



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 03:33 AM GMT

PDB ID : 2CVF
Title : Crystal structure of the RadB recombinase
Authors : Akiba, T.; Ishii, N.; Rashid, N.; Morikawa, M.; Imanaka, T.; Harata, K.
Deposited on : 2005-06-03
Resolution : 2.60 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

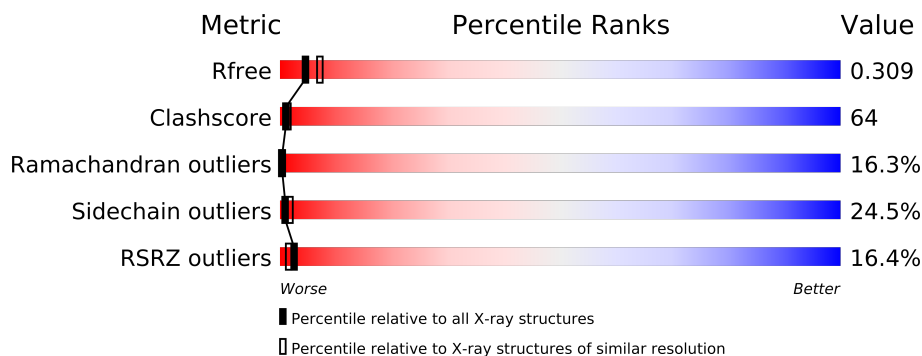
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.60 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}	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	220	
1	B	220	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3719 atoms, of which 0 are hydrogen and 0 are deuterium.

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 DNA repair and recombination protein radB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	220	Total	C	N	O	S	0	0	0
			1729	1097	308	319	5			
1	B	220	Total	C	N	O	S	0	0	0
			1729	1097	308	319	5			

- Molecule 2 is water.

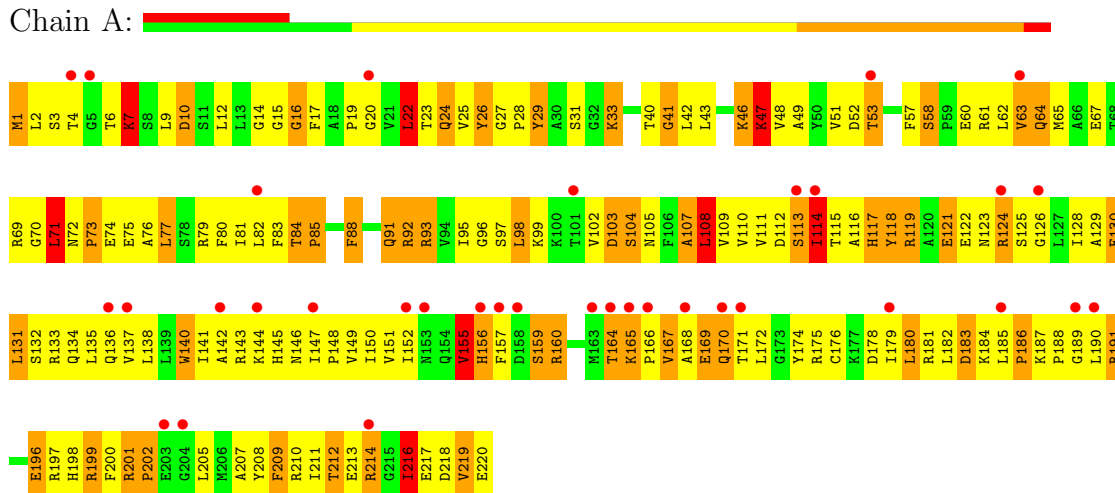
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	131	Total	O	0	0
			131	131		
2	B	130	Total	O	0	0
			130	130		

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: DNA repair and recombination protein radB

Chain A:



- Molecule 1: DNA repair and recombination protein radB

Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	46.01Å 82.47Å 111.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.60 9.99 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-2.60) 92.4 (9.99-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.37 (at 2.38Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.235 , 0.304 0.221 , 0.309	Depositor DCC
R_{free} test set	1184 reflections (9.95%)	DCC
Wilson B-factor (Å ²)	34.9	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.90 , 296.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 15802 reflections	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	3719	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality i

5.1 Standard geometry i

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	0.65	0/1759	1.04	4/2374 (0.2%)
1	B	0.63	0/1759	1.01	8/2374 (0.3%)
All	All	0.64	0/3518	1.03	12/4748 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	42	LEU	CA-CB-CG	8.66	135.21	115.30
1	A	108	LEU	CA-CB-CG	8.49	134.83	115.30
1	B	88	PHE	N-CA-C	7.51	131.28	111.00
1	B	38	LEU	CA-CB-CG	6.79	130.92	115.30
1	B	189	GLY	N-CA-C	-5.75	98.71	113.10
1	B	145	HIS	N-CA-C	-5.74	95.51	111.00
1	B	182	LEU	CA-CB-CG	5.54	128.03	115.30
1	B	31	SER	N-CA-C	5.46	125.74	111.00
1	A	22	LEU	CA-CB-CG	5.17	127.19	115.30
1	B	180	LEU	CA-CB-CG	5.12	127.06	115.30
1	A	47	LYS	N-CA-C	5.08	124.72	111.00
1	A	41	GLY	N-CA-C	5.01	125.63	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	174	TYR	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1729	0	1781	233	0
1	B	1729	0	1781	225	0
2	A	131	0	0	13	0
2	B	130	0	0	10	0
All	All	3719	0	3562	449	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 64.

