



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:43 AM GMT

PDB ID : 2DW7
Title : Crystal structure of D-tartrate dehydratase from Bradyrhizobium japonicum complexed with Mg++ and meso-tartrate
Authors : Fedorov, A.A.; Fedorov, E.V.; Yew, W.S.; Wood, B.M.; Gerlt, J.A.; Almo, S.C.
Deposited on : 2006-08-07
Resolution : 2.50 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 (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

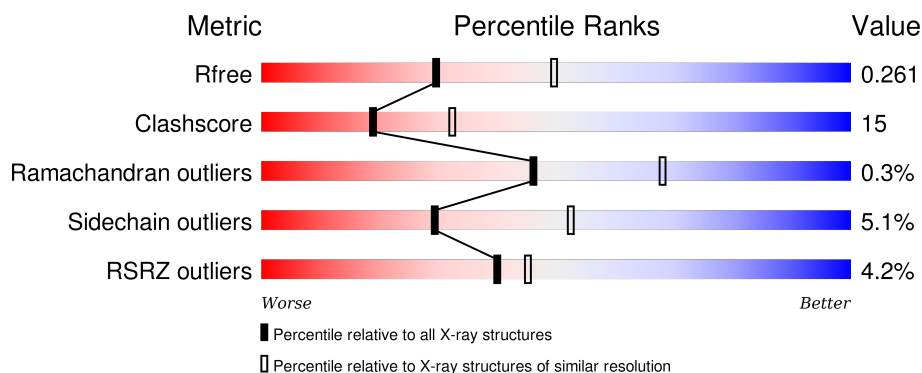
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	389	<div> <div></div> <div>74% 23% .</div> </div>
1	B	389	<div> <div>5%</div> <div>69% 29% .</div> </div>
1	C	389	<div> <div></div> <div>74% 24% .</div> </div>
1	D	389	<div> <div></div> <div>74% 23% .</div> </div>
1	E	389	<div> <div>3%</div> <div>72% 25% .</div> </div>

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Mol	Chain	Length	Quality of chain	
1	F	389		•
1	G	389		•
1	H	389		•
1	I	389		•
1	J	389		•
1	K	389		•
1	L	389		•
1	M	389		•
1	N	389		•
1	O	389		•
1	P	389		•

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
3	SRT	C	1003	-	-	-	X
3	SRT	E	1005	-	-	-	X
3	SRT	G	1007	-	-	X	X
3	SRT	I	1009	-	-	X	-
3	SRT	K	1011	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 48977 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.

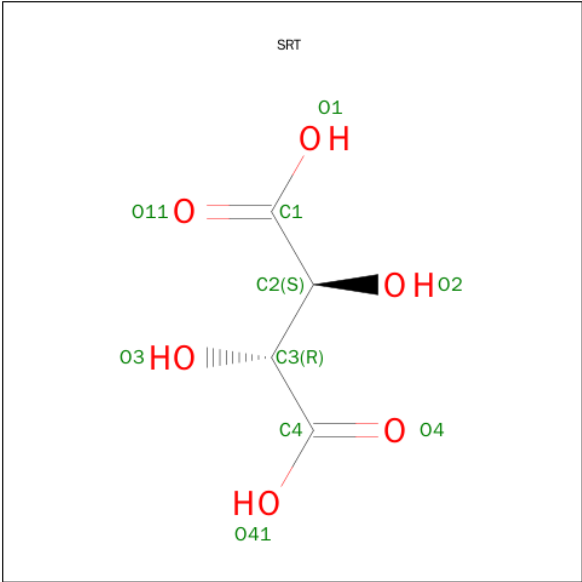
- Molecule 1 is a protein called Bll6730 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	0	0	0
			3022	1917	530	558	17			
1	B	388	Total	C	N	O	S	0	0	0
			3022	1917	530	558	17			
1	C	388	Total	C	N	O	S	0	0	0
			3022	1917	530	558	17			
1	D	388	Total	C	N	O	S	0	0	0
			3022	1917	530	558	17			
1	E	388	Total	C	N	O	S	0	0	0
			3022	1917	530	558	17			
1	F	388	Total	C	N	O	S	0	0	0
			3022	1917	530	558	17			
1	G	388	Total	C	N	O	S	0	0	0
			3022	1917	530	558	17			
1	H	388	Total	C	N	O	S	0	0	0
			3022	1917	530	558	17			
1	I	388	Total	C	N	O	S	0	0	0
			3022	1917	530	558	17			
1	J	388	Total	C	N	O	S	0	0	0
			3022	1917	530	558	17			
1	K	388	Total	C	N	O	S	0	0	0
			3022	1917	530	558	17			
1	L	388	Total	C	N	O	S	0	0	0
			3022	1917	530	558	17			
1	M	388	Total	C	N	O	S	0	0	0
			3022	1917	530	558	17			
1	N	388	Total	C	N	O	S	0	0	0
			3022	1917	530	558	17			
1	O	388	Total	C	N	O	S	0	0	0
			3022	1917	530	558	17			
1	P	388	Total	C	N	O	S	0	0	0
			3022	1917	530	558	17			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	P	1	Total	Mg	0	0
			1	1		
2	G	1	Total	Mg	0	0
			1	1		
2	J	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	K	1	Total	Mg	0	0
			1	1		
2	E	1	Total	Mg	0	0
			1	1		
2	H	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	I	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	N	1	Total	Mg	0	0
			1	1		
2	O	1	Total	Mg	0	0
			1	1		
2	L	1	Total	Mg	0	0
			1	1		
2	F	1	Total	Mg	0	0
			1	1		
2	M	1	Total	Mg	0	0
			1	1		

- Molecule 3 is S,R MESO-TARTARIC ACID (three-letter code: SRT) (formula: C₄H₆O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	4	6		
3	B	1	Total	C	O	0	0
			10	4	6		
3	C	1	Total	C	O	0	0
			10	4	6		
3	D	1	Total	C	O	0	0
			10	4	6		
3	E	1	Total	C	O	0	0
			10	4	6		
3	F	1	Total	C	O	0	0
			10	4	6		
3	G	1	Total	C	O	0	0
			10	4	6		
3	H	1	Total	C	O	0	0
			10	4	6		
3	I	1	Total	C	O	0	0
			10	4	6		
3	J	1	Total	C	O	0	0
			10	4	6		
3	K	1	Total	C	O	0	0
			10	4	6		
3	L	1	Total	C	O	0	0
			10	4	6		
3	M	1	Total	C	O	0	0
			10	4	6		
3	N	1	Total	C	O	0	0
			10	4	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	O	1	Total	C	O	0	0
			10	4	6		
3	P	1	Total	C	O	0	0
			10	4	6		

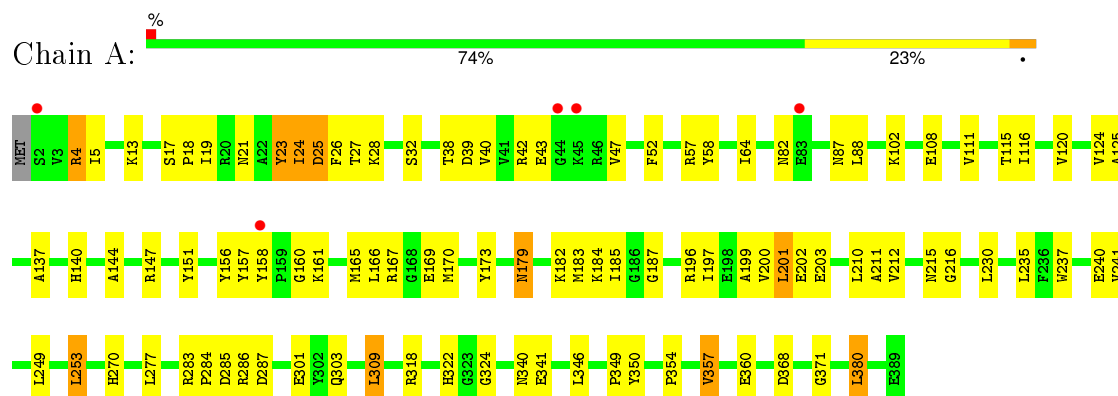
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	43	Total	O	0	0
			43	43		
4	B	21	Total	O	0	0
			21	21		
4	C	61	Total	O	0	0
			61	61		
4	D	49	Total	O	0	0
			49	49		
4	E	29	Total	O	0	0
			29	29		
4	F	53	Total	O	0	0
			53	53		
4	G	41	Total	O	0	0
			41	41		
4	H	22	Total	O	0	0
			22	22		
4	I	20	Total	O	0	0
			20	20		
4	J	12	Total	O	0	0
			12	12		
4	K	29	Total	O	0	0
			29	29		
4	L	20	Total	O	0	0
			20	20		
4	M	12	Total	O	0	0
			12	12		
4	N	20	Total	O	0	0
			20	20		
4	O	5	Total	O	0	0
			5	5		
4	P	12	Total	O	0	0
			12	12		

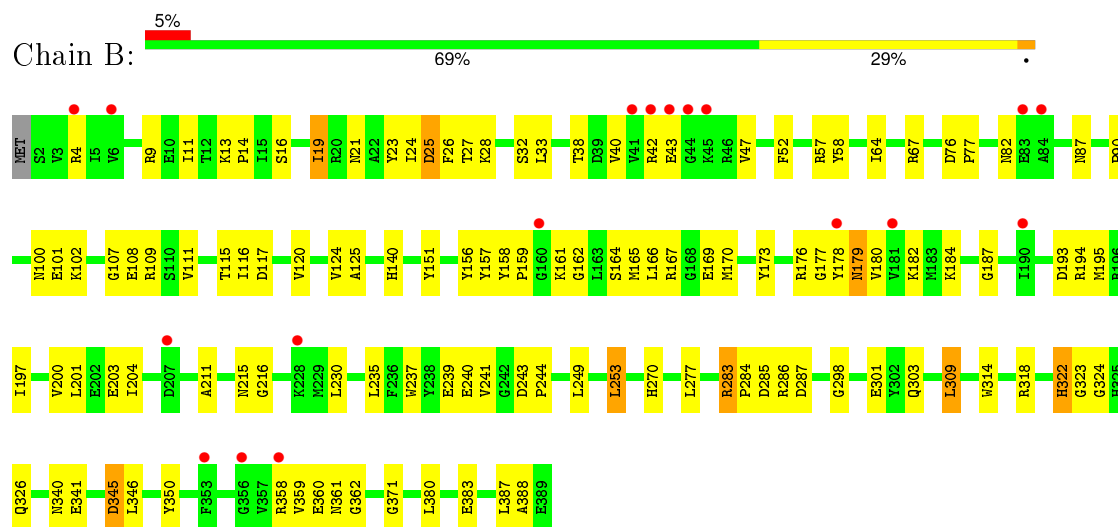
3 Residue-property plots

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 ($RSRZ > 2$). 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.

