Full wwPDB X-ray Structure Validation Report (i)

Feb 21, 2017 – 11:04 PM EST

PDB ID	:	5LOJ
Title	:	Structure of full length unliganded CodY from Bacillus subtilis
Authors	:	Wilkinson, A.J.; Levdikov, V.M.; Blagova, E.V.
Deposited on	:	2016-08-09
Resolution	:	3.71 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

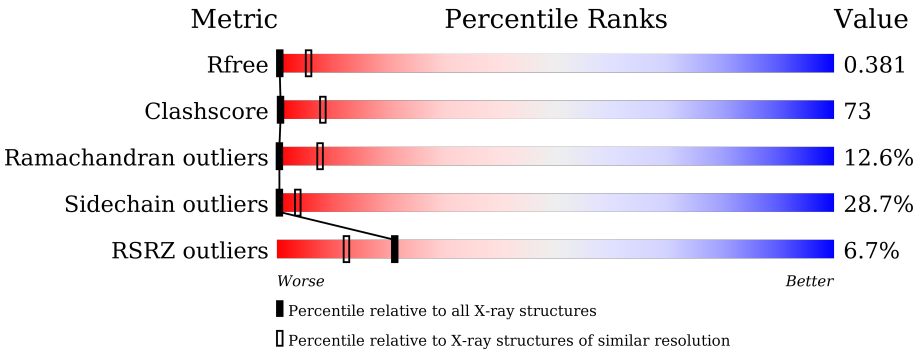
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.71 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1129 (3.94-3.50)
Clashscore	102246	1252 (3.94-3.50)
Ramachandran outliers	100387	1199 (3.94-3.50)
Sidechain outliers	100360	1197 (3.94-3.50)
RSRZ outliers	91569	1136 (3.94-3.50)

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

Mol	Chain	Length	Quality of chain
1	A	263	7% 17% 51% 26%
1	B	263	6% 21% 51% 22%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 4004 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 GTP-sensing transcriptional pleiotropic repressor CodY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	0	0
			2002	1259	341	395	7			
1	B	255	Total	C	N	O	S	0	0	0
			2002	1259	341	395	7			

There are 10 discrepancies between the modelled and reference sequences:

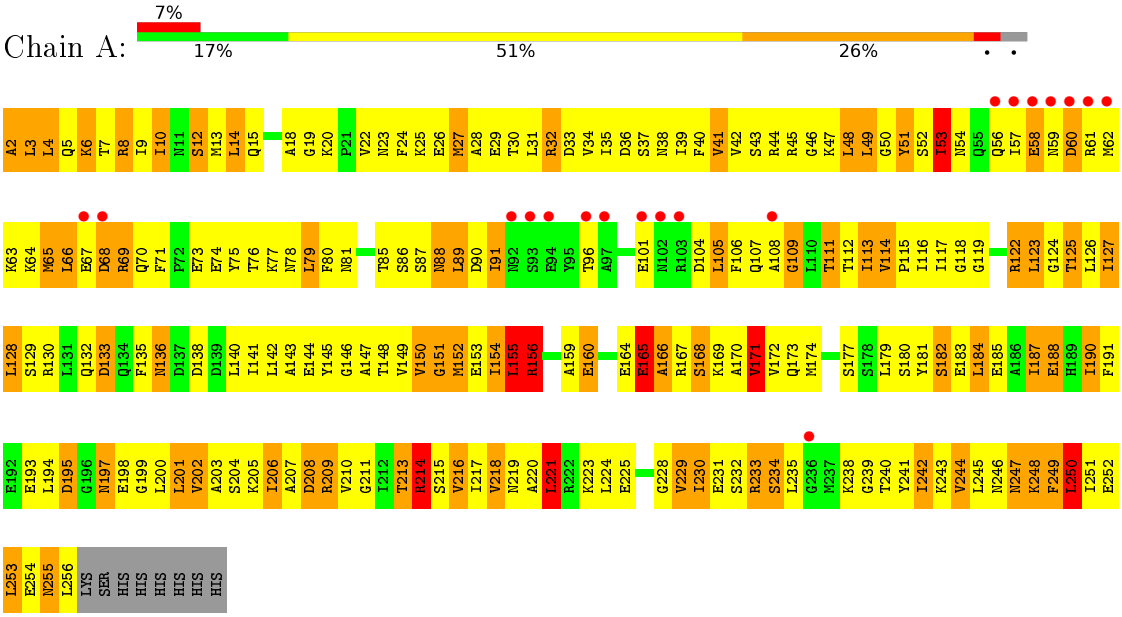
Chain	Residue	Modelled	Actual	Comment	Reference
A	260	HIS	-	expression tag	UNP P39779
A	261	HIS	-	expression tag	UNP P39779
A	262	HIS	-	expression tag	UNP P39779
A	263	HIS	-	expression tag	UNP P39779
A	264	HIS	-	expression tag	UNP P39779
B	260	HIS	-	expression tag	UNP P39779
B	261	HIS	-	expression tag	UNP P39779
B	262	HIS	-	expression tag	UNP P39779
B	263	HIS	-	expression tag	UNP P39779
B	264	HIS	-	expression tag	UNP P39779

3 Residue-property plots (i)

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

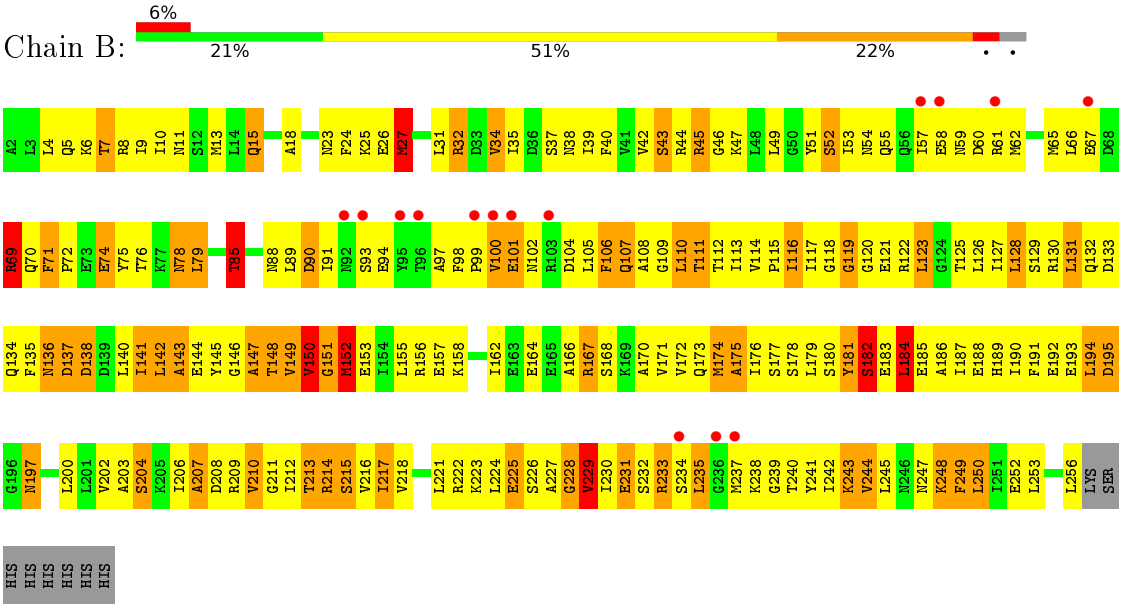
- Molecule 1: GTP-sensing transcriptional pleiotropic repressor CodY

Chain A:



- Molecule 1: GTP-sensing transcriptional pleiotropic repressor CodY

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α, β, γ	111.52Å 111.52Å 119.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.94 – 3.71 24.94 – 3.71	Depositor EDS
% Data completeness (in resolution range)	97.0 (24.94-3.71) 97.5 (24.94-3.71)	Depositor EDS
R_{merge}	5.90	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.70 (at 3.74Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.264 , 0.389 0.262 , 0.381	Depositor DCC
R_{free} test set	379 reflections (4.84%)	DCC
Wilson B-factor (Å^2)	132.2	Xtriage
Anisotropy	0.259	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 100.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	4004	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.86	1/2022 (0.0%)	1.05	5/2723 (0.2%)
1	B	0.85	0/2022	1.04	5/2723 (0.2%)
All	All	0.85	1/4044 (0.0%)	1.04	10/5446 (0.2%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	150	VAL	CA-CB	-5.06	1.44	1.54

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	184	LEU	CA-CB-CG	-6.06	101.37	115.30
1	B	123	LEU	CA-CB-CG	-5.89	101.76	115.30
1	A	156	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	A	165	GLU	N-CA-C	-5.46	96.25	111.00
1	A	250	LEU	CB-CG-CD2	5.17	119.79	111.00
1	B	229	VAL	CB-CA-C	-5.11	101.69	111.40
1	B	128	LEU	CA-CB-CG	-5.10	103.58	115.30
1	A	156	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	123	LEU	CA-CB-CG	-5.07	103.63	115.30
1	B	233	ARG	NE-CZ-NH2	5.07	122.83	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2	ALA	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2002	0	2041	299	0
1	B	2002	0	2041	310	0
All	All	4004	0	4082	593	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 73.

