



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 11, 2016 – 06:15 PM EDT

PDB ID : 5CFY
Title : CRYSTAL STRUCTURE OF GLTPH R397A IN COMPLEX WITH NA⁺ AND L-ASP
Authors : Boudker, O.; Oh, S.
Deposited on : 2015-07-08
Resolution : 3.50 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027107
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) : rb-20027107

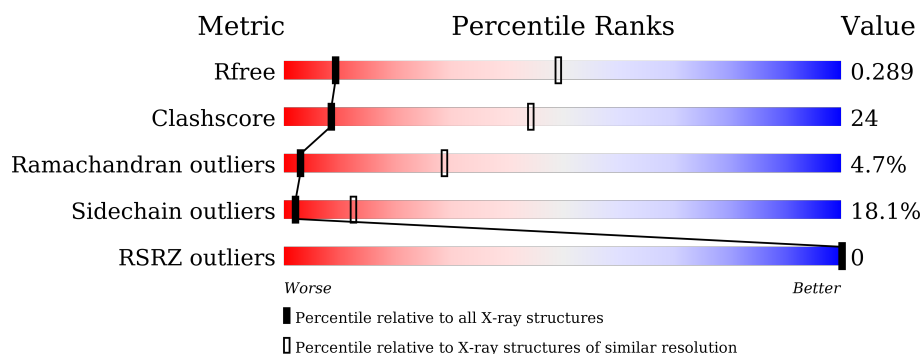
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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	425	<div> <div>48%</div> <div>39%</div> <div>10%</div> <div>.</div> </div>
1	B	425	<div> <div>46%</div> <div>39%</div> <div>11%</div> <div>..</div> </div>
1	C	425	<div> <div>51%</div> <div>37%</div> <div>8%</div> <div>.</div> </div>
1	D	425	<div> <div>48%</div> <div>40%</div> <div>8%</div> <div>..</div> </div>
1	E	425	<div> <div>50%</div> <div>39%</div> <div>7%</div> <div>.</div> </div>
1	F	425	<div> <div>44%</div> <div>42%</div> <div>11%</div> <div>..</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18240 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 425aa long hypothetical proton glutamate symport protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	S	0	0	0
			3028	1994	486	531	17			
1	B	411	Total	C	N	O	S	0	0	0
			3028	1994	486	531	17			
1	C	411	Total	C	N	O	S	0	0	0
			3028	1994	486	531	17			
1	D	411	Total	C	N	O	S	0	0	0
			3028	1994	486	531	17			
1	E	411	Total	C	N	O	S	0	0	0
			3028	1994	486	531	17			
1	F	411	Total	C	N	O	S	0	0	0
			3028	1994	486	531	17			

There are 42 discrepancies between the modelled and reference sequences:

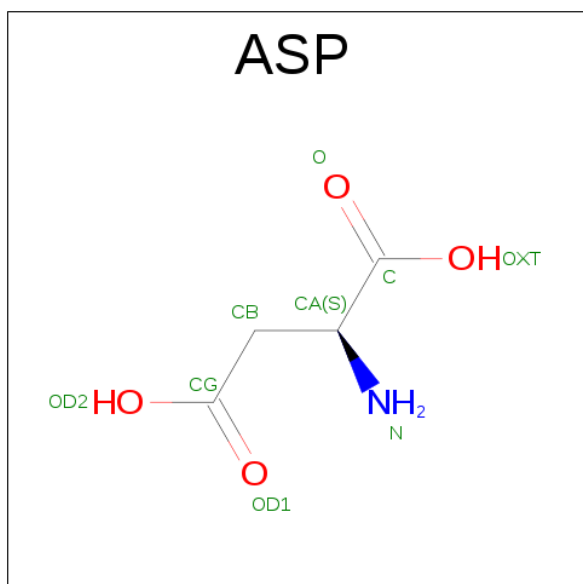
Chain	Residue	Modelled	Actual	Comment	Reference
A	37	HIS	ASP	ENGINEERED MUTATION	UNP O59010
A	40	HIS	LYS	ENGINEERED MUTATION	UNP O59010
A	132	HIS	LYS	ENGINEERED MUTATION	UNP O59010
A	223	HIS	LYS	ENGINEERED MUTATION	UNP O59010
A	264	HIS	LYS	ENGINEERED MUTATION	UNP O59010
A	368	HIS	GLU	ENGINEERED MUTATION	UNP O59010
A	397	ALA	ARG	ENGINEERED MUTATION	UNP O59010
B	37	HIS	ASP	ENGINEERED MUTATION	UNP O59010
B	40	HIS	LYS	ENGINEERED MUTATION	UNP O59010
B	132	HIS	LYS	ENGINEERED MUTATION	UNP O59010
B	223	HIS	LYS	ENGINEERED MUTATION	UNP O59010
B	264	HIS	LYS	ENGINEERED MUTATION	UNP O59010
B	368	HIS	GLU	ENGINEERED MUTATION	UNP O59010
B	397	ALA	ARG	ENGINEERED MUTATION	UNP O59010
C	37	HIS	ASP	ENGINEERED MUTATION	UNP O59010
C	40	HIS	LYS	ENGINEERED MUTATION	UNP O59010
C	132	HIS	LYS	ENGINEERED MUTATION	UNP O59010

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Chain	Residue	Modelled	Actual	Comment	Reference
C	223	HIS	LYS	ENGINEERED MUTATION	UNP O59010
C	264	HIS	LYS	ENGINEERED MUTATION	UNP O59010
C	368	HIS	GLU	ENGINEERED MUTATION	UNP O59010
C	397	ALA	ARG	ENGINEERED MUTATION	UNP O59010
D	37	HIS	ASP	ENGINEERED MUTATION	UNP O59010
D	40	HIS	LYS	ENGINEERED MUTATION	UNP O59010
D	132	HIS	LYS	ENGINEERED MUTATION	UNP O59010
D	223	HIS	LYS	ENGINEERED MUTATION	UNP O59010
D	264	HIS	LYS	ENGINEERED MUTATION	UNP O59010
D	368	HIS	GLU	ENGINEERED MUTATION	UNP O59010
D	397	ALA	ARG	ENGINEERED MUTATION	UNP O59010
E	37	HIS	ASP	ENGINEERED MUTATION	UNP O59010
E	40	HIS	LYS	ENGINEERED MUTATION	UNP O59010
E	132	HIS	LYS	ENGINEERED MUTATION	UNP O59010
E	223	HIS	LYS	ENGINEERED MUTATION	UNP O59010
E	264	HIS	LYS	ENGINEERED MUTATION	UNP O59010
E	368	HIS	GLU	ENGINEERED MUTATION	UNP O59010
E	397	ALA	ARG	ENGINEERED MUTATION	UNP O59010
F	37	HIS	ASP	ENGINEERED MUTATION	UNP O59010
F	40	HIS	LYS	ENGINEERED MUTATION	UNP O59010
F	132	HIS	LYS	ENGINEERED MUTATION	UNP O59010
F	223	HIS	LYS	ENGINEERED MUTATION	UNP O59010
F	264	HIS	LYS	ENGINEERED MUTATION	UNP O59010
F	368	HIS	GLU	ENGINEERED MUTATION	UNP O59010
F	397	ALA	ARG	ENGINEERED MUTATION	UNP O59010

- Molecule 2 is ASPARTIC ACID (three-letter code: ASP) (formula: $C_4H_7NO_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 9 4 1 4	0	0
2	B	1	Total C N O 9 4 1 4	0	0
2	C	1	Total C N O 9 4 1 4	0	0
2	D	1	Total C N O 9 4 1 4	0	0
2	E	1	Total C N O 9 4 1 4	0	0
2	F	1	Total C N O 9 4 1 4	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	2	Total Na 2 2	0	0
3	E	2	Total Na 2 2	0	0
3	B	2	Total Na 2 2	0	0
3	C	2	Total Na 2 2	0	0
3	A	2	Total Na 2 2	0	0
3	F	2	Total Na 2 2	0	0

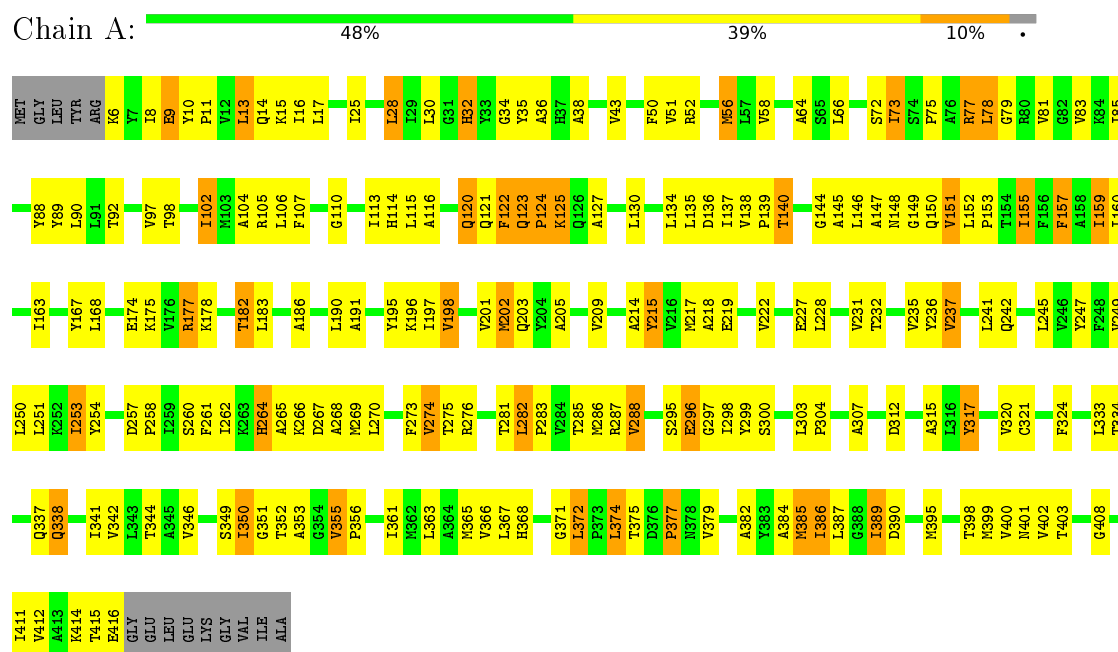
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O 1 1	0	0
4	B	1	Total O 1 1	0	0
4	C	1	Total O 1 1	0	0
4	D	1	Total O 1 1	0	0
4	E	1	Total O 1 1	0	0
4	F	1	Total O 1 1	0	0

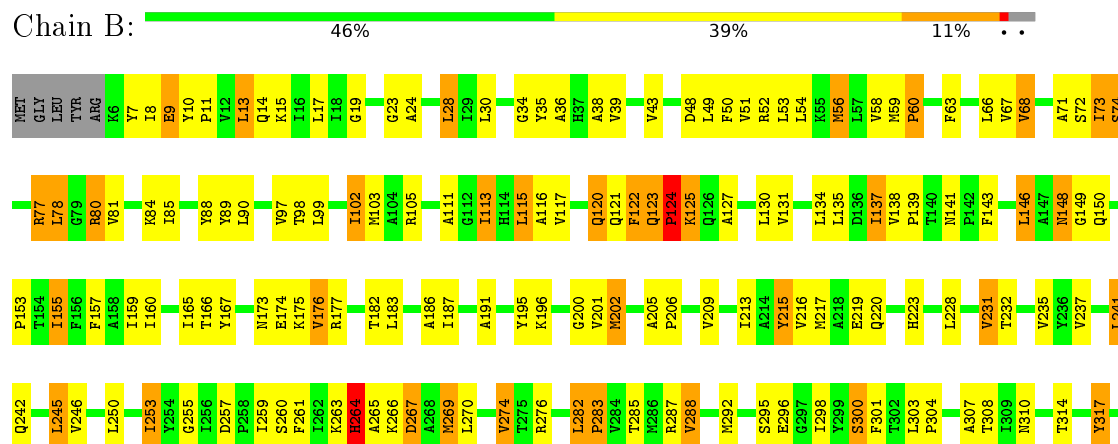
3 Residue-property plots [i](#)

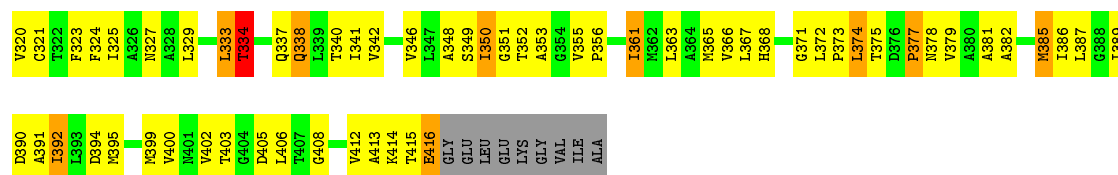
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($RSRZ > 2$). 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: 425aa long hypothetical proton glutamate symport protein



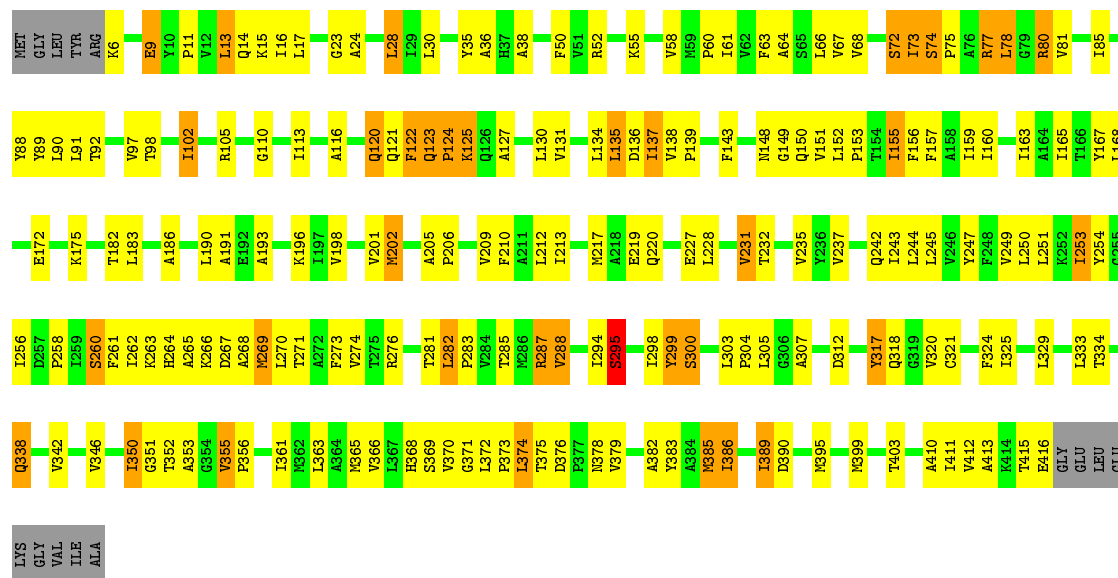
- Molecule 1: 425aa long hypothetical proton glutamate symport protein





