



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 05:17 pm BST

PDB ID : 3I7N
Title : Crystal Structure of DDB1 in Complex with the H-Box Motif of WDTC1
Authors : Li, T.; Robert, E.I.; Breugel, P.C.V.; Strubin, M.; Zheng, N.
Deposited on : 2009-07-08
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

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

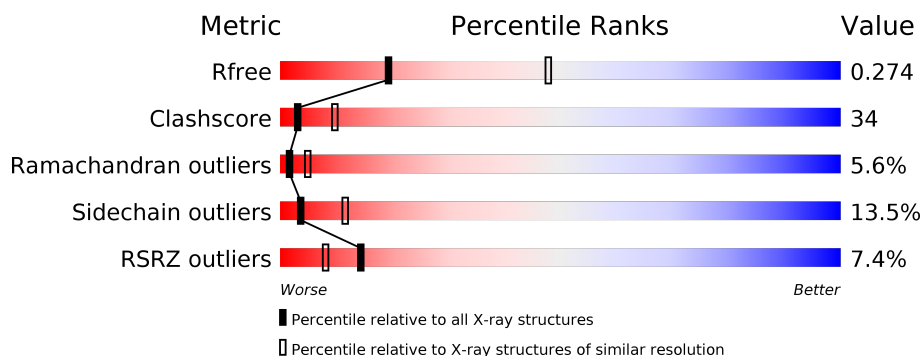
1 Overall quality at a glance

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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1143	<div> <div>7%</div> <div> <div></div> <div>46%</div> <div>41%</div> <div>9%</div> <div>..</div> </div> </div>
2	B	13	<div> <div>8%</div> <div> <div></div> <div>38%</div> <div>31%</div> <div>31%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8842 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 DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1114	Total	C	N	O	S	0	0	0
			8726	5529	1472	1677	48			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP Q16531
A	-1	SER	-	EXPRESSION TAG	UNP Q16531
A	0	HIS	-	EXPRESSION TAG	UNP Q16531
A	422	TYR	ASP	SEE REMARK 999	UNP Q16531
A	898	ASP	GLU	SEE REMARK 999	UNP Q16531
A	899	VAL	LEU	SEE REMARK 999	UNP Q16531

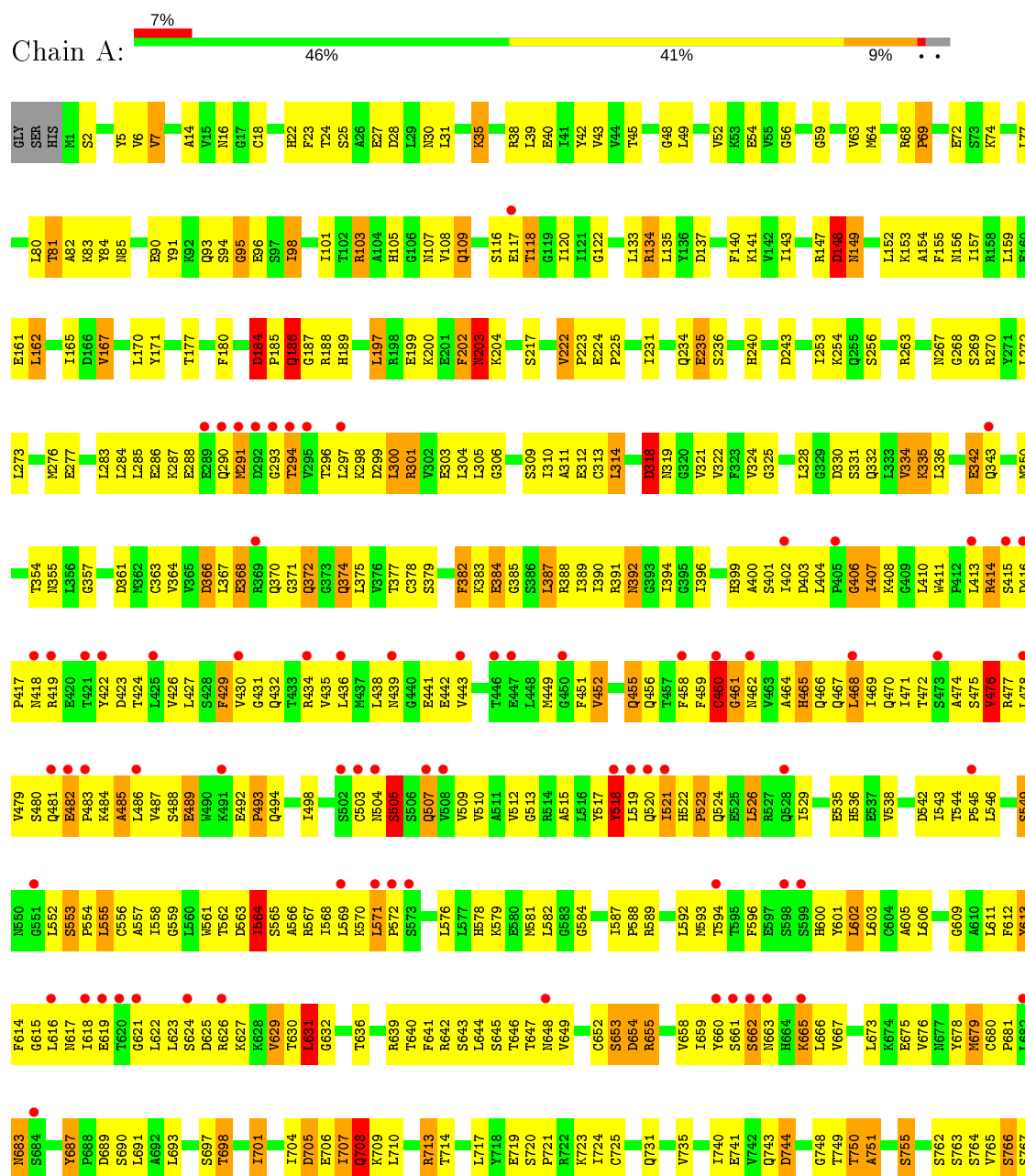
- Molecule 2 is a protein called WD and tetratricopeptide repeats protein 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	13	Total	C	N	O	0	0	0
			116	70	25	21			

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: DNA damage-binding protein 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.61Å 133.88Å 183.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.68 – 2.80 48.68 – 2.80	Depositor EDS
% Data completeness (in resolution range)	91.7 (48.68-2.80) 96.6 (48.68-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.26 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.251 , 0.290 0.249 , 0.274	Depositor DCC
R_{free} test set	1972 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	56.2	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 62.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8842	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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 ⓘ

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	0.78	7/8885 (0.1%)	0.92	24/12034 (0.2%)
2	B	1.34	1/115 (0.9%)	2.09	2/150 (1.3%)
All	All	0.79	8/9000 (0.1%)	0.94	26/12184 (0.2%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	725	CYS	CB-SG	-9.88	1.65	1.82
1	A	913	TYR	CE1-CZ	8.19	1.49	1.38
2	B	13	ARG	CZ-NH2	6.73	1.41	1.33
1	A	1008	CYS	CB-SG	-6.22	1.71	1.82
1	A	384	GLU	CG-CD	6.14	1.61	1.51
1	A	925	ASP	N-CA	6.11	1.58	1.46
1	A	924	GLY	N-CA	5.66	1.54	1.46
1	A	899	VAL	CA-CB	5.15	1.65	1.54

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	13	ARG	NE-CZ-NH1	-18.77	110.91	120.30
1	A	561	TRP	CB-CA-C	-16.97	76.47	110.40
1	A	561	TRP	N-CA-C	16.88	156.59	111.00