All (593) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:MET:CG	1:B:71:PHE:HD2	1.40	1.34
1:B:65:MET:CG	1:B:71:PHE:CD2	2.11	1.33
1:A:206:ILE:HA	1:A:209:ARG:NH1	1.52	1.25
1:A:197:ASN:O	1:A:243:LYS:HA	1.33	1.25
1:B:65:MET:HG3	1:B:71:PHE:CD2	1.73	1.21
1:B:71:PHE:CD1	1:B:72:PRO:HD2	1.80	1.16
1:B:65:MET:SD	1:B:71:PHE:CA	2.36	1.14
1:A:197:ASN:HB3	1:A:244:VAL:H	1.13	1.12
1:B:206:ILE:HG22	1:B:210:VAL:CG2	1.82	1.10
1:B:197:ASN:HB3	1:B:244:VAL:HG22	1.19	1.09
1:B:23:ASN:O	1:B:27:MET:SD	2.10	1.08
1:A:202:VAL:HA	1:A:240:THR:HG22	1.35	1.08
1:B:206:ILE:HG22	1:B:210:VAL:HG21	1.31	1.07
1:B:65:MET:SD	1:B:71:PHE:N	2.29	1.06
1:B:232:SER:HB2	1:B:242:ILE:HG22	1.11	1.05
1:A:4:LEU:CD2	1:A:8:ARG:HD2	1.85	1.05
1:B:65:MET:SD	1:B:71:PHE:HA	1.96	1.04
1:B:65:MET:HG2	1:B:71:PHE:CD2	1.91	1.01
1:A:24:PHE:O	1:A:27:MET:HB2	1.60	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ILE:HA	1:A:209:ARG:HH12	1.22	1.01
1:B:232:SER:HB2	1:B:242:ILE:CG2	1.92	1.00
1:B:24:PHE:O	1:B:27:MET:HG3	1.61	1.00
1:A:3:LEU:O	1:A:6:LYS:HB2	1.61	1.00
1:B:65:MET:HE1	1:B:71:PHE:N	1.78	0.99
1:B:65:MET:CE	1:B:71:PHE:N	2.26	0.99
1:B:38:ASN:O	1:B:128:LEU:HA	1.63	0.98
1:B:65:MET:HG3	1:B:71:PHE:HD2	0.82	0.98
1:A:152:MET:HE3	1:B:152:MET:SD	2.04	0.98
1:A:7:THR:O	1:A:10:ILE:N	1.97	0.97
1:A:114:VAL:HG23	1:A:126:LEU:HB3	1.45	0.97
1:A:32:ARG:NH2	1:A:33:ASP:OD1	1.98	0.97
1:A:59:ASN:ND2	1:A:62:MET:HG3	1.80	0.97
1:A:224:LEU:HB2	1:A:230:ILE:HD11	1.45	0.96
1:B:24:PHE:O	1:B:27:MET:CG	2.12	0.96
1:A:4:LEU:HD23	1:A:8:ARG:HD2	1.46	0.96
1:A:40:PHE:CD1	1:A:51:TYR:HB2	2.01	0.96
1:A:26:GLU:O	1:A:27:MET:HG2	1.66	0.95
1:B:128:LEU:HD12	1:B:128:LEU:N	1.79	0.95
1:B:98:PHE:HE1	1:B:102:ASN:HD22	1.14	0.95
1:A:171:VAL:HG11	1:A:246:ASN:ND2	1.81	0.95
1:A:86:SER:OG	1:A:89:LEU:HD21	1.67	0.94
1:A:22:VAL:HG23	1:A:156:ARG:HE	1.28	0.94
1:A:206:ILE:HG22	1:A:210:VAL:CG2	1.99	0.93
1:B:72:PRO:HG2	1:B:75:TYR:HD2	1.32	0.93
1:A:112:THR:HG23	1:A:113:ILE:H	1.32	0.92
1:A:13:MET:HG3	1:A:30:THR:HG21	1.51	0.92
1:A:111:THR:HG23	1:A:129:SER:HB3	1.52	0.92
1:B:38:ASN:HB3	1:B:40:PHE:HE1	1.32	0.91
1:A:146:GLY:O	1:A:150:VAL:HG23	1.70	0.91
1:B:112:THR:HG1	1:B:135:PHE:HD2	1.12	0.91
1:A:38:ASN:HB2	1:A:129:SER:O	1.71	0.90
1:A:206:ILE:HG22	1:A:210:VAL:HG21	1.52	0.90
1:B:225:GLU:HG2	1:B:230:ILE:O	1.70	0.90
1:A:200:LEU:HD12	1:A:241:TYR:HB2	1.51	0.90
1:B:59:ASN:HB2	1:B:108:ALA:HB3	1.55	0.89
1:B:79:LEU:HB2	1:B:105:LEU:HD21	1.56	0.86
1:A:197:ASN:O	1:A:243:LYS:CA	2.22	0.86
1:A:59:ASN:ND2	1:A:62:MET:CG	2.40	0.85
1:B:59:ASN:N	1:B:108:ALA:HB2	1.93	0.84
1:B:40:PHE:O	1:B:127:ILE:HD12	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:LEU:HB2	1:B:105:LEU:CD2	2.09	0.81
1:A:244:VAL:C	1:A:245:LEU:HD23	2.02	0.80
1:B:128:LEU:HD12	1:B:128:LEU:H	1.44	0.80
1:B:65:MET:HE1	1:B:71:PHE:H	1.44	0.79
1:A:71:PHE:HE2	1:A:105:LEU:HD22	1.48	0.79
1:A:43:SER:HB3	1:A:49:LEU:HD21	1.63	0.79
1:A:231:GLU:HB2	1:A:245:LEU:HD21	1.65	0.79
1:B:38:ASN:HB3	1:B:40:PHE:CE1	2.18	0.78
1:A:78:ASN:HA	1:A:81:ASN:HD22	1.48	0.77
1:A:52:SER:C	1:A:53:ILE:HG12	2.03	0.77
1:B:24:PHE:O	1:B:27:MET:HG2	1.85	0.77
1:B:65:MET:CE	1:B:69:ARG:O	2.33	0.77
1:B:151:GLY:O	1:B:153:GLU:N	2.18	0.77
1:B:72:PRO:HG2	1:B:75:TYR:CD2	2.19	0.77
1:A:3:LEU:HG	1:A:4:LEU:N	1.99	0.77
1:B:206:ILE:O	1:B:210:VAL:HG23	1.85	0.77
1:B:225:GLU:N	1:B:230:ILE:CD1	2.48	0.77
1:B:225:GLU:N	1:B:230:ILE:HD11	1.99	0.77
1:A:202:VAL:HA	1:A:240:THR:CG2	2.12	0.77
1:A:185:GLU:O	1:A:188:GLU:HB2	1.84	0.76
1:A:206:ILE:HA	1:A:209:ARG:HH11	1.45	0.76
1:A:59:ASN:HD21	1:A:62:MET:CG	1.99	0.76
1:B:25:LYS:O	1:B:27:MET:N	2.18	0.76
1:A:40:PHE:HD2	1:A:127:ILE:HG22	1.48	0.75
1:B:65:MET:HG2	1:B:71:PHE:CE2	2.22	0.75
1:B:197:ASN:CB	1:B:244:VAL:HG22	2.10	0.75
1:A:233:ARG:O	1:A:234:SER:O	2.04	0.75
1:A:9:ILE:HA	1:A:12:SER:OG	1.86	0.75
1:A:51:TYR:HD1	1:A:51:TYR:N	1.85	0.74
1:A:112:THR:CG2	1:A:113:ILE:N	2.49	0.74
1:A:13:MET:HG3	1:A:30:THR:CG2	2.17	0.74
1:A:112:THR:HG23	1:A:113:ILE:N	2.01	0.74
1:B:65:MET:SD	1:B:71:PHE:CB	2.76	0.74
1:B:109:GLY:HA2	1:B:130:ARG:O	1.88	0.73
1:A:244:VAL:HG23	1:A:246:ASN:H	1.53	0.73
1:A:38:ASN:O	1:A:128:LEU:HA	1.88	0.73
1:B:13:MET:SD	1:B:13:MET:O	2.46	0.73
1:A:44:ARG:HG2	1:A:80:PHE:HE2	1.53	0.72
1:A:63:LYS:HE3	1:A:66:LEU:HD22	1.70	0.72
1:B:75:TYR:HB3	1:B:105:LEU:HD13	1.70	0.72
1:A:88:ASN:HD21	1:A:135:PHE:H	1.36	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:LEU:HB3	1:A:230:ILE:HG13	1.71	0.72
1:A:4:LEU:HD21	1:A:8:ARG:HD2	1.68	0.72
1:A:203:ALA:O	1:A:206:ILE:HG12	1.90	0.72
1:A:202:VAL:CA	1:A:240:THR:HG22	2.17	0.72
1:B:213:THR:HB	1:B:215:SER:HB2	1.71	0.72
1:B:185:GLU:O	1:B:189:HIS:HD2	1.73	0.72
1:A:51:TYR:CD1	1:A:51:TYR:N	2.57	0.71
1:B:76:THR:O	1:B:79:LEU:HB3	1.90	0.71
1:B:170:ALA:O	1:B:174:MET:HG3	1.90	0.71
1:B:225:GLU:H	1:B:230:ILE:HD11	1.54	0.71
1:A:118:GLY:H	1:A:123:LEU:HD12	1.54	0.71
1:B:149:VAL:HG12	1:B:150:VAL:N	2.05	0.71
1:B:197:ASN:O	1:B:243:LYS:HA	1.90	0.71
1:B:65:MET:SD	1:B:70:GLN:C	2.68	0.71
1:A:59:ASN:HD21	1:A:62:MET:HG3	1.50	0.71
1:B:197:ASN:ND2	1:B:197:ASN:H	1.89	0.71
1:B:174:MET:O	1:B:177:SER:OG	2.08	0.70
1:A:38:ASN:O	1:A:39:ILE:HD13	1.91	0.70
1:A:220:ALA:O	1:A:223:LYS:HB2	1.91	0.70
1:A:152:MET:SD	1:A:155:LEU:HD12	2.32	0.70
1:A:197:ASN:HB3	1:A:244:VAL:N	1.98	0.70
1:A:152:MET:CE	1:B:152:MET:SD	2.80	0.69
1:B:65:MET:SD	1:B:71:PHE:CD2	2.86	0.69
1:A:112:THR:CG2	1:A:113:ILE:H	2.05	0.69
1:B:24:PHE:HA	1:B:27:MET:SD	2.32	0.69
1:A:197:ASN:HA	1:A:244:VAL:HG13	1.73	0.69
1:B:65:MET:HE1	1:B:70:GLN:CA	2.23	0.69
1:A:71:PHE:CE2	1:A:105:LEU:HD22	2.28	0.68
1:A:224:LEU:HB2	1:A:230:ILE:CD1	2.21	0.68
1:B:231:GLU:HB2	1:B:245:LEU:HD21	1.75	0.68
1:B:128:LEU:N	1:B:128:LEU:CD1	2.49	0.68
1:B:62:MET:HE3	1:B:71:PHE:HE2	1.59	0.68
1:A:40:PHE:CD1	1:A:51:TYR:CB	2.76	0.68
1:B:6:LYS:HB3	1:B:34:VAL:HG13	1.77	0.67
1:A:25:LYS:O	1:A:27:MET:N	2.27	0.67
1:B:208:ASP:CG	1:B:209:ARG:H	1.97	0.67
1:A:143:ALA:O	1:A:147:ALA:N	2.18	0.67
1:A:59:ASN:OD1	1:A:62:MET:HG2	1.94	0.67
1:B:98:PHE:CZ	1:B:106:PHE:HE2	2.13	0.67
1:A:206:ILE:HG22	1:A:210:VAL:HG23	1.74	0.67
1:A:63:LYS:HD2	1:A:66:LEU:HB3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:MET:O	1:A:177:SER:HB3	1.95	0.66
1:B:65:MET:HE1	1:B:70:GLN:C	2.16	0.66
1:B:71:PHE:CD1	1:B:72:PRO:CD	2.71	0.66
1:A:202:VAL:HG22	1:A:239:GLY:HA2	1.77	0.66
1:A:39:ILE:CD1	1:A:128:LEU:HD23	2.26	0.66