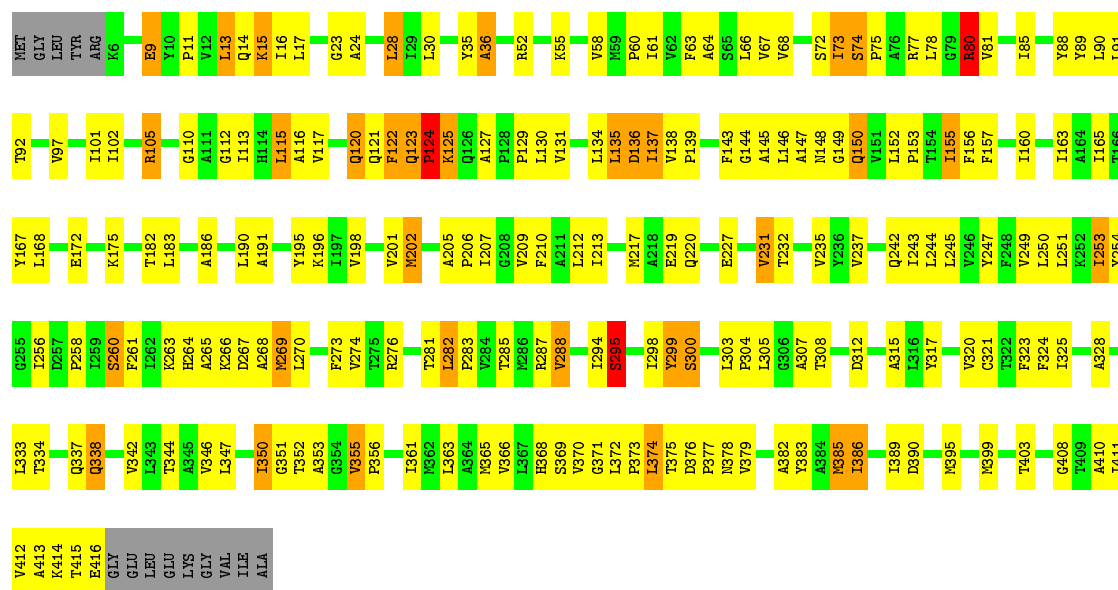
- Molecule 1: 425aa long hypothetical proton glutamate symport protein

Chain C: 51% 37% 8%



- Molecule 1: 425aa long hypothetical proton glutamate symport protein

Chain D: 48% 40% 8%



- Molecule 1: 425aa long hypothetical proton glutamate symport protein

4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	116.96Å 116.96Å 313.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 3.50 15.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	97.1 (15.00-3.50) 98.4 (15.00-3.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.249 , 0.294 0.249 , 0.289	Depositor DCC
R_{free} test set	2955 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	155.6	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 96.7	EDS
Estimated twinning fraction	0.109 for -h,-k,l 0.389 for h,-h-k,-l 0.115 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 58572 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18240	wwPDB-VP
Average B, all atoms (Å ²)	154.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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: NA

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	0.91	2/3087 (0.1%)	0.95	2/4213 (0.0%)
1	B	0.94	1/3087 (0.0%)	0.99	4/4213 (0.1%)
1	C	0.91	1/3087 (0.0%)	0.99	2/4213 (0.0%)
1	D	0.91	1/3087 (0.0%)	0.99	4/4213 (0.1%)
1	E	0.93	2/3087 (0.1%)	0.96	3/4213 (0.1%)
1	F	0.94	2/3087 (0.1%)	0.99	5/4213 (0.1%)
All	All	0.92	9/18522 (0.0%)	0.98	20/25278 (0.1%)

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
1	B	0	1
1	D	0	2
All	All	0	3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	416	GLU	CD-OE1	-8.54	1.16	1.25
1	B	416	GLU	CD-OE1	-7.77	1.17	1.25
1	C	295	SER	CB-OG	-6.87	1.33	1.42
1	D	295	SER	CB-OG	-6.82	1.33	1.42
1	E	157	PHE	CE1-CZ	5.91	1.48	1.37
1	A	157	PHE	CE1-CZ	5.72	1.48	1.37
1	F	93	SER	CB-OG	5.51	1.49	1.42
1	A	236	TYR	CG-CD1	5.15	1.45	1.39
1	E	157	PHE	CE2-CZ	5.09	1.47	1.37

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	157	PHE	CB-CG-CD1	-8.87	114.59	120.80
1	A	390	ASP	CB-CG-OD1	-8.48	110.67	118.30
1	E	177	ARG	NE-CZ-NH1	8.23	124.42	120.30
1	B	390	ASP	CB-CG-OD1	-7.76	111.32	118.30
1	A	177	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	D	136	ASP	CB-CG-OD1	6.16	123.85	118.30
1	B	267	ASP	CB-CG-OD2	6.07	123.76	118.30
1	F	390	ASP	CB-CG-OD1	-6.02	112.88	118.30
1	F	115	LEU	CA-CB-CG	5.89	128.84	115.30
1	B	115	LEU	CA-CB-CG	5.64	128.27	115.30
1	B	405	ASP	CB-CG-OD1	5.61	123.35	118.30
1	D	80	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	F	276	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	F	405	ASP	CB-CG-OD1	5.38	123.14	118.30
1	E	115	LEU	CA-CB-CG	5.20	127.25	115.30
1	C	390	ASP	CB-CG-OD1	-5.13	113.68	118.30
1	C	13	LEU	CA-CB-CG	5.10	127.02	115.30
1	F	183	LEU	CB-CG-CD1	-5.07	102.38	111.00
1	D	390	ASP	CB-CG-OD1	-5.07	113.74	118.30
1	D	80	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	124	PRO	Peptide
1	D	112	GLY	Peptide
1	D	124	PRO	Peptide

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	3028	0	3189	155	0
1	B	3028	0	3189	164	0
1	C	3028	0	3189	151	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3028	0	3189	153	0
1	E	3028	0	3189	146	0
1	F	3028	0	3189	182	0
2	A	9	0	3	1	0
2	B	9	0	3	1	0
2	C	9	0	3	0	0
2	D	9	0	3	1	0
2	E	9	0	3	2	0
2	F	9	0	3	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	1	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
All	All	18240	0	19152	896	0

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 24.