All (449) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:165:LYS:HG3	1:A:166:PRO:HD3	1.36	1.04
1:B:32:GLY:HA3	1:B:191:ARG:HH12	1.22	1.01
1:B:31:SER:HB3	1:B:34:THR:HB	1.46	0.98
1:A:135:LEU:HA	1:A:138:LEU:HB2	1.45	0.97
1:B:181:ARG:HB3	1:B:194:VAL:HG13	1.45	0.97
1:A:1:MET:HB3	1:B:68:THR:HA	1.48	0.95
1:A:112:ASP:HA	1:A:113:SER:HB2	1.52	0.91
1:A:27:GLY:HA2	1:A:156:HIS:HB3	1.54	0.88
1:A:12:LEU:HD22	1:A:207:ALA:HB3	1.59	0.85
1:B:210:ARG:NE	1:B:217:GLU:HG2	1.92	0.84
1:B:141:ILE:HG22	1:B:147:ILE:HD12	1.60	0.83
1:B:65:MET:SD	1:B:215:GLY:HA2	2.17	0.83
1:A:132:SER:O	1:A:136:GLN:HG2	1.78	0.82
1:A:61:ARG:HH22	1:A:214:ARG:H	1.27	0.82
1:B:134:GLN:O	1:B:137:VAL:HG22	1.78	0.82
1:A:131:LEU:HA	2:A:228:HOH:O	1.81	0.80
1:B:85:PRO:HG3	1:B:91:GLN:HG3	1.64	0.80
1:B:185:LEU:HD13	1:B:188:PRO:HG2	1.64	0.79
1:A:29:TYR:H	1:A:29:TYR:HD1	1.29	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:187:LYS:HZ2	1:A:190:LEU:HB2	1.45	0.78
1:B:138:LEU:HD23	1:B:151:VAL:CG2	2.14	0.78
1:B:155:VAL:HA	1:B:166:PRO:HA	1.66	0.77
1:B:192:VAL:HG13	1:B:207:ALA:O	1.83	0.77
1:B:211:ILE:CG1	1:B:216:ILE:HG12	2.15	0.77
1:A:187:LYS:HB3	1:A:190:LEU:HD13	1.66	0.76
1:A:135:LEU:HD23	1:A:138:LEU:HD13	1.67	0.75
1:B:19:PRO:HA	1:B:148:PRO:HG3	1.66	0.75
1:A:184:LYS:HA	1:A:191:ARG:HG3	1.67	0.75
1:B:198:HIS:N	1:B:202:PRO:HB3	2.02	0.75
1:A:62:LEU:HD11	1:A:77:LEU:HD22	1.66	0.75
1:A:112:ASP:CA	1:A:113:SER:HB2	2.16	0.75
1:B:156:HIS:HB2	1:B:167:VAL:HG22	1.69	0.75
1:A:24:GLN:NE2	1:A:179:ILE:HG23	2.01	0.75
1:B:109:VAL:O	1:B:149:VAL:HG13	1.87	0.75
1:A:140:TRP:HD1	1:A:141:ILE:N	1.84	0.74
1:B:210:ARG:HE	1:B:217:GLU:HG2	1.51	0.74
1:B:76:ALA:O	1:B:79:ARG:HB3	1.87	0.74
1:A:31:SER:HA	1:A:191:ARG:HD3	1.69	0.74
1:B:182:LEU:HA	1:B:192:VAL:O	1.88	0.74
1:A:19:PRO:HA	1:A:148:PRO:HG3	1.71	0.73
1:B:31:SER:HB3	1:B:34:THR:CB	2.17	0.73
1:B:22:LEU:HD12	1:B:22:LEU:H	1.54	0.73
1:B:115:THR:HG21	1:B:167:VAL:CG1	2.19	0.73
1:B:92:ARG:HA	1:B:134:GLN:HG2	1.71	0.73
1:A:217:GLU:HG3	2:A:248:HOH:O	1.87	0.73
1:A:124:ARG:O	1:A:128:ILE:HG23	1.89	0.73
1:B:13:LEU:HD22	1:B:17:PHE:O	1.88	0.72
1:B:52:ASP:HB2	1:B:84:THR:OG1	1.90	0.71
1:A:164:THR:HG22	1:A:165:LYS:HG2	1.71	0.71
1:A:140:TRP:CD1	1:A:141:ILE:HG13	2.24	0.71
1:B:51:VAL:HG22	1:B:83:PHE:HB2	1.72	0.71
1:A:82:LEU:C	1:A:83:PHE:HD2	1.94	0.71
1:B:29:TYR:HE2	2:B:267:HOH:O	1.71	0.71
1:A:187:LYS:HD2	1:A:190:LEU:HD22	1.71	0.70
1:B:197:ARG:HE	1:B:197:ARG:HA	1.56	0.70
1:A:20:GLY:O	1:A:143:ARG:HG2	1.92	0.70
1:A:98:LEU:HD13	1:A:99:LYS:N	2.07	0.69
1:A:69:ARG:NH1	1:A:214:ARG:HG3	2.07	0.69
1:B:33:LYS:HA	1:B:36:LEU:CB	2.23	0.69
1:A:88:PHE:HB2	1:A:116:ALA:CB	2.23	0.69
1:B:197:ARG:HH21	1:B:203:GLU:H	1.40	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:98:LEU:HD12	1:B:109:VAL:HG11	1.73	0.69
1:B:33:LYS:HA	1:B:36:LEU:HB3	1.73	0.68
1:A:185:LEU:HG	1:A:186:PRO:HD2	1.75	0.68
1:B:37:ALA:HB3	1:B:50:TYR:OH	1.92	0.68
1:A:53:THR:HA	1:A:85:PRO:O	1.93	0.68
1:A:135:LEU:HG	2:A:228:HOH:O	1.93	0.68
1:B:138:LEU:HD23	1:B:151:VAL:HG21	1.75	0.68
1:B:177:LYS:O	1:B:178:ASP:HB2	1.94	0.68
1:A:60:GLU:O	1:A:64:GLN:HG2	1.93	0.68
1:A:198:HIS:CE1	1:A:199:ARG:HD2	2.28	0.67
1:A:88:PHE:HB2	1:A:116:ALA:HB2	1.76	0.67
1:B:2:LEU:H	1:B:2:LEU:HD12	1.59	0.67
1:A:165:LYS:CG	1:A:166:PRO:HD3	2.17	0.67
1:B:22:LEU:CD2	1:B:138:LEU:HB3	2.24	0.67
1:B:24:GLN:HE21	1:B:179:ILE:HG23	1.58	0.67
1:B:36:LEU:HD12	1:B:182:LEU:HD11	1.75	0.67
1:B:197:ARG:HG3	1:B:198:HIS:H	1.59	0.67
1:A:76:ALA:HA	1:A:79:ARG:HD2	1.77	0.67
1:A:135:LEU:HD23	1:A:138:LEU:CD1	2.24	0.66
1:B:88:PHE:CD1	1:B:117:HIS:HB2	2.30	0.66
1:B:197:ARG:C	1:B:202:PRO:HB3	2.15	0.66
1:B:187:LYS:H	1:B:188:PRO:HD2	1.60	0.66
1:B:74:GLU:HG2	2:B:222:HOH:O	1.95	0.66
1:B:179:ILE:H	1:B:179:ILE:HD12	1.60	0.66
1:A:9:LEU:HD11	1:A:209:PHE:CD1	2.30	0.65
1:A:84:THR:HB	1:A:85:PRO:CA	2.26	0.65
1:B:98:LEU:CD1	1:B:109:VAL:HG11	2.27	0.65
1:B:89:LYS:HG3	1:B:92:ARG:HH21	1.61	0.65
1:A:48:VAL:O	1:A:80:PHE:HA	1.96	0.65
1:B:7:LYS:HD3	1:B:8:SER:N	2.11	0.65
1:A:211:ILE:HG13	1:A:211:ILE:O	1.97	0.65
1:A:219:VAL:HB	2:A:251:HOH:O	1.97	0.65
1:B:95:ILE:HG23	1:B:137:VAL:HG21	1.78	0.64
1:A:88:PHE:N	1:A:88:PHE:CD1	2.66	0.64
1:A:31:SER:HA	1:A:191:ARG:HG2	1.79	0.64
1:A:7:LYS:HA	1:A:10:ASP:HB2	1.79	0.64
1:B:22:LEU:HD22	2:B:305:HOH:O	1.96	0.63
1:B:25:VAL:CG2	1:B:150:ILE:HG23	2.28	0.63
1:A:99:LYS:HE3	1:A:109:VAL:HG11	1.80	0.63
1:B:35:THR:HA	1:B:38:LEU:HD22	1.79	0.63
1:A:141:ILE:HG23	1:A:145:HIS:CD2	2.34	0.63
1:A:88:PHE:HD1	1:A:88:PHE:H	1.46	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:211:ILE:HG13	1:B:216:ILE:HG12	1.81	0.63
1:A:213:GLU:HG2	1:A:214:ARG:NH2	2.13	0.63
1:A:64:GLN:HE21	1:A:64:GLN:HA	1.63	0.63
1:B:197:ARG:HH21	1:B:202:PRO:HB2	1.62	0.63
1:A:133:ARG:HA	1:A:136:GLN:HG2	1.82	0.62
1:B:25:VAL:HG21	1:B:150:ILE:HG23	1.81	0.62
1:A:133:ARG:HD3	1:A:136:GLN:HG3	1.81	0.62
1:B:197:ARG:NH2	1:B:202:PRO:HB2	2.15	0.62
