



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 15, 2017 – 07:59 AM EDT

PDB ID : 3H06
Title : Crystal structure of the binding domain of the AMPA subunit GluR2 bound to the willardiine antagonist, UBP282
Authors : Ahmed, A.H.; Oswald, R.E.
Deposited on : unknown
Resolution : 2.80 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

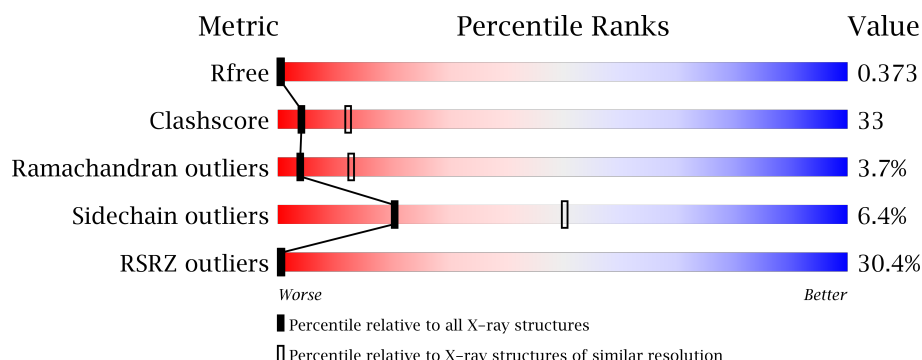
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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	B	258	<div> <div>30%</div> <div> <div>53%</div> <div>43%</div> <div>•</div> </div> </div>
1	E	258	<div> <div>36%</div> <div> <div>45%</div> <div>48%</div> <div>6%</div> </div> </div>
1	G	258	<div> <div>25%</div> <div> <div>57%</div> <div>38%</div> <div>5%</div> </div> </div>
1	H	258	<div> <div>33%</div> <div> <div>47%</div> <div>45%</div> <div>7%</div> </div> </div>
1	J	258	<div> <div>30%</div> <div> <div>51%</div> <div>43%</div> <div>5%</div> <div>•</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	L	258	
1	N	258	
1	P	258	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	VBP	B	807	X	-	-	-
2	VBP	E	808	X	-	-	-
2	VBP	G	803	X	-	-	-
2	VBP	H	806	X	-	-	-
2	VBP	J	804	X	-	-	-
2	VBP	L	801	X	-	-	-
2	VBP	N	802	X	-	-	-
2	VBP	P	805	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16564 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 Glutamate receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	257	Total	C	N	O	S	0	0	0
			2010	1280	334	382	14			
1	B	257	Total	C	N	O	S	0	0	0
			2010	1280	334	382	14			
1	E	257	Total	C	N	O	S	0	0	0
			2010	1280	334	382	14			
1	H	257	Total	C	N	O	S	0	0	0
			2010	1280	334	382	14			
1	J	257	Total	C	N	O	S	0	0	0
			2010	1280	334	382	14			
1	L	257	Total	C	N	O	S	0	0	0
			2010	1280	334	382	14			
1	N	257	Total	C	N	O	S	0	0	0
			2010	1280	334	382	14			
1	P	257	Total	C	N	O	S	0	0	0
			2010	1280	334	382	14			

There are 16 discrepancies between the modelled and reference sequences:

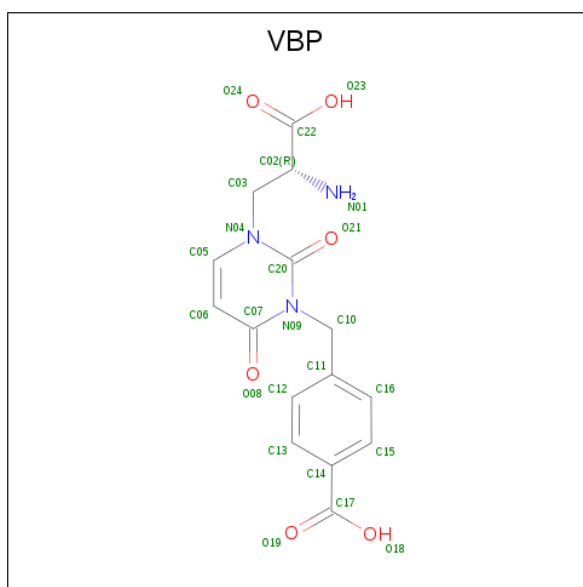
Chain	Residue	Modelled	Actual	Comment	Reference
G	118	GLY	-	LINKER	UNP P19491
G	119	THR	-	LINKER	UNP P19491
B	118	GLY	-	LINKER	UNP P19491
B	119	THR	-	LINKER	UNP P19491
E	118	GLY	-	LINKER	UNP P19491
E	119	THR	-	LINKER	UNP P19491
H	118	GLY	-	LINKER	UNP P19491
H	119	THR	-	LINKER	UNP P19491
J	118	GLY	-	LINKER	UNP P19491
J	119	THR	-	LINKER	UNP P19491
L	118	GLY	-	LINKER	UNP P19491
L	119	THR	-	LINKER	UNP P19491
N	118	GLY	-	LINKER	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
N	119	THR	-	LINKER	UNP P19491
P	118	GLY	-	LINKER	UNP P19491
P	119	THR	-	LINKER	UNP P19491

- Molecule 2 is 4-({3-[(2R)-2-amino-2-carboxyethyl]-2,6-dioxo-3,6-dihydropyrimidin-1(2H)-yl} methyl)benzoic acid (three-letter code: VBP) (formula: C₁₅H₁₅N₃O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	G	1	Total	C	N	O	0	0
			24	15	3	6		
2	B	1	Total	C	N	O	0	0
			24	15	3	6		
2	E	1	Total	C	N	O	0	0
			24	15	3	6		
2	H	1	Total	C	N	O	0	0
			24	15	3	6		
2	J	1	Total	C	N	O	0	0
			24	15	3	6		
2	L	1	Total	C	N	O	0	0
			24	15	3	6		
2	N	1	Total	C	N	O	0	0
			24	15	3	6		
2	P	1	Total	C	N	O	0	0
			24	15	3	6		

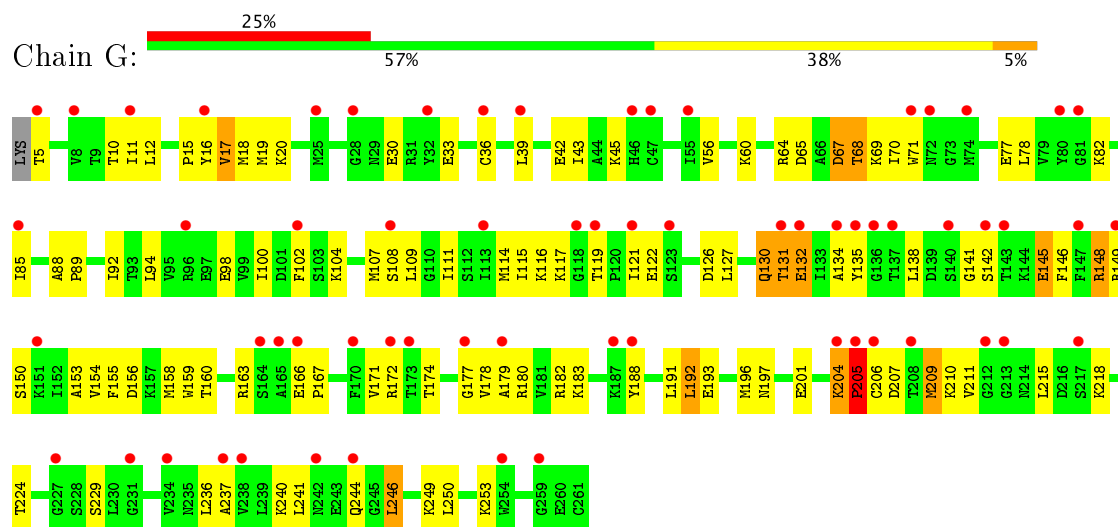
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	39	Total 39	O 39	0	0
3	B	42	Total 42	O 42	0	0
3	E	30	Total 30	O 30	0	0
3	H	30	Total 30	O 30	0	0
3	J	43	Total 43	O 43	0	0
3	L	34	Total 34	O 34	0	0
3	N	39	Total 39	O 39	0	0
3	P	35	Total 35	O 35	0	0

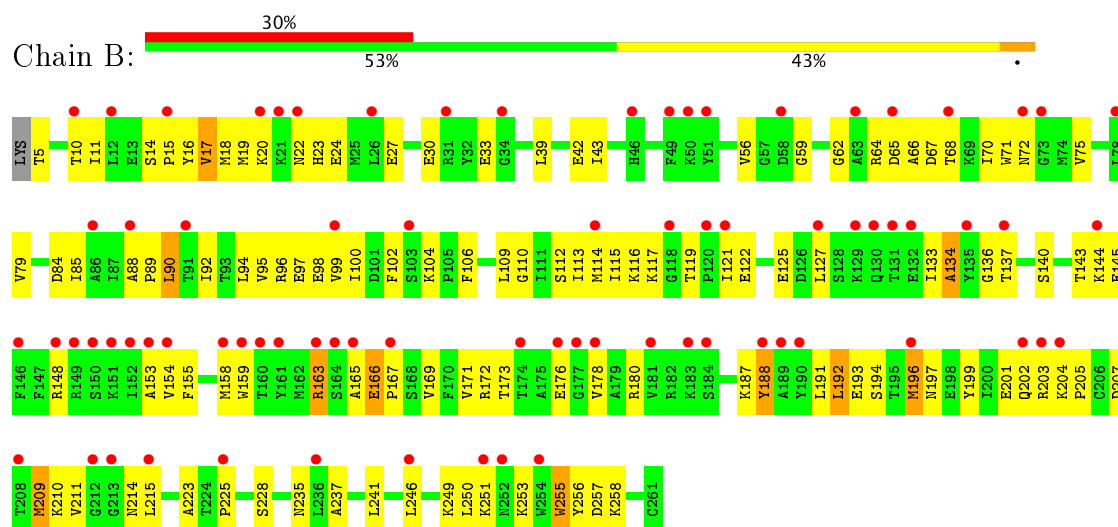
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Glutamate receptor 2

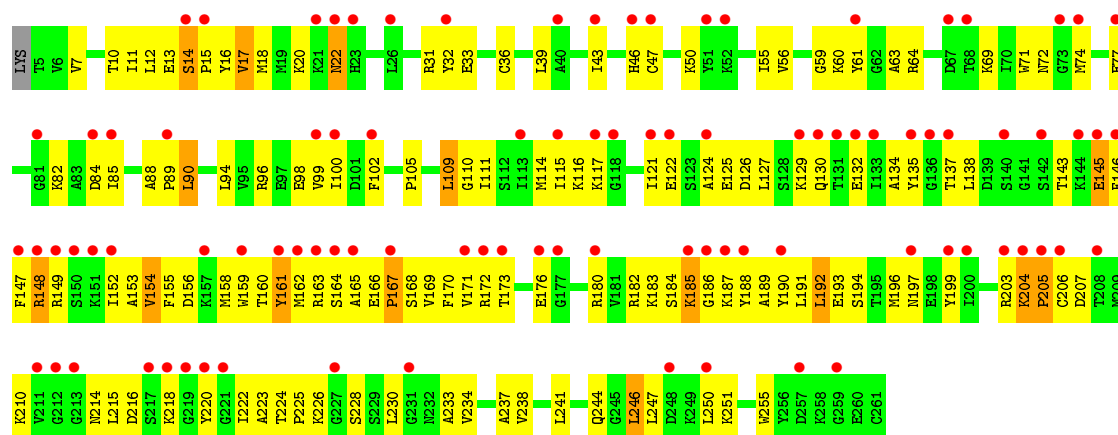


• Molecule 1: Glutamate receptor 2

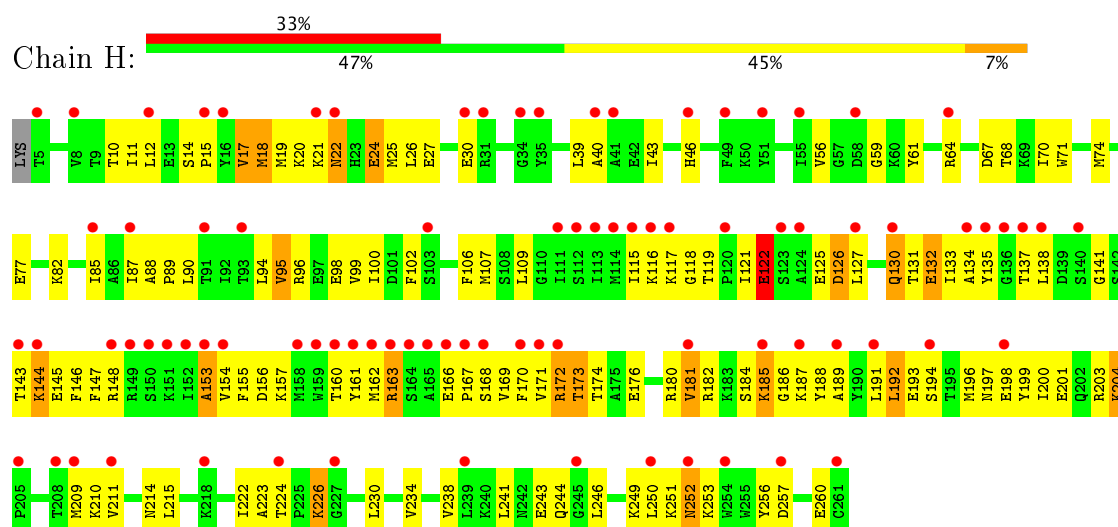


• Molecule 1: Glutamate receptor 2

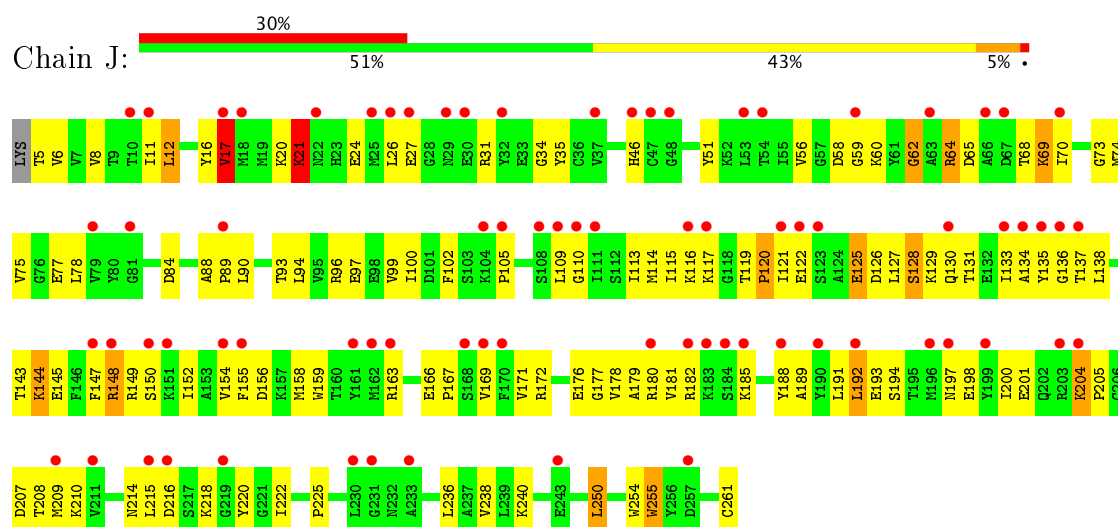




• Molecule 1: Glutamate receptor 2

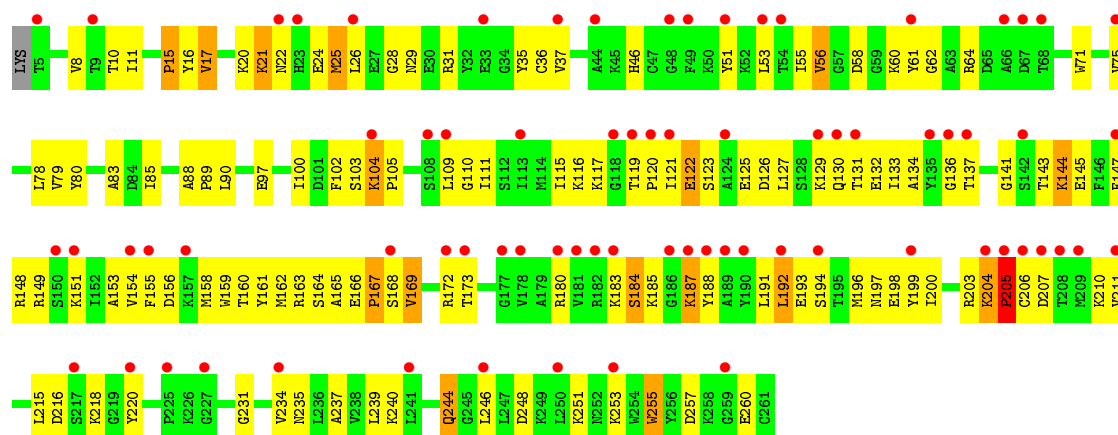


• Molecule 1: Glutamate receptor 2

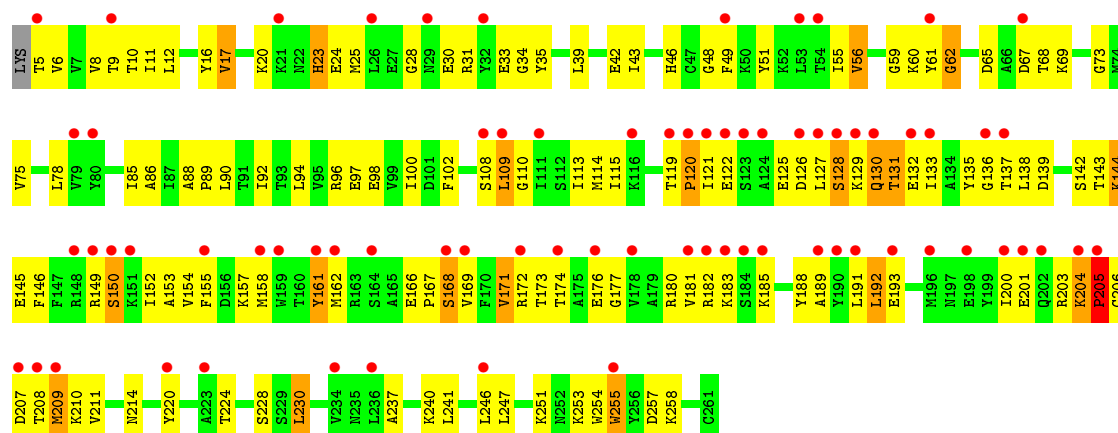


• Molecule 1: Glutamate receptor 2

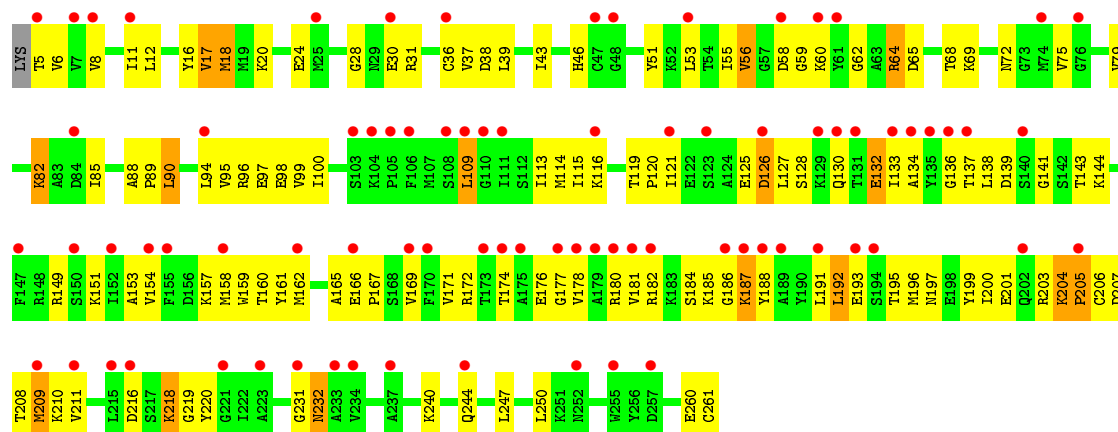




• Molecule 1: Glutamate receptor 2



• Molecule 1: Glutamate receptor 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	91.01Å 90.92Å 92.51Å 85.61° 85.52° 72.40°	Depositor
Resolution (Å)	39.71 – 2.80 39.71 – 2.78	Depositor EDS
% Data completeness (in resolution range)	93.5 (39.71-2.80) 89.8 (39.71-2.78)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	64.73 (at 2.77Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.230 , 0.295 0.375 , 0.373	Depositor DCC
R_{free} test set	3233 reflections (5.08%)	DCC
Wilson B-factor (Å ²)	39.5	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 16.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.62$, $\langle L^2 \rangle = 0.49$	Xtriage
Estimated twinning fraction	0.349 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	16564	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.87% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	B	0.41	0/2046	0.64	0/2751
1	E	0.41	0/2046	0.63	0/2751
1	G	0.41	0/2046	0.65	0/2751
1	H	0.41	0/2046	0.61	0/2751
1	J	0.40	0/2046	0.62	0/2751
1	L	0.41	0/2046	0.62	0/2751
1	N	0.39	0/2046	0.62	0/2751
1	P	0.40	0/2046	0.64	0/2751
All	All	0.40	0/16368	0.63	0/22008