1	A	342	GLU	N-CA-C	13.60	147.72	111.00
1	A	330	ASP	CB-CG-OD1	11.74	128.86	118.30
1	A	562	THR	N-CA-CB	-9.04	93.12	110.30
1	A	343	GLN	N-CA-CB	-9.01	94.38	110.60
1	A	564	ILE	N-CA-C	-8.91	86.95	111.00
2	B	13	ARG	NE-CZ-NH2	8.17	124.39	120.30
1	A	367	LEU	N-CA-C	-8.13	89.05	111.00
1	A	184	ASP	C-N-CD	-8.07	102.84	120.60
1	A	342	GLU	CB-CA-C	-7.98	94.45	110.40
1	A	187	GLY	N-CA-C	7.37	131.51	113.10
1	A	714	THR	N-CA-CB	-7.20	96.62	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	330	ASP	CB-CG-OD2	-6.85	112.13	118.30
1	A	343	GLN	N-CA-C	-6.85	92.50	111.00
1	A	388	ARG	NE-CZ-NH1	-6.25	117.18	120.30
1	A	714	THR	N-CA-C	6.20	127.75	111.00
1	A	468	LEU	CA-CB-CG	6.14	129.43	115.30
1	A	388	ARG	NE-CZ-NH2	5.85	123.23	120.30
1	A	387	LEU	N-CA-C	-5.41	96.40	111.00
1	A	924	GLY	N-CA-C	5.32	126.40	113.10
1	A	162	LEU	CA-CB-CG	5.30	127.50	115.30
1	A	367	LEU	N-CA-CB	-5.30	99.80	110.40
1	A	992	LEU	CA-CB-CG	5.23	127.34	115.30
1	A	134	ARG	NE-CZ-NH2	-5.14	117.73	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8726	0	8706	590	0
2	B	116	0	126	9	0
All	All	8842	0	8832	596	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 34.

All (596) 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:A:881:LEU:CD2	1:A:890:LEU:HD13	1.27	1.56
1:A:623:LEU:HD23	1:A:624:SER:N	1.36	1.37
1:A:617:ASN:HB2	1:A:621:GLY:N	1.45	1.31
1:A:621:GLY:C	1:A:622:LEU:HD12	1.55	1.27
1:A:614:PHE:CZ	1:A:626:ARG:HG2	1.70	1.25
1:A:706:GLU:HG2	1:A:708:GLN:OE1	1.34	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:881:LEU:CD2	1:A:890:LEU:CD1	2.21	1.19
1:A:876:PHE:CG	1:A:881:LEU:HD11	1.77	1.18
1:A:68:ARG:NH1	1:A:74:LYS:HA	1.61	1.15
1:A:614:PHE:CE2	1:A:626:ARG:HG2	1.81	1.15
1:A:881:LEU:HD23	1:A:890:LEU:HD13	1.18	1.09
1:A:881:LEU:HD23	1:A:890:LEU:CD1	1.81	1.08
1:A:614:PHE:CE2	1:A:626:ARG:CG	2.37	1.06
1:A:708:GLN:HG3	1:A:710:LEU:O	1.56	1.05
1:A:366:ASP:HB3	1:A:372:GLN:O	1.56	1.05
1:A:68:ARG:HH11	1:A:74:LYS:HA	0.91	1.04
1:A:631:LEU:H	1:A:631:LEU:HD23	1.16	1.02
1:A:660:TYR:CD1	1:A:707:ILE:HG23	1.96	1.00
1:A:870:VAL:HG11	1:A:873:MET:CE	1.93	0.98
1:A:881:LEU:HD21	1:A:890:LEU:CD1	1.87	0.98
1:A:621:GLY:O	1:A:622:LEU:HD12	1.64	0.97
1:A:660:TYR:CE2	1:A:707:ILE:HG12	1.99	0.96
1:A:1024:THR:HB	1:A:1041:THR:HG21	1.46	0.96
1:A:617:ASN:HB2	1:A:621:GLY:H	1.16	0.95
1:A:614:PHE:HE2	1:A:626:ARG:CG	1.75	0.95
1:A:920:PHE:HB3	1:A:935:TYR:HB3	1.46	0.95
1:A:881:LEU:HD21	1:A:890:LEU:HD13	0.96	0.95
1:A:661:SER:HA	1:A:666:LEU:HA	1.48	0.94
1:A:876:PHE:HB2	1:A:881:LEU:CD1	1.97	0.94
1:A:614:PHE:CD2	1:A:625:ASP:O	2.21	0.94
1:A:614:PHE:HE2	1:A:626:ARG:HG3	1.30	0.93
1:A:197:LEU:H	1:A:197:LEU:HD23	1.32	0.93
1:A:167:VAL:HG13	1:A:180:PHE:HB3	1.49	0.92
1:A:882:ALA:O	1:A:883:SER:HB3	1.67	0.92
1:A:706:GLU:O	1:A:707:ILE:HG13	1.69	0.92
1:A:614:PHE:HZ	1:A:626:ARG:HG2	1.34	0.91
1:A:68:ARG:HH11	1:A:74:LYS:CA	1.82	0.91
1:A:617:ASN:HD22	1:A:621:GLY:HA2	1.35	0.91
1:A:617:ASN:HB2	1:A:621:GLY:CA	2.00	0.91
1:A:578:HIS:NE2	1:A:623:LEU:HB2	1.86	0.91