1:A:140:TRP:CD1	1:A:141:ILE:N	2.67	0.62
1:B:138:LEU:HD23	1:B:151:VAL:HG22	1.80	0.62
1:B:88:PHE:HD1	1:B:117:HIS:HB2	1.64	0.62
1:A:88:PHE:CB	1:A:116:ALA:HB2	2.30	0.62
1:B:22:LEU:N	1:B:22:LEU:HD12	2.15	0.62
1:B:187:LYS:H	1:B:188:PRO:CD	2.13	0.62
1:A:1:MET:CB	1:B:68:THR:HA	2.27	0.62
1:A:84:THR:CB	1:A:85:PRO:HA	2.30	0.61
1:A:9:LEU:O	1:A:12:LEU:HB3	2.01	0.61
1:A:199:ARG:HG3	1:A:199:ARG:HH11	1.65	0.61
1:B:211:ILE:HG12	1:B:215:GLY:O	2.00	0.61
1:A:51:VAL:HG13	1:A:84:THR:O	2.01	0.61
1:A:180:LEU:HG	1:A:181:ARG:H	1.66	0.61
1:A:76:ALA:HA	1:A:79:ARG:CD	2.29	0.61
1:B:96:GLY:O	1:B:99:LYS:HG3	2.01	0.60
1:B:52:ASP:O	1:B:85:PRO:HD2	2.01	0.60
1:A:113:SER:HB3	1:A:152:ILE:O	2.01	0.60
1:A:52:ASP:HA	1:A:112:ASP:HB2	1.83	0.60
1:B:111:VAL:HG21	1:B:138:LEU:HD11	1.84	0.60
1:B:197:ARG:CZ	1:B:202:PRO:HG2	2.31	0.60
1:B:199:ARG:HG2	1:B:199:ARG:HH11	1.67	0.60
1:B:193:ALA:HB2	1:B:209:PHE:CE2	2.36	0.60
1:B:131:LEU:O	1:B:135:LEU:HD12	2.00	0.60
1:B:219:VAL:HG13	1:B:220:GLU:H	1.67	0.60
1:A:198:HIS:ND1	1:A:199:ARG:N	2.50	0.60
1:A:125:SER:O	1:A:128:ILE:HG12	2.02	0.59
1:A:84:THR:HB	1:A:85:PRO:HA	1.82	0.59
1:B:145:HIS:ND1	1:B:147:ILE:HD11	2.17	0.59
1:B:143:ARG:HH12	1:B:199:ARG:NH2	2.00	0.59
1:A:110:VAL:HA	1:A:150:ILE:O	2.01	0.59
1:B:58:SER:HB2	1:B:59:PRO:HD3	1.85	0.59
1:B:191:ARG:HG2	1:B:209:PHE:CE1	2.38	0.59
1:B:98:LEU:HD21	1:B:141:ILE:HG13	1.85	0.59
1:B:109:VAL:HB	1:B:149:VAL:HG22	1.84	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:201:ARG:N	1:B:202:PRO:HD3	2.17	0.59
1:B:143:ARG:HH22	1:B:199:ARG:HH22	1.51	0.59
1:B:174:TYR:O	1:B:177:LYS:HG2	2.02	0.59
1:A:118:TYR:HD1	1:A:118:TYR:N	2.01	0.59
1:B:155:VAL:HG11	1:B:181:ARG:HH22	1.68	0.58
1:A:98:LEU:O	1:A:102:VAL:HB	2.04	0.58
1:A:6:THR:CG2	1:A:216:ILE:HB	2.34	0.58
1:A:109:VAL:HB	1:A:149:VAL:HG22	1.84	0.58
1:B:115:THR:HG21	1:B:167:VAL:HG11	1.84	0.58
1:B:48:VAL:O	1:B:81:ILE:HG22	2.03	0.58
1:B:210:ARG:HG2	1:B:211:ILE:N	2.19	0.58
1:A:46:LYS:HD3	1:A:46:LYS:H	1.69	0.57
1:A:169:GLU:HG3	1:A:170:GLN:N	2.20	0.57
1:A:151:VAL:HG23	2:A:335:HOH:O	2.03	0.57
1:B:81:ILE:HG21	1:B:106:PHE:HE2	1.70	0.57
1:A:198:HIS:ND1	1:A:199:ARG:HD2	2.20	0.57
1:A:109:VAL:HB	1:A:149:VAL:HG13	1.87	0.57
1:A:118:TYR:HA	2:A:252:HOH:O	2.04	0.57
1:A:111:VAL:CG2	1:A:151:VAL:HA	2.34	0.57
1:B:32:GLY:HA3	1:B:191:ARG:NH1	2.07	0.57
1:A:31:SER:HA	1:A:191:ARG:CD	2.34	0.57
1:A:141:ILE:O	1:A:145:HIS:N	2.38	0.57
2:A:230:HOH:O	1:B:74:GLU:HB2	2.05	0.57
1:A:129:ALA:O	1:A:131:LEU:N	2.38	0.56
1:A:133:ARG:HA	1:A:136:GLN:CG	2.35	0.56
1:A:217:GLU:HG2	1:A:218:ASP:N	2.20	0.56
1:B:129:ALA:O	1:B:133:ARG:HB2	2.05	0.56
1:B:22:LEU:HA	1:B:149:VAL:O	2.06	0.56
1:A:210:ARG:HE	1:A:212:THR:HG23	1.70	0.56
1:A:118:TYR:N	1:A:118:TYR:CD1	2.72	0.56
1:B:97:SER:HA	1:B:100:LYS:HE2	1.86	0.56
1:A:98:LEU:HA	1:A:102:VAL:HG23	1.88	0.56
1:B:22:LEU:HD23	1:B:138:LEU:HB3	1.87	0.56
1:A:150:ILE:HA	2:A:335:HOH:O	2.05	0.56
1:A:114:ILE:H	1:A:114:ILE:HD13	1.71	0.56
1:B:219:VAL:HG13	1:B:220:GLU:N	2.21	0.56
1:B:45:GLY:HA2	1:B:79:ARG:NH1	2.20	0.55
1:A:12:LEU:HD22	1:A:207:ALA:CB	2.34	0.55
1:A:169:GLU:HA	1:A:172:LEU:HD12	1.88	0.55
1:A:136:GLN:HE22	1:A:175:ARG:CZ	2.19	0.55
1:B:156:HIS:O	1:B:157:PHE:HB2	2.07	0.55
1:B:38:LEU:O	1:B:42:LEU:HB2	2.06	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:141:ILE:CG2	1:B:147:ILE:HD12	2.35	0.55
1:A:61:ARG:HH22	1:A:214:ARG:N	2.03	0.55
1:A:24:GLN:HB2	1:A:176:CYS:HB3	1.89	0.55
1:A:31:SER:OG	1:A:33:LYS:HG3	2.06	0.55
1:A:88:PHE:N	1:A:88:PHE:HD1	2.04	0.55
1:B:95:ILE:CG2	1:B:137:VAL:HG21	2.36	0.55
1:B:42:LEU:CB	1:B:80:PHE:HZ	2.19	0.55
1:B:92:ARG:NH1	1:B:130:GLU:HG3	2.22	0.54
1:B:19:PRO:HB2	1:B:146:ASN:HD22	1.72	0.54
1:A:190:LEU:HG	1:A:210:ARG:HB2	1.90	0.54
1:A:111:VAL:HG23	1:A:151:VAL:HA	1.90	0.54
1:B:42:LEU:HD21	1:B:66:ALA:HB2	1.89	0.54
1:B:88:PHE:CZ	1:B:91:GLN:NE2	2.76	0.54
1:B:2:LEU:N	1:B:2:LEU:HD12	2.23	0.54
1:A:10:ASP:O	1:A:15:GLY:HA2	2.08	0.54
1:B:187:LYS:N	1:B:188:PRO:HD2	2.22	0.54
1:B:26:TYR:CE1	1:B:179:ILE:HG22	2.43	0.54
1:A:29:TYR:N	1:A:29:TYR:CD1	2.76	0.54
1:B:130:GLU:HB3	1:B:134:GLN:HE22	1.73	0.53
1:B:211:ILE:HG12	1:B:216:ILE:HG12	1.90	0.53
1:A:137:VAL:HA	1:A:140:TRP:CE2	2.44	0.53
1:A:53:THR:HB	1:A:88:PHE:CE2	2.43	0.53
1:A:25:VAL:HG13	1:A:180:LEU:CD2	2.38	0.53
1:A:169:GLU:O	1:A:171:THR:N	2.40	0.53
1:A:121:GLU:O	1:A:121:GLU:HG2	2.07	0.53
1:A:160:ARG:O	1:A:164:THR:HA	2.08	0.53
1:B:7:LYS:HG3	2:B:340:HOH:O	2.07	0.53
1:B:176:CYS:O	1:B:176:CYS:SG	2.66	0.53
1:B:219:VAL:HG22	1:B:220:GLU:H	1.73	0.53
1:A:95:ILE:HB	2:A:282:HOH:O	2.08	0.53
1:A:25:VAL:HG13	1:A:180:LEU:HD23	1.91	0.53
1:A:58:SER:HB3	1:A:61:ARG:HB3	1.91	0.53
1:B:88:PHE:HB2	1:B:117:HIS:HD2	1.72	0.53
1:B:130:GLU:HB3	1:B:134:GLN:NE2	2.24	0.53
1:A:130:GLU:O	1:A:134:GLN:HG2	2.08	0.53
1:B:88:PHE:HB2	1:B:117:HIS:CD2	2.44	0.53
1:B:118:TYR:H	1:B:118:TYR:HD2	1.55	0.52
1:B:191:ARG:HG3	1:B:192:VAL:N	2.23	0.52