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 [i](#)

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	B	2010	0	2037	133	0
1	E	2010	0	2037	140	0
1	G	2010	0	2037	116	0
1	H	2010	0	2037	139	0
1	J	2010	0	2037	134	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2010	0	2037	137	0
1	N	2010	0	2037	129	0
1	P	2010	0	2037	155	0
2	B	24	0	13	3	0
2	E	24	0	13	4	0
2	G	24	0	13	5	0
2	H	24	0	13	3	0
2	J	24	0	13	4	0
2	L	24	0	13	2	0
2	N	24	0	13	3	0
2	P	24	0	13	5	0
3	B	42	0	0	8	0
3	E	30	0	0	6	0
3	G	39	0	0	4	0
3	H	30	0	0	6	0
3	J	43	0	0	9	0
3	L	34	0	0	1	0
3	N	39	0	0	7	0
3	P	35	0	0	10	0
All	All	16564	0	16400	1065	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 33.

All (1065) 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:E:204:LYS:HB3	1:E:205:PRO:HD2	1.12	1.11
1:L:204:LYS:HB3	1:L:205:PRO:HD2	1.09	1.09
1:P:204:LYS:HB3	1:P:205:PRO:HD2	1.31	1.09
1:H:173:THR:HG23	1:H:176:GLU:HB2	1.36	1.07
1:G:204:LYS:HB3	1:G:205:PRO:HD2	1.11	1.06
1:N:204:LYS:HB3	1:N:205:PRO:HD2	1.07	1.04
1:N:204:LYS:HB3	1:N:205:PRO:CD	1.91	1.01
1:J:21:LYS:HD3	1:J:21:LYS:H	1.28	0.99
1:B:95:VAL:HG11	1:E:69:LYS:HD3	1.42	0.99
1:L:104:LYS:H	1:L:104:LYS:NZ	1.61	0.97
1:L:104:LYS:HZ3	1:L:104:LYS:H	1.01	0.96
1:L:104:LYS:N	1:L:104:LYS:HZ3	1.62	0.96
1:G:117:LYS:HE2	1:G:209:MET:HE3	1.49	0.94
1:E:185:LYS:HB2	1:E:187:LYS:HE2	1.50	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:204:LYS:HB3	1:E:205:PRO:CD	1.99	0.92
1:L:204:LYS:HB3	1:L:205:PRO:CD	1.98	0.91
1:L:130:GLN:HE21	1:L:132:GLU:HB3	1.36	0.91
1:G:114:MET:HE1	1:G:178:VAL:HG13	1.52	0.90
1:H:116:LYS:HE2	1:N:25:MET:O	1.72	0.89
1:L:204:LYS:CB	1:L:205:PRO:HD2	2.01	0.89
1:J:21:LYS:CD	1:J:21:LYS:H	1.83	0.89
1:B:121:ILE:HD13	1:B:127:LEU:HD21	1.56	0.88
1:J:117:LYS:HA	1:J:209:MET:HE3	1.53	0.88
1:L:187:LYS:HE3	1:L:188:TYR:N	1.89	0.87
1:G:204:LYS:HB3	1:G:205:PRO:CD	2.01	0.87
1:N:150:SER:HA	3:N:285:HOH:O	1.75	0.86
1:E:204:LYS:CB	1:E:205:PRO:HD2	2.01	0.85
1:N:130:GLN:NE2	1:N:132:GLU:HB3	1.89	0.85
1:P:116:LYS:HE3	1:P:207:ASP:HB2	1.56	0.84
1:G:89:PRO:HB2	2:G:803:VBP:H05	1.56	0.83
1:E:172:ARG:HB3	1:E:176:GLU:OE1	1.78	0.83
1:P:204:LYS:CB	1:P:205:PRO:HD2	2.08	0.82
1:G:204:LYS:CB	1:G:205:PRO:HD2	2.03	0.82
1:B:39:LEU:O	1:B:43:ILE:HG12	1.78	0.82
1:H:64:ARG:NH1	1:H:71:TRP:HE1	1.78	0.81
1:J:204:LYS:HB3	1:J:205:PRO:HD3	1.63	0.81
1:B:122:GLU:HA	1:B:211:VAL:HG21	1.63	0.80
1:B:89:PRO:HB2	2:B:807:VBP:H05	1.63	0.80
1:E:99:VAL:HG23	1:E:100:ILE:HG23	1.63	0.80
1:G:130:GLN:OE1	1:G:132:GLU:HB3	1.82	0.79
1:P:204:LYS:HB3	1:P:205:PRO:CD	2.12	0.79
1:E:88:ALA:HB1	1:E:89:PRO:HD2	1.62	0.79
1:H:160:THR:HA	1:H:163:ARG:NH1	1.97	0.79
1:E:152:ILE:HG22	1:E:154:VAL:HG23	1.63	0.78
1:E:10:THR:HA	1:E:74:MET:HE1	1.64	0.78
1:N:130:GLN:HE21	1:N:132:GLU:HB3	1.48	0.78
1:B:159:TRP:O	1:B:163:ARG:HB2	1.83	0.78
1:J:182:ARG:HH12	1:J:205:PRO:HB2	1.48	0.77
1:J:89:PRO:HB2	2:J:804:VBP:H05	1.66	0.76
1:P:82:LYS:NZ	1:P:82:LYS:HA	2.00	0.76
1:L:100:ILE:HD12	1:L:100:ILE:O	1.86	0.76
1:P:94:LEU:O	1:P:98:GLU:HG3	1.85	0.76
1:H:153:ALA:HA	3:H:289:HOH:O	1.85	0.76
1:E:22:ASN:H	1:E:22:ASN:HD22	1.31	0.75
1:L:22:ASN:HB2	1:L:25:MET:HG3	1.66	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:166:GLU:HA	1:J:167:PRO:C	2.07	0.75
1:G:122:GLU:HA	1:G:211:VAL:HG21	1.65	0.75
1:N:128:SER:OG	1:N:154:VAL:HG13	1.86	0.75
1:H:64:ARG:HH11	1:H:71:TRP:HE1	1.35	0.75
1:G:122:GLU:HG2	1:G:126:ASP:OD2	1.87	0.74
1:N:56:VAL:HG13	1:N:59:GLY:HA2	1.69	0.74
1:H:15:PRO:HA	1:H:18:MET:HE3	1.70	0.74
1:H:130:GLN:HE21	1:H:132:GLU:N	1.85	0.74
1:P:232:ASN:HD22	1:P:232:ASN:N	1.82	0.74
1:P:58:ASP:O	1:P:60:LYS:HG3	1.88	0.73
1:E:39:LEU:O	1:E:43:ILE:HG12	1.89	0.73
1:H:56:VAL:HG13	1:H:59:GLY:HA2	1.70	0.73
1:B:114:MET:HE1	1:B:178:VAL:HG13	1.70	0.73
1:N:115:ILE:HD13	1:N:211:VAL:HG11	1.71	0.73
1:B:140:SER:HA	1:B:144:LYS:NZ	2.03	0.73
1:H:88:ALA:HB1	1:H:89:PRO:HD2	1.69	0.73
1:L:46:HIS:CD2	1:L:240:LYS:HD2	2.24	0.73
1:P:46:HIS:CD2	1:P:240:LYS:HD2	2.24	0.73
1:B:166:GLU:HA	1:B:167:PRO:C	2.08	0.72
1:L:154:VAL:O	1:L:158:MET:HG3	1.88	0.72
1:E:224:THR:HG23	3:E:268:HOH:O	1.89	0.72
1:N:204:LYS:CB	1:N:205:PRO:HD2	2.02	0.72
1:J:148:ARG:HG3	1:J:149:ARG:N	2.04	0.72
1:B:144:LYS:HE3	1:B:148:ARG:HH22	1.54	0.71
1:L:160:THR:HA	1:L:163:ARG:NH1	2.05	0.71
1:G:68:THR:OG1	1:G:70:ILE:HB	1.91	0.71
1:H:181:VAL:O	1:H:181:VAL:HG12	1.90	0.71
1:L:111:ILE:HD11	1:L:143:THR:HA	1.73	0.71
1:E:216:ASP:OD1	1:E:218:LYS:HE3	1.91	0.71
1:G:138:LEU:HD22	2:G:803:VBP:H15	1.73	0.71
1:G:159:TRP:O	1:G:163:ARG:HB2	1.90	0.71
1:H:135:TYR:HB3	1:H:189:ALA:HB3	1.72	0.71
1:L:156:ASP:O	1:L:160:THR:HG23	1.90	0.71
1:B:241:LEU:HD22	1:B:246:LEU:CD2	2.21	0.70
1:L:21:LYS:H	1:L:21:LYS:HD3	1.56	0.70
1:B:241:LEU:HD22	1:B:246:LEU:HD23	1.74	0.70
1:E:20:LYS:HG2	1:E:31:ARG:O	1.91	0.70
1:B:20:LYS:HG2	1:B:33:GLU:CD	2.12	0.70
1:N:154:VAL:O	1:N:158:MET:HG3	1.91	0.70
1:G:145:GLU:HA	1:G:148:ARG:HG2	1.73	0.70
1:H:141:GLY:O	1:H:145:GLU:HG2	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:166:GLU:HA	1:L:167:PRO:C	2.12	0.70
1:L:192:LEU:H	1:L:192:LEU:HD12	1.57	0.70
1:P:134:ALA:N	1:P:187:LYS:O	2.25	0.70
1:E:230:LEU:O	1:E:234:VAL:HG23	1.91	0.70
1:E:50:LYS:HE2	1:E:50:LYS:HA	1.73	0.70
1:N:162:MET:HE1	1:N:191:LEU:HD12	1.73	0.70
1:J:261:CYS:HB3	3:J:300:HOH:O	1.92	0.70
1:N:135:TYR:HB3	1:N:189:ALA:HB3	1.74	0.69
1:H:10:THR:HA	1:H:74:MET:HE1	1.74	0.69
1:L:184:SER:O	1:L:187:LYS:HE2	1.92	0.69
1:P:121:ILE:HG22	1:P:126:ASP:HB3	1.73	0.69
1:E:193:GLU:HG3	3:E:279:HOH:O	1.92	0.69
1:L:187:LYS:NZ	1:L:188:TYR:HB3	2.08	0.69
1:N:137:THR:HG22	1:N:191:LEU:HB2	1.75	0.69
1:H:39:LEU:O	1:H:43:ILE:HG12	1.93	0.69
1:B:204:LYS:HB2	3:B:300:HOH:O	1.92	0.69
1:B:210:LYS:HD2	3:B:298:HOH:O	1.93	0.69
1:B:251:LYS:HE3	3:B:293:HOH:O	1.93	0.69
1:L:104:LYS:CE	1:L:104:LYS:H	2.04	0.68
1:J:134:ALA:O	1:J:188:TYR:HA	1.94	0.68
1:P:64:ARG:HD3	1:P:69:LYS:HA	1.76	0.68
1:E:172:ARG:HG2	1:E:173:THR:HG23	1.76	0.68
1:G:130:GLN:HA	1:G:130:GLN:HE21	1.58	0.68
1:L:130:GLN:NE2	1:L:133:ILE:HG13	2.07	0.68
1:H:230:LEU:O	1:H:234:VAL:HG23	1.94	0.68
1:J:185:LYS:HD2	1:J:185:LYS:N	2.09	0.67
1:L:125:GLU:OE2	1:L:154:VAL:HG21	1.93	0.67
1:N:89:PRO:HB2	2:N:802:VBP:H05	1.76	0.67
1:P:16:TYR:CD1	1:P:89:PRO:HG3	2.28	0.67
1:J:46:HIS:CD2	1:J:240:LYS:HD2	2.29	0.67
1:E:205:PRO:O	1:E:207:ASP:N	2.26	0.67
1:G:16:TYR:CD1	1:G:89:PRO:HG3	2.29	0.67
1:J:129:LYS:O	1:J:131:THR:N	2.28	0.67
1:G:193:GLU:HG3	3:G:264:HOH:O	1.94	0.66
1:E:156:ASP:O	1:E:160:THR:HG23	1.96	0.66
1:E:203:ARG:O	1:E:204:LYS:O	2.13	0.66
1:L:115:ILE:HG21	1:L:121:ILE:CD1	2.26	0.66
1:H:117:LYS:HA	1:H:209:MET:HE2	1.78	0.66
1:J:69:LYS:NZ	1:J:69:LYS:HB2	2.10	0.66
1:P:114:MET:HE1	1:P:178:VAL:HA	1.77	0.66
1:B:145:GLU:HG2	1:B:148:ARG:HH21	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:121:ILE:HG23	1:H:133:ILE:HD12	1.77	0.66
1:J:149:ARG:HG2	3:J:265:HOH:O	1.95	0.66
1:P:169:VAL:HA	1:P:180:ARG:HH12	1.61	0.66
1:P:193:GLU:H	2:P:805:VBP:H13	1.61	0.66
1:J:152:ILE:HB	1:J:155:PHE:HD2	1.60	0.66
1:E:14:SER:O	1:E:18:MET:SD	2.54	0.65
1:G:166:GLU:HA	1:G:167:PRO:C	2.17	0.65
1:G:180:ARG:HD2	1:G:188:TYR:CZ	2.31	0.65
1:L:203:ARG:O	1:L:204:LYS:O	2.15	0.65
1:L:244:GLN:HB3	1:L:246:LEU:HD13	1.79	0.65
1:N:152:ILE:HG22	3:N:280:HOH:O	1.95	0.65
1:N:110:GLY:HA3	1:N:214:ASN:HB3	1.78	0.65
1:J:35:TYR:CE1	1:J:250:LEU:HB3	2.30	0.65
1:B:251:LYS:O	1:B:255:TRP:HB2	1.97	0.65
1:N:121:ILE:HD13	1:N:127:LEU:CD2	2.27	0.65
1:B:95:VAL:HG11	1:E:69:LYS:CD	2.25	0.65
1:J:64:ARG:HD3	1:J:69:LYS:HA	1.78	0.65
1:L:164:SER:O	1:L:165:ALA:HB3	1.97	0.65
1:H:11:ILE:HG13	3:H:268:HOH:O	1.97	0.65
1:J:6:VAL:O	1:J:51:TYR:HA	1.97	0.65
1:B:154:VAL:O	1:B:158:MET:HG3	1.97	0.65
1:L:89:PRO:HB2	2:L:801:VBP:H05	1.79	0.65
1:H:197:ASN:ND2	1:H:210:LYS:HG3	2.12	0.64
1:E:154:VAL:O	1:E:158:MET:HG3	1.97	0.64
1:H:130:GLN:HG2	1:H:131:THR:N	2.11	0.64
1:H:144:LYS:HE3	1:H:148:ARG:NH2	2.13	0.64
1:J:148:ARG:HA	1:J:159:TRP:CD1	2.31	0.64
1:B:172:ARG:HB3	1:B:172:ARG:NH1	2.12	0.64
1:G:193:GLU:OE1	1:G:218:LYS:NZ	2.29	0.64
1:G:205:PRO:O	1:G:207:ASP:N	2.30	0.64
1:J:178:VAL:HG12	1:J:182:ARG:HE	1.61	0.64
1:P:138:LEU:HD11	1:P:172:ARG:O	1.97	0.64
1:G:193:GLU:HG2	2:G:803:VBP:H13	1.80	0.64
1:N:20:LYS:HG2	1:N:31:ARG:O	1.97	0.64
1:H:224:THR:HG23	3:H:287:HOH:O	1.98	0.64
1:L:10:THR:OG1	1:L:17:VAL:HG11	1.97	0.64
1:N:158:MET:O	1:N:162:MET:HG3	1.98	0.64
1:H:166:GLU:HA	1:H:167:PRO:C	2.18	0.63
1:P:116:LYS:HG3	1:P:207:ASP:O	1.98	0.63
1:B:92:ILE:HG23	1:B:102:PHE:CD2	2.32	0.63
1:J:90:LEU:O	1:J:220:TYR:HA	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:177:GLY:O	1:J:181:VAL:HG23	1.97	0.63
1:B:16:TYR:CD1	1:B:89:PRO:HG3	2.34	0.63
1:E:64:ARG:NH1	1:E:71:TRP:HE1	1.96	0.63
1:G:197:ASN:ND2	1:G:210:LYS:HG3	2.14	0.63
1:P:115:ILE:HB	1:P:119:THR:HB	1.81	0.63
1:B:19:MET:HG3	3:J:289:HOH:O	1.98	0.63
1:H:134:ALA:HB3	1:H:187:LYS:O	1.99	0.63
1:N:157:LYS:HE3	1:N:161:TYR:CE1	2.34	0.63
1:N:180:ARG:O	1:N:188:TYR:HD2	1.82	0.63
1:E:166:GLU:HA	1:E:167:PRO:C	2.20	0.62
1:G:183:LYS:H	1:G:183:LYS:HD2	1.64	0.62
1:L:103:SER:HB2	1:L:104:LYS:HZ1	1.64	0.62
1:N:16:TYR:CD1	1:N:89:PRO:HG3	2.34	0.62
1:P:199:TYR:HE1	1:P:203:ARG:NH1	1.96	0.62
1:H:163:ARG:HH11	1:H:163:ARG:CB	2.12	0.62
1:L:8:VAL:HG22	1:L:85:ILE:CG2	2.29	0.62
1:L:104:LYS:HE3	1:L:239:LEU:HG	1.81	0.62
1:H:180:ARG:HG2	1:H:188:TYR:CD2	2.34	0.62
1:L:192:LEU:HD13	1:L:197:ASN:HB2	1.82	0.62
1:B:191:LEU:N	1:B:191:LEU:HD12	2.15	0.62
1:L:137:THR:HG22	1:L:191:LEU:HB2	1.82	0.62
1:N:144:LYS:HB3	1:N:144:LYS:NZ	2.15	0.62
1:B:100:ILE:HD12	1:B:223:ALA:HB1	1.80	0.62
1:B:42:GLU:HG3	1:B:246:LEU:HD21	1.81	0.62
1:L:16:TYR:CD1	1:L:89:PRO:HG3	2.34	0.62
1:P:201:GLU:HG3	1:P:209:MET:HA	1.82	0.62
1:E:100:ILE:HD13	1:E:223:ALA:HB1	1.82	0.62
1:H:117:LYS:HG3	1:H:209:MET:HE2	1.82	0.62
1:J:110:GLY:HA3	1:J:214:ASN:HB3	1.82	0.62
1:N:251:LYS:HD2	1:N:255:TRP:CE3	2.34	0.62
1:E:138:LEU:HD22	2:E:808:VBP:H15	1.81	0.62
1:J:20:LYS:HB2	1:J:31:ARG:O	1.99	0.62
1:L:172:ARG:HG2	1:L:173:THR:HG23	1.81	0.62
1:L:24:GLU:H	1:L:24:GLU:CD	2.04	0.62
1:L:58:ASP:O	1:L:60:LYS:HG3	2.00	0.62
1:N:152:ILE:HB	1:N:155:PHE:CD2	2.35	0.62
1:P:171:VAL:HB	1:P:176:GLU:HB3	1.81	0.62
1:H:137:THR:HG22	1:H:191:LEU:HB2	1.80	0.61
1:L:104:LYS:HD2	1:L:239:LEU:HD21	1.81	0.61
1:E:183:LYS:HB2	1:E:183:LYS:NZ	2.15	0.61
1:E:204:LYS:O	1:E:205:PRO:C	2.39	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:159:TRP:HE1	1:G:163:ARG:NH1	1.97	0.61
1:H:157:LYS:HE2	1:H:161:TYR:CE1	2.35	0.61
1:B:144:LYS:HE3	1:B:148:ARG:HH12	1.65	0.61
1:E:125:GLU:N	1:E:125:GLU:OE1	2.25	0.61
1:E:169:VAL:HA	1:E:180:ARG:HH12	1.65	0.61
1:B:92:ILE:HA	1:B:102:PHE:CE2	2.35	0.61
1:H:172:ARG:HB3	1:H:176:GLU:OE1	2.00	0.61
1:N:130:GLN:HG3	1:N:133:ILE:H	1.64	0.61
1:G:240:LYS:O	1:G:244:GLN:HG3	1.99	0.61
1:P:232:ASN:N	1:P:232:ASN:ND2	2.48	0.61
1:J:148:ARG:HB2	1:J:148:ARG:HH11	1.66	0.61
1:P:79:VAL:HG22	1:P:99:VAL:HG12	1.82	0.61
1:G:172:ARG:NH1	1:G:172:ARG:HB3	2.16	0.61
1:J:222:ILE:HD13	1:J:238:VAL:HG21	1.83	0.61
1:H:10:THR:HA	1:H:74:MET:CE	2.30	0.60
1:J:121:ILE:HG13	1:J:126:ASP:HB3	1.83	0.60
1:E:155:PHE:CE1	1:E:215:LEU:HD13	2.37	0.60
1:H:147:PHE:CE2	1:H:191:LEU:HD13	2.37	0.60
1:N:166:GLU:HA	1:N:167:PRO:C	2.22	0.60
1:B:144:LYS:NZ	3:B:273:HOH:O	2.32	0.60
1:P:125:GLU:OE1	1:P:154:VAL:HG11	2.02	0.60
1:J:152:ILE:HB	1:J:155:PHE:CD2	2.36	0.60
1:P:154:VAL:O	1:P:158:MET:HG3	2.02	0.60
1:B:11:ILE:O	1:B:17:VAL:HG13	2.02	0.60
1:H:130:GLN:NE2	1:H:132:GLU:N	2.49	0.59
1:P:203:ARG:O	1:P:204:LYS:O	2.19	0.59
1:H:134:ALA:O	1:H:188:TYR:HA	2.03	0.59
1:J:114:MET:HE1	1:J:178:VAL:HA	1.84	0.59
1:L:192:LEU:N	1:L:192:LEU:HD12	2.15	0.59
1:N:130:GLN:HE21	1:N:133:ILE:H	1.50	0.59
1:B:42:GLU:CG	1:B:246:LEU:HD21	2.33	0.59
1:E:11:ILE:O	1:E:17:VAL:CG1	2.50	0.59
1:H:26:LEU:HD22	1:H:30:GLU:OE2	2.03	0.59
1:L:78:LEU:HD23	1:L:83:ALA:HB3	1.84	0.59
1:P:172:ARG:HB2	1:P:172:ARG:NH1	2.18	0.59
