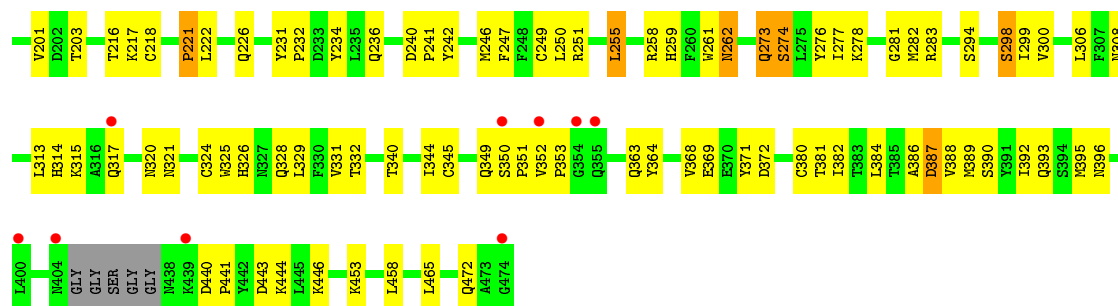


• Molecule 1: L1

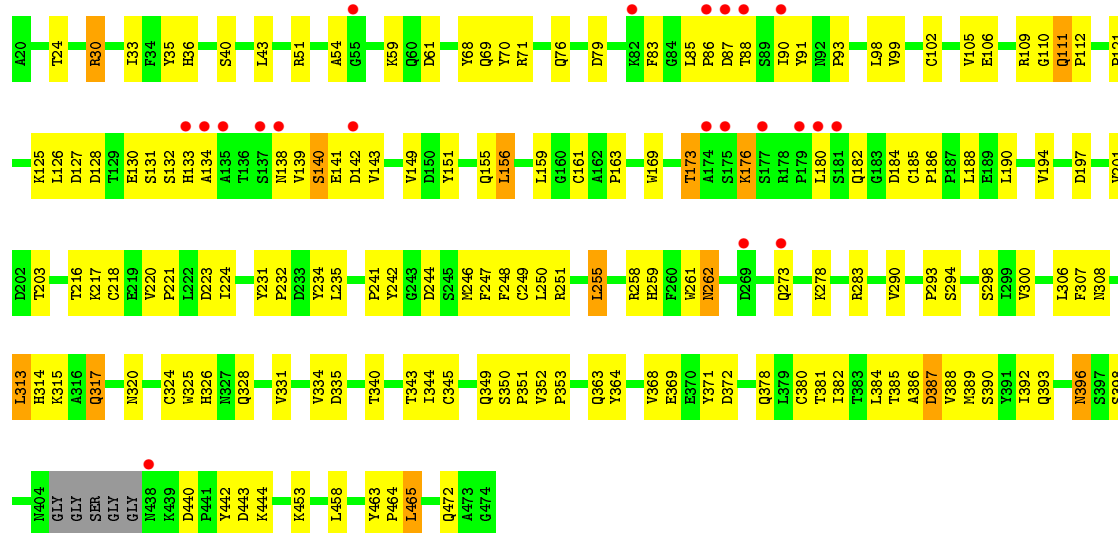


• Molecule 1: L1

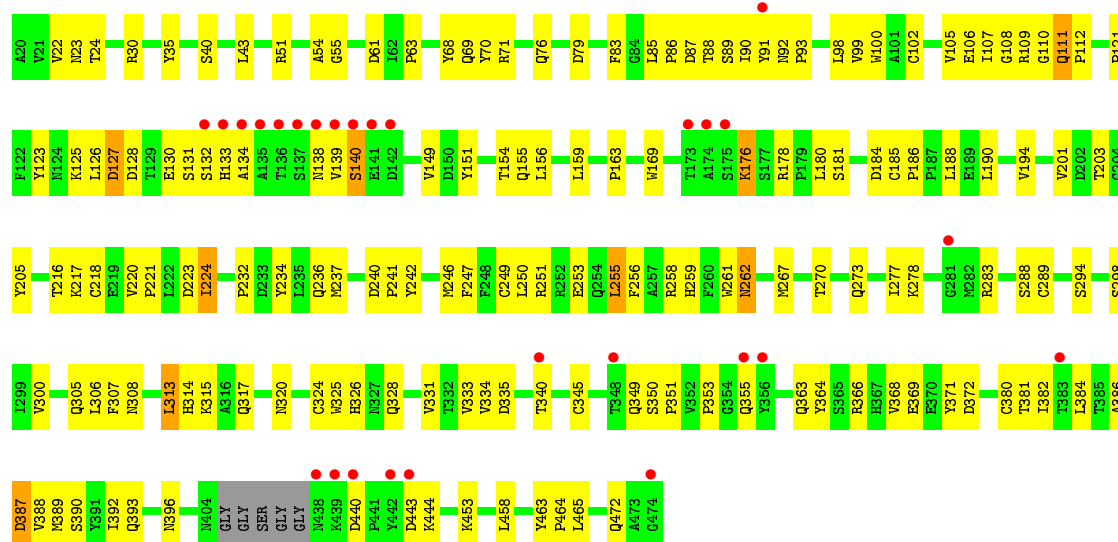




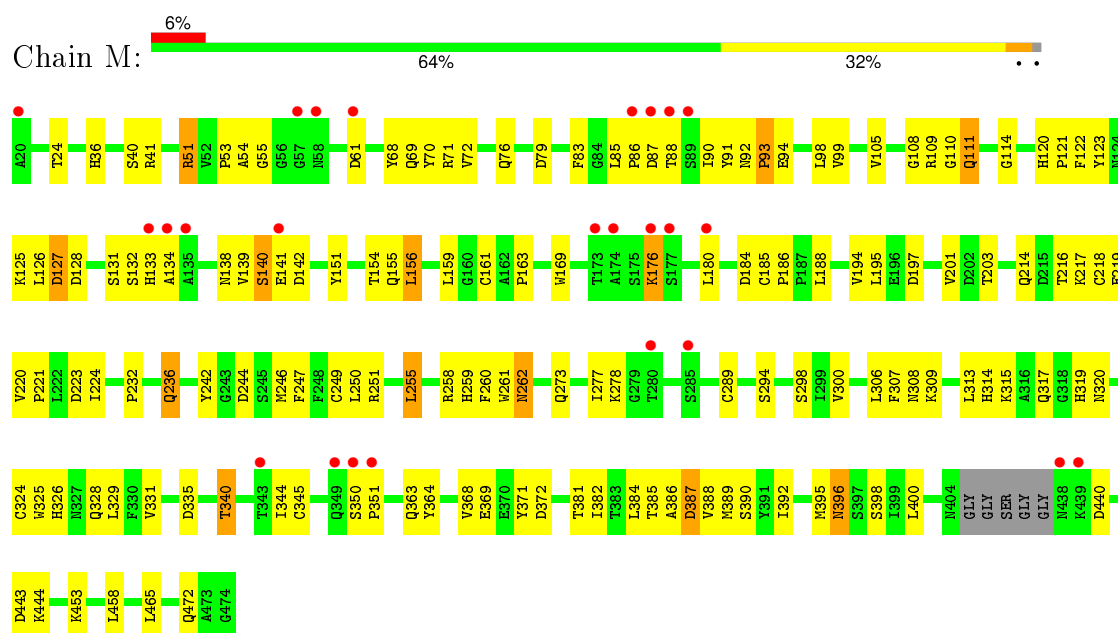
- Molecule 1: L1



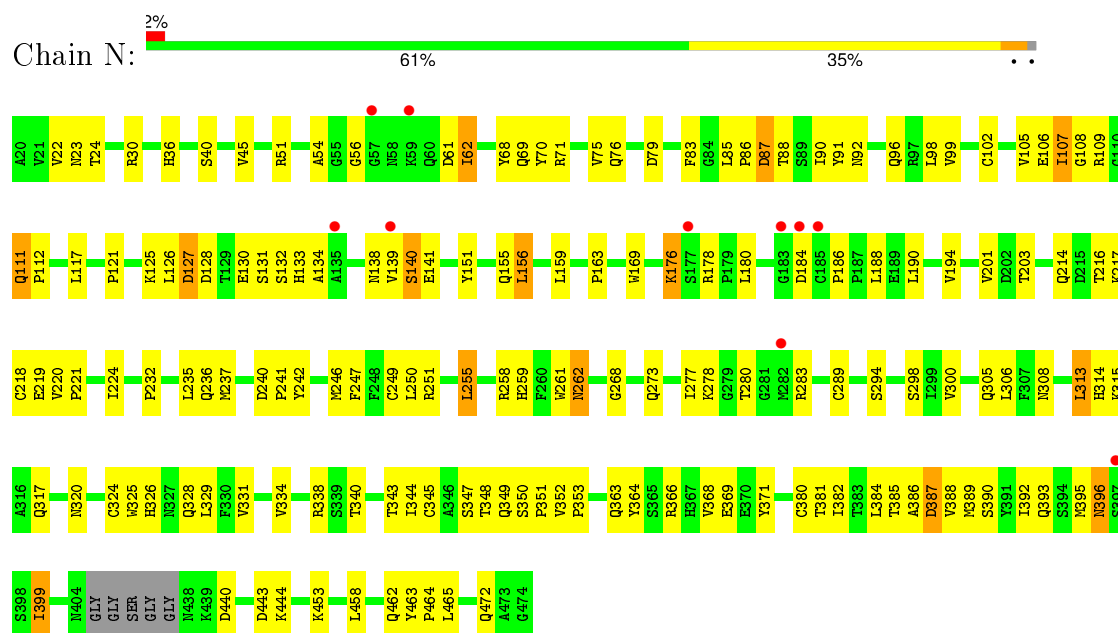
- Molecule 1: L1



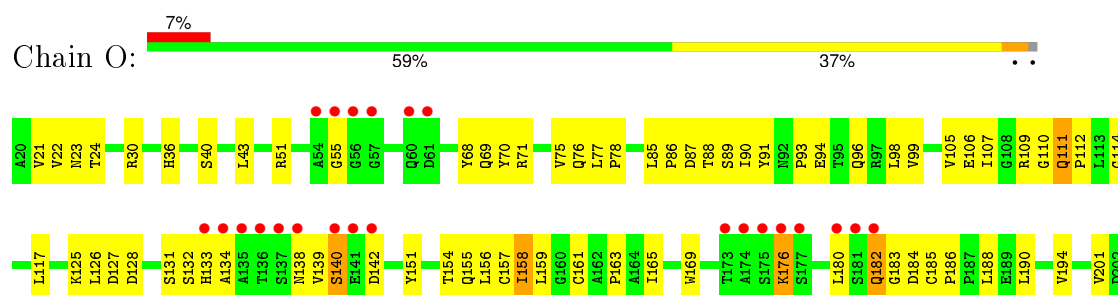
- Molecule 1: L1

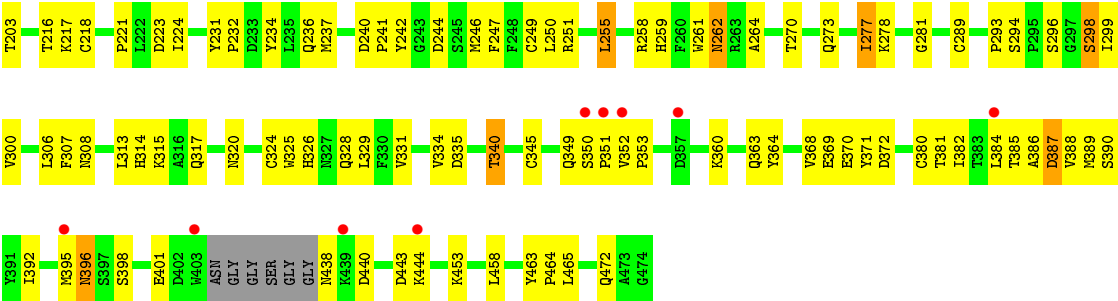


• Molecule 1: L1



• Molecule 1: L1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	80.99Å 106.49Å 237.66Å 88.46° 85.75° 69.02°	Depositor
Resolution (Å)	42.80 – 3.40 42.79 – 3.37	Depositor EDS
% Data completeness (in resolution range)	(Not available) (42.80-3.40) 84.3 (42.79-3.37)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.50 (at 3.40Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.250 , 0.281 0.251 , 0.274	Depositor DCC
R_{free} test set	4354 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	60.2	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 29.6	EDS
Estimated twinning fraction	0.017 for -h,-h+k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 92923 reflections	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	51547	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: JHM, IDS

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.76	10/3400 (0.3%)	0.77	2/4622 (0.0%)
1	B	0.63	2/3400 (0.1%)	0.67	0/4622
1	C	0.66	1/3400 (0.0%)	0.70	1/4622 (0.0%)
1	D	0.66	2/3400 (0.1%)	0.75	3/4622 (0.1%)
1	E	0.71	3/3400 (0.1%)	0.72	1/4622 (0.0%)
1	F	0.60	0/3400	0.70	0/4622
1	G	0.59	0/3400	0.70	0/4622
1	H	0.64	2/3400 (0.1%)	0.69	2/4622 (0.0%)
1	I	0.62	0/3400	0.68	0/4622
1	J	0.60	0/3400	0.69	3/4622 (0.1%)
1	K	0.61	1/3400 (0.0%)	0.69	1/4622 (0.0%)
1	L	0.58	0/3400	0.68	0/4622
1	M	0.59	0/3400	0.67	0/4622
1	N	0.60	0/3400	0.69	0/4622
1	O	0.61	0/3392	0.68	0/4611
All	All	0.63	21/50992 (0.0%)	0.70	13/69319 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	A	1	0
5	C	1	0
5	N	1	0
6	B	2	0
7	E	2	0
7	H	1	0
7	J	5	0
7	L	4	0

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	17	0

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	56	GLY	C-O	12.55	1.43	1.23
1	A	172	GLY	C-O	11.64	1.42	1.23
1	A	176	LYS	CE-NZ	-11.37	1.20	1.49
1	C	278	LYS	CE-NZ	-9.26	1.25	1.49
1	D	280	THR	CB-CG2	-8.92	1.23	1.52
1	K	30	ARG	CG-CD	-8.89	1.29	1.51
1	A	349	GLN	CD-OE1	-8.71	1.04	1.24
1	A	349	GLN	CD-NE2	-8.42	1.11	1.32
1	A	176	LYS	CD-CE	-7.75	1.31	1.51
1	A	278	LYS	CD-CE	-7.15	1.33	1.51
1	E	273	GLN	CD-OE1	-6.68	1.09	1.24
1	A	449	ASN	CG-ND2	-6.60	1.16	1.32
1	H	278	LYS	CE-NZ	-6.34	1.33	1.49
1	B	278	LYS	CE-NZ	-6.13	1.33	1.49
1	B	355	GLN	CD-OE1	-5.90	1.10	1.24
1	A	289	CYS	CB-SG	-5.86	1.72	1.81
1	H	249	CYS	CB-SG	-5.83	1.72	1.81
1	A	176	LYS	CG-CD	-5.78	1.32	1.52
1	E	444	LYS	CD-CE	-5.43	1.37	1.51
1	D	176	LYS	CB-CG	-5.13	1.38	1.52
1	A	449	ASN	CG-OD1	-5.11	1.12	1.24

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	LYS	CD-CE-NZ	-19.64	66.52	111.70
1	D	176	LYS	CA-CB-CG	12.45	140.78	113.40
1	D	278	LYS	CD-CE-NZ	-10.97	86.48	111.70
1	E	444	LYS	CD-CE-NZ	-6.82	96.02	111.70
1	D	176	LYS	CB-CA-C	-5.90	98.59	110.40
1	J	274	SER	CB-CA-C	-5.72	99.23	110.10
1	K	173	THR	CA-CB-CG2	-5.56	104.61	112.40
1	C	273	GLN	CA-C-N	-5.55	104.98	117.20
1	H	273	GLN	C-N-CA	-5.40	108.19	121.70
1	J	273	GLN	CA-CB-CG	5.38	125.23	113.40
1	J	274	SER	N-CA-CB	5.33	118.50	110.50
1	H	278	LYS	CD-CE-NZ	-5.12	99.93	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	GLY	CA-C-O	-5.01	111.58	120.60

All (17) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	518	IDS	C4
6	B	534	IDS	C4
6	B	538	IDS	C4
5	C	572	IDS	C4
7	E	548	IDS	C4
7	E	550	IDS	C4
7	H	580	IDS	C4
7	J	554	IDS	C4
7	J	556	IDS	C4
7	J	564	IDS	C4
7	J	598	IDS	C4
7	J	600	IDS	C4
7	L	614	IDS	C4
7	L	616	IDS	C4
7	L	618	IDS	C4
7	L	620	IDS	C4
5	N	608	IDS	C4

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3315	0	3178	143	0
1	B	3315	0	3181	153	0
1	C	3315	0	3181	153	0
1	D	3315	0	3181	125	0
1	E	3315	0	3181	131	0
1	F	3315	0	3181	172	0
1	G	3315	0	3181	157	1
1	H	3315	0	3181	125	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	3315	0	3181	134	0
1	J	3315	0	3181	186	2
1	K	3315	0	3181	127	1
1	L	3315	0	3181	140	1
1	M	3315	0	3181	120	4
1	N	3315	0	3181	154	1
1	O	3307	0	3175	144	6
2	E	15	0	10	8	0
3	E	45	0	17	6	0
4	C	30	0	14	0	0
4	D	120	0	55	12	0
4	E	30	0	14	3	0
4	N	30	0	14	1	0
5	A	120	0	54	1	3
5	B	60	0	26	17	0
5	C	60	0	27	5	0
5	D	60	0	26	4	2
5	E	60	0	26	5	1
5	F	60	0	27	1	1
5	N	60	0	27	18	1
5	O	60	0	26	1	0
6	B	150	0	66	9	0
6	F	150	0	66	6	4
7	E	90	0	40	5	0
7	F	90	0	40	13	0
7	H	90	0	40	10	0
7	J	270	0	120	49	0
7	L	180	0	80	17	4
All	All	51547	0	48521	2052	16