1:A:92:ARG:HG2	1:A:134:GLN:HE22	1.74	0.52
1:A:62:LEU:HD12	1:A:63:VAL:N	2.24	0.52
1:A:179:ILE:O	1:A:196:GLU:N	2.42	0.52
1:B:179:ILE:H	1:B:197:ARG:HB3	1.74	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:197:ARG:HG3	1:B:198:HIS:O	2.09	0.52
1:A:4:THR:HG23	1:A:40:THR:HA	1.92	0.52
1:B:98:LEU:HD11	1:B:141:ILE:HG13	1.92	0.52
1:B:32:GLY:O	1:B:36:LEU:N	2.42	0.52
1:B:18:ALA:HB1	1:B:21:VAL:CG1	2.39	0.52
1:A:198:HIS:CE1	1:A:200:PHE:O	2.63	0.52
1:A:134:GLN:C	1:A:138:LEU:HD12	2.29	0.52
1:B:137:VAL:HG23	1:B:138:LEU:N	2.25	0.52
1:A:65:MET:O	1:A:69:ARG:HG2	2.10	0.52
1:A:182:LEU:HD23	1:A:209:PHE:HZ	1.74	0.51
1:A:98:LEU:HA	1:A:102:VAL:CG2	2.41	0.51
1:A:6:THR:HG21	1:A:216:ILE:HB	1.92	0.51
1:B:91:GLN:NE2	1:B:114:ILE:HA	2.25	0.51
1:B:107:ALA:HB3	2:B:293:HOH:O	2.10	0.51
1:A:25:VAL:HG22	1:A:180:LEU:HD22	1.91	0.51
1:A:126:GLY:O	1:A:129:ALA:HB3	2.10	0.51
1:B:95:ILE:O	1:B:98:LEU:HB3	2.11	0.51
1:B:148:PRO:O	1:B:150:ILE:HD12	2.10	0.51
1:A:4:THR:OG1	1:B:72:ASN:HB2	2.11	0.51
1:A:130:GLU:HA	2:A:283:HOH:O	2.10	0.50
1:A:213:GLU:HG2	1:A:214:ARG:HH21	1.73	0.50
1:B:113:SER:HB2	1:B:152:ILE:O	2.12	0.50
1:B:197:ARG:CA	1:B:202:PRO:HB3	2.42	0.50
1:A:24:GLN:HE22	1:A:179:ILE:HG23	1.73	0.50
1:B:100:LYS:NZ	2:B:230:HOH:O	2.44	0.50
1:A:28:PRO:HD2	1:A:182:LEU:O	2.12	0.50
1:A:26:TYR:O	1:A:26:TYR:HD2	1.94	0.50
1:A:64:GLN:HE21	1:A:64:GLN:CA	2.24	0.50
1:A:31:SER:HA	1:A:191:ARG:CG	2.41	0.50
1:A:159:SER:O	1:A:160:ARG:HB3	2.12	0.50
1:B:215:GLY:O	1:B:216:ILE:HG12	2.12	0.50
1:B:191:ARG:HG3	1:B:192:VAL:H	1.77	0.50
1:B:179:ILE:N	1:B:179:ILE:HD12	2.26	0.50
1:A:93:ARG:O	1:A:97:SER:HB3	2.11	0.50
1:A:91:GLN:HE22	1:A:95:ILE:HD12	1.76	0.50
1:B:7:LYS:HD3	1:B:8:SER:H	1.75	0.50
1:B:42:LEU:O	1:B:79:ARG:CZ	2.60	0.50
1:B:198:HIS:HB3	1:B:200:PHE:H	1.76	0.50
1:A:4:THR:CB	1:B:73:PRO:HD2	2.42	0.50
1:B:185:LEU:HD11	1:B:192:VAL:HG23	1.94	0.49
1:A:4:THR:HB	1:B:73:PRO:HD2	1.94	0.49
1:B:210:ARG:HH11	1:B:210:ARG:HG3	1.77	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:137:VAL:O	1:B:141:ILE:HG12	2.12	0.49
1:B:190:LEU:HD23	1:B:210:ARG:HG3	1.93	0.49
1:A:125:SER:HA	1:A:128:ILE:HG12	1.93	0.49
1:A:84:THR:CB	1:A:85:PRO:CA	2.89	0.49
1:B:143:ARG:HH12	1:B:199:ARG:HH22	1.60	0.49
1:A:70:GLY:O	1:A:71:LEU:HG	2.12	0.49
1:A:142:ALA:HA	1:A:147:ILE:HG22	1.93	0.49
1:A:2:LEU:HG	1:A:19:PRO:HD3	1.93	0.49
1:A:219:VAL:HG12	1:A:220:GLU:HG2	1.95	0.49
1:B:128:ILE:H	1:B:128:ILE:HD12	1.78	0.49
1:B:185:LEU:HD11	1:B:192:VAL:CG2	2.43	0.49
1:A:12:LEU:CD1	1:A:205:LEU:HG	2.42	0.49
1:B:219:VAL:HG22	1:B:220:GLU:N	2.28	0.49
1:A:186:PRO:O	1:A:187:LYS:HG3	2.13	0.48
1:B:197:ARG:HA	1:B:202:PRO:HB3	1.95	0.48
1:A:157:PHE:CD1	1:A:165:LYS:HD2	2.48	0.48
1:A:41:GLY:HA3	1:A:48:VAL:HG21	1.95	0.48
1:B:119:ARG:O	1:B:119:ARG:HG3	2.13	0.48
1:A:1:MET:N	1:B:68:THR:O	2.43	0.48
1:A:4:THR:OG1	1:B:73:PRO:HD2	2.13	0.48
1:A:103:ASP:HB3	2:A:223:HOH:O	2.14	0.48
1:B:42:LEU:HB2	1:B:80:PHE:HZ	1.78	0.48
1:B:88:PHE:CE1	1:B:114:ILE:O	2.67	0.48
1:A:26:TYR:O	1:A:26:TYR:CD2	2.67	0.48
1:B:88:PHE:HE1	1:B:114:ILE:O	1.96	0.48
1:B:168:ALA:O	1:B:172:LEU:HB2	2.14	0.48
1:B:88:PHE:HE2	1:B:134:GLN:HE22	1.61	0.48
1:A:99:LYS:CE	1:A:109:VAL:HG11	2.44	0.48
1:A:14:GLY:HA2	1:A:201:ARG:NE	2.29	0.48
1:B:123:ASN:O	1:B:124:ARG:HB2	2.12	0.47
1:A:155:VAL:O	1:A:156:HIS:CD2	2.67	0.47
1:B:153:ASN:ND2	1:B:167:VAL:O	2.46	0.47
1:A:183:ASP:O	1:A:191:ARG:HB3	2.14	0.47
1:A:141:ILE:O	1:A:145:HIS:HB2	2.13	0.47
1:A:75:GLU:HG3	1:A:76:ALA:N	2.30	0.47
1:A:80:PHE:CD1	1:A:80:PHE:N	2.82	0.47
1:A:23:THR:HG23	1:A:178:ASP:HB3	1.96	0.47
1:B:30:ALA:O	1:B:32:GLY:N	2.48	0.47
1:B:161:THR:O	1:B:162:GLU:HB2	2.14	0.47
1:A:118:TYR:O	1:A:119:ARG:HB2	2.15	0.47
1:A:46:LYS:CD	1:A:46:LYS:H	2.27	0.47
1:B:167:VAL:O	1:B:168:ALA:HB3	2.15	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:85:PRO:HA	1:B:90:GLU:HG2	1.95	0.47
1:A:31:SER:CA	1:A:191:ARG:HG2	2.45	0.47
1:B:48:VAL:HG11	1:B:50:TYR:HD1	1.80	0.47
1:B:193:ALA:HB2	1:B:209:PHE:CD2	2.50	0.47
1:B:33:LYS:HA	1:B:36:LEU:HB2	1.97	0.47
1:A:69:ARG:NH1	1:A:214:ARG:CG	2.77	0.47
1:A:49:ALA:O	1:A:109:VAL:HA	2.15	0.47
1:B:199:ARG:HG2	1:B:199:ARG:NH1	2.30	0.47
1:A:189:GLY:C	1:A:190:LEU:HD12	2.35	0.46
1:B:115:THR:HG21	1:B:167:VAL:HG12	1.93	0.46
1:A:109:VAL:CG1	1:A:149:VAL:HG13	2.45	0.46
1:A:41:GLY:CA	1:A:48:VAL:HG21	2.45	0.46
1:B:25:VAL:HG12	1:B:180:LEU:HD23	1.96	0.46
1:A:197:ARG:O	1:A:198:HIS:HB2	2.15	0.46
1:B:27:GLY:HA2	1:B:181:ARG:NH1	2.31	0.46
1:B:61:ARG:O	1:B:63:VAL:N	2.48	0.46
1:B:33:LYS:NZ	1:B:154:GLN:OE1	2.49	0.46
1:A:187:LYS:HZ2	1:A:190:LEU:CB	2.22	0.46
1:A:157:PHE:HA	1:A:165:LYS:CB	2.46	0.46
1:B:66:ALA:O	1:B:70:GLY:N	2.49	0.46
1:A:92:ARG:HA	1:A:95:ILE:HG22	1.98	0.46
1:B:185:LEU:HD12	1:B:189:GLY:C	2.36	0.46
1:A:51:VAL:O	1:A:111:VAL:HA	2.16	0.46
1:B:210:ARG:HD2	1:B:210:ARG:C	2.36	0.45
1:A:167:VAL:O	1:A:167:VAL:CG1	2.63	0.45
1:A:40:THR:HG21	1:A:108:LEU:HD21	1.98	0.45