1:E:147:PHE:CE2	1:E:191:LEU:HD13	2.37	0.59
1:H:133:ILE:HG23	1:H:186:GLY:O	2.02	0.59
1:B:62:GLY:HA3	1:B:75:VAL:HG23	1.84	0.59
1:G:109:LEU:HD12	1:G:193:GLU:HB3	1.83	0.59
1:L:163:ARG:HG3	1:L:164:SER:N	2.17	0.59
1:L:199:TYR:O	1:L:203:ARG:HG2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:99:VAL:HG23	1:H:100:ILE:HG23	1.84	0.59
1:L:21:LYS:HG2	1:L:22:ASN:H	1.67	0.59
1:J:125:GLU:HA	1:J:128:SER:OG	2.03	0.59
1:J:121:ILE:HD13	1:J:133:ILE:HD12	1.85	0.59
1:J:194:SER:O	1:J:198:GLU:HG3	2.01	0.59
1:L:183:LYS:O	1:L:184:SER:HB3	2.02	0.59
1:L:20:LYS:HD2	1:L:26:LEU:HD12	1.85	0.59
1:E:10:THR:HA	1:E:74:MET:CE	2.31	0.59
1:E:121:ILE:HD13	1:E:127:LEU:HD21	1.85	0.59
1:L:121:ILE:HG22	1:L:126:ASP:HB3	1.85	0.59
1:N:253:LYS:HE2	1:N:258:LYS:NZ	2.18	0.59
1:P:11:ILE:O	1:P:17:VAL:HG13	2.02	0.59
1:B:115:ILE:CG2	1:B:121:ILE:HD11	2.33	0.59
1:B:144:LYS:HE3	1:B:148:ARG:NH2	2.17	0.59
1:G:171:VAL:HG11	1:G:177:GLY:HA2	1.83	0.59
1:L:155:PHE:CE1	1:L:215:LEU:HD13	2.37	0.59
1:P:46:HIS:HD2	1:P:240:LYS:HD2	1.67	0.59
1:J:117:LYS:HG2	1:J:209:MET:CE	2.33	0.58
1:N:136:GLY:HA3	1:N:169:VAL:O	2.02	0.58
1:P:53:LEU:HD11	3:P:292:HOH:O	2.02	0.58
1:B:137:THR:HG22	1:B:191:LEU:HB2	1.85	0.58
1:G:100:ILE:HD12	1:G:100:ILE:C	2.23	0.58
1:B:20:LYS:HD3	1:B:33:GLU:HB3	1.85	0.58
1:H:130:GLN:NE2	1:H:133:ILE:N	2.51	0.58
1:H:163:ARG:HB2	1:H:163:ARG:HH11	1.67	0.58
1:P:203:ARG:HD3	1:P:260:GLU:HG2	1.85	0.58
1:P:37:VAL:HG13	3:P:292:HOH:O	2.02	0.58
1:P:56:VAL:HG13	1:P:59:GLY:HA2	1.85	0.58
1:B:134:ALA:O	1:B:188:TYR:HA	2.03	0.58
1:B:225:PRO:HD2	1:B:228:SER:HB2	1.84	0.58
1:H:77:GLU:HG2	1:H:82:LYS:HB2	1.84	0.58
1:L:172:ARG:HB2	1:L:172:ARG:HH11	1.66	0.58
1:L:197:ASN:HD21	1:L:210:LYS:HA	1.69	0.58
1:N:152:ILE:HB	1:N:155:PHE:HD2	1.69	0.58
1:E:134:ALA:HA	1:E:161:TYR:OH	2.04	0.58
1:G:130:GLN:HG3	1:G:131:THR:N	2.18	0.58
1:G:154:VAL:O	1:G:158:MET:HG3	2.04	0.58
1:G:172:ARG:CZ	1:G:172:ARG:HB3	2.31	0.58
1:E:152:ILE:O	1:E:156:ASP:N	2.34	0.58
1:L:104:LYS:HB3	1:L:105:PRO:HD2	1.84	0.58
1:L:141:GLY:O	1:L:145:GLU:HG2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:21:LYS:H	1:L:21:LYS:CD	2.17	0.58
1:B:196:MET:HA	1:B:196:MET:CE	2.34	0.58
1:G:109:LEU:HD23	1:G:109:LEU:N	2.19	0.58
1:N:46:HIS:CD2	1:N:240:LYS:HD2	2.38	0.58
1:E:22:ASN:H	1:E:22:ASN:ND2	2.02	0.58
1:E:56:VAL:HG13	1:E:59:GLY:HA2	1.86	0.58
1:P:121:ILE:CG2	1:P:126:ASP:HB3	2.34	0.58
1:P:166:GLU:HA	1:P:167:PRO:C	2.23	0.58
1:G:119:THR:HG22	1:G:121:ILE:HG12	1.85	0.57
1:P:180:ARG:HD2	1:P:188:TYR:CD2	2.38	0.57
1:E:31:ARG:HH21	1:E:32:TYR:HE2	1.51	0.57
1:L:29:ASN:HB2	3:L:282:HOH:O	2.05	0.57
1:J:135:TYR:HB3	1:J:189:ALA:HB3	1.87	0.57
1:J:216:ASP:OD2	1:J:218:LYS:HE2	2.05	0.57
1:G:160:THR:O	1:G:163:ARG:HB3	2.04	0.57
1:L:11:ILE:O	1:L:17:VAL:HG13	2.04	0.57
1:N:20:LYS:HG3	1:N:30:GLU:O	2.04	0.57
1:B:192:LEU:H	1:B:192:LEU:HD12	1.69	0.57
1:E:153:ALA:HA	1:E:156:ASP:HB3	1.87	0.57
1:H:162:MET:HA	1:H:169:VAL:HG21	1.86	0.57
1:L:121:ILE:HG22	1:L:126:ASP:O	2.05	0.57
1:P:125:GLU:HA	1:P:128:SER:OG	2.04	0.57
1:P:193:GLU:OE1	1:P:218:LYS:HE2	2.04	0.57
1:E:125:GLU:O	1:E:129:LYS:HG2	2.04	0.57
1:E:192:LEU:HD13	1:E:197:ASN:HB2	1.85	0.57
1:H:160:THR:HA	1:H:163:ARG:HH11	1.67	0.57
1:N:180:ARG:HG2	1:N:188:TYR:CD2	2.40	0.57
1:N:204:LYS:O	1:N:205:PRO:C	2.42	0.57
1:N:172:ARG:HG2	1:N:173:THR:HG23	1.86	0.57
1:P:210:LYS:HE3	3:P:290:HOH:O	2.04	0.57
1:E:20:LYS:HD3	1:E:33:GLU:HB3	1.87	0.57
1:J:90:LEU:HD22	1:J:96:ARG:NH1	2.19	0.57
1:J:182:ARG:HH12	1:J:205:PRO:CB	2.16	0.56
1:N:130:GLN:O	1:N:130:GLN:HG3	2.05	0.56
1:E:152:ILE:CG2	1:E:154:VAL:HG23	2.34	0.56
1:G:246:LEU:O	1:G:250:LEU:HG	2.05	0.56
1:L:16:TYR:CG	1:L:89:PRO:HG3	2.39	0.56
1:H:130:GLN:HG2	1:H:131:THR:H	1.69	0.56
1:H:243:GLU:O	1:L:149:ARG:HD2	2.05	0.56
1:H:203:ARG:O	1:H:260:GLU:HB2	2.05	0.56
1:P:119:THR:HG22	1:P:121:ILE:HG12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:182:ARG:HG2	1:J:207:ASP:OD2	2.05	0.56
1:J:8:VAL:HG23	1:J:51:TYR:HB2	1.87	0.56
1:G:179:ALA:O	1:G:183:LYS:HD3	2.06	0.56
1:G:92:ILE:HG23	1:G:102:PHE:CD2	2.40	0.56
1:L:21:LYS:HD3	1:L:21:LYS:N	2.20	0.56
1:P:121:ILE:HD12	1:P:127:LEU:CD2	2.35	0.56
1:P:157:LYS:HD3	1:P:157:LYS:O	2.05	0.56
1:B:155:PHE:CE1	1:B:215:LEU:HD13	2.40	0.56
1:P:182:ARG:HH21	1:P:200:ILE:CG2	2.18	0.56
1:N:139:ASP:HB2	1:N:171:VAL:O	2.06	0.56
1:P:28:GLY:HA2	1:P:31:ARG:HH21	1.69	0.56
1:J:58:ASP:OD1	1:J:73:GLY:HA2	2.05	0.56
1:P:141:GLY:HA3	3:P:262:HOH:O	2.06	0.56
1:P:151:LYS:HE2	1:P:151:LYS:HA	1.88	0.56
1:L:155:PHE:HE1	1:L:215:LEU:HD13	1.68	0.56
1:L:166:GLU:CA	1:L:167:PRO:C	2.73	0.56
1:P:109:LEU:CD2	1:P:219:GLY:HA2	2.36	0.56
1:J:138:LEU:HD22	2:J:804:VBP:H15	1.87	0.56
1:N:144:LYS:HE2	1:N:144:LYS:C	2.27	0.56
1:B:20:LYS:HE2	1:B:30:GLU:O	2.06	0.55
1:B:115:ILE:C	1:B:115:ILE:HD12	2.27	0.55
1:G:156:ASP:O	1:G:160:THR:HG23	2.05	0.55
1:H:196:MET:HE2	2:H:806:VBP:H10	1.87	0.55
1:G:148:ARG:HG3	1:G:149:ARG:HG3	1.88	0.55
1:H:148:ARG:NH2	3:H:269:HOH:O	2.32	0.55
1:J:155:PHE:HE1	1:J:215:LEU:HD22	1.70	0.55
1:J:192:LEU:HD12	1:J:192:LEU:N	2.20	0.55
1:P:82:LYS:HZ2	1:P:82:LYS:HA	1.71	0.55
1:G:183:LYS:N	1:G:183:LYS:HD2	2.21	0.55
1:N:24:GLU:H	1:N:24:GLU:CD	2.10	0.55
1:B:193:GLU:H	2:B:807:VBP:H13	1.71	0.55
1:G:122:GLU:O	1:G:211:VAL:HG22	2.06	0.55
1:B:140:SER:HA	1:B:144:LYS:CE	2.36	0.55
1:B:16:TYR:CG	1:B:89:PRO:HG3	2.42	0.55
1:L:172:ARG:NH1	1:L:172:ARG:HB2	2.22	0.55
1:H:19:MET:HG3	3:P:281:HOH:O	2.05	0.55
1:L:100:ILE:HD11	1:L:102:PHE:CE2	2.42	0.55
1:L:166:GLU:HB2	1:L:168:SER:N	2.22	0.55
1:P:125:GLU:C	1:P:127:LEU:H	2.09	0.55
1:B:136:GLY:O	1:B:191:LEU:HD13	2.06	0.55
1:H:138:LEU:HD22	2:H:806:VBP:H15	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:136:GLY:HA3	1:J:169:VAL:O	2.06	0.55
1:L:147:PHE:CZ	1:L:191:LEU:HD13	2.41	0.55
1:N:247:LEU:HB2	3:N:276:HOH:O	2.07	0.55
1:P:121:ILE:HD12	1:P:127:LEU:HD23	1.88	0.55
1:P:192:LEU:HD12	1:P:192:LEU:N	2.20	0.55
1:P:195:THR:HG21	1:P:220:TYR:HE2	1.71	0.55
1:B:122:GLU:HA	1:B:211:VAL:CG2	2.35	0.55
1:B:192:LEU:HD13	1:B:197:ASN:HB2	1.89	0.55
1:H:115:ILE:O	1:H:115:ILE:HD12	2.07	0.55
1:L:205:PRO:O	1:L:207:ASP:N	2.40	0.55
1:P:208:THR:O	1:P:209:MET:HB2	2.06	0.55
1:H:201:GLU:HG3	1:H:209:MET:HA	1.89	0.55
1:H:193:GLU:H	2:H:806:VBP:H13	1.72	0.55
1:B:95:VAL:HB	1:E:64:ARG:HH21	1.71	0.54
1:N:115:ILE:CD1	1:N:211:VAL:HG11	2.36	0.54
1:G:180:ARG:HD2	1:G:188:TYR:CE2	2.41	0.54
1:N:16:TYR:HA	1:N:35:TYR:HB3	1.89	0.54
1:E:226:LYS:HE3	3:P:285:HOH:O	2.08	0.54
1:G:39:LEU:O	1:G:43:ILE:HG12	2.07	0.54
1:L:121:ILE:HD12	1:L:121:ILE:O	2.08	0.54
1:L:194:SER:O	1:L:198:GLU:HG3	2.08	0.54
1:P:182:ARG:NH1	1:P:205:PRO:HB2	2.23	0.54
1:G:148:ARG:NH1	1:G:148:ARG:HB2	2.22	0.54
1:N:185:LYS:HD2	1:N:185:LYS:N	2.23	0.54
1:H:109:LEU:HD23	1:H:109:LEU:N	2.23	0.54
1:P:192:LEU:HD13	1:P:197:ASN:HB2	1.89	0.54
1:B:180:ARG:HG2	1:B:188:TYR:CD2	2.42	0.54
1:N:88:ALA:HB1	1:N:89:PRO:CD	2.38	0.54
1:P:115:ILE:HB	1:P:119:THR:CB	2.38	0.54
1:H:27:GLU:HG2	3:H:285:HOH:O	2.07	0.54
1:N:203:ARG:O	1:N:204:LYS:O	2.26	0.54
1:N:205:PRO:O	1:N:207:ASP:N	2.33	0.54
1:N:208:THR:O	1:N:209:MET:HB3	2.07	0.54
1:B:159:TRP:NE1	1:B:163:ARG:NH1	2.56	0.54
1:L:115:ILE:HG21	1:L:121:ILE:HD13	1.89	0.54
1:N:8:VAL:HG22	1:N:85:ILE:CG2	2.38	0.54
1:H:64:ARG:NH1	1:H:71:TRP:NE1	2.49	0.53
1:J:20:LYS:HG2	1:J:26:LEU:CD1	2.37	0.53
1:B:166:GLU:H	1:B:166:GLU:CD	2.11	0.53
1:H:156:ASP:HB3	3:H:289:HOH:O	2.07	0.53
1:L:97:GLU:OE2	1:L:102:PHE:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:82:LYS:HZ3	1:P:82:LYS:HA	1.72	0.53
1:G:18:MET:N	1:G:33:GLU:O	2.32	0.53
1:N:121:ILE:HD13	1:N:127:LEU:HD21	1.91	0.53
1:G:159:TRP:HE1	1:G:163:ARG:HH11	1.57	0.53
1:L:187:LYS:HZ2	1:L:188:TYR:HB3	1.72	0.53
1:B:90:LEU:HD22	1:B:96:ARG:NH1	2.23	0.53
1:G:92:ILE:HG12	1:G:102:PHE:CG	2.44	0.53
1:J:65:ASP:O	1:J:69:LYS:HA	2.09	0.53
1:N:119:THR:HG23	1:N:133:ILE:HD13	1.90	0.53
1:P:125:GLU:C	1:P:127:LEU:N	2.62	0.53
1:P:62:GLY:HA3	1:P:75:VAL:HG23	1.91	0.53
1:E:100:ILE:HD11	1:E:102:PHE:CE2	2.44	0.53
1:H:192:LEU:HD13	1:H:197:ASN:HB2	1.91	0.53
1:N:20:LYS:O	1:N:23:HIS:HB3	2.07	0.53
1:H:118:GLY:HA2	1:N:30:GLU:CG	2.39	0.53
1:G:94:LEU:HD12	1:J:236:LEU:HD22	1.91	0.53
1:N:237:ALA:O	1:N:241:LEU:HG	2.09	0.53
1:E:246:LEU:O	1:E:250:LEU:HG	2.09	0.52
1:G:197:ASN:HD22	1:G:210:LYS:HG3	1.73	0.52
1:B:62:GLY:HA2	1:B:72:ASN:O	2.09	0.52
1:E:127:LEU:HB3	1:E:135:TYR:CE2	2.44	0.52
1:E:64:ARG:NH1	1:E:71:TRP:NE1	2.57	0.52
1:J:21:LYS:HD3	1:J:21:LYS:N	2.10	0.52
1:P:89:PRO:HB2	2:P:805:VBP:H05	1.91	0.52
1:H:17:VAL:C	1:H:18:MET:HG3	2.28	0.52
1:L:36:CYS:SG	1:L:88:ALA:HA	2.49	0.52
1:B:20:LYS:CE	1:B:30:GLU:O	2.57	0.52
1:N:125:GLU:HA	1:N:125:GLU:OE1	2.09	0.52
1:J:115:ILE:HD13	1:J:121:ILE:O	2.10	0.52
1:J:148:ARG:HG3	1:J:149:ARG:H	1.74	0.52
1:L:134:ALA:O	1:L:188:TYR:HA	2.10	0.52
1:N:20:LYS:HD3	1:N:33:GLU:HB3	1.90	0.52
1:H:115:ILE:HD12	1:H:115:ILE:C	2.30	0.52
1:B:110:GLY:HA3	1:B:214:ASN:HB3	1.91	0.52
1:G:20:LYS:NZ	1:G:30:GLU:HG2	2.25	0.52
1:H:144:LYS:HE3	1:H:148:ARG:HH21	1.73	0.52
1:L:46:HIS:HD2	1:L:240:LYS:HD2	1.75	0.52
1:P:180:ARG:O	1:P:180:ARG:HG2	2.10	0.52
1:P:199:TYR:CE1	1:P:203:ARG:NH1	2.77	0.52
1:P:232:ASN:HA	3:P:289:HOH:O	2.09	0.52
1:G:114:MET:HE2	1:G:178:VAL:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:122:GLU:HG3	1:J:126:ASP:OD2	2.10	0.52
1:P:6:VAL:O	1:P:51:TYR:HA	2.09	0.52
1:G:201:GLU:HG2	1:G:201:GLU:O	2.09	0.52
1:P:109:LEU:HD23	1:P:219:GLY:HA2	1.91	0.52
1:B:112:SER:OG	1:B:194:SER:HA	2.10	0.52
1:H:173:THR:O	1:H:176:GLU:HB3	2.10	0.52
1:J:68:THR:HB	1:J:70:ILE:HG12	1.91	0.52
1:P:193:GLU:HG2	2:P:805:VBP:H13	1.92	0.52
1:H:252:ASN:ND2	1:H:256:TYR:HB2	2.25	0.51
1:H:24:GLU:HG2	1:H:25:MET:N	2.25	0.51
1:H:21:LYS:O	1:H:22:ASN:HB3	2.10	0.51
1:J:154:VAL:O	1:J:158:MET:HG3	2.11	0.51
1:N:200:ILE:HG22	1:N:208:THR:OG1	2.09	0.51
1:P:134:ALA:O	1:P:188:TYR:HA	2.11	0.51
1:E:11:ILE:HG12	1:E:12:LEU:N	2.25	0.51
1:P:113:ILE:HG12	1:P:191:LEU:HD21	1.92	0.51
1:G:191:LEU:HD12	1:G:191:LEU:N	2.25	0.51
1:L:134:ALA:N	1:L:187:LYS:O	2.41	0.51
1:N:16:TYR:CG	1:N:89:PRO:HG3	2.45	0.51
1:B:140:SER:HA	1:B:144:LYS:HZ3	1.73	0.51
1:B:114:MET:HE2	1:B:178:VAL:HA	1.91	0.51
1:H:109:LEU:HB2	1:H:194:SER:OG	2.10	0.51
1:N:171:VAL:HG22	1:N:176:GLU:HB3	1.93	0.51
1:N:121:ILE:HD13	1:N:127:LEU:HD23	1.92	0.51
1:E:130:GLN:OE1	1:E:132:GLU:N	2.44	0.51
1:E:22:ASN:N	1:E:22:ASN:ND2	2.59	0.51
1:H:234:VAL:O	1:H:238:VAL:HG23	2.11	0.51
1:P:196:MET:HE2	2:P:805:VBP:H10	1.93	0.51
1:B:19:MET:HB3	1:B:23:HIS:CD2	2.46	0.51
1:E:135:TYR:HB3	1:E:189:ALA:HB3	1.93	0.51
1:E:225:PRO:HD2	1:E:228:SER:HB2	1.93	0.51
1:J:117:LYS:HE3	3:J:279:HOH:O	2.11	0.51
1:J:56:VAL:HG13	1:J:59:GLY:HA2	1.92	0.51
1:L:111:ILE:CD1	1:L:143:THR:HA	2.40	0.51
1:B:89:PRO:HB2	2:B:807:VBP:C05	2.38	0.50
1:J:210:LYS:HE2	3:J:267:HOH:O	2.10	0.50
1:L:79:VAL:HG12	1:L:80:TYR:CD1	2.45	0.50
1:N:142:SER:HA	1:N:145:GLU:HB2	1.93	0.50
1:P:24:GLU:H	1:P:24:GLU:CD	2.14	0.50
1:B:159:TRP:HE1	1:B:163:ARG:NH1	2.08	0.50
1:E:153:ALA:O	1:E:154:VAL:C	2.49	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:130:GLN:HE21	1:H:131:THR:C	2.13	0.50
1:J:166:GLU:HA	1:J:167:PRO:O	2.12	0.50
1:J:180:ARG:HG2	1:J:188:TYR:CD2	2.46	0.50
1:J:46:HIS:NE2	1:J:240:LYS:HD2	2.26	0.50
1:B:144:LYS:HE3	1:B:148:ARG:NH1	2.25	0.50
1:B:95:VAL:HG13	3:B:270:HOH:O	2.11	0.50
1:J:114:MET:CE	1:J:178:VAL:HA	2.42	0.50
1:P:209:MET:HG2	1:P:210:LYS:O	2.11	0.50
1:P:39:LEU:O	1:P:43:ILE:HG12	2.12	0.50
1:B:92:ILE:HA	1:B:102:PHE:CZ	2.47	0.50
1:E:11:ILE:O	1:E:17:VAL:HG11	2.10	0.50
1:E:125:GLU:H	1:E:125:GLU:CD	2.13	0.50
1:E:64:ARG:HH12	1:E:71:TRP:HE1	1.59	0.50
1:G:127:LEU:HD22	1:G:135:TYR:CD2	2.47	0.50
1:L:180:ARG:HG2	1:L:188:TYR:CD2	2.46	0.50
1:N:129:LYS:O	1:N:131:THR:N	2.44	0.50
1:E:161:TYR:CD1	1:E:161:TYR:C	2.85	0.50
1:E:18:MET:HG2	1:E:33:GLU:O	2.11	0.50
1:E:90:LEU:HD23	1:E:96:ARG:NH1	2.27	0.50
1:G:42:GLU:OE2	1:G:246:LEU:HD22	2.12	0.50
1:E:218:LYS:HD3	3:E:280:HOH:O	2.12	0.50