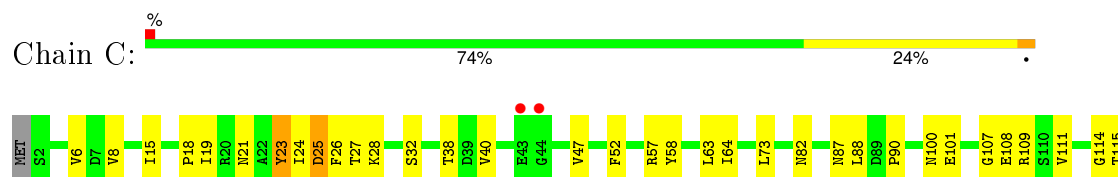
• Molecule 1: Bll6730 protein

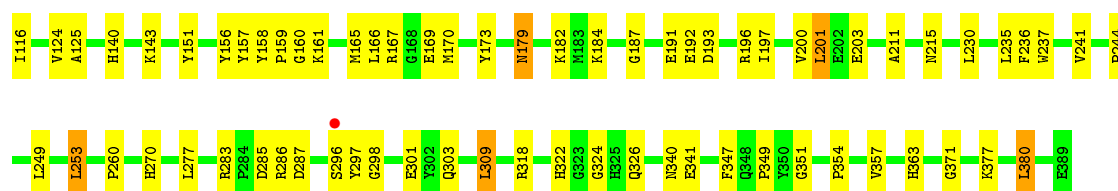


• Molecule 1: Bll6730 protein

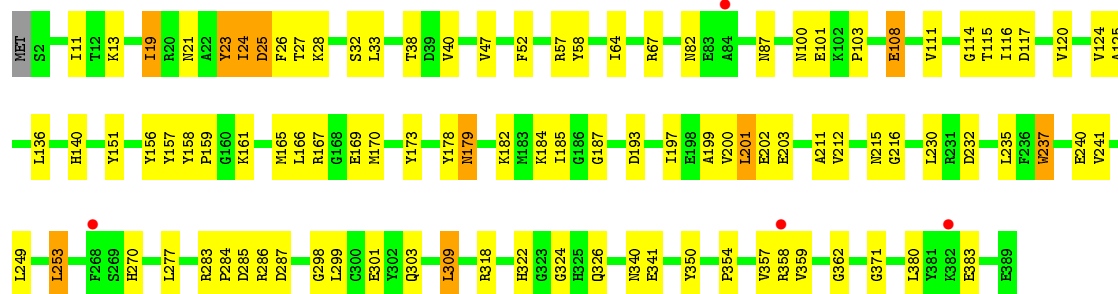


• Molecule 1: Bll6730 protein

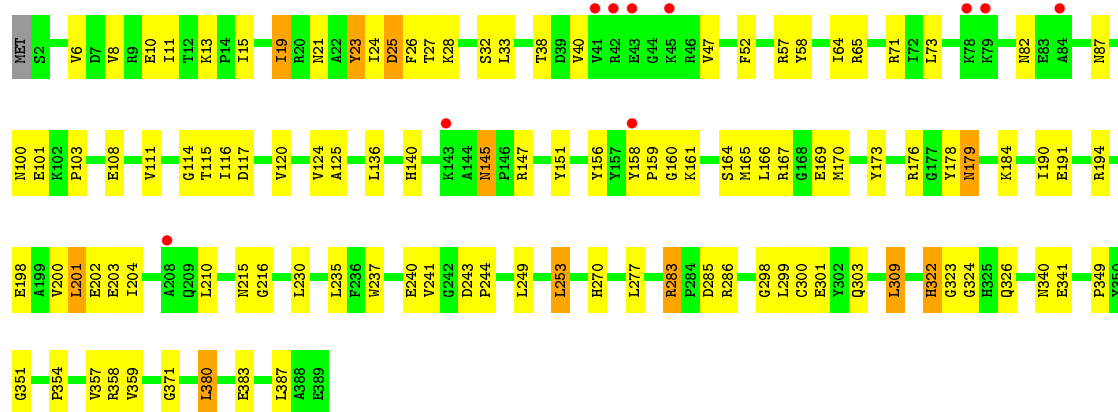




• Molecule 1: Bll6730 protein

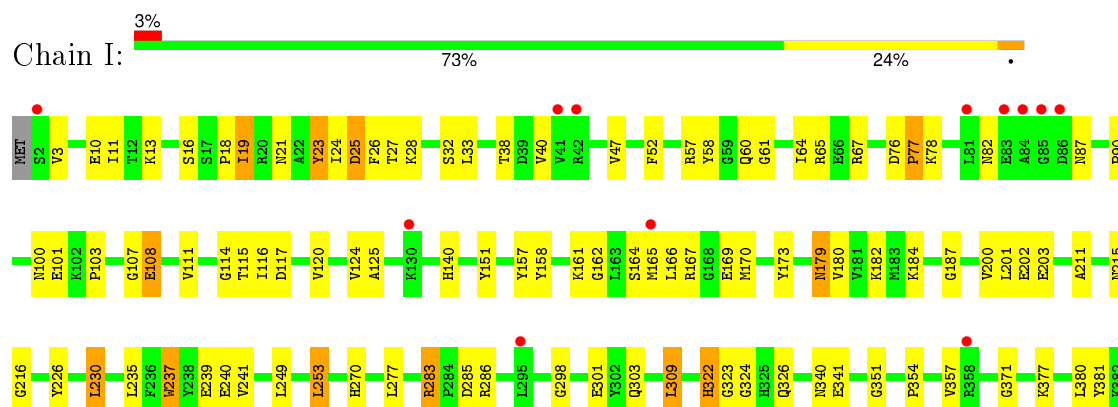


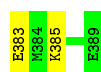
• Molecule 1: Bll6730 protein



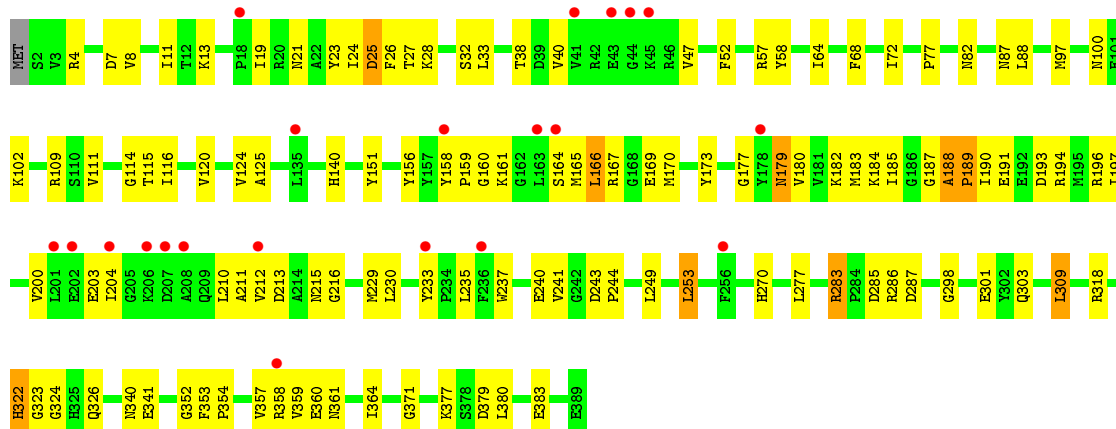
• Molecule 1: Bll6730 protein



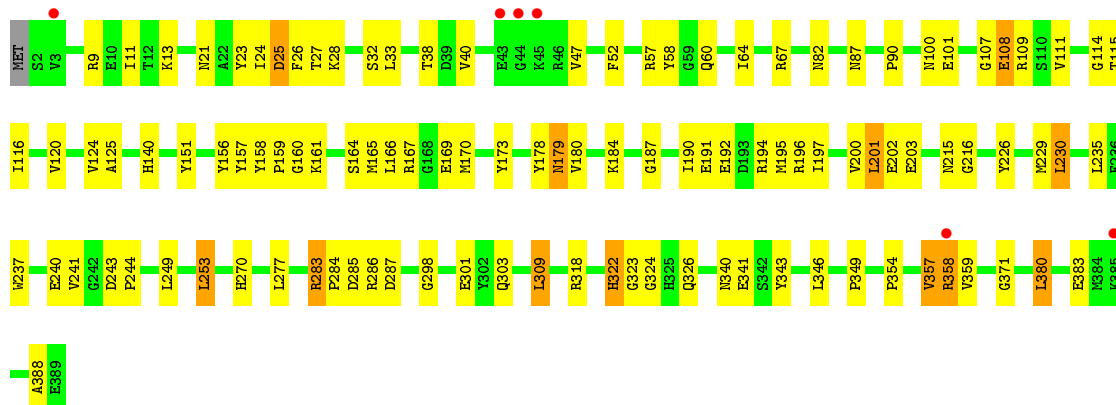




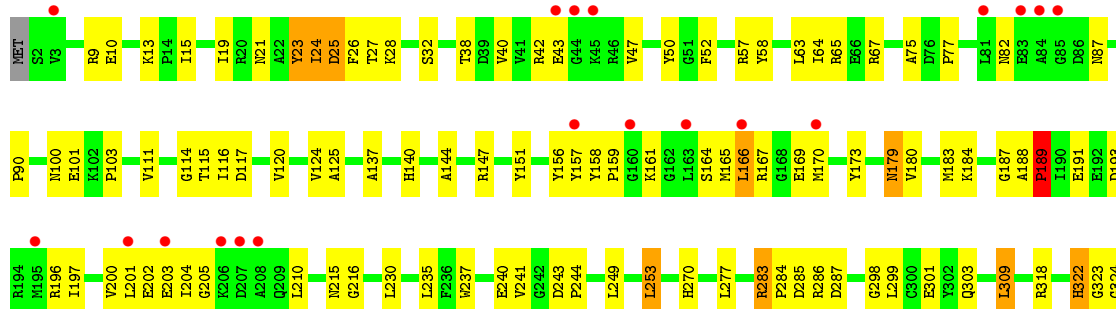
• Molecule 1: Bll6730 protein

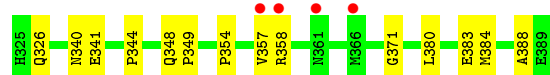


• Molecule 1: Bll6730 protein

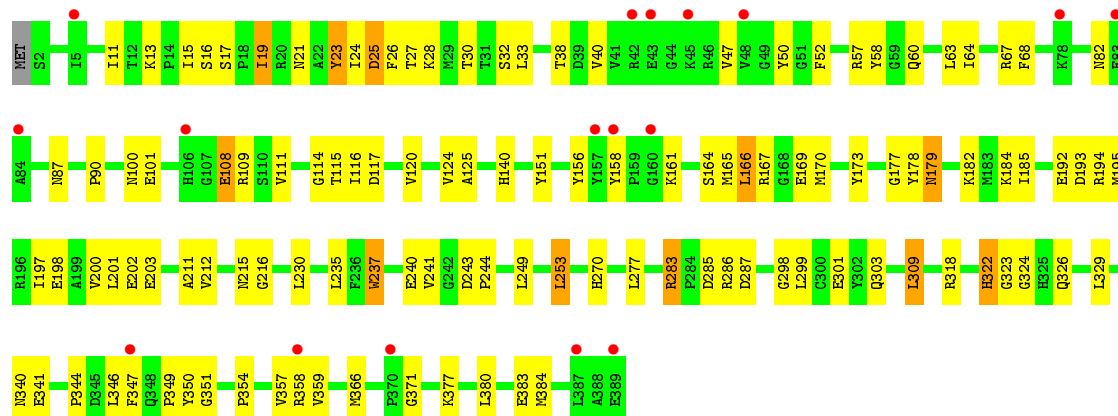


• Molecule 1: Bll6730 protein

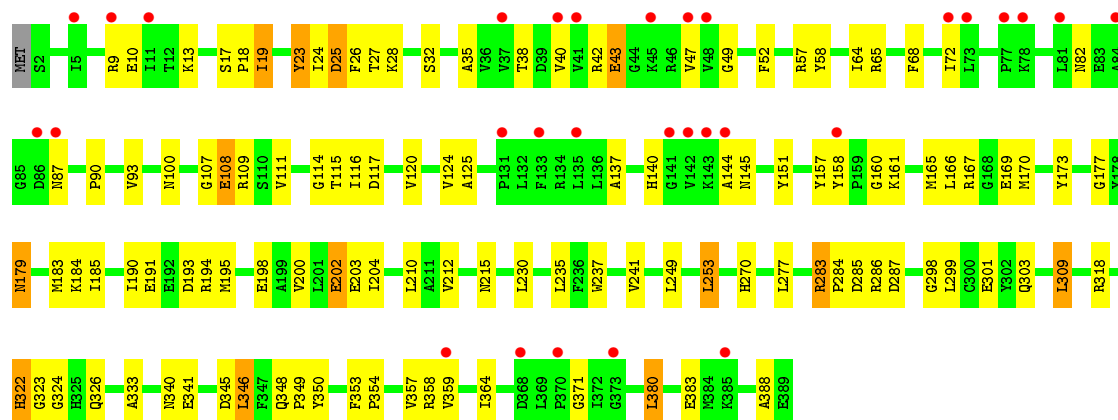




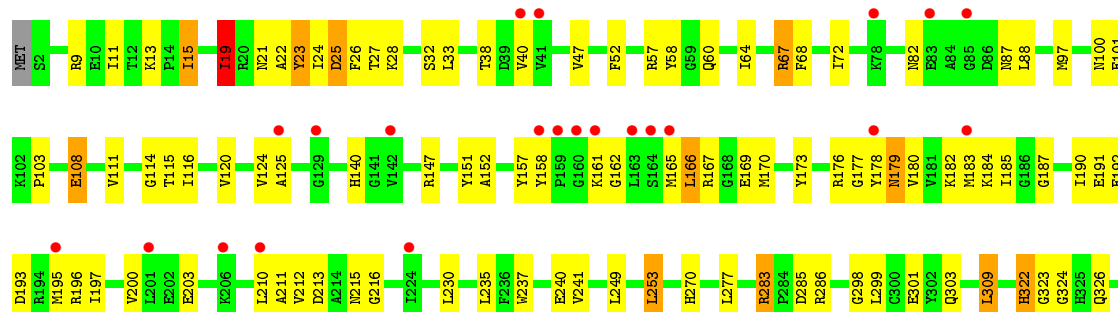
• Molecule 1: Bll6730 protein

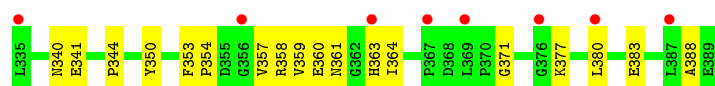


• Molecule 1: Bll6730 protein

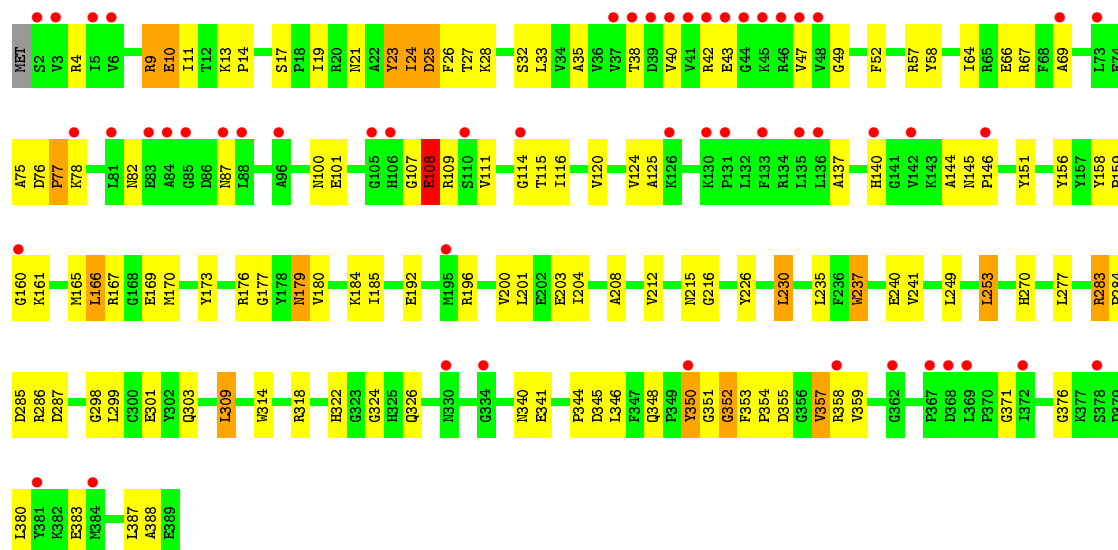


• Molecule 1: Bll6730 protein





● Molecule 1: Bll6730 protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	74.84Å 162.54Å 168.18Å 117.76° 90.03° 90.67°	Depositor
Resolution (Å)	25.00 – 2.50 39.39 – 2.49	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.50) 77.8 (39.39-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.48Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.241 , 0.265 0.238 , 0.261	Depositor DCC
R_{free} test set	11133 reflections (4.98%)	DCC
Wilson B-factor (Å ²)	35.4	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.7	EDS
Estimated twinning fraction	0.064 for h,-k,-l 0.016 for -h,k,-k-l 0.014 for -h,-k,k+l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 239187 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	48977	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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: MG, SRT

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	0.40	0/3092	0.63	0/4177
1	B	0.37	0/3092	0.61	0/4177
1	C	0.43	0/3092	0.64	0/4177
1	D	0.41	0/3092	0.64	0/4177
1	E	0.39	0/3092	0.62	0/4177
1	F	0.41	0/3092	0.64	0/4177
1	G	0.41	0/3092	0.63	0/4177
1	H	0.35	0/3092	0.61	0/4177
1	I	0.37	0/3092	0.62	0/4177
1	J	0.36	0/3092	0.61	0/4177
1	K	0.39	0/3092	0.62	0/4177
1	L	0.36	0/3092	0.61	0/4177
1	M	0.37	0/3092	0.60	0/4177
1	N	0.34	0/3092	0.61	0/4177
1	O	0.36	0/3092	0.61	0/4177
1	P	0.35	0/3092	0.60	0/4177
All	All	0.38	0/49472	0.62	0/66832

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

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	3022	0	2975	85	0
1	B	3022	0	2975	100	0
1	C	3022	0	2975	86	0
1	D	3022	0	2975	87	0
1	E	3022	0	2975	94	0
1	F	3022	0	2975	87	0
1	G	3022	0	2975	114	0
1	H	3022	0	2975	102	0
1	I	3022	0	2975	88	0
1	J	3022	0	2975	104	0
1	K	3022	0	2975	92	0
1	L	3022	0	2975	95	0
1	M	3022	0	2975	106	0
1	N	3022	0	2975	108	0
1	O	3022	0	2975	102	0
1	P	3022	0	2975	113	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
3	A	10	0	3	2	0
3	B	10	0	3	2	0
3	C	10	0	3	3	0
3	D	10	0	3	3	0
3	E	10	0	3	2	0
3	F	10	0	3	1	0
3	G	10	0	4	4	0
3	H	10	0	3	2	0
3	I	10	0	3	4	0
3	J	10	0	3	1	0
3	K	10	0	3	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	10	0	3	3	0
3	M	10	0	3	0	0
3	N	10	0	3	3	0
3	O	10	0	3	0	0
3	P	10	0	4	3	0
4	A	43	0	0	1	0
4	B	21	0	0	0	0
4	C	61	0	0	3	0
4	D	49	0	0	0	0
4	E	29	0	0	1	0
4	F	53	0	0	0	0
4	G	41	0	0	2	0
4	H	22	0	0	0	0
4	I	20	0	0	0	0
4	J	12	0	0	0	0
4	K	29	0	0	0	0
4	L	20	0	0	0	0
4	M	12	0	0	0	0
4	N	20	0	0	0	0
4	O	5	0	0	1	0
4	P	12	0	0	1	0
All	All	48977	0	47650	1472	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 15.