1:B:205:LEU:HD12	2:B:296:HOH:O	2.16	0.45
1:A:61:ARG:O	1:A:65:MET:HG2	2.17	0.45
1:A:76:ALA:O	1:A:79:ARG:HD2	2.17	0.45
1:A:155:VAL:HA	2:A:320:HOH:O	2.17	0.45
1:A:187:LYS:O	1:A:189:GLY:N	2.49	0.45
1:B:51:VAL:HA	1:B:83:PHE:O	2.17	0.45
1:A:98:LEU:HD13	1:A:99:LYS:HD3	1.99	0.45
1:A:98:LEU:HD21	1:A:99:LYS:HZ2	1.82	0.45
1:A:140:TRP:O	1:A:144:LYS:HB2	2.15	0.45
1:A:4:THR:HG22	1:A:40:THR:O	2.17	0.45
1:A:17:PHE:HD1	1:A:23:THR:HG21	1.81	0.45
1:B:33:LYS:CD	1:B:33:LYS:H	2.29	0.45
1:A:180:LEU:HG	1:A:181:ARG:N	2.31	0.45
1:B:51:VAL:HG22	1:B:83:PHE:CB	2.44	0.45
1:B:53:THR:HB	1:B:113:SER:H	1.82	0.44
1:B:131:LEU:HD23	2:B:238:HOH:O	2.16	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:98:LEU:HD23	1:B:99:LYS:N	2.31	0.44
1:B:198:HIS:HD2	1:B:201:ARG:O	2.00	0.44
1:A:92:ARG:NH1	1:A:96:GLY:HA3	2.32	0.44
1:B:159:SER:O	1:B:161:THR:N	2.50	0.44
1:B:106:PHE:N	1:B:106:PHE:CD1	2.86	0.44
1:B:33:LYS:HG2	1:B:152:ILE:HD13	1.98	0.44
1:A:171:THR:HG22	1:A:175:ARG:HG2	1.99	0.44
1:A:81:ILE:HB	2:A:308:HOH:O	2.17	0.44
1:A:190:LEU:C	1:A:191:ARG:HE	2.21	0.44
1:A:49:ALA:HA	1:A:81:ILE:HG22	1.99	0.44
1:B:191:ARG:HG2	1:B:191:ARG:HH11	1.83	0.44
1:B:6:THR:HG22	2:B:340:HOH:O	2.19	0.43
1:A:91:GLN:HB2	1:A:91:GLN:HE21	1.67	0.43
1:A:190:LEU:CD2	1:A:210:ARG:HB2	2.47	0.43
1:A:114:ILE:HG12	1:A:115:THR:N	2.33	0.43
1:B:72:ASN:HA	1:B:73:PRO:HD3	1.75	0.43
1:B:63:VAL:HG23	1:B:64:GLN:N	2.32	0.43
1:B:197:ARG:HA	1:B:202:PRO:CB	2.49	0.43
1:B:68:THR:HG21	1:B:214:ARG:HA	2.01	0.43
1:B:22:LEU:HD21	1:B:138:LEU:HB3	1.99	0.43
1:A:137:VAL:HG12	1:A:141:ILE:HD12	2.00	0.43
1:A:72:ASN:HB3	1:A:75:GLU:HG2	2.01	0.43
1:A:26:TYR:O	1:A:181:ARG:HG2	2.19	0.43
1:B:92:ARG:HH11	1:B:130:GLU:HG3	1.83	0.43
1:B:172:LEU:O	1:B:176:CYS:HB3	2.18	0.43
1:B:197:ARG:HG3	1:B:198:HIS:N	2.28	0.43
1:A:124:ARG:O	1:A:128:ILE:N	2.51	0.43
1:B:209:PHE:C	1:B:209:PHE:CD1	2.92	0.43
1:B:133:ARG:NH2	1:B:133:ARG:O	2.52	0.43
1:B:209:PHE:HD1	1:B:210:ARG:N	2.17	0.43
1:A:23:THR:HG23	1:A:178:ASP:O	2.19	0.43
1:B:31:SER:O	1:B:35:THR:HG22	2.18	0.43
1:A:43:LEU:HA	1:A:43:LEU:HD23	1.73	0.43
1:B:60:GLU:O	1:B:63:VAL:HG22	2.19	0.43
1:A:22:LEU:CD1	1:A:22:LEU:N	2.82	0.42
1:B:38:LEU:HD23	1:B:38:LEU:C	2.39	0.42
1:A:147:ILE:HA	1:A:148:PRO:HD3	1.75	0.42
1:A:83:PHE:CD2	1:A:83:PHE:N	2.87	0.42
1:A:24:GLN:HB2	1:A:176:CYS:CB	2.48	0.42
1:A:73:PRO:HG2	1:A:74:GLU:H	1.84	0.42
1:B:145:HIS:O	1:B:147:ILE:N	2.52	0.42
1:B:61:ARG:O	1:B:62:LEU:C	2.58	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:52:ASP:HA	1:A:112:ASP:OD1	2.19	0.42
1:A:84:THR:OG1	1:A:85:PRO:HA	2.20	0.42
1:A:80:PHE:H	1:A:80:PHE:HD1	1.68	0.42
1:A:201:ARG:HA	1:A:202:PRO:HD2	1.55	0.42
1:B:217:GLU:O	1:B:218:ASP:HB2	2.19	0.42
1:A:12:LEU:HD13	1:A:205:LEU:HG	2.01	0.42
1:B:26:TYR:HB2	1:B:153:ASN:O	2.20	0.42
1:A:61:ARG:HA	1:A:61:ARG:HD2	1.84	0.42
1:A:23:THR:HG23	1:A:178:ASP:CB	2.50	0.42
1:B:143:ARG:H	1:B:143:ARG:HG2	1.74	0.41
1:A:131:LEU:CD2	1:A:168:ALA:HB3	2.50	0.41
1:A:137:VAL:HG22	1:A:140:TRP:CZ2	2.55	0.41
1:B:6:THR:O	1:B:9:LEU:N	2.51	0.41
1:B:98:LEU:CD2	1:B:137:VAL:HB	2.51	0.41
1:A:109:VAL:CB	1:A:149:VAL:HG13	2.50	0.41
1:A:46:LYS:HB3	2:B:317:HOH:O	2.20	0.41
1:B:201:ARG:HB2	1:B:201:ARG:CZ	2.51	0.41
1:A:157:PHE:HA	1:A:165:LYS:HB2	2.02	0.41
1:B:183:ASP:N	1:B:192:VAL:O	2.53	0.41
1:B:29:TYR:HB3	1:B:30:ALA:H	1.78	0.41
1:A:167:VAL:O	1:A:168:ALA:HB3	2.21	0.41
1:B:98:LEU:HD21	1:B:141:ILE:CG1	2.49	0.41
1:A:104:SER:HB3	1:A:105:ASN:H	1.67	0.41
1:A:47:LYS:O	1:A:107:ALA:N	2.54	0.41
1:A:69:ARG:NH1	1:A:214:ARG:CD	2.84	0.41
1:B:202:PRO:O	1:B:204:GLY:N	2.54	0.41
1:A:43:LEU:HD13	1:B:73:PRO:HB2	2.02	0.41
1:B:6:THR:HG21	1:B:209:PHE:CB	2.51	0.41
1:B:207:ALA:C	1:B:208:TYR:CD2	2.95	0.41
1:A:208:TYR:O	1:A:209:PHE:HB3	2.20	0.41
1:B:26:TYR:CZ	1:B:179:ILE:HG21	2.55	0.41
1:A:99:LYS:HE3	1:A:109:VAL:CG1	2.48	0.41
1:A:117:HIS:C	1:A:118:TYR:HD1	2.24	0.41
1:A:22:LEU:HD21	1:A:138:LEU:O	2.20	0.41
1:A:69:ARG:CZ	1:A:214:ARG:HG3	2.51	0.41
1:A:140:TRP:HD1	1:A:141:ILE:HG13	1.80	0.41
1:A:180:LEU:HD21	1:A:182:LEU:CD1	2.51	0.40
1:A:187:LYS:NZ	1:A:187:LYS:HB2	2.36	0.40
1:A:83:PHE:HD2	1:A:83:PHE:N	2.18	0.40
1:A:43:LEU:O	1:B:73:PRO:HG2	2.21	0.40
1:B:119:ARG:O	1:B:119:ARG:CG	2.68	0.40
1:B:17:PHE:O	1:B:18:ALA:HB2	2.20	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:2:LEU:H	1:B:2:LEU:CD1	2.32	0.40
1:A:70:GLY:O	1:A:71:LEU:CG	2.69	0.40
1:B:33:LYS:CD	1:B:33:LYS:N	2.84	0.40
1:B:42:LEU:O	1:B:79:ARG:NH2	2.54	0.40
1:B:179:ILE:HB	1:B:196:GLU:HB2	2.02	0.40
1:A:6:THR:HG23	1:A:216:ILE:HD12	2.02	0.40
1:A:16:GLY:O	1:A:17:PHE:HB2	2.21	0.40
1:B:187:LYS:N	1:B:188:PRO:CD	2.79	0.40
1:B:157:PHE:HD1	1:B:158:ASP:N	2.19	0.40
1:A:48:VAL:HG22	1:A:108:LEU:HD12	2.02	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	218/220 (99%)	122 (56%)	61 (28%)	35 (16%)	0	0
1	B	218/220 (99%)	136 (62%)	46 (21%)	36 (16%)	0	0
All	All	436/440 (99%)	258 (59%)	107 (24%)	71 (16%)	0	0