1:G:88:ALA:HB1	1:G:89:PRO:CD	2.42	0.50
1:H:117:LYS:HG3	1:H:209:MET:CE	2.42	0.50
1:H:144:LYS:HD2	1:H:144:LYS:O	2.11	0.50
1:H:253:LYS:O	1:H:257:ASP:HB2	2.12	0.50
1:L:123:SER:HB3	1:L:126:ASP:OD1	2.12	0.50
1:L:204:LYS:O	1:L:205:PRO:C	2.50	0.50
1:L:110:GLY:HA3	1:L:216:ASP:O	2.11	0.50
1:E:32:TYR:HE2	3:E:287:HOH:O	1.94	0.50
1:H:143:THR:O	1:H:146:PHE:HB3	2.12	0.50
1:J:88:ALA:HB1	1:J:89:PRO:CD	2.42	0.50
1:E:196:MET:HG2	2:E:808:VBP:O08	2.12	0.49
1:H:130:GLN:OE1	1:H:133:ILE:HB	2.11	0.49
1:H:197:ASN:HD22	1:H:210:LYS:HG3	1.77	0.49
1:N:5:THR:O	1:N:5:THR:HG22	2.12	0.49
1:J:117:LYS:HG2	1:J:209:MET:HE3	1.93	0.49
1:L:103:SER:HB2	1:L:104:LYS:NZ	2.27	0.49
1:L:192:LEU:CD1	1:L:197:ASN:HB2	2.41	0.49
1:N:12:LEU:HD23	1:N:17:VAL:O	2.12	0.49
1:P:121:ILE:HG21	1:P:126:ASP:O	2.12	0.49
1:E:94:LEU:O	1:E:98:GLU:HG3	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:157:LYS:HE2	1:H:161:TYR:HE1	1.74	0.49
1:L:216:ASP:OD2	1:L:218:LYS:HE3	2.12	0.49
1:L:28:GLY:HA2	1:L:31:ARG:HH21	1.77	0.49
1:L:88:ALA:HB1	1:L:89:PRO:CD	2.43	0.49
1:P:172:ARG:HB2	1:P:172:ARG:HH11	1.78	0.49
1:P:210:LYS:HB3	1:P:210:LYS:NZ	2.28	0.49
1:B:148:ARG:HG3	1:B:159:TRP:CZ2	2.47	0.49
1:B:117:LYS:HD3	1:B:209:MET:HE3	1.93	0.49
1:J:222:ILE:N	1:J:222:ILE:HD12	2.28	0.49
1:L:160:THR:O	1:L:163:ARG:HG2	2.13	0.49
1:H:135:TYR:CB	1:H:189:ALA:HB3	2.42	0.49
1:J:185:LYS:N	1:J:185:LYS:CD	2.74	0.49
1:P:115:ILE:HG12	1:P:211:VAL:HG11	1.94	0.49
1:N:65:ASP:O	1:N:69:LYS:HA	2.12	0.49
1:N:6:VAL:O	1:N:51:TYR:HA	2.13	0.49
1:B:75:VAL:O	1:B:79:VAL:HG23	2.13	0.49
1:J:159:TRP:O	1:J:163:ARG:HB2	2.13	0.49
1:J:204:LYS:HB3	1:J:205:PRO:CD	2.38	0.49
1:B:171:VAL:HB	1:B:176:GLU:HG2	1.94	0.49
1:E:182:ARG:HG2	1:E:207:ASP:OD2	2.13	0.49
1:E:197:ASN:HD22	1:E:210:LYS:HG3	1.77	0.49
1:H:121:ILE:HD13	1:H:127:LEU:HG	1.94	0.49
1:N:108:SER:C	1:N:109:LEU:HD23	2.33	0.49
1:N:253:LYS:O	1:N:257:ASP:HB2	2.13	0.49
1:N:94:LEU:O	1:N:98:GLU:HG3	2.13	0.49
1:P:158:MET:O	1:P:162:MET:HG3	2.13	0.49
1:E:105:PRO:HA	1:E:220:TYR:O	2.13	0.49
1:H:122:GLU:OE1	1:H:126:ASP:OD2	2.31	0.49
1:H:99:VAL:O	1:H:226:LYS:HD3	2.13	0.49
1:J:148:ARG:HB2	1:J:148:ARG:NH1	2.26	0.49
1:E:244:GLN:HA	1:P:149:ARG:CD	2.43	0.49
1:B:122:GLU:O	1:B:211:VAL:HG22	2.13	0.48
1:B:241:LEU:HD22	1:B:246:LEU:HD22	1.95	0.48
1:E:159:TRP:O	1:E:163:ARG:HB2	2.13	0.48
1:B:95:VAL:CB	1:E:64:ARG:HH21	2.25	0.48
1:N:143:THR:HG21	3:N:266:HOH:O	2.13	0.48
1:P:114:MET:CE	1:P:208:THR:HG21	2.43	0.48
1:E:148:ARG:CG	1:E:148:ARG:O	2.61	0.48
1:E:77:GLU:HG2	1:E:82:LYS:HB2	1.95	0.48
1:G:11:ILE:HG13	3:G:290:HOH:O	2.12	0.48
1:L:100:ILE:HD12	1:L:100:ILE:C	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:125:GLU:O	1:P:127:LEU:N	2.46	0.48
1:P:97:GLU:HG3	1:P:97:GLU:O	2.13	0.48
1:E:137:THR:HG22	1:E:191:LEU:HB2	1.95	0.48
1:G:36:CYS:SG	1:G:88:ALA:HA	2.53	0.48
1:H:144:LYS:CE	1:H:148:ARG:NH2	2.76	0.48
1:J:27:GLU:HA	1:J:27:GLU:OE1	2.14	0.48
1:P:143:THR:HB	3:P:262:HOH:O	2.13	0.48
1:B:88:ALA:HB1	1:B:89:PRO:CD	2.43	0.48
1:H:163:ARG:NH1	1:H:163:ARG:HB2	2.27	0.48
1:H:249:LYS:HD3	1:L:151:LYS:HB3	1.95	0.48
1:J:200:ILE:HG22	1:J:208:THR:OG1	2.14	0.48
1:N:182:ARG:NH1	1:N:208:THR:HG23	2.29	0.48
1:N:193:GLU:H	2:N:802:VBP:H13	1.79	0.48
1:P:177:GLY:O	1:P:181:VAL:HG23	2.13	0.48
1:B:250:LEU:O	1:B:253:LYS:HB3	2.14	0.48
1:E:159:TRP:CE3	1:E:159:TRP:HA	2.49	0.48
1:H:162:MET:HB3	1:H:170:PHE:CZ	2.49	0.48
1:N:60:LYS:HB2	1:N:73:GLY:CA	2.44	0.48
1:P:203:ARG:HA	1:P:260:GLU:CG	2.43	0.48
1:G:237:ALA:O	1:G:241:LEU:HG	2.14	0.48
1:H:100:ILE:HD11	1:H:102:PHE:CE2	2.49	0.48
1:L:160:THR:HG22	1:L:163:ARG:HH12	1.78	0.48
1:B:199:TYR:O	1:B:203:ARG:HG2	2.14	0.48
1:B:237:ALA:O	1:B:241:LEU:HG	2.14	0.48
1:H:147:PHE:CZ	1:H:191:LEU:HD13	2.49	0.48
1:J:182:ARG:NH1	1:J:207:ASP:OD1	2.46	0.48
1:G:115:ILE:HD12	1:G:119:THR:HB	1.95	0.48
1:G:180:ARG:HD2	1:G:188:TYR:CE1	2.49	0.48
1:J:192:LEU:HD12	1:J:192:LEU:H	1.78	0.48
1:P:65:ASP:HB3	1:P:68:THR:OG1	2.14	0.48
1:J:197:ASN:ND2	1:J:210:LYS:HG3	2.29	0.48
1:P:182:ARG:HH12	1:P:205:PRO:HB2	1.79	0.48
1:B:68:THR:OG1	1:B:70:ILE:HB	2.13	0.47
1:E:234:VAL:O	1:E:237:ALA:HB3	2.14	0.47
1:E:247:LEU:HB2	3:E:286:HOH:O	2.14	0.47
1:H:181:VAL:CG1	1:H:181:VAL:O	2.62	0.47
1:H:196:MET:O	1:H:200:ILE:HG12	2.13	0.47
1:J:138:LEU:O	1:J:144:LYS:HB2	2.14	0.47
1:L:15:PRO:HD3	1:L:199:TYR:CD1	2.49	0.47
1:L:164:SER:O	1:L:165:ALA:CB	2.60	0.47
1:P:247:LEU:HB2	3:P:273:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:MET:CE	1:B:178:VAL:HA	2.44	0.47
1:E:127:LEU:HD22	1:E:135:TYR:CD2	2.49	0.47
1:L:147:PHE:CE2	1:L:191:LEU:HD13	2.49	0.47
1:P:113:ILE:HG12	1:P:191:LEU:CD2	2.44	0.47
1:P:133:ILE:HG23	1:P:187:LYS:C	2.34	0.47
1:H:192:LEU:CD1	1:H:197:ASN:HB2	2.45	0.47
1:H:249:LYS:HD3	1:L:151:LYS:CB	2.43	0.47
1:L:166:GLU:HA	1:L:167:PRO:O	2.13	0.47
1:N:144:LYS:HD3	3:N:262:HOH:O	2.15	0.47
1:B:62:GLY:HA3	1:B:75:VAL:CG2	2.43	0.47
1:H:115:ILE:HD13	1:H:119:THR:HB	1.95	0.47
1:E:13:GLU:HB3	1:E:16:TYR:HD2	1.79	0.47
1:G:182:ARG:NH1	1:G:205:PRO:HB2	2.29	0.47
1:J:145:GLU:OE1	1:J:148:ARG:HD2	2.14	0.47
1:J:16:TYR:HA	1:J:35:TYR:HB3	1.95	0.47
1:L:251:LYS:O	1:L:255:TRP:HB2	2.14	0.47
1:N:130:GLN:NE2	1:N:133:ILE:HG13	2.28	0.47
1:P:192:LEU:HD12	1:P:192:LEU:H	1.80	0.47
1:P:203:ARG:HA	1:P:260:GLU:HG3	1.96	0.47
1:B:11:ILE:O	1:B:17:VAL:CG1	2.62	0.47
1:B:97:GLU:HG3	1:B:97:GLU:O	2.13	0.47
1:E:7:VAL:HB	1:E:84:ASP:OD2	2.14	0.47
1:G:77:GLU:HG2	1:G:82:LYS:HB2	1.97	0.47
1:P:204:LYS:O	1:P:205:PRO:C	2.49	0.47
1:P:205:PRO:O	1:P:207:ASP:N	2.48	0.47
1:E:11:ILE:HG21	1:E:61:TYR:CE1	2.49	0.47
1:G:114:MET:CE	1:G:178:VAL:HA	2.44	0.47
1:G:117:LYS:HE2	1:G:209:MET:CE	2.34	0.47
1:G:130:GLN:HA	1:G:130:GLN:NE2	2.25	0.47
1:J:114:MET:HE3	1:J:178:VAL:HG13	1.96	0.47
1:J:105:PRO:HA	1:J:220:TYR:O	2.15	0.47
1:E:88:ALA:HB1	1:E:89:PRO:CD	2.39	0.47
1:J:171:VAL:HB	1:J:176:GLU:HB3	1.96	0.47
1:J:5:THR:O	1:J:5:THR:HG23	2.15	0.47
1:P:240:LYS:O	1:P:244:GLN:HG3	2.14	0.47
1:B:42:GLU:CD	1:B:246:LEU:HD21	2.35	0.47
1:E:147:PHE:CZ	1:E:191:LEU:HD13	2.49	0.47
1:E:63:ALA:N	1:E:72:ASN:OD1	2.43	0.47
1:J:113:ILE:HG22	1:J:115:ILE:HG23	1.97	0.47
1:J:137:THR:HG22	1:J:191:LEU:HB2	1.96	0.47
1:L:115:ILE:HG21	1:L:121:ILE:HD11	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:193:GLU:H	2:L:801:VBP:H13	1.80	0.47
1:N:11:ILE:O	1:N:17:VAL:HG13	2.15	0.47
1:N:130:GLN:HG2	1:N:133:ILE:HB	1.96	0.47
1:P:100:ILE:HD12	1:P:100:ILE:O	2.15	0.47
1:P:130:GLN:HE21	1:P:132:GLU:HB3	1.80	0.47
1:P:65:ASP:O	1:P:69:LYS:N	2.47	0.47
1:P:65:ASP:O	1:P:69:LYS:HA	2.15	0.47
1:B:172:ARG:CB	1:B:172:ARG:NH1	2.78	0.47
1:P:203:ARG:HA	1:P:203:ARG:HD3	1.70	0.47
1:J:62:GLY:HA3	1:J:75:VAL:HG23	1.97	0.47
1:J:99:VAL:HG23	1:J:100:ILE:HG23	1.96	0.47
1:G:115:ILE:HG22	1:G:121:ILE:HD11	1.98	0.46
1:G:182:ARG:HH12	1:G:205:PRO:HB2	1.80	0.46
1:N:113:ILE:HG22	1:N:115:ILE:HG23	1.96	0.46
1:N:182:ARG:NH1	1:N:207:ASP:OD1	2.48	0.46
1:P:75:VAL:O	1:P:79:VAL:HG23	2.14	0.46
1:B:172:ARG:CB	1:B:172:ARG:HH11	2.28	0.46
1:J:185:LYS:HD2	1:J:185:LYS:H	1.77	0.46
1:P:180:ARG:O	1:P:184:SER:HB3	2.15	0.46
1:B:155:PHE:CZ	1:B:215:LEU:HD22	2.50	0.46
1:E:22:ASN:N	1:E:22:ASN:HD22	1.96	0.46
1:E:241:LEU:HD22	1:E:246:LEU:HD22	1.98	0.46
1:N:51:TYR:N	1:N:51:TYR:CD2	2.83	0.46
1:B:133:ILE:HG23	1:B:187:LYS:HA	1.97	0.46
1:J:97:GLU:HA	1:J:97:GLU:OE2	2.16	0.46
1:N:42:GLU:HG3	1:N:246:LEU:CD2	2.45	0.46
1:P:130:GLN:HE21	1:P:130:GLN:HB3	1.57	0.46
1:N:61:TYR:CE1	2:N:802:VBP:H03A	2.50	0.46
1:G:68:THR:C	1:G:70:ILE:H	2.17	0.46
1:N:180:ARG:HG2	1:N:180:ARG:O	2.16	0.46
1:B:115:ILE:O	1:B:115:ILE:HD12	2.16	0.46
1:E:148:ARG:HA	1:E:159:TRP:CD1	2.51	0.46
1:E:169:VAL:CA	1:E:180:ARG:HH12	2.29	0.46
1:G:148:ARG:HB2	1:G:148:ARG:HH11	1.80	0.46
1:G:192:LEU:HD13	1:G:197:ASN:HB2	1.98	0.46
1:J:147:PHE:CE2	1:J:191:LEU:HD13	2.51	0.46
1:J:182:ARG:NH1	1:J:205:PRO:CB	2.78	0.46
1:P:96:ARG:C	1:P:98:GLU:H	2.19	0.46
1:H:118:GLY:HA2	1:N:30:GLU:HG3	1.96	0.46
1:P:184:SER:O	1:P:186:GLY:N	2.48	0.46
1:P:36:CYS:SG	1:P:88:ALA:HA	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:67:ASP:O	1:G:69:LYS:HD3	2.16	0.46
1:J:64:ARG:HG3	1:J:64:ARG:NH1	2.30	0.46
1:L:136:GLY:HA3	1:L:169:VAL:O	2.16	0.46
1:L:144:LYS:NZ	1:L:148:ARG:NH2	2.64	0.46
1:N:92:ILE:HG12	1:N:102:PHE:CD1	2.51	0.46
1:N:144:LYS:HB3	1:N:144:LYS:HZ3	1.80	0.46
1:P:138:LEU:HD12	1:P:139:ASP:H	1.81	0.46
1:G:111:ILE:HD12	1:G:146:PHE:CD2	2.51	0.46
1:H:14:SER:CB	1:H:18:MET:HE3	2.46	0.46
1:N:60:LYS:HB2	1:N:73:GLY:HA2	1.97	0.46
1:P:100:ILE:HD12	1:P:100:ILE:C	2.36	0.46
1:H:121:ILE:HD12	1:H:122:GLU:N	2.31	0.45
1:N:137:THR:HB	3:N:266:HOH:O	2.16	0.45
1:P:137:THR:HG22	1:P:191:LEU:HB2	1.97	0.45
1:P:62:GLY:HA3	1:P:75:VAL:CG2	2.46	0.45
1:B:211:VAL:HG13	1:B:211:VAL:O	2.16	0.45
1:E:111:ILE:O	1:E:214:ASN:HA	2.16	0.45
1:G:5:THR:N	3:G:262:HOH:O	2.49	0.45
1:H:11:ILE:O	1:H:17:VAL:HG13	2.15	0.45
1:L:121:ILE:HA	1:L:126:ASP:HB3	1.98	0.45
1:B:125:GLU:N	1:B:125:GLU:OE1	2.39	0.45
1:B:173:THR:O	1:B:176:GLU:HB3	2.16	0.45
1:H:155:PHE:CE1	1:H:215:LEU:HD13	2.51	0.45
1:J:21:LYS:CE	1:J:21:LYS:H	2.26	0.45
1:L:172:ARG:CB	1:L:172:ARG:NH1	2.80	0.45
1:N:171:VAL:CG2	1:N:176:GLU:HB3	2.46	0.45
1:N:180:ARG:O	1:N:188:TYR:CD2	2.66	0.45
1:P:180:ARG:O	1:P:184:SER:CB	2.64	0.45
1:P:197:ASN:ND2	1:P:210:LYS:HA	2.31	0.45
1:B:99:VAL:HG23	1:B:100:ILE:HG23	1.98	0.45
1:B:106:PHE:C	1:B:106:PHE:CD1	2.90	0.45
1:G:229:SER:HB2	3:G:282:HOH:O	2.17	0.45
1:L:90:LEU:O	1:L:220:TYR:HA	2.15	0.45
1:P:8:VAL:HG22	1:P:85:ILE:CG2	2.47	0.45
1:B:196:MET:HA	1:B:196:MET:HE3	1.98	0.45
1:B:205:PRO:HG2	1:B:207:ASP:OD1	2.16	0.45
1:E:11:ILE:O	1:E:17:VAL:HG13	2.15	0.45
1:H:121:ILE:CG2	1:H:133:ILE:HD12	2.46	0.45
1:J:222:ILE:HD13	1:J:238:VAL:CG2	2.46	0.45
1:L:205:PRO:O	1:L:207:ASP:OD1	2.34	0.45
1:N:172:ARG:HB3	1:N:176:GLU:OE1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:207:ASP:OD1	1:N:208:THR:HG23	2.17	0.45
1:E:147:PHE:C	1:E:149:ARG:H	2.20	0.45
1:E:171:VAL:HB	1:E:176:GLU:HB2	1.99	0.45
1:J:182:ARG:NH1	1:J:205:PRO:HB2	2.24	0.45
1:J:51:TYR:CD2	1:J:51:TYR:N	2.84	0.45
1:P:64:ARG:HG3	1:P:64:ARG:HH11	1.82	0.45
1:B:155:PHE:HE1	1:B:215:LEU:HD13	1.82	0.45
1:J:84:ASP:O	1:J:225:PRO:HD3	2.17	0.45
1:L:64:ARG:HB2	1:L:71:TRP:CE2	2.51	0.45
1:N:109:LEU:N	1:N:109:LEU:HD23	2.31	0.45
1:N:10:THR:O	1:N:55:ILE:HA	2.17	0.45
1:P:121:ILE:CB	1:P:126:ASP:HB3	2.47	0.45
1:G:159:TRP:O	1:G:163:ARG:CB	2.63	0.45
1:H:115:ILE:HB	1:H:119:THR:HB	1.98	0.45
1:J:117:LYS:HG2	1:J:209:MET:HE2	1.98	0.45
1:L:16:TYR:HA	1:L:35:TYR:HB3	1.99	0.45
1:P:64:ARG:HG3	1:P:64:ARG:NH1	2.30	0.45
1:B:159:TRP:HE1	1:B:163:ARG:HH12	1.64	0.45
1:E:251:LYS:HD3	1:E:255:TRP:CE3	2.52	0.45
1:G:19:MET:HG3	3:N:272:HOH:O	2.17	0.45
1:J:100:ILE:C	1:J:100:ILE:HD12	2.37	0.45
1:L:187:LYS:HZ2	1:L:188:TYR:CB	2.29	0.45
1:B:201:GLU:OE1	1:B:209:MET:HB2	2.16	0.44
1:B:42:GLU:OE2	1:B:246:LEU:HD21	2.18	0.44
1:E:124:ALA:O	1:E:127:LEU:N	2.50	0.44
1:H:180:ARG:C	1:H:182:ARG:H	2.20	0.44
1:L:122:GLU:HA	1:L:211:VAL:HG21	2.00	0.44
1:L:116:LYS:HE3	1:L:207:ASP:HB2	1.98	0.44
1:P:161:TYR:CD2	1:P:162:MET:N	2.86	0.44
1:P:195:THR:HG21	1:P:220:TYR:CE2	2.50	0.44
1:E:114:MET:CE	1:E:192:LEU:HD21	2.47	0.44
1:E:109:LEU:HD12	1:E:193:GLU:OE1	2.18	0.44
1:E:197:ASN:ND2	1:E:210:LYS:HA	2.32	0.44
1:G:20:LYS:HZ2	1:G:30:GLU:HG2	1.81	0.44
1:G:85:ILE:HG13	1:G:224:THR:HG22	1.99	0.44
1:J:121:ILE:CD1	1:J:133:ILE:HD12	2.47	0.44
1:J:150:SER:HA	3:J:276:HOH:O	2.17	0.44
1:J:34:GLY:HA2	1:J:254:TRP:CZ3	2.52	0.44
1:J:11:ILE:HD11	1:J:59:GLY:O	2.17	0.44
1:N:201:GLU:OE1	1:N:210:LYS:N	2.48	0.44
1:N:28:GLY:O	1:N:31:ARG:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:65:ASP:O	1:N:69:LYS:N	2.50	0.44
1:E:14:SER:HA	3:E:278:HOH:O	2.17	0.44
1:J:137:THR:HB	1:J:143:THR:HG22	1.98	0.44
1:J:24:GLU:H	1:J:24:GLU:CD	2.20	0.44
1:N:129:LYS:O	1:N:130:GLN:C	2.54	0.44
1:B:155:PHE:CZ	1:B:215:LEU:HB3	2.53	0.44
1:E:241:LEU:CD2	1:E:246:LEU:HD22	2.48	0.44