All (896) 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)
1:B:265:ALA:HB1	1:B:266:LYS:HA	1.26	1.15
1:F:265:ALA:HB1	1:F:266:LYS:HA	1.25	1.13
1:E:265:ALA:HB1	1:E:266:LYS:HA	1.20	1.12
1:A:265:ALA:HB1	1:A:266:LYS:HA	1.17	1.11
1:C:265:ALA:HB1	1:C:266:LYS:CA	1.84	1.07
1:D:265:ALA:HB1	1:D:266:LYS:CA	1.84	1.06
1:C:265:ALA:CB	1:C:266:LYS:HA	1.86	1.06
1:D:265:ALA:CB	1:D:266:LYS:HA	1.86	1.05
1:D:265:ALA:HB1	1:D:266:LYS:HA	1.06	1.05
1:A:265:ALA:HB1	1:A:266:LYS:CA	1.87	1.03
1:E:265:ALA:HB1	1:E:266:LYS:CA	1.87	1.03
1:F:265:ALA:HB1	1:F:266:LYS:CA	1.87	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:ALA:HB1	1:B:266:LYS:CA	1.87	1.02
1:C:265:ALA:HB1	1:C:266:LYS:HA	1.04	1.02
1:B:120:GLN:HB2	1:B:121:GLN:HA	1.43	1.00
1:F:120:GLN:HB2	1:F:121:GLN:HA	1.43	1.00
1:E:120:GLN:HB2	1:E:121:GLN:HA	1.45	0.99
1:F:265:ALA:CB	1:F:266:LYS:HA	1.93	0.97
1:B:265:ALA:CB	1:B:266:LYS:HA	1.94	0.96
1:D:120:GLN:HB2	1:D:121:GLN:HA	1.48	0.96
1:A:120:GLN:HB2	1:A:121:GLN:HA	1.48	0.96
1:D:264:HIS:CE1	1:D:265:ALA:HB2	2.01	0.96
1:E:265:ALA:CB	1:E:266:LYS:HA	1.97	0.95
1:A:265:ALA:CB	1:A:266:LYS:HA	1.96	0.95
1:E:264:HIS:CE1	1:E:265:ALA:HB2	2.03	0.94
1:C:120:GLN:HB2	1:C:121:GLN:HA	1.50	0.93
1:A:264:HIS:CE1	1:A:265:ALA:HB2	2.04	0.92
1:C:264:HIS:CE1	1:C:265:ALA:HB2	2.04	0.92
1:C:80:ARG:NH2	1:C:416:GLU:OE2	2.03	0.92
1:A:261:PHE:O	1:A:264:HIS:CD2	2.23	0.92
1:E:261:PHE:O	1:E:264:HIS:CD2	2.24	0.91
1:B:11:PRO:HG2	1:B:14:GLN:HG3	1.53	0.91
1:F:11:PRO:HG2	1:F:14:GLN:HG3	1.53	0.91
1:E:124:PRO:HB2	1:E:368:HIS:CE1	2.07	0.90
1:B:264:HIS:CE1	1:B:265:ALA:HB2	2.07	0.90
1:F:124:PRO:HB2	1:F:368:HIS:CE1	2.05	0.90
1:E:11:PRO:HG2	1:E:14:GLN:HG3	1.55	0.89
1:B:124:PRO:HB2	1:B:368:HIS:CE1	2.08	0.88
1:A:124:PRO:HB2	1:A:368:HIS:CE1	2.09	0.88
1:C:334:THR:O	1:C:338:GLN:HB2	1.74	0.88
1:C:124:PRO:HB2	1:C:368:HIS:CE1	2.09	0.87
1:D:334:THR:O	1:D:338:GLN:HB2	1.76	0.86
1:D:80:ARG:NH2	1:D:416:GLU:OE2	2.09	0.85
1:D:124:PRO:HB2	1:D:368:HIS:CE1	2.12	0.85
1:F:264:HIS:CE1	1:F:265:ALA:HB2	2.12	0.85
1:B:250:LEU:HA	1:B:253:ILE:HG22	1.58	0.85
1:F:235:VAL:HG22	1:F:320:VAL:HG11	1.59	0.83
1:D:36:ALA:HB1	1:D:219:GLU:HG2	1.62	0.82
1:D:269:MET:SD	1:D:403:THR:OG1	2.37	0.81
1:D:97:VAL:HG11	1:D:342:VAL:HA	1.61	0.81
1:A:36:ALA:HB1	1:A:219:GLU:HG2	1.62	0.81
1:E:36:ALA:HB1	1:E:219:GLU:HG2	1.63	0.81
1:D:261:PHE:O	1:D:264:HIS:CD2	2.34	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:VAL:HG22	1:B:320:VAL:HG11	1.64	0.80
1:C:28:LEU:HD13	1:C:217:MET:HG3	1.63	0.80
1:B:201:VAL:O	1:B:202:MET:HB2	1.82	0.79
1:F:250:LEU:HA	1:F:253:ILE:HG22	1.63	0.79
1:F:201:VAL:O	1:F:202:MET:HB2	1.82	0.79
1:A:11:PRO:HG2	1:A:14:GLN:HG3	1.65	0.79
1:D:28:LEU:HD13	1:D:217:MET:HG3	1.65	0.78
1:A:81:VAL:HG21	1:A:298:ILE:HD12	1.63	0.78
1:B:123:GLN:HG2	1:B:124:PRO:HA	1.64	0.78
1:E:81:VAL:HG21	1:E:298:ILE:HD12	1.65	0.78
1:C:261:PHE:O	1:C:264:HIS:CD2	2.37	0.77
1:D:81:VAL:HG21	1:D:298:ILE:HD12	1.65	0.77
1:D:266:LYS:CB	1:D:270:LEU:HG	2.15	0.77
1:D:201:VAL:O	1:D:202:MET:HB2	1.84	0.77
1:C:75:PRO:HG3	1:C:163:ILE:HG13	1.67	0.76
1:A:346:VAL:O	1:A:350:ILE:HG23	1.86	0.76
1:C:155:ILE:HD11	1:C:304:PRO:HB2	1.66	0.76
1:D:167:TYR:HB3	1:F:196:LYS:HE2	1.66	0.75
1:C:97:VAL:HG11	1:C:342:VAL:HA	1.67	0.75
1:F:269:MET:O	1:F:399:MET:HG3	1.86	0.75
1:E:28:LEU:HD13	1:E:217:MET:HG3	1.68	0.75
1:C:269:MET:SD	1:C:403:THR:OG1	2.43	0.75
1:B:196:LYS:HE2	1:C:167:TYR:HB3	1.70	0.74
1:D:11:PRO:HG2	1:D:14:GLN:HG3	1.68	0.74
1:F:36:ALA:HB1	1:F:219:GLU:HG2	1.67	0.74
1:C:350:ILE:N	1:C:351:GLY:HA3	2.02	0.74
1:D:121:GLN:N	1:D:122:PHE:HB3	2.03	0.73
1:A:250:LEU:HA	1:A:253:ILE:HG22	1.69	0.73
1:C:123:GLN:HG2	1:C:124:PRO:HA	1.71	0.73
1:C:266:LYS:CB	1:C:270:LEU:HG	2.18	0.73
1:A:269:MET:O	1:A:399:MET:HG3	1.88	0.73
1:A:261:PHE:O	1:A:264:HIS:HD2	1.69	0.73
1:F:123:GLN:HG2	1:F:124:PRO:HA	1.71	0.73
1:F:28:LEU:HD13	1:F:217:MET:HG3	1.69	0.72
1:D:123:GLN:HG2	1:D:124:PRO:HA	1.72	0.72
1:F:66:LEU:HD21	1:F:159:ILE:HG13	1.72	0.72
1:F:264:HIS:CE1	1:F:288:VAL:HG11	2.25	0.72
1:B:350:ILE:N	1:B:351:GLY:HA3	2.04	0.72
1:C:81:VAL:HG21	1:C:298:ILE:HD12	1.72	0.72
1:C:36:ALA:HB1	1:C:219:GLU:HG2	1.70	0.71
1:C:250:LEU:HA	1:C:253:ILE:HG22	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:382:ALA:HA	1:C:385:MET:HG3	1.73	0.71
1:F:350:ILE:N	1:F:351:GLY:HA3	2.05	0.71
1:D:350:ILE:N	1:D:351:GLY:HA3	2.05	0.71
1:A:123:GLN:HG2	1:A:124:PRO:HA	1.72	0.71
1:C:201:VAL:O	1:C:202:MET:HB2	1.91	0.71
1:F:334:THR:O	1:F:338:GLN:HB2	1.91	0.71
1:E:346:VAL:O	1:E:350:ILE:HG23	1.91	0.71
1:E:134:LEU:O	1:E:137:ILE:HG13	1.90	0.70
1:B:11:PRO:CG	1:B:14:GLN:HG3	2.21	0.70
1:C:269:MET:O	1:C:399:MET:HG3	1.91	0.70
1:D:58:VAL:HG22	1:D:283:PRO:HD3	1.72	0.70
1:F:11:PRO:CG	1:F:14:GLN:HG3	2.21	0.70
1:A:201:VAL:O	1:A:202:MET:HB2	1.91	0.70
1:F:81:VAL:HG21	1:F:298:ILE:HD12	1.72	0.70
1:B:81:VAL:HG21	1:B:298:ILE:HD12	1.74	0.70
1:D:250:LEU:HA	1:D:253:ILE:HG22	1.74	0.69
1:A:186:ALA:O	1:B:183:LEU:HD13	1.92	0.69
1:F:235:VAL:HG22	1:F:320:VAL:CG1	2.22	0.69
1:C:281:THR:HG22	1:C:285:THR:OG1	1.93	0.69
1:A:167:TYR:HB3	1:C:196:LYS:HE2	1.74	0.69
1:B:36:ALA:HB1	1:B:219:GLU:HG2	1.75	0.68
1:B:265:ALA:HB1	1:B:266:LYS:C	2.13	0.68
1:E:121:GLN:N	1:E:122:PHE:HB3	2.09	0.68
1:A:146:LEU:HD13	1:B:143:PHE:CE1	2.28	0.68
1:B:269:MET:O	1:B:399:MET:HG3	1.93	0.68
1:D:155:ILE:HD11	1:D:304:PRO:HB2	1.74	0.68
1:E:186:ALA:O	1:F:183:LEU:HD13	1.93	0.68
1:A:350:ILE:N	1:A:351:GLY:HA3	2.09	0.68
1:E:261:PHE:O	1:E:264:HIS:HD2	1.73	0.68
1:B:235:VAL:HG22	1:B:320:VAL:CG1	2.22	0.68
1:E:201:VAL:O	1:E:202:MET:HB2	1.93	0.68
1:C:121:GLN:N	1:C:122:PHE:HB3	2.09	0.67
1:E:250:LEU:HA	1:E:253:ILE:HG22	1.76	0.67
1:C:235:VAL:HG22	1:C:320:VAL:HG11	1.76	0.67
1:D:196:LYS:HE2	1:E:167:TYR:HB3	1.75	0.67
1:C:9:GLU:OE2	1:C:9:GLU:HA	1.95	0.67
1:C:366:VAL:O	1:C:369:SER:OG	2.13	0.67
1:F:265:ALA:HB1	1:F:266:LYS:C	2.14	0.67
1:C:11:PRO:HG2	1:C:14:GLN:HG3	1.77	0.67
1:F:255:GLY:O	1:F:414:LYS:HE2	1.95	0.67
1:E:231:VAL:O	1:E:235:VAL:HG23	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:VAL:HG22	1:A:320:VAL:CG1	2.25	0.67
1:B:264:HIS:CE1	1:B:288:VAL:HG11	2.30	0.67
1:D:382:ALA:HA	1:D:385:MET:HG3	1.77	0.67
1:B:265:ALA:HB1	1:B:266:LYS:O	1.95	0.66
1:B:98:THR:O	1:B:102:ILE:HB	1.95	0.66
1:D:269:MET:O	1:D:399:MET:HG3	1.95	0.66
1:E:123:GLN:HG2	1:E:124:PRO:HA	1.78	0.66
1:E:350:ILE:N	1:E:351:GLY:HA3	2.11	0.66
1:A:121:GLN:N	1:A:122:PHE:HB3	2.11	0.66
1:E:196:LYS:HE2	1:F:167:TYR:HB3	1.77	0.66
1:A:28:LEU:HD13	1:A:217:MET:HG3	1.78	0.65
1:F:265:ALA:HB1	1:F:266:LYS:O	1.97	0.65
1:D:235:VAL:HG22	1:D:320:VAL:HG11	1.79	0.65
1:E:155:ILE:HD11	1:E:304:PRO:HB2	1.79	0.64
1:D:134:LEU:O	1:D:136:ASP:N	2.30	0.64
1:D:77:ARG:HH11	1:D:416:GLU:HG3	1.63	0.64
1:A:235:VAL:HG22	1:A:320:VAL:HG11	1.80	0.64
1:D:235:VAL:HG22	1:D:320:VAL:CG1	2.28	0.64
1:E:235:VAL:HG22	1:E:320:VAL:HG11	1.80	0.64
1:E:269:MET:O	1:E:399:MET:HG3	1.98	0.64
1:E:235:VAL:HG22	1:E:320:VAL:CG1	2.27	0.64
1:C:120:GLN:CB	1:C:121:GLN:HA	2.24	0.64
1:B:255:GLY:O	1:B:414:LYS:HE2	1.96	0.64
1:C:346:VAL:O	1:C:350:ILE:HG23	1.98	0.63
1:E:261:PHE:HD2	1:E:262:ILE:HD12	1.63	0.63
1:B:334:THR:O	1:B:338:GLN:HB2	1.98	0.63
1:B:134:LEU:O	1:B:137:ILE:HG13	1.97	0.63
1:C:235:VAL:HG22	1:C:320:VAL:CG1	2.29	0.63
1:C:243:ILE:HG22	1:C:244:LEU:HD23	1.81	0.63
1:D:120:GLN:CB	1:D:121:GLN:HA	2.24	0.63
1:C:355:VAL:HB	1:C:356:PRO:CD	2.29	0.63
1:A:276:ARG:O	2:A:501:ASP:N	2.32	0.63
1:D:281:THR:HG22	1:D:285:THR:OG1	1.98	0.63
1:A:134:LEU:O	1:A:137:ILE:HG13	1.97	0.63
1:A:155:ILE:HD11	1:A:304:PRO:HB2	1.81	0.62
1:D:264:HIS:CE1	1:D:288:VAL:HG11	2.34	0.62
1:B:352:THR:HG22	1:B:353:ALA:O	1.99	0.62
1:C:264:HIS:CE1	1:C:288:VAL:HG11	2.34	0.62
1:E:269:MET:SD	1:E:403:THR:OG1	2.58	0.62
1:F:159:ILE:HD11	1:F:301:PHE:CD1	2.34	0.62
1:D:75:PRO:HG3	1:D:163:ILE:HG13	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:LEU:HD21	1:B:159:ILE:HG13	1.81	0.62
1:D:58:VAL:HG22	1:D:283:PRO:CD	2.30	0.62
1:D:9:GLU:OE2	1:D:9:GLU:HA	2.00	0.62
1:A:264:HIS:CE1	1:A:288:VAL:HG11	2.34	0.62
1:A:285:THR:HG22	1:A:303:LEU:HD13	1.82	0.62
1:D:138:VAL:HG12	1:D:138:VAL:O	1.98	0.62
1:E:146:LEU:HD13	1:F:143:PHE:CE1	2.35	0.62
1:F:63:PHE:O	1:F:67:VAL:HG23	2.00	0.62
1:B:205:ALA:N	1:B:206:PRO:HD2	2.15	0.61
1:D:125:LYS:HD3	1:D:125:LYS:N	2.15	0.61
1:A:231:VAL:O	1:A:235:VAL:HG23	2.00	0.61
1:E:50:PHE:CE1	1:E:205:ALA:HB2	2.35	0.61
1:C:254:TYR:CD2	1:C:411:ILE:HG23	2.35	0.61
1:D:254:TYR:CD2	1:D:411:ILE:HG23	2.34	0.61
1:D:261:PHE:O	1:D:264:HIS:HD2	1.81	0.61
1:D:355:VAL:HB	1:D:356:PRO:CD	2.30	0.61
1:B:123:GLN:HG2	1:B:124:PRO:CA	2.31	0.61
1:A:377:PRO:HB3	1:E:384:ALA:O	2.01	0.61
1:E:285:THR:HG22	1:E:303:LEU:HD13	1.83	0.61
1:A:52:ARG:HB3	1:B:138:VAL:HG11	1.82	0.61
1:B:121:GLN:N	1:B:122:PHE:HB3	2.16	0.61
1:D:352:THR:HG22	1:D:353:ALA:O	2.00	0.61
1:C:58:VAL:HG22	1:C:283:PRO:HD3	1.83	0.60
1:E:264:HIS:CE1	1:E:288:VAL:HG11	2.35	0.60
1:F:352:THR:HG22	1:F:353:ALA:O	2.01	0.60
1:B:314:THR:OG1	2:B:501:ASP:OD2	2.17	0.60
1:C:110:GLY:N	1:C:227:GLU:OE1	2.34	0.60
1:E:36:ALA:HB1	1:E:219:GLU:CG	2.30	0.60
1:A:209:VAL:HG13	1:A:274:VAL:HG21	1.83	0.60
1:B:324:PHE:C	1:B:324:PHE:CD2	2.74	0.60
1:F:123:GLN:HG2	1:F:124:PRO:CA	2.31	0.60
1:C:261:PHE:O	1:C:264:HIS:HD2	1.84	0.60
1:D:196:LYS:HD2	1:E:168:LEU:HD23	1.85	0.59
1:B:159:ILE:HD11	1:B:301:PHE:CD1	2.37	0.59
1:E:11:PRO:CG	1:E:14:GLN:HG3	2.30	0.59
1:C:134:LEU:O	1:C:136:ASP:N	2.35	0.59
1:E:288:VAL:O	1:E:288:VAL:HG13	2.01	0.59
1:A:414:LYS:HG3	1:A:414:LYS:O	2.02	0.59
1:A:196:LYS:HE2	1:B:167:TYR:HB3	1.83	0.59
1:C:352:THR:HG22	1:C:353:ALA:O	2.02	0.59
1:C:137:ILE:HG22	1:C:152:LEU:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:97:VAL:HG11	1:F:342:VAL:HA	1.85	0.58
1:B:269:MET:SD	1:B:403:THR:OG1	2.61	0.58
1:E:414:LYS:HG3	1:E:414:LYS:O	2.02	0.58
1:E:265:ALA:HB1	1:E:266:LYS:C	2.24	0.58
1:A:269:MET:SD	1:A:403:THR:OG1	2.60	0.58
1:B:35:TYR:O	1:B:38:ALA:N	2.37	0.58
1:D:137:ILE:HG22	1:D:152:LEU:HB3	1.86	0.58
1:F:201:VAL:O	1:F:202:MET:CB	2.50	0.58
1:E:197:ILE:HG21	1:F:160:ILE:HG21	1.84	0.58
1:D:243:ILE:HG22	1:D:244:LEU:HD23	1.85	0.58
1:B:28:LEU:HD13	1:B:217:MET:HG3	1.85	0.58
1:C:58:VAL:HG22	1:C:283:PRO:CD	2.34	0.58
1:E:9:GLU:OE2	1:E:203:GLN:NE2	2.37	0.58
1:E:197:ILE:HG21	1:F:160:ILE:CG2	2.33	0.58
1:A:125:LYS:HD3	1:A:125:LYS:N	2.19	0.57
1:B:9:GLU:OE2	1:B:9:GLU:HA	2.03	0.57
1:C:81:VAL:HG23	1:C:412:VAL:HG12	1.85	0.57
1:D:201:VAL:O	1:D:202:MET:CB	2.53	0.57
1:F:324:PHE:CD2	1:F:324:PHE:C	2.77	0.57
1:B:97:VAL:HG11	1:B:342:VAL:HA	1.86	0.57
1:D:125:LYS:HD3	1:D:125:LYS:H	1.69	0.57
1:A:36:ALA:HB1	1:A:219:GLU:CG	2.33	0.57
1:D:120:GLN:C	1:D:122:PHE:HB3	2.23	0.57
1:A:209:VAL:HA	1:A:274:VAL:HG11	1.86	0.57
1:A:247:TYR:OH	1:A:312:ASP:OD2	2.19	0.57
1:B:201:VAL:O	1:B:202:MET:CB	2.51	0.57
1:D:264:HIS:NE2	1:D:265:ALA:HB2	2.20	0.57
1:F:98:THR:O	1:F:102:ILE:HB	2.04	0.57
1:A:97:VAL:HG11	1:A:342:VAL:HA	1.86	0.57
1:C:139:PRO:HB3	1:C:153:PRO:HB3	1.86	0.57
1:D:260:SER:HA	1:D:263:LYS:CB	2.35	0.57
1:C:77:ARG:HH11	1:C:416:GLU:HG3	1.69	0.56
1:B:261:PHE:O	1:B:264:HIS:CD2	2.59	0.56
1:B:120:GLN:CB	1:B:121:GLN:HA	2.25	0.56
1:D:36:ALA:HB1	1:D:219:GLU:CG	2.35	0.56
1:C:50:PHE:HZ	1:C:271:THR:HG1	1.53	0.56
1:B:186:ALA:O	1:C:183:LEU:HD13	2.05	0.56
1:B:155:ILE:HD11	1:B:304:PRO:HB2	1.87	0.56
1:C:247:TYR:OH	1:C:312:ASP:OD2	2.20	0.56
1:F:121:GLN:N	1:F:122:PHE:HB3	2.20	0.56
1:F:261:PHE:O	1:F:264:HIS:CD2	2.58	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:VAL:O	1:B:235:VAL:HG23	2.06	0.56
1:B:325:ILE:O	1:B:329:LEU:HG	2.05	0.56
1:B:288:VAL:CG1	1:B:406:LEU:HD11	2.36	0.56
1:C:250:LEU:HA	1:C:253:ILE:CG2	2.35	0.56
1:E:58:VAL:HG22	1:E:283:PRO:HD3	1.87	0.56
1:E:247:TYR:OH	1:E:312:ASP:OD2	2.18	0.56
1:E:52:ARG:HB3	1:F:138:VAL:HG11	1.88	0.56
1:F:120:GLN:CB	1:F:121:GLN:HA	2.26	0.56
1:F:205:ALA:N	1:F:206:PRO:HD2	2.21	0.56
1:E:209:VAL:HA	1:E:274:VAL:HG11	1.87	0.56
1:E:97:VAL:HG11	1:E:342:VAL:HA	1.86	0.56
1:A:382:ALA:HA	1:A:385:MET:HG3	1.88	0.56
1:F:125:LYS:HD3	1:F:125:LYS:N	2.20	0.56
1:A:276:ARG:HD3	1:A:395:MET:CG	2.36	0.56
1:B:13:LEU:O	1:B:13:LEU:HD12	2.06	0.56
1:D:276:ARG:HG2	1:D:395:MET:HA	1.88	0.56
1:F:250:LEU:HA	1:F:253:ILE:CG2	2.35	0.56
1:B:73:ILE:HG22	1:B:78:LEU:HD22	1.87	0.55
1:B:85:ILE:HD13	1:B:408:GLY:O	2.07	0.55
1:C:249:VAL:O	1:C:253:ILE:HG22	2.06	0.55
1:D:73:ILE:HG23	1:D:74:SER:N	2.20	0.55
1:F:30:LEU:O	1:F:35:TYR:HB2	2.06	0.55
1:F:325:ILE:O	1:F:329:LEU:HG	2.06	0.55
1:A:168:LEU:HD23	1:C:196:LYS:HD2	1.88	0.55
1:B:89:TYR:CG	1:B:310:ASN:HB2	2.41	0.55
1:E:75:PRO:HG3	1:E:163:ILE:HG13	1.89	0.55
1:E:104:ALA:HB2	1:E:320:VAL:HG23	1.89	0.55
1:A:250:LEU:HA	1:A:253:ILE:CG2	2.35	0.55
1:A:352:THR:HG22	1:A:353:ALA:O	2.06	0.55
1:F:9:GLU:HA	1:F:9:GLU:OE2	2.06	0.55
1:B:123:GLN:N	1:B:124:PRO:HA	2.21	0.55
1:B:250:LEU:HA	1:B:253:ILE:CG2	2.33	0.55
1:D:346:VAL:O	1:D:350:ILE:HG23	2.07	0.55
1:A:16:ILE:HD11	1:A:205:ALA:CB	2.37	0.55
1:D:366:VAL:O	1:D:369:SER:OG	2.21	0.55
1:B:58:VAL:HG22	1:B:283:PRO:HD3	1.89	0.54
1:C:363:LEU:O	1:C:366:VAL:HG12	2.07	0.54
1:A:77:ARG:HH11	1:A:416:GLU:HG3	1.72	0.54
1:C:73:ILE:HG23	1:C:74:SER:N	2.21	0.54
1:D:137:ILE:O	1:D:139:PRO:HD3	2.07	0.54