All (1472) 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:P:353:PHE:HB2	1:P:357:VAL:HG11	1.37	1.07
1:L:184:LYS:HE3	1:L:215:ASN:HD21	1.19	1.04
1:J:167:ARG:HD3	1:J:203:GLU:HB2	1.35	1.03
1:C:100:ASN:HA	1:D:24:ILE:HG13	1.37	1.03
1:C:24:ILE:HG13	1:D:100:ASN:HA	1.39	1.02
1:G:167:ARG:HD3	1:G:203:GLU:HB2	1.40	1.02
1:L:167:ARG:HD3	1:L:203:GLU:HB2	1.42	1.02
1:H:170:MET:HG3	1:H:200:VAL:HG13	1.46	0.97
1:G:100:ASN:HA	1:H:24:ILE:HG13	1.46	0.97
1:K:100:ASN:HA	1:L:24:ILE:HG13	1.48	0.96
1:G:24:ILE:HG13	1:H:100:ASN:HA	1.47	0.96
1:L:170:MET:HG3	1:L:200:VAL:HG13	1.49	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:167:ARG:HD3	1:O:203:GLU:HB2	1.50	0.94
1:N:167:ARG:HD3	1:N:203:GLU:HB2	1.48	0.94
1:F:167:ARG:HD3	1:F:203:GLU:HB2	1.49	0.94
1:H:184:LYS:HE3	1:H:215:ASN:HD21	1.34	0.92
1:P:9:ARG:HH12	1:P:388:ALA:HB2	1.34	0.92
1:M:24:ILE:HD12	1:N:100:ASN:HA	1.50	0.92
1:A:167:ARG:HD3	1:A:203:GLU:HB2	1.52	0.91
1:E:167:ARG:HD3	1:E:203:GLU:HB2	1.52	0.91
1:P:167:ARG:HD3	1:P:203:GLU:HB2	1.52	0.90
1:O:100:ASN:HA	1:P:24:ILE:HG13	1.54	0.89
1:E:100:ASN:HA	1:F:24:ILE:HG13	1.53	0.89
1:I:100:ASN:HA	1:J:24:ILE:HG13	1.55	0.89
1:M:100:ASN:HA	1:N:24:ILE:HG13	1.54	0.88
1:I:167:ARG:HD3	1:I:203:GLU:HB2	1.56	0.88
1:M:161:LYS:HA	1:M:165:MET:HE3	1.55	0.87
1:K:167:ARG:HD3	1:K:203:GLU:HB2	1.53	0.87
1:O:184:LYS:HD2	1:O:215:ASN:HD21	1.37	0.87
1:E:170:MET:HG3	1:E:200:VAL:HG13	1.56	0.87
1:K:24:ILE:HG13	1:L:100:ASN:HA	1.57	0.87
1:J:241:VAL:HG11	1:J:253:LEU:HD21	1.56	0.86
1:M:24:ILE:HG23	1:N:100:ASN:HA	1.58	0.86
1:C:241:VAL:HG11	1:C:253:LEU:HD21	1.57	0.86
1:E:241:VAL:HG11	1:E:253:LEU:HD21	1.58	0.85
1:H:241:VAL:HG11	1:H:253:LEU:HD21	1.57	0.85
1:J:170:MET:HG3	1:J:200:VAL:HG13	1.57	0.85
1:P:353:PHE:CB	1:P:357:VAL:HG11	2.07	0.85
1:O:13:LYS:NZ	1:O:383:GLU:HG3	1.92	0.84
1:K:241:VAL:HG11	1:K:253:LEU:HD21	1.58	0.84
1:A:184:LYS:HZ3	3:A:1001:SRT:H2	1.43	0.84
1:L:241:VAL:HG11	1:L:253:LEU:HD21	1.59	0.84
1:P:241:VAL:HG11	1:P:253:LEU:HD21	1.58	0.84
1:N:241:VAL:HG11	1:N:253:LEU:HD21	1.58	0.83
1:M:241:VAL:HG11	1:M:253:LEU:HD21	1.57	0.83
1:O:241:VAL:HG11	1:O:253:LEU:HD21	1.61	0.82
1:D:167:ARG:HD3	1:D:203:GLU:HB2	1.58	0.82
1:O:184:LYS:HD2	1:O:215:ASN:ND2	1.94	0.82
1:E:184:LYS:HZ3	3:E:1005:SRT:H2	1.45	0.81
1:B:13:LYS:NZ	1:B:383:GLU:HG3	1.95	0.81
1:B:241:VAL:HG11	1:B:253:LEU:HD21	1.62	0.81
1:I:241:VAL:HG11	1:I:253:LEU:HD21	1.61	0.81
1:F:241:VAL:HG11	1:F:253:LEU:HD21	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:241:VAL:HG11	1:D:253:LEU:HD21	1.62	0.81
1:N:18:PRO:HG2	1:N:158:TYR:CE1	2.16	0.81
1:G:4:ARG:NE	1:G:77:PRO:HG3	1.94	0.81
1:A:241:VAL:HG11	1:A:253:LEU:HD21	1.63	0.80
1:G:241:VAL:HG11	1:G:253:LEU:HD21	1.62	0.80
1:H:167:ARG:HD3	1:H:203:GLU:HB2	1.64	0.80
1:P:161:LYS:HA	1:P:165:MET:HE3	1.64	0.80
1:A:147:ARG:HH21	1:A:147:ARG:HG3	1.45	0.79
1:F:184:LYS:HE2	1:F:215:ASN:HD21	1.47	0.79
1:K:161:LYS:HA	1:K:165:MET:HE3	1.64	0.79
1:G:38:THR:OG1	1:G:47:VAL:HG13	1.83	0.79
1:D:167:ARG:NH2	1:D:202:GLU:HG2	1.97	0.79
1:O:161:LYS:HA	1:O:165:MET:HE3	1.66	0.78
1:M:184:LYS:HD2	1:M:215:ASN:HD21	1.48	0.78
1:N:38:THR:OG1	1:N:47:VAL:HG13	1.83	0.78
1:G:9:ARG:HD2	1:G:388:ALA:HB2	1.65	0.78
1:F:4:ARG:HG2	1:F:77:PRO:HB3	1.66	0.78
1:D:161:LYS:HA	1:D:165:MET:HE3	1.66	0.78
1:M:24:ILE:HD12	1:N:100:ASN:CA	2.13	0.77
1:E:354:PRO:HD2	1:E:357:VAL:HG11	1.65	0.77
1:N:354:PRO:O	1:N:357:VAL:HG12	1.84	0.77
1:B:4:ARG:HG3	1:B:77:PRO:HB3	1.65	0.77
1:A:24:ILE:HG13	1:B:100:ASN:HA	1.66	0.77
1:J:353:PHE:HB2	1:J:357:VAL:HG11	1.66	0.77
1:B:179:ASN:ND2	1:B:180:VAL:HG23	2.00	0.76
1:J:184:LYS:HZ1	3:J:1010:SRT:H2	1.50	0.76
1:C:167:ARG:HD3	1:C:203:GLU:HB2	1.67	0.76
1:G:161:LYS:HA	1:G:165:MET:HE3	1.68	0.76
1:P:184:LYS:NZ	3:P:1016:SRT:H2	2.00	0.76
1:F:161:LYS:HA	1:F:165:MET:HE3	1.67	0.76
1:L:161:LYS:HA	1:L:165:MET:HE3	1.67	0.76
1:O:11:ILE:HG23	1:O:33:LEU:HB3	1.68	0.76
1:P:9:ARG:NH1	1:P:388:ALA:HB2	2.01	0.75
1:C:184:LYS:NZ	3:C:1003:SRT:H2	2.02	0.75
1:M:11:ILE:HG23	1:M:33:LEU:HB3	1.68	0.75
1:B:161:LYS:HA	1:B:165:MET:HE3	1.66	0.75
1:I:161:LYS:HA	1:I:165:MET:HE3	1.67	0.75
1:O:170:MET:HG3	1:O:200:VAL:HG13	1.67	0.75
1:H:11:ILE:HG23	1:H:33:LEU:HB3	1.67	0.75
1:I:65:ARG:HH11	1:I:65:ARG:HG3	1.51	0.75
1:J:161:LYS:HA	1:J:165:MET:HE3	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:161:LYS:HA	1:N:165:MET:HE3	1.67	0.75
1:C:100:ASN:HA	1:D:24:ILE:CG1	2.13	0.75
1:O:24:ILE:HG13	1:P:100:ASN:HA	1.69	0.75
1:E:140:HIS:HE1	1:E:303:GLN:NE2	1.85	0.75
1:A:184:LYS:NZ	3:A:1001:SRT:H2	2.01	0.75
1:M:184:LYS:HD2	1:M:215:ASN:ND2	2.02	0.75
1:P:38:THR:OG1	1:P:47:VAL:HG13	1.87	0.74
1:E:184:LYS:NZ	3:E:1005:SRT:H2	2.03	0.74
1:F:140:HIS:HE1	1:F:303:GLN:NE2	1.85	0.74
1:D:179:ASN:H	1:D:179:ASN:HD22	1.35	0.74
1:N:10:GLU:HB3	1:N:65:ARG:HH12	1.52	0.74
1:J:140:HIS:HE1	1:J:303:GLN:NE2	1.86	0.74
1:A:161:LYS:HA	1:A:165:MET:HE3	1.70	0.74
1:G:19:ILE:HG13	1:G:156:TYR:CG	2.23	0.74
1:I:140:HIS:HE1	1:I:303:GLN:NE2	1.85	0.74
1:M:170:MET:HG3	1:M:200:VAL:HG13	1.70	0.74
1:D:140:HIS:HE1	1:D:303:GLN:NE2	1.86	0.74
1:K:38:THR:OG1	1:K:47:VAL:HG13	1.87	0.74
1:P:170:MET:HG3	1:P:200:VAL:HG13	1.70	0.73
1:G:354:PRO:O	1:G:357:VAL:HG12	1.87	0.73
1:C:38:THR:OG1	1:C:47:VAL:HG13	1.89	0.73
1:J:353:PHE:CB	1:J:357:VAL:HG11	2.19	0.73
1:L:184:LYS:NZ	3:L:1012:SRT:H2	2.03	0.73
1:H:161:LYS:HA	1:H:165:MET:HE3	1.69	0.73
1:B:167:ARG:HD3	1:B:203:GLU:HB2	1.70	0.72
1:H:170:MET:HG3	1:H:200:VAL:CG1	2.19	0.72
1:N:170:MET:HG3	1:N:200:VAL:HG13	1.70	0.72
1:C:140:HIS:HE1	1:C:303:GLN:NE2	1.89	0.71
1:A:284:PRO:HG3	1:K:284:PRO:HG3	1.72	0.71
1:N:184:LYS:NZ	3:N:1014:SRT:H2	2.05	0.71
1:H:38:THR:OG1	1:H:47:VAL:HG13	1.90	0.71
1:D:184:LYS:NZ	3:D:1004:SRT:H2	2.05	0.71
1:C:161:LYS:HA	1:C:165:MET:HE3	1.70	0.71
1:B:38:THR:OG1	1:B:47:VAL:HG13	1.91	0.71
1:E:161:LYS:HA	1:E:165:MET:HE3	1.72	0.71
1:F:23:TYR:O	1:F:24:ILE:HD12	1.91	0.71
1:E:145:ASN:HD22	1:E:145:ASN:C	1.94	0.71
1:M:140:HIS:HE1	1:M:303:GLN:NE2	1.89	0.71
1:F:38:THR:OG1	1:F:47:VAL:HG13	1.91	0.70
1:K:140:HIS:HE1	1:K:303:GLN:NE2	1.90	0.70
1:A:140:HIS:HE1	1:A:303:GLN:NE2	1.89	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:152:ALA:HB3	1:G:181:VAL:HG12	1.73	0.70
1:F:195:MET:HG2	1:G:163:LEU:HG	1.74	0.70
1:N:65:ARG:HG3	1:N:65:ARG:HH11	1.56	0.70
1:G:19:ILE:HG22	1:G:26:PHE:HB2	1.72	0.70
1:O:13:LYS:HZ2	1:O:383:GLU:HG3	1.57	0.70
1:B:140:HIS:HE1	1:B:303:GLN:NE2	1.89	0.70
1:D:38:THR:OG1	1:D:47:VAL:HG13	1.91	0.70
1:J:183:MET:HG2	1:J:210:LEU:HD11	1.73	0.70
1:C:354:PRO:HG2	1:C:357:VAL:HG11	1.73	0.69
1:O:38:THR:OG1	1:O:47:VAL:HG13	1.91	0.69
1:C:24:ILE:HG13	1:D:100:ASN:CA	2.21	0.69
1:I:11:ILE:HG23	1:I:33:LEU:HB3	1.74	0.69
1:D:140:HIS:HE1	1:D:303:GLN:HE21	1.40	0.69
1:K:9:ARG:HD2	1:K:388:ALA:HB2	1.73	0.69
1:O:140:HIS:HE1	1:O:303:GLN:NE2	1.90	0.69
1:H:140:HIS:HE1	1:H:303:GLN:NE2	1.90	0.69
1:L:348:GLN:HE21	1:L:349:PRO:HA	1.58	0.69
1:O:151:TYR:HE1	1:O:182:LYS:HE2	1.56	0.69
1:J:359:VAL:HG22	1:J:364:ILE:HG22	1.74	0.68
1:D:185:ILE:HD13	1:D:212:VAL:HB	1.74	0.68
1:F:167:ARG:HH22	1:G:167:ARG:HH22	1.41	0.68
1:O:185:ILE:HD13	1:O:212:VAL:HB	1.75	0.68
1:M:167:ARG:HD3	1:M:203:GLU:HB2	1.76	0.68
1:A:368:ASP:OD2	1:J:379:ASP:HB3	1.93	0.68
1:J:193:ASP:O	1:J:197:ILE:HG13	1.93	0.68
1:F:167:ARG:NH2	1:G:167:ARG:HH22	1.91	0.68
1:I:354:PRO:O	1:I:357:VAL:HG12	1.94	0.68
1:L:184:LYS:HZ1	3:L:1012:SRT:H2	1.58	0.68
1:D:193:ASP:O	1:D:197:ILE:HG13	1.94	0.68
1:G:140:HIS:HE1	1:G:303:GLN:NE2	1.92	0.68
1:J:38:THR:OG1	1:J:47:VAL:HG13	1.94	0.68
1:G:4:ARG:HG3	1:G:77:PRO:HB3	1.75	0.68
1:K:67:ARG:HD3	1:K:101:GLU:OE2	1.94	0.67
1:C:179:ASN:HD22	1:C:179:ASN:H	1.43	0.67
1:M:38:THR:OG1	1:M:47:VAL:HG13	1.94	0.67
1:O:184:LYS:CD	1:O:215:ASN:HD21	2.07	0.67
1:E:354:PRO:O	1:E:357:VAL:HG12	1.94	0.67
1:K:179:ASN:HD22	1:K:180:VAL:HG23	1.59	0.67
1:I:277:LEU:HD11	1:I:309:LEU:HD22	1.77	0.67
1:P:177:GLY:O	1:P:359:VAL:HG12	1.94	0.67
1:N:140:HIS:HE1	1:N:303:GLN:NE2	1.92	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:277:LEU:HD11	1:C:309:LEU:HD22	1.77	0.67
1:N:137:ALA:HB2	1:N:144:ALA:HB2	1.77	0.67
1:B:170:MET:HG3	1:B:200:VAL:HG13	1.75	0.67
1:H:270:HIS:HD2	1:H:301:GLU:OE2	1.78	0.67
1:H:354:PRO:O	1:H:357:VAL:HG12	1.95	0.67
1:B:19:ILE:CD1	1:B:346:LEU:HD21	2.25	0.67
1:I:184:LYS:NZ	3:I:1009:SRT:H2	2.09	0.67
1:H:9:ARG:HG3	1:H:388:ALA:HB2	1.77	0.66
1:J:277:LEU:HD11	1:J:309:LEU:HD22	1.77	0.66
1:F:170:MET:HG3	1:F:200:VAL:HG13	1.76	0.66
1:O:178:TYR:CD1	1:O:359:VAL:HG11	2.30	0.66
1:J:353:PHE:HB2	1:J:357:VAL:CG1	2.24	0.66
1:H:324:GLY:HA2	1:H:341:GLU:O	1.95	0.66
1:G:277:LEU:HD11	1:G:309:LEU:HD22	1.78	0.66
1:E:270:HIS:HD2	1:E:301:GLU:OE2	1.77	0.66
1:I:270:HIS:HD2	1:I:301:GLU:OE2	1.79	0.66
1:K:277:LEU:HD11	1:K:309:LEU:HD22	1.78	0.66
1:B:277:LEU:HD11	1:B:309:LEU:HD22	1.78	0.66
1:O:9:ARG:HD2	1:O:388:ALA:HB2	1.77	0.66
1:E:21:ASN:HB2	1:E:215:ASN:ND2	2.10	0.66
1:G:4:ARG:CZ	1:G:77:PRO:HG3	2.25	0.66
1:M:184:LYS:CD	1:M:215:ASN:HD21	2.07	0.66
1:M:324:GLY:HA2	1:M:341:GLU:O	1.96	0.66
1:J:359:VAL:HG22	1:J:364:ILE:CG2	2.26	0.66
1:P:107:GLY:O	1:P:108:GLU:HB2	1.95	0.66
1:J:72:ILE:HD11	1:J:97:MET:HB3	1.76	0.66
1:P:177:GLY:HA3	1:P:359:VAL:O	1.97	0.65
1:F:277:LEU:HD11	1:F:309:LEU:HD22	1.78	0.65
1:M:179:ASN:H	1:M:179:ASN:HD22	1.44	0.65
1:P:324:GLY:HA2	1:P:341:GLU:O	1.96	0.65
1:E:277:LEU:HD11	1:E:309:LEU:HD22	1.77	0.65
1:L:277:LEU:HD11	1:L:309:LEU:HD22	1.77	0.65
1:O:277:LEU:HD11	1:O:309:LEU:HD22	1.77	0.65
1:M:277:LEU:HD11	1:M:309:LEU:HD22	1.77	0.65
1:G:324:GLY:HA2	1:G:341:GLU:O	1.96	0.64
1:N:324:GLY:HA2	1:N:341:GLU:O	1.97	0.64
1:H:140:HIS:HE1	1:H:303:GLN:HE21	1.46	0.64
1:E:324:GLY:HA2	1:E:341:GLU:O	1.97	0.64
1:J:11:ILE:CG2	1:J:33:LEU:HB3	2.27	0.64
1:L:173:TYR:CE1	1:L:344:PRO:HG2	2.32	0.64
1:C:170:MET:HG3	1:C:200:VAL:HG13	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:107:GLY:O	1:F:109:ARG:N	2.30	0.64
1:O:108:GLU:OE2	1:P:109:ARG:HB3	1.98	0.64
1:G:167:ARG:NH2	1:G:202:GLU:HG2	2.13	0.64
1:B:140:HIS:HE1	1:B:303:GLN:HE21	1.45	0.64
1:D:270:HIS:HD2	1:D:301:GLU:OE2	1.81	0.64
1:E:13:LYS:HE3	1:E:383:GLU:HG3	1.80	0.64
1:P:140:HIS:HE1	1:P:303:GLN:NE2	1.95	0.64
1:A:354:PRO:HD2	1:A:357:VAL:HG11	1.79	0.64
1:N:190:ILE:HG23	1:N:191:GLU:N	2.12	0.64
1:E:170:MET:HG3	1:E:200:VAL:CG1	2.27	0.64
1:P:192:GLU:O	1:P:196:ARG:HG3	1.98	0.64
1:D:184:LYS:HZ2	3:D:1004:SRT:H2	1.61	0.64
1:A:324:GLY:HA2	1:A:341:GLU:O	1.98	0.64
1:M:23:TYR:O	1:M:24:ILE:HD13	1.97	0.64
1:B:157:TYR:CE2	1:B:187:GLY:HA3	2.32	0.64
1:D:358:ARG:NH1	1:D:358:ARG:HB3	2.12	0.64
1:O:324:GLY:HA2	1:O:341:GLU:O	1.98	0.63
1:B:9:ARG:HD2	1:B:388:ALA:HB2	1.80	0.63
1:N:349:PRO:O	1:N:380:LEU:HG	1.97	0.63
1:L:270:HIS:HD2	1:L:301:GLU:OE2	1.80	0.63
1:P:270:HIS:HD2	1:P:301:GLU:OE2	1.80	0.63
1:D:277:LEU:HD11	1:D:309:LEU:HD22	1.81	0.63
1:A:277:LEU:HD11	1:A:309:LEU:HD22	1.80	0.63
1:K:111:VAL:O	1:K:115:THR:HG22	1.98	0.63
1:P:277:LEU:HD11	1:P:309:LEU:HD22	1.78	0.63
1:C:101:GLU:N	1:D:24:ILE:HD11	2.12	0.63
1:M:24:ILE:HG23	1:N:100:ASN:CA	2.28	0.63
1:D:324:GLY:HA2	1:D:341:GLU:O	1.97	0.63
1:J:177:GLY:O	1:J:359:VAL:HG12	1.98	0.63
1:E:64:ILE:HG23	1:E:116:ILE:HD11	1.81	0.63
1:A:38:THR:OG1	1:A:47:VAL:HG13	1.99	0.63
1:L:140:HIS:HE1	1:L:303:GLN:NE2	1.96	0.63
1:P:179:ASN:H	1:P:179:ASN:HD22	1.45	0.63
1:P:4:ARG:HG3	1:P:77:PRO:HG3	1.81	0.63
1:N:277:LEU:HD11	1:N:309:LEU:HD22	1.79	0.63
1:D:11:ILE:CG2	1:D:33:LEU:HB3	2.28	0.63
1:F:196:ARG:O	1:F:200:VAL:HG23	1.98	0.63
1:N:183:MET:HG2	1:N:210:LEU:HD11	1.80	0.63
1:J:111:VAL:O	1:J:115:THR:HG22	1.98	0.63
1:F:270:HIS:HD2	1:F:301:GLU:OE2	1.81	0.63
1:E:358:ARG:HB3	1:E:358:ARG:NH1	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:167:ARG:NH2	1:G:167:ARG:NH2	2.46	0.63
1:B:270:HIS:HD2	1:B:301:GLU:OE2	1.82	0.63
1:H:111:VAL:O	1:H:115:THR:HG22	1.97	0.63
1:P:23:TYR:O	1:P:24:ILE:HD12	1.99	0.62
1:M:19:ILE:HD12	1:M:346:LEU:HD21	1.81	0.62
1:K:179:ASN:ND2	1:K:180:VAL:HG23	2.13	0.62
1:O:270:HIS:HD2	1:O:301:GLU:OE2	1.80	0.62
1:B:324:GLY:HA2	1:B:341:GLU:O	1.99	0.62
1:B:197:ILE:O	1:B:201:LEU:HD23	1.99	0.62
1:O:11:ILE:CG2	1:O:33:LEU:HB3	2.30	0.62
1:I:140:HIS:HE1	1:I:303:GLN:HE21	1.47	0.62
1:L:38:THR:OG1	1:L:47:VAL:HG13	1.99	0.62
1:M:270:HIS:HD2	1:M:301:GLU:OE2	1.82	0.62
1:B:40:VAL:O	1:B:47:VAL:HG12	2.00	0.62
1:O:183:MET:HG2	1:O:210:LEU:HD11	1.80	0.62
1:K:156:TYR:HA	1:K:184:LYS:HG3	1.82	0.62
1:F:111:VAL:O	1:F:115:THR:HG22	1.99	0.62
1:D:11:ILE:HG23	1:D:33:LEU:HB3	1.80	0.62
1:A:270:HIS:HD2	1:A:301:GLU:OE2	1.83	0.62
1:E:140:HIS:HE1	1:E:303:GLN:HE21	1.47	0.61
1:K:184:LYS:NZ	3:K:1011:SRT:H2	2.15	0.61
1:H:277:LEU:HD11	1:H:309:LEU:HD22	1.81	0.61
1:C:270:HIS:HD2	1:C:301:GLU:OE2	1.83	0.61
1:A:19:ILE:HD13	1:A:346:LEU:HD23	1.81	0.61
1:I:324:GLY:HA2	1:I:341:GLU:O	1.99	0.61
1:D:40:VAL:O	1:D:47:VAL:HG12	2.00	0.61
1:A:147:ARG:NH2	1:A:147:ARG:HG3	2.15	0.61
1:F:64:ILE:HG23	1:F:116:ILE:HD11	1.82	0.61
1:B:177:GLY:HA3	1:B:359:VAL:O	2.00	0.61
1:N:270:HIS:HD2	1:N:301:GLU:OE2	1.82	0.61
1:A:170:MET:HG3	1:A:200:VAL:HG13	1.82	0.61
1:L:166:LEU:HD22	1:L:200:VAL:CG2	2.30	0.61
1:D:199:ALA:O	1:D:202:GLU:HB3	2.00	0.61
1:M:151:TYR:CZ	1:M:341:GLU:HG3	2.35	0.61
1:K:196:ARG:O	1:K:200:VAL:HG23	2.00	0.61
1:B:156:TYR:HA	1:B:184:LYS:HG3	1.81	0.61
1:P:137:ALA:HB2	1:P:144:ALA:HB2	1.81	0.61
1:G:4:ARG:HE	1:G:77:PRO:HG3	1.63	0.61
1:K:170:MET:HG3	1:K:200:VAL:HG13	1.82	0.61
1:J:270:HIS:HD2	1:J:301:GLU:OE2	1.83	0.61
1:O:21:ASN:HB2	1:O:215:ASN:ND2	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:11:ILE:CG2	1:M:33:LEU:HB3	2.31	0.61
1:B:13:LYS:HZ3	1:B:383:GLU:HG3	1.66	0.60
1:C:111:VAL:O	1:C:115:THR:HG22	2.00	0.60
1:L:324:GLY:HA2	1:L:341:GLU:O	2.00	0.60
1:A:64:ILE:HG23	1:A:116:ILE:HD11	1.81	0.60
1:M:140:HIS:HE1	1:M:303:GLN:HE21	1.49	0.60
1:J:324:GLY:HA2	1:J:341:GLU:O	2.01	0.60
1:L:21:ASN:HB2	1:L:215:ASN:ND2	2.17	0.60
1:J:354:PRO:O	1:J:357:VAL:HG12	2.01	0.60
1:L:125:ALA:HB3	1:L:371:GLY:HA2	1.82	0.60
1:C:354:PRO:HG2	1:C:357:VAL:CG1	2.31	0.60
1:C:196:ARG:O	1:C:200:VAL:HG23	2.02	0.60
1:I:21:ASN:HB2	1:I:215:ASN:ND2	2.16	0.60
1:C:157:TYR:CE2	1:C:187:GLY:HA3	2.35	0.60
1:I:157:TYR:CE2	1:I:187:GLY:HA3	2.37	0.60
1:N:9:ARG:HD2	1:N:388:ALA:HB2	1.83	0.60
1:N:23:TYR:O	1:N:24:ILE:HD12	2.01	0.60
1:C:40:VAL:O	1:C:47:VAL:HG12	2.02	0.60
1:O:111:VAL:O	1:O:115:THR:HG22	2.00	0.60
1:C:140:HIS:HE1	1:C:303:GLN:HE21	1.48	0.60
1:M:354:PRO:O	1:M:357:VAL:HG13	2.00	0.60
1:O:13:LYS:HG3	1:O:350:TYR:OH	2.02	0.60
1:B:19:ILE:HD12	1:B:346:LEU:HD21	1.83	0.60
1:C:324:GLY:HA2	1:C:341:GLU:O	2.01	0.60
1:J:140:HIS:HE1	1:J:303:GLN:HE21	1.48	0.60
1:F:140:HIS:HE1	1:F:303:GLN:HE21	1.50	0.59
1:F:11:ILE:HG23	1:F:33:LEU:HB3	1.82	0.59
1:O:13:LYS:HZ3	1:O:383:GLU:HG3	1.67	0.59
1:N:359:VAL:HG22	1:N:364:ILE:CG2	2.32	0.59
1:E:179:ASN:ND2	1:E:179:ASN:H	2.00	0.59
1:O:192:GLU:O	1:O:196:ARG:HG3	2.03	0.59
1:J:125:ALA:HB3	1:J:371:GLY:HA2	1.83	0.59
1:M:358:ARG:HB3	1:M:358:ARG:NH1	2.16	0.59
1:G:270:HIS:HD2	1:G:301:GLU:OE2	1.85	0.59
1:I:111:VAL:O	1:I:115:THR:HG22	2.02	0.59
1:M:63:LEU:HD22	1:M:67:ARG:HH21	1.66	0.59
1:A:197:ILE:HG22	1:A:201:LEU:HD22	1.85	0.59
1:I:23:TYR:C	1:I:24:ILE:HD12	2.22	0.59
1:P:32:SER:O	1:P:52:PHE:HA	2.03	0.59
1:C:184:LYS:HZ2	3:C:1003:SRT:H2	1.66	0.59
1:C:19:ILE:HG23	1:C:156:TYR:CD1	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:193:ASP:O	1:L:197:ILE:HG13	2.01	0.59
1:B:11:ILE:HG23	1:B:33:LEU:HB3	1.83	0.59
1:N:32:SER:O	1:N:52:PHE:HA	2.03	0.59
1:F:18:PRO:HG2	1:F:158:TYR:CE1	2.37	0.59
1:O:152:ALA:HB2	1:O:178:TYR:CD2	2.37	0.59
1:P:125:ALA:HB3	1:P:371:GLY:HA2	1.85	0.59
1:G:101:GLU:N	1:H:24:ILE:HD11	2.18	0.58
1:P:156:TYR:CE1	1:P:184:LYS:HE2	2.38	0.58
1:P:179:ASN:H	1:P:179:ASN:ND2	2.01	0.58
1:J:64:ILE:HG23	1:J:116:ILE:HD11	1.85	0.58
1:M:194:ARG:O	1:M:198:GLU:HG3	2.03	0.58
1:L:183:MET:HG2	1:L:210:LEU:HD11	1.85	0.58
1:J:185:ILE:HD13	1:J:212:VAL:HB	1.85	0.58
1:K:354:PRO:HD2	1:K:357:VAL:HG11	1.84	0.58
1:O:100:ASN:HA	1:P:24:ILE:CG1	2.31	0.58
1:E:103:PRO:HD3	1:F:23:TYR:CD2	2.38	0.58
1:H:10:GLU:CG	1:H:65:ARG:HH12	2.17	0.58
1:I:67:ARG:HD3	1:I:101:GLU:OE2	2.03	0.58
1:H:125:ALA:HB3	1:H:371:GLY:HA2	1.84	0.58
1:N:72:ILE:HD12	1:N:93:VAL:HG13	1.85	0.58
1:A:27:THR:HG22	1:A:28:LYS:HG2	1.86	0.58
1:O:178:TYR:CE2	1:O:344:PRO:HG2	2.39	0.58
1:N:107:GLY:O	1:N:108:GLU:HB2	2.02	0.58
1:G:340:ASN:ND2	1:G:341:GLU:H	2.01	0.58
1:N:151:TYR:CZ	1:N:341:GLU:HG3	2.38	0.58
1:J:11:ILE:HG23	1:J:33:LEU:HB3	1.83	0.58
1:F:11:ILE:CG2	1:F:387:LEU:HD13	2.34	0.58
1:A:157:TYR:CE2	1:A:187:GLY:HA3	2.39	0.58
1:M:64:ILE:HG23	1:M:116:ILE:HD11	1.86	0.58
1:I:100:ASN:CA	1:J:24:ILE:HG13	2.32	0.58
1:E:19:ILE:HG23	1:E:156:TYR:CD1	2.39	0.58
1:K:140:HIS:HE1	1:K:303:GLN:HE21	1.51	0.58
1:I:11:ILE:CG2	1:I:33:LEU:HB3	2.33	0.58
1:A:102:LYS:HG3	1:B:24:ILE:HD13	1.84	0.58
1:I:184:LYS:HZ2	3:I:1009:SRT:H2	1.68	0.58
1:B:151:TYR:CZ	1:B:341:GLU:HG3	2.39	0.58
1:M:108:GLU:OE1	1:N:109:ARG:HB3	2.04	0.58
1:E:145:ASN:ND2	1:E:147:ARG:H	2.01	0.58
1:G:151:TYR:CZ	1:G:341:GLU:HG3	2.39	0.58
1:D:151:TYR:CZ	1:D:341:GLU:HG3	2.39	0.58
1:F:324:GLY:HA2	1:F:341:GLU:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:157:TYR:CE2	1:L:187:GLY:HA3	2.39	0.58
1:C:23:TYR:O	1:C:24:ILE:HD12	2.04	0.57
1:I:64:ILE:HG23	1:I:116:ILE:HD11	1.86	0.57
1:G:24:ILE:HG13	1:H:100:ASN:CA	2.30	0.57
1:E:38:THR:OG1	1:E:47:VAL:HG13	2.04	0.57
1:K:270:HIS:HD2	1:K:301:GLU:OE2	1.85	0.57
1:O:32:SER:O	1:O:52:PHE:HA	2.04	0.57
1:P:111:VAL:O	1:P:115:THR:HG22	2.04	0.57
1:L:9:ARG:HH21	1:L:388:ALA:HA	1.68	0.57
1:N:184:LYS:HZ2	3:N:1014:SRT:H2	1.68	0.57
1:L:64:ILE:HG23	1:L:116:ILE:HD11	1.87	0.57
1:H:197:ILE:O	1:H:201:LEU:HB2	2.05	0.57
1:L:166:LEU:HD22	1:L:200:VAL:HG22	1.85	0.57
1:D:140:HIS:CE1	1:D:303:GLN:HE21	2.22	0.57
1:O:58:TYR:HB2	1:P:67:ARG:NH2	2.19	0.57
1:O:196:ARG:O	1:O:200:VAL:HG23	2.05	0.57
1:J:360:GLU:O	1:J:361:ASN:HB2	2.05	0.57
1:K:324:GLY:HA2	1:K:341:GLU:O	2.03	0.57
1:H:72:ILE:HD12	1:H:93:VAL:HG13	1.86	0.57
1:M:67:ARG:NH1	1:N:58:TYR:CD2	2.73	0.57
1:B:111:VAL:O	1:B:115:THR:HG22	2.03	0.57
1:P:184:LYS:HZ1	3:P:1016:SRT:H2	1.68	0.57
1:P:151:TYR:CZ	1:P:341:GLU:HG3	2.39	0.57
1:D:111:VAL:O	1:D:115:THR:HG22	2.04	0.57
1:N:111:VAL:O	1:N:115:THR:HG22	2.05	0.57
1:A:111:VAL:O	1:A:115:THR:HG22	2.04	0.57
1:P:27:THR:HG21	4:P:2028:HOH:O	2.03	0.57
1:F:24:ILE:HG23	1:F:25:ASP:N	2.20	0.57
1:P:184:LYS:HZ3	3:P:1016:SRT:H2	1.69	0.57
1:L:354:PRO:HD2	1:L:357:VAL:HG11	1.86	0.56
1:O:178:TYR:CE1	1:O:359:VAL:HG11	2.39	0.56
1:E:71:ARG:HH12	1:E:101:GLU:HG2	1.70	0.56
1:E:179:ASN:HD22	1:E:179:ASN:H	1.53	0.56
1:C:57:ARG:O	1:C:58:TYR:HB2	2.04	0.56
1:J:7:ASP:OD2	1:J:8:VAL:N	2.39	0.56
1:M:185:ILE:HD13	1:M:212:VAL:HB	1.87	0.56
1:G:157:TYR:CE2	1:G:187:GLY:HA3	2.40	0.56
1:L:111:VAL:O	1:L:115:THR:HG22	2.05	0.56
1:M:111:VAL:O	1:M:115:THR:HG22	2.05	0.56
1:G:111:VAL:O	1:G:115:THR:HG22	2.05	0.56
1:K:358:ARG:HG3	1:K:358:ARG:HH11	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:ASN:CA	1:D:24:ILE:HG13	2.25	0.56
1:B:340:ASN:ND2	1:B:341:GLU:H	2.04	0.56
1:E:111:VAL:O	1:E:115:THR:HG22	2.05	0.56
1:F:13:LYS:HE3	1:F:383:GLU:HG3	1.88	0.56
1:J:194:ARG:NH1	1:J:233:TYR:OH	2.38	0.56
1:I:151:TYR:CZ	1:I:341:GLU:HG3	2.41	0.56
1:G:10:GLU:HG3	1:G:61:GLY:HA2	1.87	0.56
1:F:140:HIS:CE1	1:F:303:GLN:NE2	2.72	0.56
1:D:179:ASN:H	1:D:179:ASN:ND2	2.00	0.56
1:C:354:PRO:O	1:C:357:VAL:HG13	2.06	0.56
1:O:177:GLY:HA3	1:O:359:VAL:O	2.06	0.56
1:I:23:TYR:HB3	1:I:24:ILE:HD12	1.88	0.56
1:N:27:THR:HG22	1:N:28:LYS:HG2	1.88	0.56
1:L:23:TYR:O	1:L:24:ILE:HD12	2.06	0.56
1:P:140:HIS:HE1	1:P:303:GLN:HE21	1.54	0.56
1:B:178:TYR:CZ	1:B:359:VAL:HG21	2.41	0.56
1:M:125:ALA:HB3	1:M:371:GLY:HA2	1.88	0.56
1:N:40:VAL:O	1:N:47:VAL:HG12	2.06	0.56
1:O:23:TYR:O	1:O:24:ILE:HD12	2.06	0.56
1:E:145:ASN:HD22	1:E:147:ARG:H	1.51	0.56
1:F:32:SER:O	1:F:52:PHE:HA	2.07	0.56
1:A:125:ALA:HB3	1:A:371:GLY:HA2	1.88	0.56
1:G:70:SER:O	1:G:74:GLU:HG3	2.06	0.56
1:D:57:ARG:O	1:D:58:TYR:HB2	2.06	0.55
1:D:170:MET:HG3	1:D:200:VAL:HG13	1.88	0.55
1:I:107:GLY:O	1:I:108:GLU:HB2	2.05	0.55
1:F:27:THR:HG22	1:F:28:LYS:HG2	1.89	0.55
1:D:354:PRO:HD2	1:D:357:VAL:HG21	1.88	0.55
1:C:64:ILE:HG23	1:C:116:ILE:HD11	1.88	0.55
1:K:32:SER:O	1:K:52:PHE:HA	2.07	0.55
1:P:185:ILE:HD13	1:P:212:VAL:HB	1.89	0.55
1:P:11:ILE:HG23	1:P:33:LEU:HB3	1.88	0.55
1:N:184:LYS:HD2	1:N:215:ASN:HD21	1.71	0.55
1:N:125:ALA:HB3	1:N:371:GLY:HA2	1.88	0.55
1:A:32:SER:O	1:A:52:PHE:HA	2.07	0.55
1:C:179:ASN:ND2	1:C:179:ASN:H	2.02	0.55
1:E:285:ASP:OD1	1:E:286:ARG:HG2	2.06	0.55
1:J:177:GLY:HA3	1:J:359:VAL:O	2.07	0.55
1:P:27:THR:HG22	1:P:28:LYS:HG2	1.88	0.55
1:J:27:THR:HG22	1:J:28:LYS:HG2	1.88	0.55
1:G:27:THR:HG22	1:G:28:LYS:HG2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:24:ILE:HG23	1:H:25:ASP:N	2.22	0.55
1:K:167:ARG:NH2	1:K:202:GLU:HG2	2.22	0.55
1:K:125:ALA:HB3	1:K:371:GLY:HA2	1.89	0.55
1:L:19:ILE:HG23	1:L:156:TYR:CD1	2.42	0.55
1:N:190:ILE:HG23	1:N:191:GLU:H	1.72	0.55
1:H:90:PRO:HG3	1:H:124:VAL:HG21	1.89	0.55
1:J:13:LYS:HE3	1:J:383:GLU:HG3	1.87	0.55
1:H:173:TYR:CE1	1:H:344:PRO:HG2	2.42	0.55
1:B:285:ASP:OD1	1:B:286:ARG:HG2	2.07	0.55
1:J:32:SER:O	1:J:52:PHE:HA	2.07	0.55
1:H:191:GLU:OE2	1:H:191:GLU:HA	2.06	0.55
1:O:40:VAL:O	1:O:47:VAL:HG12	2.06	0.55
1:D:27:THR:HG22	1:D:28:LYS:HG2	1.88	0.55
1:N:345:ASP:C	1:N:346:LEU:HD12	2.27	0.55
1:N:140:HIS:HE1	1:N:303:GLN:HE21	1.55	0.54
1:M:340:ASN:ND2	1:M:341:GLU:H	2.04	0.54
1:H:27:THR:HG22	1:H:28:LYS:HG2	1.89	0.54
1:C:24:ILE:HD11	1:D:101:GLU:N	2.21	0.54
1:N:18:PRO:HG2	1:N:158:TYR:CZ	2.41	0.54
1:E:151:TYR:CZ	1:E:341:GLU:HG3	2.41	0.54