1:A:623:LEU:CD2	1:A:624:SER:N	2.31	0.91
1:A:202:PHE:O	1:A:203:ASN:HB2	1.68	0.90
1:A:103:ARG:HB3	1:A:103:ARG:HH11	1.36	0.90
1:A:235:GLU:HG2	1:A:254:LYS:HZ2	1.34	0.90
1:A:660:TYR:CZ	1:A:707:ILE:HG12	2.07	0.90
1:A:374:GLN:OE1	1:A:391:ARG:HG3	1.71	0.90
1:A:23:PHE:H	1:A:30:ASN:ND2	1.69	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:978:GLN:HE21	1:A:995:VAL:HG21	1.36	0.89
1:A:660:TYR:CZ	1:A:707:ILE:CG1	2.57	0.88
1:A:706:GLU:CG	1:A:708:GLN:OE1	2.22	0.88
1:A:660:TYR:CD2	1:A:707:ILE:HG12	2.10	0.86
1:A:570:LYS:HG2	1:A:571:LEU:H	1.40	0.86
1:A:706:GLU:HG3	1:A:707:ILE:N	1.88	0.86
1:A:235:GLU:HG2	1:A:254:LYS:NZ	1.91	0.85
1:A:876:PHE:CG	1:A:881:LEU:CD1	2.59	0.85
1:A:389:ILE:HD13	1:A:713:ARG:HD3	1.59	0.85
1:A:691:LEU:O	1:A:701:ILE:HA	1.75	0.85
1:A:844:LYS:HD3	1:A:844:LYS:H	1.41	0.84
1:A:917:LYS:HG2	1:A:959:ILE:HG21	1.56	0.84
1:A:870:VAL:HG11	1:A:873:MET:HE3	1.59	0.84
1:A:414:ARG:HA	1:A:422:TYR:HA	1.58	0.84
1:A:617:ASN:CB	1:A:621:GLY:H	1.90	0.84
1:A:309:SER:H	1:A:332:GLN:HE22	1.23	0.84
1:A:309:SER:H	1:A:332:GLN:NE2	1.76	0.84
1:A:1125:THR:HB	1:A:1128:ASP:HB2	1.59	0.83
1:A:184:ASP:OD1	1:A:189:HIS:HE1	1.60	0.83
1:A:938:MET:HG2	1:A:939:GLU:H	1.43	0.83
1:A:482:GLU:HB2	1:A:483:PRO:HD3	1.60	0.83
1:A:452:VAL:HG13	1:A:477:ARG:NH1	1.94	0.83
1:A:843:PRO:HG2	1:A:869:ALA:HB2	1.60	0.83
1:A:107:ASN:OD1	1:A:109:GLN:HG2	1.79	0.83
1:A:133:LEU:HD23	1:A:135:LEU:HD21	1.60	0.82
1:A:623:LEU:HD23	1:A:624:SER:H	1.37	0.82
1:A:396:ILE:HG22	1:A:704:ILE:HD13	1.62	0.82
1:A:631:LEU:N	1:A:631:LEU:HD23	1.95	0.81
1:A:571:LEU:HB3	1:A:572:PRO:HD3	1.62	0.81
1:A:854:SER:HB2	1:A:857:LYS:HG3	1.60	0.81
1:A:413:LEU:HB3	1:A:424:THR:HB	1.61	0.81
1:A:480:SER:HB3	1:A:483:PRO:HD2	1.60	0.81
1:A:23:PHE:H	1:A:30:ASN:HD22	1.28	0.81
1:A:185:PRO:O	1:A:186:GLN:CG	2.29	0.81
1:A:876:PHE:HB2	1:A:881:LEU:HG	1.62	0.81
1:A:708:GLN:CG	1:A:710:LEU:O	2.29	0.80
1:A:1125:THR:HG22	1:A:1126:ALA:H	1.44	0.80
1:A:876:PHE:HB2	1:A:881:LEU:CG	2.11	0.80
1:A:706:GLU:HG3	1:A:707:ILE:H	1.46	0.80
1:A:563:ASP:O	1:A:563:ASP:OD1	2.01	0.79
1:A:724:ILE:HD12	1:A:735:VAL:CG2	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:ILE:HD11	1:A:471:ILE:CG1	2.13	0.78
1:A:570:LYS:NZ	1:A:572:PRO:HD2	1.99	0.78
1:A:614:PHE:CE2	1:A:626:ARG:HG3	2.12	0.77
1:A:623:LEU:HD23	1:A:623:LEU:C	2.04	0.77
1:A:288:GLU:HB3	1:A:296:THR:CG2	2.14	0.77
1:A:288:GLU:HB3	1:A:296:THR:HG23	1.68	0.76
1:A:186:GLN:CG	1:A:186:GLN:O	2.31	0.76
1:A:938:MET:HG2	1:A:939:GLU:N	2.01	0.76
1:A:185:PRO:O	1:A:186:GLN:CB	2.30	0.76
1:A:411:TRP:HB2	1:A:460:CYS:HB3	1.67	0.75
1:A:202:PHE:O	1:A:203:ASN:CB	2.30	0.75
1:A:660:TYR:CZ	1:A:707:ILE:HG13	2.21	0.75
1:A:882:ALA:O	1:A:883:SER:CB	2.30	0.75
1:A:1063:LYS:H	1:A:1063:LYS:HD3	1.51	0.75
1:A:1125:THR:HG22	1:A:1126:ALA:N	2.01	0.75
1:A:853:TYR:HA	1:A:857:LYS:O	1.87	0.75
1:A:623:LEU:HD23	1:A:624:SER:CA	2.15	0.75
1:A:876:PHE:CB	1:A:881:LEU:CD1	2.64	0.74
1:A:117:GLU:OE1	1:A:117:GLU:HA	1.86	0.74
1:A:81:THR:HG23	1:A:83:LYS:H	1.50	0.74