1:C:276:ARG:HD3	1:C:395:MET:CG	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:LYS:HD3	1:C:125:LYS:N	2.21	0.54
1:D:363:LEU:O	1:D:366:VAL:HG12	2.08	0.54
1:E:273:PHE:CE1	1:E:395:MET:HB3	2.43	0.54
1:C:190:LEU:O	1:C:191:ALA:C	2.44	0.54
1:F:125:LYS:HD3	1:F:125:LYS:H	1.73	0.54
1:A:113:ILE:HD13	1:E:113:ILE:HD13	1.88	0.54
1:E:276:ARG:HD3	1:E:395:MET:CG	2.38	0.54
1:A:197:ILE:HG21	1:B:160:ILE:HG21	1.89	0.54
1:B:77:ARG:O	1:B:78:LEU:C	2.45	0.54
1:E:367:LEU:HD22	1:E:372:LEU:HD11	1.88	0.54
1:F:215:TYR:CE1	1:F:219:GLU:OE1	2.60	0.54
1:F:257:ASP:OD2	1:F:259:ILE:HG13	2.08	0.54
1:A:201:VAL:O	1:A:202:MET:CB	2.56	0.54
1:A:288:VAL:HG13	1:A:288:VAL:O	2.07	0.54
1:B:125:LYS:HD3	1:B:125:LYS:N	2.23	0.53
1:E:352:THR:HG22	1:E:353:ALA:O	2.08	0.53
1:F:288:VAL:O	1:F:292:MET:HG2	2.08	0.53
1:C:276:ARG:HG2	1:C:395:MET:HA	1.90	0.53
1:D:23:GLY:HA2	1:D:210:PHE:CE2	2.43	0.53
1:E:209:VAL:HG13	1:E:274:VAL:HG21	1.90	0.53
1:B:257:ASP:OD2	1:B:259:ILE:HG13	2.09	0.53
1:B:39:VAL:O	1:B:43:VAL:HB	2.08	0.53
1:C:13:LEU:HD12	1:C:13:LEU:O	2.08	0.53
1:F:134:LEU:O	1:F:136:ASP:N	2.42	0.53
1:A:261:PHE:HD2	1:A:262:ILE:HD12	1.72	0.53
1:A:355:VAL:HB	1:A:356:PRO:CD	2.38	0.53
1:C:317:TYR:HD1	1:C:318:GLN:N	2.07	0.53
1:D:276:ARG:HD3	1:D:395:MET:CG	2.39	0.53
1:D:247:TYR:OH	1:D:312:ASP:OD2	2.20	0.53
1:A:276:ARG:HD3	1:A:395:MET:HG2	1.91	0.53
1:A:56:MET:HE2	1:B:157:PHE:HD1	1.73	0.53
1:F:363:LEU:O	1:F:366:VAL:HG12	2.08	0.53
1:A:81:VAL:HG23	1:A:412:VAL:HG12	1.89	0.53
1:B:215:TYR:CE1	1:B:219:GLU:OE1	2.61	0.53
1:C:264:HIS:NE2	1:C:265:ALA:HB2	2.24	0.53
1:E:334:THR:O	1:E:338:GLN:HB2	2.09	0.53
1:A:367:LEU:HD22	1:A:372:LEU:HD11	1.91	0.53
1:D:190:LEU:O	1:D:191:ALA:C	2.48	0.53
1:E:265:ALA:HB1	1:E:266:LYS:O	2.09	0.53
1:F:263:LYS:C	1:F:265:ALA:H	2.12	0.53
1:C:124:PRO:HB2	1:C:368:HIS:HE1	1.71	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:355:VAL:HB	1:E:356:PRO:CD	2.38	0.52
1:C:125:LYS:HD3	1:C:125:LYS:H	1.74	0.52
1:A:6:LYS:HA	1:A:8:ILE:HD12	1.92	0.52
1:A:104:ALA:HB2	1:A:320:VAL:HG23	1.91	0.52
1:A:123:GLN:HG2	1:A:124:PRO:CA	2.39	0.52
1:C:120:GLN:C	1:C:122:PHE:HB3	2.29	0.52
1:E:120:GLN:C	1:E:122:PHE:HB3	2.30	0.52
1:E:367:LEU:HD22	1:E:372:LEU:CD1	2.39	0.52
1:E:382:ALA:HA	1:E:385:MET:HG3	1.92	0.52
1:A:209:VAL:HG22	1:A:274:VAL:HG11	1.91	0.52
1:A:334:THR:O	1:A:338:GLN:HB2	2.09	0.52
1:F:123:GLN:N	1:F:124:PRO:HA	2.22	0.52
1:E:56:MET:CE	1:F:157:PHE:HD1	2.22	0.52
1:A:265:ALA:HB1	1:A:266:LYS:C	2.30	0.52
1:D:250:LEU:HA	1:D:253:ILE:CG2	2.39	0.52
1:B:11:PRO:HG2	1:B:14:GLN:CG	2.35	0.52
1:B:63:PHE:O	1:B:67:VAL:HG23	2.10	0.52
1:C:201:VAL:O	1:C:202:MET:CB	2.58	0.52
1:D:13:LEU:HD12	1:D:13:LEU:O	2.09	0.52
1:F:191:ALA:O	1:F:195:TYR:HD1	1.93	0.52
1:F:81:VAL:HG23	1:F:412:VAL:HG12	1.91	0.52
1:F:85:ILE:O	1:F:88:TYR:HB3	2.10	0.52
1:D:64:ALA:HB1	1:D:191:ALA:HB2	1.91	0.52
1:E:85:ILE:CD1	1:E:408:GLY:O	2.58	0.52
1:B:124:PRO:HB2	1:B:368:HIS:HE1	1.73	0.51
1:B:374:LEU:HA	1:B:379:VAL:HG11	1.92	0.51
1:A:88:TYR:CZ	1:A:92:THR:HG21	2.45	0.51
1:A:151:VAL:HG12	1:A:152:LEU:HD12	1.92	0.51
1:A:197:ILE:HG21	1:B:160:ILE:CG2	2.40	0.51
1:A:72:SER:O	1:A:73:ILE:HD12	2.11	0.51
1:E:321:CYS:HB3	1:E:363:LEU:HD21	1.93	0.51
1:E:56:MET:HE2	1:F:157:PHE:HD1	1.75	0.51
1:F:77:ARG:O	1:F:78:LEU:C	2.48	0.51
1:A:120:GLN:C	1:A:122:PHE:HB3	2.31	0.51
1:A:134:LEU:O	1:A:136:ASP:N	2.44	0.51
1:D:276:ARG:HD3	1:D:395:MET:HG2	1.93	0.51
1:D:264:HIS:CE1	1:D:265:ALA:CB	2.87	0.51
1:D:273:PHE:CE1	1:D:395:MET:HB3	2.46	0.51
1:D:55:LYS:HB2	1:E:140:THR:HG22	1.92	0.51
1:E:276:ARG:HD3	1:E:395:MET:HG2	1.93	0.51
1:B:382:ALA:HA	1:B:385:MET:HG3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:16:ILE:HD11	1:E:205:ALA:CB	2.41	0.51
1:F:276:ARG:O	1:F:356:PRO:HG3	2.10	0.51
1:F:301:PHE:O	1:F:301:PHE:CG	2.64	0.51
1:B:121:GLN:HB3	1:B:124:PRO:HD3	1.93	0.51
1:B:361:ILE:CD1	1:B:361:ILE:N	2.74	0.51
1:E:125:LYS:HD3	1:E:125:LYS:N	2.26	0.51
1:A:13:LEU:HD12	1:A:13:LEU:O	2.10	0.50
1:B:276:ARG:HD3	1:B:395:MET:HG2	1.93	0.50
1:C:156:PHE:CD2	1:C:156:PHE:O	2.64	0.50
1:D:81:VAL:HG23	1:D:412:VAL:HG12	1.93	0.50
1:E:201:VAL:O	1:E:202:MET:CB	2.60	0.50
1:F:155:ILE:HD11	1:F:304:PRO:HB2	1.93	0.50
1:D:157:PHE:HD1	1:F:56:MET:HE3	1.76	0.50
1:B:363:LEU:O	1:B:367:LEU:HG	2.12	0.50
1:D:165:ILE:O	1:D:168:LEU:N	2.44	0.50
1:D:288:VAL:O	1:D:288:VAL:HG13	2.10	0.50
1:A:136:ASP:HA	1:C:52:ARG:NH2	2.26	0.50
1:D:183:LEU:HD13	1:F:186:ALA:O	2.11	0.50
1:F:121:GLN:HB3	1:F:124:PRO:HD3	1.93	0.50
1:F:151:VAL:HG12	1:F:152:LEU:HD12	1.93	0.50
1:C:205:ALA:N	1:C:206:PRO:HD2	2.25	0.50
1:C:30:LEU:O	1:C:35:TYR:HB2	2.09	0.50
1:E:88:TYR:CZ	1:E:92:THR:HG21	2.47	0.50
1:F:173:ASN:OD1	1:F:176:VAL:HG13	2.11	0.50
1:B:298:ILE:HG21	1:B:413:ALA:HB2	1.92	0.50
1:F:77:ARG:HA	1:F:80:ARG:NH1	2.26	0.50
1:C:231:VAL:O	1:C:235:VAL:HG23	2.11	0.50
1:D:294:ILE:HG22	1:D:295:SER:N	2.26	0.50
1:D:321:CYS:SG	1:D:386:ILE:HG12	2.52	0.50
1:E:81:VAL:HG23	1:E:412:VAL:HG12	1.93	0.50
1:F:35:TYR:O	1:F:38:ALA:N	2.45	0.50
1:A:139:PRO:HB3	1:A:153:PRO:HB3	1.94	0.50
1:A:11:PRO:CG	1:A:14:GLN:HG3	2.39	0.50
1:A:408:GLY:O	1:A:412:VAL:HG23	2.12	0.50
1:C:209:VAL:HA	1:C:274:VAL:HG11	1.94	0.50
1:C:251:LEU:HD13	1:C:258:PRO:HA	1.94	0.50
1:C:324:PHE:C	1:C:324:PHE:CD2	2.85	0.50
1:C:137:ILE:O	1:C:139:PRO:HD3	2.12	0.50
1:A:264:HIS:NE2	1:A:265:ALA:HB2	2.26	0.50
1:B:125:LYS:HD3	1:B:125:LYS:H	1.76	0.50
1:B:53:LEU:O	1:B:56:MET:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:10:TYR:CD2	1:F:11:PRO:HD2	2.47	0.50
1:F:139:PRO:HB3	1:F:153:PRO:HB3	1.94	0.50
1:A:125:LYS:HD3	1:A:125:LYS:H	1.76	0.49
1:A:363:LEU:O	1:A:366:VAL:HG12	2.12	0.49
1:B:73:ILE:HG23	1:B:74:SER:N	2.27	0.49
1:C:64:ALA:HB1	1:C:191:ALA:HB2	1.94	0.49
1:A:73:ILE:HG22	1:A:78:LEU:HD22	1.93	0.49
1:B:264:HIS:NE2	1:B:265:ALA:HB2	2.27	0.49
1:C:305:LEU:HG	1:C:305:LEU:O	2.12	0.49
1:F:89:TYR:CG	1:F:310:ASN:HB2	2.47	0.49
1:A:137:ILE:O	1:A:139:PRO:HD3	2.12	0.49
1:D:249:VAL:O	1:D:253:ILE:HG22	2.12	0.49
1:F:346:VAL:O	1:F:350:ILE:HG23	2.11	0.49
1:F:414:LYS:O	1:F:414:LYS:HG3	2.13	0.49
1:B:85:ILE:O	1:B:88:TYR:HB3	2.12	0.49
1:C:260:SER:HA	1:C:263:LYS:CB	2.43	0.49
1:D:11:PRO:HG2	1:D:14:GLN:CG	2.39	0.49
1:E:276:ARG:O	2:E:501:ASP:N	2.44	0.49
1:A:195:TYR:O	1:A:198:VAL:HG12	2.13	0.49
1:A:183:LEU:HD13	1:C:186:ALA:O	2.13	0.49
1:C:24:ALA:O	1:C:28:LEU:HB2	2.11	0.49
1:F:66:LEU:HD13	1:F:300:SER:O	2.11	0.49
1:B:139:PRO:HB3	1:B:153:PRO:HB3	1.95	0.49
1:F:298:ILE:HG21	1:F:413:ALA:HB2	1.94	0.49
1:F:111:ALA:N	1:F:327:ASN:HB3	2.27	0.49
1:D:110:GLY:N	1:D:227:GLU:OE1	2.46	0.49
1:D:298:ILE:HG21	1:D:413:ALA:HB2	1.95	0.49
1:A:75:PRO:HG3	1:A:163:ILE:HG13	1.95	0.49
1:A:16:ILE:HD11	1:A:205:ALA:HB1	1.94	0.49
1:B:122:PHE:C	1:B:124:PRO:HB3	2.33	0.49
1:B:263:LYS:C	1:B:265:ALA:H	2.16	0.49
1:D:97:VAL:HG22	1:D:315:ALA:O	2.13	0.49
1:E:98:THR:O	1:E:102:ILE:HB	2.12	0.49
1:F:288:VAL:CG1	1:F:406:LEU:HD11	2.43	0.49
1:A:9:GLU:OE2	1:A:203:GLN:NE2	2.46	0.49
1:B:113:ILE:HD13	1:D:113:ILE:HD13	1.95	0.49
1:A:56:MET:CE	1:B:157:PHE:HD1	2.25	0.49
1:B:68:VAL:O	1:B:71:ALA:N	2.46	0.49
1:D:121:GLN:HB3	1:D:124:PRO:HD3	1.94	0.49
1:D:24:ALA:O	1:D:28:LEU:HB2	2.12	0.49
1:B:30:LEU:O	1:B:35:TYR:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:139:PRO:HB3	1:D:153:PRO:HB3	1.95	0.49
1:E:125:LYS:HD3	1:E:125:LYS:H	1.78	0.49
1:B:288:VAL:HG12	1:B:406:LEU:HD11	1.93	0.48
1:D:324:PHE:C	1:D:324:PHE:CD2	2.86	0.48
1:A:384:ALA:O	1:E:377:PRO:HB3	2.13	0.48
1:F:276:ARG:HD3	1:F:395:MET:HG2	1.95	0.48
1:A:10:TYR:CD2	1:A:11:PRO:HD2	2.49	0.48
1:A:321:CYS:HB3	1:A:363:LEU:HD21	1.95	0.48
1:B:266:LYS:CB	1:B:270:LEU:HG	2.43	0.48
1:B:48:ASP:O	1:B:51:VAL:N	2.46	0.48
1:E:324:PHE:CD2	1:E:324:PHE:C	2.86	0.48
1:E:77:ARG:HH11	1:E:416:GLU:HG3	1.77	0.48
1:F:322:THR:HG23	1:F:367:LEU:HD23	1.94	0.48
1:A:146:LEU:HB3	1:B:143:PHE:CD1	2.49	0.48
1:B:246:VAL:O	1:B:250:LEU:HB2	2.14	0.48
1:C:273:PHE:CE1	1:C:395:MET:HB3	2.48	0.48
1:C:321:CYS:SG	1:C:386:ILE:HG12	2.53	0.48
1:D:23:GLY:CA	1:D:210:PHE:CE2	2.96	0.48
1:E:134:LEU:O	1:E:136:ASP:N	2.47	0.48
1:E:13:LEU:O	1:E:13:LEU:HD12	2.13	0.48
1:E:197:ILE:O	1:E:200:GLY:N	2.47	0.48
1:E:250:LEU:HA	1:E:253:ILE:CG2	2.40	0.48
1:F:285:THR:HG22	1:F:303:LEU:HD13	1.96	0.48
1:A:249:VAL:O	1:A:253:ILE:HG22	2.14	0.48
1:D:282:LEU:HD13	1:D:307:ALA:HB2	1.95	0.48
1:E:123:GLN:HG2	1:E:124:PRO:CA	2.42	0.48
1:E:254:TYR:CD2	1:E:411:ILE:HG23	2.49	0.48
1:A:324:PHE:C	1:A:324:PHE:CD2	2.86	0.48
1:B:223:HIS:HD2	1:D:378:ASN:ND2	2.09	0.48
1:E:139:PRO:HB3	1:E:153:PRO:HB3	1.95	0.48
1:B:288:VAL:O	1:B:292:MET:HG2	2.14	0.48
1:E:249:VAL:O	1:E:253:ILE:HG22	2.14	0.48
1:B:60:PRO:HG3	1:C:143:PHE:CZ	2.48	0.48
1:E:6:LYS:HA	1:E:8:ILE:HD12	1.94	0.48
1:F:377:PRO:O	1:F:381:ALA:N	2.45	0.48
1:C:276:ARG:HD3	1:C:395:MET:HG2	1.96	0.48
1:F:282:LEU:HD13	1:F:307:ALA:HB2	1.94	0.48
1:A:266:LYS:CB	1:A:270:LEU:HG	2.44	0.48
1:A:35:TYR:O	1:A:38:ALA:N	2.47	0.48
1:C:138:VAL:O	1:C:138:VAL:HG12	2.12	0.48
1:D:120:GLN:HB2	1:D:121:GLN:CA	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:376:ASP:O	1:D:379:VAL:HB	2.14	0.48
1:E:195:TYR:O	1:E:198:VAL:HG12	2.14	0.48
1:F:374:LEU:HA	1:F:379:VAL:HG11	1.96	0.48
1:D:186:ALA:O	1:E:183:LEU:HD13	2.14	0.48
1:F:67:VAL:HG11	1:F:187:ILE:HD13	1.96	0.48
1:A:254:TYR:CD2	1:A:411:ILE:HG23	2.50	0.47
1:B:84:LYS:HD2	1:B:412:VAL:HG13	1.95	0.47
1:C:266:LYS:O	1:C:268:ALA:N	2.47	0.47
1:D:24:ALA:N	1:D:213:ILE:HD13	2.29	0.47
1:F:264:HIS:NE2	1:F:265:ALA:HB2	2.29	0.47
1:F:349:SER:C	1:F:351:GLY:HA3	2.34	0.47
1:D:157:PHE:HD1	1:F:56:MET:CE	2.27	0.47
1:C:165:ILE:O	1:C:168:LEU:N	2.47	0.47
1:A:235:VAL:HG22	1:A:320:VAL:HG13	1.94	0.47
1:B:120:GLN:C	1:B:122:PHE:HB3	2.34	0.47
1:F:246:VAL:O	1:F:250:LEU:HB2	2.14	0.47
1:F:99:LEU:O	1:F:103:MET:HG2	2.13	0.47
1:A:157:PHE:O	1:A:160:ILE:N	2.47	0.47
1:C:123:GLN:HG2	1:C:124:PRO:CA	2.41	0.47
1:E:121:GLN:HB3	1:E:124:PRO:HD3	1.96	0.47
1:E:134:LEU:O	1:E:137:ILE:CG1	2.60	0.47
1:E:157:PHE:O	1:E:160:ILE:N	2.48	0.47
1:F:58:VAL:HG22	1:F:283:PRO:HD3	1.95	0.47
1:F:343:LEU:HD12	1:F:347:LEU:HD23	1.96	0.47
1:C:121:GLN:HB3	1:C:124:PRO:HD3	1.96	0.47
1:C:378:ASN:OD1	1:F:385:MET:HA	2.15	0.47
1:D:124:PRO:HB2	1:D:368:HIS:HE1	1.75	0.47
1:F:263:LYS:O	1:F:265:ALA:N	2.48	0.47
1:A:56:MET:HE2	1:B:157:PHE:CD1	2.49	0.47
1:B:303:LEU:HD21	1:B:406:LEU:HD23	1.96	0.47
1:D:88:TYR:CZ	1:D:92:THR:HG21	2.50	0.47
1:F:73:ILE:HG22	1:F:78:LEU:HD22	1.95	0.47
1:B:414:LYS:HG3	1:B:414:LYS:O	2.15	0.47
1:F:84:LYS:HD2	1:F:412:VAL:HG13	1.96	0.47
1:D:136:ASP:HA	1:F:52:ARG:NH2	2.30	0.47
1:B:317:TYR:HA	1:B:320:VAL:CG1	2.45	0.47
1:D:231:VAL:O	1:D:235:VAL:HG23	2.14	0.47
1:F:231:VAL:O	1:F:235:VAL:HG23	2.15	0.47
1:B:264:HIS:CE1	1:B:265:ALA:CB	2.92	0.47
1:B:346:VAL:O	1:B:350:ILE:HG23	2.15	0.47
1:C:376:ASP:O	1:C:379:VAL:HB	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:ILE:HD11	1:D:205:ALA:CB	2.45	0.47
1:F:8:ILE:O	1:F:9:GLU:OE1	2.32	0.47
1:B:264:HIS:ND1	1:B:264:HIS:C	2.68	0.47
1:B:99:LEU:O	1:B:103:MET:HG2	2.14	0.47
1:D:251:LEU:HD13	1:D:258:PRO:HA	1.96	0.47
1:D:209:VAL:HA	1:D:274:VAL:HG11	1.97	0.47
1:E:10:TYR:CD2	1:E:11:PRO:HD2	2.50	0.47
1:A:58:VAL:HG22	1:A:283:PRO:HD3	1.96	0.47
1:B:24:ALA:N	1:B:213:ILE:HD13	2.30	0.47
1:B:66:LEU:HD13	1:B:300:SER:O	2.14	0.47
1:C:258:PRO:O	1:C:261:PHE:HB3	2.15	0.47
1:C:276:ARG:HD3	1:C:395:MET:HG3	1.97	0.47
1:D:143:PHE:CE1	1:F:146:LEU:HD13	2.50	0.47
1:F:361:ILE:N	1:F:361:ILE:CD1	2.78	0.47
1:F:73:ILE:HG23	1:F:74:SER:N	2.29	0.47
1:B:348:ALA:O	1:B:352:THR:N	2.47	0.46
1:B:81:VAL:HG23	1:B:412:VAL:HG12	1.97	0.46
1:C:288:VAL:O	1:C:288:VAL:HG13	2.15	0.46
1:D:376:ASP:O	1:D:379:VAL:N	2.49	0.46
1:A:315:ALA:HB2	1:A:349:SER:OG	2.14	0.46
1:B:173:ASN:OD1	1:B:176:VAL:HG13	2.15	0.46
1:B:78:LEU:HA	1:B:78:LEU:HD13	1.70	0.46
1:C:294:ILE:HG22	1:C:295:SER:N	2.30	0.46
1:C:63:PHE:O	1:C:67:VAL:HG23	2.15	0.46
1:D:355:VAL:O	2:D:501:ASP:N	2.49	0.46
1:C:378:ASN:ND2	1:F:223:HIS:HD2	2.12	0.46
1:E:186:ALA:O	1:F:183:LEU:CD1	2.63	0.46
1:D:266:LYS:O	1:D:268:ALA:N	2.48	0.46
1:D:66:LEU:HA	1:D:300:SER:OG	2.16	0.46
1:C:123:GLN:HG2	1:C:125:LYS:H	1.80	0.46
1:E:16:ILE:HD11	1:E:205:ALA:HB1	1.97	0.46
1:E:264:HIS:C	1:E:264:HIS:ND1	2.69	0.46
1:F:155:ILE:HG22	1:F:156:PHE:N	2.30	0.46
1:F:104:ALA:HB2	1:F:320:VAL:HG23	1.97	0.46
1:E:30:LEU:O	1:E:35:TYR:HB2	2.14	0.46
1:E:73:ILE:HG22	1:E:78:LEU:HD22	1.97	0.46
1:A:110:GLY:N	1:A:227:GLU:OE1	2.46	0.46
1:B:301:PHE:O	1:B:301:PHE:CG	2.69	0.46
1:B:35:TYR:O	1:B:38:ALA:HB3	2.16	0.46
1:C:120:GLN:HB2	1:C:121:GLN:CA	2.33	0.46
1:E:317:TYR:CD1	1:E:317:TYR:C	2.89	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:174:GLU:CD	1:F:177:ARG:HE	2.20	0.46
1:A:386:ILE:HA	1:A:389:ILE:HG22	1.96	0.46
1:C:24:ALA:N	1:C:213:ILE:HD13	2.31	0.46
1:C:85:ILE:HG13	1:C:89:TYR:CE1	2.51	0.46
1:D:115:LEU:HB2	1:D:328:ALA:O	2.16	0.46
1:E:235:VAL:HG22	1:E:320:VAL:HG13	1.98	0.46
1:B:66:LEU:HA	1:B:300:SER:OG	2.16	0.45
1:E:264:HIS:NE2	1:E:265:ALA:HB2	2.30	0.45
1:F:311:MET:CE	1:F:354:GLY:HA2	2.46	0.45
1:F:317:TYR:HA	1:F:320:VAL:CG1	2.46	0.45
1:B:363:LEU:O	1:B:366:VAL:HG12	2.15	0.45
1:B:74:SER:O	1:B:77:ARG:N	2.49	0.45
1:D:64:ALA:CB	1:D:191:ALA:HB2	2.45	0.45
1:D:265:ALA:HB1	1:D:266:LYS:C	2.35	0.45
1:E:48:ASP:O	1:E:51:VAL:N	2.49	0.45