1:K:27:THR:HG22	1:K:28:LYS:HG2	1.89	0.54
1:I:13:LYS:HE3	1:I:383:GLU:HG3	1.88	0.54
1:L:184:LYS:HE3	1:L:215:ASN:ND2	2.04	0.54
1:D:13:LYS:NZ	1:D:383:GLU:HG3	2.22	0.54
1:M:63:LEU:HD11	1:N:108:GLU:HG2	1.89	0.54
1:H:137:ALA:HB2	1:H:144:ALA:HB2	1.89	0.54
1:H:57:ARG:O	1:H:58:TYR:HB2	2.07	0.54
1:O:125:ALA:HB3	1:O:371:GLY:HA2	1.89	0.54
1:K:24:ILE:HG13	1:L:100:ASN:CA	2.34	0.54
1:F:184:LYS:CE	1:F:215:ASN:HD21	2.17	0.54
1:O:140:HIS:HE1	1:O:303:GLN:HE21	1.55	0.54
1:P:340:ASN:ND2	1:P:341:GLU:H	2.06	0.54
1:J:57:ARG:O	1:J:58:TYR:HB2	2.08	0.54
1:G:32:SER:O	1:G:52:PHE:HA	2.08	0.54
1:E:24:ILE:HD13	1:F:102:LYS:HG3	1.89	0.54
1:G:184:LYS:NZ	3:G:1007:SRT:H2	2.22	0.54
1:F:167:ARG:NH2	1:F:202:GLU:HG2	2.22	0.54
1:P:179:ASN:O	1:P:208:ALA:HA	2.07	0.54
1:G:13:LYS:HE3	1:G:383:GLU:HG3	1.90	0.54
1:K:23:TYR:HD2	1:K:24:ILE:CD1	2.20	0.54
1:G:40:VAL:O	1:G:47:VAL:HG12	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:184:LYS:HE3	1:P:215:ASN:HD21	1.71	0.54
1:I:24:ILE:HD13	1:J:102:LYS:HG2	1.90	0.54
1:M:178:TYR:OH	1:M:344:PRO:HG3	2.07	0.54
1:A:360:GLU:HG3	1:J:358:ARG:NH1	2.22	0.54
1:G:24:ILE:HD11	1:H:101:GLU:N	2.22	0.54
1:O:360:GLU:O	1:O:361:ASN:HB2	2.07	0.54
1:M:19:ILE:CD1	1:M:346:LEU:HD21	2.38	0.54
1:O:151:TYR:CE1	1:O:182:LYS:HE2	2.41	0.54
1:H:151:TYR:CZ	1:H:341:GLU:HG3	2.43	0.54
1:F:349:PRO:O	1:F:380:LEU:HG	2.08	0.54
1:D:284:PRO:HG3	1:N:284:PRO:HG3	1.89	0.54
1:P:358:ARG:HA	1:P:358:ARG:HH11	1.72	0.54
1:J:167:ARG:HD3	1:J:203:GLU:CB	2.25	0.54
1:G:151:TYR:HB2	1:G:180:VAL:HG12	1.89	0.54
1:H:65:ARG:HH11	1:H:65:ARG:HG3	1.73	0.54
1:M:57:ARG:O	1:M:58:TYR:HB2	2.07	0.54
1:H:8:VAL:HG23	1:H:73:LEU:HD21	1.89	0.54
1:H:184:LYS:NZ	3:H:1008:SRT:H2	2.23	0.54
1:A:24:ILE:HD11	1:B:101:GLU:O	2.08	0.54
1:B:11:ILE:CG2	1:B:387:LEU:HD13	2.38	0.54
1:H:17:SER:C	1:H:19:ILE:H	2.08	0.54
1:P:11:ILE:CG2	1:P:33:LEU:HB3	2.38	0.53
1:E:140:HIS:CE1	1:E:303:GLN:NE2	2.72	0.53
1:A:354:PRO:O	1:A:357:VAL:HG12	2.08	0.53
1:L:140:HIS:HE1	1:L:303:GLN:HE21	1.55	0.53
1:E:349:PRO:O	1:E:380:LEU:HG	2.08	0.53
1:M:156:TYR:CE1	1:M:184:LYS:HE2	2.43	0.53
1:M:184:LYS:HE3	1:M:215:ASN:HD21	1.74	0.53
1:J:156:TYR:CZ	1:J:184:LYS:HE3	2.44	0.53
1:C:184:LYS:HZ1	3:C:1003:SRT:H2	1.73	0.53
1:G:357:VAL:HG23	4:G:2012:HOH:O	2.09	0.53
1:P:179:ASN:HD22	1:P:179:ASN:N	2.04	0.53
1:H:65:ARG:NH1	1:H:65:ARG:HG3	2.22	0.53
1:N:198:GLU:O	1:N:202:GLU:HB2	2.08	0.53
1:B:194:ARG:HD2	1:B:195:MET:CE	2.39	0.53
1:F:57:ARG:O	1:F:58:TYR:HB2	2.08	0.53
1:I:27:THR:HG22	1:I:28:LYS:HG2	1.90	0.53
1:I:167:ARG:NH2	1:I:202:GLU:CD	2.61	0.53
1:H:158:TYR:HB3	1:H:161:LYS:HB2	1.91	0.53
1:B:27:THR:HG22	1:B:28:LYS:HG2	1.90	0.53
1:G:64:ILE:HG23	1:G:116:ILE:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:57:ARG:O	1:N:58:TYR:HB2	2.09	0.53
1:O:57:ARG:O	1:O:58:TYR:HB2	2.08	0.53
1:E:27:THR:HG22	1:E:28:LYS:HG2	1.90	0.53
1:D:32:SER:O	1:D:52:PHE:HA	2.09	0.53
1:M:158:TYR:HB3	1:M:161:LYS:HB2	1.91	0.53
1:J:158:TYR:HB3	1:J:161:LYS:HB2	1.90	0.53
1:L:179:ASN:ND2	1:L:179:ASN:H	2.06	0.53
1:K:64:ILE:HG23	1:K:116:ILE:HD11	1.91	0.53
1:O:27:THR:HG22	1:O:28:LYS:HG2	1.91	0.53
1:B:57:ARG:O	1:B:58:TYR:HB2	2.08	0.53
1:L:24:ILE:HG23	1:L:25:ASP:N	2.23	0.53
1:K:57:ARG:O	1:K:58:TYR:HB2	2.09	0.53
1:L:200:VAL:O	1:L:204:ILE:HG12	2.08	0.53
1:J:24:ILE:HG23	1:J:25:ASP:N	2.24	0.53
1:A:23:TYR:O	1:A:24:ILE:HD12	2.08	0.53
1:P:57:ARG:O	1:P:58:TYR:HB2	2.09	0.53
1:L:32:SER:O	1:L:52:PHE:HA	2.08	0.53
1:H:184:LYS:CE	1:H:215:ASN:HD21	2.14	0.52
1:B:158:TYR:HB3	1:B:161:LYS:HB2	1.91	0.52
1:L:27:THR:HG22	1:L:28:LYS:HG2	1.90	0.52
1:P:348:GLN:HE22	1:P:352:GLY:N	2.06	0.52
1:L:170:MET:HG3	1:L:200:VAL:CG1	2.32	0.52
1:M:24:ILE:HG22	1:M:25:ASP:N	2.24	0.52
1:J:19:ILE:HG23	1:J:156:TYR:CD1	2.44	0.52
1:N:340:ASN:ND2	1:N:341:GLU:H	2.06	0.52
1:A:19:ILE:HD13	1:A:346:LEU:CD2	2.39	0.52
1:A:196:ARG:O	1:A:200:VAL:HG23	2.09	0.52
1:K:107:GLY:O	1:K:109:ARG:N	2.40	0.52
1:J:140:HIS:CE1	1:J:303:GLN:NE2	2.72	0.52
1:J:340:ASN:ND2	1:J:341:GLU:H	2.07	0.52
1:J:179:ASN:ND2	1:J:180:VAL:HG23	2.24	0.52
1:H:107:GLY:O	1:H:108:GLU:HB2	2.08	0.52
1:B:179:ASN:HD22	1:B:179:ASN:H	1.57	0.52
1:B:19:ILE:HD11	1:B:346:LEU:HD21	1.91	0.52
1:H:340:ASN:ND2	1:H:341:GLU:H	2.07	0.52
1:K:23:TYR:C	1:K:24:ILE:HD12	2.30	0.52
1:M:197:ILE:O	1:M:201:LEU:HB2	2.09	0.52
1:B:64:ILE:HG23	1:B:116:ILE:HD11	1.91	0.52
1:H:40:VAL:O	1:H:47:VAL:HG12	2.10	0.52
1:E:340:ASN:ND2	1:E:341:GLU:H	2.07	0.52
1:D:157:TYR:CE2	1:D:187:GLY:HA3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:179:ASN:H	1:F:179:ASN:HD22	1.58	0.52
1:O:140:HIS:CE1	1:O:303:GLN:NE2	2.76	0.52
1:N:72:ILE:HD12	1:N:93:VAL:CG1	2.40	0.52
1:P:64:ILE:HG23	1:P:116:ILE:HD11	1.91	0.52
1:I:38:THR:OG1	1:I:47:VAL:HG13	2.10	0.52
1:H:71:ARG:HH12	1:H:101:GLU:HG2	1.75	0.52
1:M:179:ASN:ND2	1:M:179:ASN:H	2.08	0.52
1:J:4:ARG:HG3	1:J:77:PRO:HB3	1.92	0.52
1:D:23:TYR:O	1:D:24:ILE:HD12	2.10	0.52
1:K:23:TYR:CD2	1:L:103:PRO:HD3	2.45	0.52
1:E:156:TYR:CE1	1:E:184:LYS:HE3	2.45	0.52
1:N:200:VAL:O	1:N:204:ILE:HG12	2.10	0.52
1:B:170:MET:HG3	1:B:200:VAL:CG1	2.39	0.52
1:D:11:ILE:HG12	1:D:13:LYS:HE3	1.91	0.52
1:L:179:ASN:ND2	1:L:180:VAL:HG23	2.25	0.52
1:J:140:HIS:CE1	1:J:303:GLN:HE21	2.27	0.52
1:I:140:HIS:CE1	1:I:303:GLN:NE2	2.73	0.52
1:E:23:TYR:CD2	1:F:103:PRO:HD3	2.44	0.52
1:H:285:ASP:OD1	1:H:286:ARG:HG2	2.10	0.52
1:D:140:HIS:CE1	1:D:303:GLN:NE2	2.73	0.51
1:O:151:TYR:CZ	1:O:341:GLU:HG3	2.45	0.51
1:N:346:LEU:N	1:N:346:LEU:HD12	2.25	0.51
1:P:285:ASP:OD1	1:P:286:ARG:HG2	2.10	0.51
1:K:100:ASN:HA	1:L:24:ILE:CG1	2.29	0.51
1:F:340:ASN:ND2	1:F:341:GLU:H	2.08	0.51
1:O:358:ARG:HD3	1:O:360:GLU:OE2	2.10	0.51
1:C:32:SER:O	1:C:52:PHE:HA	2.11	0.51
1:K:40:VAL:O	1:K:47:VAL:HG12	2.10	0.51
1:I:354:PRO:HD2	1:I:357:VAL:HG11	1.91	0.51
1:L:340:ASN:ND2	1:L:341:GLU:H	2.07	0.51
1:K:349:PRO:O	1:K:380:LEU:HG	2.11	0.51
1:A:57:ARG:O	1:A:58:TYR:HB2	2.10	0.51
1:K:24:ILE:HD11	1:L:101:GLU:O	2.10	0.51
1:G:244:PRO:CD	1:H:103:PRO:HB2	2.40	0.51
1:G:9:ARG:NH1	1:G:388:ALA:HA	2.25	0.51
1:E:140:HIS:CE1	1:E:303:GLN:HE21	2.27	0.51
1:P:170:MET:HG3	1:P:200:VAL:CG1	2.39	0.51
1:C:140:HIS:CE1	1:C:303:GLN:NE2	2.76	0.51
1:L:179:ASN:HD22	1:L:179:ASN:H	1.57	0.51
1:C:108:GLU:OE2	1:D:67:ARG:NH2	2.42	0.51
1:N:285:ASP:OD1	1:N:286:ARG:HG2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:326:GLN:N	1:D:326:GLN:OE1	2.42	0.51
1:N:158:TYR:HB3	1:N:161:LYS:HB2	1.91	0.51
1:A:147:ARG:HH21	1:A:147:ARG:CG	2.20	0.51
1:B:179:ASN:HD22	1:B:179:ASN:N	2.08	0.51
1:F:158:TYR:HB3	1:F:161:LYS:HB2	1.92	0.51
1:E:160:GLY:O	1:E:165:MET:HE3	2.10	0.51
1:O:158:TYR:HB3	1:O:161:LYS:HB2	1.91	0.51
1:G:182:LYS:HD2	1:G:213:ASP:HB2	1.92	0.51
1:K:190:ILE:HG23	1:K:191:GLU:N	2.26	0.51
1:K:197:ILE:HG22	1:K:201:LEU:HD22	1.93	0.51
1:L:151:TYR:CZ	1:L:341:GLU:HG3	2.45	0.51
1:C:285:ASP:OD1	1:C:286:ARG:HG2	2.11	0.51
1:L:285:ASP:OD1	1:L:286:ARG:HG2	2.11	0.51
1:C:184:LYS:HD2	1:C:215:ASN:HD21	1.76	0.51
1:N:64:ILE:HG23	1:N:116:ILE:HD11	1.92	0.51
1:K:179:ASN:C	1:K:179:ASN:HD22	2.14	0.51
1:N:137:ALA:CB	1:N:144:ALA:HB2	2.41	0.51
1:E:179:ASN:HD22	1:E:179:ASN:N	2.07	0.51
1:C:8:VAL:HG23	1:C:73:LEU:HD21	1.93	0.51
1:L:40:VAL:O	1:L:47:VAL:HG12	2.11	0.51
1:G:24:ILE:CG1	1:H:100:ASN:HA	2.31	0.50
1:P:158:TYR:HB3	1:P:161:LYS:HB2	1.94	0.50
1:I:340:ASN:ND2	1:I:341:GLU:H	2.09	0.50
1:P:114:GLY:HA2	1:P:298:GLY:N	2.26	0.50
1:J:170:MET:HG3	1:J:200:VAL:CG1	2.37	0.50
1:P:40:VAL:O	1:P:47:VAL:HG12	2.11	0.50
1:D:340:ASN:ND2	1:D:341:GLU:H	2.09	0.50
1:I:24:ILE:HG13	1:J:100:ASN:HA	1.92	0.50
1:K:151:TYR:CZ	1:K:341:GLU:HG3	2.46	0.50
1:A:183:MET:HG2	1:A:210:LEU:HD11	1.93	0.50
1:H:23:TYR:O	1:H:24:ILE:HD12	2.11	0.50
1:N:24:ILE:HG23	1:N:25:ASP:N	2.25	0.50
1:G:9:ARG:HH11	1:G:388:ALA:CB	2.25	0.50
1:D:158:TYR:HB3	1:D:161:LYS:HB2	1.93	0.50
1:G:158:TYR:HB3	1:G:161:LYS:HB2	1.92	0.50
1:F:125:ALA:HB3	1:F:371:GLY:HA2	1.94	0.50
1:L:158:TYR:HB3	1:L:161:LYS:HB2	1.93	0.50
1:O:340:ASN:ND2	1:O:341:GLU:H	2.08	0.50
1:J:179:ASN:N	1:J:179:ASN:HD22	2.08	0.50
1:K:178:TYR:CZ	1:K:359:VAL:HG21	2.46	0.50
1:C:197:ILE:O	1:C:201:LEU:HD22	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:TYR:CZ	1:D:359:VAL:HG21	2.47	0.50
1:M:27:THR:HG22	1:M:28:LYS:HG2	1.93	0.50
1:E:10:GLU:OE1	1:E:65:ARG:NH1	2.44	0.50
1:G:9:ARG:HH11	1:G:388:ALA:HA	1.76	0.50
1:A:158:TYR:HB3	1:A:161:LYS:HB2	1.92	0.50
1:E:158:TYR:HB3	1:E:161:LYS:HB2	1.93	0.50
1:J:182:LYS:HA	1:J:211:ALA:O	2.11	0.50
1:J:179:ASN:H	1:J:179:ASN:HD22	1.59	0.50
1:D:125:ALA:HB3	1:D:371:GLY:HA2	1.93	0.50
1:E:100:ASN:CA	1:F:24:ILE:HG13	2.34	0.50
1:D:179:ASN:HD22	1:D:179:ASN:N	1.98	0.50
1:C:158:TYR:HB3	1:C:161:LYS:HB2	1.92	0.50
1:B:184:LYS:NZ	3:B:1002:SRT:H2	2.26	0.50
1:M:179:ASN:N	1:M:179:ASN:HD22	2.04	0.50
1:H:173:TYR:HE1	1:H:344:PRO:HG2	1.75	0.50
1:O:82:ASN:ND2	1:O:87:ASN:HB3	2.27	0.50
1:L:57:ARG:O	1:L:58:TYR:HB2	2.11	0.50
1:I:57:ARG:O	1:I:58:TYR:HB2	2.12	0.50
1:M:346:LEU:O	1:M:347:PHE:HB2	2.12	0.50
1:A:23:TYR:HD2	1:A:24:ILE:HD12	1.77	0.50
1:C:140:HIS:CE1	1:C:303:GLN:HE21	2.29	0.50
1:D:184:LYS:HD2	1:D:215:ASN:HD21	1.75	0.50
1:H:270:HIS:CD2	1:H:301:GLU:OE2	2.63	0.50
1:M:82:ASN:ND2	1:M:87:ASN:HB3	2.27	0.50
1:D:19:ILE:HG13	1:D:156:TYR:CB	2.41	0.50
1:M:184:LYS:CE	1:M:215:ASN:HD21	2.25	0.50
1:K:38:THR:HG1	1:K:47:VAL:HG13	1.77	0.50
1:K:140:HIS:CE1	1:K:303:GLN:NE2	2.76	0.50
1:O:64:ILE:HG23	1:O:116:ILE:HD11	1.92	0.50
1:E:82:ASN:ND2	1:E:87:ASN:HB3	2.27	0.50
1:L:75:ALA:O	1:L:77:PRO:HD3	2.12	0.50
1:E:11:ILE:HG23	1:E:33:LEU:HB3	1.93	0.50
1:A:184:LYS:NZ	1:A:215:ASN:HD21	2.10	0.50
1:G:17:SER:OG	1:G:19:ILE:HB	2.11	0.50
1:F:270:HIS:CD2	1:F:301:GLU:OE2	2.64	0.50
1:I:40:VAL:O	1:I:47:VAL:HG12	2.11	0.50
1:C:27:THR:HG22	1:C:28:LYS:HG2	1.93	0.50
1:K:158:TYR:HB3	1:K:161:LYS:HB2	1.94	0.49
1:I:158:TYR:HB3	1:I:161:LYS:HB2	1.94	0.49
1:M:166:LEU:HD22	1:M:200:VAL:CG2	2.41	0.49
1:M:40:VAL:O	1:M:47:VAL:HG12	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:ASN:ND2	1:A:341:GLU:H	2.10	0.49
1:O:67:ARG:HH21	1:P:58:TYR:HB2	1.76	0.49
1:D:19:ILE:HG22	1:D:26:PHE:HB2	1.94	0.49
1:J:285:ASP:OD1	1:J:286:ARG:HG2	2.12	0.49
1:I:285:ASP:OD1	1:I:286:ARG:HG2	2.11	0.49
1:F:351:GLY:O	1:F:377:LYS:HE3	2.12	0.49
1:C:326:GLN:N	1:C:326:GLN:OE1	2.43	0.49
1:O:100:ASN:CA	1:P:24:ILE:HG13	2.35	0.49
1:B:162:GLY:H	1:B:165:MET:HE3	1.78	0.49
1:G:340:ASN:HD22	1:G:341:GLU:H	1.59	0.49
1:M:178:TYR:CE2	1:M:344:PRO:HG2	2.48	0.49
1:N:145:ASN:O	1:N:333:ALA:HB1	2.12	0.49
1:D:64:ILE:HG23	1:D:116:ILE:HD11	1.94	0.49
1:K:343:TYR:HB3	1:K:346:LEU:HB2	1.95	0.49
1:P:75:ALA:O	1:P:77:PRO:HD3	2.12	0.49
1:M:285:ASP:OD1	1:M:286:ARG:HG2	2.13	0.49
1:O:193:ASP:O	1:O:197:ILE:HG13	2.12	0.49
1:N:353:PHE:HB3	1:N:354:PRO:HD2	1.95	0.49
1:G:19:ILE:HG13	1:G:156:TYR:CB	2.43	0.49
1:J:151:TYR:CZ	1:J:341:GLU:HG3	2.48	0.49
1:E:57:ARG:O	1:E:58:TYR:HB2	2.12	0.49
1:F:194:ARG:CZ	1:F:229:MET:HG2	2.42	0.49
1:G:285:ASP:OD1	1:G:286:ARG:HG2	2.13	0.49
1:L:283:ARG:N	1:L:283:ARG:HD3	2.28	0.49
1:P:357:VAL:HG22	1:P:358:ARG:N	2.27	0.49
1:A:21:ASN:HB2	1:A:215:ASN:ND2	2.28	0.49
1:M:21:ASN:HB2	1:M:215:ASN:ND2	2.28	0.49
1:A:140:HIS:HE1	1:A:303:GLN:HE21	1.57	0.49
1:N:42:ARG:O	1:N:43:GLU:HB2	2.13	0.49
1:H:32:SER:O	1:H:52:PHE:HA	2.12	0.49
1:O:285:ASP:OD1	1:O:286:ARG:HG2	2.13	0.49
1:M:101:GLU:N	1:N:24:ILE:HD11	2.28	0.49
1:K:23:TYR:O	1:K:24:ILE:HD12	2.13	0.49
1:H:11:ILE:CG2	1:H:387:LEU:HD13	2.42	0.49
1:F:40:VAL:O	1:F:47:VAL:HG12	2.13	0.49
1:M:179:ASN:N	1:M:179:ASN:ND2	2.61	0.49
1:O:162:GLY:H	1:O:165:MET:HE3	1.78	0.49
1:K:340:ASN:ND2	1:K:341:GLU:H	2.10	0.49
1:J:179:ASN:H	1:J:179:ASN:ND2	2.11	0.49
1:N:82:ASN:ND2	1:N:87:ASN:HB3	2.28	0.49
1:O:72:ILE:HD11	1:O:97:MET:SD	2.53	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:ASP:OD1	1:A:286:ARG:HG2	2.13	0.49
1:L:196:ARG:HB2	1:L:196:ARG:HH11	1.78	0.49
1:M:170:MET:HG3	1:M:200:VAL:CG1	2.42	0.49
1:H:287:ASP:O	1:H:318:ARG:HD3	2.12	0.49
1:E:125:ALA:HB3	1:E:371:GLY:HA2	1.94	0.49
1:I:140:HIS:CE1	1:I:303:GLN:HE21	2.28	0.49
1:B:184:LYS:HZ1	3:B:1002:SRT:H2	1.76	0.49
1:N:68:PHE:O	1:N:72:ILE:HG12	2.12	0.49
1:J:187:GLY:O	1:J:188:ALA:HB2	2.13	0.49
1:P:67:ARG:HD3	1:P:101:GLU:OE2	2.12	0.48
1:P:82:ASN:ND2	1:P:87:ASN:HB3	2.28	0.48
1:G:100:ASN:CA	1:H:24:ILE:HG13	2.32	0.48
1:A:151:TYR:CZ	1:A:341:GLU:HG3	2.48	0.48
1:F:194:ARG:NH1	1:F:229:MET:HG2	2.27	0.48
1:B:42:ARG:O	1:B:43:GLU:HB2	2.13	0.48
1:F:82:ASN:ND2	1:F:87:ASN:HB3	2.28	0.48
1:K:24:ILE:HD11	1:L:101:GLU:C	2.33	0.48
1:M:358:ARG:CB	1:M:358:ARG:NH1	2.76	0.48
1:I:3:VAL:HG13	1:I:40:VAL:HG21	1.95	0.48
1:O:114:GLY:HA2	1:O:298:GLY:N	2.28	0.48
1:C:125:ALA:HB3	1:C:371:GLY:HA2	1.95	0.48
1:J:82:ASN:ND2	1:J:87:ASN:HB3	2.28	0.48
1:M:100:ASN:HA	1:N:24:ILE:CG1	2.36	0.48
1:A:184:LYS:HZ2	1:A:215:ASN:HD21	1.61	0.48
1:J:21:ASN:HB2	1:J:215:ASN:ND2	2.29	0.48
1:G:140:HIS:HE1	1:G:303:GLN:HE21	1.57	0.48
1:N:157:TYR:OH	1:N:193:ASP:OD1	2.31	0.48
1:B:249:LEU:HD23	1:B:249:LEU:C	2.34	0.48
1:J:166:LEU:HD22	1:J:200:VAL:HG22	1.96	0.48
1:P:19:ILE:HG13	1:P:156:TYR:CB	2.43	0.48
1:F:140:HIS:CE1	1:F:303:GLN:HE21	2.28	0.48
1:N:184:LYS:HZ1	3:N:1014:SRT:H2	1.74	0.48
1:C:340:ASN:ND2	1:C:341:GLU:H	2.11	0.48
1:G:358:ARG:CZ	1:G:358:ARG:HB3	2.43	0.48
1:H:241:VAL:CG1	1:H:253:LEU:HD21	2.38	0.48
1:F:18:PRO:HG2	1:F:158:TYR:CZ	2.49	0.48
1:B:140:HIS:CE1	1:B:303:GLN:NE2	2.77	0.48
1:G:5:ILE:HD13	1:G:36:VAL:HG13	1.96	0.48
1:B:4:ARG:HG3	1:B:77:PRO:CB	2.41	0.48
1:C:82:ASN:ND2	1:C:87:ASN:HB3	2.29	0.48
1:A:82:ASN:ND2	1:A:87:ASN:HB3	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:103:PRO:HD3	1:F:23:TYR:CE2	2.49	0.48
1:O:11:ILE:HG12	1:O:13:LYS:HE3	1.94	0.48
1:M:19:ILE:HG12	1:M:156:TYR:CB	2.43	0.48
1:P:21:ASN:HB2	1:P:215:ASN:ND2	2.29	0.48
1:I:18:PRO:HB2	1:I:158:TYR:CE1	2.48	0.48
1:M:140:HIS:CE1	1:M:303:GLN:HE21	2.31	0.48
1:O:157:TYR:CE2	1:O:187:GLY:HA3	2.49	0.48
1:J:23:TYR:O	1:J:24:ILE:HD12	2.13	0.48
1:O:270:HIS:CD2	1:O:301:GLU:OE2	2.65	0.48
1:I:270:HIS:CD2	1:I:301:GLU:OE2	2.64	0.48
1:C:326:GLN:HG2	4:C:2041:HOH:O	2.13	0.48
1:C:249:LEU:C	1:C:249:LEU:HD23	2.34	0.48
1:B:14:PRO:HG3	1:D:159:PRO:HG3	1.96	0.47
1:J:357:VAL:O	1:J:357:VAL:HG13	2.13	0.47
1:E:179:ASN:ND2	1:E:179:ASN:N	2.61	0.47
1:I:82:ASN:ND2	1:I:87:ASN:HB3	2.28	0.47
1:N:65:ARG:CG	1:N:65:ARG:HH11	2.27	0.47
1:H:82:ASN:ND2	1:H:87:ASN:HB3	2.28	0.47
1:A:13:LYS:HG3	1:A:350:TYR:OH	2.14	0.47
1:G:57:ARG:O	1:G:58:TYR:HB2	2.14	0.47
1:H:66:GLU:HA	1:H:66:GLU:OE2	2.14	0.47
1:F:21:ASN:HB2	1:F:215:ASN:ND2	2.29	0.47
1:I:19:ILE:HD12	1:I:158:TYR:HD1	1.79	0.47
1:C:151:TYR:CZ	1:C:341:GLU:HG3	2.49	0.47
1:K:190:ILE:CG2	1:K:191:GLU:N	2.77	0.47
1:M:15:ILE:HD11	1:M:30:THR:O	2.14	0.47
1:C:349:PRO:O	1:C:380:LEU:HG	2.13	0.47
1:G:4:ARG:HG2	1:G:5:ILE:N	2.30	0.47
1:B:156:TYR:CE1	1:B:184:LYS:HD2	2.49	0.47
1:E:358:ARG:HB3	1:E:358:ARG:HH11	1.78	0.47
1:O:179:ASN:O	1:O:180:VAL:HG23	2.14	0.47
1:M:100:ASN:CA	1:N:24:ILE:HG13	2.37	0.47
1:B:345:ASP:O	1:B:346:LEU:HG	2.14	0.47
1:J:72:ILE:CD1	1:J:97:MET:HB3	2.44	0.47
1:B:270:HIS:CD2	1:B:301:GLU:OE2	2.66	0.47
1:A:249:LEU:HD23	1:A:249:LEU:C	2.34	0.47
1:C:156:TYR:CE1	1:C:184:LYS:HE3	2.50	0.47
1:D:350:TYR:OH	1:D:383:GLU:HG2	2.14	0.47
1:B:193:ASP:O	1:B:197:ILE:HG13	2.14	0.47
1:G:21:ASN:HB2	1:G:215:ASN:ND2	2.29	0.47
1:D:249:LEU:HD23	1:D:249:LEU:C	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:24:ILE:CG2	1:F:25:ASP:N	2.78	0.47
1:I:101:GLU:N	1:J:24:ILE:HD11	2.30	0.47
1:N:10:GLU:HB3	1:N:65:ARG:NH1	2.25	0.47
1:B:140:HIS:CE1	1:B:303:GLN:HE21	2.28	0.47
1:O:60:GLN:HE22	1:O:108:GLU:HG3	1.80	0.47
1:C:270:HIS:CD2	1:C:301:GLU:OE2	2.65	0.47
1:G:184:LYS:HZ3	3:G:1007:SRT:H2	1.80	0.47
1:H:107:GLY:O	1:H:108:GLU:CB	2.63	0.47
1:I:351:GLY:O	1:I:377:LYS:HE3	2.14	0.47
1:A:182:LYS:HA	1:A:211:ALA:O	2.14	0.47
1:J:190:ILE:HD11	1:J:229:MET:CB	2.44	0.47
1:I:179:ASN:HD22	1:I:179:ASN:C	2.17	0.47
1:N:179:ASN:HD22	1:N:179:ASN:H	1.62	0.47
1:H:64:ILE:HG23	1:H:116:ILE:HD11	1.95	0.47
1:H:349:PRO:O	1:H:380:LEU:HG	2.14	0.47
1:B:182:LYS:HA	1:B:211:ALA:O	2.14	0.47
1:D:25:ASP:C	1:D:25:ASP:OD1	2.53	0.47
1:B:179:ASN:ND2	1:B:179:ASN:H	2.13	0.47
1:A:160:GLY:O	1:A:165:MET:HE3	2.14	0.47
1:H:140:HIS:CE1	1:H:303:GLN:HE21	2.29	0.47
1:A:17:SER:OG	1:A:19:ILE:HG23	2.14	0.47
1:N:107:GLY:O	1:N:108:GLU:CB	2.63	0.47
1:L:179:ASN:HD22	1:L:179:ASN:N	2.10	0.47
1:H:188:ALA:HB1	1:H:189:PRO:HD2	1.97	0.47
1:H:114:GLY:HA2	1:H:298:GLY:N	2.29	0.47
1:A:179:ASN:C	1:A:179:ASN:HD22	2.18	0.47
1:J:160:GLY:O	1:J:165:MET:HE3	2.15	0.47
1:J:182:LYS:HD2	1:J:213:ASP:HB2	1.95	0.47
1:F:151:TYR:CZ	1:F:341:GLU:HG3	2.49	0.47
1:B:82:ASN:ND2	1:B:87:ASN:HB3	2.29	0.47
1:A:23:TYR:C	1:A:24:ILE:HD12	2.35	0.47
1:B:120:VAL:O	1:B:124:VAL:HG23	2.16	0.47
1:A:137:ALA:HB2	1:A:144:ALA:HB2	1.96	0.47
1:O:354:PRO:HD2	1:O:357:VAL:HG21	1.97	0.47
1:P:249:LEU:C	1:P:249:LEU:HD23	2.35	0.47
1:J:241:VAL:CG1	1:J:253:LEU:HD21	2.37	0.46
1:N:10:GLU:HG3	1:N:64:ILE:HD12	1.97	0.46
1:D:270:HIS:CD2	1:D:301:GLU:OE2	2.65	0.46
1:G:355:ASP:OD1	1:G:377:LYS:HA	2.15	0.46
1:P:169:GLU:HG2	1:P:173:TYR:CE2	2.50	0.46
1:K:160:GLY:O	1:K:165:MET:HE3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:184:LYS:NZ	1:J:215:ASN:HD21	2.13	0.46
1:N:65:ARG:HG3	1:N:65:ARG:NH1	2.29	0.46
1:J:40:VAL:O	1:J:47:VAL:HG12	2.15	0.46
1:N:179:ASN:H	1:N:179:ASN:ND2	2.13	0.46
1:L:82:ASN:ND2	1:L:87:ASN:HB3	2.30	0.46
1:G:170:MET:HG3	1:G:200:VAL:HG13	1.98	0.46
1:I:114:GLY:HA2	1:I:298:GLY:N	2.30	0.46
1:P:137:ALA:CB	1:P:144:ALA:HB2	2.45	0.46
1:C:108:GLU:CD	1:D:67:ARG:HH22	2.19	0.46
1:H:249:LEU:HD23	1:H:249:LEU:C	2.36	0.46
1:I:326:GLN:N	1:I:326:GLN:OE1	2.45	0.46
1:O:184:LYS:HD3	1:O:213:ASP:HB3	1.98	0.46
1:O:182:LYS:HA	1:O:211:ALA:O	2.16	0.46
1:B:19:ILE:HD12	1:B:346:LEU:CD2	2.46	0.46
1:D:358:ARG:CZ	1:D:358:ARG:HB3	2.45	0.46
1:K:192:GLU:O	1:K:196:ARG:HG3	2.16	0.46
1:G:358:ARG:NH1	1:G:358:ARG:HB3	2.31	0.46
1:D:287:ASP:O	1:D:318:ARG:HD3	2.16	0.46
1:K:82:ASN:ND2	1:K:87:ASN:HB3	2.30	0.46
1:A:147:ARG:NH2	1:A:147:ARG:CG	2.78	0.46
1:G:353:PHE:HB3	1:G:354:PRO:HD2	1.98	0.46
1:E:145:ASN:C	1:E:145:ASN:ND2	2.67	0.46
1:N:190:ILE:CG2	1:N:191:GLU:N	2.78	0.46
1:I:25:ASP:C	1:I:25:ASP:OD1	2.54	0.46
1:I:90:PRO:HG3	1:I:124:VAL:HG21	1.97	0.46
1:G:82:ASN:ND2	1:G:87:ASN:HB3	2.30	0.46
1:L:216:GLY:N	1:L:240:GLU:HG2	2.31	0.46
1:B:19:ILE:HG23	1:B:156:TYR:CD1	2.50	0.46
1:O:178:TYR:CE1	1:O:359:VAL:HG21	2.51	0.46
1:N:270:HIS:CD2	1:N:301:GLU:OE2	2.66	0.46
1:M:13:LYS:HE3	1:M:383:GLU:HG3	1.97	0.46
1:B:32:SER:O	1:B:52:PHE:HA	2.15	0.46
1:J:25:ASP:C	1:J:25:ASP:OD1	2.53	0.46
1:P:241:VAL:CG1	1:P:253:LEU:HD21	2.39	0.46
1:E:21:ASN:HB3	1:E:184:LYS:HG2	1.97	0.46
1:H:11:ILE:HG12	1:H:13:LYS:HE2	1.97	0.46
1:H:162:GLY:H	1:H:165:MET:HE3	1.81	0.46
1:O:22:ALA:HB2	1:O:185:ILE:O	2.16	0.46
1:M:167:ARG:NH2	1:M:202:GLU:OE1	2.48	0.46
1:B:125:ALA:HB3	1:B:371:GLY:HA2	1.97	0.46
1:E:201:LEU:HD12	1:E:201:LEU:HA	1.77	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:249:LEU:C	1:G:249:LEU:HD23	2.35	0.46
1:D:241:VAL:CG1	1:D:253:LEU:HD21	2.42	0.46
1:B:21:ASN:HB2	1:B:215:ASN:ND2	2.30	0.46
1:M:358:ARG:HB3	1:M:358:ARG:CZ	2.45	0.46
1:I:76:ASP:O	1:I:78:LYS:N	2.49	0.46
1:E:191:GLU:CD	1:E:194:ARG:HE	2.18	0.46
1:P:76:ASP:OD2	1:P:78:LYS:HB2	2.16	0.46
1:D:82:ASN:ND2	1:D:87:ASN:HB3	2.30	0.46
1:K:13:LYS:HE3	1:K:383:GLU:HG3	1.97	0.46
1:I:249:LEU:HD23	1:I:249:LEU:C	2.36	0.46
1:M:24:ILE:HG22	1:M:25:ASP:O	2.15	0.46
1:O:184:LYS:CE	1:O:215:ASN:HD21	2.28	0.46
1:O:241:VAL:CG1	1:O:253:LEU:HD21	2.40	0.46
1:C:21:ASN:HB2	1:C:215:ASN:ND2	2.31	0.46
1:K:191:GLU:O	1:K:195:MET:HG3	2.16	0.46
1:L:114:GLY:HA2	1:L:298:GLY:N	2.30	0.46
1:M:114:GLY:HA2	1:M:298:GLY:N	2.31	0.46
1:M:216:GLY:N	1:M:240:GLU:HG2	2.31	0.46
1:G:25:ASP:C	1:G:25:ASP:OD1	2.55	0.46
1:K:358:ARG:NH1	1:K:358:ARG:HG3	2.31	0.46
1:N:17:SER:OG	1:N:19:ILE:HB	2.15	0.46
1:G:197:ILE:HG22	1:G:201:LEU:HD22	1.98	0.46
1:C:6:VAL:HG12	1:C:6:VAL:O	2.15	0.46
1:L:184:LYS:CE	1:L:215:ASN:HD21	2.08	0.45
1:C:160:GLY:O	1:C:165:MET:HE3	2.17	0.45
1:H:137:ALA:CB	1:H:144:ALA:HB2	2.46	0.45
1:E:178:TYR:CZ	1:E:359:VAL:HG21	2.51	0.45
1:O:147:ARG:NH2	1:O:363:HIS:CD2	2.84	0.45
1:P:13:LYS:HE3	1:P:383:GLU:HG3	1.98	0.45
1:P:354:PRO:O	1:P:357:VAL:HG12	2.17	0.45
1:P:24:ILE:HG23	1:P:25:ASP:N	2.30	0.45
1:B:26:PHE:CD1	1:B:26:PHE:N	2.84	0.45
1:K:201:LEU:HA	1:K:201:LEU:HD12	1.78	0.45
1:L:202:GLU:O	1:L:205:GLY:N	2.46	0.45
1:H:42:ARG:O	1:H:43:GLU:HB2	2.16	0.45
1:O:184:LYS:HB3	4:O:2018:HOH:O	2.16	0.45
1:K:140:HIS:CE1	1:K:303:GLN:HE21	2.31	0.45
1:K:270:HIS:CD2	1:K:301:GLU:OE2	2.69	0.45
1:P:185:ILE:CD1	1:P:212:VAL:HB	2.46	0.45
1:E:201:LEU:HD13	1:E:210:LEU:CD2	2.46	0.45
1:B:216:GLY:N	1:B:240:GLU:HG2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:283:ARG:HD3	1:P:283:ARG:N	2.32	0.45
1:M:241:VAL:CG1	1:M:253:LEU:HD21	2.38	0.45
1:J:353:PHE:HB3	1:J:357:VAL:HG11	1.94	0.45
1:B:76:ASP:C	1:B:76:ASP:OD2	2.55	0.45
1:D:24:ILE:HG23	1:D:25:ASP:N	2.31	0.45
1:C:24:ILE:CG1	1:D:100:ASN:HA	2.28	0.45
1:K:101:GLU:N	1:L:24:ILE:HD11	2.31	0.45
1:K:100:ASN:CA	1:L:24:ILE:HG13	2.31	0.45
1:G:241:VAL:CG1	1:G:253:LEU:HD21	2.42	0.45
1:C:179:ASN:ND2	1:C:179:ASN:N	2.64	0.45
1:B:184:LYS:NZ	1:B:215:ASN:HD21	2.15	0.45
1:E:270:HIS:CD2	1:E:301:GLU:OE2	2.63	0.45
1:G:340:ASN:ND2	1:G:341:GLU:N	2.64	0.45
1:M:358:ARG:HH11	1:M:358:ARG:CB	2.29	0.45
3:G:1007:SRT:H3	1:H:102:LYS:NZ	2.30	0.45
1:B:169:GLU:HG2	1:B:173:TYR:CE2	2.51	0.45
1:G:114:GLY:HA2	1:G:298:GLY:N	2.32	0.45
1:K:243:ASP:OD1	1:K:244:PRO:HD2	2.16	0.45
1:G:100:ASN:HA	1:H:24:ILE:CG1	2.33	0.45
1:G:24:ILE:HG23	1:G:25:ASP:N	2.32	0.45