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (2052) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:561:JHM:H2A	7:J:564:IDS:C3	1.42	1.38
5:B:530:IDS:O61	1:C:274:SER:CB	1.76	1.31
1:C:95:THR:HB	5:C:572:IDS:O61	1.30	1.28
5:B:530:IDS:O61	1:C:274:SER:HB2	1.12	1.28
7:L:611:JHM:H1	7:L:614:IDS:O62	1.18	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:559:JHM:H2A	7:J:562:IDS:C6	1.67	1.23
7:J:556:IDS:C6	7:J:557:JHM:H1	1.46	1.23
1:F:178:ARG:NE	1:J:59:LYS:HB2	1.53	1.22
7:J:561:JHM:H2A	7:J:564:IDS:O3	1.41	1.21
7:J:561:JHM:C2	7:J:564:IDS:O3	1.89	1.20
1:G:217:LYS:HE3	1:G:226:GLN:NE2	1.57	1.19
1:O:182:GLN:HE21	1:O:183:GLY:N	1.46	1.12
1:F:91:TYR:C	1:O:281:GLY:HA2	1.68	1.11
7:H:577:JHM:O5	7:H:580:IDS:C3	1.96	1.11
1:N:351:PRO:HB2	5:N:607:JHM:O8	1.49	1.11
7:L:611:JHM:H1	7:L:614:IDS:C6	1.70	1.10
7:L:611:JHM:C1	7:L:614:IDS:O62	1.99	1.10
7:J:561:JHM:C2	7:J:564:IDS:H3	1.79	1.10
7:J:561:JHM:C2	7:J:564:IDS:C3	2.13	1.09
1:B:89:SER:O	1:J:281:GLY:HA3	1.53	1.08
1:O:182:GLN:NE2	1:O:183:GLY:H	1.52	1.07
4:D:504:IDS:C4	2:E:501:JHM:C1	2.32	1.07
4:D:504:IDS:C4	2:E:501:JHM:H1	1.85	1.07
7:J:561:JHM:H2A	7:J:564:IDS:H3	1.14	1.06
4:D:522:IDS:O2	5:D:523:JHM:H1	1.54	1.05
1:H:272:PRO:C	1:H:274:SER:H	1.59	1.04
1:B:217:LYS:HE3	1:B:226:GLN:NE2	1.73	1.04
1:F:277:ILE:HD11	1:J:217:LYS:HD3	1.39	1.01
7:J:556:IDS:O62	7:J:557:JHM:H1	1.59	1.01
1:H:272:PRO:O	1:H:274:SER:N	1.93	1.00
7:J:556:IDS:C6	7:J:557:JHM:C1	2.40	1.00
1:F:178:ARG:CD	1:J:59:LYS:HB2	1.93	0.99
1:D:278:LYS:HE3	5:D:523:JHM:O8	1.62	0.99
7:J:561:JHM:C1	7:J:564:IDS:O3	2.11	0.98
1:H:217:LYS:HD3	1:I:277:ILE:HD11	1.47	0.97
1:B:444:LYS:HE2	1:B:444:LYS:HA	1.47	0.96
1:J:444:LYS:HD2	7:J:563:JHM:O8	1.65	0.96
6:F:582:IDS:O2	6:F:583:JHM:H1	1.65	0.96
1:F:178:ARG:HD2	1:J:59:LYS:CD	1.96	0.96
1:F:178:ARG:HE	1:J:59:LYS:HB2	1.31	0.94
5:N:608:IDS:C6	5:N:609:JHM:H1	1.96	0.94
1:B:217:LYS:HE3	1:B:226:GLN:CD	1.85	0.94
1:O:273:GLN:HB3	5:O:604:IDS:O1S	1.66	0.94
1:G:386:ALA:HB1	1:L:355:GLN:NE2	1.83	0.94
1:F:176:LYS:H	1:F:176:LYS:HD3	1.33	0.93
1:F:179:PRO:HB2	7:F:569:JHM:O9	1.70	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:LYS:HD2	5:B:528:IDS:O2S	1.70	0.92
1:G:217:LYS:HE3	1:G:226:GLN:HE21	1.33	0.92
1:M:273:GLN:HE22	1:M:278:LYS:HE2	1.32	0.92
3:E:502:IDS:C6	3:E:505:JHM:H1	1.98	0.91
3:E:502:IDS:C6	3:E:505:JHM:C1	2.48	0.91
1:F:126:LEU:HB3	1:F:262:ASN:HB3	1.53	0.90
1:I:105:VAL:HG21	1:I:159:LEU:HD11	1.53	0.89
1:O:444:LYS:HA	1:O:444:LYS:HE2	1.52	0.89
1:J:274:SER:HB3	7:J:554:IDS:O62	1.71	0.89
1:D:444:LYS:HA	1:D:444:LYS:HE2	1.54	0.89
1:B:217:LYS:CE	1:B:226:GLN:NE2	2.34	0.89
1:F:178:ARG:CD	1:J:59:LYS:CB	2.51	0.89
1:D:105:VAL:HG21	1:D:159:LEU:HD11	1.55	0.89
1:A:444:LYS:HA	1:A:444:LYS:HE2	1.56	0.87
1:F:368:VAL:HG11	1:G:169:TRP:CZ2	2.09	0.87
7:L:611:JHM:C1	7:L:614:IDS:C6	2.48	0.86
1:O:182:GLN:NE2	1:O:183:GLY:N	2.14	0.86
1:N:273:GLN:HE22	1:N:278:LYS:HE2	1.41	0.86
7:J:561:JHM:H1	7:J:564:IDS:O3	1.76	0.85
1:I:273:GLN:HE22	1:I:278:LYS:HE2	1.39	0.85
1:N:444:LYS:HA	1:N:444:LYS:HE2	1.56	0.85
1:M:105:VAL:HG21	1:M:159:LEU:HD11	1.59	0.85
1:C:368:VAL:HG11	1:D:169:TRP:CZ2	2.11	0.84
1:C:105:VAL:HG21	1:C:159:LEU:HD11	1.59	0.84
1:A:368:VAL:HG11	1:B:169:TRP:CZ2	2.13	0.84
1:F:178:ARG:HD2	1:J:59:LYS:HD2	1.60	0.84
1:N:351:PRO:HG2	5:N:607:JHM:O6	1.78	0.84
1:B:105:VAL:HG21	1:B:159:LEU:HD11	1.58	0.83
1:D:249:CYS:O	1:D:250:LEU:HD12	1.78	0.83
1:B:217:LYS:NZ	1:B:226:GLN:NE2	2.27	0.83
1:G:250:LEU:HB3	1:G:306:LEU:HD21	1.59	0.83
7:J:595:JHM:O5	7:J:598:IDS:H3	1.72	0.82
1:J:446:LYS:NZ	7:J:599:JHM:O8	2.11	0.82
1:G:126:LEU:HB3	1:G:262:ASN:HB3	1.61	0.82
1:F:273:GLN:HE22	1:F:278:LYS:HE2	1.43	0.82
1:H:273:GLN:HE22	1:H:278:LYS:CE	1.91	0.82
1:K:273:GLN:HE22	1:K:278:LYS:HE2	1.44	0.82
1:H:444:LYS:HE2	1:H:444:LYS:HA	1.61	0.82
1:B:217:LYS:HZ2	1:B:226:GLN:NE2	1.77	0.82
1:K:444:LYS:HA	1:K:444:LYS:HE2	1.61	0.82
1:J:273:GLN:HB2	7:J:555:JHM:O1	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:178:ARG:HG3	7:L:619:JHM:O9	1.80	0.82
1:B:89:SER:HB2	1:J:282:MET:HG2	1.62	0.82
1:O:126:LEU:HB3	1:O:262:ASN:HB3	1.62	0.81
1:J:126:LEU:HB3	1:J:262:ASN:HB3	1.60	0.81
1:A:126:LEU:HB3	1:A:262:ASN:HB3	1.62	0.81
1:K:59:LYS:HD2	7:L:619:JHM:O8	1.81	0.81
1:M:300:VAL:HG13	1:N:255:LEU:HD13	1.63	0.81
1:G:105:VAL:HG21	1:G:159:LEU:HD11	1.63	0.81
1:J:444:LYS:CD	7:J:563:JHM:O8	2.28	0.81
1:D:126:LEU:HB3	1:D:262:ASN:HB3	1.61	0.81
1:C:444:LYS:HE2	1:C:444:LYS:HA	1.63	0.80
1:K:126:LEU:HB3	1:K:262:ASN:HB3	1.63	0.80
1:F:444:LYS:HE2	1:F:444:LYS:HA	1.63	0.80
1:J:444:LYS:HE2	1:J:444:LYS:HA	1.63	0.80
1:O:105:VAL:HG21	1:O:159:LEU:HD11	1.62	0.80
1:B:300:VAL:HG13	1:C:255:LEU:HD13	1.63	0.80
1:K:250:LEU:HB3	1:K:306:LEU:HD21	1.62	0.80
1:M:126:LEU:HB3	1:M:262:ASN:HB3	1.63	0.79
1:C:126:LEU:HB3	1:C:262:ASN:HB3	1.64	0.79
1:N:105:VAL:HG21	1:N:159:LEU:HD11	1.62	0.79
1:J:51:ARG:NH1	7:J:599:JHM:O1	2.14	0.79
1:L:444:LYS:HA	1:L:444:LYS:HE2	1.64	0.79
1:J:250:LEU:HB3	1:J:306:LEU:HD21	1.65	0.79
1:N:250:LEU:HB3	1:N:306:LEU:HD21	1.65	0.79
1:N:351:PRO:CB	5:N:607:JHM:O8	2.29	0.79
1:M:273:GLN:NE2	1:M:278:LYS:HE2	1.97	0.79
1:E:105:VAL:HG21	1:E:159:LEU:HD11	1.65	0.79
1:N:126:LEU:HB3	1:N:262:ASN:HB3	1.63	0.78
1:F:217:LYS:HD3	1:G:277:ILE:HD11	1.64	0.78
1:G:386:ALA:HB1	1:L:355:GLN:CD	2.02	0.78
1:I:444:LYS:HA	1:I:444:LYS:HE2	1.66	0.78
1:L:126:LEU:HB3	1:L:262:ASN:HB3	1.63	0.78
1:J:274:SER:OG	7:J:554:IDS:O61	2.01	0.78
1:J:273:GLN:HB3	7:J:555:JHM:H5	1.65	0.78
1:L:176:LYS:HA	7:L:612:IDS:H3	1.64	0.78
1:K:105:VAL:HG21	1:K:159:LEU:HD11	1.65	0.78
1:D:250:LEU:HB3	1:D:306:LEU:HD21	1.67	0.77
1:F:105:VAL:HG21	1:F:159:LEU:HD11	1.65	0.77
1:H:126:LEU:HB3	1:H:262:ASN:HB3	1.65	0.77
1:J:246:MET:HG3	1:J:246:MET:O	1.85	0.77
1:A:239:ALA:HB1	7:E:547:JHM:H6	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:LEU:HB3	1:C:306:LEU:HD21	1.65	0.77
1:E:250:LEU:HB3	1:E:306:LEU:HD21	1.67	0.77
7:J:559:JHM:H2A	7:J:562:IDS:O61	1.84	0.77
1:M:444:LYS:HA	1:M:444:LYS:HE2	1.67	0.77
5:N:609:JHM:O7	1:O:182:GLN:HB2	1.84	0.76
1:H:250:LEU:HB3	1:H:306:LEU:HD21	1.66	0.76
1:K:59:LYS:HD2	7:L:619:JHM:S	2.26	0.76
1:F:92:ASN:N	1:O:281:GLY:HA2	2.01	0.76
1:B:126:LEU:HB3	1:B:262:ASN:HB3	1.68	0.76
1:O:250:LEU:HB3	1:O:306:LEU:HD21	1.68	0.76
1:F:258:ARG:HG3	1:F:259:HIS:ND1	2.01	0.76
1:G:273:GLN:HE22	1:G:278:LYS:HE2	1.50	0.76
1:D:53:PRO:HB2	4:D:503:JHM:O8	1.85	0.75
1:B:217:LYS:HD2	5:B:529:JHM:O8	1.86	0.75
1:O:273:GLN:HE22	1:O:278:LYS:HE2	1.49	0.75
1:A:250:LEU:HB3	1:A:306:LEU:HD21	1.67	0.75
1:J:105:VAL:HG21	1:J:159:LEU:HD11	1.67	0.75
1:I:126:LEU:HB3	1:I:262:ASN:HB3	1.67	0.75
1:A:349:GLN:HE21	1:A:349:GLN:HA	1.50	0.75
1:B:121:PRO:HG3	1:C:289:CYS:SG	2.26	0.75
1:N:368:VAL:HG11	1:O:169:TRP:CZ2	2.21	0.75
1:I:369:GLU:HG3	1:I:371:TYR:HE1	1.51	0.75
1:B:226:GLN:C	5:B:528:IDS:O3	2.25	0.74
7:H:575:JHM:H1	7:H:578:IDS:O62	1.87	0.74
1:E:126:LEU:HB3	1:E:262:ASN:HB3	1.69	0.74
1:H:273:GLN:HE22	1:H:278:LYS:NZ	1.84	0.74
1:F:277:ILE:CD1	1:J:217:LYS:HD3	2.17	0.74
1:L:368:VAL:HG11	1:M:169:TRP:CZ2	2.22	0.74
1:I:273:GLN:NE2	1:I:278:LYS:HE2	2.01	0.74
1:J:273:GLN:NE2	1:J:278:LYS:HE2	2.03	0.74
1:N:351:PRO:CG	5:N:607:JHM:H4	2.17	0.73
1:L:138:ASN:ND2	1:L:140:SER:HB3	2.02	0.73
1:K:293:PRO:HB3	1:O:117:LEU:HD11	1.69	0.73
1:M:369:GLU:HG3	1:M:371:TYR:HE1	1.52	0.73
1:B:350:SER:HB3	1:B:351:PRO:HD3	1.69	0.73
1:H:272:PRO:C	1:H:274:SER:N	2.26	0.73
1:F:250:LEU:HB3	1:F:306:LEU:HD21	1.69	0.73
1:L:273:GLN:HE22	1:L:278:LYS:HE2	1.52	0.73
7:L:620:IDS:H3	7:L:621:JHM:O5	1.88	0.73
1:J:273:GLN:HE22	1:J:278:LYS:HE2	1.53	0.73
1:F:273:GLN:NE2	1:F:278:LYS:HE2	2.04	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:369:GLU:HG3	1:N:371:TYR:HE1	1.54	0.73
1:B:217:LYS:CD	5:B:529:JHM:O8	2.37	0.73
1:G:350:SER:HB3	1:G:351:PRO:HD3	1.71	0.72
1:G:109:ARG:H	1:G:308:ASN:HD21	1.35	0.72
1:G:69:GLN:NE2	1:G:71:ARG:HH22	1.87	0.72
1:I:250:LEU:HB3	1:I:306:LEU:HD21	1.70	0.72
1:C:95:THR:CB	5:C:572:IDS:O61	2.25	0.72
7:H:577:JHM:O5	7:H:580:IDS:H3	1.35	0.72
1:F:369:GLU:HG3	1:F:371:TYR:HE1	1.54	0.72
7:F:567:JHM:H2A	7:F:570:IDS:C6	2.18	0.72
1:G:70:TYR:CE1	1:G:201:VAL:HG12	2.23	0.72
1:F:179:PRO:CB	7:F:569:JHM:O9	2.36	0.72
1:A:105:VAL:HG21	1:A:159:LEU:HD11	1.70	0.72
1:J:51:ARG:HH22	7:J:599:JHM:H3	1.55	0.72
1:B:368:VAL:HG11	1:C:169:TRP:CZ2	2.25	0.72
1:F:69:GLN:NE2	1:F:71:ARG:HH22	1.88	0.72
1:J:249:CYS:O	1:J:250:LEU:HD12	1.90	0.71
1:B:250:LEU:HB3	1:B:306:LEU:HD21	1.71	0.71
1:G:220:VAL:HB	1:G:224:ILE:HD11	1.70	0.71
1:E:350:SER:HB3	1:E:351:PRO:HD3	1.71	0.71
5:B:529:JHM:O3	1:C:274:SER:HB3	1.89	0.71
1:G:217:LYS:HE3	1:G:226:GLN:HE22	1.51	0.71
1:J:176:LYS:NZ	1:J:176:LYS:HB2	2.06	0.71
1:N:273:GLN:NE2	1:N:278:LYS:HE2	2.04	0.71
1:M:249:CYS:O	1:M:250:LEU:HD12	1.90	0.71
1:H:85:LEU:HB3	1:H:86:PRO:HD2	1.73	0.71
1:D:369:GLU:HG3	1:D:371:TYR:HE1	1.55	0.71
1:D:217:LYS:HD3	1:E:277:ILE:HD11	1.71	0.71
1:D:138:ASN:ND2	1:D:140:SER:HB3	2.05	0.71
1:M:105:VAL:HG21	1:M:159:LEU:CD1	2.20	0.71
1:H:151:TYR:OH	1:H:221:PRO:HB2	1.91	0.71
1:F:91:TYR:C	1:O:281:GLY:CA	2.54	0.70
1:A:255:LEU:HD13	1:E:300:VAL:HG13	1.73	0.70
1:O:369:GLU:HG3	1:O:371:TYR:HE1	1.56	0.70
1:C:368:VAL:HG11	1:D:169:TRP:HZ2	1.53	0.70
1:F:300:VAL:HG13	1:G:255:LEU:HD13	1.73	0.70
1:I:350:SER:HB3	1:I:351:PRO:HD3	1.73	0.70
1:F:109:ARG:H	1:F:308:ASN:HD21	1.39	0.70
1:F:178:ARG:NE	1:J:59:LYS:CB	2.43	0.70
1:E:41:ARG:HB2	7:E:548:IDS:O2S	1.92	0.70
1:H:300:VAL:HG13	1:I:255:LEU:HD13	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:180:LEU:HD21	1:I:186:PRO:HA	1.72	0.70
1:G:444:LYS:HA	1:G:444:LYS:HE2	1.72	0.70
1:G:226:GLN:NE2	7:H:578:IDS:O2S	2.25	0.70
1:A:369:GLU:HG3	1:A:371:TYR:HE1	1.56	0.70
1:L:350:SER:HB3	1:L:351:PRO:HD3	1.72	0.70
1:F:138:ASN:ND2	1:F:140:SER:HB3	2.07	0.70
1:F:99:VAL:HG21	1:F:382:ILE:CD1	2.22	0.70
1:A:70:TYR:CE1	1:A:201:VAL:HG12	2.27	0.70
1:J:273:GLN:HB3	7:J:555:JHM:C5	2.22	0.70
1:L:178:ARG:CG	7:L:619:JHM:O9	2.40	0.70
1:I:109:ARG:H	1:I:308:ASN:HD21	1.40	0.70
1:H:369:GLU:HG3	1:H:371:TYR:HE1	1.57	0.69
1:J:69:GLN:NE2	1:J:71:ARG:HH22	1.90	0.69
1:L:368:VAL:HG11	1:M:169:TRP:HZ2	1.56	0.69
1:B:369:GLU:HG3	1:B:371:TYR:HE1	1.57	0.69
1:J:70:TYR:CE1	1:J:201:VAL:HG12	2.26	0.69
1:M:368:VAL:HG11	1:N:169:TRP:CZ2	2.27	0.69
1:N:109:ARG:H	1:N:308:ASN:HD21	1.38	0.69
1:N:368:VAL:HG11	1:O:169:TRP:HZ2	1.56	0.69
1:I:69:GLN:NE2	1:I:71:ARG:HH22	1.90	0.69
1:A:258:ARG:HG3	1:A:259:HIS:ND1	2.07	0.69
1:L:105:VAL:HG21	1:L:159:LEU:HD11	1.74	0.69
4:D:504:IDS:C4	2:E:501:JHM:O1	2.41	0.69
1:C:369:GLU:HG3	1:C:371:TYR:HE1	1.58	0.69
1:C:159:LEU:CD2	1:C:331:VAL:HG22	2.22	0.69
1:M:159:LEU:CD2	1:M:331:VAL:HG22	2.22	0.69
1:A:350:SER:HB3	1:A:351:PRO:HD3	1.75	0.69
1:M:246:MET:O	1:M:246:MET:HG3	1.91	0.69
1:N:249:CYS:O	1:N:250:LEU:HD12	1.93	0.69
1:C:69:GLN:NE2	1:C:71:ARG:HH22	1.90	0.69
1:H:105:VAL:HG21	1:H:159:LEU:HD11	1.74	0.68
1:C:300:VAL:HG13	1:D:255:LEU:HD13	1.75	0.68
1:J:273:GLN:HB2	7:J:554:IDS:H3	1.73	0.68
1:E:384:LEU:HB3	1:E:389:MET:CE	2.24	0.68
1:O:350:SER:HB3	1:O:351:PRO:HD3	1.75	0.68
1:A:352:VAL:CG1	5:B:529:JHM:O9	2.41	0.68
1:K:273:GLN:NE2	1:K:278:LYS:HE2	2.08	0.68
1:H:138:ASN:ND2	1:H:140:SER:HB3	2.09	0.68
1:N:70:TYR:CE1	1:N:201:VAL:HG12	2.29	0.68
1:A:109:ARG:H	1:A:308:ASN:HD21	1.41	0.68
1:C:273:GLN:NE2	1:C:278:LYS:NZ	2.42	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:178:ARG:CD	1:J:59:LYS:HD2	2.24	0.68
1:G:273:GLN:NE2	1:G:278:LYS:HE2	2.09	0.68
1:N:188:LEU:HD22	1:N:188:LEU:N	2.09	0.68
1:G:70:TYR:OH	1:G:232:PRO:HD3	1.93	0.68
1:L:70:TYR:CE1	1:L:201:VAL:HG12	2.30	0.67
1:J:45:VAL:HG12	1:J:368:VAL:HG22	1.77	0.67
1:H:350:SER:HB3	1:H:351:PRO:HD3	1.77	0.67
1:F:70:TYR:OH	1:F:232:PRO:HD3	1.94	0.67
1:D:246:MET:HG3	1:D:246:MET:O	1.93	0.67
1:K:246:MET:O	1:K:246:MET:HG3	1.94	0.67
1:L:188:LEU:N	1:L:188:LEU:HD22	2.09	0.67
1:M:151:TYR:CD2	1:M:203:THR:HB	2.30	0.67
7:J:559:JHM:C2	7:J:562:IDS:C6	2.60	0.67
1:I:105:VAL:HG21	1:I:159:LEU:CD1	2.24	0.67
1:J:350:SER:HB3	1:J:351:PRO:HD3	1.75	0.67
1:B:105:VAL:HG21	1:B:159:LEU:CD1	2.25	0.67
1:K:169:TRP:HZ2	1:O:368:VAL:HG11	1.59	0.67
1:L:345:CYS:HB3	1:L:363:GLN:NE2	2.10	0.67
1:L:109:ARG:H	1:L:308:ASN:HD21	1.42	0.67
1:F:180:LEU:HD21	1:F:186:PRO:HA	1.76	0.67
1:F:178:ARG:HD2	1:J:59:LYS:CB	2.25	0.67
1:F:178:ARG:HD2	1:J:59:LYS:HD3	1.76	0.66
1:L:159:LEU:CD2	1:L:331:VAL:HG22	2.25	0.66
1:N:300:VAL:HG13	1:O:255:LEU:HD13	1.76	0.66
1:N:99:VAL:HG21	1:N:382:ILE:CD1	2.25	0.66
1:B:70:TYR:OH	1:B:232:PRO:HD3	1.94	0.66
1:G:386:ALA:CB	1:L:355:GLN:CD	2.63	0.66
1:G:99:VAL:CG2	1:G:382:ILE:HD13	2.25	0.66
1:K:369:GLU:HG3	1:K:371:TYR:HE1	1.60	0.66
1:F:126:LEU:HG	1:F:127:ASP:OD2	1.95	0.66
1:G:180:LEU:HD21	1:G:186:PRO:HA	1.77	0.66
1:I:368:VAL:HG11	1:J:169:TRP:CZ2	2.31	0.66
1:D:384:LEU:HD22	1:D:389:MET:HG3	1.77	0.66
1:K:99:VAL:HG21	1:K:382:ILE:CD1	2.25	0.66
1:D:109:ARG:H	1:D:308:ASN:HD21	1.41	0.66
1:M:99:VAL:HG21	1:M:382:ILE:CD1	2.25	0.66
1:B:159:LEU:CD2	1:B:331:VAL:HG22	2.26	0.66
1:L:258:ARG:HG3	1:L:259:HIS:ND1	2.11	0.66
1:H:180:LEU:HD21	1:H:186:PRO:HA	1.75	0.66
1:O:249:CYS:O	1:O:250:LEU:HD12	1.96	0.66
1:J:109:ARG:H	1:J:308:ASN:HD21	1.42	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:347:SER:O	1:O:182:GLN:NE2	2.29	0.66
1:D:70:TYR:OH	1:D:232:PRO:HD3	1.96	0.66
1:D:151:TYR:CD2	1:D:203:THR:HB	2.31	0.66
1:O:151:TYR:OH	1:O:221:PRO:HB2	1.96	0.66
1:J:138:ASN:ND2	1:J:140:SER:HB3	2.11	0.66
7:J:597:JHM:H2A	7:J:600:IDS:O62	1.96	0.66
1:J:274:SER:HB3	7:J:554:IDS:C6	2.26	0.65
1:B:70:TYR:CE1	1:B:201:VAL:HG12	2.31	0.65
1:L:250:LEU:HB3	1:L:306:LEU:HD21	1.76	0.65
1:A:368:VAL:HG11	1:B:169:TRP:HZ2	1.61	0.65
1:N:105:VAL:HG21	1:N:159:LEU:CD1	2.25	0.65
1:G:386:ALA:HB2	1:L:355:GLN:HB2	1.78	0.65
1:K:151:TYR:CD2	1:K:203:THR:HB	2.32	0.65
1:A:384:LEU:HB3	1:A:389:MET:CE	2.27	0.65
1:I:188:LEU:N	1:I:188:LEU:HD22	2.12	0.65
1:I:369:GLU:HG3	1:I:371:TYR:CE1	2.32	0.65
7:F:567:JHM:C1	7:F:570:IDS:C6	2.75	0.65
1:O:151:TYR:CD2	1:O:203:THR:HB	2.31	0.65
1:B:188:LEU:N	1:B:188:LEU:HD22	2.11	0.65
1:N:69:GLN:NE2	1:N:71:ARG:HH22	1.93	0.65
1:G:217:LYS:CE	1:G:226:GLN:NE2	2.48	0.65
1:G:217:LYS:HD2	7:H:578:IDS:O3S	1.97	0.65
1:F:350:SER:HB3	1:F:351:PRO:HD3	1.79	0.65
1:C:350:SER:HB3	1:C:351:PRO:HD3	1.78	0.65
1:C:188:LEU:HD22	1:C:188:LEU:N	2.12	0.65
1:K:249:CYS:O	1:K:250:LEU:HD12	1.97	0.65
1:J:384:LEU:HD22	1:J:389:MET:HG3	1.78	0.65
1:L:273:GLN:NE2	1:L:278:LYS:HE2	2.10	0.65
1:C:273:GLN:HE22	1:C:278:LYS:NZ	1.95	0.65
1:J:151:TYR:OH	1:J:221:PRO:HB2	1.97	0.65
1:E:369:GLU:HG3	1:E:371:TYR:HE1	1.62	0.65
1:C:314:HIS:O	1:C:315:LYS:HG3	1.97	0.65
1:M:69:GLN:NE2	1:M:71:ARG:HH22	1.94	0.65
1:E:384:LEU:HB3	1:E:389:MET:HE1	1.78	0.65
1:C:99:VAL:HG21	1:C:382:ILE:CD1	2.27	0.65
1:F:41:ARG:NH1	1:G:190:LEU:HD23	2.12	0.64
1:L:369:GLU:HG3	1:L:371:TYR:HE1	1.61	0.64
1:H:99:VAL:CG2	1:H:382:ILE:HD13	2.28	0.64
1:G:151:TYR:CD2	1:G:203:THR:HB	2.33	0.64
1:C:176:LYS:HB2	1:C:176:LYS:HZ2	1.61	0.64
1:B:109:ARG:H	1:B:308:ASN:HD21	1.44	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:GLN:HE22	1:C:280:THR:HG23	1.61	0.64
1:K:176:LYS:NZ	1:K:176:LYS:HB2	2.13	0.64
1:A:99:VAL:CG2	1:A:382:ILE:HD13	2.28	0.64
1:G:258:ARG:HG3	1:G:259:HIS:ND1	2.13	0.64
1:O:99:VAL:HG21	1:O:382:ILE:CD1	2.26	0.64
1:J:45:VAL:N	7:J:598:IDS:O61	2.30	0.64
1:A:138:ASN:ND2	1:A:140:SER:HB3	2.11	0.64
1:C:109:ARG:H	1:C:308:ASN:HD21	1.44	0.64
1:M:369:GLU:HG3	1:M:371:TYR:CE1	2.32	0.64
7:H:577:JHM:O5	7:H:580:IDS:O3	2.16	0.64
1:M:250:LEU:HB3	1:M:306:LEU:HD21	1.78	0.64
1:J:258:ARG:HG3	1:J:259:HIS:ND1	2.12	0.64
4:D:522:IDS:H3	5:D:523:JHM:O5	1.89	0.64
1:B:368:VAL:HG11	1:C:169:TRP:HZ2	1.62	0.64
1:D:369:GLU:HG3	1:D:371:TYR:CE1	2.33	0.64
1:O:76:GLN:HG3	1:O:453:LYS:HE3	1.79	0.64
1:K:69:GLN:NE2	1:K:71:ARG:HH22	1.95	0.64
1:O:258:ARG:HG3	1:O:259:HIS:ND1	2.13	0.64
1:K:159:LEU:CD2	1:K:331:VAL:HG22	2.28	0.64
1:H:314:HIS:O	1:H:315:LYS:HG3	1.98	0.64
1:B:99:VAL:CG2	1:B:382:ILE:HD13	2.27	0.64
1:A:69:GLN:NE2	1:A:71:ARG:HH22	1.96	0.64
1:F:188:LEU:HD22	1:F:188:LEU:N	2.13	0.64
1:O:109:ARG:H	1:O:308:ASN:HD21	1.46	0.63
1:E:109:ARG:H	1:E:308:ASN:HD21	1.46	0.63
1:F:345:CYS:HB3	1:F:363:GLN:NE2	2.12	0.63
1:G:369:GLU:HG3	1:G:371:TYR:HE1	1.62	0.63
6:B:536:IDS:O62	6:B:537:JHM:O5	2.16	0.63
1:E:216:THR:HG22	1:E:218:CYS:HB2	1.79	0.63
1:E:88:THR:O	1:E:88:THR:HG22	1.98	0.63
1:G:216:THR:HG22	1:G:218:CYS:HB2	1.80	0.63
1:L:151:TYR:OH	1:L:221:PRO:HB2	1.99	0.63
1:G:368:VAL:HG11	1:H:169:TRP:CZ2	2.33	0.63
1:B:138:ASN:ND2	1:B:140:SER:HB3	2.14	0.63
1:O:188:LEU:N	1:O:188:LEU:HD22	2.14	0.63
1:B:89:SER:C	1:J:281:GLY:HA3	2.18	0.63
1:I:216:THR:HG22	1:I:218:CYS:HB2	1.81	0.63
1:C:176:LYS:NZ	1:C:176:LYS:HB2	2.14	0.63
1:O:85:LEU:HB3	1:O:86:PRO:HD2	1.81	0.63
6:F:584:IDS:C6	6:F:585:JHM:H1	2.28	0.63
1:B:176:LYS:NZ	1:B:176:LYS:HB2	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:ASN:ND2	5:C:572:IDS:O62	2.31	0.63
1:E:249:CYS:O	1:E:250:LEU:HD12	1.99	0.63
1:N:85:LEU:HB3	1:N:86:PRO:HD2	1.81	0.63
1:O:99:VAL:CG2	1:O:382:ILE:HD12	2.28	0.63
1:D:159:LEU:CD2	1:D:331:VAL:HG22	2.29	0.63
1:H:159:LEU:CD2	1:H:331:VAL:HG22	2.28	0.63
1:E:69:GLN:NE2	1:E:71:ARG:HH22	1.97	0.63
1:N:88:THR:O	1:N:88:THR:HG22	1.99	0.63
1:N:351:PRO:HG2	5:N:607:JHM:H4	1.80	0.62
1:K:140:SER:OG	1:K:141:GLU:N	2.32	0.62
1:H:70:TYR:CE1	1:H:201:VAL:HG12	2.34	0.62
1:F:99:VAL:HG21	1:F:382:ILE:HD11	1.81	0.62
1:A:99:VAL:HG23	1:A:382:ILE:HD13	1.80	0.62
1:O:70:TYR:CE1	1:O:201:VAL:HG12	2.34	0.62
1:A:352:VAL:HG11	5:B:529:JHM:O9	1.99	0.62
1:D:105:VAL:HG21	1:D:159:LEU:CD1	2.26	0.62
1:M:350:SER:HB3	1:M:351:PRO:HD3	1.80	0.62
1:K:300:VAL:HG13	1:L:255:LEU:HD13	1.81	0.62
1:I:69:GLN:HE21	1:I:71:ARG:HH12	1.47	0.62
1:M:85:LEU:HB3	1:M:86:PRO:HD2	1.82	0.62
1:I:246:MET:O	1:I:246:MET:HG3	1.98	0.62
1:H:99:VAL:HG23	1:H:382:ILE:HD13	1.82	0.62
1:K:258:ARG:HG3	1:K:259:HIS:ND1	2.14	0.62
1:K:169:TRP:CZ2	1:O:368:VAL:HG11	2.33	0.62
1:A:169:TRP:CZ2	1:E:368:VAL:HG11	2.35	0.62
1:B:388:VAL:O	1:B:392:ILE:HG13	1.99	0.62
1:E:151:TYR:CD2	1:E:203:THR:HB	2.35	0.62
1:H:246:MET:O	1:H:246:MET:HG3	1.99	0.62
1:N:369:GLU:HG3	1:N:371:TYR:CE1	2.34	0.62
1:C:121:PRO:HG3	1:D:289:CYS:SG	2.40	0.62
1:F:85:LEU:HB3	1:F:86:PRO:HD2	1.81	0.62
1:I:384:LEU:HB3	1:I:389:MET:CE	2.29	0.62
7:J:561:JHM:C3	7:J:564:IDS:H3	2.30	0.62
1:A:369:GLU:HG3	1:A:371:TYR:CE1	2.34	0.62
1:F:99:VAL:CG2	1:F:382:ILE:HD12	2.29	0.62
1:K:368:VAL:HG11	1:L:169:TRP:CZ2	2.34	0.62
1:J:273:GLN:N	7:J:554:IDS:O2S	2.32	0.62
1:E:188:LEU:HD22	1:E:188:LEU:N	2.15	0.62
5:B:530:IDS:C6	1:C:274:SER:CB	2.74	0.62
1:F:178:ARG:HG3	1:F:178:ARG:NH1	2.15	0.62
1:F:179:PRO:HB2	7:F:569:JHM:S	2.40	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:314:HIS:O	1:L:315:LYS:HG3	2.00	0.62
1:G:368:VAL:HG11	1:H:169:TRP:HZ2	1.65	0.61
1:J:99:VAL:HG23	1:J:382:ILE:HD13	1.82	0.61
1:D:69:GLN:NE2	1:D:71:ARG:HH22	1.98	0.61
1:I:151:TYR:OH	1:I:221:PRO:HB2	1.99	0.61
1:N:351:PRO:HG3	5:N:607:JHM:H4	1.80	0.61
1:H:258:ARG:NH1	1:I:130:GLU:OE1	2.32	0.61
1:C:88:THR:O	1:C:88:THR:HG22	1.99	0.61
1:F:178:ARG:HG3	1:F:178:ARG:HH11	1.65	0.61
1:C:99:VAL:CG2	1:C:382:ILE:HD12	2.30	0.61
1:K:176:LYS:HZ2	1:K:176:LYS:HB2	1.65	0.61
1:M:258:ARG:HG3	1:M:259:HIS:ND1	2.15	0.61
1:N:325:TRP:O	1:N:326:HIS:HB2	2.00	0.61
1:J:188:LEU:N	1:J:188:LEU:HD22	2.15	0.61
1:F:99:VAL:HG23	1:F:382:ILE:HD12	1.83	0.61
1:D:314:HIS:O	1:D:315:LYS:HG3	2.00	0.61
1:F:159:LEU:CD2	1:F:331:VAL:HG22	2.31	0.61
1:N:111:GLN:HB3	1:N:112:PRO:HD2	1.82	0.61
1:B:217:LYS:NZ	1:B:226:GLN:HE21	1.96	0.61
1:C:95:THR:HB	5:C:572:IDS:C6	2.23	0.61
1:F:369:GLU:HG3	1:F:371:TYR:CE1	2.34	0.61
1:O:105:VAL:HG21	1:O:159:LEU:CD1	2.30	0.61
1:M:99:VAL:CG2	1:M:382:ILE:HD12	2.31	0.61
1:C:111:GLN:HB3	1:C:112:PRO:HD2	1.83	0.61
1:O:159:LEU:CD2	1:O:331:VAL:HG22	2.29	0.61
1:B:249:CYS:O	1:B:250:LEU:HD12	2.01	0.61
1:H:151:TYR:CD2	1:H:203:THR:HB	2.36	0.61
1:N:99:VAL:CG2	1:N:382:ILE:HD12	2.31	0.61
1:J:151:TYR:CD2	1:J:203:THR:HB	2.36	0.61
1:E:258:ARG:HG3	1:E:259:HIS:ND1	2.16	0.61
1:O:111:GLN:HB3	1:O:112:PRO:HD2	1.83	0.61
1:A:151:TYR:OH	1:A:221:PRO:HB2	2.01	0.61
5:N:609:JHM:S	1:O:182:GLN:HB2	2.40	0.61
1:O:273:GLN:NE2	1:O:278:LYS:HE2	2.16	0.61
1:B:369:GLU:HG3	1:B:371:TYR:CE1	2.36	0.61
1:F:221:PRO:HD2	1:F:224:ILE:HD11	1.83	0.61
1:D:188:LEU:HD22	1:D:188:LEU:N	2.16	0.61
1:D:151:TYR:OH	1:D:221:PRO:HB2	2.01	0.61
1:K:70:TYR:OH	1:K:232:PRO:HD3	2.00	0.61
1:I:159:LEU:CD2	1:I:331:VAL:HG22	2.31	0.60
1:J:369:GLU:HG3	1:J:371:TYR:HE1	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:99:VAL:CG2	1:K:382:ILE:HD12	2.30	0.60
1:I:138:ASN:ND2	1:I:140:SER:HB3	2.16	0.60
1:E:99:VAL:CG2	1:E:382:ILE:HD13	2.31	0.60
1:A:188:LEU:HD22	1:A:188:LEU:N	2.16	0.60
1:A:349:GLN:HE21	1:A:349:GLN:CA	2.12	0.60
1:I:140:SER:OG	1:I:141:GLU:N	2.35	0.60
1:C:105:VAL:HG21	1:C:159:LEU:CD1	2.30	0.60
1:M:396:ASN:ND2	1:M:398:SER:OG	2.35	0.60
1:N:351:PRO:HB2	5:N:607:JHM:S	2.41	0.60
1:E:105:VAL:HG21	1:E:159:LEU:CD1	2.32	0.60
1:K:396:ASN:ND2	1:K:398:SER:OG	2.34	0.60
6:B:540:IDS:O62	6:B:541:JHM:H1	2.01	0.60
1:G:384:LEU:HD22	1:G:389:MET:HG3	1.84	0.60
1:A:246:MET:HG3	1:A:246:MET:O	2.02	0.60
1:N:99:VAL:HG23	1:N:382:ILE:HD12	1.84	0.60
1:N:345:CYS:HB3	1:N:363:GLN:NE2	2.16	0.60
1:M:109:ARG:H	1:M:308:ASN:HD21	1.48	0.60
1:C:246:MET:O	1:C:246:MET:HG3	2.02	0.60
1:H:278:LYS:NZ	7:H:580:IDS:O1S	2.34	0.60
1:N:69:GLN:HE21	1:N:71:ARG:HH12	1.47	0.60
1:N:151:TYR:OH	1:N:221:PRO:HB2	2.01	0.60
1:L:300:VAL:HG13	1:M:255:LEU:HD13	1.82	0.60
1:B:258:ARG:HG3	1:B:259:HIS:ND1	2.15	0.60
1:E:138:ASN:ND2	1:E:140:SER:HB3	2.16	0.60
1:A:355:GLN:HE22	1:C:280:THR:CG2	2.14	0.60
6:B:540:IDS:O62	6:B:541:JHM:C1	2.49	0.60
1:M:217:LYS:HD3	1:N:277:ILE:HD11	1.84	0.60
1:J:70:TYR:OH	1:J:232:PRO:HD3	2.02	0.60
1:M:99:VAL:HG23	1:M:382:ILE:HD12	1.83	0.60
1:B:151:TYR:OH	1:B:221:PRO:HB2	2.02	0.60
1:K:111:GLN:HB3	1:K:112:PRO:HD2	1.84	0.60
1:F:280:THR:HG23	1:I:355:GLN:HE22	1.66	0.60
1:I:125:LYS:HD2	1:I:261:TRP:NE1	2.16	0.60
1:M:121:PRO:HG3	1:N:289:CYS:SG	2.42	0.60
1:B:85:LEU:HB3	1:B:86:PRO:HD2	1.83	0.60
1:H:105:VAL:HG21	1:H:159:LEU:CD1	2.31	0.60
1:O:99:VAL:HG23	1:O:382:ILE:HD12	1.83	0.60
1:E:325:TRP:O	1:E:326:HIS:HB2	2.01	0.60
1:M:70:TYR:CE1	1:M:201:VAL:HG12	2.37	0.60
1:J:216:THR:HG22	1:J:218:CYS:HB2	1.84	0.59
1:D:85:LEU:HB3	1:D:86:PRO:HD2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:388:VAL:O	1:G:392:ILE:HG13	2.02	0.59
1:H:69:GLN:NE2	1:H:71:ARG:HH22	2.00	0.59
1:N:350:SER:HB3	1:N:351:PRO:HD3	1.83	0.59
1:I:368:VAL:HG11	1:J:169:TRP:HZ2	1.67	0.59
1:H:368:VAL:HG11	1:I:169:TRP:CZ2	2.37	0.59
1:H:258:ARG:HG3	1:H:259:HIS:ND1	2.17	0.59
1:D:240:ASP:OD1	1:D:241:PRO:HD2	2.01	0.59
1:D:180:LEU:HD21	1:D:186:PRO:HA	1.83	0.59
1:G:246:MET:O	1:G:246:MET:HG3	2.02	0.59
1:M:151:TYR:OH	1:M:221:PRO:HB2	2.02	0.59
1:J:99:VAL:CG2	1:J:382:ILE:HD13	2.31	0.59
1:H:216:THR:HG22	1:H:218:CYS:HB2	1.84	0.59
1:M:345:CYS:HB3	1:M:363:GLN:NE2	2.16	0.59
1:M:176:LYS:NZ	1:M:176:LYS:HB2	2.16	0.59
1:J:99:VAL:HG23	1:J:382:ILE:CD1	2.32	0.59
1:C:151:TYR:OH	1:C:221:PRO:HB2	2.02	0.59
1:J:180:LEU:HD21	1:J:186:PRO:HA	1.84	0.59
1:G:384:LEU:HB3	1:G:389:MET:HE1	1.84	0.59
1:O:69:GLN:NE2	1:O:71:ARG:HH22	2.00	0.59
1:J:388:VAL:O	1:J:392:ILE:HG13	2.02	0.59
1:B:99:VAL:HG23	1:B:382:ILE:HD13	1.85	0.59
1:F:76:GLN:HG3	1:F:453:LYS:HE3	1.83	0.59
1:I:88:THR:HG22	1:I:88:THR:O	2.02	0.59
1:F:180:LEU:C	7:F:569:JHM:O8	2.41	0.59
7:H:575:JHM:C1	7:H:578:IDS:O62	2.51	0.59
1:H:99:VAL:CG2	1:H:382:ILE:CD1	2.80	0.59
1:G:105:VAL:HG21	1:G:159:LEU:CD1	2.31	0.59
1:B:121:PRO:CG	1:C:289:CYS:SG	2.90	0.59
1:A:384:LEU:HB3	1:A:389:MET:HE1	1.85	0.59
1:D:325:TRP:O	1:D:326:HIS:HB2	2.03	0.59
1:M:384:LEU:HD22	1:M:389:MET:HG3	1.85	0.59
1:E:151:TYR:OH	1:E:221:PRO:HB2	2.03	0.59
1:H:384:LEU:HB3	1:H:389:MET:CE	2.33	0.59
1:N:68:TYR:CE2	1:N:151:TYR:HB2	2.38	0.59
1:H:109:ARG:H	1:H:308:ASN:HD21	1.49	0.59
1:I:85:LEU:HB3	1:I:86:PRO:HD2	1.84	0.59
1:M:188:LEU:HD22	1:M:188:LEU:N	2.18	0.59
1:G:384:LEU:HB3	1:G:389:MET:CE	2.33	0.58
1:K:440:ASP:HB3	1:K:443:ASP:CG	2.22	0.58
1:A:159:LEU:CD2	1:A:331:VAL:HG22	2.33	0.58
1:O:369:GLU:HG3	1:O:371:TYR:CE1	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:VAL:HG23	1:C:382:ILE:HD12	1.84	0.58
1:B:99:VAL:CG2	1:B:382:ILE:CD1	2.81	0.58
1:O:87:ASP:O	1:O:90:ILE:HG12	2.02	0.58
1:N:216:THR:HG22	1:N:218:CYS:HB2	1.84	0.58
1:A:151:TYR:CD2	1:A:203:THR:HB	2.38	0.58
1:F:151:TYR:CD2	1:F:203:THR:HB	2.38	0.58
1:F:384:LEU:HB3	1:F:389:MET:CE	2.32	0.58
1:D:99:VAL:CG2	1:D:382:ILE:HD13	2.33	0.58
1:I:70:TYR:CE1	1:I:201:VAL:HG12	2.39	0.58
1:J:111:GLN:HB3	1:J:112:PRO:HD2	1.85	0.58
1:L:125:LYS:HD2	1:L:261:TRP:NE1	2.19	0.58
1:A:390:SER:O	1:A:393:GLN:HB3	2.04	0.58
1:J:69:GLN:HE21	1:J:71:ARG:HH12	1.51	0.58
1:E:99:VAL:HG23	1:E:382:ILE:HD13	1.84	0.58
1:E:99:VAL:CG2	1:E:382:ILE:CD1	2.81	0.58
1:G:24:THR:CG2	1:G:320:ASN:HA	2.33	0.58
1:H:188:LEU:N	1:H:188:LEU:HD22	2.19	0.58
1:F:70:TYR:CE1	1:F:201:VAL:HG12	2.39	0.58
1:I:324:CYS:SG	1:I:329:LEU:HD13	2.43	0.58
1:K:86:PRO:HB3	1:K:458:LEU:HD11	1.86	0.58
1:B:325:TRP:O	1:B:326:HIS:HB2	2.02	0.58
1:C:369:GLU:HG3	1:C:371:TYR:CE1	2.38	0.58
1:K:151:TYR:OH	1:K:221:PRO:HB2	2.03	0.58
1:E:324:CYS:SG	1:E:329:LEU:HD13	2.44	0.58
1:L:88:THR:HG22	1:L:88:THR:O	2.04	0.58
1:F:99:VAL:CG2	1:F:382:ILE:CD1	2.81	0.58
1:K:369:GLU:HG3	1:K:371:TYR:CE1	2.38	0.58
1:L:151:TYR:CD2	1:L:203:THR:HB	2.38	0.58
1:K:258:ARG:NH1	1:L:130:GLU:OE1	2.37	0.58
1:H:325:TRP:O	1:H:326:HIS:HB2	2.04	0.58
1:N:258:ARG:HG3	1:N:259:HIS:ND1	2.18	0.58
1:L:384:LEU:HD22	1:L:389:MET:HG3	1.85	0.58
1:D:345:CYS:HB3	1:D:363:GLN:NE2	2.19	0.58
1:F:169:TRP:CZ2	1:J:368:VAL:HG11	2.38	0.58
1:F:249:CYS:O	1:F:250:LEU:HD12	2.03	0.58
6:F:584:IDS:O62	6:F:585:JHM:H1	2.03	0.58
1:J:99:VAL:CG2	1:J:382:ILE:CD1	2.81	0.58
1:I:151:TYR:CD2	1:I:203:THR:HB	2.39	0.58
1:B:226:GLN:O	5:B:528:IDS:O3	2.20	0.57
1:L:181:SER:HA	7:L:614:IDS:O2S	2.04	0.57
1:F:216:THR:HG22	1:F:218:CYS:HB2	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:567:JHM:C2	7:F:570:IDS:C6	2.82	0.57
1:A:68:TYR:CE2	1:A:151:TYR:HB2	2.39	0.57
1:K:70:TYR:CE1	1:K:201:VAL:HG12	2.39	0.57
1:B:151:TYR:CD2	1:B:203:THR:HB	2.39	0.57
1:C:92:ASN:HD22	1:C:95:THR:HG22	1.68	0.57
1:H:369:GLU:HG3	1:H:371:TYR:CE1	2.38	0.57
1:D:99:VAL:HG23	1:D:382:ILE:HD13	1.85	0.57
1:K:368:VAL:HG11	1:L:169:TRP:HZ2	1.69	0.57
1:C:87:ASP:O	1:C:90:ILE:HG12	2.03	0.57
1:I:440:ASP:HB3	1:I:443:ASP:CG	2.24	0.57
1:G:240:ASP:OD1	1:G:241:PRO:HD2	2.05	0.57
1:L:221:PRO:HD2	1:L:224:ILE:HD11	1.86	0.57
1:M:180:LEU:HD21	1:M:186:PRO:HA	1.86	0.57
1:M:99:VAL:CG2	1:M:382:ILE:CD1	2.82	0.57
1:K:68:TYR:CE2	1:K:151:TYR:HB2	2.40	0.57
1:A:99:VAL:HG23	1:A:382:ILE:CD1	2.35	0.57
1:K:216:THR:HG22	1:K:218:CYS:HB2	1.86	0.57
1:L:217:LYS:HD3	1:M:277:ILE:HD11	1.86	0.57
1:D:350:SER:HB3	1:D:351:PRO:HD3	1.86	0.57
1:G:99:VAL:HG23	1:G:382:ILE:HD13	1.86	0.57
1:F:151:TYR:OH	1:F:221:PRO:HB2	2.04	0.57
1:A:314:HIS:O	1:A:315:LYS:HG3	2.04	0.57
1:L:180:LEU:HD21	1:L:186:PRO:HA	1.86	0.57
1:K:384:LEU:HB3	1:K:389:MET:CE	2.34	0.57
1:H:176:LYS:NZ	1:H:176:LYS:HB2	2.19	0.57
1:H:273:GLN:HE22	1:H:278:LYS:HE3	1.69	0.57
1:M:86:PRO:HB3	1:M:458:LEU:HD11	1.87	0.57
1:H:241:PRO:HG2	1:H:242:TYR:H	1.70	0.57
1:O:384:LEU:HB3	1:O:389:MET:CE	2.35	0.57
1:F:87:ASP:O	1:F:90:ILE:HG12	2.04	0.57
1:O:246:MET:HG3	1:O:246:MET:O	2.03	0.57
1:J:45:VAL:HG12	1:J:368:VAL:HG13	1.87	0.57
1:L:369:GLU:HG3	1:L:371:TYR:CE1	2.40	0.57
1:M:69:GLN:HE21	1:M:71:ARG:HH12	1.51	0.57
1:A:277:ILE:HD11	1:E:217:LYS:HD3	1.85	0.57
1:J:110:GLY:O	1:J:111:GLN:O	2.23	0.57
1:N:214:GLN:OE1	1:N:219:GLU:HB2	2.05	0.57
1:K:180:LEU:HD21	1:K:186:PRO:HA	1.86	0.57
1:A:180:LEU:HD21	1:A:186:PRO:HA	1.87	0.57
1:K:188:LEU:HD22	1:K:188:LEU:N	2.20	0.57
7:J:559:JHM:H2A	7:J:562:IDS:O62	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:159:LEU:CD2	1:E:331:VAL:HG22	2.35	0.57
1:E:99:VAL:HG23	1:E:382:ILE:CD1	2.35	0.57
1:G:125:LYS:HD2	1:G:261:TRP:NE1	2.20	0.57
1:C:180:LEU:HD21	1:C:186:PRO:HA	1.86	0.57
7:H:575:JHM:C1	7:H:578:IDS:C6	2.83	0.56
1:M:99:VAL:HG21	1:M:382:ILE:HD11	1.87	0.56
1:E:163:PRO:HB2	1:E:194:VAL:HG13	1.87	0.56
1:A:352:VAL:HG12	5:B:529:JHM:O9	2.04	0.56
1:I:217:LYS:HD3	1:J:277:ILE:HD11	1.88	0.56
1:O:169:TRP:CZ2	1:O:190:LEU:HD13	2.40	0.56
1:J:384:LEU:HB3	1:J:389:MET:CE	2.35	0.56
1:B:176:LYS:HZ2	1:B:176:LYS:HB2	1.68	0.56
1:O:240:ASP:OD1	1:O:241:PRO:HD2	2.05	0.56
1:E:246:MET:HG3	1:E:246:MET:O	2.05	0.56
1:J:276:TYR:O	7:J:555:JHM:O9	2.23	0.56
1:N:126:LEU:HG	1:N:127:ASP:OD2	2.04	0.56
1:L:105:VAL:HG21	1:L:159:LEU:CD1	2.34	0.56
1:E:369:GLU:HG3	1:E:371:TYR:CE1	2.39	0.56
1:H:99:VAL:HG23	1:H:382:ILE:CD1	2.36	0.56
1:E:68:TYR:CE2	1:E:151:TYR:HB2	2.40	0.56
1:O:69:GLN:HE21	1:O:71:ARG:HH12	1.53	0.56
1:C:85:LEU:HB3	1:C:86:PRO:HD2	1.86	0.56
1:C:24:THR:CG2	1:C:320:ASN:HA	2.35	0.56
1:D:258:ARG:HG3	1:D:259:HIS:ND1	2.20	0.56
7:E:550:IDS:O2	7:E:551:JHM:H1	2.05	0.56
1:C:128:ASP:O	1:C:132:SER:HB3	2.05	0.56
1:L:99:VAL:CG2	1:L:382:ILE:HD13	2.35	0.56
1:G:128:ASP:O	1:G:132:SER:HB3	2.04	0.56
1:J:274:SER:CB	7:J:554:IDS:C6	2.82	0.56
1:B:169:TRP:CZ2	1:B:190:LEU:HD13	2.40	0.56
1:F:258:ARG:NH1	1:G:130:GLU:OE1	2.39	0.56
1:I:249:CYS:O	1:I:250:LEU:HD12	2.05	0.56
7:F:567:JHM:H1	7:F:570:IDS:O5	2.02	0.56
1:L:68:TYR:CE2	1:L:151:TYR:HB2	2.40	0.56
7:L:613:JHM:O5	7:L:616:IDS:H3	2.06	0.56
1:K:325:TRP:O	1:K:326:HIS:HB2	2.05	0.56
1:K:105:VAL:HG21	1:K:159:LEU:CD1	2.35	0.56
1:F:105:VAL:HG21	1:F:159:LEU:CD1	2.34	0.56
1:A:99:VAL:CG2	1:A:382:ILE:CD1	2.84	0.56
1:H:163:PRO:HB2	1:H:194:VAL:HG13	1.86	0.56
1:A:283:ARG:HD2	1:E:142:ASP:CG	2.25	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:176:LYS:HB2	1:N:176:LYS:NZ	2.21	0.56
1:O:176:LYS:NZ	1:O:176:LYS:HB2	2.20	0.56
1:L:138:ASN:HD22	1:L:140:SER:HB3	1.71	0.56
1:N:169:TRP:CZ2	1:N:190:LEU:HD13	2.40	0.56
1:M:70:TYR:OH	1:M:232:PRO:HD3	2.05	0.56
1:K:85:LEU:HB3	1:K:86:PRO:HD2	1.86	0.56
1:G:324:CYS:HB3	1:G:328:GLN:O	2.06	0.56
1:O:138:ASN:ND2	1:O:140:SER:HB3	2.20	0.56
5:B:530:IDS:O61	1:C:274:SER:HB3	1.93	0.56
1:F:109:ARG:H	1:F:308:ASN:ND2	2.03	0.56
1:B:99:VAL:HG23	1:B:382:ILE:CD1	2.36	0.56
1:C:214:GLN:OE1	1:C:219:GLU:HB2	2.05	0.56
1:A:85:LEU:HB3	1:A:86:PRO:HD2	1.87	0.56
1:F:187:PRO:HD3	7:J:596:IDS:O61	2.05	0.56
1:J:369:GLU:HG3	1:J:371:TYR:CE1	2.41	0.56
1:N:246:MET:HG3	1:N:246:MET:O	2.05	0.56
1:K:344:ILE:HD12	1:K:344:ILE:N	2.20	0.56
1:O:388:VAL:O	1:O:392:ILE:HG13	2.04	0.56
1:C:76:GLN:HG3	1:C:453:LYS:HE3	1.88	0.56
1:H:217:LYS:HD3	1:I:277:ILE:CD1	2.28	0.56
3:E:502:IDS:C6	3:E:505:JHM:H2A	2.36	0.56
1:J:105:VAL:HG21	1:J:159:LEU:CD1	2.35	0.56
1:D:99:VAL:HG23	1:D:382:ILE:CD1	2.35	0.56
1:N:138:ASN:ND2	1:N:140:SER:HB3	2.20	0.56
1:E:70:TYR:CE1	1:E:201:VAL:HG12	2.41	0.56
1:E:220:VAL:HB	1:E:224:ILE:HD11	1.88	0.56
1:F:368:VAL:HG11	1:G:169:TRP:HZ2	1.63	0.56
1:D:70:TYR:CE1	1:D:201:VAL:HG12	2.41	0.56
1:D:300:VAL:HG13	1:E:255:LEU:HD13	1.88	0.56
1:I:300:VAL:HG13	1:J:255:LEU:HD13	1.87	0.56
1:M:138:ASN:ND2	1:M:140:SER:HB3	2.20	0.56
1:E:384:LEU:HD22	1:E:389:MET:HG3	1.88	0.55
1:K:99:VAL:HG21	1:K:382:ILE:HD11	1.87	0.55
1:F:59:LYS:HE3	6:F:584:IDS:O61	2.06	0.55
1:D:99:VAL:CG2	1:D:382:ILE:CD1	2.83	0.55
1:J:85:LEU:HB3	1:J:86:PRO:HD2	1.88	0.55
1:G:111:GLN:HB3	1:G:112:PRO:HD2	1.88	0.55
1:J:176:LYS:CB	1:J:176:LYS:NZ	2.68	0.55
1:G:368:VAL:HG12	1:G:369:GLU:N	2.20	0.55
1:B:217:LYS:HD3	5:B:529:JHM:O8	2.05	0.55
1:L:99:VAL:HG23	1:L:382:ILE:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:ASP:O	1:B:132:SER:HB3	2.06	0.55
1:B:180:LEU:HD21	1:B:186:PRO:HA	1.87	0.55
7:J:556:IDS:O62	7:J:557:JHM:C1	2.45	0.55
3:E:502:IDS:C6	3:E:505:JHM:C2	2.84	0.55
1:A:368:VAL:HG12	1:A:369:GLU:N	2.20	0.55
1:H:76:GLN:HG3	1:H:453:LYS:HE3	1.88	0.55
1:D:111:GLN:HB3	1:D:112:PRO:HD2	1.88	0.55
1:C:384:LEU:HB3	1:C:389:MET:CE	2.36	0.55
1:H:273:GLN:NE2	1:H:278:LYS:NZ	2.53	0.55
1:F:176:LYS:CD	1:F:176:LYS:H	2.13	0.55
1:I:109:ARG:H	1:I:308:ASN:ND2	2.03	0.55
1:D:87:ASP:O	1:D:90:ILE:HG12	2.07	0.55
1:C:138:ASN:ND2	1:C:140:SER:HB3	2.20	0.55
1:H:111:GLN:HB3	1:H:112:PRO:HD2	1.88	0.55
1:G:188:LEU:N	1:G:188:LEU:HD22	2.21	0.55
6:F:582:IDS:C2	6:F:583:JHM:H1	2.36	0.55
1:L:176:LYS:NZ	1:L:176:LYS:HB2	2.21	0.55
1:A:69:GLN:HE21	1:A:71:ARG:HH12	1.55	0.55
1:E:86:PRO:HB3	1:E:458:LEU:HD11	1.87	0.55
1:F:69:GLN:HE21	1:F:71:ARG:HH12	1.55	0.55
1:K:176:LYS:NZ	1:K:176:LYS:CB	2.70	0.55
1:A:163:PRO:HB2	1:A:194:VAL:HG13	1.88	0.55
1:I:99:VAL:CG2	1:I:382:ILE:HD13	2.37	0.55
1:C:70:TYR:CE1	1:C:201:VAL:HG12	2.42	0.55
1:E:111:GLN:HB3	1:E:112:PRO:HD2	1.89	0.55
1:L:87:ASP:O	1:L:90:ILE:HG12	2.07	0.55
1:G:99:VAL:CG2	1:G:382:ILE:CD1	2.85	0.55
1:D:163:PRO:HB2	1:D:194:VAL:HG13	1.89	0.55
1:F:163:PRO:HB2	1:F:194:VAL:HG13	1.88	0.55
1:K:217:LYS:HD3	1:L:277:ILE:HD11	1.89	0.55
1:J:345:CYS:HB3	1:J:363:GLN:NE2	2.21	0.55
1:D:324:CYS:SG	1:D:329:LEU:HD13	2.47	0.55
1:M:24:THR:CG2	1:M:320:ASN:HA	2.37	0.55
1:M:163:PRO:HB2	1:M:194:VAL:HG13	1.89	0.55
1:K:364:TYR:CD2	1:L:185:CYS:HB2	2.42	0.55
1:N:384:LEU:HB3	1:N:389:MET:CE	2.36	0.55
1:N:99:VAL:HG21	1:N:382:ILE:HD11	1.88	0.55
1:I:384:LEU:HB3	1:I:389:MET:HE1	1.88	0.55
1:D:324:CYS:HB3	1:D:328:GLN:O	2.06	0.55
1:N:324:CYS:SG	1:N:329:LEU:HD13	2.47	0.55
1:L:111:GLN:HB3	1:L:112:PRO:HD2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:385:THR:OG1	1:H:388:VAL:HG23	2.07	0.55
1:E:180:LEU:HD21	1:E:186:PRO:HA	1.89	0.54
1:H:390:SER:O	1:H:393:GLN:HB3	2.08	0.54
1:D:440:ASP:HB3	1:D:443:ASP:CG	2.27	0.54
1:C:258:ARG:HG3	1:C:259:HIS:ND1	2.22	0.54
1:M:88:THR:HG22	1:M:88:THR:O	2.07	0.54
1:H:140:SER:OG	1:H:141:GLU:N	2.40	0.54
1:N:99:VAL:CG2	1:N:382:ILE:CD1	2.84	0.54
1:G:151:TYR:OH	1:G:221:PRO:HB2	2.06	0.54
1:H:240:ASP:OD1	1:H:241:PRO:HD2	2.06	0.54
1:A:210:PHE:HE1	1:A:229:CYS:HG	1.55	0.54
1:M:325:TRP:O	1:M:326:HIS:HB2	2.08	0.54
1:G:226:GLN:HG3	1:H:275:LEU:HD23	1.90	0.54
1:F:91:TYR:O	1:O:281:GLY:HA2	2.05	0.54
1:J:163:PRO:HB2	1:J:194:VAL:HG13	1.89	0.54
1:D:216:THR:HG22	1:D:218:CYS:HB2	1.89	0.54
1:B:387:ASP:HA	1:B:390:SER:OG	2.06	0.54
1:N:180:LEU:HD21	1:N:186:PRO:HA	1.88	0.54
1:G:369:GLU:HG3	1:G:371:TYR:CE1	2.41	0.54
1:N:324:CYS:HB3	1:N:328:GLN:O	2.08	0.54
3:E:502:IDS:O61	3:E:505:JHM:H1	2.06	0.54
1:D:249:CYS:C	1:D:250:LEU:HD12	2.28	0.54
1:J:159:LEU:CD2	1:J:331:VAL:HG22	2.38	0.54
1:H:70:TYR:OH	1:H:232:PRO:HD3	2.07	0.54
1:K:345:CYS:HB3	1:K:363:GLN:NE2	2.23	0.54
1:F:246:MET:HG3	1:F:246:MET:O	2.07	0.54
1:G:140:SER:OG	1:G:141:GLU:N	2.33	0.54
1:C:169:TRP:CZ2	1:C:190:LEU:HD13	2.43	0.54
1:A:300:VAL:HG13	1:B:255:LEU:HD13	1.90	0.54
1:J:173:THR:HG21	7:J:559:JHM:H6A	1.90	0.54
1:N:109:ARG:H	1:N:308:ASN:ND2	2.02	0.54
1:N:86:PRO:HB3	1:N:458:LEU:HD11	1.90	0.54
1:K:350:SER:HB3	1:K:351:PRO:HD3	1.90	0.54
1:I:111:GLN:HB3	1:I:112:PRO:HD2	1.89	0.54
1:B:384:LEU:HD22	1:B:389:MET:HG3	1.90	0.54
1:F:111:GLN:HB3	1:F:112:PRO:HD2	1.88	0.54
1:C:99:VAL:CG2	1:C:382:ILE:CD1	2.85	0.54
1:I:24:THR:CG2	1:I:320:ASN:HA	2.37	0.54
1:G:85:LEU:C	1:G:87:ASP:H	2.11	0.54
1:I:76:GLN:HG3	1:I:453:LYS:HE3	1.88	0.54
1:D:88:THR:O	1:D:88:THR:HG22	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:87:ASP:O	1:M:90:ILE:HG12	2.07	0.54
1:A:240:ASP:OD1	1:A:241:PRO:HD2	2.07	0.54
1:A:440:ASP:HB3	1:A:443:ASP:CG	2.28	0.54
1:G:217:LYS:HG2	1:G:226:GLN:NE2	2.22	0.53
1:K:99:VAL:CG2	1:K:382:ILE:CD1	2.86	0.53
1:A:355:GLN:NE2	1:C:280:THR:HG23	2.22	0.53
1:K:69:GLN:HE21	1:K:71:ARG:HH12	1.56	0.53
1:H:69:GLN:HE21	1:H:71:ARG:HH12	1.56	0.53
1:H:324:CYS:HB3	1:H:328:GLN:O	2.08	0.53
1:B:345:CYS:HB3	1:B:363:GLN:NE2	2.23	0.53
7:F:565:JHM:O9	7:F:568:IDS:O2S	2.27	0.53
1:J:176:LYS:HB2	1:J:176:LYS:HZ2	1.72	0.53
1:D:368:VAL:HG11	1:E:169:TRP:CZ2	2.43	0.53
1:B:176:LYS:CB	1:B:176:LYS:NZ	2.70	0.53
1:E:140:SER:OG	1:E:141:GLU:N	2.37	0.53
1:I:99:VAL:HG23	1:I:382:ILE:HD13	1.90	0.53
1:O:163:PRO:HB2	1:O:194:VAL:HG13	1.90	0.53
1:L:223:ASP:OD1	1:L:224:ILE:HG23	2.08	0.53
1:F:68:TYR:CE2	1:F:151:TYR:HB2	2.44	0.53
1:C:163:PRO:HB2	1:C:194:VAL:HG13	1.90	0.53
1:O:88:THR:O	1:O:88:THR:HG22	2.09	0.53
1:A:349:GLN:HB2	1:A:353:PRO:HD3	1.91	0.53
1:B:258:ARG:NH1	1:C:130:GLU:OE1	2.41	0.53
1:N:140:SER:OG	1:N:141:GLU:N	2.39	0.53
1:L:163:PRO:HB2	1:L:194:VAL:HG13	1.89	0.53
1:E:273:GLN:OE1	1:E:278:LYS:HE2	2.08	0.53
1:K:388:VAL:O	1:K:392:ILE:HG13	2.08	0.53
1:K:163:PRO:HB2	1:K:194:VAL:HG13	1.90	0.53
1:B:440:ASP:HB3	1:B:443:ASP:OD1	2.09	0.53
1:M:314:HIS:O	1:M:315:LYS:HG3	2.08	0.53
1:F:178:ARG:CD	1:J:59:LYS:HB3	2.37	0.53
1:A:387:ASP:HA	1:A:390:SER:OG	2.09	0.53
1:L:246:MET:O	1:L:246:MET:HG3	2.09	0.53
1:K:109:ARG:H	1:K:308:ASN:HD21	1.56	0.53
1:G:76:GLN:HG3	1:G:453:LYS:HE3	1.89	0.53
1:L:107:ILE:N	1:L:107:ILE:HD12	2.24	0.53
7:H:575:JHM:H1	7:H:578:IDS:C6	2.38	0.53
1:H:273:GLN:HE22	1:H:278:LYS:CD	2.22	0.53
1:H:121:PRO:HG3	1:I:289:CYS:SG	2.49	0.53
1:C:325:TRP:O	1:C:326:HIS:HB2	2.08	0.53
1:N:388:VAL:O	1:N:392:ILE:HG13	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:368:VAL:HG12	1:F:369:GLU:N	2.24	0.53
1:D:109:ARG:H	1:D:308:ASN:ND2	2.05	0.53
1:F:130:GLU:OE1	1:J:258:ARG:NH1	2.41	0.53
6:B:540:IDS:O62	6:B:541:JHM:O5	2.27	0.53
1:N:151:TYR:CD2	1:N:203:THR:HB	2.44	0.53
1:E:86:PRO:HB3	1:E:458:LEU:CD1	2.39	0.53
1:E:85:LEU:HB3	1:E:86:PRO:HD2	1.90	0.53
1:E:128:ASP:O	1:E:132:SER:HB3	2.09	0.53
1:A:239:ALA:HB1	7:E:547:JHM:C6	2.35	0.53
1:B:68:TYR:CE2	1:B:151:TYR:HB2	2.44	0.53
1:L:216:THR:HG22	1:L:218:CYS:SG	2.48	0.53
1:O:216:THR:HG22	1:O:218:CYS:HB2	1.91	0.53
1:L:102:CYS:SG	1:L:313:LEU:HD11	2.49	0.53
1:L:54:ALA:HB2	1:L:61:ASP:CG	2.30	0.53
1:N:76:GLN:HG3	1:N:453:LYS:HE3	1.90	0.53
1:N:159:LEU:CD2	1:N:331:VAL:HG22	2.39	0.53
1:H:249:CYS:O	1:H:250:LEU:HD12	2.09	0.53
1:C:140:SER:OG	1:C:141:GLU:N	2.40	0.53
1:B:440:ASP:HB3	1:B:443:ASP:CG	2.29	0.53
1:H:364:TYR:CE2	1:I:268:GLY:HA3	2.42	0.53
1:B:217:LYS:NZ	1:C:274:SER:O	2.41	0.53
7:L:618:IDS:H3	7:L:619:JHM:O5	2.08	0.53
1:N:300:VAL:CG1	1:O:255:LEU:HD13	2.39	0.53
1:F:324:CYS:SG	1:F:329:LEU:HD13	2.49	0.53
1:I:384:LEU:HD22	1:I:389:MET:HG3	1.90	0.52
1:M:384:LEU:HB3	1:M:389:MET:CE	2.39	0.52
1:N:217:LYS:HD3	1:O:277:ILE:HD11	1.92	0.52
1:M:140:SER:OG	1:M:141:GLU:N	2.42	0.52
1:E:390:SER:O	1:E:393:GLN:HB3	2.09	0.52
1:G:109:ARG:H	1:G:308:ASN:ND2	2.04	0.52
1:H:86:PRO:HB3	1:H:458:LEU:HD11	1.91	0.52
1:H:41:ARG:NH1	1:I:190:LEU:HD23	2.24	0.52
1:A:102:CYS:SG	1:A:313:LEU:HD11	2.50	0.52
1:L:463:TYR:HB3	1:L:464:PRO:HD2	1.91	0.52
1:I:258:ARG:HG3	1:I:259:HIS:ND1	2.24	0.52
1:O:180:LEU:HD21	1:O:186:PRO:HA	1.90	0.52
1:J:349:GLN:HB2	1:J:353:PRO:HD3	1.90	0.52
1:J:444:LYS:HD2	7:J:563:JHM:S	2.48	0.52
1:L:249:CYS:O	1:L:250:LEU:HD12	2.09	0.52
1:N:220:VAL:HB	1:N:224:ILE:HD11	1.91	0.52
1:C:68:TYR:CE2	1:C:151:TYR:HB2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:390:SER:O	1:F:393:GLN:HB3	2.10	0.52
1:K:128:ASP:O	1:K:132:SER:HB3	2.10	0.52
1:J:273:GLN:CB	7:J:555:JHM:O1	2.53	0.52
1:N:462:GLN:HE22	1:O:21:VAL:HB	1.74	0.52
1:G:217:LYS:NZ	1:H:274:SER:O	2.41	0.52
1:J:277:ILE:HA	7:J:555:JHM:O9	2.09	0.52
1:K:99:VAL:HG23	1:K:382:ILE:HD12	1.90	0.52
1:A:384:LEU:HD22	1:A:389:MET:HG3	1.91	0.52
1:G:163:PRO:HB2	1:G:194:VAL:HG13	1.90	0.52
1:C:344:ILE:N	1:C:344:ILE:HD12	2.24	0.52
1:O:387:ASP:HA	1:O:390:SER:OG	2.10	0.52
1:F:128:ASP:O	1:F:132:SER:HB3	2.10	0.52
1:G:88:THR:HG22	1:G:88:THR:O	2.10	0.52
1:K:384:LEU:HD22	1:K:389:MET:HG3	1.91	0.52
1:G:324:CYS:SG	1:G:329:LEU:HD13	2.50	0.52
1:I:142:ASP:CG	1:J:283:ARG:HD2	2.29	0.52
1:O:396:ASN:ND2	1:O:398:SER:OG	2.43	0.52
1:O:314:HIS:O	1:O:315:LYS:HG3	2.09	0.52
1:A:111:GLN:HB3	1:A:112:PRO:HD2	1.91	0.52
1:A:110:GLY:O	1:A:111:GLN:O	2.27	0.52
1:B:217:LYS:HZ2	1:B:226:GLN:HE21	1.49	0.52
1:J:249:CYS:C	1:J:250:LEU:HD12	2.30	0.52
1:E:156:LEU:HA	1:E:250:LEU:O	2.10	0.52
1:G:99:VAL:HG21	1:G:382:ILE:HD13	1.91	0.52
1:K:343:THR:C	1:K:344:ILE:HD12	2.29	0.52
1:C:232:PRO:HB2	1:C:234:TYR:CE1	2.44	0.52
1:K:364:TYR:CG	1:L:185:CYS:HB2	2.45	0.52
1:N:387:ASP:HA	1:N:390:SER:OG	2.10	0.52
1:F:342:LEU:HD22	1:G:208:MET:SD	2.50	0.52
1:F:182:GLN:O	7:F:567:JHM:O9	2.28	0.52
1:D:68:TYR:CE2	1:D:151:TYR:HB2	2.45	0.52
1:H:99:VAL:HG21	1:H:382:ILE:CD1	2.40	0.52
1:O:384:LEU:HD22	1:O:389:MET:HG3	1.91	0.52
1:A:24:THR:CG2	1:A:320:ASN:HA	2.40	0.52
1:L:388:VAL:O	1:L:392:ILE:HG13	2.10	0.52
1:A:273:GLN:NE2	4:D:510:IDS:O2S	2.43	0.52
1:M:54:ALA:HB2	1:M:61:ASP:CG	2.29	0.52
1:N:351:PRO:CG	5:N:608:IDS:C1	2.87	0.52
1:J:273:GLN:HB2	7:J:554:IDS:C3	2.40	0.52
1:C:273:GLN:NE2	1:C:278:LYS:HZ2	2.07	0.52
1:O:86:PRO:HB3	1:O:458:LEU:HD11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:344:ILE:N	1:N:344:ILE:HD12	2.24	0.52
1:I:99:VAL:CG2	1:I:382:ILE:CD1	2.88	0.52
1:E:76:GLN:HG3	1:E:453:LYS:HE3	1.92	0.52
1:I:325:TRP:O	1:I:326:HIS:HB2	2.09	0.52
1:F:217:LYS:HE3	1:F:226:GLN:NE2	2.25	0.51
5:E:513:JHM:O5	4:E:516:IDS:O62	2.27	0.51
1:F:223:ASP:OD1	1:F:224:ILE:HG23	2.10	0.51
1:K:384:LEU:HB3	1:K:389:MET:HE1	1.91	0.51
1:F:324:CYS:HB3	1:F:328:GLN:O	2.11	0.51
1:B:123:TYR:HD2	1:B:125:LYS:HB2	1.76	0.51
1:B:79:ASP:O	1:B:83:PHE:HB2	2.10	0.51
1:J:387:ASP:HA	1:J:390:SER:OG	2.10	0.51
1:G:30:ARG:HG2	1:G:380:CYS:SG	2.50	0.51
1:C:92:ASN:ND2	1:C:95:THR:HG22	2.25	0.51
1:B:87:ASP:O	1:B:90:ILE:HG12	2.10	0.51
1:H:384:LEU:HD22	1:H:389:MET:HG3	1.92	0.51
1:G:138:ASN:ND2	1:G:140:SER:HB3	2.25	0.51
1:B:324:CYS:HB3	1:B:328:GLN:O	2.10	0.51
1:L:70:TYR:OH	1:L:232:PRO:HD3	2.09	0.51
1:D:86:PRO:HB3	1:D:458:LEU:HD11	1.92	0.51
1:B:390:SER:O	1:B:393:GLN:HB3	2.11	0.51
1:G:87:ASP:O	1:G:90:ILE:HG12	2.10	0.51
1:F:79:ASP:O	1:F:83:PHE:HB2	2.10	0.51
1:L:178:ARG:HG3	7:L:619:JHM:S	2.50	0.51
1:K:368:VAL:HG12	1:K:369:GLU:N	2.25	0.51
1:G:242:TYR:CZ	1:G:395:MET:HA	2.45	0.51
5:E:513:JHM:O5	4:E:516:IDS:C6	2.58	0.51
1:E:124:ASN:OD1	1:E:264:ALA:HB3	2.11	0.51
1:A:87:ASP:O	1:A:90:ILE:HG12	2.10	0.51
1:A:72:VAL:HG22	1:A:332:THR:HG23	1.93	0.51
1:I:220:VAL:HB	1:I:224:ILE:HD11	1.93	0.51
1:O:24:THR:CG2	1:O:320:ASN:HA	2.41	0.51
1:O:155:GLN:HA	1:O:334:VAL:O	2.11	0.51
1:C:176:LYS:NZ	1:C:176:LYS:CB	2.72	0.51
1:G:85:LEU:HB3	1:G:86:PRO:HD2	1.92	0.51
1:D:54:ALA:HB2	1:D:61:ASP:CG	2.31	0.51
1:O:307:PHE:HE1	1:O:335:ASP:HB2	1.76	0.51
1:E:126:LEU:HG	1:E:127:ASP:OD2	2.11	0.51
1:L:109:ARG:H	1:L:308:ASN:ND2	2.06	0.51
1:K:86:PRO:HB3	1:K:458:LEU:CD1	2.40	0.51
1:B:142:ASP:CG	1:C:283:ARG:HD2	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:240:ASP:OD1	1:N:241:PRO:HD2	2.11	0.51
1:F:388:VAL:O	1:F:392:ILE:HG13	2.10	0.51
1:F:384:LEU:HD22	1:F:389:MET:HG3	1.92	0.51
1:G:349:GLN:HB2	1:G:353:PRO:HD3	1.92	0.51
1:B:163:PRO:HB2	1:B:194:VAL:HG13	1.93	0.51
1:N:163:PRO:HB2	1:N:194:VAL:HG13	1.92	0.51
1:N:156:LEU:HA	1:N:250:LEU:O	2.11	0.51
1:N:45:VAL:HG12	1:N:368:VAL:HG22	1.92	0.51
1:G:108:GLY:HA2	1:G:308:ASN:ND2	2.26	0.51
1:A:105:VAL:HG21	1:A:159:LEU:CD1	2.39	0.51
1:O:70:TYR:CZ	1:O:201:VAL:HG12	2.45	0.51
1:B:246:MET:HG3	1:B:246:MET:O	2.10	0.51
1:C:324:CYS:SG	1:C:329:LEU:HD13	2.51	0.51
1:F:283:ARG:HD2	1:J:142:ASP:CG	2.30	0.51
1:J:88:THR:O	1:J:88:THR:HG22	2.11	0.51
1:N:107:ILE:HD13	1:N:107:ILE:N	2.26	0.51
1:F:178:ARG:NH1	1:J:59:LYS:HD2	2.26	0.51
1:C:99:VAL:HG21	1:C:382:ILE:HD11	1.92	0.51
1:E:70:TYR:OH	1:E:232:PRO:HD3	2.11	0.51
1:I:99:VAL:HG23	1:I:382:ILE:CD1	2.40	0.51
1:C:70:TYR:OH	1:C:232:PRO:HD3	2.11	0.51
1:N:384:LEU:HD22	1:N:389:MET:HG3	1.92	0.51
1:L:107:ILE:H	1:L:107:ILE:HD12	1.76	0.51
1:N:314:HIS:CG	1:N:315:LYS:H	2.29	0.51
1:E:176:LYS:NZ	1:E:176:LYS:HB2	2.26	0.51
1:I:368:VAL:HG12	1:I:369:GLU:N	2.26	0.50
1:D:140:SER:OG	1:D:141:GLU:N	2.44	0.50
1:I:70:TYR:OH	1:I:232:PRO:HD3	2.11	0.50
1:O:241:PRO:HG2	1:O:242:TYR:H	1.76	0.50
1:J:86:PRO:HB3	1:J:458:LEU:CD1	2.42	0.50
1:L:69:GLN:NE2	1:L:71:ARG:HH22	2.08	0.50
1:G:387:ASP:HB3	1:N:280:THR:HG22	1.92	0.50
1:N:102:CYS:SG	1:N:313:LEU:HD11	2.51	0.50
1:B:300:VAL:CG1	1:C:255:LEU:HD13	2.38	0.50
1:F:217:LYS:HD3	1:G:277:ILE:CD1	2.38	0.50
7:F:567:JHM:H1	7:F:570:IDS:C6	2.34	0.50
1:J:109:ARG:H	1:J:308:ASN:ND2	2.09	0.50
1:H:123:TYR:HD2	1:H:125:LYS:HB2	1.77	0.50
1:J:30:ARG:HG2	1:J:380:CYS:SG	2.51	0.50
1:I:128:ASP:O	1:I:132:SER:HB3	2.11	0.50
1:J:324:CYS:HB3	1:J:328:GLN:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:387:ASP:HA	1:M:390:SER:OG	2.11	0.50
1:J:440:ASP:HB3	1:J:443:ASP:CG	2.31	0.50
1:B:43:LEU:HD12	1:B:369:GLU:O	2.12	0.50
1:H:87:ASP:O	1:H:90:ILE:HG12	2.11	0.50
1:B:109:ARG:H	1:B:308:ASN:ND2	2.09	0.50
1:B:99:VAL:HG21	1:B:382:ILE:CD1	2.42	0.50
1:E:108:GLY:HA2	1:E:308:ASN:ND2	2.27	0.50
1:C:151:TYR:CD2	1:C:203:THR:HB	2.46	0.50
1:L:99:VAL:CG2	1:L:382:ILE:CD1	2.89	0.50
1:N:241:PRO:HG2	1:N:242:TYR:H	1.76	0.50
1:O:325:TRP:O	1:O:326:HIS:HB2	2.12	0.50
5:N:608:IDS:O62	5:N:609:JHM:H1	2.08	0.50
7:F:567:JHM:H2A	7:F:570:IDS:O61	2.12	0.50
1:N:70:TYR:OH	1:N:232:PRO:HD3	2.11	0.50
1:D:384:LEU:HB3	1:D:389:MET:CE	2.41	0.50
1:L:261:TRP:CZ3	1:L:294:SER:HB3	2.46	0.50
1:L:325:TRP:O	1:L:326:HIS:HB2	2.11	0.50
1:N:56:GLY:O	4:N:601:JHM:H2	2.11	0.50
1:F:325:TRP:O	1:F:326:HIS:HB2	2.11	0.50
1:M:76:GLN:HG3	1:M:453:LYS:HE3	1.94	0.50
1:B:349:GLN:HB2	1:B:353:PRO:HD3	1.92	0.50
1:C:440:ASP:HB3	1:C:443:ASP:CG	2.32	0.50
1:B:90:ILE:C	1:J:281:GLY:HA2	2.31	0.50
1:M:151:TYR:CG	1:M:203:THR:HB	2.46	0.50
1:J:140:SER:OG	1:J:141:GLU:N	2.44	0.50
1:N:121:PRO:HG3	1:O:289:CYS:SG	2.52	0.50
1:G:216:THR:O	1:G:217:LYS:HB2	2.10	0.50