1:A:317:TYR:C	1:A:317:TYR:CD1	2.90	0.45
1:D:123:GLN:HG2	1:D:124:PRO:CA	2.42	0.45
1:F:282:LEU:HB3	1:F:283:PRO:HD3	1.99	0.45
1:A:50:PHE:CE1	1:A:205:ALA:HB2	2.51	0.45
1:C:265:ALA:HB1	1:C:266:LYS:C	2.35	0.45
1:F:288:VAL:HG12	1:F:406:LEU:HD11	1.97	0.45
1:B:317:TYR:O	1:B:321:CYS:N	2.47	0.45
1:B:85:ILE:CD1	1:B:408:GLY:O	2.64	0.45
1:E:209:VAL:HG22	1:E:274:VAL:HG11	1.97	0.45
1:F:120:GLN:C	1:F:122:PHE:HB3	2.37	0.45
1:F:190:LEU:O	1:F:193:ALA:N	2.49	0.45
1:F:72:SER:O	1:F:73:ILE:HD12	2.16	0.45
1:F:85:ILE:HD13	1:F:408:GLY:O	2.16	0.45
1:D:144:GLY:O	1:D:147:ALA:N	2.49	0.45
1:E:266:LYS:CB	1:E:270:LEU:HG	2.47	0.45
1:F:333:LEU:HD22	1:F:341:ILE:HD11	1.98	0.45
1:F:303:LEU:HD21	1:F:406:LEU:HD23	1.99	0.45
1:F:53:LEU:O	1:F:56:MET:HB3	2.16	0.45
1:A:266:LYS:O	1:A:268:ALA:N	2.50	0.45
1:D:134:LEU:C	1:D:136:ASP:N	2.70	0.45
1:F:66:LEU:CD2	1:F:159:ILE:HG13	2.45	0.45
1:F:78:LEU:HD13	1:F:78:LEU:HA	1.75	0.45
1:A:276:ARG:HD3	1:A:395:MET:HG3	1.99	0.45
1:A:30:LEU:O	1:A:35:TYR:HB2	2.16	0.45
1:B:400:VAL:O	1:B:400:VAL:HG12	2.17	0.45
1:C:298:ILE:HG21	1:C:413:ALA:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:89:TYR:CD2	1:F:310:ASN:HB2	2.52	0.45
1:D:145:ALA:O	1:D:150:GLN:HB2	2.17	0.45
1:F:178:LYS:O	1:F:182:THR:OG1	2.35	0.45
1:D:256:ILE:HD13	1:D:410:ALA:HB1	1.98	0.45
1:F:209:VAL:HG13	1:F:274:VAL:HG21	1.98	0.45
1:F:41:THR:HG22	1:F:42:TYR:CD1	2.52	0.45
1:D:212:LEU:CB	1:D:274:VAL:HG13	2.46	0.44
1:D:305:LEU:HG	1:D:305:LEU:O	2.17	0.44
1:A:262:ILE:O	1:A:265:ALA:HB3	2.17	0.44
1:F:122:PHE:C	1:F:124:PRO:HB3	2.37	0.44
1:F:273:PHE:CE1	1:F:395:MET:HB3	2.52	0.44
1:B:111:ALA:N	1:B:327:ASN:HB3	2.33	0.44
1:B:282:LEU:HD13	1:B:307:ALA:HB2	1.98	0.44
1:B:276:ARG:HD3	1:B:395:MET:CG	2.47	0.44
1:B:77:ARG:HA	1:B:80:ARG:NH1	2.32	0.44
1:D:374:LEU:HA	1:D:379:VAL:HG11	1.99	0.44
1:E:146:LEU:HB3	1:F:143:PHE:CD1	2.53	0.44
1:E:216:VAL:HG12	1:E:392:ILE:HD12	2.00	0.44
1:F:13:LEU:HD12	1:F:13:LEU:O	2.17	0.44
1:F:264:HIS:CE1	1:F:265:ALA:CB	2.94	0.44
1:F:382:ALA:HA	1:F:385:MET:HG3	1.97	0.44
1:B:191:ALA:O	1:B:195:TYR:HD1	1.99	0.44
1:B:81:VAL:HG21	1:B:298:ILE:HG23	1.99	0.44
1:C:317:TYR:C	1:C:317:TYR:CD1	2.91	0.44
1:C:77:ARG:O	1:C:78:LEU:C	2.56	0.44
1:D:264:HIS:ND1	1:D:264:HIS:C	2.70	0.44
1:D:30:LEU:O	1:D:35:TYR:HB2	2.17	0.44
1:F:333:LEU:HD12	1:F:333:LEU:H	1.83	0.44
1:A:144:GLY:O	1:A:147:ALA:N	2.50	0.44
1:A:265:ALA:HB1	1:A:266:LYS:O	2.17	0.44
1:A:273:PHE:CE1	1:A:395:MET:HB3	2.53	0.44
1:D:414:LYS:HG3	1:D:414:LYS:O	2.17	0.44
1:F:337:GLN:O	1:F:341:ILE:N	2.48	0.44
1:A:231:VAL:HG23	1:A:320:VAL:HG22	1.99	0.44
1:B:349:SER:C	1:B:351:GLY:HA3	2.37	0.44
1:B:67:VAL:HG11	1:B:187:ILE:HD13	2.00	0.44
1:C:198:VAL:HG13	1:C:287:ARG:HD3	2.00	0.44
1:D:282:LEU:HB3	1:D:283:PRO:HD3	2.00	0.44
1:D:285:THR:HG22	1:D:303:LEU:HD13	1.99	0.44
1:F:81:VAL:HG21	1:F:298:ILE:HG23	2.00	0.44
1:F:48:ASP:O	1:F:49:LEU:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:THR:HG22	1:C:55:LYS:HB2	1.99	0.44
1:B:377:PRO:O	1:B:381:ALA:N	2.48	0.44
1:D:325:ILE:HD11	1:D:383:TYR:HA	1.99	0.44
1:D:52:ARG:NH2	1:E:136:ASP:HA	2.32	0.44
1:E:315:ALA:HB2	1:E:349:SER:OG	2.18	0.44
1:F:124:PRO:HB2	1:F:368:HIS:NE2	2.32	0.44
1:F:77:ARG:HA	1:F:80:ARG:HH12	1.83	0.44
1:D:134:LEU:O	1:D:135:LEU:C	2.55	0.44
1:E:394:ASP:OD1	2:E:501:ASP:N	2.51	0.44
1:B:10:TYR:CD2	1:B:11:PRO:HD2	2.53	0.43
1:A:281:THR:O	1:A:283:PRO:N	2.51	0.43
1:E:50:PHE:CZ	1:E:54:LEU:HD11	2.52	0.43
1:F:23:GLY:HA2	1:F:210:PHE:CE2	2.53	0.43
1:A:107:PHE:HE1	1:A:237:VAL:HG11	1.84	0.43
1:C:72:SER:O	1:C:73:ILE:HD12	2.18	0.43
1:D:63:PHE:O	1:D:67:VAL:HG23	2.19	0.43
1:E:191:ALA:O	1:E:195:TYR:HD1	2.01	0.43
1:E:205:ALA:N	1:E:206:PRO:HD2	2.33	0.43
1:F:48:ASP:O	1:F:51:VAL:N	2.52	0.43
1:A:228:LEU:HB3	1:A:389:ILE:HD13	1.99	0.43
1:C:325:ILE:O	1:C:329:LEU:HG	2.18	0.43
1:C:374:LEU:HA	1:C:379:VAL:HG11	2.00	0.43
1:D:146:LEU:HD13	1:E:143:PHE:CE1	2.53	0.43
1:E:123:GLN:N	1:E:124:PRO:HA	2.33	0.43
1:E:15:LYS:HZ2	1:E:206:PRO:HG3	1.83	0.43
1:E:311:MET:CE	1:E:354:GLY:HA2	2.48	0.43
1:A:264:HIS:C	1:A:264:HIS:ND1	2.72	0.43
1:A:282:LEU:HD13	1:A:307:ALA:HB2	2.01	0.43
1:B:263:LYS:O	1:B:265:ALA:N	2.52	0.43
1:C:262:ILE:O	1:C:265:ALA:HB3	2.19	0.43
1:D:157:PHE:O	1:D:160:ILE:N	2.50	0.43
1:C:73:ILE:CG2	1:C:74:SER:N	2.81	0.43
1:F:202:MET:HA	1:F:205:ALA:HB2	2.01	0.43
1:C:317:TYR:HD1	1:C:317:TYR:C	2.22	0.43
1:D:134:LEU:C	1:D:136:ASP:H	2.22	0.43
1:E:9:GLU:OE2	1:E:9:GLU:HA	2.18	0.43
1:A:367:LEU:HD22	1:A:372:LEU:CD1	2.48	0.43
1:A:85:ILE:HG13	1:A:89:TYR:CE1	2.54	0.43
1:B:50:PHE:CZ	1:B:54:LEU:HD11	2.54	0.43
1:C:134:LEU:O	1:C:135:LEU:C	2.57	0.43
1:C:134:LEU:O	1:C:137:ILE:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:321:CYS:HB3	1:D:363:LEU:HD21	2.01	0.43
1:F:28:LEU:HA	1:F:28:LEU:HD12	1.87	0.43
1:A:297:GLY:O	1:A:298:ILE:HD13	2.19	0.43
1:C:253:ILE:HG23	1:C:254:TYR:HD1	1.84	0.43
1:F:391:ALA:HA	1:F:394:ASP:CB	2.49	0.43
1:B:7:TYR:HD2	1:B:9:GLU:OE2	2.02	0.42
1:D:294:ILE:HG22	1:D:295:SER:H	1.83	0.42
1:E:337:GLN:O	1:E:341:ILE:N	2.52	0.42
1:F:68:VAL:O	1:F:71:ALA:N	2.52	0.42
1:A:228:LEU:HB3	1:A:389:ILE:CD1	2.50	0.42
1:A:374:LEU:HA	1:A:379:VAL:HG11	2.01	0.42
1:B:48:ASP:O	1:B:49:LEU:C	2.57	0.42
1:D:101:ILE:O	1:D:105:ARG:HG2	2.18	0.42
1:E:317:TYR:HD1	1:E:317:TYR:C	2.23	0.42
1:E:72:SER:O	1:E:73:ILE:HD12	2.19	0.42
1:A:251:LEU:HD13	1:A:258:PRO:HA	2.01	0.42
1:C:157:PHE:O	1:C:160:ILE:N	2.51	0.42
1:E:276:ARG:HD3	1:E:395:MET:HG3	2.00	0.42
1:F:134:LEU:O	1:F:137:ILE:HG13	2.18	0.42
1:F:228:LEU:HB3	1:F:389:ILE:CD1	2.50	0.42
1:F:74:SER:O	1:F:77:ARG:N	2.52	0.42
1:A:32:HIS:HB2	1:A:222:VAL:HG12	2.01	0.42
1:A:400:VAL:O	1:A:400:VAL:HG12	2.20	0.42
1:B:117:VAL:CG1	1:B:378:ASN:HB2	2.49	0.42
1:C:264:HIS:C	1:C:264:HIS:ND1	2.72	0.42
1:C:282:LEU:HD13	1:C:307:ALA:HB2	2.01	0.42
1:C:66:LEU:HA	1:C:300:SER:OG	2.20	0.42
1:D:134:LEU:O	1:D:137:ILE:HG13	2.20	0.42
1:B:385:MET:HA	1:D:378:ASN:OD1	2.19	0.42
1:E:281:THR:O	1:E:283:PRO:N	2.52	0.42
1:E:56:MET:HE2	1:F:157:PHE:CD1	2.54	0.42
1:F:382:ALA:O	1:F:385:MET:HG3	2.19	0.42
1:B:123:GLN:N	1:B:124:PRO:CA	2.82	0.42
1:B:276:ARG:O	1:B:356:PRO:HG3	2.18	0.42
1:B:58:VAL:HG22	1:B:283:PRO:CD	2.49	0.42
1:C:134:LEU:C	1:C:136:ASP:N	2.72	0.42
1:E:24:ALA:N	1:E:213:ILE:HD13	2.35	0.42
1:E:58:VAL:HG22	1:E:283:PRO:CD	2.49	0.42
1:F:134:LEU:O	1:F:135:LEU:C	2.56	0.42
1:A:98:THR:O	1:A:102:ILE:HB	2.18	0.42
1:B:228:LEU:HB3	1:B:389:ILE:CD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:258:PRO:O	1:D:261:PHE:HB3	2.18	0.42
1:D:408:GLY:O	1:D:412:VAL:HG23	2.20	0.42
1:F:263:LYS:C	1:F:265:ALA:N	2.73	0.42
1:F:348:ALA:O	1:F:352:THR:N	2.52	0.42
1:C:64:ALA:CB	1:C:191:ALA:HB2	2.49	0.42
1:D:253:ILE:HG23	1:D:254:TYR:HD1	1.84	0.42
1:E:7:TYR:N	1:E:8:ILE:HA	2.34	0.42
1:F:216:VAL:HG12	1:F:392:ILE:HD12	2.02	0.42
1:F:24:ALA:O	1:F:28:LEU:HB2	2.20	0.42
1:F:84:LYS:NZ	1:F:416:GLU:OE1	2.49	0.42
1:A:113:ILE:HD12	1:A:114:HIS:H	1.85	0.42
1:A:28:LEU:HA	1:A:28:LEU:HD12	1.86	0.42
1:A:79:GLY:O	1:A:83:VAL:HG23	2.20	0.42
1:B:209:VAL:HG22	1:B:274:VAL:HG11	2.02	0.42
1:C:285:THR:HG22	1:C:303:LEU:HD13	2.00	0.42
1:F:39:VAL:O	1:F:43:VAL:HB	2.20	0.42
1:A:190:LEU:O	1:A:191:ALA:C	2.56	0.42
1:B:337:GLN:O	1:B:341:ILE:N	2.50	0.42
1:C:81:VAL:HG23	1:C:412:VAL:CG1	2.48	0.42
1:F:59:MET:CE	1:F:146:LEU:HA	2.50	0.42
1:F:276:ARG:HD3	1:F:395:MET:CG	2.50	0.42
1:A:317:TYR:HD1	1:A:317:TYR:C	2.24	0.42
1:B:89:TYR:CD2	1:B:310:ASN:HB2	2.55	0.42
1:E:250:LEU:CA	1:E:253:ILE:HG22	2.49	0.42
1:E:297:GLY:O	1:E:298:ILE:HD13	2.20	0.42
1:E:64:ALA:CB	1:E:191:ALA:HB2	2.50	0.42
1:F:134:LEU:C	1:F:136:ASP:N	2.74	0.42
1:F:391:ALA:HA	1:F:394:ASP:HB3	2.01	0.42
1:F:7:TYR:CD2	1:F:9:GLU:OE2	2.73	0.42
1:C:295:SER:OG	1:C:298:ILE:HG12	2.20	0.41
1:A:138:VAL:HG11	1:C:52:ARG:HB3	2.02	0.41
1:C:75:PRO:HG3	1:C:163:ILE:CG1	2.45	0.41
1:D:156:PHE:O	1:D:156:PHE:CD2	2.73	0.41
1:E:137:ILE:O	1:E:139:PRO:HD3	2.20	0.41
1:E:28:LEU:HD12	1:E:28:LEU:HA	1.89	0.41
1:F:363:LEU:O	1:F:367:LEU:HG	2.20	0.41
1:F:7:TYR:HD2	1:F:9:GLU:OE2	2.02	0.41
1:A:144:GLY:O	1:A:145:ALA:C	2.59	0.41
1:A:146:LEU:O	1:B:141:ASN:ND2	2.49	0.41
1:B:216:VAL:HG12	1:B:392:ILE:HD12	2.02	0.41
1:B:56:MET:HE3	1:C:157:PHE:HD1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:115:LEU:HD22	1:F:378:ASN:ND2	2.34	0.41
1:F:24:ALA:N	1:F:213:ILE:HD13	2.35	0.41
1:B:333:LEU:HD12	1:B:333:LEU:H	1.86	0.41
1:C:202:MET:HA	1:C:205:ALA:HB2	2.01	0.41
1:E:113:ILE:HD12	1:E:114:HIS:H	1.85	0.41
1:E:89:TYR:CD2	1:E:310:ASN:HB2	2.55	0.41
1:B:52:ARG:NH2	1:C:136:ASP:HA	2.36	0.41
1:C:317:TYR:CD1	1:C:318:GLN:N	2.88	0.41
1:C:228:LEU:HB3	1:C:389:ILE:HD13	2.02	0.41
1:D:209:VAL:HG13	1:D:274:VAL:HG21	2.02	0.41
1:E:66:LEU:HD21	1:E:159:ILE:HG13	2.03	0.41
1:E:228:LEU:HB3	1:E:389:ILE:CD1	2.51	0.41
1:F:264:HIS:ND1	1:F:264:HIS:C	2.73	0.41
1:A:174:GLU:OE1	1:A:177:ARG:NE	2.53	0.41
1:B:146:LEU:O	1:B:148:ASN:N	2.53	0.41
1:C:77:ARG:HA	1:C:80:ARG:NH1	2.36	0.41
1:D:205:ALA:N	1:D:206:PRO:HD2	2.34	0.41
1:A:337:GLN:O	1:A:341:ILE:N	2.53	0.41
1:A:398:THR:HA	1:A:401:ASN:ND2	2.36	0.41
1:A:66:LEU:HA	1:A:300:SER:OG	2.21	0.41
1:B:59:MET:CE	1:B:146:LEU:HA	2.51	0.41
1:C:209:VAL:HG13	1:C:274:VAL:HG21	2.02	0.41
1:C:212:LEU:CB	1:C:274:VAL:HG13	2.50	0.41
1:C:261:PHE:HD2	1:C:262:ILE:HD12	1.85	0.41
1:E:124:PRO:CB	1:E:368:HIS:CE1	2.92	0.41
1:E:398:THR:HA	1:E:401:ASN:ND2	2.36	0.41
1:F:123:GLN:N	1:F:124:PRO:CA	2.84	0.41
1:F:110:GLY:N	1:F:227:GLU:OE1	2.48	0.41
1:F:9:GLU:OE2	1:F:203:GLN:NE2	2.54	0.41
1:A:43:VAL:HG11	1:A:214:ALA:CB	2.50	0.41
1:A:78:LEU:HD13	1:A:78:LEU:HA	1.82	0.41
1:C:193:ALA:O	1:C:196:LYS:HB2	2.21	0.41
1:D:299:TYR:C	1:D:299:TYR:CD2	2.94	0.41
1:E:111:ALA:N	1:E:327:ASN:HB3	2.35	0.41
1:E:159:ILE:HD11	1:E:301:PHE:CD1	2.56	0.41
1:F:190:LEU:O	1:F:193:ALA:HB3	2.21	0.41
1:A:51:VAL:HG22	1:A:275:THR:HG23	2.02	0.41
1:A:346:VAL:O	1:A:350:ILE:CG2	2.65	0.41
1:B:165:ILE:O	1:B:166:THR:C	2.59	0.41
1:B:391:ALA:HA	1:B:394:ASP:HB3	2.02	0.41
1:D:123:GLN:HG2	1:D:125:LYS:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:344:THR:HA	1:D:347:LEU:HB2	2.03	0.41
1:E:183:LEU:HG	1:E:187:ILE:HD12	2.02	0.41
1:E:15:LYS:NZ	1:E:206:PRO:HG3	2.35	0.41
1:A:66:LEU:HD21	1:A:159:ILE:HG13	2.03	0.41
1:C:256:ILE:HD13	1:C:410:ALA:HB1	2.03	0.41
1:C:325:ILE:HD11	1:C:383:TYR:HA	2.02	0.41
1:D:77:ARG:HA	1:D:80:ARG:NH1	2.36	0.41
1:A:123:GLN:N	1:A:124:PRO:HA	2.36	0.41
1:A:178:LYS:O	1:A:182:THR:OG1	2.39	0.41
1:A:85:ILE:CD1	1:A:408:GLY:O	2.69	0.41
1:B:77:ARG:HH11	1:B:416:GLU:HG3	1.85	0.41
1:B:7:TYR:CD2	1:B:9:GLU:OE2	2.74	0.41
1:C:11:PRO:HG2	1:C:14:GLN:CG	2.47	0.41
1:C:23:GLY:HA2	1:C:210:PHE:CE2	2.55	0.41
1:C:88:TYR:CZ	1:C:92:THR:HG21	2.56	0.41
1:E:228:LEU:HB3	1:E:389:ILE:HD13	2.03	0.41
1:F:317:TYR:O	1:F:321:CYS:N	2.50	0.41
1:A:9:GLU:HA	1:A:9:GLU:OE2	2.21	0.41
1:B:19:GLY:O	1:B:23:GLY:N	2.51	0.41
1:B:49:LEU:O	1:B:52:ARG:HB2	2.21	0.41
1:D:276:ARG:HD3	1:D:395:MET:HG3	2.02	0.41
1:D:281:THR:O	1:D:282:LEU:C	2.59	0.41
1:D:117:VAL:CG1	1:D:378:ASN:HB2	2.51	0.41
1:E:322:THR:HG21	1:E:341:ILE:CD1	2.51	0.41
1:F:248:PHE:O	1:F:252:LYS:HB2	2.21	0.41
1:F:314:THR:HG22	1:F:318:GLN:NE2	2.36	0.41
1:A:286:MET:HA	1:A:303:LEU:HD12	2.03	0.40
1:B:7:TYR:HB2	1:B:8:ILE:O	2.21	0.40
1:C:16:ILE:HD11	1:C:205:ALA:CB	2.51	0.40
1:C:97:VAL:HB	1:C:342:VAL:HG22	2.03	0.40
1:C:350:ILE:N	1:C:351:GLY:CA	2.81	0.40
1:D:15:LYS:HZ2	1:D:206:PRO:HG3	1.86	0.40
1:D:212:LEU:HB2	1:D:274:VAL:HG13	2.02	0.40
1:E:400:VAL:HG12	1:E:400:VAL:O	2.21	0.40
1:E:197:ILE:CG2	1:F:160:ILE:CG2	2.99	0.40
1:F:257:ASP:HA	1:F:258:PRO:HD3	1.93	0.40
1:F:73:ILE:CG2	1:F:74:SER:N	2.84	0.40
1:A:11:PRO:HG2	1:A:14:GLN:CG	2.45	0.40
1:A:64:ALA:CB	1:A:191:ALA:HB2	2.52	0.40
1:A:215:TYR:O	1:A:218:ALA:N	2.54	0.40
1:B:137:ILE:O	1:B:139:PRO:HD3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:GLU:CD	1:B:177:ARG:HE	2.24	0.40
1:B:209:VAL:HG13	1:B:274:VAL:HG21	2.03	0.40
1:B:265:ALA:CB	1:B:266:LYS:O	2.68	0.40
1:C:35:TYR:O	1:C:38:ALA:N	2.54	0.40
1:D:85:ILE:HG13	1:D:89:TYR:CE1	2.56	0.40
1:F:103:MET:HE1	1:F:241:LEU:HD22	2.03	0.40
1:D:143:PHE:CZ	1:F:60:PRO:HG3	2.55	0.40
1:B:7:TYR:HB2	1:B:8:ILE:C	2.41	0.40
1:C:123:GLN:N	1:C:124:PRO:HA	2.36	0.40
1:C:299:TYR:CD2	1:C:299:TYR:C	2.95	0.40
1:F:261:PHE:O	1:F:264:HIS:HD2	2.02	0.40
1:F:311:MET:HE1	1:F:354:GLY:HA2	2.03	0.40
1:C:98:THR:O	1:C:102:ILE:HB	2.22	0.40
1:C:16:ILE:HD11	1:C:205:ALA:HB3	2.04	0.40
1:D:337:GLN:O	1:D:338:GLN:C	2.60	0.40
1:A:134:LEU:O	1:A:137:ILE:CG1	2.66	0.40
1:A:257:ASP:HA	1:A:258:PRO:HD3	1.98	0.40
1:A:296:GLU:HA	1:A:299:TYR:CE1	2.56	0.40
1:B:241:LEU:O	1:B:245:LEU:HB2	2.22	0.40
1:B:285:THR:HG22	1:B:303:LEU:HD13	2.04	0.40
1:B:402:VAL:HG22	4:B:601:HOH:O	2.22	0.40
1:D:195:TYR:O	1:D:198:VAL:HG12	2.22	0.40
1:F:237:VAL:O	1:F:241:LEU:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	409/425 (96%)	330 (81%)	63 (15%)	16 (4%)	4	34
1	B	409/425 (96%)	326 (80%)	59 (14%)	24 (6%)	2	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	409/425 (96%)	328 (80%)	63 (15%)	18 (4%)	3	30
1	D	409/425 (96%)	331 (81%)	56 (14%)	22 (5%)	2	25
1	E	409/425 (96%)	328 (80%)	68 (17%)	13 (3%)	5	40
1	F	409/425 (96%)	321 (78%)	66 (16%)	22 (5%)	2	25
All	All	2454/2550 (96%)	1964 (80%)	375 (15%)	115 (5%)	3	29