1:A:480:SER:CB	1:A:483:PRO:HD2	2.16	0.74
1:A:197:LEU:H	1:A:197:LEU:CD2	1.99	0.74
1:A:660:TYR:CE2	1:A:707:ILE:CG1	2.69	0.74
1:A:38:ARG:HD2	1:A:54:GLU:OE1	1.88	0.73
1:A:59:GLY:HA2	1:A:1073:TRP:CZ3	2.23	0.73
1:A:407:ILE:HG21	1:A:410:LEU:HD23	1.70	0.73
1:A:621:GLY:C	1:A:622:LEU:CD1	2.48	0.73
1:A:662:SER:HB3	1:A:665:LYS:HB2	1.71	0.72
1:A:969:GLU:O	1:A:971:ALA:N	2.22	0.72
1:A:654:ASP:HA	1:A:675:GLU:HG3	1.71	0.72
1:A:143:ILE:HG12	1:A:154:ALA:HB2	1.72	0.72
1:A:116:SER:OG	1:A:134:ARG:CZ	2.37	0.71
1:A:980:ASP:HB2	1:A:993:GLN:OE1	1.90	0.71
1:A:909:ILE:HG21	1:A:927:MET:HG2	1.70	0.71
1:A:909:ILE:HG22	1:A:925:ASP:OD2	1.90	0.71
1:A:623:LEU:CD2	1:A:624:SER:O	2.39	0.71
1:A:1057:ARG:HD2	1:A:1108:VAL:O	1.91	0.71
1:A:614:PHE:CE2	1:A:625:ASP:O	2.44	0.71
1:A:660:TYR:CE1	1:A:707:ILE:HG12	2.24	0.71
1:A:910:MET:HE1	2:B:6:ILE:HD13	1.71	0.71
1:A:165:ILE:HG12	1:A:188:ARG:HH21	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:GLN:O	1:A:526:LEU:HA	1.90	0.70
1:A:641:PHE:CZ	1:A:648:ASN:HB2	2.26	0.70
1:A:885:ASN:O	1:A:886:SER:CB	2.37	0.70
1:A:184:ASP:OD1	1:A:189:HIS:CE1	2.44	0.70
1:A:876:PHE:CD2	1:A:881:LEU:HD11	2.27	0.70
1:A:24:THR:H	1:A:30:ASN:HD21	1.40	0.69
1:A:659:ILE:HA	1:A:667:VAL:O	1.92	0.69
1:A:16:ASN:ND2	1:A:35:LYS:O	2.25	0.69
1:A:876:PHE:CB	1:A:881:LEU:HD11	2.22	0.69
1:A:536:HIS:CD2	1:A:563:ASP:OD2	2.45	0.69
1:A:884:ILE:O	1:A:886:SER:N	2.25	0.69
1:A:613:TYR:CZ	1:A:627:LYS:HB2	2.28	0.69
2:B:16:LYS:CG	2:B:17:GLU:H	2.05	0.68
1:A:570:LYS:HZ3	1:A:572:PRO:HD2	1.58	0.68
1:A:364:VAL:HG22	1:A:375:LEU:HD12	1.75	0.68
1:A:909:ILE:HD13	1:A:928:ARG:HD3	1.74	0.68
1:A:469:ILE:HD11	1:A:471:ILE:HG12	1.75	0.68
1:A:701:ILE:HD13	1:A:701:ILE:N	2.08	0.68
1:A:743:GLN:HG2	1:A:783:GLY:N	2.09	0.68
1:A:81:THR:HG22	1:A:85:ASN:H	1.60	0.67
1:A:542:ASP:OD2	1:A:593:MET:N	2.25	0.67
1:A:870:VAL:CG1	1:A:873:MET:HE3	2.25	0.67
1:A:844:LYS:HD3	1:A:844:LYS:N	2.10	0.67
1:A:926:LEU:HG	1:A:927:MET:N	2.10	0.67
1:A:719:GLU:OE2	1:A:755:SER:HB2	1.96	0.66
1:A:617:ASN:HD22	1:A:621:GLY:CA	2.08	0.66
1:A:917:LYS:CG	1:A:959:ILE:HG21	2.23	0.66
1:A:921:ILE:C	1:A:922:LEU:HD12	2.16	0.66
1:A:876:PHE:CZ	1:A:920:PHE:HA	2.30	0.66
1:A:631:LEU:H	1:A:631:LEU:CD2	1.99	0.66
1:A:385:GLY:HA3	1:A:719:GLU:O	1.96	0.66
1:A:1024:THR:HB	1:A:1041:THR:CG2	2.23	0.65
1:A:482:GLU:CB	1:A:483:PRO:HD3	2.27	0.65
1:A:449:MET:HB3	1:A:485:ALA:HA	1.78	0.65
1:A:185:PRO:O	1:A:186:GLN:HB3	1.96	0.65
1:A:660:TYR:CG	1:A:707:ILE:HG12	2.31	0.65
1:A:708:GLN:NE2	1:A:710:LEU:O	2.30	0.65
1:A:622:LEU:HD12	1:A:622:LEU:N	2.10	0.65
1:A:660:TYR:CE1	1:A:707:ILE:CG1	2.80	0.65
1:A:830:ILE:HG12	1:A:850:VAL:HG22	1.79	0.65
1:A:1011:SER:OG	1:A:1013:VAL:HG23	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:658:VAL:HG11	1:A:660:TYR:CD1	2.32	0.65
1:A:724:ILE:HD12	1:A:735:VAL:HG22	1.80	0.64
1:A:1014:MET:HG3	1:A:1015:GLN:N	2.10	0.64
1:A:623:LEU:HD21	1:A:624:SER:O	1.96	0.64
1:A:596:PHE:HD1	1:A:601:TYR:CE1	2.16	0.64
1:A:874:VAL:HG22	1:A:875:GLU:N	2.12	0.64