All (71) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	LYS
1	A	71	LEU
1	A	84	THR
1	A	107	ALA
1	A	113	SER
1	A	124	ARG
1	A	130	GLU
1	A	160	ARG
1	A	165	LYS
1	A	169	GLU

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Mol	Chain	Res	Type
1	A	170	GLN
1	A	186	PRO
1	A	214	ARG
1	B	25	VAL
1	B	31	SER
1	B	59	PRO
1	B	88	PHE
1	B	102	VAL
1	B	157	PHE
1	B	178	ASP
1	B	187	LYS
1	B	202	PRO
1	B	218	ASP
1	A	103	ASP
1	A	104	SER
1	A	119	ARG
1	A	131	LEU
1	A	146	ASN
1	A	155	VAL
1	A	156	HIS
1	A	164	THR
1	B	7	LYS
1	B	53	THR
1	B	62	LEU
1	B	160	ARG
1	B	162	GLU
1	B	164	THR
1	A	7	LYS
1	A	73	PRO
1	A	122	GLU
1	A	159	SER
1	A	216	ILE
1	A	219	VAL
1	B	20	GLY
1	B	29	TYR
1	B	107	ALA
1	B	177	LYS
1	B	186	PRO
1	A	16	GLY
1	B	139	LEU
1	B	159	SER
1	B	219	VAL