All (115) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	116	ALA
1	A	124	PRO
1	A	127	ALA
1	A	267	ASP
1	B	68	VAL
1	B	124	PRO
1	B	127	ALA
1	B	282	LEU
1	C	116	ALA
1	C	124	PRO
1	C	127	ALA
1	C	130	LEU
1	C	135	LEU
1	C	267	ASP
1	C	282	LEU
1	D	124	PRO
1	D	127	ALA
1	D	130	LEU
1	D	135	LEU
1	D	267	ASP
1	E	116	ALA
1	E	124	PRO
1	E	127	ALA
1	E	149	GLY
1	E	267	ASP
1	E	282	LEU
1	F	68	VAL
1	F	124	PRO
1	F	127	ALA
1	F	267	ASP
1	F	282	LEU
1	A	130	LEU

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Mol	Chain	Res	Type
1	A	135	LEU
1	A	149	GLY
1	A	150	GLN
1	A	282	LEU
1	B	56	MET
1	B	115	LEU
1	B	116	ALA
1	B	130	LEU
1	B	149	GLY
1	B	200	GLY
1	B	202	MET
1	B	264	HIS
1	B	267	ASP
1	C	149	GLY
1	C	172	GLU
1	C	202	MET
1	D	116	ALA
1	D	149	GLY
1	D	202	MET
1	D	282	LEU
1	E	130	LEU
1	E	135	LEU
1	E	150	GLN
1	F	34	GLY
1	F	115	LEU
1	F	116	ALA
1	F	130	LEU
1	F	149	GLY
1	F	155	ILE
1	F	202	MET
1	F	264	HIS
1	B	155	ILE
1	C	155	ILE
1	C	220	GLN
1	D	155	ILE
1	E	34	GLY
1	E	56	MET
1	E	202	MET
1	F	135	LEU
1	F	150	GLN
1	F	200	GLY
1	F	334	THR