1:H:96:ARG:O	1:H:100:ILE:HG13	2.17	0.44
1:H:106:PHE:CD1	1:H:106:PHE:C	2.91	0.44
1:J:115:ILE:CD1	1:J:121:ILE:O	2.64	0.44
1:J:178:VAL:CG1	1:J:182:ARG:HE	2.28	0.44
1:P:113:ILE:HD13	1:P:127:LEU:CD1	2.47	0.44
1:P:169:VAL:HA	1:P:180:ARG:NH1	2.31	0.44
1:B:104:LYS:HG2	1:B:235:ASN:OD1	2.18	0.44
1:E:234:VAL:O	1:E:238:VAL:HG23	2.17	0.44
1:H:68:THR:O	1:H:70:ILE:HG13	2.18	0.44
1:J:121:ILE:HG12	1:J:127:LEU:HD23	1.98	0.44
1:J:179:ALA:HA	1:J:182:ARG:HD2	1.99	0.44
1:J:69:LYS:HB2	1:J:69:LYS:HZ3	1.80	0.44
1:J:73:GLY:O	1:J:77:GLU:HG2	2.17	0.44
1:L:161:TYR:HD2	1:L:162:MET:HG3	1.83	0.44
1:P:109:LEU:N	1:P:109:LEU:HD23	2.32	0.44
1:P:130:GLN:NE2	1:P:132:GLU:HB3	2.32	0.44
1:P:204:LYS:CB	1:P:205:PRO:CD	2.87	0.44
1:E:162:MET:HB3	1:E:170:PHE:CZ	2.53	0.44
1:E:197:ASN:ND2	1:E:210:LYS:HG3	2.33	0.44
1:H:122:GLU:HB3	1:H:211:VAL:HG21	1.99	0.44
1:J:152:ILE:N	1:J:152:ILE:HD12	2.32	0.44
1:J:74:MET:O	1:J:77:GLU:HB2	2.18	0.44
1:N:183:LYS:O	1:N:185:LYS:HD2	2.18	0.44
1:P:38:ASP:HB3	1:P:250:LEU:HD11	1.99	0.44
1:H:107:MET:HE1	1:H:251:LYS:HG2	2.00	0.44
1:H:20:LYS:CE	1:H:30:GLU:O	2.66	0.44
1:L:196:MET:HE2	1:L:200:ILE:HG12	1.99	0.44
1:P:136:GLY:HA2	1:P:162:MET:SD	2.58	0.44
1:B:165:ALA:HB2	3:B:290:HOH:O	2.17	0.43
1:E:185:LYS:HB3	1:E:186:GLY:H	1.68	0.43
1:E:193:GLU:H	2:E:808:VBP:H13	1.82	0.43
1:G:179:ALA:O	1:G:183:LYS:CD	2.66	0.43
1:N:9:THR:O	1:N:86:ALA:HA	2.18	0.43
1:B:136:GLY:HA3	1:B:169:VAL:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:155:PHE:CZ	1:G:215:LEU:HD22	2.52	0.43
1:G:68:THR:C	1:G:70:ILE:N	2.72	0.43
1:N:114:MET:CE	1:N:192:LEU:HD21	2.48	0.43
1:P:260:GLU:O	1:P:261:CYS:SG	2.76	0.43
1:P:60:LYS:HD3	1:P:72:ASN:ND2	2.33	0.43
1:B:115:ILE:HG22	1:B:121:ILE:HD11	2.00	0.43
1:B:14:SER:HB2	3:B:279:HOH:O	2.17	0.43
1:B:56:VAL:HG13	1:B:59:GLY:HA2	2.01	0.43
1:E:12:LEU:HD13	1:E:55:ILE:CD1	2.48	0.43
1:G:11:ILE:HG12	1:G:12:LEU:N	2.33	0.43
1:H:201:GLU:CG	1:H:209:MET:HA	2.48	0.43
1:H:94:LEU:O	1:H:98:GLU:HG3	2.17	0.43
1:J:143:THR:HB	3:J:288:HOH:O	2.19	0.43
1:P:137:THR:HB	1:P:143:THR:HG22	2.00	0.43
1:L:125:GLU:C	1:L:127:LEU:N	2.70	0.43
1:B:67:ASP:OD2	1:B:68:THR:HG23	2.18	0.43
1:G:121:ILE:HD13	1:G:127:LEU:HD21	1.99	0.43
1:H:121:ILE:HG23	1:H:133:ILE:CD1	2.46	0.43
1:H:153:ALA:O	1:H:154:VAL:C	2.57	0.43
1:J:113:ILE:N	3:J:287:HOH:O	2.48	0.43
1:E:47:CYS:SG	1:E:233:ALA:HB1	2.58	0.43
1:G:193:GLU:CD	1:G:218:LYS:HZ2	2.18	0.43
1:G:16:TYR:CG	1:G:89:PRO:HG3	2.53	0.43
1:H:100:ILE:HD13	1:H:223:ALA:HB1	1.99	0.43
1:H:11:ILE:HG12	1:H:12:LEU:N	2.33	0.43
1:J:119:THR:HA	1:J:120:PRO:HD3	1.84	0.43
1:L:159:TRP:HA	1:L:159:TRP:CE3	2.54	0.43
1:B:143:THR:HG21	1:B:191:LEU:O	2.19	0.43
1:B:94:LEU:O	1:B:98:GLU:HG3	2.17	0.43
1:E:115:ILE:CG2	1:E:121:ILE:HD11	2.49	0.43
1:E:183:LYS:HB2	1:E:183:LYS:HZ2	1.83	0.43
1:G:11:ILE:CG1	1:G:12:LEU:N	2.82	0.43
1:J:20:LYS:HB2	1:J:31:ARG:C	2.39	0.43
1:L:184:SER:HB2	1:L:187:LYS:NZ	2.33	0.43
1:N:143:THR:O	1:N:146:PHE:HB3	2.18	0.43
1:N:253:LYS:HE2	1:N:258:LYS:HZ3	1.84	0.43
1:E:116:LYS:NZ	1:E:185:LYS:HA	2.32	0.43
1:E:159:TRP:HA	1:E:159:TRP:HE3	1.82	0.43
1:G:236:LEU:HD22	1:J:94:LEU:CD1	2.49	0.43
1:H:144:LYS:NZ	1:H:148:ARG:NH2	2.67	0.43
1:H:20:LYS:HZ2	1:H:30:GLU:HG2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:5:THR:N	3:J:291:HOH:O	2.51	0.43
1:N:130:GLN:HE21	1:N:132:GLU:CB	2.25	0.43
1:P:193:GLU:HG2	2:P:805:VBP:C13	2.48	0.43
1:B:10:THR:OG1	1:B:11:ILE:N	2.48	0.43
1:B:84:ASP:O	1:B:85:ILE:HB	2.18	0.43
1:G:122:GLU:HA	1:G:211:VAL:CG2	2.41	0.43
1:G:64:ARG:HG3	1:G:71:TRP:CE2	2.54	0.43
1:L:37:VAL:HG13	1:L:53:LEU:HD11	2.00	0.43
1:N:130:GLN:HE21	1:N:133:ILE:N	2.16	0.43
1:P:197:ASN:HD21	1:P:210:LYS:HA	1.84	0.43
1:B:92:ILE:HG12	1:B:102:PHE:CG	2.54	0.42
1:E:115:ILE:HG22	1:E:121:ILE:HD11	2.00	0.42
1:E:161:TYR:O	1:E:165:ALA:HB2	2.18	0.42
1:E:180:ARG:HD3	1:E:188:TYR:CE2	2.54	0.42
1:H:172:ARG:HG2	1:H:173:THR:N	2.34	0.42
1:H:250:LEU:O	1:H:253:LYS:HB3	2.19	0.42
1:H:40:ALA:HA	1:H:87:ILE:HD13	2.01	0.42
1:L:55:ILE:O	1:L:56:VAL:C	2.58	0.42
1:N:100:ILE:HD12	1:N:100:ILE:C	2.40	0.42
1:N:65:ASP:HB3	1:N:68:THR:OG1	2.18	0.42
1:P:12:LEU:HD22	1:P:18:MET:HA	2.00	0.42
1:B:171:VAL:HB	1:B:176:GLU:CG	2.48	0.42
1:H:118:GLY:HA2	1:N:30:GLU:HG2	2.01	0.42
1:H:184:SER:O	1:H:186:GLY:N	2.53	0.42
1:P:250:LEU:HA	1:P:250:LEU:HD23	1.78	0.42
1:J:12:LEU:HD12	1:J:17:VAL:O	2.20	0.42
1:J:116:LYS:HG3	1:J:207:ASP:O	2.19	0.42
1:J:16:TYR:CE1	1:J:255:TRP:HH2	2.37	0.42
1:P:181:VAL:HG22	1:P:188:TYR:O	2.18	0.42
1:P:16:TYR:CE1	1:P:89:PRO:HG3	2.54	0.42
1:P:96:ARG:C	1:P:98:GLU:N	2.73	0.42
1:E:145:GLU:O	1:E:146:PHE:C	2.58	0.42
1:J:60:LYS:HB2	1:J:73:GLY:CA	2.50	0.42
1:L:21:LYS:HG2	1:L:22:ASN:N	2.33	0.42
1:P:114:MET:HE2	1:P:208:THR:HG21	2.01	0.42
1:P:88:ALA:HB1	1:P:89:PRO:CD	2.49	0.42
1:B:203:ARG:NH1	1:B:258:LYS:O	2.52	0.42
1:G:130:GLN:HG3	1:G:131:THR:H	1.84	0.42
1:L:11:ILE:HG21	1:L:61:TYR:CE1	2.54	0.42
1:E:100:ILE:HD13	1:E:223:ALA:CB	2.50	0.42
1:H:100:ILE:HD12	1:H:100:ILE:C	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:11:ILE:HG21	1:H:61:TYR:CE1	2.55	0.42
1:J:68:THR:CB	1:J:70:ILE:HG12	2.49	0.42
1:N:122:GLU:HA	1:N:211:VAL:CG2	2.49	0.42
1:P:125:GLU:OE2	1:P:125:GLU:N	2.52	0.42
1:P:159:TRP:O	1:P:160:THR:C	2.57	0.42
1:P:216:ASP:OD2	1:P:218:LYS:HD2	2.20	0.42
1:B:24:GLU:N	1:B:24:GLU:OE1	2.43	0.42
1:E:172:ARG:N	1:E:176:GLU:OE2	2.42	0.42
1:E:210:LYS:HB3	1:E:210:LYS:NZ	2.34	0.42
1:B:116:LYS:O	1:B:117:LYS:C	2.58	0.42
1:G:196:MET:CE	1:G:196:MET:HA	2.50	0.42
1:L:8:VAL:HG13	1:L:85:ILE:HG23	2.02	0.42
1:E:192:LEU:CD1	1:E:197:ASN:HB2	2.48	0.42
1:H:11:ILE:O	1:H:17:VAL:CG1	2.68	0.42
1:G:104:LYS:NZ	1:J:102:PHE:O	2.36	0.42
1:J:64:ARG:HG3	1:J:64:ARG:HH11	1.83	0.42
1:L:119:THR:HA	1:L:120:PRO:HD3	1.86	0.42
1:L:144:LYS:NZ	1:L:148:ARG:HH21	2.18	0.42
1:N:90:LEU:O	1:N:220:TYR:HA	2.19	0.42
1:P:79:VAL:HG22	1:P:99:VAL:CG1	2.50	0.42
1:P:16:TYR:CG	1:P:89:PRO:HG3	2.55	0.42
1:B:119:THR:HG22	1:B:121:ILE:H	1.85	0.42
1:E:110:GLY:O	1:E:194:SER:N	2.38	0.42
1:G:246:LEU:O	1:G:249:LYS:HB3	2.19	0.42
1:G:94:LEU:O	1:G:98:GLU:HG3	2.19	0.42
1:H:116:LYS:HG3	1:H:185:LYS:O	2.18	0.42
1:H:201:GLU:O	1:H:201:GLU:HG2	2.20	0.42
1:H:20:LYS:C	1:H:22:ASN:H	2.22	0.42
1:J:193:GLU:H	2:J:804:VBP:H13	1.84	0.42
1:B:246:LEU:O	1:B:249:LYS:HB3	2.21	0.41
1:E:116:LYS:O	1:E:117:LYS:C	2.58	0.41
1:G:10:THR:O	1:G:56:VAL:HG12	2.20	0.41
1:H:171:VAL:HB	1:H:176:GLU:OE2	2.20	0.41
1:H:46:HIS:CE1	1:H:241:LEU:HD21	2.54	0.41
1:H:88:ALA:O	1:H:90:LEU:N	2.52	0.41
1:L:234:VAL:O	1:L:237:ALA:HB3	2.20	0.41
1:B:19:MET:HA	1:B:19:MET:HE3	2.02	0.41
1:E:20:LYS:HB3	1:E:22:ASN:ND2	2.35	0.41
1:G:116:LYS:O	1:G:117:LYS:C	2.58	0.41
1:G:134:ALA:O	1:G:188:TYR:HA	2.20	0.41
1:G:141:GLY:O	1:G:142:SER:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:11:ILE:O	1:G:17:VAL:HG13	2.21	0.41
1:H:121:ILE:C	1:H:122:GLU:HG3	2.41	0.41
1:H:214:ASN:N	1:H:214:ASN:HD22	2.17	0.41
1:J:93:THR:OG1	1:J:96:ARG:HD2	2.20	0.41
1:N:119:THR:HA	1:N:120:PRO:HD3	1.82	0.41
1:N:127:LEU:O	1:N:128:SER:C	2.58	0.41
1:N:167:PRO:O	1:N:168:SER:C	2.58	0.41
1:B:92:ILE:HG12	1:B:102:PHE:CD1	2.56	0.41
1:B:166:GLU:N	1:B:166:GLU:CD	2.73	0.41
1:E:190:TYR:CD2	1:E:192:LEU:HG	2.55	0.41
1:L:21:LYS:N	1:L:21:LYS:CD	2.82	0.41
1:N:97:GLU:O	1:N:97:GLU:HG3	2.19	0.41
1:G:121:ILE:CD1	1:G:127:LEU:HD21	2.50	0.41
1:G:127:LEU:O	1:G:130:GLN:HB3	2.21	0.41
1:G:193:GLU:H	2:G:803:VBP:H13	1.84	0.41
1:N:122:GLU:HA	1:N:211:VAL:HG21	2.02	0.41
1:P:137:THR:HB	1:P:143:THR:CG2	2.50	0.41
1:B:15:PRO:HB3	1:B:199:TYR:CE1	2.55	0.41
1:B:113:ILE:C	1:B:197:ASN:HD21	2.23	0.41
1:L:121:ILE:HG22	1:L:126:ASP:C	2.41	0.41
1:N:62:GLY:HA3	1:N:75:VAL:CG2	2.51	0.41
1:P:20:LYS:NZ	1:P:30:GLU:O	2.45	0.41
1:B:109:LEU:HB2	1:B:194:SER:OG	2.20	0.41
1:E:143:THR:O	1:E:146:PHE:HB3	2.20	0.41
1:E:60:LYS:HD2	1:E:72:ASN:ND2	2.36	0.41
1:H:125:GLU:OE1	1:H:125:GLU:N	2.38	0.41
1:H:15:PRO:HA	1:H:18:MET:CE	2.43	0.41
1:L:204:LYS:HG2	1:L:260:GLU:OE1	2.21	0.41
1:N:138:LEU:HA	1:N:138:LEU:HD12	1.95	0.41
1:B:65:ASP:HB3	1:B:68:THR:OG1	2.20	0.41
1:E:148:ARG:HG3	1:E:148:ARG:O	2.21	0.41
1:B:95:VAL:HG12	1:E:69:LYS:HB3	2.03	0.41
1:G:119:THR:CG2	1:G:121:ILE:HG12	2.50	0.41
1:G:15:PRO:HA	1:G:18:MET:SD	2.60	0.41
1:G:209:MET:HE3	1:G:209:MET:HB3	1.93	0.41
1:G:65:ASP:HB3	1:G:68:THR:HG23	2.03	0.41
1:H:169:VAL:HA	1:H:180:ARG:HH22	1.85	0.41
1:H:85:ILE:HD11	1:H:222:ILE:HG21	2.02	0.41
1:P:171:VAL:HB	1:P:176:GLU:CB	2.46	0.41
1:P:55:ILE:O	1:P:56:VAL:C	2.59	0.41
1:B:95:VAL:CG1	1:E:69:LYS:HB3	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:109:LEU:HD23	1:J:109:LEU:N	2.35	0.41
1:L:62:GLY:HA3	1:L:75:VAL:HG23	2.03	0.41
1:N:136:GLY:HA2	1:N:162:MET:HE2	2.03	0.41
1:N:177:GLY:O	1:N:181:VAL:HG23	2.21	0.41
1:B:256:TYR:O	1:B:257:ASP:C	2.59	0.41
1:E:148:ARG:HB2	1:E:159:TRP:CE2	2.55	0.41
1:G:205:PRO:O	1:G:207:ASP:OD1	2.39	0.41
1:H:211:VAL:HG13	1:H:211:VAL:O	2.20	0.41
1:H:88:ALA:HB1	1:H:89:PRO:CD	2.45	0.41
1:J:155:PHE:O	1:J:158:MET:HB2	2.21	0.41
1:L:130:GLN:NE2	1:L:132:GLU:HB3	2.19	0.41
1:N:96:ARG:O	1:N:100:ILE:HG13	2.20	0.41
1:E:192:LEU:N	1:E:192:LEU:HD12	2.36	0.41
1:E:16:TYR:HB3	1:E:36:CYS:SG	2.61	0.41
1:G:130:GLN:CG	1:G:131:THR:N	2.83	0.41
1:G:204:LYS:O	1:G:205:PRO:C	2.56	0.41
1:J:21:LYS:CD	1:J:21:LYS:N	2.63	0.41
1:L:161:TYR:O	1:L:164:SER:O	2.38	0.41
1:L:187:LYS:C	1:L:187:LYS:HE3	2.39	0.41
1:P:115:ILE:HD12	1:P:119:THR:HB	2.03	0.41
1:E:110:GLY:HA3	1:E:214:ASN:HB3	2.03	0.41
1:E:199:TYR:CE1	1:E:203:ARG:NE	2.89	0.41
1:G:148:ARG:HB3	1:G:159:TRP:CZ2	2.55	0.41
1:J:201:GLU:HG3	1:J:209:MET:HA	2.02	0.41
1:J:68:THR:O	1:J:69:LYS:HB3	2.20	0.41
1:L:159:TRP:O	1:L:160:THR:C	2.60	0.41
1:N:204:LYS:CB	1:N:205:PRO:CD	2.77	0.41
1:N:34:GLY:HA2	1:N:254:TRP:CZ3	2.56	0.41
1:P:144:LYS:HZ2	1:P:159:TRP:HH2	1.69	0.41
1:E:164:SER:O	1:E:165:ALA:HB2	2.21	0.40
1:E:85:ILE:HD11	1:E:222:ILE:CG2	2.51	0.40
1:G:250:LEU:O	1:G:253:LYS:HB3	2.22	0.40
1:H:198:GLU:O	1:H:199:TYR:C	2.59	0.40
1:H:203:ARG:HB3	1:H:204:LYS:H	1.65	0.40
1:L:119:THR:HG22	1:L:121:ILE:HG13	2.03	0.40
1:L:131:THR:O	1:L:132:GLU:C	2.59	0.40
1:L:8:VAL:HG23	1:L:51:TYR:HB2	2.02	0.40
1:L:79:VAL:HG12	1:L:80:TYR:CE1	2.56	0.40
1:P:119:THR:HG22	1:P:121:ILE:CG1	2.51	0.40
1:P:192:LEU:CD1	1:P:197:ASN:HB2	2.50	0.40
1:P:201:GLU:CG	1:P:209:MET:HA	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:90:LEU:O	1:P:220:TYR:HA	2.21	0.40
1:B:67:ASP:N	1:B:67:ASP:OD2	2.53	0.40
1:J:89:PRO:HB2	2:J:804:VBP:C05	2.44	0.40
1:P:180:ARG:HD2	1:P:188:TYR:CE2	2.55	0.40
1:B:201:GLU:HG2	1:B:202:GLN:NE2	2.36	0.40
1:B:5:THR:N	3:B:262:HOH:O	2.54	0.40
1:G:146:PHE:O	1:G:150:SER:HB2	2.22	0.40
1:J:201:GLU:OE1	1:J:210:LYS:N	2.48	0.40
1:L:253:LYS:HA	1:L:257:ASP:HB2	2.02	0.40
1:P:133:ILE:HG23	1:P:187:LYS:O	2.21	0.40
1:B:64:ARG:HG3	1:B:71:TRP:CZ2	2.56	0.40
1:J:204:LYS:O	1:J:205:PRO:C	2.60	0.40
1:J:20:LYS:HG2	1:J:26:LEU:HD12	2.04	0.40
1:H:244:GLN:O	1:L:149:ARG:HG2	2.20	0.40
1:L:166:GLU:HB2	1:L:167:PRO:CA	2.52	0.40
1:N:11:ILE:O	1:N:17:VAL:CG1	2.69	0.40
1:N:228:SER:OG	1:N:230:LEU:HD12	2.21	0.40
1:E:89:PRO:HB2	2:E:808:VBP:H05	2.04	0.40
1:G:107:MET:HG2	1:G:108:SER:N	2.36	0.40
1:G:193:GLU:HG2	2:G:803:VBP:C13	2.51	0.40
1:H:130:GLN:HE22	1:H:133:ILE:N	2.17	0.40
1:N:127:LEU:O	1:N:129:LYS:N	2.55	0.40
1:N:136:GLY:HA2	1:N:162:MET:CE	2.51	0.40
1:N:39:LEU:O	1:N:43:ILE:HG12	2.20	0.40
1:N:49:PHE:CD1	1:N:49:PHE:C	2.95	0.40
1:P:5:THR:N	3:P:283:HOH:O	2.54	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	B	255/258 (99%)	227 (89%)	23 (9%)	5 (2%)	9	28
1	E	255/258 (99%)	222 (87%)	20 (8%)	13 (5%)	2	7
1	G	255/258 (99%)	223 (88%)	27 (11%)	5 (2%)	9	28
1	H	255/258 (99%)	211 (83%)	35 (14%)	9 (4%)	4	14
1	J	255/258 (99%)	228 (89%)	19 (8%)	8 (3%)	5	16
1	L	255/258 (99%)	212 (83%)	32 (12%)	11 (4%)	3	10
1	N	255/258 (99%)	220 (86%)	23 (9%)	12 (5%)	3	8
1	P	255/258 (99%)	206 (81%)	37 (14%)	12 (5%)	3	8
All	All	2040/2064 (99%)	1749 (86%)	216 (11%)	75 (4%)	4	13