1:A:65:MET:HG3	1:A:71:PHE:HB2	1.77	0.66
1:B:126:LEU:HD12	1:B:127:ILE:N	2.11	0.66
1:A:109:GLY:CA	1:A:130:ARG:O	2.44	0.66
1:A:51:TYR:HD1	1:A:51:TYR:H	1.42	0.66
1:B:126:LEU:HD12	1:B:127:ILE:H	1.61	0.66
1:B:65:MET:HE3	1:B:69:ARG:C	2.17	0.66
1:A:26:GLU:O	1:A:27:MET:CG	2.43	0.66
1:A:88:ASN:ND2	1:A:135:PHE:H	1.95	0.65
1:A:144:GLU:O	1:A:148:THR:OG1	2.08	0.65
1:A:216:VAL:O	1:A:219:ASN:N	2.30	0.65
1:B:75:TYR:HB3	1:B:105:LEU:CD1	2.27	0.65
1:A:109:GLY:HA3	1:A:130:ARG:O	1.97	0.64
1:B:65:MET:HE1	1:B:69:ARG:O	1.97	0.64
1:B:98:PHE:HE1	1:B:102:ASN:ND2	1.92	0.64
1:A:112:THR:N	1:A:128:LEU:O	2.30	0.64
1:B:171:VAL:O	1:B:174:MET:HB2	1.97	0.64
1:A:206:ILE:CA	1:A:209:ARG:HH12	2.06	0.64
1:B:4:LEU:HD23	1:B:5:GLN:N	2.11	0.64
1:B:72:PRO:CG	1:B:75:TYR:HD2	2.09	0.64
1:A:118:GLY:H	1:A:123:LEU:CD1	2.11	0.64
1:A:151:GLY:O	1:A:153:GLU:N	2.26	0.64
1:A:150:VAL:O	1:A:154:ILE:HD11	1.98	0.64
1:B:217:ILE:HG22	1:B:218:VAL:N	2.12	0.64
1:A:170:ALA:O	1:A:174:MET:HG2	1.97	0.64
1:B:227:ALA:O	1:B:229:VAL:N	2.29	0.64
1:A:65:MET:HE2	1:A:69:ARG:HA	1.78	0.63
1:B:65:MET:HE3	1:B:69:ARG:O	1.97	0.63
1:A:231:GLU:O	1:A:242:ILE:HG22	1.97	0.63
1:B:138:ASP:HA	1:B:141:ILE:HB	1.81	0.63
1:B:65:MET:CE	1:B:69:ARG:C	2.67	0.63
1:B:144:GLU:O	1:B:145:TYR:C	2.37	0.63
1:B:168:SER:O	1:B:171:VAL:HG12	1.99	0.63
1:A:190:ILE:HG22	1:A:191:PHE:N	2.12	0.62
1:A:171:VAL:O	1:A:174:MET:HB2	1.97	0.62
1:A:122:ARG:HD2	1:A:124:GLY:O	1.98	0.62
1:A:71:PHE:CE2	1:A:75:TYR:HB3	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:VAL:HG11	1:A:246:ASN:HD22	1.65	0.62
1:B:231:GLU:O	1:B:243:LYS:HG2	1.98	0.62
1:A:188:GLU:OE1	1:A:188:GLU:HA	1.99	0.62
1:A:71:PHE:HE2	1:A:75:TYR:HB3	1.63	0.62
1:B:149:VAL:C	1:B:151:GLY:N	2.51	0.62
1:B:230:ILE:HD12	1:B:230:ILE:O	1.99	0.62
1:B:4:LEU:HD21	1:B:8:ARG:CZ	2.29	0.62
1:A:59:ASN:CG	1:A:62:MET:HG2	2.20	0.62
1:B:197:ASN:HB3	1:B:244:VAL:CG2	2.13	0.62
1:B:138:ASP:HA	1:B:141:ILE:HD12	1.81	0.62
1:B:191:PHE:HA	1:B:194:LEU:HB2	1.82	0.62
1:B:224:LEU:HB2	1:B:230:ILE:CG1	2.29	0.62
1:A:9:ILE:O	1:A:12:SER:OG	2.17	0.61
1:B:59:ASN:HB2	1:B:108:ALA:CB	2.28	0.61
1:B:79:LEU:O	1:B:79:LEU:HD22	2.00	0.61
1:A:111:THR:HA	1:A:129:SER:HA	1.81	0.61
1:B:151:GLY:C	1:B:153:GLU:H	2.01	0.61
1:A:245:LEU:N	1:A:245:LEU:HD23	2.15	0.61
1:B:137:ASP:HB3	1:B:138:ASP:OD1	2.00	0.61
1:B:149:VAL:HG12	1:B:150:VAL:H	1.64	0.61
1:A:171:VAL:HG11	1:A:246:ASN:HD21	1.61	0.61
1:A:250:LEU:O	1:A:254:GLU:HG3	2.01	0.61
1:A:44:ARG:HG3	1:A:122:ARG:O	2.01	0.61
1:B:187:ILE:HA	1:B:190:ILE:HD12	1.82	0.60
1:B:59:ASN:CG	1:B:107:GLN:HB3	2.22	0.60
1:B:147:ALA:O	1:B:150:VAL:HG23	2.02	0.60
1:B:213:THR:HB	1:B:215:SER:CB	2.32	0.60
1:B:138:ASP:OD1	1:B:138:ASP:N	2.33	0.60
1:B:62:MET:CE	1:B:71:PHE:CE2	2.84	0.60
1:B:193:GLU:O	1:B:194:LEU:HD12	2.00	0.60
1:B:65:MET:CE	1:B:71:PHE:H	2.01	0.60
1:A:59:ASN:ND2	1:A:62:MET:HG2	2.17	0.60
1:B:112:THR:OG1	1:B:135:PHE:HD2	1.82	0.60
1:B:228:GLY:O	1:B:245:LEU:HD12	2.02	0.60
1:A:136:ASN:ND2	1:A:138:ASP:H	2.00	0.59
1:A:209:ARG:HB3	1:A:209:ARG:HH11	1.66	0.59
1:A:41:VAL:HG23	1:A:50:GLY:O	2.02	0.59
1:B:225:GLU:N	1:B:230:ILE:HD12	2.17	0.59
1:A:23:ASN:ND2	1:A:26:GLU:HB2	2.17	0.59
1:B:23:ASN:O	1:B:27:MET:CG	2.51	0.59
1:B:147:ALA:O	1:B:149:VAL:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:ALA:HB1	1:B:212:ILE:O	2.02	0.59
1:B:224:LEU:HB2	1:B:230:ILE:HD11	1.85	0.59
1:A:152:MET:CE	1:B:152:MET:HE1	2.33	0.59
1:B:51:TYR:O	1:B:52:SER:HB2	2.02	0.59
1:A:159:ALA:O	1:A:160:GLU:C	2.41	0.59
1:B:185:GLU:O	1:B:189:HIS:CD2	2.53	0.59
1:B:182:SER:O	1:B:185:GLU:N	2.36	0.58
1:B:200:LEU:HB2	1:B:241:TYR:HD2	1.68	0.58
1:A:152:MET:HE1	1:A:155:LEU:HD12	1.85	0.58
1:B:149:VAL:CG1	1:B:150:VAL:N	2.66	0.58
1:B:162:ILE:C	1:B:164:GLU:H	2.07	0.58
1:A:144:GLU:OE1	1:B:8:ARG:HG3	2.03	0.58
1:A:46:GLY:HA3	1:A:76:THR:HG21	1.85	0.58
1:A:51:TYR:CD1	1:A:51:TYR:O	2.57	0.58
1:A:214:ARG:O	1:A:217:ILE:N	2.36	0.58
1:B:59:ASN:N	1:B:108:ALA:CB	2.64	0.58
1:B:136:ASN:O	1:B:137:ASP:C	2.42	0.58
1:B:208:ASP:CG	1:B:209:ARG:N	2.57	0.58
1:A:132:GLN:HG3	1:A:133:ASP:H	1.69	0.57
1:A:216:VAL:O	1:A:217:ILE:C	2.40	0.57
1:A:232:SER:HB2	1:A:241:TYR:O	2.04	0.57
1:A:40:PHE:HD1	1:A:51:TYR:CB	2.16	0.57
1:B:62:MET:CE	1:B:71:PHE:HE2	2.16	0.57
1:A:202:VAL:HG13	1:A:239:GLY:C	2.24	0.57
1:A:3:LEU:HD23	1:B:141:ILE:HD13	1.85	0.57
1:B:197:ASN:N	1:B:197:ASN:ND2	2.50	0.57
1:A:86:SER:HB3	1:A:89:LEU:HD11	1.87	0.57
1:A:152:MET:HG3	1:B:152:MET:CE	2.35	0.57
1:A:38:ASN:OD1	1:A:53:ILE:HG23	2.04	0.57
1:B:59:ASN:HA	1:B:107:GLN:HG2	1.85	0.57
1:A:200:LEU:HD12	1:A:241:TYR:CB	2.31	0.57
1:A:7:THR:OG1	1:A:8:ARG:N	2.37	0.57
1:A:247:ASN:H	1:A:247:ASN:HD22	1.53	0.56
1:A:4:LEU:HD12	1:B:137:ASP:O	2.05	0.56
1:B:197:ASN:HA	1:B:244:VAL:HG13	1.87	0.56
1:A:194:LEU:HG	1:A:195:ASP:H	1.69	0.56
1:B:206:ILE:CG2	1:B:210:VAL:HG21	2.21	0.56
1:A:122:ARG:HG3	1:A:124:GLY:H	1.70	0.56
1:A:179:LEU:HD23	1:A:223:LYS:HD3	1.86	0.56
1:B:116:ILE:HG23	1:B:147:ALA:HB1	1.87	0.56
1:A:9:ILE:CA	1:A:12:SER:OG	2.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:VAL:HG12	1:A:172:VAL:N	2.21	0.56
1:A:23:ASN:HD21	1:A:26:GLU:HB2	1.71	0.56
1:B:214:ARG:O	1:B:215:SER:C	2.44	0.56
1:A:240:THR:O	1:A:240:THR:HG23	2.06	0.56
1:A:71:PHE:CE2	1:A:75:TYR:CB	2.89	0.56
1:B:118:GLY:H	1:B:123:LEU:HD12	1.71	0.56
1:B:145:TYR:O	1:B:148:THR:HB	2.06	0.56
1:B:191:PHE:CE2	1:B:249:PHE:HE2	2.24	0.56
1:A:78:ASN:O	1:A:81:ASN:N	2.39	0.56
1:B:207:ALA:O	1:B:211:GLY:N	2.38	0.56
1:A:249:PHE:O	1:A:250:LEU:C	2.44	0.55
1:A:90:ASP:CG	1:A:91:ILE:H	2.09	0.55
1:B:4:LEU:C	1:B:4:LEU:HD23	2.26	0.55
1:A:213:THR:OG1	1:A:215:SER:HB2	2.05	0.55
1:A:215:SER:O	1:A:218:VAL:HB	2.05	0.55
1:A:141:ILE:HD11	1:B:4:LEU:HB2	1.88	0.55
1:A:48:LEU:H	1:A:65:MET:CE	2.19	0.55
1:B:49:LEU:N	1:B:49:LEU:HD23	2.22	0.55
1:A:65:MET:C	1:A:67:GLU:H	2.10	0.55
1:A:7:THR:C	1:A:9:ILE:N	2.59	0.55
1:B:98:PHE:CD1	1:B:102:ASN:HB3	2.42	0.55
1:A:41:VAL:HG13	1:A:126:LEU:HD13	1.89	0.55
1:B:212:ILE:CG2	1:B:216:VAL:HG23	2.37	0.55
1:A:152:MET:CE	1:A:155:LEU:HD12	2.38	0.54
1:A:4:LEU:HB2	1:B:141:ILE:HD11	1.90	0.54
1:B:61:ARG:HG2	1:B:104:ASP:O	2.08	0.54
1:B:214:ARG:O	1:B:216:VAL:N	2.40	0.54
1:B:32:ARG:NH1	1:B:54:ASN:HB3	2.22	0.54
1:A:197:ASN:C	1:A:243:LYS:HA	2.21	0.54
1:B:112:THR:HG22	1:B:113:ILE:N	2.23	0.54
1:A:252:GLU:O	1:A:255:ASN:N	2.40	0.54
1:A:166:ALA:HA	1:A:169:LYS:HB2	1.90	0.54