1:I:241:VAL:CG1	1:I:253:LEU:HD21	2.41	0.45
1:O:166:LEU:HD22	1:O:200:VAL:HG22	1.99	0.45
1:P:270:HIS:CD2	1:P:301:GLU:OE2	2.65	0.45
1:F:179:ASN:HD22	1:F:179:ASN:N	2.13	0.45
1:J:287:ASP:O	1:J:318:ARG:HD3	2.17	0.45
1:G:199:ALA:O	1:G:202:GLU:HB3	2.17	0.45
1:A:140:HIS:CE1	1:A:303:GLN:NE2	2.77	0.45
1:O:140:HIS:CE1	1:O:303:GLN:HE21	2.32	0.45
1:C:192:GLU:O	1:C:196:ARG:HG3	2.16	0.45
1:J:270:HIS:CD2	1:J:301:GLU:OE2	2.67	0.45
1:J:151:TYR:HE1	1:J:182:LYS:HE2	1.82	0.45
1:K:285:ASP:OD1	1:K:286:ARG:HG2	2.16	0.45
1:L:10:GLU:OE1	1:L:65:ARG:NH1	2.49	0.45
1:B:360:GLU:O	1:B:361:ASN:HB2	2.16	0.45
1:L:358:ARG:HB3	1:L:358:ARG:NH1	2.31	0.45
1:P:10:GLU:CD	1:P:10:GLU:C	2.75	0.45
1:G:17:SER:C	1:G:19:ILE:H	2.20	0.45
1:B:19:ILE:HG22	1:B:26:PHE:CD1	2.52	0.45
1:B:16:SER:HB2	1:B:26:PHE:O	2.16	0.45
1:I:32:SER:O	1:I:52:PHE:HA	2.17	0.45
1:J:326:GLN:OE1	1:J:326:GLN:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:VAL:CG1	1:A:253:LEU:HD21	2.42	0.45
1:F:195:MET:HG2	1:G:163:LEU:CG	2.44	0.45
1:N:177:GLY:HA3	1:N:359:VAL:O	2.17	0.45
1:P:351:GLY:O	1:P:352:GLY:O	2.35	0.45
1:M:169:GLU:HG2	1:M:173:TYR:CE2	2.51	0.45
1:C:90:PRO:HG3	1:C:124:VAL:HG21	1.99	0.45
1:H:4:ARG:HB2	1:H:77:PRO:HB3	1.99	0.45
1:M:326:GLN:OE1	1:M:326:GLN:N	2.48	0.45
1:K:241:VAL:CG1	1:K:253:LEU:HD21	2.38	0.45
1:M:140:HIS:CE1	1:M:303:GLN:NE2	2.78	0.45
1:M:193:ASP:O	1:M:197:ILE:HG13	2.17	0.45
1:F:179:ASN:H	1:F:179:ASN:ND2	2.14	0.45
1:I:179:ASN:ND2	1:I:180:VAL:HG23	2.31	0.45
1:O:190:ILE:HG23	1:O:191:GLU:H	1.82	0.45
1:K:249:LEU:C	1:K:249:LEU:HD23	2.37	0.45
1:H:25:ASP:OD1	1:H:25:ASP:C	2.54	0.44
1:O:103:PRO:HD3	1:P:23:TYR:CD2	2.52	0.44
1:L:241:VAL:CG1	1:L:253:LEU:HD21	2.40	0.44
1:E:184:LYS:NZ	1:E:215:ASN:HD21	2.15	0.44
1:A:25:ASP:OD1	1:A:25:ASP:C	2.56	0.44
1:A:18:PRO:HG2	1:A:158:TYR:CE1	2.51	0.44
1:B:200:VAL:O	1:B:204:ILE:HG12	2.16	0.44
1:L:196:ARG:CB	1:L:196:ARG:HH11	2.30	0.44
1:D:285:ASP:OD1	1:D:286:ARG:HG2	2.17	0.44
1:P:326:GLN:OE1	1:P:326:GLN:N	2.48	0.44
1:O:25:ASP:OD1	1:O:25:ASP:C	2.56	0.44
1:B:11:ILE:HG22	1:B:387:LEU:HD13	1.98	0.44
1:G:176:ARG:O	1:G:359:VAL:HB	2.18	0.44
1:K:169:GLU:HG2	1:K:173:TYR:CE2	2.52	0.44
1:I:65:ARG:HG3	1:I:65:ARG:NH1	2.24	0.44
1:K:21:ASN:HB2	1:K:215:ASN:ND2	2.33	0.44
1:G:200:VAL:O	1:G:204:ILE:HG12	2.18	0.44
1:J:216:GLY:N	1:J:240:GLU:HG2	2.32	0.44
1:F:285:ASP:OD1	1:F:286:ARG:HG2	2.16	0.44
1:H:63:LEU:CD2	1:H:67:ARG:HH21	2.30	0.44
1:J:169:GLU:HG2	1:J:173:TYR:CE2	2.52	0.44
1:K:283:ARG:HD3	1:K:283:ARG:N	2.32	0.44
1:P:25:ASP:C	1:P:25:ASP:OD1	2.56	0.44
1:E:19:ILE:HG22	1:E:26:PHE:CD1	2.53	0.44
1:F:76:ASP:HA	1:F:77:PRO:HD2	1.85	0.44
1:N:140:HIS:CE1	1:N:303:GLN:HE21	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:19:ILE:HG22	1:L:26:PHE:CD1	2.52	0.44
1:O:179:ASN:C	1:O:179:ASN:HD22	2.21	0.44
1:O:216:GLY:N	1:O:240:GLU:HG2	2.33	0.44
1:F:239:GLU:OE2	3:F:1006:SRT:O1	2.36	0.44
1:J:196:ARG:O	1:J:200:VAL:HG23	2.17	0.44
1:L:26:PHE:N	1:L:26:PHE:CD1	2.86	0.44
1:E:32:SER:O	1:E:52:PHE:HA	2.17	0.44
1:F:169:GLU:HG2	1:F:173:TYR:CE2	2.52	0.44
1:M:26:PHE:CD1	1:M:26:PHE:N	2.85	0.44
1:E:326:GLN:OE1	1:E:326:GLN:N	2.46	0.44
1:N:184:LYS:HD2	1:N:215:ASN:ND2	2.32	0.44
1:H:19:ILE:HG22	1:H:26:PHE:HB2	1.99	0.44
1:F:45:LYS:HZ1	1:F:389:GLU:HG3	1.82	0.44
1:O:26:PHE:N	1:O:26:PHE:CD1	2.85	0.44
1:A:199:ALA:O	1:A:202:GLU:HB3	2.17	0.44
1:O:101:GLU:N	1:P:24:ILE:HD11	2.32	0.44
1:G:4:ARG:NH2	1:G:77:PRO:HG3	2.32	0.44
1:A:24:ILE:HD13	1:B:102:LYS:HA	2.00	0.44
1:A:346:LEU:HD12	1:A:346:LEU:N	2.33	0.44
1:K:157:TYR:CE2	1:K:187:GLY:HA3	2.53	0.44
1:M:351:GLY:O	1:M:377:LYS:HE3	2.17	0.44
1:E:114:GLY:HA2	1:E:298:GLY:N	2.33	0.44
1:M:32:SER:O	1:M:52:PHE:HA	2.17	0.44
1:C:351:GLY:O	1:C:377:LYS:HE3	2.18	0.44
1:G:283:ARG:HD3	1:G:283:ARG:N	2.33	0.44
1:P:11:ILE:HB	1:P:387:LEU:HD13	2.00	0.44
1:F:241:VAL:CG1	1:F:253:LEU:HD21	2.40	0.44
1:J:156:TYR:CE1	1:J:184:LYS:HE3	2.53	0.44
1:E:136:LEU:HD21	1:E:299:LEU:HD21	2.00	0.44
1:D:184:LYS:HZ1	3:D:1004:SRT:H2	1.81	0.44
1:P:140:HIS:CE1	1:P:303:GLN:HE21	2.35	0.44
1:L:270:HIS:CD2	1:L:301:GLU:OE2	2.65	0.44
1:C:197:ILE:HG22	1:C:201:LEU:CD2	2.48	0.44
1:D:114:GLY:HA2	1:D:298:GLY:N	2.33	0.44
1:N:169:GLU:HG2	1:N:173:TYR:CE2	2.52	0.44
1:O:353:PHE:CE1	1:O:364:ILE:HG21	2.52	0.44
1:J:283:ARG:HD3	1:J:283:ARG:N	2.32	0.44
1:C:143:LYS:HD3	1:C:143:LYS:HA	1.75	0.44
1:L:25:ASP:C	1:L:25:ASP:OD1	2.55	0.44
1:M:25:ASP:C	1:M:25:ASP:OD1	2.56	0.44
1:E:101:GLU:N	1:F:24:ILE:HD11	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:26:PHE:N	1:E:26:PHE:CD1	2.86	0.44
1:B:241:VAL:CG1	1:B:253:LEU:HD21	2.41	0.44
1:E:158:TYR:CG	1:E:159:PRO:HD2	2.53	0.44
1:E:40:VAL:O	1:E:47:VAL:HG12	2.18	0.44
1:C:107:GLY:O	1:C:109:ARG:N	2.49	0.44
1:L:50:TYR:CD1	1:L:384:MET:HB3	2.53	0.44
1:P:355:ASP:HB2	1:P:376:GLY:O	2.17	0.44
1:N:326:GLN:OE1	1:N:326:GLN:N	2.49	0.44
1:H:179:ASN:ND2	1:H:179:ASN:H	2.16	0.44
1:E:249:LEU:C	1:E:249:LEU:HD23	2.37	0.44
1:I:26:PHE:CD1	1:I:26:PHE:N	2.86	0.43
1:A:140:HIS:CE1	1:A:303:GLN:HE21	2.35	0.43
1:O:178:TYR:CZ	1:O:359:VAL:HG21	2.53	0.43
1:H:26:PHE:N	1:H:26:PHE:CD1	2.86	0.43
1:E:120:VAL:O	1:E:124:VAL:HG23	2.18	0.43
1:K:108:GLU:CD	1:L:67:ARG:HH22	2.21	0.43
1:G:179:ASN:HD22	1:G:179:ASN:C	2.21	0.43
1:N:283:ARG:HD3	1:N:283:ARG:N	2.33	0.43
1:E:200:VAL:O	1:E:204:ILE:HG12	2.19	0.43
1:P:200:VAL:O	1:P:204:ILE:HG12	2.18	0.43
1:E:326:GLN:NE2	1:E:351:GLY:O	2.51	0.43
1:K:120:VAL:O	1:K:124:VAL:HG23	2.18	0.43
1:M:68:PHE:CZ	1:M:109:ARG:HB2	2.53	0.43
1:J:26:PHE:CD1	1:J:26:PHE:N	2.86	0.43
1:O:249:LEU:C	1:O:249:LEU:HD23	2.39	0.43
1:D:21:ASN:HB2	1:D:215:ASN:ND2	2.34	0.43
1:I:184:LYS:HZ1	3:I:1009:SRT:H2	1.82	0.43
1:M:340:ASN:HD22	1:M:341:GLU:H	1.66	0.43
1:P:140:HIS:CE1	1:P:303:GLN:NE2	2.82	0.43
1:A:270:HIS:CD2	1:A:301:GLU:OE2	2.67	0.43
1:D:216:GLY:N	1:D:240:GLU:HG2	2.34	0.43
1:J:249:LEU:C	1:J:249:LEU:HD23	2.38	0.43
1:P:26:PHE:CD1	1:P:26:PHE:N	2.87	0.43
1:E:167:ARG:NH2	1:E:202:GLU:OE2	2.52	0.43
1:H:11:ILE:CG1	1:H:13:LYS:HE2	2.49	0.43
1:D:358:ARG:NH1	1:D:358:ARG:CB	2.79	0.43
1:A:40:VAL:O	1:A:47:VAL:HG12	2.17	0.43
1:H:173:TYR:CE1	1:H:344:PRO:CG	3.01	0.43
1:D:26:PHE:CD1	1:D:26:PHE:N	2.87	0.43
1:A:169:GLU:HG2	1:A:173:TYR:CE2	2.54	0.43
1:O:283:ARG:N	1:O:283:ARG:HD3	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:120:VAL:O	1:M:124:VAL:HG23	2.19	0.43
1:A:287:ASP:O	1:A:318:ARG:HD3	2.18	0.43
1:O:178:TYR:HE2	1:O:344:PRO:HG2	1.80	0.43
1:P:13:LYS:HG3	1:P:350:TYR:OH	2.19	0.43
1:N:185:ILE:HD13	1:N:212:VAL:HB	2.00	0.43
1:B:284:PRO:HG3	1:L:284:PRO:HG3	1.99	0.43
1:C:241:VAL:CG1	1:C:253:LEU:HD21	2.38	0.43
1:P:21:ASN:HB3	1:P:184:LYS:HE3	2.01	0.43
1:F:11:ILE:HG22	1:F:387:LEU:HD13	2.00	0.43
1:J:114:GLY:HA2	1:J:298:GLY:N	2.34	0.43
1:F:120:VAL:O	1:F:124:VAL:HG23	2.18	0.43
1:M:24:ILE:CG2	1:M:25:ASP:N	2.81	0.43
1:B:4:ARG:NE	1:B:77:PRO:HG3	2.34	0.43
1:D:184:LYS:HD2	1:D:215:ASN:ND2	2.34	0.43
1:C:161:LYS:HB3	4:C:2034:HOH:O	2.17	0.43
1:J:13:LYS:CE	1:J:383:GLU:HG3	2.49	0.43
1:H:169:GLU:HG2	1:H:173:TYR:CE2	2.54	0.43
1:N:179:ASN:HD22	1:N:179:ASN:N	2.15	0.43
1:C:114:GLY:HA2	1:C:298:GLY:N	2.33	0.43
1:E:216:GLY:N	1:E:240:GLU:HG2	2.34	0.43
1:N:26:PHE:CD1	1:N:26:PHE:N	2.87	0.43
1:E:241:VAL:CG1	1:E:253:LEU:HD21	2.38	0.43
1:P:19:ILE:HG13	1:P:156:TYR:CG	2.54	0.43
1:I:19:ILE:HD12	1:I:158:TYR:CD1	2.54	0.43
1:I:10:GLU:HG3	1:I:64:ILE:HD12	2.01	0.43
1:I:182:LYS:HA	1:I:211:ALA:O	2.18	0.43
1:A:185:ILE:HG21	1:A:212:VAL:HB	2.00	0.43
1:C:169:GLU:HG2	1:C:173:TYR:CE2	2.54	0.43
1:E:169:GLU:HG2	1:E:173:TYR:CE2	2.53	0.43
1:M:249:LEU:HD23	1:M:249:LEU:C	2.39	0.43
1:E:283:ARG:N	1:E:283:ARG:HD3	2.34	0.43
1:L:184:LYS:HZ2	3:L:1012:SRT:H2	1.82	0.43
1:C:158:TYR:CG	1:C:159:PRO:HD2	2.54	0.43
1:G:140:HIS:CE1	1:G:303:GLN:HE21	2.36	0.43
1:P:64:ILE:O	1:P:69:ALA:HB3	2.19	0.43
1:H:3:VAL:O	1:H:81:LEU:HD21	2.18	0.43
1:F:50:TYR:CD1	1:F:384:MET:HB3	2.54	0.43
1:N:114:GLY:HA2	1:N:298:GLY:N	2.34	0.43
1:L:191:GLU:OE2	1:L:191:GLU:HA	2.19	0.43
1:H:184:LYS:HZ2	3:H:1008:SRT:H2	1.83	0.43
1:B:350:TYR:OH	1:B:383:GLU:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:179:ASN:ND2	1:D:362:GLY:HA3	2.33	0.43
1:L:169:GLU:HG2	1:L:173:TYR:CE2	2.53	0.43
1:N:13:LYS:NZ	1:N:383:GLU:HG3	2.34	0.43
1:O:68:PHE:O	1:O:72:ILE:HG13	2.18	0.43
1:N:90:PRO:HG3	1:N:124:VAL:HG21	2.00	0.43
1:M:322:HIS:CG	1:M:323:GLY:N	2.86	0.43
1:M:182:LYS:HA	1:M:211:ALA:O	2.19	0.43
1:I:216:GLY:N	1:I:240:GLU:HG2	2.34	0.43
1:G:67:ARG:HG2	4:G:2043:HOH:O	2.19	0.43
1:L:137:ALA:HB2	1:L:144:ALA:HB2	2.01	0.43
1:E:6:VAL:HG12	1:E:6:VAL:O	2.18	0.43
1:A:24:ILE:HD11	1:B:101:GLU:C	2.39	0.42
1:I:61:GLY:O	1:I:65:ARG:HB2	2.18	0.42
1:G:26:PHE:N	1:G:26:PHE:CD1	2.87	0.42
1:B:164:SER:O	1:B:167:ARG:HB2	2.19	0.42
1:E:201:LEU:HD13	1:E:210:LEU:HD22	2.01	0.42
1:L:322:HIS:CG	1:L:323:GLY:N	2.87	0.42
1:L:287:ASP:O	1:L:318:ARG:HD3	2.19	0.42
1:O:169:GLU:HG2	1:O:173:TYR:CE2	2.53	0.42
1:D:201:LEU:HD12	1:D:201:LEU:HA	1.87	0.42
1:G:140:HIS:CE1	1:G:303:GLN:NE2	2.79	0.42
1:N:140:HIS:CE1	1:N:303:GLN:NE2	2.79	0.42
1:I:24:ILE:CD1	1:J:102:LYS:HA	2.49	0.42
1:G:244:PRO:HD3	1:H:103:PRO:HB2	2.01	0.42
1:H:179:ASN:HD22	1:H:179:ASN:H	1.66	0.42
1:M:243:ASP:OD1	1:M:244:PRO:HD2	2.20	0.42
1:G:120:VAL:O	1:G:124:VAL:HG23	2.19	0.42
1:P:216:GLY:N	1:P:240:GLU:HG2	2.34	0.42
1:G:125:ALA:HB3	1:G:371:GLY:HA2	2.01	0.42
1:I:170:MET:HG3	1:I:200:VAL:HG13	2.00	0.42
1:L:120:VAL:O	1:L:124:VAL:HG23	2.19	0.42
1:G:23:TYR:O	1:G:24:ILE:HD12	2.18	0.42
1:H:7:ASP:OD1	1:H:9:ARG:NE	2.51	0.42
1:I:239:GLU:OE2	3:I:1009:SRT:O1	2.36	0.42
1:N:340:ASN:HD22	1:N:341:GLU:H	1.67	0.42
1:P:179:ASN:N	1:P:179:ASN:ND2	2.63	0.42
1:K:21:ASN:HB3	1:K:184:LYS:HD3	2.00	0.42
1:H:19:ILE:HG13	1:H:156:TYR:CB	2.49	0.42
1:D:169:GLU:HG2	1:D:173:TYR:CE2	2.54	0.42
1:O:120:VAL:O	1:O:124:VAL:HG23	2.19	0.42
1:F:236:PHE:O	1:F:260:PRO:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:299:LEU:HD22	1:H:327:MET:CE	2.49	0.42
1:G:188:ALA:HB1	1:G:189:PRO:HD2	2.02	0.42
1:P:35:ALA:HA	1:P:49:GLY:O	2.20	0.42
1:A:26:PHE:CD1	1:A:26:PHE:N	2.87	0.42
1:P:9:ARG:NH1	1:P:387:LEU:O	2.52	0.42
1:K:25:ASP:C	1:K:25:ASP:OD1	2.58	0.42
1:G:160:GLY:O	1:G:165:MET:HE3	2.19	0.42
1:G:299:LEU:O	1:G:303:GLN:HG3	2.20	0.42
1:E:358:ARG:HH11	1:E:358:ARG:CB	2.32	0.42
1:B:340:ASN:ND2	1:B:341:GLU:N	2.66	0.42
1:L:197:ILE:O	1:L:201:LEU:HB2	2.18	0.42
1:M:216:GLY:CA	1:M:240:GLU:HG2	2.50	0.42
1:K:11:ILE:CG2	1:K:33:LEU:HB3	2.49	0.42
1:P:120:VAL:O	1:P:124:VAL:HG23	2.20	0.42
1:F:287:ASP:O	1:F:318:ARG:HD3	2.19	0.42
1:A:4:ARG:HB2	1:A:39:ASP:OD1	2.18	0.42
1:C:236:PHE:O	1:C:260:PRO:HG2	2.20	0.42
1:L:249:LEU:C	1:L:249:LEU:HD23	2.38	0.42
1:G:196:ARG:O	1:G:199:ALA:HB3	2.18	0.42
1:I:100:ASN:HA	1:J:24:ILE:CG1	2.38	0.42
1:J:200:VAL:O	1:J:204:ILE:HG12	2.19	0.42
1:L:348:GLN:HA	1:L:348:GLN:NE2	2.34	0.42
1:M:270:HIS:CD2	1:M:301:GLU:OE2	2.67	0.42
1:D:136:LEU:HD21	1:D:299:LEU:HD21	2.02	0.42
1:C:63:LEU:HD11	1:D:108:GLU:HG2	2.00	0.42
1:M:177:GLY:HA3	1:M:359:VAL:O	2.19	0.42
1:K:216:GLY:N	1:K:240:GLU:HG2	2.35	0.42
1:A:108:GLU:OE2	1:B:67:ARG:NH2	2.40	0.42
1:K:26:PHE:CD1	1:K:26:PHE:N	2.88	0.42
1:E:25:ASP:OD1	1:E:25:ASP:C	2.57	0.42
1:N:249:LEU:C	1:N:249:LEU:HD23	2.40	0.42
1:G:167:ARG:HH22	1:G:202:GLU:HG2	1.83	0.42
1:P:9:ARG:HB2	1:P:9:ARG:HH11	1.85	0.42
1:G:241:VAL:HG21	1:G:253:LEU:HD23	2.01	0.42
1:C:18:PRO:HB2	1:C:158:TYR:CE1	2.55	0.42
1:O:60:GLN:NE2	1:O:108:GLU:HG3	2.34	0.42
1:B:216:GLY:CA	1:B:240:GLU:HG2	2.49	0.42
1:J:216:GLY:CA	1:J:240:GLU:HG2	2.50	0.42
1:G:350:TYR:N	1:G:350:TYR:CD1	2.86	0.42
1:G:169:GLU:HG2	1:G:173:TYR:CE2	2.55	0.42
1:H:15:ILE:HD13	1:H:31:THR:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:194:ARG:HD2	1:N:195:MET:CE	2.50	0.42
1:F:326:GLN:N	1:F:326:GLN:OE1	2.47	0.42
1:A:24:ILE:HG23	1:A:25:ASP:N	2.35	0.42
1:H:40:VAL:HB	1:H:47:VAL:CG1	2.49	0.42
1:M:340:ASN:ND2	1:M:341:GLU:N	2.67	0.42
1:L:299:LEU:O	1:L:303:GLN:HG3	2.20	0.42
1:B:197:ILE:O	1:B:201:LEU:CD2	2.67	0.42
1:B:182:LYS:HG3	1:B:211:ALA:HB3	2.02	0.42
1:K:108:GLU:HG2	1:L:63:LEU:HD11	2.02	0.42
1:B:287:ASP:O	1:B:318:ARG:HD3	2.19	0.42
1:C:182:LYS:HA	1:C:211:ALA:O	2.19	0.42
1:O:326:GLN:OE1	1:O:326:GLN:N	2.47	0.42
1:G:287:ASP:O	1:G:318:ARG:HD3	2.19	0.42
1:F:25:ASP:OD1	1:F:25:ASP:C	2.58	0.42
1:D:158:TYR:CG	1:D:159:PRO:HD2	2.55	0.42
1:N:340:ASN:ND2	1:N:341:GLU:N	2.68	0.42
1:H:349:PRO:HD2	1:H:350:TYR:CE1	2.55	0.42
1:O:190:ILE:HG23	1:O:191:GLU:N	2.35	0.42
1:P:287:ASP:O	1:P:318:ARG:HD3	2.20	0.42
1:K:287:ASP:O	1:K:318:ARG:HD3	2.19	0.42
1:D:232:ASP:OD2	1:P:160:GLY:HA2	2.19	0.42
1:J:352:GLY:HA3	1:J:377:LYS:HE3	2.01	0.42
1:M:287:ASP:O	1:M:318:ARG:HD3	2.20	0.42
1:J:191:GLU:OE1	1:J:191:GLU:N	2.33	0.42
1:E:21:ASN:CB	1:E:215:ASN:ND2	2.82	0.42
1:B:179:ASN:ND2	1:B:362:GLY:HA3	2.35	0.42
1:I:10:GLU:OE1	1:I:65:ARG:NH2	2.52	0.42
1:P:348:GLN:HE22	1:P:352:GLY:CA	2.33	0.42
1:G:182:LYS:HA	1:G:211:ALA:O	2.19	0.42
1:O:191:GLU:O	1:O:195:MET:HG2	2.20	0.42
1:D:216:GLY:CA	1:D:240:GLU:HG2	2.50	0.42
1:P:216:GLY:CA	1:P:240:GLU:HG2	2.50	0.42
1:I:125:ALA:HB3	1:I:371:GLY:HA2	2.02	0.42
1:E:300:CYS:HB3	4:E:2025:HOH:O	2.19	0.42
1:L:326:GLN:N	1:L:326:GLN:OE1	2.48	0.42
1:H:326:GLN:OE1	1:H:326:GLN:N	2.49	0.42
1:D:358:ARG:CB	1:D:358:ARG:HH11	2.32	0.42
1:N:349:PRO:HD2	1:N:350:TYR:CE1	2.55	0.42
1:H:87:ASN:OD1	1:H:88:LEU:N	2.53	0.42
1:I:120:VAL:O	1:I:124:VAL:HG23	2.19	0.42
1:K:114:GLY:HA2	1:K:298:GLY:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:326:GLN:N	1:G:326:GLN:OE1	2.50	0.42
1:F:216:GLY:N	1:F:240:GLU:HG2	2.35	0.42
1:F:243:ASP:OD1	1:F:244:PRO:HD2	2.20	0.42
1:N:241:VAL:CG1	1:N:253:LEU:HD21	2.39	0.41
1:F:160:GLY:O	1:F:165:MET:HE3	2.20	0.41
1:B:158:TYR:CG	1:B:159:PRO:HD2	2.55	0.41
1:J:322:HIS:CG	1:J:323:GLY:N	2.87	0.41
1:K:226:TYR:O	1:K:230:LEU:HB2	2.19	0.41
1:P:158:TYR:CG	1:P:159:PRO:HD2	2.55	0.41
1:G:9:ARG:HB3	1:G:387:LEU:HD11	2.03	0.41
1:I:162:GLY:H	1:I:165:MET:HE3	1.84	0.41
1:H:140:HIS:CE1	1:H:303:GLN:NE2	2.79	0.41
1:P:340:ASN:ND2	1:P:341:GLU:N	2.68	0.41
1:B:197:ILE:HG22	1:B:201:LEU:CD2	2.50	0.41
1:F:151:TYR:HE1	1:F:182:LYS:HE2	1.85	0.41
1:A:87:ASN:OD1	1:A:88:LEU:N	2.53	0.41
1:G:108:GLU:OE2	1:H:67:ARG:NH2	2.52	0.41
1:B:107:GLY:O	1:B:109:ARG:N	2.53	0.41
1:G:236:PHE:O	1:G:260:PRO:HG2	2.20	0.41
1:L:42:ARG:O	1:L:43:GLU:HB2	2.20	0.41
1:P:145:ASN:HA	1:P:146:PRO:HD3	1.85	0.41
1:C:100:ASN:CA	1:D:24:ILE:CG1	2.93	0.41
1:N:160:GLY:O	1:N:165:MET:HE3	2.20	0.41
1:N:287:ASP:O	1:N:318:ARG:HD3	2.20	0.41
1:F:178:TYR:CZ	1:F:359:VAL:HG21	2.56	0.41
1:I:169:GLU:HG2	1:I:173:TYR:CE2	2.55	0.41
1:L:164:SER:O	1:L:167:ARG:HB2	2.20	0.41
1:C:179:ASN:HD22	1:C:179:ASN:N	2.06	0.41
1:I:24:ILE:CG2	1:I:25:ASP:N	2.83	0.41
1:I:226:TYR:O	1:I:230:LEU:HB2	2.21	0.41
1:P:176:ARG:NH2	1:P:345:ASP:OD1	2.50	0.41
1:P:166:LEU:HD22	1:P:200:VAL:CG2	2.50	0.41
1:N:299:LEU:O	1:N:303:GLN:HG3	2.21	0.41
1:N:348:GLN:HB3	1:N:349:PRO:HA	2.03	0.41
1:C:87:ASN:OD1	1:C:88:LEU:N	2.53	0.41
1:E:176:ARG:O	1:E:359:VAL:HB	2.21	0.41
1:K:90:PRO:HG3	1:K:124:VAL:HG21	2.01	0.41
1:P:42:ARG:O	1:P:43:GLU:HB2	2.21	0.41
1:K:194:ARG:CZ	1:K:229:MET:HG2	2.50	0.41
1:A:349:PRO:O	1:A:380:LEU:HG	2.21	0.41
1:I:322:HIS:CG	1:I:323:GLY:N	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:226:TYR:O	1:P:230:LEU:HB2	2.21	0.41
1:A:42:ARG:O	1:A:43:GLU:HB2	2.20	0.41
1:E:322:HIS:CG	1:E:323:GLY:N	2.88	0.41
1:C:363:HIS:HB2	4:C:2058:HOH:O	2.20	0.41
1:P:237:TRP:C	1:P:237:TRP:CD1	2.94	0.41
1:C:25:ASP:OD1	1:C:25:ASP:C	2.58	0.41
1:C:26:PHE:N	1:C:26:PHE:CD1	2.88	0.41
1:N:25:ASP:OD1	1:N:25:ASP:C	2.59	0.41
1:L:241:VAL:HG21	1:L:253:LEU:HD23	2.03	0.41
1:I:19:ILE:HG22	1:I:26:PHE:CD1	2.56	0.41
1:O:299:LEU:O	1:O:303:GLN:HG3	2.21	0.41
1:O:340:ASN:HD22	1:O:341:GLU:H	1.69	0.41
1:J:340:ASN:HD22	1:J:341:GLU:H	1.68	0.41
1:H:10:GLU:HB3	1:H:65:ARG:NH2	2.36	0.41
1:E:194:ARG:O	1:E:198:GLU:HG3	2.20	0.41
1:B:284:PRO:HB3	1:B:314:TRP:CE2	2.56	0.41
1:K:216:GLY:CA	1:K:240:GLU:HG2	2.51	0.41
1:K:322:HIS:CG	1:K:323:GLY:N	2.87	0.41
1:A:283:ARG:HD3	1:A:283:ARG:N	2.36	0.41
1:E:164:SER:O	1:E:167:ARG:HB2	2.20	0.41
1:P:177:GLY:C	1:P:359:VAL:HG12	2.41	0.41
1:M:60:GLN:OE1	1:M:108:GLU:HG3	2.21	0.41
1:E:11:ILE:HG22	1:E:387:LEU:HD13	2.03	0.41
1:C:287:ASP:O	1:C:318:ARG:HD3	2.21	0.41
1:M:329:LEU:HB3	1:M:366:MET:SD	2.61	0.41
1:A:120:VAL:O	1:A:124:VAL:HG23	2.21	0.41
1:F:114:GLY:HA2	1:F:298:GLY:N	2.35	0.41
1:I:103:PRO:HB2	1:J:244:PRO:CD	2.49	0.41
1:G:63:LEU:HD13	1:G:109:ARG:HA	2.02	0.41
1:M:283:ARG:N	1:M:283:ARG:HD3	2.36	0.41
1:D:237:TRP:CD1	1:D:237:TRP:C	2.94	0.41
1:B:283:ARG:HD3	1:B:283:ARG:N	2.35	0.41
1:G:167:ARG:HD3	1:G:203:GLU:CB	2.30	0.41
1:A:241:VAL:HG21	1:A:253:LEU:HD23	2.03	0.41
1:G:270:HIS:CD2	1:G:301:GLU:OE2	2.69	0.41
1:J:188:ALA:O	1:J:189:PRO:C	2.58	0.41
1:M:16:SER:HA	1:M:26:PHE:O	2.21	0.41
1:O:19:ILE:HG22	1:O:26:PHE:CD1	2.56	0.41
1:G:54:SER:HB3	1:G:323:GLY:HA2	2.03	0.41
1:A:216:GLY:N	1:A:240:GLU:HG2	2.35	0.41
1:P:284:PRO:HB3	1:P:314:TRP:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:192:GLU:O	1:M:195:MET:HB2	2.21	0.41
1:E:243:ASP:OD1	1:E:244:PRO:HD2	2.20	0.41
1:C:191:GLU:HA	1:C:191:GLU:OE2	2.21	0.41
1:G:101:GLU:C	1:H:24:ILE:HD11	2.41	0.41
1:I:241:VAL:HG21	1:I:253:LEU:HD23	2.02	0.41
1:F:156:TYR:CZ	1:F:184:LYS:NZ	2.88	0.41
1:K:158:TYR:CG	1:K:159:PRO:HD2	2.55	0.41
1:G:9:ARG:HH11	1:G:388:ALA:CA	2.33	0.41
1:H:9:ARG:HB3	1:H:387:LEU:HD11	2.02	0.41
1:F:299:LEU:O	1:F:303:GLN:HG3	2.21	0.41
1:M:299:LEU:O	1:M:303:GLN:HG3	2.20	0.41
1:N:190:ILE:CG2	1:N:191:GLU:H	2.33	0.41
1:P:179:ASN:HD22	1:P:180:VAL:N	2.19	0.41
1:B:340:ASN:HD22	1:B:341:GLU:H	1.67	0.41
1:H:10:GLU:HB3	1:H:65:ARG:NH1	2.36	0.41
1:G:243:ASP:HA	1:G:244:PRO:HD3	1.97	0.41
1:J:87:ASN:OD1	1:J:88:LEU:N	2.54	0.41
1:B:182:LYS:HZ2	1:B:239:GLU:CD	2.22	0.41
1:G:355:ASP:OD1	1:G:378:SER:N	2.45	0.41
1:I:76:ASP:HA	1:I:77:PRO:HD2	1.90	0.41
1:O:216:GLY:CA	1:O:240:GLU:HG2	2.51	0.41
1:M:90:PRO:HG3	1:M:124:VAL:HG21	2.03	0.41
1:I:216:GLY:CA	1:I:240:GLU:HG2	2.51	0.41
1:P:344:PRO:O	1:P:345:ASP:C	2.57	0.41
1:J:243:ASP:OD1	1:J:244:PRO:HD2	2.21	0.41
1:A:216:GLY:CA	1:A:240:GLU:HG2	2.50	0.41
1:J:68:PHE:CZ	1:J:109:ARG:HB2	2.55	0.41
1:K:326:GLN:OE1	1:K:326:GLN:N	2.49	0.41
1:L:243:ASP:HA	1:L:244:PRO:HD3	1.93	0.41
1:O:322:HIS:CG	1:O:323:GLY:N	2.88	0.41
1:F:26:PHE:N	1:F:26:PHE:CD1	2.88	0.41
1:B:326:GLN:OE1	1:B:326:GLN:N	2.50	0.41
1:I:237:TRP:C	1:I:237:TRP:CD1	2.94	0.41
1:C:296:SER:O	1:C:297:TYR:HB2	2.21	0.41
1:M:24:ILE:HD12	1:N:100:ASN:C	2.41	0.41
1:N:24:ILE:CG2	1:N:25:ASP:N	2.83	0.41
1:I:164:SER:O	1:I:167:ARG:HB2	2.21	0.41
1:A:156:TYR:CE1	1:A:184:LYS:HE3	2.57	0.41
1:I:60:GLN:HG3	1:I:111:VAL:HB	2.03	0.41
1:O:87:ASN:OD1	1:O:88:LEU:N	2.54	0.41
1:A:5:ILE:HD11	1:A:88:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:120:VAL:O	1:N:124:VAL:HG23	2.21	0.41
1:G:349:PRO:HD2	1:G:350:TYR:CE1	2.55	0.41
1:F:216:GLY:CA	1:F:240:GLU:HG2	2.51	0.41
1:D:120:VAL:O	1:D:124:VAL:HG23	2.20	0.41
1:J:164:SER:O	1:J:167:ARG:HB2	2.21	0.40
1:F:340:ASN:ND2	1:F:341:GLU:N	2.69	0.40
1:E:190:ILE:HG23	1:E:191:GLU:N	2.36	0.40
1:E:216:GLY:CA	1:E:240:GLU:HG2	2.50	0.40
1:L:90:PRO:HG3	1:L:124:VAL:HG21	2.02	0.40
1:F:190:ILE:HG23	1:F:191:GLU:N	2.36	0.40
1:E:8:VAL:HG23	1:E:73:LEU:HD21	2.03	0.40
1:F:226:TYR:O	1:F:230:LEU:HB2	2.21	0.40
1:K:164:SER:O	1:K:167:ARG:HB2	2.22	0.40
1:A:184:LYS:HD2	1:A:215:ASN:HD21	1.84	0.40
1:M:17:SER:C	1:M:19:ILE:H	2.24	0.40
1:C:184:LYS:HD2	1:C:215:ASN:ND2	2.34	0.40
1:H:11:ILE:HG23	1:H:11:ILE:O	2.21	0.40
1:J:158:TYR:CG	1:J:159:PRO:HD2	2.56	0.40
1:N:65:ARG:CG	1:N:65:ARG:NH1	2.84	0.40
1:K:60:GLN:O	1:K:64:ILE:HG13	2.21	0.40
1:L:216:GLY:CA	1:L:240:GLU:HG2	2.50	0.40
1:M:349:PRO:O	1:M:351:GLY:N	2.53	0.40
1:L:188:ALA:O	1:L:189:PRO:C	2.59	0.40
1:N:35:ALA:HA	1:N:49:GLY:O	2.21	0.40
1:F:237:TRP:C	1:F:237:TRP:CD1	2.94	0.40
1:I:381:TYR:CE2	1:I:385:LYS:HD3	2.57	0.40
1:B:117:ASP:CG	1:B:298:GLY:HA3	2.42	0.40
1:K:24:ILE:CG2	1:K:25:ASP:N	2.84	0.40
1:L:158:TYR:CG	1:L:159:PRO:HD2	2.57	0.40
1:H:158:TYR:CG	1:H:159:PRO:HD2	2.57	0.40
1:P:299:LEU:O	1:P:303:GLN:HG3	2.21	0.40
1:H:120:VAL:O	1:H:124:VAL:HG23	2.22	0.40
1:G:184:LYS:NZ	3:G:1007:SRT:O41	2.54	0.40
1:H:349:PRO:HB3	1:H:379:ASP:OD2	2.21	0.40
1:O:353:PHE:O	1:O:377:LYS:HD2	2.21	0.40
1:N:322:HIS:CG	1:N:323:GLY:N	2.89	0.40
1:B:322:HIS:CG	1:B:323:GLY:N	2.89	0.40
1:B:243:ASP:OD1	1:B:244:PRO:HD2	2.21	0.40
1:F:322:HIS:CG	1:F:323:GLY:N	2.89	0.40
1:J:120:VAL:O	1:J:124:VAL:HG23	2.21	0.40
1:H:358:ARG:HB3	1:H:358:ARG:CZ	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:241:VAL:HG21	1:K:253:LEU:HD23	2.04	0.40
1:F:158:TYR:CG	1:F:159:PRO:HD2	2.56	0.40
1:E:299:LEU:O	1:E:303:GLN:HG3	2.21	0.40
1:N:184:LYS:HD3	1:N:184:LYS:HA	1.90	0.40
1:M:164:SER:O	1:M:167:ARG:HB2	2.21	0.40
1:N:350:TYR:OH	1:N:383:GLU:HG2	2.21	0.40
1:I:24:ILE:HD11	1:J:102:LYS:HA	2.04	0.40
1:K:354:PRO:O	1:K:357:VAL:HG13	2.21	0.40
1:I:179:ASN:C	1:I:179:ASN:ND2	2.74	0.40
1:A:240:GLU:HG3	4:A:2034:HOH:O	2.22	0.40
1:C:244:PRO:CD	1:D:103:PRO:HB2	2.51	0.40
1:D:182:LYS:HA	1:D:211:ALA:O	2.21	0.40
1:I:283:ARG:HD3	1:I:283:ARG:N	2.36	0.40
1:M:237:TRP:CD1	1:M:237:TRP:C	2.95	0.40
1:L:24:ILE:CG2	1:L:25:ASP:N	2.83	0.40
1:P:4:ARG:HG2	1:P:77:PRO:HB3	2.04	0.40
1:A:19:ILE:CD1	1:A:346:LEU:HD23	2.50	0.40
1:C:193:ASP:O	1:C:197:ILE:HG13	2.21	0.40
1:E:11:ILE:CG2	1:E:387:LEU:HD13	2.51	0.40
1:B:90:PRO:HG3	1:B:124:VAL:HG21	2.03	0.40
1:G:332:ALA:HA	1:G:337:LEU:HG	2.02	0.40
1:L:13:LYS:HE2	1:L:383:GLU:HG3	2.03	0.40
1:M:50:TYR:CD1	1:M:384:MET:HB3	2.57	0.40
1:B:25:ASP:C	1:B:25:ASP:OD1	2.58	0.40
1:O:15:ILE:HG13	1:O:15:ILE:O	2.21	0.40