All (75) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	205	PRO
1	G	206	CYS
1	B	163	ARG
1	E	14	SER
1	E	185	LYS
1	E	204	LYS
1	E	205	PRO
1	E	206	CYS
1	H	22	ASN
1	H	122	GLU
1	H	153	ALA
1	J	130	GLN
1	J	204	LYS
1	L	184	SER
1	L	204	LYS
1	L	205	PRO
1	L	206	CYS
1	N	130	GLN
1	N	204	LYS
1	N	205	PRO
1	N	206	CYS
1	P	153	ALA
1	P	165	ALA
1	P	204	LYS
1	P	205	PRO
1	G	204	LYS
1	B	66	ALA

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Mol	Chain	Res	Type
1	E	148	ARG
1	E	184	SER
1	J	120	PRO
1	J	128	SER
1	L	153	ALA
1	N	153	ALA
1	N	168	SER
1	P	206	CYS
1	G	153	ALA
1	B	153	ALA
1	E	15	PRO
1	H	172	ARG
1	H	185	LYS
1	J	21	LYS
1	N	128	SER
1	P	132	GLU
1	B	134	ALA
1	E	46	HIS
1	E	122	GLU
1	E	168	SER
1	H	132	GLU
1	H	168	SER
1	L	117	LYS
1	L	167	PRO
1	L	185	LYS
1	P	120	PRO
1	P	185	LYS
1	P	209	MET
1	G	131	THR
1	L	122	GLU
1	L	231	GLY
1	N	209	MET
1	P	126	ASP
1	B	188	TYR
1	J	172	ARG
1	L	56	VAL
1	N	120	PRO
1	H	181	VAL
1	J	17	VAL
1	J	62	GLY
1	P	56	VAL
1	E	154	VAL