1:G:99:VAL:HG21	1:G:382:ILE:CD1	2.42	0.50
1:I:24:THR:HG23	1:I:320:ASN:HA	1.94	0.50
1:N:24:THR:CG2	1:N:320:ASN:HA	2.41	0.50
1:C:364:TYR:CG	1:D:185:CYS:HB2	2.46	0.50
1:N:390:SER:O	1:N:393:GLN:HB3	2.12	0.50
1:E:174:ALA:N	5:E:511:JHM:O8	2.43	0.50
1:O:324:CYS:HB3	1:O:328:GLN:O	2.10	0.50
1:D:77:LEU:HB3	1:D:78:PRO:HD2	1.93	0.50
1:D:155:GLN:HA	1:D:334:VAL:O	2.12	0.50
1:A:325:TRP:O	1:A:326:HIS:HB2	2.12	0.50
1:C:368:VAL:HG12	1:C:369:GLU:N	2.27	0.50
1:O:156:LEU:HA	1:O:250:LEU:O	2.11	0.50
1:M:214:GLN:OE1	1:M:219:GLU:HB2	2.12	0.50
1:I:77:LEU:HB3	1:I:78:PRO:HD2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:142:ASP:CG	1:L:283:ARG:HD2	2.32	0.50
1:E:169:TRP:CZ2	1:E:190:LEU:HD13	2.46	0.50
1:H:138:ASN:HD22	1:H:140:SER:HB3	1.76	0.50
1:L:24:THR:CG2	1:L:320:ASN:HA	2.42	0.50
1:G:345:CYS:HB3	1:G:363:GLN:NE2	2.27	0.50
1:K:121:PRO:HG3	1:L:289:CYS:SG	2.52	0.50
1:B:98:LEU:HD23	1:B:381:THR:HG22	1.94	0.50
4:D:504:IDS:H3	2:E:501:JHM:O5	2.12	0.49
1:C:324:CYS:HB3	1:C:328:GLN:O	2.11	0.49
1:K:255:LEU:HD13	1:O:300:VAL:HG13	1.93	0.49
1:D:390:SER:O	1:D:393:GLN:HB3	2.13	0.49
1:H:349:GLN:HB2	1:H:353:PRO:HD3	1.94	0.49
1:A:128:ASP:O	1:A:132:SER:HB3	2.11	0.49
1:K:24:THR:CG2	1:K:320:ASN:HA	2.41	0.49
1:A:59:LYS:HG2	1:A:60:GLN:N	2.26	0.49
1:H:273:GLN:HE22	1:H:278:LYS:HD3	1.77	0.49
1:K:156:LEU:HA	1:K:250:LEU:O	2.11	0.49
1:A:130:GLU:OE1	1:E:258:ARG:NH1	2.45	0.49
1:O:110:GLY:O	1:O:111:GLN:O	2.30	0.49
1:G:390:SER:O	1:G:393:GLN:HB3	2.11	0.49
1:B:76:GLN:HG3	1:B:453:LYS:HE3	1.93	0.49
1:M:324:CYS:HB3	1:M:328:GLN:O	2.12	0.49
1:L:349:GLN:HB2	1:L:353:PRO:HD3	1.94	0.49
1:C:216:THR:HG22	1:C:218:CYS:HB2	1.94	0.49
1:A:462:GLN:HE22	1:B:21:VAL:H	1.60	0.49
1:N:444:LYS:HA	1:N:444:LYS:CE	2.38	0.49
1:I:68:TYR:CE2	1:I:151:TYR:HB2	2.47	0.49
1:E:99:VAL:HG21	1:E:382:ILE:CD1	2.43	0.49
1:K:24:THR:HG23	1:K:320:ASN:HA	1.94	0.49
1:K:387:ASP:HA	1:K:390:SER:OG	2.12	0.49
1:A:107:ILE:HD13	1:A:107:ILE:N	2.28	0.49
1:G:217:LYS:HG2	1:G:226:GLN:HE22	1.78	0.49
1:B:156:LEU:HA	1:B:250:LEU:O	2.13	0.49
1:A:109:ARG:H	1:A:308:ASN:ND2	2.08	0.49
1:J:87:ASP:O	1:J:90:ILE:HG12	2.12	0.49
1:C:125:LYS:HD2	1:C:261:TRP:NE1	2.26	0.49
1:E:214:GLN:OE1	1:E:219:GLU:HB2	2.12	0.49
1:G:70:TYR:CZ	1:G:201:VAL:HG12	2.47	0.49
1:A:169:TRP:HZ2	1:E:368:VAL:HG11	1.76	0.49
6:B:540:IDS:C6	6:B:541:JHM:C1	2.90	0.49
1:M:109:ARG:H	1:M:308:ASN:ND2	2.09	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:280:THR:CG2	1:I:355:GLN:HE22	2.25	0.49
1:H:220:VAL:HB	1:H:224:ILE:HD11	1.95	0.49
1:F:88:THR:HG22	1:F:88:THR:O	2.11	0.49
1:N:105:VAL:HG12	1:N:106:GLU:N	2.27	0.49
1:A:357:ASP:HA	1:B:141:GLU:HG3	1.94	0.49
1:H:128:ASP:O	1:H:132:SER:HB3	2.13	0.49
1:M:142:ASP:CG	1:N:283:ARG:HD2	2.33	0.49
1:F:36:HIS:ND1	1:F:36:HIS:C	2.65	0.49
1:H:176:LYS:NZ	1:H:176:LYS:CB	2.75	0.49
1:C:384:LEU:HB3	1:C:389:MET:HE1	1.95	0.49
1:C:102:CYS:SG	1:C:313:LEU:HD11	2.53	0.49
1:C:349:GLN:HB2	1:C:353:PRO:HD3	1.94	0.49
1:N:349:GLN:HB2	1:N:353:PRO:HD3	1.95	0.49
1:N:249:CYS:C	1:N:250:LEU:HD12	2.33	0.49
1:E:249:CYS:C	1:E:250:LEU:HD12	2.32	0.49
1:J:169:TRP:CZ2	1:J:190:LEU:HD13	2.47	0.49
1:G:108:GLY:HA2	1:G:308:ASN:HD22	1.78	0.49
1:G:24:THR:HG21	1:G:320:ASN:HA	1.95	0.49
1:L:99:VAL:HG23	1:L:382:ILE:CD1	2.42	0.49
1:D:440:ASP:HB3	1:D:443:ASP:OD1	2.13	0.49
1:J:24:THR:CG2	1:J:320:ASN:HA	2.42	0.49
1:L:121:PRO:HG3	1:M:289:CYS:SG	2.52	0.49
1:H:88:THR:O	1:H:88:THR:HG22	2.12	0.49
1:K:36:HIS:ND1	1:K:36:HIS:C	2.66	0.49
1:B:444:LYS:HE2	1:B:444:LYS:CA	2.30	0.49
1:G:249:CYS:O	1:G:250:LEU:HD12	2.13	0.49
1:G:69:GLN:HE21	1:G:71:ARG:HH12	1.61	0.49
1:M:86:PRO:HB3	1:M:458:LEU:CD1	2.43	0.49
1:H:384:LEU:HB3	1:H:389:MET:HE2	1.95	0.49
1:B:384:LEU:HB3	1:B:389:MET:CE	2.42	0.49
1:H:364:TYR:CZ	1:I:268:GLY:HA3	2.48	0.49
1:G:216:THR:CG2	1:G:218:CYS:HB2	2.43	0.49
1:A:300:VAL:O	1:A:300:VAL:HG13	2.12	0.49
1:H:92:ASN:O	1:H:94:GLU:N	2.46	0.49
1:A:41:ARG:NH2	1:B:233:ASP:OD2	2.46	0.49
1:F:121:PRO:HG3	1:G:289:CYS:SG	2.52	0.49
1:I:364:TYR:CD2	1:J:185:CYS:HB2	2.48	0.49
1:F:43:LEU:HD21	1:G:169:TRP:HH2	1.78	0.48
1:F:105:VAL:HG12	1:F:106:GLU:N	2.27	0.48
1:N:188:LEU:CD2	1:N:188:LEU:N	2.74	0.48
1:G:99:VAL:HG23	1:G:382:ILE:CD1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:368:VAL:HG12	1:E:369:GLU:N	2.28	0.48
1:E:109:ARG:H	1:E:308:ASN:ND2	2.11	0.48
1:E:440:ASP:HB3	1:E:443:ASP:CG	2.34	0.48
1:D:388:VAL:O	1:D:392:ILE:HG13	2.13	0.48
1:E:123:TYR:HD2	1:E:125:LYS:HB2	1.78	0.48
1:I:345:CYS:HB3	1:I:363:GLN:NE2	2.28	0.48
1:G:143:VAL:HG12	1:G:143:VAL:O	2.13	0.48
1:C:105:VAL:HG12	1:C:106:GLU:N	2.28	0.48
1:J:51:ARG:NH2	7:J:599:JHM:H3	2.26	0.48
1:J:384:LEU:HB3	1:J:389:MET:HE2	1.95	0.48
1:F:344:ILE:HD12	1:F:344:ILE:N	2.28	0.48
1:F:384:LEU:HB3	1:F:389:MET:HE2	1.93	0.48
1:L:387:ASP:HA	1:L:390:SER:OG	2.13	0.48
1:E:87:ASP:O	1:E:90:ILE:HG12	2.13	0.48
1:J:76:GLN:HG3	1:J:453:LYS:HE3	1.95	0.48
1:D:125:LYS:HD2	1:D:261:TRP:NE1	2.27	0.48
1:J:128:ASP:O	1:J:132:SER:HB3	2.13	0.48
1:C:109:ARG:H	1:C:308:ASN:ND2	2.08	0.48
1:C:388:VAL:O	1:C:392:ILE:HG13	2.13	0.48
1:G:300:VAL:O	1:G:300:VAL:HG13	2.13	0.48
1:L:128:ASP:O	1:L:132:SER:HB3	2.13	0.48
1:J:344:ILE:N	1:J:344:ILE:HD12	2.28	0.48
1:E:216:THR:O	1:E:217:LYS:HB2	2.13	0.48
1:L:300:VAL:O	1:L:300:VAL:HG13	2.14	0.48
1:L:384:LEU:HB3	1:L:389:MET:CE	2.43	0.48
1:C:86:PRO:HB3	1:C:458:LEU:HD11	1.94	0.48
1:E:344:ILE:HG22	1:E:345:CYS:N	2.28	0.48
1:F:364:TYR:CE2	1:G:268:GLY:HA3	2.49	0.48
1:O:161:CYS:SG	1:O:244:ASP:HB3	2.53	0.48
1:F:314:HIS:O	1:F:315:LYS:HG3	2.13	0.48
1:L:241:PRO:HG2	1:L:242:TYR:H	1.79	0.48
1:B:111:GLN:HB3	1:B:112:PRO:HD2	1.95	0.48
1:B:227:SER:OG	5:B:528:IDS:H3	2.14	0.48
1:F:178:ARG:CZ	1:J:59:LYS:HD2	2.43	0.48
1:D:169:TRP:CZ2	1:D:190:LEU:HD13	2.49	0.48
1:H:79:ASP:O	1:H:83:PHE:HB2	2.12	0.48
1:G:364:TYR:CG	1:H:185:CYS:HB2	2.48	0.48
1:O:76:GLN:CG	1:O:453:LYS:HE3	2.42	0.48
1:I:344:ILE:HG22	1:I:345:CYS:N	2.28	0.48
1:M:122:PHE:O	1:M:218:CYS:HB3	2.13	0.48
1:H:165:ILE:HD12	1:H:237:MET:HG2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:155:GLN:HA	1:N:334:VAL:O	2.14	0.48
1:J:79:ASP:O	1:J:83:PHE:HB2	2.14	0.48
1:A:76:GLN:HG3	1:A:453:LYS:HE3	1.96	0.48
1:E:349:GLN:HB2	1:E:353:PRO:HD3	1.95	0.48
1:F:72:VAL:HG21	1:F:195:LEU:O	2.14	0.48
1:K:324:CYS:HB3	1:K:328:GLN:O	2.12	0.48
1:J:59:LYS:O	7:J:596:IDS:O3	2.17	0.48
1:A:70:TYR:OH	1:A:232:PRO:HD3	2.13	0.48
1:O:68:TYR:CE2	1:O:151:TYR:HB2	2.48	0.48
1:F:357:ASP:OD2	1:G:141:GLU:HG3	2.13	0.48
1:C:217:LYS:HE3	1:C:226:GLN:NE2	2.28	0.48
1:N:128:ASP:O	1:N:132:SER:HB3	2.14	0.48
1:K:125:LYS:HD2	1:K:261:TRP:NE1	2.29	0.48
1:M:300:VAL:CG1	1:N:255:LEU:HD13	2.38	0.48
1:D:138:ASN:HD22	1:D:140:SER:HB3	1.75	0.48
1:L:188:LEU:N	1:L:188:LEU:CD2	2.76	0.48
1:D:151:TYR:CG	1:D:203:THR:HB	2.48	0.48
1:O:232:PRO:HB2	1:O:234:TYR:CE1	2.49	0.48
1:G:300:VAL:HG13	1:H:255:LEU:HD13	1.94	0.48
1:B:102:CYS:SG	1:B:313:LEU:HD11	2.54	0.48
1:N:92:ASN:O	1:N:96:GLN:HG2	2.13	0.48
1:N:117:LEU:HD11	1:O:293:PRO:HB3	1.96	0.48
1:G:176:LYS:NZ	1:G:176:LYS:HB2	2.28	0.48
1:A:357:ASP:OD2	1:B:141:GLU:HG3	2.14	0.48
1:B:138:ASN:HD22	1:B:140:SER:HB3	1.79	0.48
1:M:176:LYS:NZ	1:M:176:LYS:CB	2.76	0.48
1:A:86:PRO:HB3	1:A:458:LEU:HD11	1.96	0.48
1:G:35:TYR:OH	1:G:86:PRO:HD3	2.13	0.48
1:I:396:ASN:ND2	1:I:398:SER:OG	2.47	0.48
1:F:241:PRO:HG2	1:F:242:TYR:H	1.79	0.48
1:O:349:GLN:HB2	1:O:353:PRO:HD3	1.95	0.48
1:J:126:LEU:HG	1:J:127:ASP:OD2	2.14	0.48
1:A:239:ALA:CB	7:E:547:JHM:H6	2.41	0.48
1:J:232:PRO:HB2	1:J:234:TYR:CE1	2.49	0.48
1:D:108:GLY:HA2	1:D:308:ASN:ND2	2.29	0.48
1:E:108:GLY:HA2	1:E:308:ASN:HD22	1.79	0.48
1:O:385:THR:OG1	1:O:388:VAL:HG23	2.14	0.48
1:D:92:ASN:O	1:D:94:GLU:N	2.47	0.48
1:O:345:CYS:HB3	1:O:363:GLN:NE2	2.29	0.48
1:N:305:GLN:HA	1:N:305:GLN:NE2	2.29	0.48
1:L:155:GLN:HA	1:L:334:VAL:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:344:ILE:N	1:D:344:ILE:HD12	2.29	0.48
1:C:92:ASN:ND2	5:C:572:IDS:C6	2.76	0.47
1:F:187:PRO:CD	7:J:596:IDS:O61	2.62	0.47
1:M:176:LYS:HZ2	1:M:176:LYS:HB2	1.79	0.47
1:J:86:PRO:HB3	1:J:458:LEU:HD11	1.95	0.47
1:L:69:GLN:HE21	1:L:71:ARG:HH12	1.62	0.47
1:K:463:TYR:HB3	1:K:464:PRO:HD2	1.96	0.47
1:K:349:GLN:HB2	1:K:353:PRO:HD3	1.96	0.47
1:K:87:ASP:O	1:K:90:ILE:HG12	2.14	0.47
1:A:88:THR:HG22	1:A:88:THR:O	2.14	0.47
1:A:366:ARG:HA	1:A:366:ARG:HD3	1.76	0.47
1:J:368:VAL:HG12	1:J:369:GLU:N	2.28	0.47
1:H:169:TRP:CZ2	1:H:190:LEU:HD13	2.49	0.47
1:K:440:ASP:HB3	1:K:443:ASP:OD1	2.13	0.47
1:L:85:LEU:C	1:L:87:ASP:H	2.15	0.47
1:A:223:ASP:OD1	1:A:224:ILE:HG23	2.14	0.47
1:F:98:LEU:HD23	1:F:381:THR:HG22	1.96	0.47
1:O:440:ASP:HB3	1:O:443:ASP:CG	2.34	0.47
1:B:114:GLY:HA3	1:B:340:THR:HG23	1.96	0.47
1:F:126:LEU:CB	1:F:262:ASN:HB3	2.35	0.47
1:B:45:VAL:HG12	1:B:368:VAL:HG22	1.97	0.47
1:J:151:TYR:CG	1:J:203:THR:HB	2.49	0.47
1:K:138:ASN:ND2	1:K:140:SER:HB3	2.29	0.47
1:O:70:TYR:OH	1:O:232:PRO:HD3	2.14	0.47
1:J:325:TRP:O	1:J:326:HIS:HB2	2.15	0.47
1:D:76:GLN:HG3	1:D:453:LYS:HE3	1.96	0.47
1:C:107:ILE:N	1:C:107:ILE:HD12	2.29	0.47
1:J:441:PRO:O	7:J:563:JHM:H2A	2.14	0.47
1:H:68:TYR:CE2	1:H:151:TYR:HB2	2.50	0.47
1:B:188:LEU:N	1:B:188:LEU:CD2	2.76	0.47
5:E:513:JHM:H6A	4:E:516:IDS:O61	2.15	0.47
1:J:98:LEU:HD23	1:J:381:THR:HG22	1.97	0.47
1:D:24:THR:CG2	1:D:320:ASN:HA	2.44	0.47
1:D:128:ASP:O	1:D:132:SER:HB3	2.15	0.47
1:J:36:HIS:C	1:J:36:HIS:ND1	2.67	0.47
1:E:300:VAL:HG13	1:E:300:VAL:O	2.15	0.47
1:A:24:THR:HG23	1:A:320:ASN:HA	1.96	0.47
1:F:242:TYR:CZ	1:F:395:MET:HA	2.49	0.47
1:A:345:CYS:HB3	1:A:363:GLN:NE2	2.29	0.47
1:A:214:GLN:OE1	1:A:219:GLU:HB2	2.14	0.47
1:F:156:LEU:HA	1:F:250:LEU:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:85:LEU:C	1:H:87:ASP:H	2.17	0.47
1:D:86:PRO:HB3	1:D:458:LEU:CD1	2.44	0.47
1:F:349:GLN:HB2	1:F:353:PRO:HD3	1.97	0.47
1:B:396:ASN:ND2	1:B:398:SER:OG	2.47	0.47
1:L:76:GLN:HG3	1:L:453:LYS:HE3	1.96	0.47
1:A:55:GLY:HA2	1:A:58:ASN:O	2.13	0.47
1:M:128:ASP:O	1:M:132:SER:HB3	2.14	0.47
1:F:178:ARG:HH11	1:F:178:ARG:CG	2.25	0.47
1:J:274:SER:OG	7:J:554:IDS:C6	2.63	0.47
1:K:105:VAL:HG12	1:K:106:GLU:N	2.30	0.47
1:A:249:CYS:O	1:A:250:LEU:HD12	2.14	0.47
1:J:105:VAL:HG12	1:J:106:GLU:N	2.30	0.47
1:I:262:ASN:HA	1:I:262:ASN:HD22	1.45	0.47
1:F:140:SER:OG	1:F:141:GLU:N	2.48	0.47
1:O:109:ARG:H	1:O:308:ASN:ND2	2.11	0.47
1:M:85:LEU:C	1:M:87:ASP:N	2.68	0.47
1:H:109:ARG:H	1:H:308:ASN:ND2	2.12	0.47
1:G:24:THR:HG23	1:G:320:ASN:HA	1.95	0.47
1:F:283:ARG:HD2	1:J:142:ASP:OD1	2.15	0.47
1:O:300:VAL:O	1:O:300:VAL:HG13	2.15	0.47
1:B:69:GLN:NE2	1:B:71:ARG:HH22	2.13	0.47
1:J:125:LYS:HD2	1:J:261:TRP:NE1	2.29	0.47
1:C:79:ASP:O	1:C:83:PHE:HB2	2.15	0.47
1:A:293:PRO:HB3	1:E:117:LEU:HD11	1.97	0.47
1:D:349:GLN:HB2	1:D:353:PRO:HD3	1.97	0.47
1:K:30:ARG:HG2	1:K:380:CYS:SG	2.54	0.47
1:O:223:ASP:OD1	1:O:224:ILE:HG23	2.14	0.47
1:M:364:TYR:CE2	1:N:268:GLY:HA3	2.50	0.47
1:K:307:PHE:HE1	1:K:335:ASP:HB2	1.80	0.47
1:D:97:ARG:HE	1:D:403:TRP:HB3	1.79	0.47
1:M:249:CYS:C	1:M:250:LEU:HD12	2.34	0.47
1:F:138:ASN:HD22	1:F:140:SER:HB3	1.76	0.47
1:N:85:LEU:C	1:N:87:ASP:H	2.18	0.47
1:G:125:LYS:HG3	1:G:261:TRP:CG	2.50	0.47
1:G:86:PRO:HB3	1:G:458:LEU:HD11	1.96	0.47
1:C:386:ALA:CB	1:G:355:GLN:NE2	2.78	0.47
1:E:314:HIS:O	1:E:315:LYS:HG3	2.15	0.47
1:K:161:CYS:SG	1:K:244:ASP:HB3	2.54	0.47
1:O:36:HIS:C	1:O:36:HIS:ND1	2.69	0.47
5:B:527:JHM:O5	5:B:530:IDS:C6	2.63	0.47
1:N:351:PRO:HG2	5:N:607:JHM:C4	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:176:LYS:CB	1:J:176:LYS:HZ3	2.27	0.47
1:D:368:VAL:HG12	1:D:369:GLU:N	2.30	0.47
1:L:232:PRO:HB2	1:L:234:TYR:CE1	2.50	0.47
1:I:261:TRP:CZ3	1:I:294:SER:HB3	2.49	0.47
1:H:176:LYS:HB2	1:H:176:LYS:HZ2	1.79	0.47
1:C:59:LYS:O	1:C:60:GLN:HB3	2.14	0.47
1:B:307:PHE:HE1	1:B:335:ASP:HB2	1.80	0.47
1:B:24:THR:CG2	1:B:320:ASN:HA	2.45	0.47
1:G:54:ALA:HB2	1:G:61:ASP:CG	2.36	0.47
1:O:22:VAL:HG12	1:O:23:ASN:N	2.30	0.47
1:B:54:ALA:HB2	1:B:61:ASP:CG	2.35	0.47
1:L:305:GLN:HA	1:L:305:GLN:NE2	2.30	0.47
1:J:274:SER:HG	7:J:554:IDS:C6	2.20	0.47
1:O:249:CYS:C	1:O:250:LEU:HD12	2.36	0.47
1:A:349:GLN:NE2	1:A:349:GLN:HA	2.25	0.47
1:N:368:VAL:HG12	1:N:369:GLU:N	2.30	0.47
1:O:77:LEU:HB3	1:O:78:PRO:HD2	1.96	0.47
1:G:155:GLN:HA	1:G:334:VAL:O	2.15	0.47
1:C:463:TYR:HB3	1:C:464:PRO:HD2	1.97	0.47
1:K:79:ASP:O	1:K:83:PHE:HB2	2.14	0.47
1:J:75:VAL:HB	1:J:329:LEU:HB3	1.97	0.47
1:I:163:PRO:HB2	1:I:194:VAL:HG13	1.96	0.47
1:E:24:THR:CG2	1:E:320:ASN:HA	2.44	0.47
1:J:59:LYS:O	1:J:60:GLN:HB3	2.15	0.46
1:I:105:VAL:HG12	1:I:106:GLU:N	2.30	0.46
1:H:156:LEU:HA	1:H:250:LEU:O	2.15	0.46
1:H:369:GLU:CG	1:H:371:TYR:HE1	2.27	0.46
1:J:68:TYR:CE2	1:J:151:TYR:HB2	2.50	0.46
1:O:99:VAL:CG2	1:O:382:ILE:CD1	2.87	0.46
1:G:45:VAL:HG12	1:G:368:VAL:HG22	1.97	0.46
1:K:231:TYR:CE1	1:O:112:PRO:HB3	2.50	0.46
1:G:261:TRP:CZ3	1:G:294:SER:HB3	2.51	0.46
1:D:75:VAL:HB	1:D:329:LEU:HB3	1.96	0.46
1:A:463:TYR:HB3	1:A:464:PRO:HD2	1.96	0.46
1:C:114:GLY:HA3	1:C:340:THR:HG23	1.96	0.46
1:K:314:HIS:CG	1:K:315:LYS:H	2.33	0.46
1:N:36:HIS:C	1:N:36:HIS:ND1	2.67	0.46
1:C:36:HIS:ND1	1:C:36:HIS:C	2.68	0.46
1:G:105:VAL:HG12	1:G:106:GLU:N	2.30	0.46
1:M:369:GLU:CG	1:M:371:TYR:HE1	2.26	0.46
1:F:182:GLN:NE2	1:F:182:GLN:HA	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:VAL:HG12	1:A:106:GLU:N	2.30	0.46
1:L:108:GLY:HA2	1:L:308:ASN:ND2	2.30	0.46
1:F:86:PRO:HB3	1:F:458:LEU:HD11	1.97	0.46
1:K:35:TYR:OH	1:K:86:PRO:HD3	2.15	0.46
1:I:364:TYR:CG	1:J:185:CYS:HB2	2.49	0.46
1:D:117:LEU:HD11	1:E:293:PRO:HB3	1.97	0.46
1:D:220:VAL:HB	1:D:224:ILE:HD11	1.98	0.46
1:N:364:TYR:CD2	1:O:185:CYS:HB2	2.51	0.46
1:M:36:HIS:ND1	1:M:36:HIS:C	2.69	0.46
1:I:216:THR:O	1:I:217:LYS:HB2	2.14	0.46
1:F:249:CYS:C	1:F:250:LEU:HD12	2.36	0.46
1:I:108:GLY:HA2	1:I:308:ASN:ND2	2.30	0.46
1:H:368:VAL:HG12	1:H:369:GLU:N	2.29	0.46
1:I:149:VAL:HG21	1:I:294:SER:HB2	1.96	0.46
1:D:387:ASP:HA	1:D:390:SER:OG	2.14	0.46
1:F:154:THR:HG22	1:F:155:GLN:N	2.30	0.46
1:B:241:PRO:HG2	1:B:242:TYR:H	1.80	0.46
1:A:216:THR:HG22	1:A:218:CYS:HB2	1.96	0.46
5:N:609:JHM:O9	1:O:182:GLN:HB2	2.16	0.46
1:J:70:TYR:CZ	1:J:201:VAL:HG12	2.50	0.46
1:D:108:GLY:HA2	1:D:308:ASN:HD22	1.81	0.46
1:A:357:ASP:HA	1:B:141:GLU:CG	2.45	0.46
1:O:188:LEU:N	1:O:188:LEU:CD2	2.78	0.46
1:F:59:LYS:O	1:F:60:GLN:HB3	2.15	0.46
1:C:24:THR:HG23	1:C:320:ASN:HA	1.96	0.46
1:O:176:LYS:CB	1:O:176:LYS:NZ	2.79	0.46
1:G:344:ILE:N	1:G:344:ILE:HD12	2.31	0.46
1:H:223:ASP:OD1	1:H:224:ILE:HG23	2.15	0.46
1:A:122:PHE:O	1:A:218:CYS:HB3	2.16	0.46
1:N:98:LEU:HD23	1:N:381:THR:HG22	1.96	0.46
1:I:385:THR:OG1	1:I:388:VAL:HG23	2.16	0.46
1:B:36:HIS:C	1:B:36:HIS:ND1	2.69	0.46
1:D:444:LYS:CA	1:D:444:LYS:HE2	2.37	0.46
1:K:249:CYS:C	1:K:250:LEU:HD12	2.36	0.46
1:H:387:ASP:HA	1:H:390:SER:OG	2.14	0.46
1:J:123:TYR:HD2	1:J:125:LYS:HB2	1.81	0.46
1:F:440:ASP:HB3	1:F:443:ASP:CG	2.36	0.46
1:C:223:ASP:OD1	1:C:224:ILE:HG23	2.15	0.46
1:K:220:VAL:HB	1:K:224:ILE:HD11	1.98	0.46
1:F:91:TYR:O	1:O:281:GLY:CA	2.63	0.46
1:A:262:ASN:HD22	1:A:262:ASN:HA	1.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:262:ASN:HD22	1:N:262:ASN:HA	1.46	0.46
1:O:151:TYR:CG	1:O:203:THR:HB	2.50	0.46
1:B:108:GLY:HA2	1:B:308:ASN:HD22	1.80	0.46
1:N:87:ASP:O	1:N:90:ILE:HG12	2.16	0.46
1:D:85:LEU:C	1:D:87:ASP:H	2.19	0.46
1:O:176:LYS:HZ2	1:O:176:LYS:HB2	1.80	0.46
1:N:314:HIS:CG	1:N:315:LYS:N	2.83	0.46
1:H:24:THR:CG2	1:H:320:ASN:HA	2.46	0.46
1:G:156:LEU:HA	1:G:250:LEU:O	2.16	0.46
1:K:231:TYR:CD1	1:O:112:PRO:HB3	2.51	0.46
1:D:99:VAL:HG21	1:D:382:ILE:CD1	2.46	0.46
1:N:75:VAL:HB	1:N:329:LEU:HB3	1.98	0.46
1:H:125:LYS:HD2	1:H:261:TRP:NE1	2.31	0.46
1:C:123:TYR:HD2	1:C:125:LYS:HB2	1.80	0.46
1:B:154:THR:HG23	1:B:253:GLU:HB3	1.97	0.46
1:C:155:GLN:HA	1:C:334:VAL:O	2.15	0.46
1:M:79:ASP:O	1:M:83:PHE:HB2	2.16	0.46
1:G:236:GLN:O	1:G:236:GLN:HG3	2.15	0.46
1:I:176:LYS:NZ	1:I:176:LYS:HB2	2.31	0.46
5:B:530:IDS:O61	1:C:274:SER:OG	2.31	0.46
1:I:108:GLY:HA2	1:I:308:ASN:HD22	1.81	0.46
1:K:440:ASP:HB3	1:K:443:ASP:OD2	2.15	0.46
1:L:390:SER:O	1:L:393:GLN:HB3	2.15	0.46
1:L:24:THR:HG23	1:L:320:ASN:HA	1.98	0.46
1:K:314:HIS:CG	1:K:315:LYS:N	2.84	0.46
1:G:325:TRP:O	1:G:326:HIS:HB2	2.15	0.46
1:E:241:PRO:HG2	1:E:242:TYR:H	1.80	0.46
1:B:88:THR:HG22	1:B:88:THR:O	2.15	0.46
1:E:99:VAL:HG21	1:E:382:ILE:HD11	1.98	0.46
1:D:363:GLN:HB3	1:E:290:VAL:HG21	1.97	0.46
1:I:440:ASP:HB3	1:I:443:ASP:OD2	2.16	0.46
1:A:86:PRO:HB3	1:A:458:LEU:CD1	2.46	0.46
1:A:242:TYR:CZ	1:A:395:MET:HA	2.50	0.46
1:E:314:HIS:CG	1:E:315:LYS:H	2.33	0.46
1:O:125:LYS:HD2	1:O:261:TRP:NE1	2.29	0.46
1:A:307:PHE:HE1	1:A:335:ASP:HB2	1.81	0.46
1:F:97:ARG:HE	1:F:403:TRP:HB3	1.80	0.46
1:C:30:ARG:HG2	1:C:380:CYS:SG	2.56	0.46
1:N:351:PRO:O	1:N:352:VAL:HB	2.16	0.46
1:D:156:LEU:HA	1:D:250:LEU:O	2.16	0.46
1:O:368:VAL:HG12	1:O:369:GLU:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:169:TRP:CZ2	1:L:190:LEU:HD13	2.51	0.46
1:M:344:ILE:HG22	1:M:345:CYS:N	2.31	0.46
1:I:86:PRO:HB3	1:I:458:LEU:HD11	1.98	0.46
1:L:86:PRO:HB3	1:L:458:LEU:HD11	1.98	0.46
1:L:85:LEU:C	1:L:87:ASP:N	2.70	0.46
1:F:387:ASP:HA	1:F:390:SER:OG	2.16	0.46
1:N:364:TYR:CG	1:O:185:CYS:HB2	2.51	0.46
1:O:98:LEU:HD23	1:O:381:THR:HG22	1.97	0.46
1:C:307:PHE:HE1	1:C:335:ASP:HB2	1.80	0.46
1:I:277:ILE:N	1:I:277:ILE:CD1	2.78	0.45
1:C:249:CYS:O	1:C:250:LEU:HD12	2.16	0.45
1:J:138:ASN:HD22	1:J:140:SER:HB3	1.79	0.45
1:L:156:LEU:HA	1:L:250:LEU:O	2.17	0.45
1:N:86:PRO:HB3	1:N:458:LEU:CD1	2.45	0.45
1:E:324:CYS:HB3	1:E:328:GLN:O	2.16	0.45
1:C:85:LEU:C	1:C:87:ASP:H	2.18	0.45
1:L:35:TYR:OH	1:L:86:PRO:HD3	2.15	0.45
1:L:79:ASP:O	1:L:83:PHE:HB2	2.15	0.45
1:K:155:GLN:HA	1:K:334:VAL:O	2.15	0.45
1:I:36:HIS:ND1	1:I:36:HIS:C	2.68	0.45
1:A:349:GLN:NE2	1:A:349:GLN:CA	2.77	0.45
1:E:384:LEU:HB3	1:E:389:MET:HE2	1.98	0.45
1:N:300:VAL:O	1:N:300:VAL:HG13	2.17	0.45
1:I:188:LEU:CD2	1:I:188:LEU:N	2.78	0.45
1:C:188:LEU:CD2	1:C:188:LEU:N	2.78	0.45
1:B:108:GLY:HA2	1:B:308:ASN:ND2	2.32	0.45
1:O:85:LEU:C	1:O:87:ASP:N	2.70	0.45
1:M:85:LEU:C	1:M:87:ASP:H	2.19	0.45
1:J:99:VAL:HG21	1:J:382:ILE:CD1	2.45	0.45
1:I:125:LYS:HG3	1:I:261:TRP:CG	2.50	0.45
1:F:76:GLN:CG	1:F:453:LYS:HE3	2.46	0.45
1:G:79:ASP:O	1:G:83:PHE:HB2	2.17	0.45
1:D:307:PHE:HE1	1:D:335:ASP:HB2	1.81	0.45
1:M:385:THR:OG1	1:M:388:VAL:HG23	2.16	0.45
1:L:307:PHE:HE1	1:L:335:ASP:HB2	1.81	0.45
1:D:105:VAL:HG12	1:D:106:GLU:N	2.31	0.45
1:B:368:VAL:HG12	1:B:369:GLU:N	2.30	0.45
1:L:345:CYS:CB	1:L:363:GLN:NE2	2.79	0.45
1:O:242:TYR:CZ	1:O:395:MET:HA	2.51	0.45
1:A:124:ASN:OD1	1:A:264:ALA:HB3	2.16	0.45
1:I:114:GLY:HA3	1:I:340:THR:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:277:ILE:N	1:F:277:ILE:CD1	2.79	0.45
1:B:262:ASN:HD22	1:B:262:ASN:HA	1.47	0.45
1:K:440:ASP:OD1	1:K:442:TYR:HB2	2.16	0.45
1:G:75:VAL:HB	1:G:329:LEU:HB3	1.99	0.45
1:N:242:TYR:CZ	1:N:395:MET:HA	2.52	0.45
1:L:324:CYS:HB3	1:L:328:GLN:O	2.17	0.45
1:N:440:ASP:HB3	1:N:443:ASP:CG	2.37	0.45
1:N:22:VAL:HG12	1:N:23:ASN:N	2.31	0.45
1:M:110:GLY:O	1:M:111:GLN:O	2.34	0.45
1:N:62:ILE:CD1	1:N:62:ILE:N	2.79	0.45
1:O:384:LEU:HB3	1:O:389:MET:HE2	1.97	0.45
1:N:314:HIS:O	1:N:315:LYS:HG3	2.16	0.45
1:J:300:VAL:HG13	1:J:300:VAL:O	2.17	0.45
1:H:54:ALA:HB2	1:H:61:ASP:CG	2.37	0.45
1:K:59:LYS:HB2	7:L:619:JHM:O9	2.16	0.45
1:I:156:LEU:HA	1:I:250:LEU:O	2.17	0.45
1:M:368:VAL:HG11	1:N:169:TRP:HZ2	1.77	0.45
1:O:99:VAL:HG21	1:O:382:ILE:HD11	1.97	0.45
1:N:343:THR:C	1:N:344:ILE:HD12	2.37	0.45
1:E:463:TYR:HB3	1:E:464:PRO:HD2	1.99	0.45
1:A:165:ILE:HD12	1:A:237:MET:HG2	1.99	0.45
1:C:305:GLN:NE2	1:C:305:GLN:HA	2.32	0.45
1:F:178:ARG:CD	1:J:59:LYS:CD	2.79	0.45
1:F:262:ASN:HD22	1:F:262:ASN:HA	1.49	0.45
1:C:156:LEU:HA	1:C:250:LEU:O	2.16	0.45
1:G:68:TYR:CE2	1:G:151:TYR:HB2	2.52	0.45
1:J:85:LEU:C	1:J:87:ASP:H	2.19	0.45
1:O:24:THR:HG23	1:O:320:ASN:HA	1.98	0.45
1:E:173:THR:HG23	5:E:511:JHM:O6	2.16	0.45
1:C:390:SER:O	1:C:393:GLN:HB3	2.17	0.45
1:D:463:TYR:HB3	1:D:464:PRO:HD2	1.98	0.45
1:I:314:HIS:CG	1:I:315:LYS:H	2.34	0.45
1:K:54:ALA:HB2	1:K:61:ASP:CG	2.37	0.45
1:A:125:LYS:HD2	1:A:261:TRP:NE1	2.31	0.45
1:M:223:ASP:OD1	1:M:224:ILE:HG23	2.17	0.45
1:G:72:VAL:HG22	1:G:332:THR:HG23	1.98	0.45
1:K:88:THR:HG22	1:K:88:THR:O	2.17	0.45
1:D:278:LYS:CE	5:D:523:JHM:O8	2.50	0.45
1:F:43:LEU:HD12	1:F:369:GLU:O	2.17	0.45
1:H:151:TYR:OH	1:H:221:PRO:CB	2.64	0.45
1:L:216:THR:HG22	1:L:218:CYS:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:85:LEU:C	1:G:87:ASP:N	2.70	0.45
1:E:314:HIS:CG	1:E:315:LYS:N	2.85	0.45
1:N:62:ILE:N	1:N:62:ILE:HD13	2.32	0.45
1:J:61:ASP:O	1:J:63:PRO:HD3	2.17	0.45
1:G:467:ARG:O	1:G:471:VAL:HG23	2.17	0.45
1:D:114:GLY:HA3	1:D:340:THR:HG23	1.98	0.45
4:D:504:IDS:C3	2:E:501:JHM:C1	2.92	0.45
1:C:45:VAL:HG12	1:C:368:VAL:HG22	1.98	0.45
1:M:258:ARG:NH1	1:N:130:GLU:OE1	2.49	0.45
1:C:385:THR:OG1	1:C:388:VAL:HG23	2.17	0.45
1:M:114:GLY:HA3	1:M:340:THR:HG23	1.98	0.45
1:E:54:ALA:HB2	1:E:61:ASP:CG	2.37	0.45
1:E:307:PHE:HE1	1:E:335:ASP:HB2	1.82	0.45
1:E:161:CYS:SG	1:E:244:ASP:HB3	2.57	0.45
1:N:366:ARG:HA	1:N:366:ARG:HD3	1.77	0.45
1:D:368:VAL:HG11	1:E:169:TRP:HZ2	1.82	0.45
1:H:384:LEU:HB3	1:H:389:MET:HE1	1.98	0.45
1:L:123:TYR:HD2	1:L:125:LYS:HB2	1.81	0.45
1:A:325:TRP:HB3	1:A:399:ILE:HD13	1.99	0.45
1:M:324:CYS:SG	1:M:329:LEU:HD13	2.57	0.45
1:H:92:ASN:C	1:H:94:GLU:H	2.20	0.45
1:B:240:ASP:OD1	1:B:241:PRO:HD2	2.17	0.45
1:C:77:LEU:HB3	1:C:78:PRO:HD2	1.99	0.45
1:H:97:ARG:HE	1:H:403:TRP:HB3	1.82	0.45
1:G:107:ILE:N	1:G:107:ILE:HD12	2.32	0.45
1:F:220:VAL:HB	1:F:224:ILE:HD11	1.98	0.44
1:L:216:THR:O	1:L:217:LYS:HB2	2.17	0.44
1:E:223:ASP:OD1	1:E:224:ILE:HG23	2.17	0.44
1:B:384:LEU:HB3	1:B:389:MET:HE1	1.99	0.44
1:D:92:ASN:C	1:D:94:GLU:H	2.19	0.44
1:M:92:ASN:HA	1:M:93:PRO:HD2	1.86	0.44
1:F:355:GLN:HE22	1:H:280:THR:HG23	1.82	0.44
1:I:214:GLN:OE1	1:I:219:GLU:HB2	2.18	0.44
1:E:385:THR:OG1	1:E:388:VAL:HG23	2.17	0.44
1:L:205:TYR:CD2	1:L:220:VAL:HG12	2.52	0.44
1:E:155:GLN:HA	1:E:334:VAL:O	2.17	0.44
1:G:216:THR:HG22	1:G:218:CYS:CB	2.46	0.44
1:F:169:TRP:HZ2	1:J:368:VAL:HG11	1.81	0.44
1:H:262:ASN:HA	1:H:262:ASN:HD22	1.51	0.44
1:M:156:LEU:HA	1:M:250:LEU:O	2.17	0.44
1:N:176:LYS:CB	1:N:176:LYS:NZ	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:385:THR:OG1	1:K:388:VAL:HG23	2.18	0.44
1:K:149:VAL:HG21	1:K:294:SER:HB2	1.99	0.44
1:K:283:ARG:HD2	1:O:142:ASP:CG	2.37	0.44
1:F:108:GLY:HA2	1:F:308:ASN:ND2	2.33	0.44
1:A:70:TYR:CZ	1:A:201:VAL:HG12	2.52	0.44
1:C:69:GLN:HE21	1:C:71:ARG:HH22	1.63	0.44
1:D:85:LEU:C	1:D:87:ASP:N	2.69	0.44
1:M:24:THR:HG23	1:M:320:ASN:HA	1.98	0.44
1:B:314:HIS:O	1:B:315:LYS:HG3	2.18	0.44
1:B:333:VAL:HG12	1:B:334:VAL:N	2.32	0.44
1:F:268:GLY:HA3	1:J:364:TYR:CE2	2.51	0.44
1:E:262:ASN:HD22	1:E:262:ASN:HA	1.47	0.44
1:I:123:TYR:HD2	1:I:125:LYS:HB2	1.83	0.44
1:O:75:VAL:HB	1:O:329:LEU:HB3	1.99	0.44
1:O:114:GLY:HA3	1:O:340:THR:HG23	1.99	0.44
1:K:235:LEU:HD12	1:O:370:GLU:OE2	2.17	0.44
1:J:143:VAL:O	1:J:143:VAL:HG12	2.16	0.44
1:N:348:THR:O	1:O:182:GLN:HG3	2.17	0.44
1:H:126:LEU:HG	1:H:127:ASP:OD2	2.16	0.44
1:G:223:ASP:OD1	1:G:224:ILE:HG23	2.18	0.44
1:D:440:ASP:OD1	1:D:442:TYR:HB2	2.17	0.44
1:N:385:THR:OG1	1:N:388:VAL:HG23	2.18	0.44
1:B:261:TRP:CZ3	1:B:294:SER:HB3	2.53	0.44
1:E:343:THR:C	1:E:344:ILE:HD13	2.38	0.44
1:D:366:ARG:HD3	1:D:366:ARG:HA	1.78	0.44
1:I:143:VAL:O	1:I:143:VAL:HG12	2.18	0.44
1:A:342:LEU:HD22	1:B:208:MET:SD	2.58	0.44
1:I:324:CYS:HB3	1:I:328:GLN:O	2.16	0.44
1:C:86:PRO:HB3	1:C:458:LEU:CD1	2.47	0.44
1:L:54:ALA:HB2	1:L:61:ASP:OD1	2.18	0.44
1:K:290:VAL:HG21	1:O:363:GLN:HB3	1.99	0.44
1:B:214:GLN:OE1	1:B:219:GLU:HB2	2.18	0.44
1:B:92:ASN:HD21	1:B:95:THR:HG23	1.83	0.44
1:M:72:VAL:HG21	1:M:195:LEU:O	2.17	0.44
1:O:463:TYR:HB3	1:O:464:PRO:HD2	1.99	0.44
1:L:176:LYS:NZ	1:L:176:LYS:CB	2.80	0.44
1:O:43:LEU:HD12	1:O:369:GLU:O	2.17	0.44
1:A:99:VAL:HG21	1:A:382:ILE:CD1	2.48	0.44
1:O:86:PRO:HB3	1:O:458:LEU:CD1	2.47	0.44
1:M:121:PRO:CG	1:N:289:CYS:SG	3.06	0.44
1:A:241:PRO:HG2	1:A:242:TYR:H	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:ASN:O	1:A:399:ILE:HG13	2.18	0.44
1:B:69:GLN:HE21	1:B:71:ARG:HH12	1.65	0.44
1:H:24:THR:HG23	1:H:320:ASN:HA	2.00	0.44
1:C:387:ASP:HA	1:C:390:SER:OG	2.18	0.44
1:K:241:PRO:HG2	1:K:242:TYR:H	1.83	0.44
1:J:44:THR:O	1:J:44:THR:HG23	2.18	0.44
1:K:182:GLN:NE2	1:K:182:GLN:HA	2.32	0.44
1:A:138:ASN:HD22	1:A:140:SER:HB3	1.82	0.44
1:C:76:GLN:CG	1:C:453:LYS:HE3	2.48	0.44
1:E:85:LEU:C	1:E:87:ASP:H	2.21	0.44
1:M:24:THR:HG23	1:M:319:HIS:O	2.17	0.44
1:A:324:CYS:HB3	1:A:328:GLN:O	2.17	0.44
1:G:463:TYR:HB3	1:G:464:PRO:HD2	2.00	0.44
1:F:125:LYS:HD2	1:F:261:TRP:NE1	2.32	0.44
1:G:217:LYS:CE	1:G:226:GLN:HE22	2.25	0.44
1:J:216:THR:O	1:J:217:LYS:HB2	2.17	0.44
3:E:502:IDS:O5	3:E:505:JHM:H1	2.06	0.44
1:E:69:GLN:HE21	1:E:71:ARG:HH12	1.66	0.44
1:I:75:VAL:HB	1:I:329:LEU:HB3	2.00	0.44
1:M:24:THR:HG21	1:M:320:ASN:HA	1.99	0.44
1:C:216:THR:O	1:C:217:LYS:HB2	2.18	0.44
1:L:240:ASP:OD1	1:L:241:PRO:HD2	2.18	0.44
1:K:464:PRO:HG2	1:K:465:LEU:H	1.81	0.44
1:C:307:PHE:O	1:C:309:LYS:HG3	2.17	0.44
1:F:123:TYR:HD2	1:F:125:LYS:HB2	1.83	0.44
1:D:124:ASN:OD1	1:D:264:ALA:HB3	2.18	0.44
1:I:67:ALA:HB2	1:I:367:HIS:CE1	2.53	0.44
1:G:386:ALA:CB	1:L:355:GLN:NE2	2.69	0.43
1:G:277:ILE:CD1	1:G:277:ILE:N	2.81	0.43
1:L:368:VAL:HG12	1:L:369:GLU:N	2.33	0.43
1:C:273:GLN:HE22	1:C:278:LYS:HZ3	1.66	0.43
1:F:188:LEU:N	1:F:188:LEU:CD2	2.80	0.43
6:B:536:IDS:O62	6:B:537:JHM:C1	2.65	0.43
1:O:277:ILE:N	1:O:277:ILE:CD1	2.81	0.43
1:H:76:GLN:CG	1:H:453:LYS:HE3	2.48	0.43
1:D:125:LYS:HG3	1:D:261:TRP:CG	2.53	0.43
1:B:24:THR:HG23	1:B:320:ASN:HA	2.00	0.43
1:K:223:ASP:OD1	1:K:224:ILE:HG23	2.18	0.43
1:O:261:TRP:CZ3	1:O:294:SER:HB3	2.52	0.43
1:F:255:LEU:HD13	1:J:300:VAL:HG13	1.99	0.43
5:A:517:JHM:O8	1:E:57:GLY:O	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:155:GLN:HA	1:I:334:VAL:O	2.18	0.43
1:I:217:LYS:HE3	1:I:226:GLN:NE2	2.32	0.43
7:L:620:IDS:H3	7:L:621:JHM:C5	2.48	0.43
1:D:384:LEU:HB3	1:D:389:MET:HE2	1.99	0.43
1:J:35:TYR:OH	1:J:86:PRO:HD3	2.18	0.43
1:I:223:ASP:OD1	1:I:224:ILE:HG23	2.18	0.43
1:H:261:TRP:CZ3	1:H:294:SER:HB3	2.53	0.43
1:J:24:THR:HG23	1:J:320:ASN:HA	2.00	0.43
1:D:123:TYR:HD2	1:D:125:LYS:HB2	1.82	0.43
1:E:72:VAL:HG22	1:E:332:THR:HG23	2.00	0.43
1:E:79:ASP:O	1:E:83:PHE:HB2	2.18	0.43
1:B:30:ARG:HG2	1:B:380:CYS:SG	2.58	0.43
1:A:54:ALA:HB2	1:A:61:ASP:CG	2.39	0.43
1:G:366:ARG:HA	1:G:366:ARG:HD3	1.82	0.43
1:F:92:ASN:O	1:F:96:GLN:HG2	2.17	0.43
1:B:369:GLU:CG	1:B:371:TYR:HE1	2.28	0.43
1:F:108:GLY:HA2	1:F:308:ASN:HD22	1.82	0.43
1:H:99:VAL:HG21	1:H:382:ILE:HD11	1.99	0.43
1:A:151:TYR:CG	1:A:203:THR:HB	2.53	0.43
1:N:344:ILE:HG22	1:N:345:CYS:N	2.32	0.43
1:K:110:GLY:O	1:K:111:GLN:O	2.36	0.43
1:A:440:ASP:HB3	1:A:443:ASP:OD1	2.19	0.43
1:K:390:SER:O	1:K:393:GLN:HB3	2.18	0.43
1:D:385:THR:OG1	1:D:388:VAL:HG23	2.18	0.43
1:D:24:THR:HG23	1:D:320:ASN:HA	1.99	0.43
1:N:396:ASN:O	1:N:399:ILE:HG13	2.18	0.43
1:N:351:PRO:HG2	5:N:607:JHM:C6	2.48	0.43
4:D:504:IDS:C3	2:E:501:JHM:O1	2.66	0.43
1:G:169:TRP:CZ2	1:G:190:LEU:HD13	2.53	0.43
1:H:45:VAL:HG12	1:H:368:VAL:HG22	2.00	0.43
1:L:108:GLY:HA2	1:L:308:ASN:HD22	1.83	0.43
1:D:188:LEU:CD2	1:D:188:LEU:N	2.82	0.43
1:C:440:ASP:OD1	1:C:442:TYR:HB2	2.18	0.43
1:C:72:VAL:HG22	1:C:332:THR:HG23	2.01	0.43
1:F:24:THR:CG2	1:F:320:ASN:HA	2.48	0.43
1:M:440:ASP:HB3	1:M:443:ASP:CG	2.38	0.43
1:M:123:TYR:HD2	1:M:125:LYS:HB2	1.82	0.43
1:E:366:ARG:HA	1:E:366:ARG:HD3	1.76	0.43
1:I:216:THR:CG2	1:I:218:CYS:HB2	2.48	0.43
1:J:273:GLN:CB	7:J:555:JHM:H5	2.40	0.43
1:O:126:LEU:HD13	1:O:264:ALA:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:LEU:HG	1:A:127:ASP:OD2	2.19	0.43
1:N:108:GLY:HA2	1:N:308:ASN:ND2	2.34	0.43
1:L:105:VAL:HG12	1:L:106:GLU:N	2.34	0.43
1:F:351:PRO:O	1:F:352:VAL:HB	2.18	0.43
1:E:345:CYS:HB3	1:E:363:GLN:NE2	2.33	0.43
1:B:314:HIS:ND1	1:B:314:HIS:N	2.65	0.43
1:I:390:SER:O	1:I:393:GLN:HB3	2.19	0.43
1:I:92:ASN:C	1:I:94:GLU:H	2.21	0.43
1:A:364:TYR:CE2	1:B:268:GLY:HA3	2.53	0.43
1:K:33:ILE:HD12	1:K:33:ILE:N	2.34	0.43
1:G:126:LEU:HG	1:G:127:ASP:OD2	2.18	0.43
1:E:105:VAL:HG12	1:E:106:GLU:N	2.32	0.43
1:H:85:LEU:C	1:H:87:ASP:N	2.71	0.43
1:N:108:GLY:HA2	1:N:308:ASN:HD22	1.84	0.43
1:E:151:TYR:CG	1:E:203:THR:HB	2.52	0.43
1:M:384:LEU:HB3	1:M:389:MET:HE1	1.99	0.43
1:E:267:MET:SD	1:E:290:VAL:HG23	2.58	0.43
1:J:74:ARG:HH22	1:J:440:ASP:CG	2.22	0.43
1:L:333:VAL:HG12	1:L:334:VAL:N	2.33	0.43
1:J:98:LEU:CD2	1:J:381:THR:HG22	2.48	0.43
1:I:59:LYS:O	1:I:60:GLN:HB3	2.19	0.43
1:A:92:ASN:C	1:A:94:GLU:H	2.22	0.43
1:M:307:PHE:HE1	1:M:335:ASP:HB2	1.84	0.43
1:A:79:ASP:O	1:A:83:PHE:HB2	2.19	0.43
1:B:178:ARG:NH2	6:B:534:IDS:O2S	2.50	0.43
1:M:242:TYR:CZ	1:M:395:MET:HA	2.54	0.43
1:O:30:ARG:HG2	1:O:380:CYS:SG	2.58	0.43
1:C:92:ASN:C	1:C:94:GLU:H	2.21	0.43
1:B:90:ILE:O	1:B:90:ILE:HG22	2.19	0.43
4:D:504:IDS:C4	2:E:501:JHM:O5	2.67	0.43
1:F:277:ILE:HD13	1:J:217:LYS:HB2	2.00	0.43
1:E:351:PRO:O	1:E:352:VAL:HB	2.18	0.43
1:B:140:SER:OG	1:B:141:GLU:N	2.49	0.43
1:D:69:GLN:HE21	1:D:71:ARG:HH12	1.67	0.43
1:C:85:LEU:C	1:C:87:ASP:N	2.71	0.43
1:O:307:PHE:CE1	1:O:335:ASP:HB2	2.54	0.43
1:A:107:ILE:CD1	1:A:107:ILE:N	2.82	0.43
1:C:97:ARG:HE	1:C:403:TRP:HB3	1.83	0.43
1:K:317:GLN:C	1:K:317:GLN:NE2	2.72	0.43
1:J:217:LYS:HE3	1:J:226:GLN:NE2	2.33	0.43
1:N:216:THR:CG2	1:N:218:CYS:HB2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:THR:HG21	1:C:320:ASN:HA	1.99	0.43
1:C:74:ARG:HH22	1:C:440:ASP:CG	2.22	0.43
1:A:92:ASN:OD1	1:A:94:GLU:HB2	2.18	0.43
6:B:534:IDS:O3	6:B:535:JHM:H1	1.72	0.43
1:E:77:LEU:HB3	1:E:78:PRO:HD2	2.00	0.43
1:N:54:ALA:HB2	1:N:61:ASP:CG	2.39	0.43
1:L:92:ASN:HA	1:L:93:PRO:HD2	1.84	0.43
1:G:62:ILE:N	1:G:62:ILE:HD13	2.34	0.43
1:A:97:ARG:HE	1:A:403:TRP:HB3	1.84	0.43
1:F:216:THR:O	1:F:217:LYS:HB2	2.18	0.43
1:M:68:TYR:CE2	1:M:151:TYR:HB2	2.53	0.43
1:J:99:VAL:HG21	1:J:382:ILE:HD11	2.01	0.43
1:I:440:ASP:HB3	1:I:443:ASP:OD1	2.19	0.43
1:E:81:ASN:C	1:E:83:PHE:H	2.22	0.43
1:G:62:ILE:N	1:G:62:ILE:CD1	2.82	0.43
1:M:98:LEU:HD23	1:M:381:THR:HG22	2.01	0.43
1:J:92:ASN:HA	1:J:93:PRO:HD2	1.88	0.43
1:E:36:HIS:ND1	1:E:36:HIS:C	2.71	0.43
1:C:143:VAL:O	1:C:143:VAL:HG12	2.19	0.43
1:J:222:LEU:HD12	1:J:222:LEU:HA	1.87	0.43
1:N:351:PRO:CG	5:N:607:JHM:O6	2.57	0.43
1:J:384:LEU:HB3	1:J:389:MET:HE1	2.01	0.43
1:A:140:SER:OG	1:A:141:GLU:N	2.49	0.43
1:M:108:GLY:HA2	1:M:308:ASN:HD22	1.84	0.43
1:N:216:THR:O	1:N:217:LYS:HB2	2.18	0.43
1:L:125:LYS:HG3	1:L:261:TRP:CG	2.54	0.43
1:L:384:LEU:HB3	1:L:389:MET:HE2	2.01	0.43
1:N:384:LEU:HB3	1:N:389:MET:HE1	2.00	0.43
1:F:110:GLY:O	1:F:111:GLN:O	2.36	0.43
1:K:255:LEU:HD13	1:O:300:VAL:CG1	2.49	0.43
1:J:125:LYS:HG3	1:J:261:TRP:CG	2.53	0.43
1:I:314:HIS:CG	1:I:315:LYS:N	2.87	0.43
1:M:92:ASN:C	1:M:94:GLU:H	2.22	0.43
1:K:76:GLN:HG3	1:K:453:LYS:HE3	2.01	0.43
1:A:385:THR:OG1	1:A:388:VAL:HG23	2.19	0.43
1:O:107:ILE:HD12	1:O:107:ILE:N	2.34	0.43
1:N:235:LEU:HA	1:N:235:LEU:HD23	1.90	0.43
1:F:366:ARG:HD3	1:F:366:ARG:HA	1.81	0.43
1:F:91:TYR:CA	1:O:281:GLY:HA2	2.45	0.42
1:B:70:TYR:CZ	1:B:201:VAL:HG12	2.53	0.42
1:K:151:TYR:CG	1:K:203:THR:HB	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:314:HIS:N	1:D:314:HIS:ND1	2.67	0.42
1:M:389:MET:HG2	1:M:400:LEU:HD21	2.00	0.42
1:F:261:TRP:CZ3	1:F:294:SER:HB3	2.53	0.42
1:F:214:GLN:OE1	1:F:219:GLU:HB2	2.19	0.42
1:N:261:TRP:CZ3	1:N:294:SER:HB3	2.53	0.42
1:C:317:GLN:NE2	1:C:317:GLN:C	2.73	0.42
1:J:45:VAL:CG1	1:J:368:VAL:HG22	2.47	0.42
1:B:126:LEU:HG	1:B:127:ASP:OD2	2.19	0.42
1:H:105:VAL:HG12	1:H:106:GLU:N	2.34	0.42
1:E:188:LEU:CD2	1:E:188:LEU:N	2.81	0.42
1:H:71:ARG:HA	1:H:197:ASP:OD1	2.19	0.42
1:E:24:THR:HG23	1:E:320:ASN:HA	2.01	0.42
1:L:440:ASP:HB3	1:L:443:ASP:CG	2.40	0.42
1:J:72:VAL:HG22	1:J:332:THR:HG23	2.01	0.42
1:B:364:TYR:CG	1:C:185:CYS:HB2	2.54	0.42
1:M:260:PHE:N	1:M:260:PHE:CD2	2.85	0.42
1:F:178:ARG:HD2	1:J:59:LYS:HB3	1.99	0.42
6:F:584:IDS:C6	6:F:585:JHM:C1	2.97	0.42
1:E:75:VAL:HB	1:E:329:LEU:HB3	2.01	0.42
1:L:237:MET:HB3	1:L:246:MET:HG2	2.00	0.42
1:A:58:ASN:N	1:A:58:ASN:OD1	2.52	0.42
1:M:125:LYS:HD2	1:M:261:TRP:NE1	2.34	0.42
1:E:157:CYS:C	1:E:158:ILE:HG12	2.37	0.42
1:M:154:THR:HG22	1:M:155:GLN:N	2.34	0.42
1:I:79:ASP:O	1:I:83:PHE:HB2	2.19	0.42
1:L:22:VAL:HG12	1:L:23:ASN:N	2.35	0.42
1:K:98:LEU:HD23	1:K:381:THR:HG22	2.01	0.42
1:I:98:LEU:HD23	1:I:381:THR:HG22	2.01	0.42
1:F:30:ARG:HD3	1:F:378:GLN:OE1	2.19	0.42
1:H:345:CYS:HB3	1:H:363:GLN:NE2	2.33	0.42
1:B:91:TYR:N	1:J:281:GLY:HA2	2.35	0.42
1:L:43:LEU:HD12	1:L:369:GLU:O	2.19	0.42
1:O:85:LEU:C	1:O:87:ASP:H	2.22	0.42
1:I:384:LEU:HB3	1:I:389:MET:HE2	1.99	0.42
1:J:188:LEU:N	1:J:188:LEU:CD2	2.81	0.42
1:A:188:LEU:CD2	1:A:188:LEU:N	2.81	0.42
1:G:355:GLN:OE1	1:G:355:GLN:HA	2.19	0.42
1:A:216:THR:O	1:A:217:LYS:HB2	2.19	0.42
1:M:220:VAL:HB	1:M:224:ILE:HD11	2.02	0.42
1:I:54:ALA:HB2	1:I:61:ASP:CG	2.40	0.42
1:O:128:ASP:O	1:O:132:SER:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:98:LEU:HD23	1:L:381:THR:HG22	2.00	0.42
1:H:74:ARG:HH22	1:H:440:ASP:CG	2.23	0.42
1:A:289:CYS:SG	1:E:121:PRO:HG3	2.59	0.42
1:J:242:TYR:CZ	1:J:395:MET:HA	2.54	0.42
1:G:249:CYS:C	1:G:250:LEU:HD12	2.40	0.42
1:M:126:LEU:HG	1:M:127:ASP:OD2	2.20	0.42
1:D:369:GLU:CG	1:D:371:TYR:HE1	2.28	0.42
1:M:120:HIS:HA	1:M:121:PRO:HD3	1.86	0.42
1:J:390:SER:O	1:J:393:GLN:HB3	2.20	0.42
1:O:324:CYS:SG	1:O:329:LEU:HD13	2.60	0.42
1:C:125:LYS:HG3	1:C:261:TRP:CG	2.54	0.42
1:O:349:GLN:CG	1:O:360:LYS:HE2	2.49	0.42
1:B:124:ASN:OD1	1:B:264:ALA:HB3	2.19	0.42
1:G:165:ILE:HD12	1:G:237:MET:HG2	2.01	0.42
1:H:98:LEU:HD23	1:H:381:THR:HG22	2.01	0.42
1:E:149:VAL:HG21	1:E:294:SER:HB2	2.01	0.42
1:J:21:VAL:HG12	1:J:22:VAL:N	2.34	0.42
1:E:114:GLY:HA3	1:E:340:THR:HG23	2.01	0.42
1:N:30:ARG:HG2	1:N:380:CYS:SG	2.59	0.42
1:L:366:ARG:HA	1:L:366:ARG:HD3	1.86	0.42
1:G:159:LEU:HB2	1:G:248:PHE:HB3	2.01	0.42
1:B:351:PRO:O	1:B:352:VAL:HB	2.20	0.42
1:I:249:CYS:C	1:I:250:LEU:HD12	2.38	0.42
1:K:71:ARG:HA	1:K:197:ASP:OD1	2.20	0.42
1:K:109:ARG:H	1:K:308:ASN:ND2	2.17	0.42
1:C:344:ILE:HG22	1:C:345:CYS:N	2.33	0.42
1:B:125:LYS:HD2	1:B:261:TRP:NE1	2.35	0.42
1:M:216:THR:HG22	1:M:218:CYS:HB2	2.02	0.42
1:I:92:ASN:OD1	1:I:94:GLU:HB2	2.19	0.42
1:N:79:ASP:O	1:N:83:PHE:HB2	2.19	0.42
1:G:92:ASN:C	1:G:94:GLU:H	2.23	0.42
1:E:22:VAL:HG12	1:E:23:ASN:N	2.34	0.42
1:J:314:HIS:CG	1:J:315:LYS:H	2.37	0.42
1:O:157:CYS:C	1:O:158:ILE:HG12	2.40	0.42
1:K:159:LEU:HB2	1:K:248:PHE:HB3	2.00	0.42
1:I:369:GLU:CG	1:I:371:TYR:HE1	2.28	0.42
1:C:300:VAL:CG1	1:D:255:LEU:HD13	2.46	0.42
1:B:232:PRO:HB2	1:B:234:TYR:CE1	2.54	0.42
1:K:43:LEU:HD12	1:K:369:GLU:O	2.19	0.42
1:I:151:TYR:CG	1:I:203:THR:HB	2.54	0.42
1:L:389:MET:O	1:L:393:GLN:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:99:VAL:HG21	1:I:382:ILE:CD1	2.50	0.42
1:H:440:ASP:HB3	1:H:443:ASP:CG	2.40	0.42
1:J:22:VAL:HG12	1:J:23:ASN:N	2.34	0.42
1:I:23:ASN:O	1:I:25:ASP:N	2.52	0.42
1:F:107:ILE:N	1:F:107:ILE:HD12	2.35	0.42
1:D:273:GLN:HE22	1:D:278:LYS:CE	2.32	0.42
1:A:43:LEU:HD21	1:B:169:TRP:HH2	1.84	0.42
1:K:169:TRP:CZ2	1:K:190:LEU:HD13	2.55	0.42
1:D:232:PRO:HB2	1:D:234:TYR:CE1	2.55	0.42
1:K:130:GLU:OE1	1:O:259:HIS:HE1	2.03	0.42
1:F:344:ILE:HG22	1:F:345:CYS:N	2.35	0.42
1:F:280:THR:HG23	1:I:355:GLN:NE2	2.32	0.42
1:G:344:ILE:HG22	1:G:345:CYS:N	2.34	0.42
1:I:387:ASP:HA	1:I:390:SER:OG	2.20	0.42
1:G:98:LEU:HD23	1:G:381:THR:HG22	2.01	0.42
1:G:114:GLY:HA3	1:G:340:THR:HG23	2.02	0.42
1:H:154:THR:HG22	1:H:155:GLN:N	2.35	0.42
1:I:352:VAL:HA	1:I:353:PRO:HD2	1.85	0.42
1:B:85:LEU:C	1:B:87:ASP:H	2.23	0.42
1:C:69:GLN:HE21	1:C:71:ARG:HH12	1.68	0.42
1:G:151:TYR:CG	1:G:203:THR:HB	2.54	0.42
1:G:385:THR:OG1	1:G:388:VAL:HG23	2.20	0.42
1:J:85:LEU:C	1:J:87:ASP:N	2.73	0.42
1:C:75:VAL:HB	1:C:329:LEU:HB3	2.01	0.42
1:K:261:TRP:CZ3	1:K:294:SER:HB3	2.55	0.42
1:L:154:THR:HG23	1:L:253:GLU:HB3	2.02	0.42
1:F:161:CYS:SG	1:F:244:ASP:HB3	2.60	0.42
1:M:161:CYS:SG	1:M:244:ASP:HB3	2.60	0.42
1:L:267:MET:SD	1:L:288:SER:HA	2.59	0.42
1:B:169:TRP:CE2	1:B:190:LEU:HD13	2.54	0.42
1:F:216:THR:CG2	1:F:218:CYS:HB2	2.50	0.42
1:N:169:TRP:CE2	1:N:190:LEU:HD13	2.54	0.42
1:F:86:PRO:HB3	1:F:458:LEU:CD1	2.49	0.42
1:I:232:PRO:HB2	1:I:234:TYR:CE1	2.54	0.42
1:A:315:LYS:HA	1:A:321:ASN:HD21	1.85	0.42
1:D:154:THR:HG22	1:D:155:GLN:N	2.35	0.42
1:E:345:CYS:HA	1:E:362:LYS:O	2.19	0.42
1:A:21:VAL:HG12	1:A:22:VAL:N	2.35	0.42
1:K:102:CYS:SG	1:K:313:LEU:HD11	2.60	0.42
1:D:260:PHE:CD2	1:D:260:PHE:N	2.87	0.42
1:J:444:LYS:HA	1:J:444:LYS:CE	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:368:VAL:HG11	1:I:169:TRP:HZ2	1.84	0.41
1:M:41:ARG:NH1	1:N:190:LEU:HD23	2.35	0.41
1:L:99:VAL:HG21	1:L:382:ILE:CD1	2.50	0.41
1:B:396:ASN:O	1:B:399:ILE:HG13	2.19	0.41
1:M:92:ASN:O	1:M:94:GLU:N	2.53	0.41
1:E:260:PHE:N	1:E:260:PHE:CD2	2.85	0.41
1:L:176:LYS:HZ2	1:L:176:LYS:HB2	1.85	0.41
1:A:156:LEU:HA	1:A:250:LEU:O	2.20	0.41
1:F:351:PRO:HD2	5:F:591:JHM:O7	2.19	0.41
1:F:345:CYS:CB	1:F:363:GLN:NE2	2.81	0.41
1:G:123:TYR:HD2	1:G:125:LYS:HB2	1.85	0.41
1:A:283:ARG:HD2	1:E:142:ASP:OD1	2.19	0.41
1:I:76:GLN:CG	1:I:453:LYS:HE3	2.50	0.41
1:K:352:VAL:HA	1:K:353:PRO:HD2	1.85	0.41
1:J:315:LYS:HA	1:J:321:ASN:HD21	1.85	0.41
1:I:349:GLN:HB2	1:I:353:PRO:HD3	2.01	0.41
1:E:30:ARG:HG2	1:E:380:CYS:SG	2.60	0.41
1:C:233:ASP:CG	1:C:236:GLN:HB3	2.41	0.41
1:H:222:LEU:HD12	1:H:222:LEU:HA	1.83	0.41
1:B:465:LEU:HD23	1:B:465:LEU:O	2.20	0.41
1:O:105:VAL:HG12	1:O:106:GLU:N	2.34	0.41
1:N:85:LEU:C	1:N:87:ASP:N	2.72	0.41
1:H:232:PRO:HB2	1:H:234:TYR:CE1	2.55	0.41
1:M:108:GLY:HA2	1:M:308:ASN:ND2	2.35	0.41
1:L:99:VAL:HG12	1:L:100:TRP:N	2.35	0.41
1:D:440:ASP:HB3	1:D:443:ASP:OD2	2.20	0.41
1:M:314:HIS:CG	1:M:315:LYS:H	2.39	0.41
1:C:345:CYS:HB3	1:C:363:GLN:NE2	2.35	0.41
1:O:352:VAL:HA	1:O:353:PRO:HD2	1.84	0.41
1:J:261:TRP:CZ3	1:J:294:SER:HB3	2.55	0.41
1:A:123:TYR:HD2	1:A:125:LYS:HB2	1.85	0.41
1:F:355:GLN:NE2	1:H:280:THR:HG23	2.34	0.41
1:L:364:TYR:CG	1:M:185:CYS:HB2	2.55	0.41
1:E:98:LEU:HD23	1:E:381:THR:HG22	2.02	0.41
1:J:43:LEU:HD12	1:J:369:GLU:O	2.20	0.41
1:G:159:LEU:CD2	1:G:331:VAL:HG22	2.50	0.41
1:C:151:TYR:CG	1:C:203:THR:HB	2.56	0.41
1:G:149:VAL:HG21	1:G:294:SER:HB2	2.02	0.41
1:G:110:GLY:O	1:G:111:GLN:O	2.39	0.41
1:C:343:THR:C	1:C:344:ILE:HD12	2.40	0.41
1:C:364:TYR:CD1	1:D:185:CYS:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:333:VAL:HG12	1:D:334:VAL:N	2.34	0.41
1:N:125:LYS:HD2	1:N:261:TRP:NE1	2.36	0.41
1:I:242:TYR:CZ	1:I:395:MET:HA	2.56	0.41
1:H:114:GLY:HA3	1:H:340:THR:HG23	2.02	0.41
1:D:142:ASP:CG	1:E:283:ARG:HD2	2.40	0.41
1:H:107:ILE:HD12	1:H:107:ILE:N	2.35	0.41
1:O:96:GLN:HE21	1:O:96:GLN:HB3	1.59	0.41
1:I:366:ARG:HD3	1:I:366:ARG:HA	1.76	0.41
1:B:105:VAL:HG12	1:B:106:GLU:N	2.36	0.41
1:G:351:PRO:O	1:G:352:VAL:HB	2.20	0.41
1:D:43:LEU:HD12	1:D:369:GLU:O	2.20	0.41
1:L:159:LEU:HD23	1:L:331:VAL:HG22	2.01	0.41
1:D:99:VAL:HG21	1:D:382:ILE:HD11	2.02	0.41
1:L:149:VAL:HG21	1:L:294:SER:HB2	2.02	0.41
1:G:214:GLN:OE1	1:G:219:GLU:HB2	2.21	0.41
1:F:51:ARG:O	1:F:53:PRO:HD3	2.20	0.41
1:O:298:SER:OG	1:O:299:ILE:N	2.53	0.41
1:G:314:HIS:O	1:G:315:LYS:HG3	2.20	0.41
1:N:338:ARG:HG3	1:N:338:ARG:HH11	1.85	0.41
1:H:36:HIS:ND1	1:H:36:HIS:C	2.74	0.41
1:N:351:PRO:HG3	5:N:608:IDS:C1	2.51	0.41
1:L:178:ARG:NE	7:L:619:JHM:O9	2.54	0.41
1:D:241:PRO:HG2	1:D:242:TYR:H	1.85	0.41
1:N:24:THR:HG23	1:N:320:ASN:HA	2.02	0.41
1:A:396:ASN:HB3	1:A:399:ILE:HG13	2.02	0.41
1:F:27:TYR:CD1	1:F:28:VAL:HG23	2.56	0.41
1:N:463:TYR:HB3	1:N:464:PRO:HD2	2.03	0.41
1:F:178:ARG:HA	1:F:179:PRO:HD2	1.60	0.41
1:N:352:VAL:HA	1:N:353:PRO:HD2	1.85	0.41
1:C:126:LEU:HG	1:C:127:ASP:OD2	2.20	0.41
1:H:86:PRO:HB3	1:H:458:LEU:CD1	2.50	0.41
1:O:216:THR:HG22	1:O:218:CYS:CB	2.50	0.41
1:G:387:ASP:HA	1:G:390:SER:OG	2.20	0.41
1:C:440:ASP:HB3	1:C:443:ASP:OD2	2.21	0.41
1:C:217:LYS:HD3	1:D:277:ILE:HD11	2.02	0.41
1:B:396:ASN:HB3	1:B:399:ILE:HG13	2.03	0.41
1:K:30:ARG:HD3	1:K:378:GLN:OE1	2.20	0.41
1:I:92:ASN:HA	1:I:93:PRO:HD2	1.90	0.41
1:J:240:ASP:OD1	1:J:241:PRO:HD2	2.20	0.41
1:C:92:ASN:HA	1:C:93:PRO:HD2	1.90	0.41
1:J:273:GLN:N	7:J:554:IDS:O2	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:159:LEU:O	1:M:246:MET:HA	2.21	0.41
1:J:151:TYR:OH	1:J:221:PRO:CB	2.67	0.41
1:L:85:LEU:HB3	1:L:86:PRO:HD2	2.02	0.41
1:O:216:THR:O	1:O:217:LYS:HB2	2.20	0.41
1:A:261:TRP:CZ3	1:A:294:SER:HB3	2.55	0.41
1:M:261:TRP:CZ3	1:M:294:SER:HB3	2.55	0.41
1:G:22:VAL:HG12	1:G:23:ASN:N	2.35	0.41
1:J:120:HIS:HA	1:J:121:PRO:HD3	1.94	0.41
1:O:165:ILE:HD12	1:O:237:MET:HG2	2.03	0.41
1:E:254:GLN:HG3	1:E:254:GLN:O	2.20	0.41
1:J:107:ILE:N	1:J:107:ILE:HD12	2.35	0.41
5:N:608:IDS:C6	5:N:609:JHM:C1	2.83	0.41
1:A:45:VAL:HG12	1:A:368:VAL:HG22	2.03	0.41
1:L:126:LEU:HG	1:L:127:ASP:OD2	2.20	0.41
1:H:249:CYS:C	1:H:250:LEU:HD12	2.40	0.41
1:C:169:TRP:CE2	1:C:190:LEU:HD13	2.56	0.41
1:I:307:PHE:O	1:I:308:ASN:HB2	2.21	0.41
1:L:255:LEU:HD22	1:L:256:PHE:N	2.36	0.41
1:C:121:PRO:CG	1:D:289:CYS:SG	3.06	0.41
1:I:138:ASN:C	1:I:140:SER:H	2.22	0.41
1:G:241:PRO:HG2	1:G:242:TYR:H	1.86	0.41
1:O:384:LEU:HB3	1:O:389:MET:HE1	2.02	0.41
1:L:110:GLY:O	1:L:111:GLN:O	2.39	0.41
1:J:352:VAL:HA	1:J:353:PRO:HD2	1.90	0.41
1:G:162:ALA:O	1:G:163:PRO:C	2.60	0.41
1:O:154:THR:HG22	1:O:155:GLN:N	2.35	0.41
1:M:142:ASP:OD1	1:N:283:ARG:HD2	2.21	0.41
1:N:96:GLN:HB3	1:N:96:GLN:HE21	1.54	0.41
1:A:22:VAL:HG12	1:A:23:ASN:N	2.36	0.41
1:G:314:HIS:CG	1:G:315:LYS:H	2.39	0.41
1:A:98:LEU:HD23	1:A:381:THR:HG22	2.03	0.41
1:B:122:PHE:O	1:B:218:CYS:HB3	2.21	0.41
1:D:22:VAL:HG12	1:D:23:ASN:N	2.35	0.41
1:G:120:HIS:HA	1:G:121:PRO:HD3	1.93	0.41
1:F:67:ALA:HB2	1:F:367:HIS:CE1	2.56	0.41
1:G:59:LYS:O	1:G:60:GLN:HB3	2.21	0.41
1:A:260:PHE:N	1:A:260:PHE:CD2	2.87	0.41
1:I:182:GLN:HA	1:I:182:GLN:NE2	2.35	0.41
1:J:298:SER:OG	1:J:299:ILE:N	2.53	0.41
1:D:79:ASP:O	1:D:83:PHE:HB2	2.21	0.41
1:D:233:ASP:CG	1:D:236:GLN:HB3	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:44:THR:O	1:I:44:THR:HG23	2.20	0.41
1:M:236:GLN:HG3	1:M:236:GLN:O	2.19	0.41
1:C:96:GLN:HB3	1:C:383:THR:HA	2.02	0.41
1:J:176:LYS:HG2	1:J:176:LYS:H	1.70	0.41
1:D:217:LYS:HD3	1:E:277:ILE:CD1	2.44	0.41
1:L:151:TYR:CG	1:L:203:THR:HB	2.55	0.41
1:B:385:THR:OG1	1:B:388:VAL:HG23	2.20	0.41
1:L:86:PRO:HB3	1:L:458:LEU:CD1	2.51	0.41
1:M:314:HIS:CG	1:M:315:LYS:N	2.89	0.41
1:F:121:PRO:CG	1:G:289:CYS:SG	3.08	0.41
1:E:74:ARG:HH22	1:E:440:ASP:CG	2.24	0.41
1:B:92:ASN:ND2	1:B:95:THR:OG1	2.54	0.41
1:M:307:PHE:CE1	1:M:335:ASP:HB2	2.56	0.41
1:E:102:CYS:SG	1:E:313:LEU:HD11	2.61	0.41
4:D:504:IDS:O3	2:E:501:JHM:O1	2.28	0.40
1:J:216:THR:CG2	1:J:218:CYS:HB2	2.51	0.40
1:F:182:GLN:O	7:F:567:JHM:S	2.80	0.40
1:B:249:CYS:C	1:B:250:LEU:HD12	2.42	0.40
1:H:351:PRO:O	1:H:352:VAL:HB	2.21	0.40
1:E:45:VAL:HG12	1:E:368:VAL:HG22	2.02	0.40
1:M:71:ARG:HA	1:M:197:ASP:OD1	2.21	0.40
1:N:221:PRO:HD2	1:N:224:ILE:HD11	2.03	0.40
1:N:237:MET:HB3	1:N:246:MET:HG2	2.03	0.40
1:J:33:ILE:CG2	1:J:35:TYR:HE1	2.33	0.40
1:C:107:ILE:HD12	1:C:107:ILE:H	1.85	0.40
1:B:242:TYR:CZ	1:B:395:MET:HA	2.56	0.40
1:J:92:ASN:C	1:J:94:GLU:H	2.24	0.40
1:K:185:CYS:HB2	1:O:364:TYR:CG	2.56	0.40
1:J:156:LEU:HA	1:J:250:LEU:O	2.21	0.40
1:C:351:PRO:O	1:C:352:VAL:HB	2.22	0.40
1:N:216:THR:HG22	1:N:218:CYS:CB	2.51	0.40
1:F:357:ASP:HA	1:G:141:GLU:HG3	2.03	0.40
1:A:112:PRO:HB3	1:B:231:TYR:CD1	2.57	0.40
1:A:462:GLN:NE2	1:B:21:VAL:H	2.18	0.40
1:I:396:ASN:O	1:I:399:ILE:HG13	2.21	0.40
1:C:159:LEU:HD23	1:C:331:VAL:HG22	2.02	0.40
1:K:232:PRO:HB2	1:K:234:TYR:CE1	2.56	0.40
1:I:85:LEU:C	1:I:87:ASP:N	2.75	0.40
1:I:86:PRO:HB3	1:I:458:LEU:CD1	2.52	0.40
1:E:85:LEU:C	1:E:87:ASP:N	2.74	0.40
1:I:112:PRO:HB3	1:J:231:TYR:CE1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:86:PRO:HB3	1:G:458:LEU:CD1	2.51	0.40
1:L:61:ASP:O	1:L:63:PRO:HD3	2.21	0.40
1:K:314:HIS:O	1:K:315:LYS:HG3	2.22	0.40
1:E:240:ASP:OD1	1:E:241:PRO:HD2	2.22	0.40
1:B:333:VAL:CG1	1:B:334:VAL:N	2.84	0.40
1:G:314:HIS:N	1:G:314:HIS:ND1	2.69	0.40
1:A:96:GLN:HB3	1:A:383:THR:HA	2.02	0.40
1:E:92:ASN:HA	1:E:93:PRO:HD2	1.89	0.40
1:B:143:VAL:HG12	1:B:143:VAL:O	2.21	0.40
1:C:366:ARG:HD3	1:C:366:ARG:HA	1.78	0.40
1:D:273:GLN:HE22	1:D:278:LYS:HE3	1.87	0.40
1:A:368:VAL:CG1	1:A:369:GLU:N	2.84	0.40
1:L:138:ASN:C	1:L:140:SER:H	2.25	0.40
1:I:307:PHE:HE1	1:I:335:ASP:HB2	1.86	0.40
1:I:69:GLN:HE21	1:I:71:ARG:HH22	1.69	0.40
1:J:108:GLY:HA2	1:J:308:ASN:ND2	2.36	0.40
1:A:169:TRP:CZ2	1:A:190:LEU:HD13	2.57	0.40
1:L:314:HIS:CG	1:L:315:LYS:N	2.90	0.40
1:N:112:PRO:HB3	1:O:231:TYR:CD1	2.57	0.40
1:J:440:ASP:HB3	1:J:443:ASP:OD1	2.21	0.40
1:F:255:LEU:HD22	1:F:256:PHE:N	2.36	0.40
1:B:30:ARG:HD3	1:B:378:GLN:OE1	2.21	0.40
1:M:307:PHE:O	1:M:309:LYS:HG3	2.22	0.40
6:B:534:IDS:O3	6:B:535:JHM:C1	2.48	0.40
1:G:307:PHE:C	1:G:309:LYS:H	2.25	0.40
1:B:75:VAL:HB	1:B:329:LEU:HB3	2.03	0.40
1:H:102:CYS:SG	1:H:313:LEU:HD11	2.62	0.40
1:C:92:ASN:O	1:C:94:GLU:N	2.55	0.40
1:F:45:VAL:HG12	1:F:368:VAL:HG22	2.04	0.40
1:F:258:ARG:HG3	1:F:259:HIS:CE1	2.54	0.40
1:A:159:LEU:O	1:A:246:MET:HA	2.22	0.40
1:B:151:TYR:CG	1:B:203:THR:HB	2.56	0.40
1:M:188:LEU:N	1:M:188:LEU:CD2	2.85	0.40
1:B:237:MET:HB3	1:B:246:MET:HG2	2.03	0.40
1:L:30:ARG:HG2	1:L:380:CYS:SG	2.62	0.40
1:D:72:VAL:HG22	1:D:332:THR:HG23	2.04	0.40
1:B:338:ARG:HH11	1:B:338:ARG:HG3	1.87	0.40
1:K:143:VAL:O	1:K:143:VAL:HG12	2.21	0.40