There are no symmetry-related clashes.

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	386/389 (99%)	370 (96%)	16 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	386/389 (99%)	366 (95%)	20 (5%)	0	100	100
1	C	386/389 (99%)	373 (97%)	11 (3%)	2 (0%)	34	55
1	D	386/389 (99%)	374 (97%)	12 (3%)	0	100	100
1	E	386/389 (99%)	367 (95%)	18 (5%)	1 (0%)	46	68
1	F	386/389 (99%)	367 (95%)	18 (5%)	1 (0%)	46	68
1	G	386/389 (99%)	371 (96%)	14 (4%)	1 (0%)	46	68
1	H	386/389 (99%)	369 (96%)	17 (4%)	0	100	100
1	I	386/389 (99%)	367 (95%)	18 (5%)	1 (0%)	46	68
1	J	386/389 (99%)	367 (95%)	18 (5%)	1 (0%)	46	68
1	K	386/389 (99%)	371 (96%)	15 (4%)	0	100	100
1	L	386/389 (99%)	358 (93%)	26 (7%)	2 (0%)	34	55
1	M	386/389 (99%)	365 (95%)	20 (5%)	1 (0%)	46	68
1	N	386/389 (99%)	365 (95%)	21 (5%)	0	100	100
1	O	386/389 (99%)	367 (95%)	17 (4%)	2 (0%)	34	55
1	P	386/389 (99%)	363 (94%)	15 (4%)	8 (2%)	9	14
All	All	6176/6224 (99%)	5880 (95%)	276 (4%)	20 (0%)	46	68