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Mol	Chain	Res	Type
1	A	34	GLY
1	A	115	LEU
1	A	202	MET
1	B	150	GLN
1	B	334	THR
1	C	68	VAL
1	C	150	GLN
1	D	172	GLU
1	D	220	GLN
1	F	56	MET
1	F	220	GLN
1	A	56	MET
1	B	34	GLY
1	B	135	LEU
1	B	146	LEU
1	B	220	GLN
1	D	36	ALA
1	D	115	LEU
1	D	150	GLN
1	F	352	THR
1	C	60	PRO
1	D	371	GLY
1	A	377	PRO
1	C	370	VAL
1	F	222	VAL
1	B	60	PRO
1	B	371	GLY
1	C	371	GLY
1	C	373	PRO
1	D	60	PRO
1	D	68	VAL
1	D	370	VAL
1	F	60	PRO
1	B	377	PRO
1	D	129	PRO
1	D	373	PRO
1	A	155	ILE
1	A	371	GLY
1	D	377	PRO
1	B	373	PRO
1	E	370	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	316/330 (96%)	260 (82%)	56 (18%)	2	13
1	B	316/330 (96%)	254 (80%)	62 (20%)	1	9
1	C	316/330 (96%)	261 (83%)	55 (17%)	2	14
1	D	316/330 (96%)	262 (83%)	54 (17%)	2	15
1	E	316/330 (96%)	259 (82%)	57 (18%)	2	12
1	F	316/330 (96%)	256 (81%)	60 (19%)	2	10
All	All	1896/1980 (96%)	1552 (82%)	344 (18%)	2	12