All (16) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:53:PRO:CB	6:F:583:JHM:O7[1_655]	1.52	0.68
1:M:61:ASP:OD1	6:F:584:IDS:O2S[1_655]	1.81	0.39
1:O:86:PRO:O	5:A:519:JHM:O7[1_666]	1.83	0.37
1:L:89:SER:CB	7:L:613:JHM:O9[1_655]	1.89	0.31
1:K:173:THR:CG2	5:E:514:IDS:O1S[1_566]	1.95	0.25
1:O:401:GLU:O	7:L:616:IDS:O61[1_565]	1.98	0.22
1:O:438:ASN:OD1	7:L:615:JHM:C1[1_565]	1.98	0.22
1:O:89:SER:OG	5:A:518:IDS:O1S[1_666]	2.01	0.19
1:N:92:ASN:ND2	5:N:608:IDS:O3[1_655]	2.02	0.18
1:M:51:ARG:CD	6:F:584:IDS:O1S[1_655]	2.06	0.14
1:J:181:SER:OG	5:D:526:IDS:O2S[1_565]	2.11	0.09
1:J:182:GLN:O	5:D:526:IDS:O1S[1_565]	2.12	0.08
1:M:61:ASP:CG	6:F:584:IDS:O2S[1_655]	2.13	0.07
1:G:86:PRO:CA	5:F:594:IDS:O3[1_655]	2.15	0.05
1:O:94:GLU:OE1	7:L:611:JHM:C4[1_565]	2.18	0.02
1:O:90:ILE:CD1	5:A:518:IDS:O3[1_666]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	418/427 (98%)	366 (88%)	40 (10%)	12 (3%)	6	40
1	B	418/427 (98%)	368 (88%)	41 (10%)	9 (2%)	8	46
1	C	418/427 (98%)	364 (87%)	44 (10%)	10 (2%)	7	44
1	D	418/427 (98%)	366 (88%)	43 (10%)	9 (2%)	8	46
1	E	418/427 (98%)	368 (88%)	41 (10%)	9 (2%)	8	46
1	F	418/427 (98%)	364 (87%)	44 (10%)	10 (2%)	7	44
1	G	418/427 (98%)	366 (88%)	42 (10%)	10 (2%)	7	44
1	H	418/427 (98%)	367 (88%)	39 (9%)	12 (3%)	6	40
1	I	418/427 (98%)	367 (88%)	40 (10%)	11 (3%)	7	42
1	J	418/427 (98%)	363 (87%)	44 (10%)	11 (3%)	7	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	418/427 (98%)	366 (88%)	43 (10%)	9 (2%)	8	46
1	L	418/427 (98%)	370 (88%)	39 (9%)	9 (2%)	8	46
1	M	418/427 (98%)	365 (87%)	43 (10%)	10 (2%)	7	44
1	N	418/427 (98%)	365 (87%)	45 (11%)	8 (2%)	10	49
1	O	417/427 (98%)	362 (87%)	44 (11%)	11 (3%)	7	42
All	All	6269/6405 (98%)	5487 (88%)	632 (10%)	150 (2%)	7	44