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Mol	Chain	Res	Type
1	P	231	GLY
1	N	48	GLY
1	N	56	VAL
1	N	62	GLY
1	H	95	VAL
1	E	167	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	216/217 (100%)	206 (95%)	10 (5%)	31	65
1	E	216/217 (100%)	207 (96%)	9 (4%)	34	68
1	G	216/217 (100%)	201 (93%)	15 (7%)	18	46
1	H	216/217 (100%)	199 (92%)	17 (8%)	14	38
1	J	216/217 (100%)	203 (94%)	13 (6%)	22	54
1	L	216/217 (100%)	200 (93%)	16 (7%)	16	42
1	N	216/217 (100%)	198 (92%)	18 (8%)	13	36
1	P	216/217 (100%)	204 (94%)	12 (6%)	25	57
All	All	1728/1736 (100%)	1618 (94%)	110 (6%)	20	50

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	17	VAL
1	G	45	LYS
1	G	60	LYS
1	G	67	ASP
1	G	68	THR
1	G	78	LEU
1	G	130	GLN
1	G	132	GLU
1	G	145	GLU

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Mol	Chain	Res	Type
1	G	148	ARG
1	G	174	THR
1	G	192	LEU
1	G	205	PRO
1	G	209	MET
1	G	246	LEU
1	B	17	VAL
1	B	18	MET
1	B	22	ASN
1	B	27	GLU
1	B	90	LEU
1	B	166	GLU
1	B	192	LEU
1	B	196	MET
1	B	209	MET
1	B	255	TRP
1	E	17	VAL
1	E	22	ASN
1	E	90	LEU
1	E	109	LEU
1	E	126	ASP
1	E	145	GLU
1	E	161	TYR
1	E	192	LEU
1	E	246	LEU
1	H	17	VAL
1	H	18	MET
1	H	24	GLU
1	H	67	ASP
1	H	95	VAL
1	H	122	GLU
1	H	126	ASP
1	H	130	GLN
1	H	144	LYS
1	H	163	ARG
1	H	173	THR
1	H	174	THR
1	H	192	LEU
1	H	204	LYS
1	H	226	LYS
1	H	246	LEU
1	H	252	ASN

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Mol	Chain	Res	Type
1	J	12	LEU
1	J	17	VAL
1	J	21	LYS
1	J	64	ARG
1	J	69	LYS
1	J	78	LEU
1	J	125	GLU
1	J	144	LYS
1	J	148	ARG
1	J	156	ASP
1	J	192	LEU
1	J	250	LEU
1	J	255	TRP
1	L	15	PRO
1	L	17	VAL
1	L	21	LYS
1	L	25	MET
1	L	104	LYS
1	L	109	LEU
1	L	129	LYS
1	L	144	LYS
1	L	169	VAL
1	L	187	LYS
1	L	192	LEU
1	L	205	PRO
1	L	235	ASN
1	L	244	GLN
1	L	248	ASP
1	L	255	TRP
1	N	17	VAL
1	N	23	HIS
1	N	67	ASP
1	N	78	LEU
1	N	109	LEU
1	N	126	ASP
1	N	131	THR
1	N	144	LYS
1	N	149	ARG
1	N	150	SER
1	N	161	TYR
1	N	171	VAL
1	N	174	THR

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Mol	Chain	Res	Type
1	N	192	LEU
1	N	205	PRO
1	N	224	THR
1	N	230	LEU
1	N	255	TRP
1	P	17	VAL
1	P	18	MET
1	P	64	ARG
1	P	82	LYS
1	P	90	LEU
1	P	95	VAL
1	P	109	LEU
1	P	174	THR
1	P	187	LYS
1	P	192	LEU
1	P	218	LYS
1	P	232	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	46	HIS
1	B	46	HIS
1	B	130	GLN
1	B	244	GLN
1	E	22	ASN
1	E	46	HIS
1	E	197	ASN
1	E	244	GLN
1	H	130	GLN
1	H	197	ASN
1	H	214	ASN
1	H	244	GLN
1	H	252	ASN
1	J	130	GLN
1	J	244	GLN
1	L	46	HIS
1	L	130	GLN
1	L	197	ASN
1	L	252	ASN
1	N	46	HIS
1	N	130	GLN

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Mol	Chain	Res	Type
1	N	197	ASN
1	N	244	GLN
1	P	46	HIS
1	P	130	GLN
1	P	197	ASN
1	P	232	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 ⓘ

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	VBP	B	807	-	14,25,25	6.48	11 (78%)	15,35,35	1.49	1 (6%)
2	VBP	E	808	-	14,25,25	6.55	11 (78%)	15,35,35	1.60	1 (6%)
2	VBP	G	803	-	14,25,25	6.64	11 (78%)	15,35,35	1.65	1 (6%)
2	VBP	H	806	-	14,25,25	6.32	11 (78%)	15,35,35	1.76	2 (13%)
2	VBP	J	804	-	14,25,25	6.46	12 (85%)	15,35,35	1.54	1 (6%)
2	VBP	L	801	-	14,25,25	6.55	12 (85%)	15,35,35	1.52	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	VBP	N	802	-	14,25,25	6.43	12 (85%)	15,35,35	1.41	1 (6%)
2	VBP	P	805	-	14,25,25	6.80	11 (78%)	15,35,35	1.35	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	VBP	B	807	-	1/1/3/3	0/7/16/16	0/2/2/2
2	VBP	E	808	-	1/1/3/3	0/7/16/16	0/2/2/2
2	VBP	G	803	-	1/1/3/3	0/7/16/16	0/2/2/2
2	VBP	H	806	-	1/1/3/3	0/7/16/16	0/2/2/2
2	VBP	J	804	-	1/1/3/3	0/7/16/16	0/2/2/2
2	VBP	L	801	-	1/1/3/3	0/7/16/16	0/2/2/2
2	VBP	N	802	-	1/1/3/3	0/7/16/16	0/2/2/2
2	VBP	P	805	-	1/1/3/3	0/7/16/16	0/2/2/2

All (91) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	806	VBP	C03-N04	-6.04	1.42	1.48
2	N	802	VBP	C03-N04	-5.92	1.42	1.48
2	G	803	VBP	C03-N04	-5.55	1.42	1.48
2	B	807	VBP	C03-N04	-5.30	1.42	1.48
2	E	808	VBP	C03-N04	-5.20	1.43	1.48
2	J	804	VBP	C03-N04	-4.82	1.43	1.48
2	L	801	VBP	C03-N04	-4.72	1.43	1.48
2	P	805	VBP	C03-N04	-4.57	1.43	1.48
2	L	801	VBP	C10-N09	-2.36	1.44	1.48
2	N	802	VBP	C10-N09	-2.29	1.44	1.48
2	J	804	VBP	C10-N09	-2.17	1.44	1.48
2	N	802	VBP	C05-C06	5.37	1.49	1.38
2	J	804	VBP	C05-C06	5.47	1.49	1.38
2	H	806	VBP	C05-C06	5.50	1.49	1.38
2	P	805	VBP	C05-C06	5.51	1.49	1.38
2	G	803	VBP	C05-C06	5.51	1.50	1.38
2	B	807	VBP	C05-C06	5.65	1.50	1.38
2	L	801	VBP	C05-C06	5.73	1.50	1.38
2	E	808	VBP	C05-C06	5.75	1.50	1.38
2	H	806	VBP	O08-C07	6.04	1.39	1.24
2	B	807	VBP	O08-C07	6.05	1.39	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	802	VBP	O08-C07	6.14	1.39	1.24
2	G	803	VBP	O08-C07	6.41	1.40	1.24
2	J	804	VBP	O08-C07	6.45	1.40	1.24
2	P	805	VBP	O08-C07	6.48	1.40	1.24
2	E	808	VBP	O08-C07	6.51	1.40	1.24
2	J	804	VBP	C13-C14	6.61	1.53	1.39
2	N	802	VBP	C12-C11	6.61	1.52	1.38
2	H	806	VBP	C12-C11	6.61	1.52	1.38
2	H	806	VBP	C13-C14	6.62	1.53	1.39
2	G	803	VBP	C13-C14	6.66	1.53	1.39
2	N	802	VBP	C13-C14	6.67	1.53	1.39
2	L	801	VBP	O08-C07	6.70	1.41	1.24
2	P	805	VBP	C13-C14	6.75	1.53	1.39
2	B	807	VBP	C12-C11	6.80	1.53	1.38
2	J	804	VBP	C12-C11	6.82	1.53	1.38
2	L	801	VBP	C13-C14	6.83	1.53	1.39
2	B	807	VBP	C13-C14	6.85	1.53	1.39
2	L	801	VBP	C12-C11	6.88	1.53	1.38
2	H	806	VBP	C07-N09	6.97	1.48	1.38
2	P	805	VBP	C12-C11	6.98	1.53	1.38
2	E	808	VBP	C05-N04	6.98	1.48	1.36
2	L	801	VBP	C16-C11	6.99	1.53	1.38
2	N	802	VBP	C15-C14	7.05	1.54	1.39
2	E	808	VBP	C13-C14	7.12	1.54	1.39
2	E	808	VBP	C12-C11	7.12	1.53	1.38
2	J	804	VBP	C16-C11	7.14	1.53	1.38
2	G	803	VBP	C12-C11	7.15	1.53	1.38
2	N	802	VBP	C16-C11	7.22	1.53	1.38
2	L	801	VBP	C15-C14	7.22	1.54	1.39
2	B	807	VBP	C16-C11	7.32	1.54	1.38
2	H	806	VBP	C05-N04	7.35	1.48	1.36
2	H	806	VBP	C16-C11	7.37	1.54	1.38
2	G	803	VBP	C16-C11	7.40	1.54	1.38
2	J	804	VBP	C15-C14	7.47	1.55	1.39
2	B	807	VBP	C15-C14	7.49	1.55	1.39
2	B	807	VBP	C05-N04	7.51	1.49	1.36
2	H	806	VBP	C15-C14	7.54	1.55	1.39
2	G	803	VBP	C15-C14	7.57	1.55	1.39
2	P	805	VBP	C16-C11	7.61	1.54	1.38
2	E	808	VBP	C16-C11	7.66	1.54	1.38
2	N	802	VBP	C07-N09	7.69	1.49	1.38
2	L	801	VBP	C05-N04	7.75	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	804	VBP	C05-N04	7.79	1.49	1.36
2	E	808	VBP	C15-C14	7.81	1.55	1.39
2	P	805	VBP	C15-C14	7.86	1.56	1.39
2	G	803	VBP	C05-N04	7.93	1.49	1.36
2	J	804	VBP	C07-N09	7.95	1.50	1.38
2	E	808	VBP	C07-N09	7.97	1.50	1.38
2	P	805	VBP	C05-N04	8.07	1.49	1.36
2	N	802	VBP	C05-N04	8.12	1.50	1.36
2	B	807	VBP	C07-N09	8.25	1.50	1.38
2	G	803	VBP	C07-N09	8.29	1.50	1.38
2	L	801	VBP	C07-N09	8.48	1.50	1.38
2	N	802	VBP	C12-C13	8.51	1.54	1.38
2	H	806	VBP	C12-C13	8.51	1.54	1.38
2	E	808	VBP	C12-C13	8.74	1.54	1.38
2	B	807	VBP	C12-C13	8.78	1.54	1.38
2	J	804	VBP	C12-C13	8.80	1.54	1.38
2	H	806	VBP	C16-C15	8.88	1.54	1.38
2	L	801	VBP	C16-C15	9.06	1.55	1.38
2	B	807	VBP	C16-C15	9.12	1.55	1.38
2	G	803	VBP	C16-C15	9.15	1.55	1.38
2	N	802	VBP	C16-C15	9.18	1.55	1.38
2	P	805	VBP	C07-N09	9.18	1.51	1.38
2	L	801	VBP	C12-C13	9.22	1.55	1.38
2	P	805	VBP	C12-C13	9.27	1.55	1.38
2	J	804	VBP	C16-C15	9.29	1.55	1.38
2	E	808	VBP	C16-C15	9.32	1.55	1.38
2	G	803	VBP	C12-C13	9.36	1.55	1.38
2	P	805	VBP	C16-C15	10.06	1.56	1.38

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	806	VBP	C16-C11-C12	2.16	121.59	118.16
2	P	805	VBP	C10-N09-C20	4.02	122.63	117.92
2	N	802	VBP	C10-N09-C20	4.23	122.88	117.92
2	J	804	VBP	C10-N09-C20	4.64	123.35	117.92
2	L	801	VBP	C10-N09-C20	4.85	123.59	117.92
2	B	807	VBP	C10-N09-C20	4.87	123.63	117.92
2	E	808	VBP	C10-N09-C20	5.08	123.87	117.92
2	G	803	VBP	C10-N09-C20	5.24	124.05	117.92
2	H	806	VBP	C10-N09-C20	5.62	124.50	117.92

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	H	806	VBP	C02
2	E	808	VBP	C02
2	N	802	VBP	C02
2	B	807	VBP	C02
2	P	805	VBP	C02
2	J	804	VBP	C02
2	G	803	VBP	C02
2	L	801	VBP	C02

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	807	VBP	3	0
2	E	808	VBP	4	0
2	G	803	VBP	5	0
2	H	806	VBP	3	0
2	J	804	VBP	4	0
2	L	801	VBP	2	0
2	N	802	VBP	3	0
2	P	805	VBP	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	B	257/258 (99%)	1.53	77 (29%) 1 0	12, 32, 65, 76	0
1	E	257/258 (99%)	1.75	93 (36%) 0 0	17, 37, 70, 91	0
1	G	257/258 (99%)	1.47	64 (24%) 1 0	14, 34, 61, 71	0
1	H	257/258 (99%)	1.68	86 (33%) 0 0	13, 36, 72, 89	0
1	J	257/258 (99%)	1.60	77 (29%) 1 0	18, 35, 60, 68	0
1	L	257/258 (99%)	1.62	74 (28%) 1 0	18, 36, 64, 74	0
1	N	257/258 (99%)	1.62	73 (28%) 1 0	16, 35, 65, 74	0
1	P	257/258 (99%)	1.77	80 (31%) 0 0	17, 36, 63, 73	0
All	All	2056/2064 (99%)	1.63	624 (30%) 0 0	12, 35, 65, 91	0

All (624) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	121	ILE	10.8
1	H	164	SER	9.8
1	E	147	PHE	9.4
1	E	219	GLY	8.6
1	J	109	LEU	8.3
1	P	121	ILE	8.3
1	N	183	LYS	8.0
1	E	151	LYS	7.7
1	J	147	PHE	7.5
1	P	223	ALA	7.5
1	G	164	SER	7.5
1	L	108	SER	7.3
1	J	47	CYS	7.1
1	E	122	GLU	6.7
1	L	190	TYR	6.5
1	B	164	SER	6.4

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Mol	Chain	Res	Type	RSRZ
1	P	188	TYR	6.4
1	N	136	GLY	6.3
1	H	153	ALA	6.3
1	L	49	PHE	6.2
1	B	161	TYR	6.2
1	N	161	TYR	6.2
1	H	135	TYR	6.2
1	H	154	VAL	6.1
1	N	124	ALA	6.0
1	B	151	LYS	6.0
1	E	167	PRO	6.0
1	L	246	LEU	5.9
1	E	205	PRO	5.9
1	N	121	ILE	5.8
1	H	148	ARG	5.8
1	E	204	LYS	5.7
1	N	159	TRP	5.6
1	P	11	ILE	5.6
1	N	148	ARG	5.5
1	J	135	TYR	5.5
1	G	118	GLY	5.5
1	G	136	GLY	5.5
1	H	167	PRO	5.4
1	E	213	GLY	5.4
1	N	80	TYR	5.4
1	L	150	SER	5.4
1	P	108	SER	5.4
1	H	149	ARG	5.3
1	N	209	MET	5.3
1	L	205	PRO	5.3
1	H	5	THR	5.3
1	H	144	LYS	5.3
1	L	5	THR	5.3
1	L	207	ASP	5.3
1	E	190	TYR	5.2
1	H	150	SER	5.2
1	J	121	ILE	5.1
1	H	114	MET	5.1
1	H	161	TYR	5.1
1	E	212	GLY	5.0
1	E	188	TYR	5.0
1	B	212	GLY	5.0

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Mol	Chain	Res	Type	RSRZ
1	J	188	TYR	4.9
1	P	182	ARG	4.9
1	G	205	PRO	4.8
1	P	136	GLY	4.8
1	L	157	LYS	4.8
1	N	162	MET	4.8
1	J	134	ALA	4.7
1	J	79	VAL	4.7
1	P	126	ASP	4.7
1	B	114	MET	4.7
1	L	204	LYS	4.7
1	J	48	GLY	4.7
1	G	151	LYS	4.7
1	P	134	ALA	4.7
1	E	26	LEU	4.6
1	L	137	THR	4.6
1	B	130	GLN	4.6
1	G	16	TYR	4.6
1	H	151	LYS	4.6
1	G	165	ALA	4.6
1	G	212	GLY	4.6
1	J	123	SER	4.5
1	G	80	TYR	4.5
1	L	48	GLY	4.5
1	H	127	LEU	4.5
1	B	153	ALA	4.5
1	E	164	SER	4.5
1	N	149	ARG	4.5
1	P	110	GLY	4.4
1	J	151	LYS	4.4
1	P	7	VAL	4.4
1	B	150	SER	4.4
1	N	223	ALA	4.4
1	L	211	VAL	4.4
1	N	155	PHE	4.4
1	H	159	TRP	4.3
1	N	185	LYS	4.3
1	B	51	TYR	4.3
1	P	174	THR	4.3
1	N	130	GLN	4.3
1	L	129	LYS	4.3
1	P	180	ARG	4.3