1:A:1065:VAL:C	1:A:1067:LYS:H	1.99	0.64
1:A:882:ALA:O	1:A:914:LEU:HD11	1.98	0.64
1:A:953:TRP:HB2	1:A:970:ASN:HB2	1.78	0.64
1:A:1041:THR:HG22	1:A:1042:SER:N	2.13	0.64
1:A:1011:SER:OG	1:A:1013:VAL:CG2	2.46	0.63
1:A:1125:THR:CG2	1:A:1126:ALA:H	2.10	0.63
1:A:361:ASP:OD1	1:A:723:LYS:HD2	1.98	0.63
1:A:498:ILE:HG23	1:A:510:VAL:HB	1.78	0.63
1:A:660:TYR:CD1	1:A:707:ILE:HG12	2.33	0.63
1:A:1065:VAL:O	1:A:1067:LYS:N	2.32	0.62
1:A:1102:ARG:N	1:A:1103:PRO:HD2	2.13	0.62
1:A:536:HIS:CD2	1:A:563:ASP:CG	2.72	0.62
1:A:6:VAL:HG12	1:A:1040:VAL:HG22	1.81	0.62
1:A:18:CYS:N	1:A:313:CYS:SG	2.72	0.62
1:A:477:ARG:HH21	1:A:486:LEU:HD13	1.63	0.62
1:A:424:THR:HA	1:A:436:LEU:O	2.00	0.62
1:A:641:PHE:HA	1:A:681:PRO:HG3	1.81	0.62
1:A:617:ASN:ND2	1:A:621:GLY:HA2	2.10	0.62
1:A:926:LEU:O	1:A:953:TRP:HA	1.99	0.62
1:A:570:LYS:HG2	1:A:571:LEU:N	2.13	0.62
1:A:426:VAL:HB	1:A:460:CYS:SG	2.39	0.61
1:A:1055:GLN:HG2	1:A:1093:LEU:HD12	1.82	0.61
1:A:22:HIS:CD2	1:A:28:ASP:O	2.53	0.61
1:A:415:SER:HB2	1:A:423:ASP:OD2	1.99	0.61
1:A:322:VAL:HB	1:A:334:VAL:HG12	1.82	0.61
1:A:509:VAL:O	1:A:509:VAL:HG12	2.00	0.61
1:A:985:THR:HB	1:A:989:ARG:HE	1.66	0.61
2:B:16:LYS:HG2	2:B:17:GLU:H	1.64	0.61
1:A:309:SER:N	1:A:332:GLN:HE22	1.97	0.61
1:A:592:LEU:O	1:A:602:LEU:HA	2.01	0.61
1:A:929:SER:HB3	1:A:952:ASN:HB2	1.82	0.61
1:A:641:PHE:O	1:A:647:THR:HB	2.00	0.61
1:A:103:ARG:HB3	1:A:103:ARG:NH1	2.13	0.60
1:A:186:GLN:O	1:A:186:GLN:HG3	2.00	0.60
1:A:578:HIS:CE1	1:A:623:LEU:HB2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:596:PHE:HZ	1:A:649:VAL:HG23	1.66	0.60
1:A:335:LYS:HB2	1:A:350:MET:SD	2.40	0.60
1:A:482:GLU:HB2	1:A:483:PRO:CD	2.29	0.60
1:A:72:GLU:OE1	1:A:103:ARG:NH2	2.35	0.60
1:A:396:ILE:HG12	1:A:673:LEU:HD11	1.83	0.59
1:A:498:ILE:HD13	1:A:510:VAL:HG11	1.83	0.59
1:A:234:GLN:C	1:A:235:GLU:HG3	2.22	0.59
1:A:5:TYR:CE2	1:A:7:VAL:HG22	2.37	0.59
1:A:833:THR:O	1:A:834:ALA:HB2	2.02	0.59
1:A:917:LYS:O	1:A:919:ASP:N	2.35	0.59
1:A:458:PHE:O	1:A:459:PHE:HB2	2.03	0.59
1:A:105:HIS:HA	1:A:152:LEU:HD12	1.85	0.58
1:A:459:PHE:CD2	1:A:460:CYS:N	2.71	0.58
1:A:1127:ASP:O	1:A:1130:ILE:HG22	2.03	0.58
1:A:922:LEU:N	1:A:922:LEU:HD12	2.18	0.58
1:A:492:GLU:O	1:A:494:GLN:N	2.34	0.58
1:A:1041:THR:HG22	1:A:1042:SER:H	1.68	0.58
1:A:1093:LEU:O	1:A:1096:SER:HB3	2.04	0.58
1:A:701:ILE:HD13	1:A:701:ILE:H	1.66	0.58
1:A:375:LEU:HB2	1:A:1012:LEU:HD21	1.85	0.58
1:A:427:LEU:O	1:A:427:LEU:HD12	2.04	0.58
1:A:475:SER:HA	1:A:498:ILE:HD12	1.85	0.58
1:A:679:MET:C	1:A:679:MET:SD	2.82	0.58
1:A:396:ILE:HG22	1:A:704:ILE:CD1	2.33	0.58
1:A:741:GLU:HG2	1:A:751:ALA:HA	1.86	0.58
1:A:617:ASN:HB2	1:A:621:GLY:HA2	1.84	0.58
1:A:864:LYS:NZ	1:A:899:VAL:O	2.29	0.58
1:A:469:ILE:HD11	1:A:471:ILE:HG13	1.84	0.58
1:A:1139:ILE:HG22	1:A:1139:ILE:O	2.04	0.58
1:A:81:THR:HB	1:A:85:ASN:HB2	1.85	0.58
1:A:413:LEU:C	1:A:422:TYR:HB3	2.25	0.57
1:A:876:PHE:CD1	1:A:881:LEU:HD11	2.34	0.57
1:A:1125:THR:CB	1:A:1128:ASP:HB2	2.32	0.57
1:A:642:ARG:HH22	1:A:683:ASN:CG	2.08	0.57