1:A:205:LYS:O	1:A:208:ASP:OD1	2.26	0.54
1:A:76:THR:O	1:A:79:LEU:HB3	2.08	0.54
1:B:25:LYS:C	1:B:27:MET:H	2.09	0.54
1:A:165:GLU:HG2	1:A:248:LYS:NZ	2.23	0.54
1:A:198:GLU:HG2	1:A:243:LYS:HG3	1.89	0.54
1:A:22:VAL:HG23	1:A:156:ARG:NE	2.10	0.54
1:A:25:LYS:O	1:A:28:ALA:N	2.41	0.54
1:B:23:ASN:O	1:B:27:MET:HG2	2.08	0.54
1:A:88:ASN:ND2	1:A:135:PHE:HB2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:GLU:O	1:A:255:ASN:HB2	2.08	0.54
1:A:78:ASN:C	1:A:80:PHE:N	2.58	0.54
1:B:89:LEU:O	1:B:110:LEU:HD23	2.07	0.54
1:A:221:LEU:O	1:A:230:ILE:HD11	2.07	0.53
1:B:7:THR:O	1:B:10:ILE:HB	2.08	0.53
1:A:43:SER:CB	1:A:49:LEU:HD21	2.37	0.53
1:A:232:SER:CB	1:A:241:TYR:O	2.56	0.53
1:B:206:ILE:HD13	1:B:206:ILE:N	2.23	0.53
1:A:199:GLY:N	1:A:242:ILE:O	2.40	0.53
1:A:187:ILE:HG22	1:A:253:LEU:HD11	1.90	0.53
1:B:126:LEU:HG	1:B:128:LEU:HD11	1.90	0.53
1:A:147:ALA:O	1:A:151:GLY:N	2.42	0.53
1:A:152:MET:HG3	1:B:152:MET:HE1	1.90	0.53
1:B:109:GLY:CA	1:B:130:ARG:O	2.55	0.53
1:B:34:VAL:HG12	1:B:142:LEU:HD13	1.91	0.53
1:A:187:ILE:HG22	1:A:253:LEU:CD1	2.39	0.53
1:A:26:GLU:C	1:A:27:MET:HG2	2.29	0.52
1:A:7:THR:O	1:A:9:ILE:N	2.42	0.52
1:B:173:GLN:HE22	1:B:252:GLU:CD	2.11	0.52
1:A:51:TYR:CD1	1:A:51:TYR:C	2.81	0.52
1:B:172:VAL:HG11	1:B:249:PHE:HA	1.90	0.52
1:B:4:LEU:HD21	1:B:8:ARG:NH1	2.23	0.52
1:A:48:LEU:H	1:A:65:MET:HE1	1.74	0.52
1:B:115:PRO:HB3	1:B:122:ARG:CZ	2.39	0.52
1:B:157:GLU:OE2	1:B:158:LYS:HG2	2.10	0.52
1:B:34:VAL:O	1:B:34:VAL:HG13	2.09	0.52
1:A:182:SER:O	1:A:183:GLU:C	2.48	0.52
1:B:112:THR:OG1	1:B:135:PHE:CD2	2.52	0.52
1:B:208:ASP:N	1:B:208:ASP:OD1	2.42	0.52
1:B:38:ASN:HB2	1:B:129:SER:OG	2.10	0.52
1:B:65:MET:CE	1:B:70:GLN:C	2.78	0.52
1:A:217:ILE:O	1:A:219:ASN:N	2.42	0.52
1:B:206:ILE:C	1:B:210:VAL:HG23	2.29	0.52
1:B:195:ASP:N	1:B:195:ASP:OD1	2.42	0.52
1:A:217:ILE:C	1:A:219:ASN:H	2.13	0.51
1:B:79:LEU:CB	1:B:105:LEU:HD21	2.34	0.51
1:B:223:LYS:O	1:B:226:SER:HB3	2.10	0.51
1:B:13:MET:SD	1:B:13:MET:C	2.88	0.51
1:B:34:VAL:CG1	1:B:34:VAL:O	2.58	0.51
1:B:60:ASP:H	1:B:107:GLN:NE2	2.09	0.51
1:A:141:ILE:HD11	1:B:4:LEU:CA	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:PRO:C	1:B:101:GLU:H	2.15	0.51
1:B:207:ALA:CB	1:B:212:ILE:O	2.59	0.51
1:B:200:LEU:HA	1:B:240:THR:O	2.10	0.51
1:A:206:ILE:CG2	1:A:210:VAL:HG21	2.35	0.51
1:B:200:LEU:HD12	1:B:241:TYR:HB2	1.92	0.50
1:A:59:ASN:N	1:A:108:ALA:HB3	2.26	0.50
1:B:181:TYR:C	1:B:181:TYR:CD1	2.83	0.50
1:B:61:ARG:NH2	1:B:104:ASP:OD2	2.45	0.50
1:A:181:TYR:O	1:A:185:GLU:HB2	2.11	0.50
1:A:63:LYS:HE3	1:A:66:LEU:HB3	1.93	0.50
1:A:39:ILE:HD13	1:A:128:LEU:HD23	1.93	0.50
1:B:221:LEU:O	1:B:222:ARG:C	2.49	0.50
1:B:34:VAL:CG1	1:B:142:LEU:HD13	2.42	0.50
1:B:216:VAL:O	1:B:217:ILE:C	2.49	0.50
1:A:249:PHE:O	1:A:251:ILE:N	2.45	0.50
1:A:91:ILE:HG12	1:A:91:ILE:O	2.11	0.50
1:A:199:GLY:O	1:A:241:TYR:HA	2.12	0.50
1:A:171:VAL:CG1	1:A:246:ASN:ND2	2.66	0.50
1:B:167:ARG:O	1:B:170:ALA:HB3	2.12	0.50
1:A:74:GLU:HA	1:A:77:LYS:HD2	1.93	0.49
1:B:112:THR:CG2	1:B:113:ILE:N	2.74	0.49
1:B:35:ILE:HD11	1:B:143:ALA:N	2.27	0.49
1:B:119:GLY:N	1:B:155:LEU:HD11	2.27	0.49
1:B:31:LEU:HB3	1:B:39:ILE:HD12	1.94	0.49
1:B:231:GLU:HB3	1:B:243:LYS:CG	2.42	0.49
1:A:149:VAL:HG12	1:A:150:VAL:N	2.27	0.49
1:B:187:ILE:O	1:B:190:ILE:HB	2.12	0.49
1:B:247:ASN:OD1	1:B:248:LYS:HD2	2.12	0.49
1:A:115:PRO:HB2	1:A:117:ILE:HD11	1.95	0.49
1:B:180:SER:OG	1:B:182:SER:OG	2.23	0.49
1:B:186:ALA:O	1:B:187:ILE:C	2.50	0.49
1:B:85:THR:HA	1:B:113:ILE:O	2.13	0.49
1:B:197:ASN:N	1:B:197:ASN:HD22	2.10	0.49
1:B:213:THR:HG22	1:B:214:ARG:NH1	2.28	0.49
1:A:232:SER:HB2	1:A:242:ILE:HG23	1.93	0.49
1:A:54:ASN:N	1:A:54:ASN:OD1	2.46	0.49
1:A:165:GLU:O	1:A:167:ARG:N	2.46	0.48
1:B:225:GLU:HG2	1:B:230:ILE:HD12	1.95	0.48
1:B:130:ARG:HD2	1:B:135:PHE:CE1	2.48	0.48
1:B:224:LEU:HB2	1:B:230:ILE:CD1	2.43	0.48
1:B:32:ARG:O	1:B:32:ARG:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:PHE:HD2	1:A:127:ILE:CG2	2.24	0.48
1:A:61:ARG:NH2	1:A:104:ASP:OD2	2.42	0.48
1:A:156:ARG:C	1:A:156:ARG:HD2	2.34	0.48
1:B:78:ASN:HB2	1:B:102:ASN:ND2	2.29	0.48
1:B:174:MET:O	1:B:175:ALA:C	2.51	0.48
1:B:191:PHE:CE2	1:B:249:PHE:CE2	3.02	0.48
1:B:203:ALA:HA	1:B:206:ILE:HG12	1.95	0.48
1:A:40:PHE:CD2	1:A:127:ILE:HG22	2.39	0.48
1:A:150:VAL:O	1:A:154:ILE:CD1	2.61	0.48
1:A:7:THR:O	1:A:8:ARG:C	2.51	0.48
1:B:150:VAL:O	1:B:151:GLY:O	2.32	0.48
1:B:71:PHE:HE1	1:B:75:TYR:HB3	1.78	0.48
1:A:37:SER:OG	1:A:128:LEU:HB3	2.14	0.48
1:B:149:VAL:O	1:B:150:VAL:C	2.52	0.48
1:B:191:PHE:HD2	1:B:253:LEU:HD22	1.78	0.47
1:B:190:ILE:HG22	1:B:191:PHE:N	2.28	0.47
1:B:229:VAL:HG12	1:B:229:VAL:O	2.13	0.47
1:B:65:MET:HE1	1:B:69:ARG:C	2.35	0.47
1:A:180:SER:N	1:A:183:GLU:OE1	2.36	0.47
1:A:184:LEU:O	1:A:188:GLU:HG2	2.14	0.47
1:A:224:LEU:CB	1:A:230:ILE:HG13	2.41	0.47
1:A:39:ILE:HG23	1:A:126:LEU:HD11	1.96	0.47
1:A:3:LEU:O	1:A:6:LYS:CB	2.47	0.47
1:B:98:PHE:CZ	1:B:106:PHE:CE2	3.00	0.47
1:A:117:ILE:O	1:A:117:ILE:HG22	2.14	0.47
1:A:148:THR:HG21	1:B:145:TYR:OH	2.15	0.47
1:A:14:LEU:O	1:A:15:GLN:C	2.52	0.47
1:A:167:ARG:O	1:A:170:ALA:N	2.48	0.47
1:A:201:LEU:HG	1:A:205:LYS:HD2	1.96	0.47
1:A:6:LYS:O	1:A:9:ILE:HB	2.14	0.47
1:B:118:GLY:H	1:B:123:LEU:CD1	2.27	0.47
1:B:242:ILE:O	1:B:242:ILE:HD12	2.13	0.47
1:A:219:ASN:O	1:A:220:ALA:C	2.50	0.47
1:A:31:LEU:HD21	1:A:146:GLY:HA3	1.95	0.47
1:A:167:ARG:O	1:A:168:SER:C	2.53	0.47
1:A:52:SER:O	1:A:53:ILE:HG12	2.14	0.47
1:B:174:MET:O	1:B:177:SER:N	2.47	0.47
1:B:71:PHE:HD1	1:B:72:PRO:HD2	1.66	0.47
1:A:10:ILE:HD12	1:A:10:ILE:HA	1.83	0.47
1:A:36:ASP:O	1:A:130:ARG:NE	2.46	0.47
1:A:56:GLN:C	1:A:57:ILE:HG13	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:LEU:HD12	1:A:184:LEU:HB2	1.96	0.47
1:B:15:GLN:H	1:B:15:GLN:HG2	1.57	0.47
1:B:191:PHE:HE2	1:B:249:PHE:CE2	2.33	0.47
1:A:184:LEU:HD12	1:A:188:GLU:HG2	1.97	0.47
1:B:118:GLY:O	1:B:121:GLU:N	2.48	0.47
1:B:145:TYR:O	1:B:146:GLY:C	2.53	0.47
1:B:206:ILE:HG22	1:B:210:VAL:HG23	1.84	0.47
1:A:2:ALA:O	1:A:5:GLN:OE1	2.33	0.46
1:B:183:GLU:O	1:B:186:ALA:HB3	2.15	0.46
1:B:24:PHE:HA	1:B:27:MET:CG	2.45	0.46
1:A:151:GLY:O	1:A:154:ILE:HD12	2.14	0.46
1:A:213:THR:O	1:A:217:ILE:HG13	2.14	0.46
1:B:190:ILE:HG22	1:B:191:PHE:CD1	2.50	0.46
1:A:63:LYS:HD2	1:A:66:LEU:CB	2.44	0.46
1:B:136:ASN:OD1	1:B:138:ASP:N	2.48	0.46
1:A:171:VAL:HG12	1:A:172:VAL:HG23	1.97	0.46
1:A:40:PHE:CE1	1:A:51:TYR:HB2	2.50	0.46
1:B:65:MET:SD	1:B:71:PHE:CG	3.08	0.46