All (344) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLU
1	A	13	LEU
1	A	15	LYS
1	A	17	LEU
1	A	25	ILE
1	A	28	LEU
1	A	32	HIS
1	A	73	ILE
1	A	77	ARG
1	A	78	LEU
1	A	90	LEU
1	A	102	ILE
1	A	105	ARG
1	A	106	LEU
1	A	120	GLN
1	A	122	PHE
1	A	123	GLN
1	A	125	LYS
1	A	140	THR
1	A	148	ASN
1	A	151	VAL
1	A	159	ILE

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Mol	Chain	Res	Type
1	A	175	LYS
1	A	182	THR
1	A	198	VAL
1	A	215	TYR
1	A	232	THR
1	A	237	VAL
1	A	241	LEU
1	A	242	GLN
1	A	245	LEU
1	A	253	ILE
1	A	260	SER
1	A	264	HIS
1	A	274	VAL
1	A	287	ARG
1	A	288	VAL
1	A	295	SER
1	A	296	GLU
1	A	317	TYR
1	A	333	LEU
1	A	338	GLN
1	A	344	THR
1	A	350	ILE
1	A	355	VAL
1	A	361	ILE
1	A	365	MET
1	A	372	LEU
1	A	374	LEU
1	A	375	THR
1	A	385	MET
1	A	386	ILE
1	A	387	LEU
1	A	389	ILE
1	A	402	VAL
1	A	415	THR
1	B	9	GLU
1	B	13	LEU
1	B	15	LYS
1	B	17	LEU
1	B	28	LEU
1	B	72	SER
1	B	73	ILE
1	B	74	SER

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Mol	Chain	Res	Type
1	B	77	ARG
1	B	78	LEU
1	B	80	ARG
1	B	90	LEU
1	B	102	ILE
1	B	105	ARG
1	B	113	ILE
1	B	120	GLN
1	B	122	PHE
1	B	123	GLN
1	B	125	LYS
1	B	131	VAL
1	B	137	ILE
1	B	148	ASN
1	B	175	LYS
1	B	176	VAL
1	B	182	THR
1	B	215	TYR
1	B	231	VAL
1	B	232	THR
1	B	237	VAL
1	B	241	LEU
1	B	242	GLN
1	B	245	LEU
1	B	253	ILE
1	B	260	SER
1	B	264	HIS
1	B	269	MET
1	B	274	VAL
1	B	283	PRO
1	B	287	ARG
1	B	288	VAL
1	B	295	SER
1	B	296	GLU
1	B	300	SER
1	B	308	THR
1	B	317	TYR
1	B	323	PHE
1	B	333	LEU
1	B	334	THR
1	B	338	GLN
1	B	340	THR

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Mol	Chain	Res	Type
1	B	350	ILE
1	B	355	VAL
1	B	361	ILE
1	B	365	MET
1	B	372	LEU
1	B	374	LEU
1	B	375	THR
1	B	385	MET
1	B	386	ILE
1	B	387	LEU
1	B	392	ILE
1	B	415	THR
1	C	6	LYS
1	C	9	GLU
1	C	15	LYS
1	C	17	LEU
1	C	28	LEU
1	C	61	ILE
1	C	72	SER
1	C	73	ILE
1	C	74	SER
1	C	77	ARG
1	C	78	LEU
1	C	80	ARG
1	C	90	LEU
1	C	91	LEU
1	C	102	ILE
1	C	105	ARG
1	C	113	ILE
1	C	120	GLN
1	C	122	PHE
1	C	123	GLN
1	C	125	LYS
1	C	131	VAL
1	C	137	ILE
1	C	148	ASN
1	C	151	VAL
1	C	159	ILE
1	C	175	LYS
1	C	182	THR
1	C	231	VAL
1	C	232	THR

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Mol	Chain	Res	Type
1	C	237	VAL
1	C	242	GLN
1	C	245	LEU
1	C	253	ILE
1	C	260	SER
1	C	269	MET
1	C	287	ARG
1	C	288	VAL
1	C	295	SER
1	C	299	TYR
1	C	300	SER
1	C	317	TYR
1	C	333	LEU
1	C	338	GLN
1	C	350	ILE
1	C	355	VAL
1	C	361	ILE
1	C	365	MET
1	C	372	LEU
1	C	374	LEU
1	C	375	THR
1	C	385	MET
1	C	386	ILE
1	C	389	ILE
1	C	415	THR
1	D	9	GLU
1	D	13	LEU
1	D	15	LYS
1	D	17	LEU
1	D	28	LEU
1	D	61	ILE
1	D	72	SER
1	D	73	ILE
1	D	74	SER
1	D	78	LEU
1	D	80	ARG
1	D	90	LEU
1	D	91	LEU
1	D	102	ILE
1	D	105	ARG
1	D	120	GLN
1	D	122	PHE

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Mol	Chain	Res	Type
1	D	123	GLN
1	D	125	LYS
1	D	131	VAL
1	D	137	ILE
1	D	148	ASN
1	D	175	LYS
1	D	182	THR
1	D	207	ILE
1	D	231	VAL
1	D	232	THR
1	D	237	VAL
1	D	242	GLN
1	D	245	LEU
1	D	253	ILE
1	D	260	SER
1	D	269	MET
1	D	287	ARG
1	D	288	VAL
1	D	295	SER
1	D	299	TYR
1	D	300	SER
1	D	308	THR
1	D	317	TYR
1	D	323	PHE
1	D	333	LEU
1	D	338	GLN
1	D	350	ILE
1	D	355	VAL
1	D	361	ILE
1	D	365	MET
1	D	372	LEU
1	D	374	LEU
1	D	375	THR
1	D	385	MET
1	D	386	ILE
1	D	389	ILE
1	D	415	THR
1	E	9	GLU
1	E	15	LYS
1	E	17	LEU
1	E	25	ILE
1	E	28	LEU

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Mol	Chain	Res	Type
1	E	32	HIS
1	E	73	ILE
1	E	77	ARG
1	E	78	LEU
1	E	80	ARG
1	E	90	LEU
1	E	99	LEU
1	E	102	ILE
1	E	105	ARG
1	E	106	LEU
1	E	120	GLN
1	E	122	PHE
1	E	123	GLN
1	E	125	LYS
1	E	137	ILE
1	E	140	THR
1	E	148	ASN
1	E	151	VAL
1	E	159	ILE
1	E	175	LYS
1	E	178	LYS
1	E	182	THR
1	E	215	TYR
1	E	232	THR
1	E	237	VAL
1	E	241	LEU
1	E	242	GLN
1	E	245	LEU
1	E	253	ILE
1	E	260	SER
1	E	264	HIS
1	E	274	VAL
1	E	287	ARG
1	E	288	VAL
1	E	295	SER
1	E	296	GLU
1	E	317	TYR
1	E	333	LEU
1	E	334	THR
1	E	338	GLN
1	E	344	THR
1	E	350	ILE

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Mol	Chain	Res	Type
1	E	355	VAL
1	E	365	MET
1	E	372	LEU
1	E	374	LEU
1	E	375	THR
1	E	385	MET
1	E	386	ILE
1	E	387	LEU
1	E	389	ILE
1	E	415	THR
1	F	9	GLU
1	F	13	LEU
1	F	15	LYS
1	F	17	LEU
1	F	28	LEU
1	F	52	ARG
1	F	73	ILE
1	F	77	ARG
1	F	78	LEU
1	F	80	ARG
1	F	90	LEU
1	F	102	ILE
1	F	105	ARG
1	F	113	ILE
1	F	120	GLN
1	F	122	PHE
1	F	123	GLN
1	F	125	LYS
1	F	135	LEU
1	F	137	ILE
1	F	140	THR
1	F	148	ASN
1	F	175	LYS
1	F	176	VAL
1	F	182	THR
1	F	215	TYR
1	F	231	VAL
1	F	232	THR
1	F	237	VAL
1	F	241	LEU
1	F	242	GLN
1	F	245	LEU

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Mol	Chain	Res	Type
1	F	253	ILE
1	F	260	SER
1	F	264	HIS
1	F	269	MET
1	F	274	VAL
1	F	287	ARG
1	F	288	VAL
1	F	295	SER
1	F	296	GLU
1	F	300	SER
1	F	317	TYR
1	F	323	PHE
1	F	333	LEU
1	F	334	THR
1	F	338	GLN
1	F	350	ILE
1	F	355	VAL
1	F	361	ILE
1	F	365	MET
1	F	372	LEU
1	F	374	LEU
1	F	375	THR
1	F	385	MET
1	F	386	ILE
1	F	387	LEU
1	F	389	ILE
1	F	392	ILE
1	F	415	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	GLN
1	A	203	GLN
1	A	223	HIS
1	A	242	GLN
1	A	264	HIS
1	A	310	ASN
1	A	368	HIS
1	B	121	GLN
1	B	203	GLN
1	B	223	HIS

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Mol	Chain	Res	Type
1	B	242	GLN
1	B	310	ASN
1	B	368	HIS
1	C	150	GLN
1	C	242	GLN
1	C	264	HIS
1	C	310	ASN
1	C	368	HIS
1	D	242	GLN
1	D	264	HIS
1	D	368	HIS
1	E	203	GLN
1	E	223	HIS
1	E	242	GLN
1	E	264	HIS
1	E	368	HIS
1	F	203	GLN
1	F	223	HIS
1	F	242	GLN
1	F	310	ASN

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 for Mogul analysis.

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	ASP	A	501	-	2,8,8	0.21	0	1,10,10	0.14	0
2	ASP	B	501	-	2,8,8	0.27	0	1,10,10	0.01	0
2	ASP	C	501	-	2,8,8	0.25	0	1,10,10	0.47	0
2	ASP	D	501	-	2,8,8	0.40	0	1,10,10	0.36	0
2	ASP	E	501	-	2,8,8	0.07	0	1,10,10	0.18	0
2	ASP	F	501	-	2,8,8	0.25	0	1,10,10	0.01	0

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	ASP	A	501	-	-	0/2/8/8	0/0/0/0
2	ASP	B	501	-	-	0/2/8/8	0/0/0/0
2	ASP	C	501	-	-	0/2/8/8	0/0/0/0
2	ASP	D	501	-	-	0/2/8/8	0/0/0/0
2	ASP	E	501	-	-	0/2/8/8	0/0/0/0
2	ASP	F	501	-	-	0/2/8/8	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	ASP	1	0
2	B	501	ASP	1	0
2	D	501	ASP	1	0
2	E	501	ASP	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	411/425 (96%)	-0.29	0 100 100	117, 165, 200, 226	0
1	B	411/425 (96%)	-0.29	0 100 100	108, 147, 181, 213	0
1	C	411/425 (96%)	-0.28	0 100 100	108, 147, 182, 215	0
1	D	411/425 (96%)	-0.28	0 100 100	111, 147, 182, 217	0
1	E	411/425 (96%)	-0.31	0 100 100	119, 165, 200, 224	0
1	F	411/425 (96%)	-0.28	0 100 100	105, 146, 182, 211	0
All	All	2466/2550 (96%)	-0.29	0 100 100	105, 153, 190, 226	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

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
3	NA	A	503	1/1	0.98	0.24	1.61	155,155,155,155	0
3	NA	C	503	1/1	0.99	0.23	0.81	137,137,137,137	0
3	NA	E	503	1/1	0.99	0.16	-0.15	155,155,155,155	0
3	NA	B	503	1/1	0.99	0.16	-0.45	140,140,140,140	0
2	ASP	E	501	9/9	0.96	0.15	-0.56	132,140,145,148	0
3	NA	D	503	1/1	0.99	0.14	-0.99	132,132,132,132	0
3	NA	F	503	1/1	0.98	0.13	-1.04	140,140,140,140	0
3	NA	B	502	1/1	0.96	0.11	-1.14	105,105,105,105	0
3	NA	A	502	1/1	0.95	0.12	-1.14	124,124,124,124	0
2	ASP	A	501	9/9	0.95	0.12	-1.15	135,140,146,150	0
2	ASP	C	501	9/9	0.86	0.14	-1.37	122,127,130,136	0
2	ASP	F	501	9/9	0.92	0.11	-1.42	125,127,130,132	0
3	NA	D	502	1/1	0.93	0.08	-1.45	106,106,106,106	0
2	ASP	D	501	9/9	0.83	0.13	-1.48	122,128,130,137	0
3	NA	C	502	1/1	0.95	0.11	-1.50	106,106,106,106	0
3	NA	E	502	1/1	0.96	0.07	-1.55	123,123,123,123	0
2	ASP	B	501	9/9	0.92	0.10	-1.57	124,127,131,132	0
3	NA	F	502	1/1	0.89	0.07	-1.89	108,108,108,108	0

6.5 Other polymers [i](#)

There are no such residues in this entry.