1:A:571:LEU:CB	1:A:572:PRO:HD3	2.32	0.57
1:A:917:LYS:HG2	1:A:959:ILE:CG2	2.32	0.57
1:A:593:MET:HA	1:A:601:TYR:O	2.05	0.57
1:A:602:LEU:HD23	1:A:614:PHE:HB2	1.86	0.57
1:A:68:ARG:HD3	1:A:74:LYS:C	2.25	0.57
1:A:507:GLN:HE22	1:A:553:SER:N	2.01	0.57
1:A:630:THR:O	1:A:631:LEU:O	2.23	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1014:MET:O	1:A:1015:GLN:C	2.42	0.57
1:A:882:ALA:O	1:A:914:LEU:CD1	2.53	0.56
1:A:631:LEU:N	1:A:631:LEU:CD2	2.65	0.56
1:A:391:ARG:NH2	1:A:705:ASP:OD2	2.39	0.56
1:A:919:ASP:CG	1:A:920:PHE:H	2.09	0.56
1:A:559:GLY:HA2	1:A:565:SER:O	2.06	0.56
1:A:1011:SER:HG	1:A:1013:VAL:CG2	2.19	0.56
1:A:623:LEU:CD2	1:A:623:LEU:C	2.71	0.56
1:A:938:MET:CG	1:A:939:GLU:H	2.13	0.56
1:A:844:LYS:H	1:A:844:LYS:CD	2.17	0.56
1:A:293:GLY:O	1:A:294:THR:C	2.44	0.55
1:A:910:MET:CE	2:B:6:ILE:HD13	2.36	0.55
1:A:263:ARG:HH11	1:A:263:ARG:HG2	1.72	0.55
1:A:452:VAL:HG13	1:A:477:ARG:HH11	1.70	0.55
1:A:660:TYR:CD1	1:A:707:ILE:CG2	2.83	0.55
1:A:879:LYS:HB2	1:A:890:LEU:HD11	1.87	0.55
1:A:451:PHE:CD1	1:A:479:VAL:HG21	2.41	0.55
1:A:234:GLN:O	1:A:235:GLU:HG3	2.06	0.55
1:A:378:CYS:SG	1:A:724:ILE:HB	2.47	0.55
1:A:687:TYR:O	1:A:690:SER:HB3	2.07	0.55
1:A:708:GLN:HG3	1:A:710:LEU:C	2.25	0.55
1:A:2:SER:CB	1:A:995:VAL:HG23	2.37	0.55
1:A:932:LEU:HD22	1:A:965:PHE:HE1	1.71	0.55
2:B:6:ILE:HA	2:B:9:ASP:OD2	2.07	0.55
1:A:133:LEU:HB3	1:A:135:LEU:HD22	1.88	0.55
1:A:658:VAL:HG11	1:A:660:TYR:CE1	2.42	0.55
1:A:936:LYS:O	1:A:938:MET:N	2.36	0.55
1:A:324:VAL:HB	1:A:332:GLN:HG2	1.89	0.54
1:A:81:THR:HG21	1:A:85:ASN:OD1	2.07	0.54
1:A:22:HIS:HD2	1:A:28:ASP:O	1.89	0.54
1:A:301:ARG:NH1	1:A:303:GLU:OE2	2.41	0.54
1:A:1044:SER:OG	1:A:1047:TRP:HB2	2.08	0.54
1:A:639:ARG:HG3	1:A:640:THR:N	2.22	0.54
1:A:549:SER:HB2	1:A:552:LEU:O	2.07	0.54
1:A:690:SER:OG	1:A:701:ILE:HB	2.08	0.54
1:A:165:ILE:HG12	1:A:188:ARG:NH2	2.21	0.54
1:A:594:THR:OG1	1:A:601:TYR:HB2	2.09	0.53
1:A:704:ILE:HG22	1:A:705:ASP:N	2.22	0.53
1:A:713:ARG:CG	1:A:713:ARG:HH11	2.22	0.53
1:A:881:LEU:HD23	1:A:890:LEU:HD12	1.82	0.53
1:A:520:GLN:NE2	1:A:529:ILE:HD11	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:767:SER:O	1:A:768:SER:O	2.27	0.53
1:A:366:ASP:N	1:A:366:ASP:OD1	2.30	0.53
1:A:492:GLU:C	1:A:494:GLN:H	2.11	0.53
1:A:579:LYS:NZ	1:A:581:MET:SD	2.81	0.53
1:A:765:VAL:HG22	1:A:766:SER:H	1.74	0.53
1:A:184:ASP:OD2	1:A:189:HIS:CE1	2.62	0.53
1:A:518:TYR:C	1:A:518:TYR:CD2	2.83	0.53
1:A:876:PHE:HB2	1:A:881:LEU:HD12	1.84	0.53
1:A:93:GLN:O	1:A:95:GLY:N	2.42	0.53
1:A:1063:LYS:H	1:A:1063:LYS:CD	2.21	0.53
1:A:185:PRO:O	1:A:186:GLN:HG2	2.05	0.53
1:A:469:ILE:HG12	1:A:470:GLN:N	2.24	0.52
1:A:498:ILE:CG2	1:A:510:VAL:HB	2.39	0.52
1:A:614:PHE:HB3	1:A:624:SER:HG	1.74	0.52
1:A:596:PHE:CE2	1:A:648:ASN:HA	2.45	0.52
1:A:383:LYS:NZ	1:A:384:GLU:OE2	2.34	0.52
1:A:518:TYR:C	1:A:518:TYR:HD2	2.12	0.52
1:A:701:ILE:N	1:A:701:ILE:CD1	2.73	0.52
1:A:596:PHE:HE2	1:A:648:ASN:HA	1.74	0.52
1:A:922:LEU:CD1	1:A:922:LEU:N	2.73	0.52