1:A:65:MET:HE3	1:A:69:ARG:O	2.16	0.46
1:B:37:SER:HB2	1:B:130:ARG:HG3	1.98	0.46
1:A:249:PHE:O	1:A:252:GLU:N	2.48	0.46
1:A:24:PHE:O	1:A:25:LYS:C	2.54	0.46
1:B:212:ILE:CG2	1:B:216:VAL:CG2	2.93	0.46
1:A:116:ILE:HG13	1:A:124:GLY:O	2.15	0.45
1:A:122:ARG:HE	1:A:125:THR:HG23	1.80	0.45
1:B:59:ASN:H	1:B:108:ALA:CB	2.29	0.45
1:B:43:SER:OG	1:B:49:LEU:HD21	2.16	0.45
1:A:9:ILE:C	1:A:12:SER:OG	2.55	0.45
1:A:136:ASN:HD21	1:A:138:ASP:H	1.63	0.45
1:B:224:LEU:CB	1:B:230:ILE:HG13	2.46	0.45
1:B:230:ILE:HG22	1:B:243:LYS:O	2.16	0.45
1:B:5:GLN:C	1:B:9:ILE:HD12	2.36	0.45
1:A:10:ILE:HD12	1:A:30:THR:HG22	1.97	0.45
1:A:191:PHE:HA	1:A:194:LEU:HB3	1.99	0.45
1:A:250:LEU:HD13	1:A:254:GLU:OE2	2.17	0.45
1:A:40:PHE:HZ	1:A:53:ILE:HD13	1.82	0.45
1:B:118:GLY:N	1:B:123:LEU:HD12	2.31	0.45
1:B:71:PHE:CE1	1:B:75:TYR:HB3	2.52	0.45
1:B:167:ARG:O	1:B:168:SER:C	2.54	0.45
1:B:38:ASN:HB2	1:B:129:SER:O	2.17	0.45
1:B:71:PHE:HE1	1:B:75:TYR:CB	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:ILE:CG2	1:B:210:VAL:CG2	2.75	0.45
1:B:212:ILE:HG22	1:B:213:THR:N	2.31	0.45
1:B:221:LEU:HD12	1:B:221:LEU:HA	1.64	0.45
1:B:4:LEU:HD11	1:B:8:ARG:NH2	2.32	0.45
1:A:40:PHE:HE1	1:A:51:TYR:HD2	1.65	0.44
1:A:5:GLN:C	1:A:9:ILE:HD12	2.38	0.44
1:B:31:LEU:HA	1:B:31:LEU:HD23	1.63	0.44
1:B:79:LEU:C	1:B:79:LEU:HD22	2.37	0.44
1:B:213:THR:O	1:B:214:ARG:C	2.55	0.44
1:B:59:ASN:HA	1:B:107:GLN:HB3	1.99	0.44
1:A:253:LEU:HA	1:A:256:LEU:HD12	2.00	0.44
1:A:152:MET:CE	1:B:152:MET:CE	2.96	0.44
1:A:32:ARG:CZ	1:A:33:ASP:OD1	2.63	0.44
1:A:6:LYS:HD2	1:A:34:VAL:HG13	1.99	0.44
1:A:155:LEU:HA	1:A:155:LEU:HD22	1.86	0.44
1:A:209:ARG:NH1	1:A:209:ARG:HB3	2.32	0.44
1:A:214:ARG:O	1:A:218:VAL:HG23	2.18	0.44
1:B:155:LEU:HA	1:B:155:LEU:HD23	1.84	0.44
1:B:78:ASN:OD1	1:B:78:ASN:N	2.50	0.44
1:A:151:GLY:C	1:A:153:GLU:H	2.17	0.44
1:B:147:ALA:O	1:B:148:THR:C	2.56	0.44
1:A:78:ASN:C	1:A:80:PHE:H	2.20	0.44
1:B:24:PHE:O	1:B:25:LYS:C	2.56	0.44
1:B:213:THR:CB	1:B:215:SER:HB2	2.44	0.44
1:A:152:MET:HE2	1:B:152:MET:HE1	1.99	0.44
1:B:221:LEU:N	1:B:221:LEU:CD1	2.79	0.44
1:A:224:LEU:CB	1:A:230:ILE:CG1	2.96	0.43
1:A:53:ILE:HG21	1:A:57:ILE:HD11	1.99	0.43
1:B:32:ARG:HD3	1:B:52:SER:OG	2.18	0.43
1:B:65:MET:CG	1:B:71:PHE:CE2	2.83	0.43
1:A:154:ILE:H	1:A:154:ILE:HG13	1.52	0.43
1:A:4:LEU:HD21	1:A:8:ARG:CD	2.44	0.43
1:B:71:PHE:CE1	1:B:72:PRO:HD2	2.43	0.43
1:A:154:ILE:O	1:A:155:LEU:C	2.55	0.43
1:A:170:ALA:O	1:A:171:VAL:C	2.56	0.43
1:A:200:LEU:HD23	1:A:200:LEU:C	2.38	0.43
1:A:228:GLY:O	1:A:229:VAL:C	2.57	0.43
1:A:63:LYS:CD	1:A:66:LEU:HB3	2.47	0.43
1:B:116:ILE:C	1:B:117:ILE:HG13	2.38	0.43
1:A:40:PHE:HB3	1:A:48:LEU:CD1	2.48	0.43
1:A:6:LYS:N	1:A:9:ILE:HD12	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:VAL:O	1:B:151:GLY:N	2.51	0.43
1:B:11:ASN:O	1:B:15:GLN:HG2	2.19	0.43
1:B:243:LYS:HG3	1:B:245:LEU:HD21	2.00	0.43
1:A:214:ARG:O	1:A:215:SER:C	2.57	0.43
1:A:3:LEU:C	1:A:3:LEU:HD12	2.39	0.43
1:A:78:ASN:HA	1:A:81:ASN:ND2	2.26	0.43
1:B:182:SER:O	1:B:183:GLU:C	2.56	0.43
1:B:225:GLU:CA	1:B:230:ILE:HD12	2.49	0.43
1:B:71:PHE:CE1	1:B:75:TYR:CB	3.02	0.43
1:B:130:ARG:HB3	1:B:131:LEU:H	1.62	0.43
1:B:203:ALA:O	1:B:204:SER:C	2.56	0.43
1:A:5:GLN:H	1:A:5:GLN:CD	2.22	0.43
1:B:71:PHE:CE1	1:B:105:LEU:HD12	2.53	0.43
1:B:235:LEU:HD22	1:B:239:GLY:O	2.19	0.43
1:A:14:LEU:HD12	1:A:149:VAL:HG13	2.01	0.43
1:A:247:ASN:N	1:A:247:ASN:HD22	2.17	0.43
1:B:206:ILE:O	1:B:207:ALA:C	2.57	0.43
1:A:140:LEU:O	1:A:141:ILE:C	2.57	0.43
1:A:228:GLY:O	1:A:230:ILE:N	2.52	0.43
1:B:184:LEU:O	1:B:185:GLU:C	2.57	0.43
1:B:32:ARG:N	1:B:39:ILE:HG13	2.34	0.43
1:B:45:ARG:HD3	1:B:45:ARG:H	1.84	0.43
1:B:65:MET:HE2	1:B:71:PHE:HB2	2.01	0.43
1:A:57:ILE:HG22	1:A:58:GLU:H	1.84	0.42
1:B:151:GLY:C	1:B:153:GLU:N	2.67	0.42
1:A:149:VAL:C	1:A:151:GLY:N	2.73	0.42
1:B:249:PHE:CD2	1:B:250:LEU:N	2.88	0.42
1:A:4:LEU:HD11	1:B:140:LEU:HB2	2.00	0.42
1:B:118:GLY:O	1:B:119:GLY:C	2.58	0.42
1:B:65:MET:SD	1:B:71:PHE:HB2	2.58	0.42
1:A:91:ILE:O	1:A:91:ILE:CG1	2.66	0.42
1:B:58:GLU:C	1:B:108:ALA:HB2	2.39	0.42
1:B:118:GLY:C	1:B:120:GLY:N	2.72	0.42
1:A:19:GLY:O	1:A:20:LYS:C	2.58	0.42
1:B:132:GLN:HG3	1:B:133:ASP:N	2.34	0.42
1:B:136:ASN:ND2	1:B:137:ASP:HB3	2.35	0.42
1:A:132:GLN:HG3	1:A:133:ASP:OD1	2.18	0.42
1:B:136:ASN:CG	1:B:138:ASP:H	2.22	0.42
1:B:146:GLY:O	1:B:150:VAL:HG23	2.19	0.42
1:B:176:ILE:O	1:B:179:LEU:HB2	2.20	0.42
1:A:22:VAL:HG22	1:A:153:GLU:OE1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:LYS:HA	1:A:65:MET:HE3	2.02	0.42
1:B:224:LEU:HB2	1:B:230:ILE:HG13	2.02	0.42
1:A:207:ALA:O	1:A:211:GLY:N	2.48	0.41
1:B:88:ASN:ND2	1:B:135:PHE:HB2	2.35	0.41
1:B:46:GLY:HA3	1:B:76:THR:HG21	2.02	0.41
1:A:60:ASP:H	1:A:107:GLN:NE2	2.19	0.41
1:A:152:MET:HA	1:A:155:LEU:HB2	2.01	0.41
1:B:206:ILE:O	1:B:209:ARG:N	2.53	0.41
1:B:25:LYS:C	1:B:27:MET:N	2.72	0.41
1:A:213:THR:O	1:A:216:VAL:HG23	2.21	0.41
1:B:182:SER:O	1:B:185:GLU:CB	2.68	0.41
1:A:136:ASN:OD1	1:A:138:ASP:HB2	2.21	0.41
1:A:23:ASN:C	1:A:23:ASN:OD1	2.58	0.41
1:B:222:ARG:O	1:B:223:LYS:C	2.58	0.41
1:A:141:ILE:HD11	1:B:4:LEU:CB	2.51	0.41
1:A:35:ILE:HG23	1:A:142:LEU:HD12	2.02	0.41
1:B:60:ASP:H	1:B:107:GLN:HE21	1.66	0.41
1:A:114:VAL:CG2	1:A:126:LEU:HB3	2.33	0.41
1:A:80:PHE:C	1:A:80:PHE:CD1	2.94	0.41
1:B:89:LEU:H	1:B:110:LEU:CD2	2.33	0.41
1:B:252:GLU:OE1	1:B:256:LEU:HD11	2.20	0.41
1:B:72:PRO:C	1:B:74:GLU:H	2.24	0.41
1:A:10:ILE:HD13	1:A:34:VAL:HG21	2.03	0.41
1:B:24:PHE:CD2	1:B:49:LEU:HB3	2.56	0.41
1:A:68:ASP:C	1:A:70:GLN:H	2.24	0.41
1:A:71:PHE:CE2	1:A:105:LEU:CD2	2.99	0.41
1:A:29:GLU:O	1:A:30:THR:C	2.59	0.40
1:A:41:VAL:CG2	1:A:50:GLY:O	2.68	0.40
1:B:59:ASN:OD1	1:B:107:GLN:HB3	2.21	0.40
1:B:10:ILE:O	1:B:11:ASN:C	2.58	0.40
1:B:111:THR:HG23	1:B:129:SER:HB3	2.03	0.40
1:B:231:GLU:HB3	1:B:243:LYS:HE2	2.02	0.40
1:B:42:VAL:HA	1:B:47:LYS:O	2.22	0.40
1:B:88:ASN:ND2	1:B:135:PHE:H	2.20	0.40
1:A:164:GLU:OE2	1:A:167:ARG:CD	2.69	0.40
1:A:165:GLU:C	1:A:167:ARG:H	2.24	0.40
1:A:173:GLN:HE22	1:A:252:GLU:CG	2.34	0.40
1:A:38:ASN:O	1:A:128:LEU:HB3	2.22	0.40
1:B:152:MET:HE3	1:B:152:MET:HB3	1.74	0.40
1:A:63:LYS:CE	1:A:66:LEU:HB3	2.52	0.40
1:B:62:MET:SD	1:B:71:PHE:CZ	3.15	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	253/263 (96%)	154 (61%)	68 (27%)	31 (12%)	0 8
1	B	253/263 (96%)	147 (58%)	73 (29%)	33 (13%)	0 7
All	All	506/526 (96%)	301 (60%)	141 (28%)	64 (13%)	0 8