All (150) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	B	131	SER
1	B	140	SER
1	B	298	SER
1	C	131	SER
1	C	134	ALA
1	C	298	SER
1	D	131	SER
1	D	298	SER
1	E	40	SER
1	E	131	SER
1	E	140	SER
1	F	40	SER
1	F	298	SER
1	G	40	SER
1	G	131	SER
1	G	140	SER
1	G	298	SER
1	H	40	SER
1	H	131	SER
1	H	273	GLN
1	I	134	ALA
1	I	298	SER
1	J	131	SER
1	J	134	ALA
1	J	140	SER
1	J	298	SER
1	K	140	SER
1	K	298	SER
1	L	131	SER

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Mol	Chain	Res	Type
1	L	140	SER
1	L	298	SER
1	M	40	SER
1	M	131	SER
1	M	298	SER
1	N	298	SER
1	O	131	SER
1	O	298	SER
1	O	386	ALA
1	A	40	SER
1	A	131	SER
1	A	134	ALA
1	A	140	SER
1	A	298	SER
1	B	40	SER
1	B	134	ALA
1	B	386	ALA
1	C	40	SER
1	C	140	SER
1	D	40	SER
1	D	134	ALA
1	D	140	SER
1	D	386	ALA
1	E	134	ALA
1	E	298	SER
1	E	386	ALA
1	F	131	SER
1	F	134	ALA
1	F	140	SER
1	F	177	SER
1	G	134	ALA
1	G	386	ALA
1	H	134	ALA
1	H	140	SER
1	H	298	SER
1	H	386	ALA
1	I	40	SER
1	I	131	SER
1	I	140	SER
1	I	386	ALA
1	J	40	SER
1	J	386	ALA