1:A:120:ILE:HG12	1:A:135:LEU:HD12	1.92	0.52
1:A:966:LEU:HD11	1:A:1040:VAL:HG21	1.91	0.52
1:A:570:LYS:HZ1	1:A:572:PRO:HD2	1.72	0.51
1:A:1054:MET:SD	1:A:1129:LEU:HD12	2.51	0.51
1:A:2:SER:HB2	1:A:995:VAL:HG23	1.93	0.51
1:A:731:GLN:HA	1:A:796:GLN:NE2	2.24	0.51
1:A:844:LYS:HE2	1:A:845:GLN:HG3	1.92	0.51
1:A:881:LEU:HD23	1:A:890:LEU:HA	1.92	0.51
1:A:199:GLU:O	1:A:200:LYS:HB2	2.09	0.51
1:A:765:VAL:HG22	1:A:766:SER:N	2.25	0.51
1:A:313:CYS:HB3	1:A:325:GLY:HA3	1.92	0.51
1:A:884:ILE:C	1:A:886:SER:H	2.13	0.51
1:A:185:PRO:O	1:A:186:GLN:CD	2.48	0.51
1:A:622:LEU:CD1	1:A:622:LEU:N	2.72	0.51
1:A:961:ASP:C	1:A:961:ASP:OD2	2.49	0.51
1:A:518:TYR:HD2	1:A:519:LEU:N	2.09	0.51
1:A:660:TYR:HB2	1:A:667:VAL:HB	1.92	0.51
1:A:141:LYS:HE2	1:A:156:ASN:ND2	2.25	0.51
1:A:538:VAL:HG13	1:A:558:ILE:HD11	1.93	0.51
1:A:617:ASN:CB	1:A:621:GLY:HA2	2.41	0.51
1:A:750:THR:O	1:A:751:ALA:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:LEU:HD12	1:A:177:THR:HG22	1.92	0.51
1:A:460:CYS:O	1:A:461:GLY:O	2.29	0.51
1:A:185:PRO:O	1:A:186:GLN:OE1	2.29	0.50
1:A:293:GLY:O	1:A:294:THR:O	2.29	0.50
1:A:932:LEU:HD22	1:A:965:PHE:CE1	2.46	0.50
1:A:197:LEU:N	1:A:197:LEU:HD23	2.13	0.50
1:A:438:LEU:HD23	1:A:443:VAL:HA	1.92	0.50
1:A:482:GLU:CB	1:A:483:PRO:CD	2.89	0.50
1:A:328:LEU:HD21	2:B:15:ILE:HG23	1.92	0.50
1:A:411:TRP:CZ2	1:A:459:PHE:HA	2.47	0.50
1:A:707:ILE:O	1:A:708:GLN:O	2.29	0.50
1:A:81:THR:CG2	1:A:83:LYS:H	2.22	0.50
1:A:276:MET:O	1:A:310:ILE:HD12	2.12	0.50
1:A:378:CYS:HB3	1:A:721:PRO:HB2	1.94	0.50
1:A:466:GLN:HB3	1:A:481:GLN:HB2	1.93	0.50
1:A:617:ASN:CB	1:A:621:GLY:CA	2.84	0.50
1:A:1090:ASP:HB2	1:A:1092:ASP:HB2	1.94	0.50
1:A:821:LEU:O	1:A:824:ASP:HB3	2.12	0.50
1:A:1033:VAL:CG1	1:A:1033:VAL:O	2.60	0.50
1:A:1105:MET:SD	1:A:1130:ILE:HD12	2.51	0.50
1:A:885:ASN:O	1:A:886:SER:HB2	2.11	0.50
1:A:876:PHE:HZ	1:A:920:PHE:HA	1.75	0.50
1:A:225:PRO:HG2	1:A:267:ASN:HA	1.94	0.50
1:A:438:LEU:HD23	1:A:442:GLU:O	2.12	0.50
1:A:731:GLN:C	1:A:796:GLN:HE21	2.14	0.50
1:A:484:LYS:O	1:A:484:LYS:HG3	2.12	0.49
1:A:304:LEU:HD12	1:A:306:GLY:H	1.77	0.49
1:A:616:LEU:HG	1:A:617:ASN:H	1.77	0.49
1:A:874:VAL:CG2	1:A:875:GLU:N	2.75	0.49
1:A:276:MET:SD	1:A:276:MET:O	2.70	0.49
1:A:615:GLY:H	1:A:624:SER:CB	2.25	0.49
1:A:564:ILE:HD13	1:A:584:GLY:O	2.12	0.49
1:A:913:TYR:O	1:A:914:LEU:HD23	2.12	0.49
1:A:290:GLN:O	1:A:291:MET:O	2.30	0.49
1:A:653:SER:HB3	1:A:655:ARG:H	1.78	0.49
1:A:231:ILE:HD13	1:A:240:HIS:CD2	2.48	0.49
1:A:488:SER:O	1:A:489:GLU:HB2	2.13	0.49
1:A:521:ILE:HD13	1:A:526:LEU:CD2	2.42	0.49
1:A:81:THR:HG23	1:A:82:ALA:N	2.28	0.49
1:A:969:GLU:OE2	1:A:971:ALA:HB3	2.13	0.49
1:A:133:LEU:HD23	1:A:135:LEU:CD2	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:GLN:HG3	1:A:290:GLN:O	2.12	0.49
1:A:1000:LEU:HD13	1:A:1002:GLU:HB2	1.95	0.48
1:A:63:VAL:HG11	1:A:122:GLY:HA3	1.93	0.48
1:A:639:ARG:HG3	1:A:640:THR:H	1.78	0.48
1:A:1033:VAL:HG12	1:A:1033:VAL:O	2.13	0.48
1:A:155:PHE:HE1	1:A:157:ILE:HD11	1.78	0.48
1:A:296:THR:OG1	1:A:297:LEU:N	2.43	0.48