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	27	MET
1	A	152	MET
1	A	168	SER
1	A	171	VAL
1	A	218	VAL
1	A	229	VAL
1	A	234	SER
1	B	18	ALA
1	B	91	ILE
1	B	107	GLN
1	B	137	ASP
1	B	148	THR
1	B	152	MET
1	B	182	SER
1	B	215	SER
1	A	4	LEU
1	A	8	ARG
1	A	88	ASN
1	A	119	GLY
1	A	155	LEU
1	A	188	GLU

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Mol	Chain	Res	Type
1	B	52	SER
1	B	90	ASP
1	B	97	ALA
1	B	100	VAL
1	B	151	GLY
1	B	166	ALA
1	B	175	ALA
1	B	207	ALA
1	B	228	GLY
1	B	229	VAL
1	A	6	LYS
1	A	73	GLU
1	A	166	ALA
1	A	221	LEU
1	A	255	ASN
1	B	26	GLU
1	B	69	ARG
1	B	85	THR
1	B	143	ALA
1	B	147	ALA
1	B	150	VAL
1	B	174	MET
1	B	249	PHE
1	A	32	ARG
1	A	66	LEU
1	A	109	GLY
1	A	151	GLY
1	A	214	ARG
1	A	249	PHE
1	B	217	ILE
1	A	18	ALA
1	A	187	ILE
1	B	27	MET
1	B	141	ILE
1	B	142	LEU
1	B	188	GLU
1	B	237	MET
1	A	160	GLU
1	A	190	ILE
1	A	53	ILE
1	B	119	GLY
1	A	91	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	221/229 (96%)	156 (71%)	65 (29%)	0 4
1	B	221/229 (96%)	159 (72%)	62 (28%)	0 4
All	All	442/458 (96%)	315 (71%)	127 (29%)	0 4