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Mol	Chain	Res	Type
1	K	40	SER
1	K	131	SER
1	K	134	ALA
1	K	386	ALA
1	L	40	SER
1	L	134	ALA
1	L	386	ALA
1	M	134	ALA
1	M	140	SER
1	N	40	SER
1	N	131	SER
1	N	134	ALA
1	N	140	SER
1	N	386	ALA
1	O	40	SER
1	O	134	ALA
1	O	140	SER
1	A	386	ALA
1	H	55	GLY
1	H	316	ALA
1	J	111	GLN
1	L	55	GLY
1	M	386	ALA
1	O	111	GLN
1	A	111	GLN
1	C	55	GLY
1	C	111	GLN
1	C	386	ALA
1	D	93	PRO
1	F	386	ALA
1	G	111	GLN
1	H	93	PRO
1	I	24	THR
1	I	139	VAL
1	K	111	GLN
1	L	139	VAL
1	M	55	GLY
1	B	296	SER
1	F	111	GLN
1	G	87	ASP
1	I	111	GLN
1	J	139	VAL

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Mol	Chain	Res	Type
1	L	111	GLN
1	M	93	PRO
1	M	111	GLN
1	N	111	GLN
1	A	221	PRO
1	A	316	ALA
1	D	111	GLN
1	E	93	PRO
1	E	139	VAL
1	F	179	PRO
1	H	111	GLN
1	J	93	PRO
1	O	296	SER
1	A	93	PRO
1	A	139	VAL
1	F	139	VAL
1	G	93	PRO
1	G	139	VAL
1	H	139	VAL
1	K	139	VAL
1	M	139	VAL
1	N	139	VAL
1	O	55	GLY
1	B	93	PRO
1	C	139	VAL
1	D	55	GLY
1	I	55	GLY
1	J	221	PRO
1	B	139	VAL
1	C	93	PRO
1	E	221	PRO
1	I	93	PRO
1	J	55	GLY
1	K	93	PRO
1	O	93	PRO
1	O	139	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	369/370 (100%)	343 (93%)	26 (7%)	19	58
1	B	369/370 (100%)	347 (94%)	22 (6%)	24	64
1	C	369/370 (100%)	343 (93%)	26 (7%)	19	58
1	D	369/370 (100%)	348 (94%)	21 (6%)	25	65
1	E	369/370 (100%)	342 (93%)	27 (7%)	17	56
1	F	369/370 (100%)	341 (92%)	28 (8%)	16	54
1	G	369/370 (100%)	345 (94%)	24 (6%)	21	61
1	H	369/370 (100%)	346 (94%)	23 (6%)	23	63
1	I	369/370 (100%)	345 (94%)	24 (6%)	21	61
1	J	369/370 (100%)	348 (94%)	21 (6%)	25	65
1	K	369/370 (100%)	350 (95%)	19 (5%)	29	69
1	L	369/370 (100%)	348 (94%)	21 (6%)	25	65
1	M	369/370 (100%)	348 (94%)	21 (6%)	25	65
1	N	369/370 (100%)	345 (94%)	24 (6%)	21	61
1	O	368/370 (100%)	345 (94%)	23 (6%)	22	62
All	All	5534/5550 (100%)	5184 (94%)	350 (6%)	22	62

All (350) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	ARG
1	A	60	GLN
1	A	91	TYR
1	A	107	ILE
1	A	127	ASP
1	A	133	HIS
1	A	158	ILE
1	A	176	LYS
1	A	178	ARG
1	A	236	GLN
1	A	247	PHE
1	A	251	ARG
1	A	255	LEU
1	A	262	ASN
1	A	270	THR

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Mol	Chain	Res	Type
1	A	313	LEU
1	A	317	GLN
1	A	340	THR
1	A	349	GLN
1	A	372	ASP
1	A	387	ASP
1	A	392	ILE
1	A	396	ASN
1	A	399	ILE
1	A	465	LEU
1	A	472	GLN
1	B	51	ARG
1	B	91	TYR
1	B	127	ASP
1	B	133	HIS
1	B	156	LEU
1	B	176	LYS
1	B	178	ARG
1	B	184	ASP
1	B	247	PHE
1	B	251	ARG
1	B	255	LEU
1	B	262	ASN
1	B	270	THR
1	B	313	LEU
1	B	317	GLN
1	B	340	THR
1	B	372	ASP
1	B	387	ASP
1	B	396	ASN
1	B	399	ILE
1	B	465	LEU
1	B	472	GLN
1	C	51	ARG
1	C	91	TYR
1	C	127	ASP
1	C	133	HIS
1	C	156	LEU
1	C	176	LYS
1	C	178	ARG
1	C	184	ASP
1	C	185	CYS

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Mol	Chain	Res	Type
1	C	215	ASP
1	C	236	GLN
1	C	247	PHE
1	C	251	ARG
1	C	255	LEU
1	C	262	ASN
1	C	270	THR
1	C	273	GLN
1	C	274	SER
1	C	313	LEU
1	C	317	GLN
1	C	340	THR
1	C	372	ASP
1	C	387	ASP
1	C	396	ASN
1	C	465	LEU
1	C	472	GLN
1	D	51	ARG
1	D	91	TYR
1	D	127	ASP
1	D	133	HIS
1	D	176	LYS
1	D	178	ARG
1	D	184	ASP
1	D	236	GLN
1	D	247	PHE
1	D	251	ARG
1	D	255	LEU
1	D	262	ASN
1	D	278	LYS
1	D	313	LEU
1	D	317	GLN
1	D	340	THR
1	D	372	ASP
1	D	387	ASP
1	D	396	ASN
1	D	465	LEU
1	D	472	GLN
1	E	51	ARG
1	E	91	TYR
1	E	127	ASP
1	E	133	HIS

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Mol	Chain	Res	Type
1	E	156	LEU
1	E	158	ILE
1	E	176	LYS
1	E	178	ARG
1	E	184	ASP
1	E	215	ASP
1	E	236	GLN
1	E	247	PHE
1	E	251	ARG
1	E	255	LEU
1	E	262	ASN
1	E	270	THR
1	E	273	GLN
1	E	277	ILE
1	E	313	LEU
1	E	317	GLN
1	E	340	THR
1	E	372	ASP
1	E	387	ASP
1	E	392	ILE
1	E	396	ASN
1	E	465	LEU
1	E	472	GLN
1	F	51	ARG
1	F	91	TYR
1	F	127	ASP
1	F	133	HIS
1	F	156	LEU
1	F	176	LYS
1	F	178	ARG
1	F	180	LEU
1	F	181	SER
1	F	184	ASP
1	F	185	CYS
1	F	224	ILE
1	F	236	GLN
1	F	247	PHE
1	F	251	ARG
1	F	255	LEU
1	F	262	ASN
1	F	270	THR
1	F	277	ILE

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Mol	Chain	Res	Type
1	F	293	PRO
1	F	313	LEU
1	F	317	GLN
1	F	340	THR
1	F	372	ASP
1	F	387	ASP
1	F	396	ASN
1	F	465	LEU
1	F	472	GLN
1	G	51	ARG
1	G	62	ILE
1	G	91	TYR
1	G	127	ASP
1	G	133	HIS
1	G	176	LYS
1	G	178	ARG
1	G	184	ASP
1	G	215	ASP
1	G	227	SER
1	G	236	GLN
1	G	247	PHE
1	G	251	ARG
1	G	255	LEU
1	G	262	ASN
1	G	277	ILE
1	G	313	LEU
1	G	317	GLN
1	G	340	THR
1	G	372	ASP
1	G	387	ASP
1	G	396	ASN
1	G	465	LEU
1	G	472	GLN
1	H	51	ARG
1	H	91	TYR
1	H	127	ASP
1	H	133	HIS
1	H	156	LEU
1	H	176	LYS
1	H	184	ASP
1	H	215	ASP
1	H	247	PHE

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Mol	Chain	Res	Type
1	H	251	ARG
1	H	255	LEU
1	H	262	ASN
1	H	277	ILE
1	H	278	LYS
1	H	313	LEU
1	H	317	GLN
1	H	340	THR
1	H	372	ASP
1	H	387	ASP
1	H	392	ILE
1	H	396	ASN
1	H	465	LEU
1	H	472	GLN
1	I	51	ARG
1	I	87	ASP
1	I	91	TYR
1	I	127	ASP
1	I	133	HIS
1	I	156	LEU
1	I	176	LYS
1	I	178	ARG
1	I	184	ASP
1	I	247	PHE
1	I	251	ARG
1	I	255	LEU
1	I	262	ASN
1	I	270	THR
1	I	277	ILE
1	I	313	LEU
1	I	317	GLN
1	I	340	THR
1	I	372	ASP
1	I	387	ASP
1	I	392	ILE
1	I	396	ASN
1	I	465	LEU
1	I	472	GLN
1	J	51	ARG
1	J	91	TYR
1	J	127	ASP
1	J	133	HIS

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Mol	Chain	Res	Type
1	J	156	LEU
1	J	176	LYS
1	J	178	ARG
1	J	184	ASP
1	J	236	GLN
1	J	247	PHE
1	J	251	ARG
1	J	255	LEU
1	J	262	ASN
1	J	313	LEU
1	J	317	GLN
1	J	340	THR
1	J	372	ASP
1	J	387	ASP
1	J	396	ASN
1	J	465	LEU
1	J	472	GLN
1	K	51	ARG
1	K	91	TYR
1	K	127	ASP
1	K	133	HIS
1	K	156	LEU
1	K	176	LYS
1	K	184	ASP
1	K	247	PHE
1	K	251	ARG
1	K	255	LEU
1	K	262	ASN
1	K	313	LEU
1	K	317	GLN
1	K	340	THR
1	K	372	ASP
1	K	387	ASP
1	K	396	ASN
1	K	465	LEU
1	K	472	GLN
1	L	51	ARG
1	L	91	TYR
1	L	127	ASP
1	L	133	HIS
1	L	176	LYS
1	L	184	ASP

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Mol	Chain	Res	Type
1	L	224	ILE
1	L	236	GLN
1	L	247	PHE
1	L	251	ARG
1	L	255	LEU
1	L	262	ASN
1	L	270	THR
1	L	313	LEU
1	L	317	GLN
1	L	340	THR
1	L	372	ASP
1	L	387	ASP
1	L	396	ASN
1	L	465	LEU
1	L	472	GLN
1	M	51	ARG
1	M	91	TYR
1	M	127	ASP
1	M	133	HIS
1	M	156	LEU
1	M	176	LYS
1	M	184	ASP
1	M	236	GLN
1	M	247	PHE
1	M	251	ARG
1	M	255	LEU
1	M	262	ASN
1	M	313	LEU
1	M	317	GLN
1	M	340	THR
1	M	372	ASP
1	M	387	ASP
1	M	392	ILE
1	M	396	ASN
1	M	465	LEU
1	M	472	GLN
1	N	51	ARG
1	N	62	ILE
1	N	87	ASP
1	N	91	TYR
1	N	107	ILE
1	N	127	ASP

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Mol	Chain	Res	Type
1	N	133	HIS
1	N	156	LEU
1	N	176	LYS
1	N	178	ARG
1	N	184	ASP
1	N	236	GLN
1	N	247	PHE
1	N	251	ARG
1	N	255	LEU
1	N	262	ASN
1	N	313	LEU
1	N	317	GLN
1	N	340	THR
1	N	387	ASP
1	N	396	ASN
1	N	399	ILE
1	N	465	LEU
1	N	472	GLN
1	O	51	ARG
1	O	91	TYR
1	O	127	ASP
1	O	133	HIS
1	O	158	ILE
1	O	176	LYS
1	O	182	GLN
1	O	184	ASP
1	O	236	GLN
1	O	247	PHE
1	O	251	ARG
1	O	255	LEU
1	O	262	ASN
1	O	270	THR
1	O	277	ILE
1	O	313	LEU
1	O	317	GLN
1	O	340	THR
1	O	372	ASP
1	O	387	ASP
1	O	396	ASN
1	O	465	LEU
1	O	472	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (237) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	69	GLN
1	A	138	ASN
1	A	153	GLN
1	A	182	GLN
1	A	262	ASN
1	A	308	ASN
1	A	317	GLN
1	A	321	ASN
1	A	326	HIS
1	A	341	ASN
1	A	355	GLN
1	A	363	GLN
1	A	367	HIS
1	A	396	ASN
1	A	462	GLN
1	B	69	GLN
1	B	138	ASN
1	B	153	GLN
1	B	182	GLN
1	B	226	GLN
1	B	262	ASN
1	B	273	GLN
1	B	308	ASN
1	B	317	GLN
1	B	321	ASN
1	B	341	ASN
1	B	349	GLN
1	B	363	GLN
1	B	367	HIS
1	B	396	ASN
1	B	462	GLN
1	C	69	GLN
1	C	138	ASN
1	C	153	GLN
1	C	182	GLN
1	C	262	ASN
1	C	273	GLN
1	C	308	ASN
1	C	317	GLN
1	C	321	ASN
1	C	326	HIS

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Mol	Chain	Res	Type
1	C	341	ASN
1	C	349	GLN
1	C	363	GLN
1	C	367	HIS
1	C	396	ASN
1	C	462	GLN
1	D	69	GLN
1	D	138	ASN
1	D	153	GLN
1	D	182	GLN
1	D	262	ASN
1	D	273	GLN
1	D	308	ASN
1	D	317	GLN
1	D	321	ASN
1	D	326	HIS
1	D	341	ASN
1	D	363	GLN
1	D	367	HIS
1	D	396	ASN
1	D	462	GLN
1	E	69	GLN
1	E	138	ASN
1	E	153	GLN
1	E	182	GLN
1	E	254	GLN
1	E	262	ASN
1	E	308	ASN
1	E	317	GLN
1	E	321	ASN
1	E	341	ASN
1	E	363	GLN
1	E	367	HIS
1	E	396	ASN
1	E	462	GLN
1	F	69	GLN
1	F	138	ASN
1	F	153	GLN
1	F	182	GLN
1	F	254	GLN
1	F	262	ASN
1	F	273	GLN

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Mol	Chain	Res	Type
1	F	308	ASN
1	F	317	GLN
1	F	321	ASN
1	F	341	ASN
1	F	363	GLN
1	F	367	HIS
1	F	396	ASN
1	F	462	GLN
1	G	69	GLN
1	G	138	ASN
1	G	153	GLN
1	G	182	GLN
1	G	226	GLN
1	G	254	GLN
1	G	262	ASN
1	G	273	GLN
1	G	308	ASN
1	G	317	GLN
1	G	321	ASN
1	G	326	HIS
1	G	341	ASN
1	G	363	GLN
1	G	367	HIS
1	G	396	ASN
1	G	462	GLN
1	H	69	GLN
1	H	138	ASN
1	H	153	GLN
1	H	182	GLN
1	H	254	GLN
1	H	262	ASN
1	H	273	GLN
1	H	308	ASN
1	H	317	GLN
1	H	321	ASN
1	H	326	HIS
1	H	341	ASN
1	H	363	GLN
1	H	367	HIS
1	H	396	ASN
1	H	462	GLN
1	I	69	GLN

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Mol	Chain	Res	Type
1	I	138	ASN
1	I	153	GLN
1	I	182	GLN
1	I	254	GLN
1	I	262	ASN
1	I	273	GLN
1	I	308	ASN
1	I	317	GLN
1	I	321	ASN
1	I	341	ASN
1	I	363	GLN
1	I	367	HIS
1	I	396	ASN
1	I	462	GLN
1	J	69	GLN
1	J	138	ASN
1	J	153	GLN
1	J	182	GLN
1	J	192	ASN
1	J	254	GLN
1	J	262	ASN
1	J	273	GLN
1	J	308	ASN
1	J	317	GLN
1	J	321	ASN
1	J	326	HIS
1	J	341	ASN
1	J	349	GLN
1	J	363	GLN
1	J	367	HIS
1	J	396	ASN
1	J	462	GLN
1	K	69	GLN
1	K	138	ASN
1	K	153	GLN
1	K	182	GLN
1	K	254	GLN
1	K	262	ASN
1	K	273	GLN
1	K	308	ASN
1	K	317	GLN
1	K	321	ASN

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Continued from previous page...

Mol	Chain	Res	Type
1	K	341	ASN
1	K	363	GLN
1	K	367	HIS
1	K	396	ASN
1	K	462	GLN
1	L	69	GLN
1	L	138	ASN
1	L	153	GLN
1	L	182	GLN
1	L	254	GLN
1	L	262	ASN
1	L	273	GLN
1	L	308	ASN
1	L	317	GLN
1	L	321	ASN
1	L	326	HIS
1	L	341	ASN
1	L	349	GLN
1	L	363	GLN
1	L	367	HIS
1	L	396	ASN
1	L	462	GLN
1	M	69	GLN
1	M	138	ASN
1	M	153	GLN
1	M	182	GLN
1	M	254	GLN
1	M	262	ASN
1	M	273	GLN
1	M	308	ASN
1	M	317	GLN
1	M	321	ASN
1	M	327	ASN
1	M	341	ASN
1	M	363	GLN
1	M	367	HIS
1	M	393	GLN
1	M	396	ASN
1	M	462	GLN
1	N	69	GLN
1	N	138	ASN
1	N	153	GLN

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Mol	Chain	Res	Type
1	N	182	GLN
1	N	254	GLN
1	N	262	ASN
1	N	273	GLN
1	N	308	ASN
1	N	317	GLN
1	N	326	HIS
1	N	341	ASN
1	N	349	GLN
1	N	363	GLN
1	N	367	HIS
1	N	396	ASN
1	N	462	GLN
1	O	69	GLN
1	O	138	ASN
1	O	153	GLN
1	O	182	GLN
1	O	262	ASN
1	O	273	GLN
1	O	308	ASN
1	O	317	GLN
1	O	321	ASN
1	O	341	ASN
1	O	363	GLN
1	O	367	HIS
1	O	396	ASN
1	O	462	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