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Mol	Chain	Res	Type	RSRZ
1	J	211	VAL	4.2
1	B	176	GLU	4.2
1	H	257	ASP	4.2
1	G	227	GLY	4.2
1	B	127	LEU	4.2
1	B	154	VAL	4.2
1	P	169	VAL	4.2
1	N	172	ARG	4.2
1	B	144	LYS	4.2
1	N	182	ARG	4.1
1	P	109	LEU	4.1
1	B	78	LEU	4.1
1	E	199	TYR	4.1
1	P	155	PHE	4.1
1	P	233	ALA	4.0
1	E	142	SER	4.0
1	P	189	ALA	4.0
1	J	130	GLN	4.0
1	J	209	MET	4.0
1	B	129	LYS	4.0
1	P	170	PHE	4.0
1	H	261	CYS	4.0
1	N	109	LEU	4.0
1	E	81	GLY	4.0
1	L	136	GLY	4.0
1	J	154	VAL	4.0
1	H	112	SER	4.0
1	N	26	LEU	4.0
1	H	250	LEU	3.9
1	G	213	GLY	3.9
1	E	248	ASP	3.9
1	P	137	THR	3.9
1	E	171	VAL	3.9
1	L	120	PRO	3.9
1	E	162	MET	3.9
1	P	187	LYS	3.8
1	J	110	GLY	3.8
1	N	126	ASP	3.8
1	N	168	SER	3.8
1	H	152	ILE	3.8
1	H	168	SER	3.8
1	J	11	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	J	197	ASN	3.8
1	B	137	THR	3.7
1	G	142	SER	3.7
1	H	120	PRO	3.7
1	B	152	ILE	3.7
1	N	158	MET	3.7
1	J	204	LYS	3.7
1	L	109	LEU	3.7
1	P	30	GLU	3.7
1	L	208	THR	3.7
1	N	137	THR	3.7
1	E	21	LYS	3.7
1	L	75	VAL	3.7
1	B	149	ARG	3.7
1	L	189	ALA	3.7
1	J	137	THR	3.7
1	B	181	VAL	3.7
1	B	159	TRP	3.7
1	G	46	HIS	3.7
1	B	49	PHE	3.7
1	N	54	THR	3.7
1	B	50	LYS	3.7
1	E	159	TRP	3.7
1	H	137	THR	3.7
1	P	150	SER	3.6
1	P	193	GLU	3.6
1	P	135	TYR	3.6
1	J	81	GLY	3.6
1	B	203	ARG	3.6
1	E	163	ARG	3.6
1	L	181	VAL	3.6
1	E	144	LYS	3.6
1	G	113	ILE	3.6
1	P	105	PRO	3.6
1	P	173	THR	3.6
1	L	177	GLY	3.6
1	P	215	LEU	3.6
1	H	58	ASP	3.5
1	L	147	PHE	3.5
1	B	213	GLY	3.5
1	E	118	GLY	3.5
1	L	194	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	N	176	GLU	3.5
1	B	196	MET	3.5
1	N	53	LEU	3.5
1	N	204	LYS	3.5
1	J	219	GLY	3.5
1	G	188	TYR	3.5
1	E	211	VAL	3.5
1	N	123	SER	3.5
1	N	196	MET	3.5
1	L	178	VAL	3.5
1	G	96	ARG	3.4
1	G	134	ALA	3.4
1	J	66	ALA	3.4
1	N	5	THR	3.4
1	B	26	LEU	3.4
1	P	5	THR	3.4
1	N	234	VAL	3.4
1	J	185	LYS	3.4
1	P	131	THR	3.4
1	B	99	VAL	3.3
1	J	215	LEU	3.3
1	H	162	MET	3.3
1	P	178	VAL	3.3
1	H	172	ARG	3.3
1	J	105	PRO	3.3
1	P	202	GLN	3.3
1	G	173	THR	3.3
1	E	257	ASP	3.3
1	E	51	TYR	3.3
1	H	51	TYR	3.3
1	H	252	ASN	3.3
1	N	246	LEU	3.3
1	J	122	GLU	3.3
1	J	148	ARG	3.3
1	L	26	LEU	3.3
1	E	136	GLY	3.3
1	J	230	LEU	3.3
1	P	181	VAL	3.2
1	P	94	LEU	3.2
1	G	147	PHE	3.2
1	P	48	GLY	3.2
1	G	231	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	J	257	ASP	3.2
1	E	23	HIS	3.2
1	H	227	GLY	3.2
1	J	111	ILE	3.2
1	P	36	CYS	3.2
1	N	174	THR	3.2
1	L	188	TYR	3.2
1	N	127	LEU	3.2
1	E	14	SER	3.2
1	J	26	LEU	3.2
1	J	216	ASP	3.2
1	L	142	SER	3.2
1	P	140	SER	3.2
1	H	158	MET	3.2
1	P	53	LEU	3.2
1	E	121	ILE	3.1
1	G	81	GLY	3.1
1	B	177	GLY	3.1
1	H	163	ARG	3.1
1	E	131	THR	3.1
1	N	208	THR	3.1
1	G	11	ILE	3.1
1	E	99	VAL	3.1
1	L	130	GLN	3.1
1	L	209	MET	3.1
1	E	40	ALA	3.1
1	B	204	LYS	3.1
1	E	102	PHE	3.1
1	E	146	PHE	3.1
1	E	150	SER	3.0
1	B	158	MET	3.0
1	P	186	GLY	3.0
1	N	122	GLU	3.0
1	P	123	SER	3.0
1	L	119	THR	3.0
1	H	181	VAL	3.0
1	B	63	ALA	3.0
1	G	25	MET	3.0
1	G	32	TYR	3.0
1	P	106	PHE	3.0
1	H	30	GLU	3.0
1	J	199	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	P	191	LEU	3.0
1	E	186	GLY	3.0
1	B	184	SER	3.0
1	E	208	THR	3.0
1	P	237	ALA	2.9
1	J	53	LEU	2.9
1	E	129	LYS	2.9
1	J	27	GLU	2.9
1	E	32	TYR	2.9
1	E	148	ARG	2.9
1	B	120	PRO	2.9
1	H	254	TRP	2.9
1	N	129	LYS	2.9
1	H	8	VAL	2.9
1	N	220	TYR	2.9
1	E	130	GLN	2.9
1	L	22	ASN	2.9
1	L	183	LYS	2.9
1	N	150	SER	2.9
1	B	135	TYR	2.9
1	J	22	ASN	2.9
1	E	67	ASP	2.9
1	E	84	ASP	2.9
1	E	85	ILE	2.9
1	G	254	TRP	2.9
1	J	59	GLY	2.9
1	H	189	ALA	2.9
1	P	60	LYS	2.9
1	G	74	MET	2.9
1	L	118	GLY	2.9
1	E	149	ARG	2.9
1	E	250	LEU	2.9
1	G	137	THR	2.9
1	E	117	LYS	2.9
1	G	28	GLY	2.9
1	J	108	SER	2.8
1	B	118	GLY	2.8
1	H	171	VAL	2.8
1	L	154	VAL	2.8
1	J	89	PRO	2.8
1	J	190	TYR	2.8
1	P	234	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	68	THR	2.8
1	G	108	SER	2.8
1	E	43	ILE	2.8
1	H	111	ILE	2.8
1	G	47	CYS	2.8
1	B	86	ALA	2.8
1	B	160	THR	2.8
1	L	113	ILE	2.8
1	E	133	ILE	2.8
1	N	178	VAL	2.8
1	E	52	LYS	2.8
1	L	187	LYS	2.8
1	N	116	LYS	2.8
1	H	194	SER	2.8
1	P	216	ASP	2.8
1	P	25	MET	2.8
1	B	46	HIS	2.8
1	H	117	LYS	2.8
1	H	166	GLU	2.8
1	G	237	ALA	2.8
1	H	134	ALA	2.8
1	H	113	ILE	2.7
1	J	180	ARG	2.7
1	H	138	LEU	2.7
1	L	37	VAL	2.7
1	N	79	VAL	2.7
1	G	135	TYR	2.7
1	J	37	VAL	2.7
1	P	154	VAL	2.7
1	N	190	TYR	2.7
1	G	149	ARG	2.7
1	B	246	LEU	2.7
1	J	17	VAL	2.7
1	N	132	GLU	2.7
1	E	115	ILE	2.7
1	B	15	PRO	2.7
1	G	217	SER	2.7
1	L	217	SER	2.7
1	N	119	THR	2.7
1	N	200	ILE	2.7
1	J	30	GLU	2.7
1	E	221	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	227	GLY	2.7
1	J	32	TYR	2.7
1	H	239	LEU	2.7
1	E	140	SER	2.7
1	B	121	ILE	2.7
1	L	61	TYR	2.7
1	N	49	PHE	2.7
1	N	61	TYR	2.7
1	P	47	CYS	2.7
1	E	22	ASN	2.7
1	P	257	ASP	2.7
1	J	203	ARG	2.7
1	B	132	GLU	2.6
1	E	145	GLU	2.6
1	G	72	ASN	2.6
1	G	119	THR	2.6
1	N	108	SER	2.6
1	B	148	ARG	2.6
1	J	67	ASP	2.6
1	L	259	GLY	2.6
1	B	88	ALA	2.6
1	H	22	ASN	2.6
1	B	21	LYS	2.6
1	B	236	LEU	2.6
1	H	116	LYS	2.6
1	L	206	CYS	2.6
1	B	22	ASN	2.6
1	H	124	ALA	2.6
1	P	179	ALA	2.6
1	E	185	LYS	2.6
1	B	165	ALA	2.6
1	H	64	ARG	2.6
1	L	131	THR	2.6
1	B	146	PHE	2.6
1	E	231	GLY	2.5
1	J	136	GLY	2.5
1	J	18	MET	2.5
1	J	196	MET	2.5
1	P	103	SER	2.5
1	N	189	ALA	2.5
1	B	215	LEU	2.5
1	L	173	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	L	220	TYR	2.5
1	G	242	ASN	2.5
1	G	172	ARG	2.5
1	E	113	ILE	2.5
1	P	252	ASN	2.5
1	B	254	TRP	2.5
1	P	74	MET	2.5
1	P	175	ALA	2.5
1	H	87	ILE	2.5
1	G	170	PHE	2.5
1	J	184	SER	2.5
1	N	133	ILE	2.5
1	L	53	LEU	2.5
1	N	198	GLU	2.5
1	B	167	PRO	2.5
1	N	236	LEU	2.5
1	G	206	CYS	2.5
1	G	179	ALA	2.5
1	E	46	HIS	2.5
1	H	130	GLN	2.5
1	B	251	LYS	2.5
1	E	152	ILE	2.5
1	P	111	ILE	2.5
1	H	31	ARG	2.5
1	N	169	VAL	2.5
1	P	244	GLN	2.5
1	G	143	THR	2.5
1	G	204	LYS	2.5
1	H	115	ILE	2.5
1	B	163	ARG	2.4
1	E	132	GLU	2.4
1	H	123	SER	2.4
1	N	67	ASP	2.4
1	L	227	GLY	2.4
1	P	162	MET	2.4
1	N	151	LYS	2.4
1	J	162	MET	2.4
1	G	187	LYS	2.4
1	E	61	TYR	2.4
1	E	137	THR	2.4
1	J	170	PHE	2.4
1	B	73	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	L	66	ALA	2.4
1	J	117	LYS	2.4
1	N	202	GLN	2.4
1	N	191	LEU	2.4
1	B	131	THR	2.4
1	E	73	GLY	2.4
1	N	181	VAL	2.4
1	G	102	PHE	2.4
1	E	161	TYR	2.4
1	H	35	TYR	2.4
1	P	130	GLN	2.4
1	J	150	SER	2.4
1	B	12	LEU	2.4
1	L	104	LYS	2.4
1	L	172	ARG	2.4
1	E	89	PRO	2.4
1	P	211	VAL	2.4
1	G	131	THR	2.4
1	H	160	THR	2.4
1	H	209	MET	2.4
1	P	209	MET	2.4
1	L	192	LEU	2.4
1	E	177	GLY	2.3
1	H	16	TYR	2.3
1	E	157	LYS	2.3
1	H	55	ILE	2.3
1	J	29	ASN	2.3
1	G	132	GLU	2.3
1	H	91	THR	2.3
1	G	71	TRP	2.3
1	J	70	ILE	2.3
1	N	201	GLU	2.3
1	B	65	ASP	2.3
1	E	197	ASN	2.3
1	E	200	ILE	2.3
1	P	194	SER	2.3
1	B	34	GLY	2.3
1	E	259	GLY	2.3
1	P	221	GLY	2.3
1	L	180	ARG	2.3
1	L	234	VAL	2.3
1	B	188	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	77	GLU	2.3
1	J	25	MET	2.3
1	B	91	THR	2.3
1	J	54	THR	2.3
1	L	168	SER	2.3
1	H	143	THR	2.3
1	J	155	PHE	2.3
1	P	116	LYS	2.3
1	P	129	LYS	2.3
1	G	39	LEU	2.3
1	G	121	ILE	2.3
1	L	182	ARG	2.3
1	H	170	PHE	2.3
1	H	21	LYS	2.3
1	G	123	SER	2.3
1	E	74	MET	2.3
1	J	243	GLU	2.3
1	G	259	GLY	2.2
1	E	165	ALA	2.2
1	L	51	TYR	2.2
1	P	152	ILE	2.2
1	N	29	ASN	2.2
1	G	36	CYS	2.2
1	J	182	ARG	2.2
1	H	187	LYS	2.2
1	L	253	LYS	2.2
1	L	54	THR	2.2
1	H	136	GLY	2.2
1	L	44	ALA	2.2
1	L	225	PRO	2.2
1	N	205	PRO	2.2
1	E	206	CYS	2.2
1	G	8	VAL	2.2
1	G	140	SER	2.2
1	H	198	GLU	2.2
1	N	9	THR	2.2
1	P	58	ASP	2.2
1	P	205	PRO	2.2
1	H	93	THR	2.2
1	L	250	LEU	2.2
1	E	15	PRO	2.2
1	P	76	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	233	ALA	2.2
1	L	155	PHE	2.2
1	E	176	GLU	2.2
1	B	183	LYS	2.2
1	L	124	ALA	2.2
1	B	174	THR	2.2
1	B	225	PRO	2.2
1	E	173	THR	2.2
1	N	128	SER	2.2
1	P	61	TYR	2.2
1	E	203	ARG	2.2
1	P	231	GLY	2.2
1	N	255	TRP	2.2
1	B	202	GLN	2.2
1	J	133	ILE	2.2
1	P	133	ILE	2.2
1	H	218	LYS	2.2
1	L	241	LEU	2.1
1	G	244	GLN	2.1
1	B	189	ALA	2.1
1	B	252	ASN	2.1
1	J	116	LYS	2.1
1	E	217	SER	2.1
1	H	205	PRO	2.1
1	G	208	THR	2.1
1	B	10	THR	2.1
1	J	46	HIS	2.1
1	L	68	THR	2.1
1	N	32	TYR	2.1
1	E	124	ALA	2.1
1	H	40	ALA	2.1
1	H	165	ALA	2.1
1	H	46	HIS	2.1
1	G	5	THR	2.1
1	G	234	VAL	2.1
1	J	10	THR	2.1
1	L	135	TYR	2.1
1	N	207	ASP	2.1
1	P	147	PHE	2.1
1	E	172	ARG	2.1
1	P	158	MET	2.1
1	G	177	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	P	8	VAL	2.1
1	B	208	THR	2.1
1	N	21	LYS	2.1
1	G	166	GLU	2.1
1	E	180	ARG	2.1
1	H	85	ILE	2.1
1	B	20	LYS	2.1
1	H	34	GLY	2.1
1	J	231	GLY	2.1
1	P	104	LYS	2.1
1	B	58	ASP	2.1
1	H	12	LEU	2.1
1	E	220	TYR	2.1
1	H	208	THR	2.1
1	L	9	THR	2.1
1	L	67	ASP	2.1
1	J	63	ALA	2.1
1	B	72	ASN	2.1
1	H	245	GLY	2.1
1	H	211	VAL	2.1
1	L	23	HIS	2.1
1	N	164	SER	2.1
1	E	187	LYS	2.1
1	E	100	ILE	2.1
1	N	111	ILE	2.1
1	P	84	ASP	2.1
1	P	166	GLU	2.1
1	J	183	LYS	2.1
1	P	255	TRP	2.0
1	E	135	TYR	2.0
1	E	47	CYS	2.0
1	P	177	GLY	2.0
1	E	218	LYS	2.0
1	J	169	VAL	2.0
1	H	191	LEU	2.0
1	G	55	ILE	2.0
1	B	190	TYR	2.0
1	H	224	THR	2.0
1	L	33	GLU	2.0
1	L	151	LYS	2.0
1	L	186	GLY	2.0
1	L	199	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	H	15	PRO	2.0
1	N	120	PRO	2.0
1	B	103	SER	2.0
1	H	103	SER	2.0
1	J	104	LYS	2.0
1	J	168	SER	2.0
1	N	193	GLU	2.0
1	J	161	TYR	2.0
1	G	238	VAL	2.0
1	J	163	ARG	2.0
1	J	192	LEU	2.0
1	G	85	ILE	2.0
1	H	41	ALA	2.0
1	H	140	SER	2.0
1	N	184	SER	2.0
1	B	31	ARG	2.0
1	B	68	THR	2.0
1	B	178	VAL	2.0
1	H	49	PHE	2.0
1	H	185	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
2	VBP	B	807	24/24	0.75	0.31	0.33	22,26,35,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	VBP	J	804	24/24	0.74	0.33	0.33	27,30,34,38	0
2	VBP	G	803	24/24	0.82	0.33	0.13	18,28,38,43	0
2	VBP	P	805	24/24	0.79	0.33	0.08	18,27,38,40	0
2	VBP	N	802	24/24	0.76	0.32	-0.09	21,25,38,38	0
2	VBP	E	808	24/24	0.77	0.30	-0.39	25,30,38,42	0
2	VBP	L	801	24/24	0.82	0.28	-0.58	22,25,31,38	0
2	VBP	H	806	24/24	0.78	0.28	-0.80	25,30,35,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.