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	12	SER
1	A	14	LEU
1	A	41	VAL
1	A	42	VAL
1	A	45	ARG
1	A	48	LEU
1	A	49	LEU
1	A	51	TYR
1	A	53	ILE
1	A	58	GLU
1	A	60	ASP
1	A	64	LYS
1	A	65	MET
1	A	68	ASP
1	A	69	ARG
1	A	79	LEU
1	A	85	THR
1	A	87	SER
1	A	89	LEU
1	A	96	THR
1	A	101	GLU
1	A	105	LEU
1	A	106	PHE
1	A	111	THR
1	A	113	ILE
1	A	114	VAL

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Mol	Chain	Res	Type
1	A	122	ARG
1	A	125	THR
1	A	127	ILE
1	A	128	LEU
1	A	133	ASP
1	A	136	ASN
1	A	145	TYR
1	A	154	ILE
1	A	155	LEU
1	A	156	ARG
1	A	165	GLU
1	A	171	VAL
1	A	182	SER
1	A	184	LEU
1	A	193	GLU
1	A	195	ASP
1	A	197	ASN
1	A	201	LEU
1	A	202	VAL
1	A	204	SER
1	A	206	ILE
1	A	208	ASP
1	A	209	ARG
1	A	213	THR
1	A	214	ARG
1	A	216	VAL
1	A	221	LEU
1	A	225	GLU
1	A	230	ILE
1	A	233	ARG
1	A	235	LEU
1	A	238	LYS
1	A	242	ILE
1	A	244	VAL
1	A	247	ASN
1	A	248	LYS
1	A	250	LEU
1	A	253	LEU
1	B	7	THR
1	B	15	GLN
1	B	27	MET
1	B	32	ARG