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	108	GLU
1	J	188	ALA
1	M	350	TYR
1	P	66	GLU
1	P	352	GLY
1	P	357	VAL
1	C	347	PHE
1	L	189	PRO
1	P	346	LEU
1	P	14	PRO
1	P	350	TYR
1	C	15	ILE
1	P	108	GLU
1	I	77	PRO
1	L	15	ILE
1	E	15	ILE
1	O	15	ILE

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Mol	Chain	Res	Type
1	P	77	PRO
1	G	15	ILE
1	O	19	ILE

5.3.2 Protein sidechains [i](#)

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	308/309 (100%)	293 (95%)	15 (5%)	31	55
1	B	308/309 (100%)	291 (94%)	17 (6%)	27	48
1	C	308/309 (100%)	295 (96%)	13 (4%)	36	62
1	D	308/309 (100%)	291 (94%)	17 (6%)	27	48
1	E	308/309 (100%)	291 (94%)	17 (6%)	27	48
1	F	308/309 (100%)	292 (95%)	16 (5%)	29	51
1	G	308/309 (100%)	294 (96%)	14 (4%)	34	59
1	H	308/309 (100%)	293 (95%)	15 (5%)	31	55
1	I	308/309 (100%)	291 (94%)	17 (6%)	27	48
1	J	308/309 (100%)	296 (96%)	12 (4%)	39	66
1	K	308/309 (100%)	293 (95%)	15 (5%)	31	55
1	L	308/309 (100%)	292 (95%)	16 (5%)	29	51
1	M	308/309 (100%)	293 (95%)	15 (5%)	31	55
1	N	308/309 (100%)	289 (94%)	19 (6%)	23	41
1	O	308/309 (100%)	292 (95%)	16 (5%)	29	51
1	P	308/309 (100%)	290 (94%)	18 (6%)	25	45
All	All	4928/4944 (100%)	4676 (95%)	252 (5%)	29	52

All (252) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG

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Mol	Chain	Res	Type
1	A	23	TYR
1	A	24	ILE
1	A	25	ASP
1	A	166	LEU
1	A	179	ASN
1	A	201	LEU
1	A	230	LEU
1	A	235	LEU
1	A	237	TRP
1	A	253	LEU
1	A	309	LEU
1	A	322	HIS
1	A	357	VAL
1	A	380	LEU
1	B	19	ILE
1	B	23	TYR
1	B	25	ASP
1	B	108	GLU
1	B	166	LEU
1	B	176	ARG
1	B	179	ASN
1	B	230	LEU
1	B	235	LEU
1	B	237	TRP
1	B	253	LEU
1	B	283	ARG
1	B	309	LEU
1	B	322	HIS
1	B	345	ASP
1	B	358	ARG
1	B	380	LEU
1	C	23	TYR
1	C	25	ASP
1	C	166	LEU
1	C	179	ASN
1	C	201	LEU
1	C	230	LEU
1	C	235	LEU
1	C	237	TRP
1	C	253	LEU
1	C	283	ARG
1	C	309	LEU

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Mol	Chain	Res	Type
1	C	322	HIS
1	C	380	LEU
1	D	19	ILE
1	D	23	TYR
1	D	24	ILE
1	D	25	ASP
1	D	108	GLU
1	D	117	ASP
1	D	166	LEU
1	D	179	ASN
1	D	201	LEU
1	D	230	LEU
1	D	235	LEU
1	D	237	TRP
1	D	253	LEU
1	D	283	ARG
1	D	309	LEU
1	D	322	HIS
1	D	380	LEU
1	E	19	ILE
1	E	23	TYR
1	E	25	ASP
1	E	108	GLU
1	E	117	ASP
1	E	145	ASN
1	E	166	LEU
1	E	179	ASN
1	E	201	LEU
1	E	230	LEU
1	E	235	LEU
1	E	237	TRP
1	E	253	LEU
1	E	283	ARG
1	E	309	LEU
1	E	322	HIS
1	E	380	LEU
1	F	4	ARG
1	F	16	SER
1	F	25	ASP
1	F	70	SER
1	F	166	LEU
1	F	179	ASN