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Mol	Chain	Res	Type
1	A	201	ARG
1	A	202	PRO
1	A	209	PHE
1	B	28	PRO
1	B	121	GLU
1	B	122	GLU
1	B	126	GLY
1	A	3	SER
1	B	71	LEU
1	B	77	LEU
1	B	124	ARG
1	A	188	PRO
1	B	18	ALA
1	B	167	VAL
1	A	114	ILE
1	B	55	GLY
1	B	15	GLY
1	B	216	ILE
1	A	85	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	A	188/188 (100%)	149 (79%)	39 (21%)	2	3
1	B	188/188 (100%)	135 (72%)	53 (28%)	0	1
All	All	376/376 (100%)	284 (76%)	92 (24%)	1	2

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	7	LYS
1	A	10	ASP
1	A	22	LEU
1	A	24	GLN
1	A	26	TYR

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Mol	Chain	Res	Type
1	A	29	TYR
1	A	33	LYS
1	A	42	LEU
1	A	46	LYS
1	A	53	THR
1	A	57	PHE
1	A	58	SER
1	A	63	VAL
1	A	64	GLN
1	A	67	GLU
1	A	71	LEU
1	A	77	LEU
1	A	88	PHE
1	A	91	GLN
1	A	92	ARG
1	A	93	ARG
1	A	98	LEU
1	A	108	LEU
1	A	114	ILE
1	A	117	HIS
1	A	118	TYR
1	A	121	GLU
1	A	123	ASN
1	A	140	TRP
1	A	155	VAL
1	A	167	VAL
1	A	180	LEU
1	A	183	ASP
1	A	191	ARG
1	A	196	GLU
1	A	199	ARG
1	A	212	THR
1	A	216	ILE
1	B	1	MET
1	B	7	LYS
1	B	8	SER
1	B	13	LEU
1	B	17	PHE
1	B	22	LEU
1	B	24	GLN
1	B	25	VAL
1	B	26	TYR