121 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	JHM	A	517	5	15,15,15	1.14	2 (13%)	20,22,22	1.25	3 (15%)
5	IDS	A	518	5	12,15,17	2.16	1 (8%)	12,22,26	1.05	1 (8%)
5	JHM	A	519	5	15,15,15	1.16	2 (13%)	20,22,22	1.25	3 (15%)
5	IDS	A	520	5	12,15,17	2.16	1 (8%)	12,22,26	1.05	1 (8%)
5	JHM	A	543	5	15,15,15	1.13	2 (13%)	20,22,22	1.24	3 (15%)
5	IDS	A	544	5	12,15,17	2.17	1 (8%)	12,22,26	1.04	1 (8%)
5	JHM	A	545	5	15,15,15	1.16	2 (13%)	20,22,22	1.25	3 (15%)
5	IDS	A	546	5	12,15,17	2.14	1 (8%)	12,22,26	1.07	1 (8%)
5	JHM	B	527	5	15,15,15	1.14	2 (13%)	20,22,22	1.23	3 (15%)
5	IDS	B	528	5	12,15,17	2.15	1 (8%)	12,22,26	1.05	1 (8%)
5	JHM	B	529	5	15,15,15	1.14	2 (13%)	20,22,22	1.25	3 (15%)
5	IDS	B	530	5	12,15,17	2.14	1 (8%)	12,22,26	1.05	1 (8%)
6	JHM	B	533	6	15,15,15	1.17	2 (13%)	20,22,22	1.25	3 (15%)
6	IDS	B	534	6	12,15,17	2.17	1 (8%)	12,22,26	1.06	1 (8%)
6	JHM	B	535	6	15,15,15	1.15	2 (13%)	20,22,22	1.25	3 (15%)
6	IDS	B	536	6	12,15,17	2.16	1 (8%)	12,22,26	1.05	1 (8%)
6	JHM	B	537	6	15,15,15	1.16	2 (13%)	20,22,22	1.24	3 (15%)
6	IDS	B	538	6	12,15,17	2.15	1 (8%)	12,22,26	1.05	1 (8%)
6	JHM	B	539	6	15,15,15	1.15	2 (13%)	20,22,22	1.25	3 (15%)
6	IDS	B	540	6	12,15,17	2.16	1 (8%)	12,22,26	1.06	1 (8%)
6	JHM	B	541	6	15,15,15	1.15	2 (13%)	20,22,22	1.24	3 (15%)
6	IDS	B	542	6	12,15,17	2.14	1 (8%)	12,22,26	1.06	1 (8%)
4	JHM	C	531	4	15,15,15	1.14	2 (13%)	20,22,22	1.24	3 (15%)
4	IDS	C	532	4	12,15,17	2.14	1 (8%)	12,22,26	1.05	1 (8%)
5	JHM	C	571	5	15,15,15	1.14	2 (13%)	20,22,22	1.24	3 (15%)
5	IDS	C	572	5	12,15,17	2.15	1 (8%)	12,22,26	1.06	1 (8%)
5	JHM	C	573	5	15,15,15	1.13	2 (13%)	20,22,22	1.24	3 (15%)
5	IDS	C	574	5	12,15,17	2.15	1 (8%)	12,22,26	1.06	1 (8%)
4	JHM	D	503	4	15,15,15	1.14	2 (13%)	20,22,22	1.24	3 (15%)
4	IDS	D	504	4	12,15,17	2.14	1 (8%)	12,22,26	1.06	1 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	JHM	D	507	4	15,15,15	1.16	2 (13%)	20,22,22	1.25	3 (15%)
4	IDS	D	508	4	12,15,17	2.15	1 (8%)	12,22,26	1.06	1 (8%)
4	JHM	D	509	4	15,15,15	1.15	2 (13%)	20,22,22	1.25	3 (15%)
4	IDS	D	510	4	12,15,17	2.14	1 (8%)	12,22,26	1.06	1 (8%)
4	JHM	D	521	4	15,15,15	1.15	2 (13%)	20,22,22	1.25	3 (15%)
4	IDS	D	522	5,4	12,15,17	2.16	1 (8%)	12,22,26	1.05	1 (8%)
5	JHM	D	523	5,4	15,15,15	1.14	2 (13%)	20,22,22	1.25	3 (15%)
5	IDS	D	524	5	12,15,17	2.16	1 (8%)	12,22,26	1.06	1 (8%)
5	JHM	D	525	5	15,15,15	1.17	2 (13%)	20,22,22	1.25	3 (15%)
5	IDS	D	526	5	12,15,17	2.17	1 (8%)	12,22,26	1.05	1 (8%)
3	IDS	E	502	3,2	12,15,17	2.14	1 (8%)	12,22,26	1.05	1 (8%)
3	JHM	E	505	3	15,15,15	1.14	2 (13%)	20,22,22	1.24	3 (15%)
3	IDS	E	506	3	12,15,17	2.15	1 (8%)	12,22,26	1.07	1 (8%)
5	JHM	E	511	5	15,15,15	1.14	2 (13%)	20,22,22	1.24	3 (15%)
5	IDS	E	512	5	12,15,17	2.14	1 (8%)	12,22,26	1.05	1 (8%)
5	JHM	E	513	5	15,15,15	1.14	2 (13%)	20,22,22	1.24	3 (15%)
5	IDS	E	514	5	12,15,17	2.14	1 (8%)	12,22,26	1.06	1 (8%)
4	JHM	E	515	4	15,15,15	1.13	2 (13%)	20,22,22	1.25	3 (15%)
4	IDS	E	516	4	12,15,17	2.14	1 (8%)	12,22,26	1.05	1 (8%)
7	JHM	E	547	7	15,15,15	1.14	2 (13%)	20,22,22	1.24	3 (15%)
7	IDS	E	548	7	12,15,17	2.15	1 (8%)	12,22,26	1.05	1 (8%)
7	JHM	E	549	7	15,15,15	1.14	2 (13%)	20,22,22	1.25	3 (15%)
7	IDS	E	550	7	12,15,17	2.15	1 (8%)	12,22,26	1.05	1 (8%)
7	JHM	E	551	7	15,15,15	1.14	2 (13%)	20,22,22	1.25	3 (15%)
7	IDS	E	552	7	12,15,17	2.14	1 (8%)	12,22,26	1.06	1 (8%)
7	JHM	F	565	7	15,15,15	1.14	2 (13%)	20,22,22	1.24	3 (15%)
7	IDS	F	566	7	12,15,17	2.16	1 (8%)	12,22,26	1.05	1 (8%)
7	JHM	F	567	7	15,15,15	1.14	2 (13%)	20,22,22	1.23	3 (15%)
7	IDS	F	568	7	12,15,17	2.16	1 (8%)	12,22,26	1.05	1 (8%)
7	JHM	F	569	7	15,15,15	1.13	2 (13%)	20,22,22	1.24	3 (15%)
7	IDS	F	570	7	12,15,17	2.16	1 (8%)	12,22,26	1.06	1 (8%)
6	JHM	F	581	6	15,15,15	1.15	2 (13%)	20,22,22	1.25	3 (15%)
6	IDS	F	582	6	12,15,17	2.16	1 (8%)	12,22,26	1.05	1 (8%)
6	JHM	F	583	6	15,15,15	1.15	2 (13%)	20,22,22	1.24	3 (15%)
6	IDS	F	584	6	12,15,17	2.15	1 (8%)	12,22,26	1.04	1 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	JHM	F	585	6	15,15,15	1.13	2 (13%)	20,22,22	1.25	3 (15%)
6	IDS	F	586	6	12,15,17	2.16	1 (8%)	12,22,26	1.05	1 (8%)
6	JHM	F	587	6	15,15,15	1.15	2 (13%)	20,22,22	1.24	3 (15%)
6	IDS	F	588	6	12,15,17	2.14	1 (8%)	12,22,26	1.05	1 (8%)
6	JHM	F	589	6	15,15,15	1.14	2 (13%)	20,22,22	1.25	3 (15%)
6	IDS	F	590	6	12,15,17	2.15	1 (8%)	12,22,26	1.05	1 (8%)
5	JHM	F	591	5	15,15,15	1.14	2 (13%)	20,22,22	1.24	3 (15%)
5	IDS	F	592	5	12,15,17	2.15	1 (8%)	12,22,26	1.05	1 (8%)
5	JHM	F	593	5	15,15,15	1.13	2 (13%)	20,22,22	1.24	3 (15%)
5	IDS	F	594	5	12,15,17	2.17	1 (8%)	12,22,26	1.06	1 (8%)
7	JHM	H	575	7	15,15,15	1.16	2 (13%)	20,22,22	1.24	3 (15%)
7	IDS	H	576	7	12,15,17	2.15	1 (8%)	12,22,26	1.05	1 (8%)
7	JHM	H	577	7	15,15,15	1.14	2 (13%)	20,22,22	1.23	3 (15%)
7	IDS	H	578	7	12,15,17	2.15	1 (8%)	12,22,26	1.05	1 (8%)
7	JHM	H	579	7	15,15,15	1.16	2 (13%)	20,22,22	1.24	3 (15%)
7	IDS	H	580	7	12,15,17	2.15	1 (8%)	12,22,26	1.06	1 (8%)
7	JHM	J	553	7	15,15,15	1.14	2 (13%)	20,22,22	1.25	3 (15%)
7	IDS	J	554	7	12,15,17	2.14	1 (8%)	12,22,26	1.05	1 (8%)
7	JHM	J	555	7	15,15,15	1.14	2 (13%)	20,22,22	1.24	3 (15%)
7	IDS	J	556	7	12,15,17	2.14	1 (8%)	12,22,26	1.05	1 (8%)
7	JHM	J	557	7	15,15,15	1.13	2 (13%)	20,22,22	1.24	3 (15%)
7	IDS	J	558	7	12,15,17	2.16	1 (8%)	12,22,26	1.05	1 (8%)
7	JHM	J	559	7	15,15,15	1.13	2 (13%)	20,22,22	1.23	3 (15%)
7	IDS	J	560	7	12,15,17	2.14	1 (8%)	12,22,26	1.07	1 (8%)
7	JHM	J	561	7	15,15,15	1.14	2 (13%)	20,22,22	1.24	3 (15%)
7	IDS	J	562	7	12,15,17	2.15	1 (8%)	12,22,26	1.05	1 (8%)
7	JHM	J	563	7	15,15,15	1.15	2 (13%)	20,22,22	1.24	3 (15%)
7	IDS	J	564	7	12,15,17	2.13	1 (8%)	12,22,26	1.06	1 (8%)
7	JHM	J	595	7	15,15,15	1.14	2 (13%)	20,22,22	1.24	3 (15%)
7	IDS	J	596	7	12,15,17	2.18	1 (8%)	12,22,26	1.04	1 (8%)
7	JHM	J	597	7	15,15,15	1.14	2 (13%)	20,22,22	1.24	3 (15%)
7	IDS	J	598	7	12,15,17	2.17	1 (8%)	12,22,26	1.05	1 (8%)
7	JHM	J	599	7	15,15,15	1.15	2 (13%)	20,22,22	1.24	3 (15%)
7	IDS	J	600	7	12,15,17	2.13	1 (8%)	12,22,26	1.06	1 (8%)
7	JHM	L	611	7	15,15,15	1.15	2 (13%)	20,22,22	1.24	3 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	IDS	L	612	7	12,15,17	2.15	1 (8%)	12,22,26	1.05	1 (8%)
7	JHM	L	613	7	15,15,15	1.14	2 (13%)	20,22,22	1.24	3 (15%)
7	IDS	L	614	7	12,15,17	2.15	1 (8%)	12,22,26	1.05	1 (8%)
7	JHM	L	615	7	15,15,15	1.15	2 (13%)	20,22,22	1.23	3 (15%)
7	IDS	L	616	7	12,15,17	2.16	1 (8%)	12,22,26	1.06	1 (8%)
7	JHM	L	617	7	15,15,15	1.14	2 (13%)	20,22,22	1.24	3 (15%)
7	IDS	L	618	7	12,15,17	2.16	1 (8%)	12,22,26	1.04	1 (8%)
7	JHM	L	619	7	15,15,15	1.14	2 (13%)	20,22,22	1.24	3 (15%)
7	IDS	L	620	7	12,15,17	2.17	1 (8%)	12,22,26	1.05	1 (8%)
7	JHM	L	621	7	15,15,15	1.15	2 (13%)	20,22,22	1.24	3 (15%)
7	IDS	L	622	7	12,15,17	2.14	1 (8%)	12,22,26	1.06	1 (8%)
4	JHM	N	601	4	15,15,15	1.14	2 (13%)	20,22,22	1.24	3 (15%)
4	IDS	N	602	4	12,15,17	2.14	1 (8%)	12,22,26	1.04	1 (8%)
5	JHM	N	607	5	15,15,15	1.14	2 (13%)	20,22,22	1.24	3 (15%)
5	IDS	N	608	5	12,15,17	2.16	1 (8%)	12,22,26	1.05	1 (8%)
5	JHM	N	609	5	15,15,15	1.14	2 (13%)	20,22,22	1.24	3 (15%)
5	IDS	N	610	5	12,15,17	2.15	1 (8%)	12,22,26	1.05	1 (8%)
5	JHM	O	603	5	15,15,15	1.13	2 (13%)	20,22,22	1.23	3 (15%)
5	IDS	O	604	5	12,15,17	2.16	1 (8%)	12,22,26	1.04	1 (8%)
5	JHM	O	605	5	15,15,15	1.13	2 (13%)	20,22,22	1.24	3 (15%)
5	IDS	O	606	5	12,15,17	2.14	1 (8%)	12,22,26	1.05	1 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	JHM	A	517	5	-	0/6/22/22	0/1/1/1
5	IDS	A	518	5	1/1/5/7	0/5/22/29	0/1/1/1
5	JHM	A	519	5	-	0/6/22/22	0/1/1/1
5	IDS	A	520	5	-	0/5/22/29	0/1/1/1
5	JHM	A	543	5	-	0/6/22/22	0/1/1/1
5	IDS	A	544	5	-	0/5/22/29	0/1/1/1
5	JHM	A	545	5	-	0/6/22/22	0/1/1/1
5	IDS	A	546	5	-	0/5/22/29	0/1/1/1
5	JHM	B	527	5	-	0/6/22/22	0/1/1/1
5	IDS	B	528	5	-	0/5/22/29	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	JHM	B	529	5	-	0/6/22/22	0/1/1/1
5	IDS	B	530	5	-	0/5/22/29	0/1/1/1
6	JHM	B	533	6	-	0/6/22/22	0/1/1/1
6	IDS	B	534	6	1/1/5/7	0/5/22/29	0/1/1/1
6	JHM	B	535	6	-	0/6/22/22	0/1/1/1
6	IDS	B	536	6	-	0/5/22/29	0/1/1/1
6	JHM	B	537	6	-	0/6/22/22	0/1/1/1
6	IDS	B	538	6	1/1/5/7	0/5/22/29	0/1/1/1
6	JHM	B	539	6	-	0/6/22/22	0/1/1/1
6	IDS	B	540	6	-	0/5/22/29	0/1/1/1
6	JHM	B	541	6	-	0/6/22/22	0/1/1/1
6	IDS	B	542	6	-	0/5/22/29	0/1/1/1
4	JHM	C	531	4	-	0/6/22/22	0/1/1/1
4	IDS	C	532	4	-	0/5/22/29	0/1/1/1
5	JHM	C	571	5	-	0/6/22/22	0/1/1/1
5	IDS	C	572	5	1/1/5/7	0/5/22/29	0/1/1/1
5	JHM	C	573	5	-	0/6/22/22	0/1/1/1
5	IDS	C	574	5	-	0/5/22/29	0/1/1/1
4	JHM	D	503	4	-	0/6/22/22	0/1/1/1
4	IDS	D	504	4	-	0/5/22/29	0/1/1/1
4	JHM	D	507	4	-	0/6/22/22	0/1/1/1
4	IDS	D	508	4	-	0/5/22/29	0/1/1/1
4	JHM	D	509	4	-	0/6/22/22	0/1/1/1
4	IDS	D	510	4	-	0/5/22/29	0/1/1/1
4	JHM	D	521	4	-	0/6/22/22	0/1/1/1
4	IDS	D	522	5,4	-	0/5/22/29	0/1/1/1
5	JHM	D	523	5,4	-	0/6/22/22	0/1/1/1
5	IDS	D	524	5	-	0/5/22/29	0/1/1/1
5	JHM	D	525	5	-	0/6/22/22	0/1/1/1
5	IDS	D	526	5	-	0/5/22/29	0/1/1/1
3	IDS	E	502	3,2	-	0/5/22/29	0/1/1/1
3	JHM	E	505	3	-	0/6/22/22	0/1/1/1
3	IDS	E	506	3	-	0/5/22/29	0/1/1/1
5	JHM	E	511	5	-	0/6/22/22	0/1/1/1
5	IDS	E	512	5	-	0/5/22/29	0/1/1/1
5	JHM	E	513	5	-	0/6/22/22	0/1/1/1
5	IDS	E	514	5	-	0/5/22/29	0/1/1/1
4	JHM	E	515	4	-	0/6/22/22	0/1/1/1
4	IDS	E	516	4	-	0/5/22/29	0/1/1/1
7	JHM	E	547	7	-	0/6/22/22	0/1/1/1
7	IDS	E	548	7	1/1/5/7	0/5/22/29	0/1/1/1
7	JHM	E	549	7	-	0/6/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	IDS	E	550	7	1/1/5/7	0/5/22/29	0/1/1/1
7	JHM	E	551	7	-	0/6/22/22	0/1/1/1
7	IDS	E	552	7	-	0/5/22/29	0/1/1/1
7	JHM	F	565	7	-	0/6/22/22	0/1/1/1
7	IDS	F	566	7	-	0/5/22/29	0/1/1/1
7	JHM	F	567	7	-	0/6/22/22	0/1/1/1
7	IDS	F	568	7	-	0/5/22/29	0/1/1/1
7	JHM	F	569	7	-	0/6/22/22	0/1/1/1
7	IDS	F	570	7	-	0/5/22/29	0/1/1/1
6	JHM	F	581	6	-	0/6/22/22	0/1/1/1
6	IDS	F	582	6	-	0/5/22/29	0/1/1/1
6	JHM	F	583	6	-	0/6/22/22	0/1/1/1
6	IDS	F	584	6	-	0/5/22/29	0/1/1/1
6	JHM	F	585	6	-	0/6/22/22	0/1/1/1
6	IDS	F	586	6	-	0/5/22/29	0/1/1/1
6	JHM	F	587	6	-	0/6/22/22	0/1/1/1
6	IDS	F	588	6	-	0/5/22/29	0/1/1/1
6	JHM	F	589	6	-	0/6/22/22	0/1/1/1
6	IDS	F	590	6	-	0/5/22/29	0/1/1/1
5	JHM	F	591	5	-	0/6/22/22	0/1/1/1
5	IDS	F	592	5	-	0/5/22/29	0/1/1/1
5	JHM	F	593	5	-	0/6/22/22	0/1/1/1
5	IDS	F	594	5	-	0/5/22/29	0/1/1/1
7	JHM	H	575	7	-	0/6/22/22	0/1/1/1
7	IDS	H	576	7	-	0/5/22/29	0/1/1/1
7	JHM	H	577	7	-	0/6/22/22	0/1/1/1
7	IDS	H	578	7	-	0/5/22/29	0/1/1/1
7	JHM	H	579	7	-	0/6/22/22	0/1/1/1
7	IDS	H	580	7	1/1/5/7	0/5/22/29	0/1/1/1
7	JHM	J	553	7	-	0/6/22/22	0/1/1/1
7	IDS	J	554	7	1/1/5/7	0/5/22/29	0/1/1/1
7	JHM	J	555	7	-	0/6/22/22	0/1/1/1
7	IDS	J	556	7	1/1/5/7	0/5/22/29	0/1/1/1
7	JHM	J	557	7	-	0/6/22/22	0/1/1/1
7	IDS	J	558	7	-	0/5/22/29	0/1/1/1
7	JHM	J	559	7	-	0/6/22/22	0/1/1/1
7	IDS	J	560	7	-	0/5/22/29	0/1/1/1
7	JHM	J	561	7	-	0/6/22/22	0/1/1/1
7	IDS	J	562	7	-	0/5/22/29	0/1/1/1
7	JHM	J	563	7	-	0/6/22/22	0/1/1/1
7	IDS	J	564	7	1/1/5/7	0/5/22/29	0/1/1/1
7	JHM	J	595	7	-	0/6/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	IDS	J	596	7	-	0/5/22/29	0/1/1/1
7	JHM	J	597	7	-	0/6/22/22	0/1/1/1
7	IDS	J	598	7	1/1/5/7	0/5/22/29	0/1/1/1
7	JHM	J	599	7	-	0/6/22/22	0/1/1/1
7	IDS	J	600	7	1/1/5/7	0/5/22/29	0/1/1/1
7	JHM	L	611	7	-	0/6/22/22	0/1/1/1
7	IDS	L	612	7	-	0/5/22/29	0/1/1/1
7	JHM	L	613	7	-	0/6/22/22	0/1/1/1
7	IDS	L	614	7	1/1/5/7	0/5/22/29	0/1/1/1
7	JHM	L	615	7	-	0/6/22/22	0/1/1/1
7	IDS	L	616	7	1/1/5/7	0/5/22/29	0/1/1/1
7	JHM	L	617	7	-	0/6/22/22	0/1/1/1
7	IDS	L	618	7	1/1/5/7	0/5/22/29	0/1/1/1
7	JHM	L	619	7	-	0/6/22/22	0/1/1/1
7	IDS	L	620	7	1/1/5/7	0/5/22/29	0/1/1/1
7	JHM	L	621	7	-	0/6/22/22	0/1/1/1
7	IDS	L	622	7	-	0/5/22/29	0/1/1/1
4	JHM	N	601	4	-	0/6/22/22	0/1/1/1
4	IDS	N	602	4	-	0/5/22/29	0/1/1/1
5	JHM	N	607	5	-	0/6/22/22	0/1/1/1
5	IDS	N	608	5	1/1/5/7	0/5/22/29	0/1/1/1
5	JHM	N	609	5	-	0/6/22/22	0/1/1/1
5	IDS	N	610	5	-	0/5/22/29	0/1/1/1
5	JHM	O	603	5	-	0/6/22/22	0/1/1/1
5	IDS	O	604	5	-	0/5/22/29	0/1/1/1
5	JHM	O	605	5	-	0/6/22/22	0/1/1/1
5	IDS	O	606	5	-	0/5/22/29	0/1/1/1

All (181) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	594	IDS	O2-C2	-6.76	1.37	1.47
7	J	596	IDS	O2-C2	-6.76	1.37	1.47
5	A	544	IDS	O2-C2	-6.74	1.37	1.47
7	J	598	IDS	O2-C2	-6.73	1.37	1.47
5	D	526	IDS	O2-C2	-6.72	1.37	1.47
7	L	620	IDS	O2-C2	-6.72	1.37	1.47
7	F	570	IDS	O2-C2	-6.72	1.37	1.47
5	A	518	IDS	O2-C2	-6.72	1.37	1.47
7	J	558	IDS	O2-C2	-6.71	1.37	1.47
4	D	522	IDS	O2-C2	-6.71	1.37	1.47
6	B	534	IDS	O2-C2	-6.71	1.37	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	524	IDS	O2-C2	-6.71	1.37	1.47
6	B	540	IDS	O2-C2	-6.70	1.37	1.47
7	F	568	IDS	O2-C2	-6.70	1.37	1.47
6	B	536	IDS	O2-C2	-6.69	1.37	1.47
6	F	582	IDS	O2-C2	-6.69	1.37	1.47
5	O	604	IDS	O2-C2	-6.69	1.37	1.47
6	F	586	IDS	O2-C2	-6.69	1.37	1.47
7	L	618	IDS	O2-C2	-6.68	1.37	1.47
7	E	550	IDS	O2-C2	-6.68	1.37	1.47
4	D	508	IDS	O2-C2	-6.68	1.37	1.47
7	F	566	IDS	O2-C2	-6.68	1.37	1.47
7	L	612	IDS	O2-C2	-6.68	1.37	1.47
5	C	574	IDS	O2-C2	-6.68	1.37	1.47
7	L	616	IDS	O2-C2	-6.68	1.37	1.47
7	E	548	IDS	O2-C2	-6.67	1.37	1.47
6	F	584	IDS	O2-C2	-6.67	1.37	1.47
5	N	608	IDS	O2-C2	-6.67	1.37	1.47
5	B	528	IDS	O2-C2	-6.67	1.37	1.47
7	H	576	IDS	O2-C2	-6.67	1.37	1.47
5	A	520	IDS	O2-C2	-6.66	1.37	1.47
7	H	580	IDS	O2-C2	-6.66	1.37	1.47
5	N	610	IDS	O2-C2	-6.66	1.37	1.47
7	H	578	IDS	O2-C2	-6.66	1.37	1.47
7	L	614	IDS	O2-C2	-6.66	1.37	1.47
7	J	562	IDS	O2-C2	-6.65	1.37	1.47
5	F	592	IDS	O2-C2	-6.65	1.37	1.47
5	C	572	IDS	O2-C2	-6.65	1.37	1.47
6	B	538	IDS	O2-C2	-6.64	1.37	1.47
6	F	590	IDS	O2-C2	-6.64	1.37	1.47
3	E	506	IDS	O2-C2	-6.64	1.37	1.47
3	E	502	IDS	O2-C2	-6.63	1.37	1.47
7	E	552	IDS	O2-C2	-6.63	1.37	1.47
7	J	554	IDS	O2-C2	-6.63	1.37	1.47
5	E	514	IDS	O2-C2	-6.63	1.37	1.47
5	E	512	IDS	O2-C2	-6.63	1.37	1.47
7	J	560	IDS	O2-C2	-6.63	1.37	1.47
4	D	504	IDS	O2-C2	-6.63	1.37	1.47
5	A	546	IDS	O2-C2	-6.62	1.37	1.47
4	D	510	IDS	O2-C2	-6.62	1.37	1.47
7	L	622	IDS	O2-C2	-6.61	1.37	1.47
6	F	588	IDS	O2-C2	-6.61	1.37	1.47
5	O	606	IDS	O2-C2	-6.61	1.37	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	530	IDS	O2-C2	-6.60	1.37	1.47
4	E	516	IDS	O2-C2	-6.60	1.37	1.47
4	N	602	IDS	O2-C2	-6.60	1.37	1.47
7	J	564	IDS	O2-C2	-6.60	1.37	1.47
7	J	556	IDS	O2-C2	-6.59	1.37	1.47
4	C	532	IDS	O2-C2	-6.59	1.37	1.47
6	B	542	IDS	O2-C2	-6.57	1.37	1.47
7	J	600	IDS	O2-C2	-6.56	1.37	1.47
7	L	617	JHM	C3-C4	2.11	1.55	1.52
5	E	511	JHM	C3-C4	2.18	1.55	1.52
5	C	573	JHM	C3-C4	2.19	1.55	1.52
7	J	559	JHM	C3-C4	2.20	1.55	1.52
5	O	605	JHM	C3-C4	2.20	1.55	1.52
7	L	621	JHM	C3-C4	2.21	1.55	1.52
6	F	589	JHM	C3-C4	2.21	1.55	1.52
7	H	577	JHM	C3-C4	2.21	1.55	1.52
5	N	609	JHM	C3-C4	2.21	1.55	1.52
7	J	555	JHM	C3-C4	2.21	1.55	1.52
7	E	551	JHM	C3-C4	2.22	1.55	1.52
5	O	603	JHM	C3-C4	2.22	1.55	1.52
7	L	611	JHM	C3-C4	2.22	1.55	1.52
5	N	607	JHM	C3-C4	2.23	1.55	1.52
4	N	601	JHM	C3-C4	2.23	1.55	1.52
7	L	619	JHM	C3-C4	2.23	1.55	1.52
5	F	593	JHM	C3-C4	2.23	1.55	1.52
7	F	569	JHM	C3-C4	2.23	1.55	1.52
7	J	595	JHM	C3-C4	2.23	1.55	1.52
5	A	543	JHM	C3-C4	2.23	1.55	1.52
7	L	615	JHM	C3-C4	2.24	1.55	1.52
5	B	527	JHM	C3-C4	2.24	1.55	1.52
6	B	535	JHM	C3-C4	2.24	1.55	1.52
7	E	549	JHM	C3-C4	2.25	1.55	1.52
6	B	541	JHM	C3-C4	2.25	1.55	1.52
4	E	515	JHM	C3-C4	2.25	1.55	1.52
7	J	561	JHM	C3-C4	2.25	1.55	1.52
3	E	505	JHM	C3-C4	2.26	1.55	1.52
5	F	591	JHM	C3-C4	2.26	1.55	1.52
6	F	585	JHM	C3-C4	2.26	1.55	1.52
7	F	567	JHM	C3-C4	2.26	1.55	1.52
7	J	557	JHM	C3-C4	2.26	1.55	1.52
5	B	529	JHM	C3-C4	2.26	1.55	1.52
5	A	517	JHM	C3-C4	2.27	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	531	JHM	C3-C4	2.27	1.55	1.52
5	D	523	JHM	C3-C4	2.27	1.55	1.52
4	D	521	JHM	C3-C4	2.27	1.55	1.52
7	J	597	JHM	C3-C4	2.27	1.55	1.52
7	L	613	JHM	C3-C4	2.28	1.55	1.52
7	E	547	JHM	C3-C4	2.28	1.55	1.52
6	F	583	JHM	C3-C4	2.28	1.55	1.52
5	E	513	JHM	C3-C4	2.29	1.55	1.52
6	F	587	JHM	C3-C4	2.29	1.55	1.52
5	C	571	JHM	C3-C4	2.29	1.55	1.52
4	D	509	JHM	C3-C4	2.29	1.55	1.52
4	D	503	JHM	C3-C4	2.29	1.55	1.52
7	H	575	JHM	C3-C4	2.29	1.55	1.52
7	J	553	JHM	C3-C4	2.29	1.55	1.52
7	F	565	JHM	C3-C4	2.29	1.55	1.52
7	H	579	JHM	C3-C4	2.30	1.55	1.52
6	B	539	JHM	C3-C4	2.31	1.55	1.52
6	F	581	JHM	C3-C4	2.32	1.55	1.52
6	B	537	JHM	C3-C4	2.33	1.55	1.52
4	D	507	JHM	C3-C4	2.33	1.55	1.52
7	J	599	JHM	C3-C4	2.34	1.55	1.52
6	B	533	JHM	C3-C4	2.34	1.55	1.52
5	A	545	JHM	C3-C4	2.37	1.55	1.52
7	J	563	JHM	C3-C4	2.37	1.55	1.52
5	D	525	JHM	C3-C4	2.40	1.55	1.52
5	A	519	JHM	C3-C4	2.41	1.55	1.52
6	F	585	JHM	O1-C1	2.54	1.45	1.39
7	J	553	JHM	O1-C1	2.54	1.45	1.39
6	F	583	JHM	O1-C1	2.54	1.45	1.39
7	E	547	JHM	O1-C1	2.55	1.45	1.39
7	J	555	JHM	O1-C1	2.56	1.45	1.39
5	F	593	JHM	O1-C1	2.56	1.45	1.39
7	L	613	JHM	O1-C1	2.56	1.45	1.39
5	D	523	JHM	O1-C1	2.56	1.45	1.39
7	E	549	JHM	O1-C1	2.56	1.45	1.39
5	B	529	JHM	O1-C1	2.56	1.45	1.39
5	O	603	JHM	O1-C1	2.57	1.45	1.39
5	D	525	JHM	O1-C1	2.57	1.45	1.39
6	B	541	JHM	O1-C1	2.57	1.45	1.39
7	J	597	JHM	O1-C1	2.57	1.45	1.39
7	F	565	JHM	O1-C1	2.57	1.45	1.39
6	B	535	JHM	O1-C1	2.57	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	619	JHM	O1-C1	2.57	1.45	1.39
5	N	607	JHM	O1-C1	2.57	1.45	1.39
6	F	587	JHM	O1-C1	2.57	1.45	1.39
7	F	569	JHM	O1-C1	2.58	1.45	1.39
4	N	601	JHM	O1-C1	2.58	1.45	1.39
5	A	543	JHM	O1-C1	2.58	1.45	1.39
6	F	589	JHM	O1-C1	2.58	1.45	1.39
5	O	605	JHM	O1-C1	2.58	1.45	1.39
7	H	577	JHM	O1-C1	2.58	1.45	1.39
7	J	557	JHM	O1-C1	2.58	1.45	1.39
4	C	531	JHM	O1-C1	2.58	1.45	1.39
5	A	517	JHM	O1-C1	2.58	1.45	1.39
6	F	581	JHM	O1-C1	2.58	1.45	1.39
4	D	509	JHM	O1-C1	2.59	1.45	1.39
7	J	599	JHM	O1-C1	2.59	1.45	1.39
7	H	579	JHM	O1-C1	2.59	1.45	1.39
5	F	591	JHM	O1-C1	2.59	1.45	1.39
7	J	559	JHM	O1-C1	2.59	1.45	1.39
7	J	561	JHM	O1-C1	2.59	1.45	1.39
7	F	567	JHM	O1-C1	2.59	1.45	1.39
5	A	519	JHM	O1-C1	2.59	1.45	1.39
5	C	573	JHM	O1-C1	2.59	1.45	1.39
7	J	563	JHM	O1-C1	2.60	1.45	1.39
7	J	595	JHM	O1-C1	2.60	1.45	1.39
4	D	503	JHM	O1-C1	2.60	1.45	1.39
7	L	611	JHM	O1-C1	2.60	1.45	1.39
7	E	551	JHM	O1-C1	2.60	1.45	1.39
5	A	545	JHM	O1-C1	2.60	1.45	1.39
5	C	571	JHM	O1-C1	2.61	1.45	1.39
6	B	539	JHM	O1-C1	2.61	1.45	1.39
5	N	609	JHM	O1-C1	2.61	1.45	1.39
7	L	617	JHM	O1-C1	2.61	1.45	1.39
4	E	515	JHM	O1-C1	2.61	1.45	1.39
4	D	507	JHM	O1-C1	2.61	1.45	1.39
5	E	513	JHM	O1-C1	2.62	1.45	1.39
3	E	505	JHM	O1-C1	2.62	1.45	1.39
4	D	521	JHM	O1-C1	2.62	1.45	1.39
7	L	615	JHM	O1-C1	2.62	1.45	1.39
5	E	511	JHM	O1-C1	2.63	1.45	1.39
7	L	621	JHM	O1-C1	2.63	1.45	1.39
7	H	575	JHM	O1-C1	2.64	1.45	1.39
6	B	533	JHM	O1-C1	2.64	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	527	JHM	O1-C1	2.65	1.45	1.39
6	B	537	JHM	O1-C1	2.66	1.45	1.39