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Mol	Chain	Res	Type
1	F	201	LEU
1	F	230	LEU
1	F	235	LEU
1	F	237	TRP
1	F	253	LEU
1	F	283	ARG
1	F	309	LEU
1	F	322	HIS
1	F	357	VAL
1	F	380	LEU
1	G	25	ASP
1	G	108	GLU
1	G	166	LEU
1	G	179	ASN
1	G	201	LEU
1	G	230	LEU
1	G	235	LEU
1	G	237	TRP
1	G	253	LEU
1	G	283	ARG
1	G	309	LEU
1	G	322	HIS
1	G	340	ASN
1	G	380	LEU
1	H	24	ILE
1	H	25	ASP
1	H	43	GLU
1	H	108	GLU
1	H	166	LEU
1	H	179	ASN
1	H	230	LEU
1	H	235	LEU
1	H	237	TRP
1	H	253	LEU
1	H	283	ARG
1	H	309	LEU
1	H	322	HIS
1	H	347	PHE
1	H	380	LEU
1	I	16	SER
1	I	19	ILE
1	I	23	TYR

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Mol	Chain	Res	Type
1	I	25	ASP
1	I	108	GLU
1	I	117	ASP
1	I	166	LEU
1	I	179	ASN
1	I	201	LEU
1	I	230	LEU
1	I	235	LEU
1	I	237	TRP
1	I	253	LEU
1	I	283	ARG
1	I	309	LEU
1	I	322	HIS
1	I	380	LEU
1	J	25	ASP
1	J	166	LEU
1	J	179	ASN
1	J	189	PRO
1	J	230	LEU
1	J	235	LEU
1	J	237	TRP
1	J	253	LEU
1	J	283	ARG
1	J	309	LEU
1	J	322	HIS
1	J	380	LEU
1	K	25	ASP
1	K	108	GLU
1	K	166	LEU
1	K	179	ASN
1	K	201	LEU
1	K	230	LEU
1	K	235	LEU
1	K	237	TRP
1	K	253	LEU
1	K	283	ARG
1	K	309	LEU
1	K	322	HIS
1	K	357	VAL
1	K	358	ARG
1	K	380	LEU
1	L	23	TYR

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Mol	Chain	Res	Type
1	L	24	ILE
1	L	25	ASP
1	L	117	ASP
1	L	147	ARG
1	L	166	LEU
1	L	179	ASN
1	L	189	PRO
1	L	230	LEU
1	L	235	LEU
1	L	237	TRP
1	L	253	LEU
1	L	283	ARG
1	L	309	LEU
1	L	322	HIS
1	L	380	LEU
1	M	19	ILE
1	M	23	TYR
1	M	25	ASP
1	M	108	GLU
1	M	117	ASP
1	M	166	LEU
1	M	179	ASN
1	M	230	LEU
1	M	235	LEU
1	M	237	TRP
1	M	253	LEU
1	M	283	ARG
1	M	309	LEU
1	M	322	HIS
1	M	380	LEU
1	N	19	ILE
1	N	23	TYR
1	N	25	ASP
1	N	43	GLU
1	N	108	GLU
1	N	117	ASP
1	N	166	LEU
1	N	179	ASN
1	N	202	GLU
1	N	230	LEU
1	N	235	LEU
1	N	237	TRP

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Mol	Chain	Res	Type
1	N	253	LEU
1	N	283	ARG
1	N	309	LEU
1	N	322	HIS
1	N	346	LEU
1	N	358	ARG
1	N	380	LEU
1	O	19	ILE
1	O	23	TYR
1	O	25	ASP
1	O	67	ARG
1	O	108	GLU
1	O	166	LEU
1	O	176	ARG
1	O	179	ASN
1	O	230	LEU
1	O	235	LEU
1	O	237	TRP
1	O	253	LEU
1	O	283	ARG
1	O	309	LEU
1	O	322	HIS
1	O	380	LEU
1	P	9	ARG
1	P	10	GLU
1	P	17	SER
1	P	23	TYR
1	P	24	ILE
1	P	25	ASP
1	P	108	GLU
1	P	166	LEU
1	P	179	ASN
1	P	201	LEU
1	P	230	LEU
1	P	235	LEU
1	P	237	TRP
1	P	253	LEU
1	P	283	ARG
1	P	309	LEU
1	P	322	HIS
1	P	380	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (109) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	HIS
1	A	179	ASN
1	A	215	ASN
1	A	250	GLN
1	A	270	HIS
1	A	303	GLN
1	A	340	ASN
1	B	140	HIS
1	B	179	ASN
1	B	215	ASN
1	B	270	HIS
1	B	303	GLN
1	B	340	ASN
1	C	140	HIS
1	C	179	ASN
1	C	215	ASN
1	C	250	GLN
1	C	270	HIS
1	C	303	GLN
1	C	340	ASN
1	D	140	HIS
1	D	179	ASN
1	D	215	ASN
1	D	250	GLN
1	D	270	HIS
1	D	303	GLN
1	D	340	ASN
1	E	140	HIS
1	E	145	ASN
1	E	179	ASN
1	E	215	ASN
1	E	250	GLN
1	E	270	HIS
1	E	303	GLN
1	E	340	ASN
1	F	140	HIS
1	F	179	ASN
1	F	215	ASN
1	F	270	HIS
1	F	303	GLN
1	F	340	ASN
1	G	140	HIS

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Mol	Chain	Res	Type
1	G	179	ASN
1	G	215	ASN
1	G	250	GLN
1	G	270	HIS
1	G	303	GLN
1	G	340	ASN
1	H	140	HIS
1	H	179	ASN
1	H	215	ASN
1	H	250	GLN
1	H	270	HIS
1	H	303	GLN
1	H	340	ASN
1	I	140	HIS
1	I	179	ASN
1	I	215	ASN
1	I	270	HIS
1	I	303	GLN
1	I	340	ASN
1	J	140	HIS
1	J	179	ASN
1	J	215	ASN
1	J	270	HIS
1	J	303	GLN
1	J	340	ASN
1	K	140	HIS
1	K	179	ASN
1	K	215	ASN
1	K	250	GLN
1	K	270	HIS
1	K	303	GLN
1	K	340	ASN
1	L	140	HIS
1	L	179	ASN
1	L	215	ASN
1	L	250	GLN
1	L	270	HIS
1	L	303	GLN
1	L	340	ASN
1	L	348	GLN
1	M	140	HIS
1	M	179	ASN

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Mol	Chain	Res	Type
1	M	215	ASN
1	M	250	GLN
1	M	270	HIS
1	M	303	GLN
1	M	340	ASN
1	N	140	HIS
1	N	179	ASN
1	N	215	ASN
1	N	270	HIS
1	N	303	GLN
1	N	340	ASN
1	O	140	HIS
1	O	179	ASN
1	O	215	ASN
1	O	250	GLN
1	O	270	HIS
1	O	303	GLN
1	O	340	ASN
1	P	140	HIS
1	P	179	ASN
1	P	215	ASN
1	P	250	GLN
1	P	270	HIS
1	P	303	GLN
1	P	340	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 32 ligands modelled in this entry, 16 are monoatomic - leaving 16 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
3	SRT	A	1001	2	3,9,9	0.65	0	6,12,12	1.02	0
3	SRT	B	1002	2	3,9,9	0.59	0	6,12,12	0.94	0
3	SRT	C	1003	2	3,9,9	0.81	0	6,12,12	1.10	0
3	SRT	D	1004	2	3,9,9	0.89	0	6,12,12	0.96	0
3	SRT	E	1005	2	3,9,9	0.84	0	6,12,12	0.99	0
3	SRT	F	1006	2	3,9,9	0.83	0	6,12,12	1.06	0
3	SRT	G	1007	2	3,9,9	0.84	0	6,12,12	1.14	1 (16%)
3	SRT	H	1008	2	3,9,9	0.75	0	6,12,12	0.98	0
3	SRT	I	1009	2	3,9,9	0.54	0	6,12,12	0.91	0
3	SRT	J	1010	2	3,9,9	0.79	0	6,12,12	0.91	0
3	SRT	K	1011	2	3,9,9	0.85	0	6,12,12	1.00	0
3	SRT	L	1012	2	3,9,9	0.75	0	6,12,12	0.88	0
3	SRT	M	1013	2	3,9,9	0.82	0	6,12,12	0.88	0
3	SRT	N	1014	2	3,9,9	0.62	0	6,12,12	0.92	0
3	SRT	O	1015	2	3,9,9	0.68	0	6,12,12	0.94	0
3	SRT	P	1016	2	3,9,9	0.73	0	6,12,12	0.92	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
3	SRT	A	1001	2	-	0/4/12/12	0/0/0/0
3	SRT	B	1002	2	-	0/4/12/12	0/0/0/0
3	SRT	C	1003	2	-	0/4/12/12	0/0/0/0
3	SRT	D	1004	2	-	0/4/12/12	0/0/0/0
3	SRT	E	1005	2	-	0/4/12/12	0/0/0/0
3	SRT	F	1006	2	-	0/4/12/12	0/0/0/0
3	SRT	G	1007	2	-	0/4/12/12	0/0/0/0
3	SRT	H	1008	2	-	0/4/12/12	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SRT	I	1009	2	-	0/4/12/12	0/0/0/0
3	SRT	J	1010	2	-	0/4/12/12	0/0/0/0
3	SRT	K	1011	2	-	0/4/12/12	0/0/0/0
3	SRT	L	1012	2	-	0/4/12/12	0/0/0/0
3	SRT	M	1013	2	-	0/4/12/12	0/0/0/0
3	SRT	N	1014	2	-	0/4/12/12	0/0/0/0
3	SRT	O	1015	2	-	0/4/12/12	0/0/0/0
3	SRT	P	1016	2	-	0/4/12/12	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1007	SRT	C4-C3-C2	-2.04	109.17	113.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	SRT	2	0
3	B	1002	SRT	2	0
3	C	1003	SRT	3	0
3	D	1004	SRT	3	0
3	E	1005	SRT	2	0
3	F	1006	SRT	1	0
3	G	1007	SRT	4	0
3	H	1008	SRT	2	0
3	I	1009	SRT	4	0
3	J	1010	SRT	1	0
3	K	1011	SRT	1	0
3	L	1012	SRT	3	0
3	N	1014	SRT	3	0
3	P	1016	SRT	3	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 ⓘ

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	388/389 (99%)	-0.13	5 (1%) 79 82	14, 34, 57, 76	0
1	B	388/389 (99%)	0.42	18 (4%) 36 41	21, 49, 68, 84	0
1	C	388/389 (99%)	-0.15	3 (0%) 87 89	13, 30, 48, 77	0
1	D	388/389 (99%)	-0.19	4 (1%) 84 86	13, 32, 50, 73	0
1	E	388/389 (99%)	0.15	10 (2%) 59 63	16, 43, 66, 89	0
1	F	388/389 (99%)	-0.09	3 (0%) 87 89	11, 34, 64, 77	0
1	G	388/389 (99%)	0.12	11 (2%) 56 61	14, 41, 69, 81	0
1	H	388/389 (99%)	0.35	13 (3%) 49 54	18, 49, 67, 82	0
1	I	388/389 (99%)	0.18	12 (3%) 52 57	22, 43, 71, 90	0
1	J	388/389 (99%)	0.40	21 (5%) 29 33	19, 49, 70, 78	0
1	K	388/389 (99%)	-0.06	6 (1%) 76 79	14, 38, 63, 84	0
1	L	388/389 (99%)	0.46	23 (5%) 26 29	20, 53, 72, 83	0
1	M	388/389 (99%)	0.36	17 (4%) 38 43	24, 53, 69, 89	0
1	N	388/389 (99%)	0.45	30 (7%) 16 18	26, 58, 77, 87	0
1	O	388/389 (99%)	0.59	30 (7%) 16 18	34, 56, 72, 83	0
1	P	388/389 (99%)	0.89	53 (13%) 4 4	30, 62, 80, 94	0
All	All	6208/6224 (99%)	0.23	259 (4%) 40 45	11, 45, 71, 94	0

All (259) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	44	GLY	13.5
1	P	78	LYS	5.7
1	L	44	GLY	5.5
1	O	158	TYR	5.4
1	P	146	PRO	5.3

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Mol	Chain	Res	Type	RSRZ
1	P	84	ALA	5.2
1	I	2	SER	5.1
1	P	3	VAL	5.1
1	P	5	ILE	4.9
1	P	45	LYS	4.8
1	B	84	ALA	4.7
1	P	42	ARG	4.7
1	P	358	ARG	4.7
1	I	84	ALA	4.5
1	E	41	VAL	4.5
1	H	41	VAL	4.5
1	E	43	GLU	4.3
1	P	40	VAL	4.3
1	O	195	MET	4.2
1	P	368	ASP	4.2
1	E	84	ALA	4.2
1	P	6	VAL	4.1
1	P	73	LEU	4.1
1	J	158	TYR	4.1
1	L	84	ALA	4.0
1	N	45	LYS	3.9
1	B	45	LYS	3.9
1	F	79	LYS	3.9
1	L	166	LEU	3.7
1	L	83	GLU	3.6
1	N	47	VAL	3.6
1	A	44	GLY	3.6
1	G	81	LEU	3.6
1	P	48	VAL	3.5
1	O	178	TYR	3.5
1	G	43	GLU	3.5
1	J	206	LYS	3.5
1	M	45	LYS	3.5
1	L	163	LEU	3.4
1	N	84	ALA	3.4
1	L	3	VAL	3.3
1	M	84	ALA	3.3
1	L	208	ALA	3.2
1	M	5	ILE	3.2
1	P	85	GLY	3.2
1	B	83	GLU	3.2
1	G	3	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	I	42	ARG	3.2
1	N	37	VAL	3.1
1	P	195	MET	3.1
1	L	357	VAL	3.1
1	L	358	ARG	3.1
1	O	210	LEU	3.1
1	P	37	VAL	3.1
1	B	356	GLY	3.1
1	L	43	GLU	3.0
1	M	160	GLY	3.0
1	G	80	LEU	3.0
1	J	164	SER	3.0
1	O	163	LEU	3.0
1	C	44	GLY	3.0
1	H	350	TYR	3.0
1	K	3	VAL	2.9
1	P	367	PRO	2.9
1	O	160	GLY	2.9
1	P	83	GLU	2.8
1	B	207	ASP	2.8
1	L	201	LEU	2.8
1	L	206	LYS	2.8
1	O	165	MET	2.8
1	E	42	ARG	2.8
1	M	358	ARG	2.8
1	P	133	PHE	2.8
1	O	376	GLY	2.8
1	P	96	ALA	2.8
1	P	362	GLY	2.8
1	O	387	LEU	2.8
1	I	85	GLY	2.8
1	K	43	GLU	2.8
1	G	40	VAL	2.8
1	D	84	ALA	2.8
1	N	9	ARG	2.8
1	J	201	LEU	2.7
1	L	160	GLY	2.7
1	O	367	PRO	2.7
1	J	45	LYS	2.7
1	P	130	LYS	2.7
1	N	86	ASP	2.7
1	M	158	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	190	ILE	2.7
1	H	165	MET	2.7
1	P	47	VAL	2.7
1	E	78	LYS	2.7
1	N	73	LEU	2.7
1	L	170	MET	2.7
1	G	2	SER	2.6
1	N	385	LYS	2.6
1	P	126	LYS	2.6
1	A	158	TYR	2.6
1	J	233	TYR	2.6
1	D	358	ARG	2.6
1	A	45	LYS	2.6
1	E	45	LYS	2.6
1	N	41	VAL	2.6
1	N	143	LYS	2.6
1	J	135	LEU	2.6
1	P	135	LEU	2.6
1	P	38	THR	2.6
1	H	347	PHE	2.6
1	N	133	PHE	2.6
1	O	125	ALA	2.6
1	G	37	VAL	2.6
1	H	233	TYR	2.6
1	P	369	LEU	2.6
1	P	136	LEU	2.6
1	P	106	HIS	2.6
1	A	2	SER	2.5
1	O	201	LEU	2.5
1	J	256	PHE	2.5
1	M	43	GLU	2.5
1	P	2	SER	2.5
1	J	178	TYR	2.5
1	H	45	LYS	2.5
1	O	159	PRO	2.5
1	O	335	LEU	2.5
1	N	5	ILE	2.5
1	M	389	GLU	2.5
1	P	46	ARG	2.5
1	K	385	LYS	2.5
1	O	78	LYS	2.5
1	J	44	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	P	110	SER	2.5
1	B	6	VAL	2.5
1	P	131	PRO	2.5
1	J	163	LEU	2.5
1	O	369	LEU	2.5
1	B	178	TYR	2.5
1	P	39	ASP	2.5
1	I	295	LEU	2.5
1	P	330	ASN	2.5
1	G	6	VAL	2.4
1	E	208	ALA	2.4
1	K	45	LYS	2.4
1	L	207	ASP	2.4
1	O	85	GLY	2.4
1	P	160	GLY	2.4
1	N	48	VAL	2.4
1	F	84	ALA	2.4
1	E	158	TYR	2.4
1	J	18	PRO	2.4
1	P	87	ASN	2.4
1	P	334	GLY	2.4
1	M	83	GLU	2.4
1	F	4	ARG	2.4
1	I	41	VAL	2.4
1	O	206	LYS	2.4
1	O	183	MET	2.4
1	O	363	HIS	2.4
1	P	69	ALA	2.4
1	E	79	LYS	2.3
1	H	353	PHE	2.3
1	M	78	LYS	2.3
1	B	43	GLU	2.3
1	O	164	SER	2.3
1	H	388	ALA	2.3
1	N	370	PRO	2.3
1	P	88	LEU	2.3
1	K	44	GLY	2.3
1	N	373	GLY	2.3
1	J	207	ASP	2.3
1	O	161	LYS	2.3
1	L	157	TYR	2.3
1	K	358	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	I	83	GLU	2.3
1	N	135	LEU	2.3
1	N	158	TYR	2.3
1	B	160	GLY	2.3
1	H	362	GLY	2.3
1	O	142	VAL	2.3
1	L	361	ASN	2.3
1	J	358	ARG	2.3
1	N	87	ASN	2.2
1	P	140	HIS	2.2
1	G	44	GLY	2.2
1	B	358	ARG	2.2
1	J	212	VAL	2.2
1	P	41	VAL	2.2
1	I	165	MET	2.2
1	P	384	MET	2.2
1	B	41	VAL	2.2
1	N	78	LYS	2.2
1	I	86	ASP	2.2
1	P	378	SER	2.2
1	O	83	GLU	2.2
1	B	353	PHE	2.2
1	A	83	GLU	2.2
1	J	204	ILE	2.2
1	N	72	ILE	2.2
1	O	224	ILE	2.2
1	P	114	GLY	2.2
1	M	347	PHE	2.2
1	H	163	LEU	2.2
1	J	43	GLU	2.2
1	L	203	GLU	2.2
1	N	359	VAL	2.2
1	I	130	LYS	2.2
1	M	42	ARG	2.2
1	I	358	ARG	2.2
1	M	370	PRO	2.2
1	N	131	PRO	2.2
1	P	381	TYR	2.2
1	O	129	GLY	2.2
1	N	81	LEU	2.2
1	N	142	VAL	2.1
1	O	41	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	P	372	ILE	2.1
1	D	382	LYS	2.1
1	B	4	ARG	2.1
1	G	88	LEU	2.1
1	O	380	LEU	2.1
1	M	106	HIS	2.1
1	C	296	SER	2.1
1	P	105	GLY	2.1
1	J	236	PHE	2.1
1	C	43	GLU	2.1
1	O	40	VAL	2.1
1	L	366	MET	2.1
1	H	43	GLU	2.1
1	N	368	ASP	2.1
1	G	45	LYS	2.1
1	M	387	LEU	2.1
1	P	81	LEU	2.1
1	H	84	ALA	2.1
1	J	41	VAL	2.1
1	M	48	VAL	2.1
1	P	142	VAL	2.1
1	B	228	LYS	2.1
1	M	157	TYR	2.1
1	I	81	LEU	2.1
1	B	44	GLY	2.1
1	O	356	GLY	2.1
1	P	43	GLU	2.1
1	J	208	ALA	2.1
1	B	181	VAL	2.1
1	P	350	TYR	2.1
1	D	268	PHE	2.1
1	E	143	LYS	2.1
1	L	81	LEU	2.1
1	J	202	GLU	2.0
1	L	85	GLY	2.0
1	N	141	GLY	2.0
1	N	77	PRO	2.0
1	H	6	VAL	2.0
1	N	11	ILE	2.0
1	N	144	ALA	2.0
1	L	195	MET	2.0
1	N	40	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	42	ARG	2.0
1	L	45	LYS	2.0

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(Å ²)	Q<0.9
3	SRT	G	1007	10/10	0.84	0.22	2.91	32,36,40,41	0
3	SRT	E	1005	10/10	0.90	0.22	2.46	45,47,50,51	0
3	SRT	C	1003	10/10	0.88	0.20	2.20	18,28,38,45	0
3	SRT	K	1011	10/10	0.92	0.23	2.01	24,28,35,36	0
3	SRT	A	1001	10/10	0.89	0.16	1.97	26,30,32,36	0
3	SRT	D	1004	10/10	0.93	0.17	1.82	21,34,38,43	0
3	SRT	H	1008	10/10	0.91	0.22	1.79	50,54,56,57	0
2	MG	C	2003	1/1	0.97	0.16	1.65	26,26,26,26	0
3	SRT	I	1009	10/10	0.92	0.18	1.12	20,33,36,36	0
2	MG	D	2004	1/1	0.98	0.15	0.96	27,27,27,27	0
2	MG	P	2016	1/1	0.97	0.15	0.71	45,45,45,45	0
3	SRT	P	1016	10/10	0.87	0.18	0.50	51,54,55,57	0
3	SRT	F	1006	10/10	0.91	0.17	0.38	25,33,37,38	0
3	SRT	B	1002	10/10	0.89	0.19	0.35	44,49,53,54	0
3	SRT	N	1014	10/10	0.93	0.16	0.29	49,51,52,53	0
3	SRT	J	1010	10/10	0.90	0.16	0.01	45,47,52,53	0
2	MG	B	2002	1/1	0.96	0.15	-0.44	62,62,62,62	0
2	MG	H	2008	1/1	0.92	0.15	-0.45	42,42,42,42	0
3	SRT	M	1013	10/10	0.93	0.15	-0.53	47,51,52,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	SRT	L	1012	10/10	0.91	0.15	-0.63	43,46,48,49	0
2	MG	I	2009	1/1	0.92	0.12	-1.04	25,25,25,25	0
2	MG	E	2005	1/1	0.95	0.11	-1.08	39,39,39,39	0
3	SRT	O	1015	10/10	0.89	0.17	-1.10	50,52,56,58	0
2	MG	K	2011	1/1	0.95	0.14	-1.11	15,15,15,15	0
2	MG	A	2001	1/1	0.92	0.11	-1.30	20,20,20,20	0
2	MG	M	2013	1/1	0.97	0.10	-1.57	36,36,36,36	0
2	MG	L	2012	1/1	0.97	0.10	-1.87	42,42,42,42	0
2	MG	J	2010	1/1	0.93	0.08	-1.93	41,41,41,41	0
2	MG	O	2015	1/1	0.88	0.08	-2.84	43,43,43,43	0
2	MG	N	2014	1/1	0.95	0.09	-2.98	27,27,27,27	0
2	MG	F	2006	1/1	0.85	0.16	-	19,19,19,19	0
2	MG	G	2007	1/1	0.93	0.10	-	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.