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Mol	Chain	Res	Type
1	B	34	VAL
1	B	43	SER
1	B	44	ARG
1	B	45	ARG
1	B	53	ILE
1	B	55	GLN
1	B	57	ILE
1	B	66	LEU
1	B	67	GLU
1	B	69	ARG
1	B	71	PHE
1	B	74	GLU
1	B	78	ASN
1	B	79	LEU
1	B	85	THR
1	B	90	ASP
1	B	93	SER
1	B	94	GLU
1	B	100	VAL
1	B	101	GLU
1	B	106	PHE
1	B	110	LEU
1	B	111	THR
1	B	114	VAL
1	B	116	ILE
1	B	125	THR
1	B	131	LEU
1	B	134	GLN
1	B	136	ASN
1	B	138	ASP
1	B	149	VAL
1	B	150	VAL
1	B	152	MET
1	B	156	ARG
1	B	167	ARG
1	B	178	SER
1	B	181	TYR
1	B	182	SER
1	B	184	LEU
1	B	192	GLU
1	B	194	LEU
1	B	195	ASP

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Mol	Chain	Res	Type
1	B	197	ASN
1	B	202	VAL
1	B	204	SER
1	B	210	VAL
1	B	213	THR
1	B	214	ARG
1	B	225	GLU
1	B	231	GLU
1	B	233	ARG
1	B	234	SER
1	B	235	LEU
1	B	238	LYS
1	B	243	LYS
1	B	244	VAL
1	B	248	LYS
1	B	250	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	56	GLN
1	A	78	ASN
1	A	81	ASN
1	A	88	ASN
1	A	107	GLN
1	A	173	GLN
1	A	197	ASN
1	A	247	ASN
1	B	88	ASN
1	B	102	ASN
1	B	107	GLN
1	B	189	HIS
1	B	197	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

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, 95^{th} 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	255/263 (96%)	-0.09	19 (7%)	17	11	21, 73, 199, 276	0
1	B	255/263 (96%)	-0.22	15 (5%)	26	16	20, 65, 180, 216	0
All	All	510/526 (96%)	-0.15	34 (6%)	21	12	20, 69, 187, 276	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	100	VAL	9.9
1	A	57	ILE	7.8
1	A	96	THR	7.5
1	A	93	SER	5.8
1	B	57	ILE	5.4
1	A	61	ARG	5.0
1	A	92	ASN	4.9
1	A	60	ASP	4.4
1	B	237	MET	4.1
1	A	103	ARG	4.1
1	A	94	GLU	3.9
1	B	61	ARG	3.9
1	A	56	GLN	3.7
1	A	59	ASN	3.6
1	A	101	GLU	3.6
1	B	234	SER	3.3
1	B	103	ARG	3.3
1	A	97	ALA	3.1
1	A	62	MET	3.1
1	B	95	TYR	3.0
1	A	102	ASN	2.9
1	A	58	GLU	2.9
1	B	67	GLU	2.8
1	A	236	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	99	PRO	2.7
1	B	236	GLY	2.7
1	A	68	ASP	2.6
1	A	67	GLU	2.6
1	B	96	THR	2.5
1	B	92	ASN	2.5
1	B	101	GLU	2.3
1	A	108	ALA	2.3
1	B	93	SER	2.2
1	B	58	GLU	2.1

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.