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Mol	Chain	Res	Type
1	B	29	TYR
1	B	33	LYS
1	B	35	THR
1	B	36	LEU
1	B	38	LEU
1	B	39	GLN
1	B	42	LEU
1	B	50	TYR
1	B	62	LEU
1	B	78	SER
1	B	79	ARG
1	B	87	ASP
1	B	88	PHE
1	B	93	ARG
1	B	98	LEU
1	B	106	PHE
1	B	114	ILE
1	B	115	THR
1	B	124	ARG
1	B	128	ILE
1	B	133	ARG
1	B	136	GLN
1	B	143	ARG
1	B	145	HIS
1	B	161	THR
1	B	171	THR
1	B	174	TYR
1	B	175	ARG
1	B	177	LYS
1	B	179	ILE
1	B	181	ARG
1	B	182	LEU
1	B	183	ASP
1	B	184	LYS
1	B	185	LEU
1	B	194	VAL
1	B	197	ARG
1	B	198	HIS
1	B	200	PHE
1	B	205	LEU
1	B	206	MET
1	B	208	TYR

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Mol	Chain	Res	Type
1	B	210	ARG
1	B	211	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	64	GLN
1	A	91	GLN
1	A	123	ASN
1	A	134	GLN
1	A	136	GLN
1	B	39	GLN
1	B	64	GLN
1	B	91	GLN
1	B	134	GLN
1	B	146	ASN
1	B	198	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no ligands in this entry.

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	220/220 (100%)	0.82	35 (15%) 3 1	17, 42, 65, 88	0
1	B	220/220 (100%)	0.84	37 (16%) 2 1	16, 45, 68, 101	0
All	All	440/440 (100%)	0.83	72 (16%) 2 1	16, 43, 67, 101	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	15	GLY	10.5
1	A	204	GLY	6.5
1	A	142	ALA	5.4
1	A	157	PHE	5.4
1	A	5	GLY	5.0
1	B	71	LEU	4.9
1	A	20	GLY	4.6
1	A	156	HIS	4.5
1	A	165	LYS	4.4
1	B	14	GLY	4.4
1	A	114	ILE	4.3
1	B	128	ILE	4.3
1	B	127	LEU	4.1
1	B	129	ALA	3.4
1	A	189	GLY	3.4
1	B	16	GLY	3.3
1	A	214	ARG	3.2
1	A	153	ASN	3.2
1	B	77	LEU	3.1
1	A	163	MET	3.1
1	A	126	GLY	3.1
1	A	53	THR	3.1
1	A	164	THR	3.0
1	B	3	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	171	THR	3.0
1	A	152	ILE	3.0
1	B	72	ASN	3.0
1	A	137	VAL	2.9
1	B	122	GLU	2.9
1	B	120	ALA	2.9
1	A	147	ILE	2.9
1	B	52	ASP	2.8
1	B	29	TYR	2.8
1	A	158	ASP	2.8
1	B	70	GLY	2.8
1	B	78	SER	2.8
1	B	201	ARG	2.7
1	B	214	ARG	2.7
1	B	163	MET	2.7
1	A	82	LEU	2.6
1	B	1	MET	2.5
1	A	185	LEU	2.5
1	B	162	GLU	2.5
1	B	124	ARG	2.5
1	A	101	THR	2.5
1	B	4	THR	2.5
1	B	67	GLU	2.4
1	B	10	ASP	2.4
1	B	35	THR	2.4
1	B	66	ALA	2.4
1	B	121	GLU	2.4
1	A	170	GLN	2.4
1	A	113	SER	2.4
1	A	144	LYS	2.4
1	A	124	ARG	2.4
1	B	186	PRO	2.4
1	A	203	GLU	2.4
1	A	4	THR	2.4
1	B	212	THR	2.4
1	B	117	HIS	2.3
1	A	136	GLN	2.2
1	B	133	ARG	2.2
1	A	168	ALA	2.2
1	A	166	PRO	2.2
1	B	141	ILE	2.2
1	B	202	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	63	VAL	2.1
1	A	190	LEU	2.1
1	B	208	TYR	2.1
1	B	9	LEU	2.1
1	B	140	TRP	2.1
1	A	179	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.