All (241) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	535	JHM	C3-C4-C5	-3.27	106.64	109.93
5	A	545	JHM	C3-C4-C5	-3.26	106.65	109.93
5	D	523	JHM	C3-C4-C5	-3.25	106.65	109.93
6	B	533	JHM	C3-C4-C5	-3.25	106.65	109.93
5	D	525	JHM	C3-C4-C5	-3.25	106.66	109.93
4	E	515	JHM	C3-C4-C5	-3.23	106.67	109.93
4	D	521	JHM	C3-C4-C5	-3.23	106.68	109.93
4	D	507	JHM	C3-C4-C5	-3.22	106.69	109.93
5	A	519	JHM	C3-C4-C5	-3.22	106.69	109.93
7	E	547	JHM	C3-C4-C5	-3.22	106.69	109.93
7	L	611	JHM	C3-C4-C5	-3.21	106.70	109.93
4	D	509	JHM	C3-C4-C5	-3.21	106.70	109.93
6	F	581	JHM	C3-C4-C5	-3.20	106.70	109.93
6	B	537	JHM	C3-C4-C5	-3.20	106.71	109.93
5	A	517	JHM	C3-C4-C5	-3.20	106.71	109.93
7	E	551	JHM	C3-C4-C5	-3.20	106.71	109.93
6	B	539	JHM	C3-C4-C5	-3.19	106.72	109.93
7	J	599	JHM	C3-C4-C5	-3.19	106.72	109.93
7	L	613	JHM	C3-C4-C5	-3.19	106.72	109.93
7	H	575	JHM	C3-C4-C5	-3.19	106.72	109.93
7	H	579	JHM	C3-C4-C5	-3.18	106.72	109.93
4	N	601	JHM	C3-C4-C5	-3.18	106.72	109.93
5	C	573	JHM	C3-C4-C5	-3.18	106.72	109.93
7	L	621	JHM	C3-C4-C5	-3.18	106.73	109.93
7	J	597	JHM	C3-C4-C5	-3.18	106.73	109.93
4	D	503	JHM	C3-C4-C5	-3.18	106.73	109.93
7	J	563	JHM	C3-C4-C5	-3.18	106.73	109.93
7	L	615	JHM	C3-C4-C5	-3.18	106.73	109.93
7	E	549	JHM	C3-C4-C5	-3.18	106.73	109.93
5	E	511	JHM	C3-C4-C5	-3.17	106.74	109.93
7	J	595	JHM	C3-C4-C5	-3.17	106.74	109.93
6	F	589	JHM	C3-C4-C5	-3.17	106.74	109.93
5	O	605	JHM	C3-C4-C5	-3.17	106.74	109.93
7	J	553	JHM	C3-C4-C5	-3.16	106.75	109.93
6	F	585	JHM	C3-C4-C5	-3.16	106.75	109.93
5	N	609	JHM	C3-C4-C5	-3.16	106.75	109.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	J	555	JHM	C3-C4-C5	-3.16	106.75	109.93
7	L	619	JHM	C3-C4-C5	-3.16	106.75	109.93
5	N	607	JHM	C3-C4-C5	-3.16	106.75	109.93
5	B	529	JHM	C3-C4-C5	-3.16	106.75	109.93
5	C	571	JHM	C3-C4-C5	-3.16	106.75	109.93
6	B	541	JHM	C3-C4-C5	-3.15	106.75	109.93
5	F	593	JHM	C3-C4-C5	-3.15	106.75	109.93
7	F	567	JHM	C3-C4-C5	-3.15	106.75	109.93
7	F	565	JHM	C3-C4-C5	-3.15	106.76	109.93
3	E	505	JHM	C3-C4-C5	-3.15	106.76	109.93
4	C	531	JHM	C3-C4-C5	-3.15	106.76	109.93
5	A	543	JHM	C3-C4-C5	-3.15	106.76	109.93
7	F	569	JHM	C3-C4-C5	-3.14	106.77	109.93
5	E	513	JHM	C3-C4-C5	-3.14	106.77	109.93
7	L	617	JHM	C3-C4-C5	-3.14	106.77	109.93
7	J	559	JHM	C3-C4-C5	-3.13	106.78	109.93
6	F	587	JHM	C3-C4-C5	-3.13	106.78	109.93
5	B	527	JHM	C3-C4-C5	-3.12	106.78	109.93
5	O	603	JHM	C3-C4-C5	-3.12	106.79	109.93
7	H	577	JHM	C3-C4-C5	-3.12	106.79	109.93
5	F	591	JHM	C3-C4-C5	-3.11	106.80	109.93
6	F	583	JHM	C3-C4-C5	-3.11	106.80	109.93
7	J	561	JHM	C3-C4-C5	-3.11	106.80	109.93
7	J	557	JHM	C3-C4-C5	-3.10	106.81	109.93
7	J	553	JHM	C2-C3-C4	-2.52	107.13	110.56
6	F	585	JHM	C2-C3-C4	-2.52	107.13	110.56
7	F	569	JHM	C2-C3-C4	-2.51	107.14	110.56
5	O	605	JHM	C2-C3-C4	-2.51	107.14	110.56
6	F	589	JHM	C2-C3-C4	-2.51	107.15	110.56
6	F	583	JHM	C2-C3-C4	-2.51	107.15	110.56
4	D	507	JHM	C2-C3-C4	-2.50	107.15	110.56
5	O	603	JHM	C2-C3-C4	-2.50	107.15	110.56
7	H	575	JHM	C2-C3-C4	-2.50	107.16	110.56
5	E	511	JHM	C1-C2-C3	-2.50	106.95	111.23
5	B	529	JHM	C2-C3-C4	-2.50	107.16	110.56
7	J	561	JHM	C2-C3-C4	-2.50	107.16	110.56
5	F	591	JHM	C2-C3-C4	-2.50	107.16	110.56
4	E	515	JHM	C2-C3-C4	-2.49	107.16	110.56
6	F	587	JHM	C2-C3-C4	-2.49	107.17	110.56
5	E	513	JHM	C1-C2-C3	-2.49	106.96	111.23
6	B	535	JHM	C1-C2-C3	-2.49	106.96	111.23
7	J	557	JHM	C2-C3-C4	-2.49	107.17	110.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	531	JHM	C2-C3-C4	-2.49	107.17	110.56
5	F	593	JHM	C2-C3-C4	-2.49	107.17	110.56
4	E	515	JHM	C1-C2-C3	-2.49	106.97	111.23
5	A	519	JHM	C2-C3-C4	-2.49	107.17	110.56
7	J	599	JHM	C2-C3-C4	-2.49	107.17	110.56
5	A	543	JHM	C2-C3-C4	-2.49	107.17	110.56
7	E	549	JHM	C2-C3-C4	-2.48	107.17	110.56
5	C	571	JHM	C2-C3-C4	-2.48	107.18	110.56
7	J	563	JHM	C2-C3-C4	-2.48	107.18	110.56
5	D	525	JHM	C2-C3-C4	-2.48	107.18	110.56
7	H	577	JHM	C2-C3-C4	-2.48	107.18	110.56
7	E	551	JHM	C1-C2-C3	-2.48	106.98	111.23
7	F	565	JHM	C2-C3-C4	-2.48	107.19	110.56
6	F	583	JHM	C1-C2-C3	-2.48	106.99	111.23
5	C	573	JHM	C1-C2-C3	-2.47	106.99	111.23
7	J	597	JHM	C1-C2-C3	-2.47	106.99	111.23
5	A	545	JHM	C2-C3-C4	-2.47	107.19	110.56
4	D	507	JHM	C1-C2-C3	-2.47	106.99	111.23
5	E	513	JHM	C2-C3-C4	-2.47	107.19	110.56
7	L	617	JHM	C1-C2-C3	-2.47	106.99	111.23
7	H	579	JHM	C2-C3-C4	-2.47	107.19	110.56
6	B	539	JHM	C1-C2-C3	-2.47	107.00	111.23
5	D	523	JHM	C2-C3-C4	-2.47	107.19	110.56
6	B	537	JHM	C2-C3-C4	-2.47	107.20	110.56
7	E	547	JHM	C2-C3-C4	-2.47	107.20	110.56
5	A	517	JHM	C2-C3-C4	-2.47	107.20	110.56
4	D	509	JHM	C1-C2-C3	-2.47	107.00	111.23
5	E	511	JHM	C2-C3-C4	-2.47	107.20	110.56
6	B	539	JHM	C2-C3-C4	-2.47	107.20	110.56
7	J	559	JHM	C2-C3-C4	-2.47	107.20	110.56
7	L	619	JHM	C2-C3-C4	-2.46	107.20	110.56
6	B	541	JHM	C2-C3-C4	-2.46	107.20	110.56
4	D	509	JHM	C2-C3-C4	-2.46	107.20	110.56
4	D	521	JHM	C1-C2-C3	-2.46	107.01	111.23
5	B	527	JHM	C2-C3-C4	-2.46	107.21	110.56
5	A	517	JHM	C1-C2-C3	-2.46	107.01	111.23
4	N	601	JHM	C2-C3-C4	-2.46	107.21	110.56
7	L	613	JHM	C2-C3-C4	-2.46	107.21	110.56
4	D	503	JHM	C1-C2-C3	-2.46	107.01	111.23
7	J	561	JHM	C1-C2-C3	-2.46	107.01	111.23
6	F	581	JHM	C2-C3-C4	-2.46	107.21	110.56
3	E	505	JHM	C2-C3-C4	-2.46	107.21	110.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	607	JHM	C2-C3-C4	-2.46	107.21	110.56
5	F	591	JHM	C1-C2-C3	-2.46	107.02	111.23
7	J	557	JHM	C1-C2-C3	-2.46	107.02	111.23
5	D	525	JHM	C1-C2-C3	-2.46	107.02	111.23
4	D	503	JHM	C2-C3-C4	-2.46	107.21	110.56
7	F	565	JHM	C1-C2-C3	-2.46	107.02	111.23
6	B	537	JHM	C1-C2-C3	-2.45	107.02	111.23
3	E	505	JHM	C1-C2-C3	-2.45	107.02	111.23
7	E	547	JHM	C1-C2-C3	-2.45	107.03	111.23
7	L	617	JHM	C2-C3-C4	-2.45	107.22	110.56
7	J	555	JHM	C1-C2-C3	-2.45	107.03	111.23
5	N	609	JHM	C2-C3-C4	-2.45	107.22	110.56
7	E	549	JHM	C1-C2-C3	-2.45	107.03	111.23
4	D	521	JHM	C2-C3-C4	-2.45	107.22	110.56
5	D	523	JHM	C1-C2-C3	-2.45	107.03	111.23
7	H	579	JHM	C1-C2-C3	-2.45	107.03	111.23
6	F	587	JHM	C1-C2-C3	-2.45	107.03	111.23
7	E	551	JHM	C2-C3-C4	-2.45	107.23	110.56
7	J	595	JHM	C2-C3-C4	-2.45	107.23	110.56
5	A	519	JHM	C1-C2-C3	-2.45	107.04	111.23
7	J	595	JHM	C1-C2-C3	-2.45	107.04	111.23
4	N	601	JHM	C1-C2-C3	-2.45	107.04	111.23
5	B	529	JHM	C1-C2-C3	-2.44	107.04	111.23
5	C	571	JHM	C1-C2-C3	-2.44	107.04	111.23
6	F	581	JHM	C1-C2-C3	-2.44	107.04	111.23
5	A	545	JHM	C1-C2-C3	-2.44	107.04	111.23
7	F	569	JHM	C1-C2-C3	-2.44	107.04	111.23
6	B	533	JHM	C2-C3-C4	-2.44	107.23	110.56
7	L	615	JHM	C2-C3-C4	-2.44	107.23	110.56
5	N	609	JHM	C1-C2-C3	-2.44	107.04	111.23
7	F	567	JHM	C2-C3-C4	-2.44	107.23	110.56
6	F	589	JHM	C1-C2-C3	-2.44	107.05	111.23
6	B	541	JHM	C1-C2-C3	-2.44	107.05	111.23
5	F	593	JHM	C1-C2-C3	-2.44	107.05	111.23
6	B	535	JHM	C2-C3-C4	-2.44	107.24	110.56
7	J	553	JHM	C1-C2-C3	-2.44	107.05	111.23
7	L	621	JHM	C2-C3-C4	-2.44	107.24	110.56
6	F	585	JHM	C1-C2-C3	-2.43	107.06	111.23
5	A	543	JHM	C1-C2-C3	-2.43	107.06	111.23
7	L	611	JHM	C2-C3-C4	-2.43	107.24	110.56
5	B	527	JHM	C1-C2-C3	-2.43	107.06	111.23
7	F	567	JHM	C1-C2-C3	-2.43	107.06	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	573	JHM	C2-C3-C4	-2.43	107.25	110.56
6	B	533	JHM	C1-C2-C3	-2.43	107.06	111.23
7	J	555	JHM	C2-C3-C4	-2.43	107.25	110.56
7	J	597	JHM	C2-C3-C4	-2.43	107.25	110.56
5	O	603	JHM	C1-C2-C3	-2.43	107.07	111.23
7	H	575	JHM	C1-C2-C3	-2.42	107.08	111.23
7	L	619	JHM	C1-C2-C3	-2.42	107.08	111.23
5	N	607	JHM	C1-C2-C3	-2.42	107.08	111.23
7	J	599	JHM	C1-C2-C3	-2.42	107.08	111.23
7	L	613	JHM	C1-C2-C3	-2.42	107.08	111.23
7	H	577	JHM	C1-C2-C3	-2.42	107.08	111.23
7	L	621	JHM	C1-C2-C3	-2.41	107.09	111.23
7	J	563	JHM	C1-C2-C3	-2.41	107.10	111.23
7	L	615	JHM	C1-C2-C3	-2.41	107.10	111.23
4	C	531	JHM	C1-C2-C3	-2.41	107.10	111.23
7	J	559	JHM	C1-C2-C3	-2.40	107.11	111.23
7	L	611	JHM	C1-C2-C3	-2.40	107.11	111.23
5	O	605	JHM	C1-C2-C3	-2.38	107.15	111.23
4	N	602	IDS	C1-C2-C3	2.73	113.62	109.89
7	J	596	IDS	C1-C2-C3	2.74	113.63	109.89
6	F	584	IDS	C1-C2-C3	2.74	113.63	109.89
5	O	604	IDS	C1-C2-C3	2.75	113.65	109.89
5	A	544	IDS	C1-C2-C3	2.75	113.65	109.89
5	N	610	IDS	C1-C2-C3	2.76	113.66	109.89
7	E	550	IDS	C1-C2-C3	2.76	113.66	109.89
7	J	598	IDS	C1-C2-C3	2.76	113.66	109.89
6	F	582	IDS	C1-C2-C3	2.76	113.66	109.89
7	L	614	IDS	C1-C2-C3	2.76	113.66	109.89
5	B	528	IDS	C1-C2-C3	2.76	113.66	109.89
7	L	618	IDS	C1-C2-C3	2.77	113.67	109.89
7	H	578	IDS	C1-C2-C3	2.77	113.67	109.89
7	E	548	IDS	C1-C2-C3	2.77	113.68	109.89
5	F	592	IDS	C1-C2-C3	2.77	113.68	109.89
5	A	518	IDS	C1-C2-C3	2.77	113.68	109.89
7	F	568	IDS	C1-C2-C3	2.78	113.68	109.89
5	E	512	IDS	C1-C2-C3	2.78	113.69	109.89
3	E	502	IDS	C1-C2-C3	2.78	113.69	109.89
6	F	586	IDS	C1-C2-C3	2.78	113.69	109.89
4	E	516	IDS	C1-C2-C3	2.78	113.69	109.89
7	H	576	IDS	C1-C2-C3	2.78	113.69	109.89
7	J	562	IDS	C1-C2-C3	2.78	113.69	109.89
6	F	588	IDS	C1-C2-C3	2.78	113.69	109.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	530	IDS	C1-C2-C3	2.78	113.70	109.89
7	L	620	IDS	C1-C2-C3	2.78	113.70	109.89
5	D	526	IDS	C1-C2-C3	2.78	113.70	109.89
6	F	590	IDS	C1-C2-C3	2.78	113.70	109.89
6	B	538	IDS	C1-C2-C3	2.79	113.70	109.89
7	F	566	IDS	C1-C2-C3	2.79	113.70	109.89
6	B	536	IDS	C1-C2-C3	2.79	113.70	109.89
7	J	558	IDS	C1-C2-C3	2.79	113.70	109.89
5	N	608	IDS	C1-C2-C3	2.79	113.70	109.89
4	C	532	IDS	C1-C2-C3	2.79	113.70	109.89
7	L	612	IDS	C1-C2-C3	2.79	113.70	109.89
5	A	520	IDS	C1-C2-C3	2.79	113.71	109.89
5	F	594	IDS	C1-C2-C3	2.79	113.71	109.89
4	D	522	IDS	C1-C2-C3	2.79	113.71	109.89
7	L	622	IDS	C1-C2-C3	2.80	113.71	109.89
7	J	556	IDS	C1-C2-C3	2.80	113.71	109.89
7	F	570	IDS	C1-C2-C3	2.80	113.71	109.89
7	H	580	IDS	C1-C2-C3	2.80	113.72	109.89
7	E	552	IDS	C1-C2-C3	2.81	113.72	109.89
5	O	606	IDS	C1-C2-C3	2.81	113.73	109.89
7	J	564	IDS	C1-C2-C3	2.81	113.73	109.89
4	D	510	IDS	C1-C2-C3	2.81	113.73	109.89
6	B	540	IDS	C1-C2-C3	2.81	113.73	109.89
5	C	574	IDS	C1-C2-C3	2.81	113.73	109.89
7	J	554	IDS	C1-C2-C3	2.82	113.74	109.89
4	D	504	IDS	C1-C2-C3	2.82	113.74	109.89
5	D	524	IDS	C1-C2-C3	2.82	113.74	109.89
5	A	546	IDS	C1-C2-C3	2.82	113.75	109.89
3	E	506	IDS	C1-C2-C3	2.82	113.75	109.89
5	C	572	IDS	C1-C2-C3	2.82	113.75	109.89
6	B	534	IDS	C1-C2-C3	2.82	113.75	109.89
6	B	542	IDS	C1-C2-C3	2.82	113.75	109.89
5	E	514	IDS	C1-C2-C3	2.83	113.76	109.89
7	J	600	IDS	C1-C2-C3	2.83	113.76	109.89
4	D	508	IDS	C1-C2-C3	2.83	113.76	109.89
7	L	616	IDS	C1-C2-C3	2.84	113.77	109.89
7	J	560	IDS	C1-C2-C3	2.85	113.78	109.89

All (17) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	J	556	IDS	C4

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Mol	Chain	Res	Type	Atom
7	L	614	IDS	C4
7	L	616	IDS	C4
7	J	554	IDS	C4
7	L	620	IDS	C4
7	J	600	IDS	C4
5	C	572	IDS	C4
5	A	518	IDS	C4
6	B	534	IDS	C4
7	L	618	IDS	C4
6	B	538	IDS	C4
7	E	548	IDS	C4
7	E	550	IDS	C4
7	J	598	IDS	C4
7	J	564	IDS	C4
5	N	608	IDS	C4
7	H	580	IDS	C4

There are no torsion outliers.

There are no ring outliers.

75 monomers are involved in 194 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	517	JHM	1	0
5	A	518	IDS	0	2
5	A	519	JHM	0	1
5	B	527	JHM	1	0
5	B	528	IDS	4	0
5	B	529	JHM	7	0
5	B	530	IDS	6	0
6	B	534	IDS	3	0
6	B	535	JHM	2	0
6	B	536	IDS	2	0
6	B	537	JHM	2	0
6	B	540	IDS	4	0
6	B	541	JHM	4	0
5	C	572	IDS	5	0
4	D	503	JHM	1	0
4	D	504	IDS	8	0
4	D	510	IDS	1	0
4	D	522	IDS	2	0
5	D	523	JHM	4	0
5	D	526	IDS	0	2

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	502	IDS	6	0
3	E	505	JHM	6	0
5	E	511	JHM	2	0
5	E	513	JHM	3	0
5	E	514	IDS	0	1
4	E	516	IDS	3	0
7	E	547	JHM	3	0
7	E	548	IDS	1	0
7	E	550	IDS	1	0
7	E	551	JHM	1	0
7	F	565	JHM	1	0
7	F	567	JHM	8	0
7	F	568	IDS	1	0
7	F	569	JHM	4	0
7	F	570	IDS	6	0
6	F	582	IDS	2	0
6	F	583	JHM	2	1
6	F	584	IDS	4	3
6	F	585	JHM	3	0
5	F	591	JHM	1	0
5	F	594	IDS	0	1
7	H	575	JHM	4	0
7	H	577	JHM	3	0
7	H	578	IDS	6	0
7	H	580	IDS	4	0
7	J	554	IDS	10	0
7	J	555	JHM	7	0
7	J	556	IDS	4	0
7	J	557	JHM	4	0
7	J	559	JHM	5	0
7	J	561	JHM	9	0
7	J	562	IDS	4	0
7	J	563	JHM	4	0
7	J	564	IDS	9	0
7	J	595	JHM	1	0
7	J	596	IDS	3	0
7	J	597	JHM	1	0
7	J	598	IDS	2	0
7	J	599	JHM	4	0
7	J	600	IDS	1	0
7	L	611	JHM	4	1
7	L	612	IDS	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	L	613	JHM	1	1
7	L	614	IDS	5	0
7	L	615	JHM	0	1
7	L	616	IDS	1	1
7	L	618	IDS	1	0
7	L	619	JHM	8	0
7	L	620	IDS	2	0
7	L	621	JHM	2	0
4	N	601	JHM	1	0
5	N	607	JHM	10	0
5	N	608	IDS	5	1
5	N	609	JHM	6	0
5	O	604	IDS	1	0

5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	JHM	E	501	3	15,15,15	1.15	2 (13%)	20,22,22	1.24	3 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	JHM	E	501	3	-	0/6/22/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	501	JHM	C3-C4	2.29	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	501	JHM	O1-C1	2.62	1.45	1.39

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	501	JHM	C3-C4-C5	-3.16	106.75	109.93
2	E	501	JHM	C2-C3-C4	-2.50	107.16	110.56
2	E	501	JHM	C1-C2-C3	-2.45	107.03	111.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	501	JHM	8	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	422/427 (98%)	-0.01	18 (4%)	39	34	13, 51, 103, 135	0
1	B	422/427 (98%)	0.08	24 (5%)	27	25	12, 49, 101, 134	0
1	C	422/427 (98%)	-0.01	18 (4%)	39	34	11, 44, 102, 137	0
1	D	422/427 (98%)	-0.03	14 (3%)	50	45	11, 43, 96, 137	0
1	E	422/427 (98%)	-0.09	15 (3%)	46	41	11, 44, 101, 137	0
1	F	422/427 (98%)	-0.07	11 (2%)	59	54	13, 51, 103, 143	0
1	G	422/427 (98%)	0.13	27 (6%)	23	21	15, 52, 102, 124	0
1	H	422/427 (98%)	0.01	17 (4%)	42	37	11, 42, 99, 141	0
1	I	422/427 (98%)	-0.09	18 (4%)	39	34	12, 43, 97, 135	0
1	J	422/427 (98%)	0.10	24 (5%)	27	25	11, 48, 102, 131	0
1	K	422/427 (98%)	0.06	21 (4%)	32	29	14, 52, 99, 140	0
1	L	422/427 (98%)	0.25	27 (6%)	23	21	14, 50, 104, 131	0
1	M	422/427 (98%)	0.11	25 (5%)	26	23	12, 50, 101, 130	0
1	N	422/427 (98%)	-0.02	10 (2%)	62	57	16, 55, 99, 135	0
1	O	421/427 (98%)	0.13	32 (7%)	17	16	12, 51, 102, 136	0
All	All	6329/6405 (98%)	0.04	301 (4%)	34	31	11, 48, 102, 143	0

All (301) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	138	ASN	13.4
1	L	136	THR	11.2
1	L	137	SER	11.0
1	H	177	SER	9.0
1	L	135	ALA	8.9
1	G	174	ALA	8.8
1	C	136	THR	8.8

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Mol	Chain	Res	Type	RSRZ
1	H	135	ALA	8.4
1	D	134	ALA	8.0
1	M	173	THR	7.6
1	L	134	ALA	7.5
1	H	176	LYS	7.2
1	C	141	GLU	7.1
1	L	139	VAL	7.1
1	G	175	SER	7.0
1	M	174	ALA	6.7
1	G	176	LYS	6.6
1	M	57	GLY	6.4
1	O	135	ALA	6.4
1	L	140	SER	6.4
1	F	133	HIS	6.2
1	B	177	SER	6.2
1	E	177	SER	6.2
1	M	134	ALA	6.2
1	C	134	ALA	6.1
1	F	134	ALA	6.0
1	A	137	SER	6.0
1	H	137	SER	6.0
1	H	136	THR	5.9
1	G	177	SER	5.8
1	M	135	ALA	5.8
1	D	135	ALA	5.7
1	H	138	ASN	5.5
1	L	141	GLU	5.5
1	C	177	SER	5.5
1	N	135	ALA	5.5
1	B	350	SER	5.4
1	C	137	SER	5.4
1	B	173	THR	5.4
1	D	176	LYS	5.4
1	G	140	SER	5.3
1	C	135	ALA	5.1
1	O	55	GLY	5.1
1	L	474	GLY	5.1
1	O	351	PRO	5.0
1	G	173	THR	4.9
1	O	138	ASN	4.9
1	A	136	THR	4.8
1	E	438	ASN	4.7

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Mol	Chain	Res	Type	RSRZ
1	J	90	ILE	4.7
1	O	56	GLY	4.7
1	B	175	SER	4.6
1	G	88	THR	4.6
1	L	438	ASN	4.6
1	C	140	SER	4.6
1	A	174	ALA	4.6
1	E	175	SER	4.6
1	O	141	GLU	4.5
1	D	133	HIS	4.5
1	A	177	SER	4.5
1	M	439	LYS	4.4
1	B	56	GLY	4.4
1	H	134	ALA	4.4
1	G	318	GLY	4.4
1	C	176	LYS	4.3
1	O	177	SER	4.2
1	G	384	LEU	4.2
1	H	179	PRO	4.2
1	K	88	THR	4.2
1	G	137	SER	4.2
1	M	438	ASN	4.2
1	J	89	SER	4.1
1	O	173	THR	4.1
1	O	134	ALA	4.1
1	B	438	ASN	4.1
1	L	173	THR	4.0
1	M	58	ASN	4.0
1	I	173	THR	4.0
1	K	138	ASN	4.0
1	F	135	ALA	4.0
1	H	178	ARG	3.9
1	C	88	THR	3.9
1	O	350	SER	3.8
1	E	141	GLU	3.8
1	O	54	ALA	3.8
1	C	133	HIS	3.8
1	B	179	PRO	3.8
1	H	175	SER	3.8
1	N	184	ASP	3.8
1	D	175	SER	3.7
1	J	177	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	G	55	GLY	3.7
1	M	88	THR	3.7
1	J	175	SER	3.7
1	O	133	HIS	3.7
1	G	141	GLU	3.7
1	B	134	ALA	3.7
1	C	438	ASN	3.7
1	C	350	SER	3.6
1	B	138	ASN	3.6
1	A	176	LYS	3.6
1	I	90	ILE	3.5
1	M	351	PRO	3.5
1	O	352	VAL	3.5
1	C	174	ALA	3.5
1	J	179	PRO	3.5
1	E	474	GLY	3.5
1	A	86	PRO	3.5
1	E	314	HIS	3.5
1	M	86	PRO	3.4
1	M	133	HIS	3.4
1	O	61	ASP	3.4
1	E	134	ALA	3.4
1	F	173	THR	3.4
1	K	82	LYS	3.4
1	O	57	GLY	3.4
1	G	179	PRO	3.4
1	E	178	ARG	3.4
1	O	136	THR	3.4
1	J	174	ALA	3.3
1	O	142	ASP	3.3
1	D	177	SER	3.3
1	I	87	ASP	3.3
1	J	317	GLN	3.2
1	K	174	ALA	3.2
1	B	137	SER	3.2
1	O	174	ALA	3.2
1	C	139	VAL	3.2
1	E	133	HIS	3.2
1	J	137	SER	3.2
1	M	87	ASP	3.2
1	K	181	SER	3.2
1	B	392	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	L	439	LYS	3.2
1	E	439	LYS	3.1
1	G	383	THR	3.1
1	H	174	ALA	3.1
1	K	273	GLN	3.1
1	I	89	SER	3.1
1	E	179	PRO	3.1
1	J	86	PRO	3.1
1	J	173	THR	3.0
1	L	440	ASP	3.0
1	K	137	SER	3.0
1	K	133	HIS	3.0
1	B	395	MET	3.0
1	L	175	SER	3.0
1	I	174	ALA	3.0
1	E	182	GLN	3.0
1	H	141	GLU	3.0
1	L	356	TYR	3.0
1	B	136	THR	3.0
1	G	134	ALA	3.0
1	J	136	THR	3.0
1	M	350	SER	2.9
1	B	396	ASN	2.9
1	F	177	SER	2.9
1	L	355	GLN	2.9
1	C	138	ASN	2.9
1	D	174	ALA	2.9
1	L	174	ALA	2.9
1	M	343	THR	2.9
1	O	181	SER	2.9
1	A	141	GLU	2.8
1	J	354	GLY	2.8
1	I	350	SER	2.8
1	O	137	SER	2.8
1	B	133	HIS	2.8
1	D	350	SER	2.8
1	G	135	ALA	2.8
1	E	443	ASP	2.8
1	F	56	GLY	2.8
1	H	55	GLY	2.7
1	G	91	TYR	2.7
1	H	315	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	K	179	PRO	2.7
1	I	314	HIS	2.7
1	L	91	TYR	2.7
1	O	60	GLN	2.7
1	K	180	LEU	2.7
1	A	179	PRO	2.7
1	O	175	SER	2.7
1	J	355	GLN	2.7
1	B	176	LYS	2.6
1	B	172	GLY	2.6
1	F	176	LYS	2.6
1	G	289	CYS	2.6
1	C	349	GLN	2.6
1	O	182	GLN	2.6
1	L	348	THR	2.6
1	I	86	PRO	2.6
1	K	438	ASN	2.6
1	A	315	LYS	2.6
1	F	438	ASN	2.6
1	I	135	ALA	2.6
1	A	314	HIS	2.6
1	C	314	HIS	2.6
1	M	141	GLU	2.6
1	B	88	THR	2.6
1	B	61	ASP	2.6
1	N	185	CYS	2.6
1	M	177	SER	2.6
1	I	269	ASP	2.6
1	D	141	GLU	2.6
1	M	180	LEU	2.5
1	A	138	ASN	2.5
1	A	139	VAL	2.5
1	K	134	ALA	2.5
1	I	438	ASN	2.5
1	M	89	SER	2.5
1	I	315	LYS	2.5
1	I	439	LYS	2.5
1	I	88	THR	2.5
1	M	280	THR	2.5
1	L	133	HIS	2.5
1	G	94	GLU	2.5
1	J	135	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	K	175	SER	2.5
1	D	180	LEU	2.5
1	O	176	LYS	2.5
1	F	282	MET	2.4
1	H	133	HIS	2.4
1	A	57	GLY	2.4
1	L	142	ASP	2.4
1	J	88	THR	2.4
1	J	400	LEU	2.4
1	K	135	ALA	2.4
1	E	315	LYS	2.4
1	G	60	GLN	2.4
1	B	135	ALA	2.4
1	K	177	SER	2.4
1	L	442	TYR	2.4
1	O	180	LEU	2.4
1	G	59	LYS	2.4
1	G	439	LYS	2.4
1	L	340	THR	2.4
1	N	57	GLY	2.4
1	O	444	LYS	2.4
1	I	387	ASP	2.3
1	B	174	ALA	2.3
1	J	55	GLY	2.3
1	J	352	VAL	2.3
1	G	86	PRO	2.3
1	A	175	SER	2.3
1	M	349	GLN	2.3
1	H	348	THR	2.3
1	B	139	VAL	2.3
1	I	186	PRO	2.3
1	B	398	SER	2.3
1	K	90	ILE	2.3
1	N	59	LYS	2.3
1	N	139	VAL	2.3
1	D	172	GLY	2.2
1	J	87	ASP	2.2
1	G	138	ASN	2.2
1	F	55	GLY	2.2
1	I	183	GLY	2.2
1	M	176	LYS	2.2
1	K	55	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	350	SER	2.2
1	N	282	MET	2.2
1	O	140	SER	2.2
1	G	315	LYS	2.2
1	L	281	GLY	2.2
1	K	87	ASP	2.2
1	L	443	ASP	2.2
1	O	439	LYS	2.1
1	G	133	HIS	2.1
1	J	439	LYS	2.1
1	D	138	ASN	2.1
1	K	142	ASP	2.1
1	M	61	ASP	2.1
1	O	395	MET	2.1
1	C	175	SER	2.1
1	E	135	ALA	2.1
1	G	56	GLY	2.1
1	J	474	GLY	2.1
1	J	178	ARG	2.1
1	I	134	ALA	2.1
1	O	403	TRP	2.1
1	A	87	ASP	2.1
1	M	285	SER	2.1
1	N	397	SER	2.1
1	H	88	THR	2.1
1	A	133	HIS	2.1
1	N	183	GLY	2.1
1	L	383	THR	2.1
1	K	86	PRO	2.1
1	M	20	ALA	2.1
1	A	60	GLN	2.1
1	O	384	LEU	2.1
1	A	173	THR	2.0
1	D	88	THR	2.0
1	F	127	ASP	2.0
1	B	60	GLN	2.0
1	K	269	ASP	2.0
1	J	404	ASN	2.0
1	O	357	ASP	2.0
1	L	132	SER	2.0
1	N	177	SER	2.0
1	D	137	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	IDS	F	590	15/17	0.73	0.64	22.41	26,28,35,39	0
7	JHM	E	547	15/15	0.54	0.81	20.45	42,62,84,85	0
5	JHM	A	519	15/15	0.71	0.56	15.51	42,62,84,85	0
7	IDS	E	548	15/17	0.79	0.67	13.33	26,28,35,39	0
5	JHM	N	607	15/15	0.55	0.66	10.22	42,62,84,85	0
7	IDS	J	554	15/17	0.76	0.52	9.86	26,28,35,39	0
7	IDS	J	598	15/17	0.72	0.65	9.54	26,28,35,39	0
7	JHM	H	575	15/15	0.25	0.87	9.03	42,62,84,85	0
7	JHM	J	555	15/15	0.51	0.68	8.28	42,62,84,85	0
7	JHM	J	597	15/15	0.68	0.47	8.10	42,62,84,85	0
6	IDS	F	584	15/17	0.44	0.82	7.64	26,28,35,39	0
5	IDS	A	518	15/17	0.87	0.58	7.26	26,28,35,39	0
7	IDS	H	578	15/17	0.59	0.72	7.03	26,28,35,39	0
5	JHM	E	511	15/15	0.74	0.64	6.27	42,62,84,85	0
7	JHM	H	577	15/15	0.60	0.66	6.20	42,62,84,85	0
4	JHM	D	509	15/15	0.50	0.55	5.48	42,62,84,85	0
5	JHM	B	529	15/15	0.47	0.74	5.07	42,62,84,85	0
7	JHM	F	567	15/15	0.63	0.50	4.80	42,62,84,85	0
7	IDS	F	570	15/17	0.77	0.64	4.33	26,28,35,39	0
4	JHM	N	601	15/15	0.67	0.64	4.21	42,62,84,85	0
7	JHM	L	615	15/15	0.56	0.65	4.16	42,62,84,85	0
5	IDS	N	608	15/17	0.68	0.63	4.00	26,28,35,39	0
5	JHM	C	571	15/15	0.63	0.52	3.47	42,62,84,85	0
5	JHM	B	527	15/15	0.69	0.49	3.46	42,62,84,85	0
7	JHM	L	613	15/15	0.63	0.44	3.11	42,62,84,85	0
5	IDS	B	528	15/17	0.69	0.45	3.04	26,28,35,39	0
5	JHM	A	517	15/15	0.69	0.46	2.71	42,62,84,85	0
5	IDS	F	594	15/17	0.70	0.58	2.53	26,28,35,39	0
7	IDS	J	596	15/17	0.77	0.54	2.21	26,28,35,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	IDS	L	616	15/17	0.38	0.45	2.07	26,28,35,39	0
5	IDS	F	592	15/17	0.74	0.56	1.68	26,28,35,39	0
5	JHM	N	609	15/15	0.74	0.61	1.57	42,62,84,85	0
5	JHM	F	591	15/15	0.48	0.52	1.00	42,62,84,85	0
5	IDS	B	530	15/17	0.78	0.52	-	26,28,35,39	0
5	JHM	E	513	15/15	0.60	0.65	-	42,62,84,85	0
5	JHM	D	523	15/15	0.68	0.57	-	42,62,84,85	0
3	JHM	E	505	15/15	0.72	0.53	-	42,62,84,85	0
7	IDS	L	622	15/17	0.67	0.68	-	26,28,35,39	0
6	JHM	B	533	15/15	0.77	0.87	-	42,62,84,85	0
7	IDS	L	620	15/17	0.68	0.62	-	26,28,35,39	0
7	IDS	J	560	15/17	0.74	0.59	-	26,28,35,39	0
6	JHM	F	585	15/15	0.71	0.70	-	42,62,84,85	0
6	IDS	B	536	15/17	0.78	0.69	-	26,28,35,39	0
4	JHM	E	515	15/15	0.70	0.52	-	42,62,84,85	0
6	JHM	F	581	15/15	0.64	0.69	-	42,62,84,85	0
7	IDS	H	576	15/17	0.63	0.65	-	26,28,35,39	0
6	JHM	F	587	15/15	0.59	0.59	-	42,62,84,85	0
5	IDS	D	526	15/17	0.74	0.52	-	26,28,35,39	0
7	IDS	J	600	15/17	0.80	0.50	-	26,28,35,39	0
5	IDS	C	572	15/17	0.68	0.64	-	26,28,35,39	0
6	IDS	B	540	15/17	0.69	0.54	-	26,28,35,39	0
7	JHM	L	617	15/15	0.73	0.45	-	42,62,84,85	0
7	JHM	J	559	15/15	0.74	0.68	-	42,62,84,85	0
7	JHM	J	557	15/15	0.65	0.73	-	42,62,84,85	0
4	IDS	D	504	15/17	0.75	0.53	-	26,28,35,39	0
6	IDS	B	534	15/17	0.78	0.57	-	26,28,35,39	0
7	JHM	J	561	15/15	0.68	0.52	-	42,62,84,85	0
7	JHM	E	551	15/15	0.54	0.77	-	42,62,84,85	0
7	JHM	F	565	15/15	0.59	0.61	-	42,62,84,85	0
5	JHM	D	525	15/15	0.56	0.46	-	42,62,84,85	0
7	JHM	L	621	15/15	0.62	0.55	-	42,62,84,85	0
4	IDS	D	522	15/17	0.75	0.57	-	26,28,35,39	0
7	IDS	L	618	15/17	0.74	0.56	-	26,28,35,39	0
5	IDS	A	546	15/17	0.71	0.56	-	26,28,35,39	0
3	IDS	E	506	15/17	0.75	0.65	-	26,28,35,39	0
5	JHM	O	605	15/15	0.65	0.78	-	42,62,84,85	0
7	JHM	E	549	15/15	0.61	0.72	-	42,62,84,85	0
6	JHM	B	541	15/15	0.51	0.49	-	42,62,84,85	0
7	JHM	H	579	15/15	0.59	0.59	-	42,62,84,85	0
6	IDS	F	586	15/17	0.84	0.52	-	26,28,35,39	0
6	IDS	B	538	15/17	0.66	0.61	-	26,28,35,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	IDS	F	588	15/17	0.79	0.50	-	26,28,35,39	0
6	JHM	F	589	15/15	0.69	0.78	-	42,62,84,85	0
7	JHM	J	595	15/15	0.64	0.55	-	42,62,84,85	0
5	IDS	D	524	15/17	0.62	0.49	-	26,28,35,39	0
7	IDS	L	614	15/17	0.74	0.46	-	26,28,35,39	0
5	JHM	F	593	15/15	0.72	0.61	-	42,62,84,85	0
7	IDS	J	562	15/17	0.69	0.56	-	26,28,35,39	0
4	JHM	D	507	15/15	0.71	0.62	-	42,62,84,85	0
5	JHM	C	573	15/15	0.69	0.71	-	42,62,84,85	0
5	IDS	E	514	15/17	0.75	0.63	-	26,28,35,39	0
4	IDS	N	602	15/17	0.76	0.63	-	26,28,35,39	0
5	IDS	O	606	15/17	0.66	0.59	-	26,28,35,39	0
4	JHM	C	531	15/15	0.50	0.60	-	42,62,84,85	0
3	IDS	E	502	15/17	0.83	0.45	-	26,28,35,39	0
7	JHM	J	553	15/15	0.59	0.67	-	42,62,84,85	0
7	IDS	E	550	15/17	0.60	0.64	-	26,28,35,39	0
6	IDS	B	542	15/17	0.74	0.67	-	26,28,35,39	0
5	IDS	A	544	15/17	0.68	0.53	-	26,28,35,39	0
7	JHM	F	569	15/15	0.56	0.55	-	42,62,84,85	0
6	JHM	B	537	15/15	0.55	0.60	-	42,62,84,85	0
5	IDS	C	574	15/17	0.65	0.61	-	26,28,35,39	0
4	IDS	C	532	15/17	0.72	0.75	-	26,28,35,39	0
7	IDS	E	552	15/17	0.74	0.53	-	26,28,35,39	0
6	JHM	B	535	15/15	0.53	0.66	-	42,62,84,85	0
5	IDS	E	512	15/17	0.85	0.68	-	26,28,35,39	0
4	IDS	E	516	15/17	0.67	0.58	-	26,28,35,39	0
5	JHM	O	603	15/15	0.61	0.85	-	42,62,84,85	0
5	IDS	O	604	15/17	0.60	0.85	-	26,28,35,39	0
4	IDS	D	510	15/17	0.67	0.82	-	26,28,35,39	0
5	IDS	N	610	15/17	0.76	0.64	-	26,28,35,39	0
7	IDS	F	568	15/17	0.68	0.67	-	26,28,35,39	0
7	IDS	F	566	15/17	0.77	0.61	-	26,28,35,39	0
7	JHM	L	619	15/15	0.69	0.58	-	42,62,84,85	0
7	IDS	L	612	15/17	0.81	0.44	-	26,28,35,39	0
4	JHM	D	521	15/15	0.52	0.68	-	42,62,84,85	0
7	IDS	J	564	15/17	0.72	0.51	-	26,28,35,39	0
5	JHM	A	545	15/15	0.69	0.61	-	42,62,84,85	0
7	JHM	J	599	15/15	0.70	0.49	-	42,62,84,85	0
7	JHM	L	611	15/15	0.67	0.53	-	42,62,84,85	0
6	IDS	F	582	15/17	0.76	0.64	-	26,28,35,39	0
6	JHM	B	539	15/15	0.55	0.59	-	42,62,84,85	0
4	IDS	D	508	15/17	0.74	0.53	-	26,28,35,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	IDS	J	558	15/17	0.56	0.80	-	26,28,35,39	0
7	JHM	J	563	15/15	0.71	0.54	-	42,62,84,85	0
7	IDS	J	556	15/17	0.76	0.75	-	26,28,35,39	0
6	JHM	F	583	15/15	0.62	0.71	-	42,62,84,85	0
7	IDS	H	580	15/17	0.61	0.66	-	26,28,35,39	0
5	JHM	A	543	15/15	0.64	0.51	-	42,62,84,85	0
5	IDS	A	520	15/17	0.81	0.48	-	26,28,35,39	0
4	JHM	D	503	15/15	0.54	0.73	-	42,62,84,85	0

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	JHM	E	501	15/15	0.74	0.47	-	42,62,84,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.