1:A:432:GLN:O	1:A:456:GLN:HA	2.14	0.48
1:A:614:PHE:HB3	1:A:624:SER:OG	2.13	0.48
1:A:676:VAL:HG11	1:A:693:LEU:HD23	1.96	0.48
1:A:939:GLU:HG3	1:A:941:ASN:HB2	1.95	0.48
1:A:1065:VAL:C	1:A:1067:LYS:N	2.66	0.48
1:A:379:SER:O	1:A:385:GLY:HA2	2.12	0.48
1:A:522:HIS:O	1:A:524:GLN:N	2.46	0.48
1:A:69:PRO:HD2	1:A:72:GLU:HG3	1.95	0.48
1:A:117:GLU:OE1	1:A:117:GLU:CA	2.60	0.48
1:A:400:ALA:H	1:A:701:ILE:HD11	1.79	0.48
1:A:469:ILE:CG1	1:A:470:GLN:N	2.75	0.48
1:A:535:GLU:HB3	1:A:536:HIS:CD2	2.48	0.48
1:A:708:GLN:CD	1:A:710:LEU:O	2.51	0.48
1:A:843:PRO:CG	1:A:869:ALA:HB2	2.38	0.48
1:A:120:ILE:HG12	1:A:135:LEU:CD1	2.44	0.48
1:A:140:PHE:HB2	1:A:159:LEU:HD12	1.96	0.48
1:A:43:VAL:HG23	1:A:52:VAL:HG21	1.96	0.48
1:A:184:ASP:CG	1:A:189:HIS:CE1	2.87	0.48
1:A:290:GLN:O	1:A:291:MET:C	2.51	0.48
1:A:478:LEU:HB3	1:A:488:SER:H	1.78	0.48
1:A:997:LEU:HB3	1:A:1076:PHE:CD1	2.49	0.48
1:A:64:MET:HG3	1:A:77:LEU:HD11	1.95	0.47
1:A:1091:GLY:HA2	1:A:1094:ILE:HB	1.96	0.47
1:A:149:ASN:OD1	1:A:153:LYS:N	2.44	0.47
1:A:615:GLY:N	1:A:624:SER:OG	2.42	0.47
1:A:318:ASP:HB3	1:A:319:ASN:H	1.57	0.47
1:A:893:TRP:CE3	1:A:899:VAL:HG13	2.49	0.47
1:A:159:LEU:HD22	1:A:161:GLU:O	2.15	0.47
1:A:451:PHE:CE1	1:A:479:VAL:HG21	2.49	0.47
1:A:558:ILE:O	1:A:566:ALA:HA	2.15	0.47
1:A:697:SER:O	1:A:698:THR:CB	2.62	0.47
1:A:741:GLU:HB3	1:A:749:THR:HB	1.97	0.47
1:A:80:LEU:HD12	1:A:85:ASN:O	2.15	0.47
1:A:116:SER:OG	1:A:134:ARG:NE	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:630:THR:O	1:A:631:LEU:C	2.52	0.47
1:A:414:ARG:HG2	1:A:414:ARG:HH11	1.80	0.47
1:A:985:THR:OG1	1:A:985:THR:O	2.32	0.47
1:A:471:ILE:HG12	1:A:476:VAL:HB	1.95	0.47
1:A:744:ASP:N	1:A:748:GLY:O	2.37	0.47
1:A:1013:VAL:O	1:A:1014:MET:O	2.33	0.47
1:A:141:LYS:HE2	1:A:156:ASN:HD21	1.79	0.47
1:A:286:GLU:N	1:A:299:ASP:O	2.48	0.47
1:A:462:ASN:O	1:A:505:SER:OG	2.24	0.47
1:A:658:VAL:CG1	1:A:659:ILE:N	2.76	0.47
1:A:920:PHE:O	1:A:934:ALA:HA	2.14	0.47
1:A:186:GLN:O	1:A:186:GLN:HG2	2.13	0.46
1:A:588:PRO:HA	1:A:606:LEU:HD23	1.96	0.46
1:A:750:THR:O	1:A:751:ALA:CB	2.64	0.46
1:A:159:LEU:HD23	1:A:161:GLU:H	1.80	0.46
1:A:546:LEU:HD22	1:A:600:HIS:ND1	2.30	0.46
1:A:63:VAL:CG2	1:A:80:LEU:HB3	2.46	0.46
1:A:923:VAL:HG12	1:A:959:ILE:HD11	1.97	0.46
1:A:39:LEU:CD1	1:A:64:MET:SD	3.04	0.46
1:A:706:GLU:CG	1:A:707:ILE:H	2.14	0.46
1:A:90:GLU:HB3	1:A:101:ILE:HG22	1.98	0.46
1:A:426:VAL:HG22	1:A:435:VAL:HG13	1.97	0.46
1:A:555:LEU:H	1:A:555:LEU:HD23	1.81	0.46
1:A:984:THR:O	1:A:986:ASP:N	2.47	0.46
1:A:368:GLU:HB2	1:A:370:GLN:HG3	1.98	0.46
1:A:408:LYS:HA	1:A:678:TYR:CE1	2.50	0.46
1:A:59:GLY:HA2	1:A:1073:TRP:CE3	2.51	0.46
1:A:355:ASN:ND2	1:A:357:GLY:HA2	2.31	0.46
1:A:617:ASN:CB	1:A:621:GLY:N	2.39	0.46
1:A:80:LEU:HD21	1:A:135:LEU:HD11	1.97	0.46
1:A:404:LEU:HB2	1:A:407:ILE:HD11	1.96	0.46
1:A:644:LEU:HG	1:A:645:SER:N	2.30	0.46
1:A:876:PHE:CD1	1:A:881:LEU:CD1	2.96	0.46
1:A:923:VAL:HA	1:A:931:LEU:O	2.16	0.46
1:A:399:HIS:HB2	1:A:701:ILE:HG12	1.97	0.46
1:A:960:LEU:HD21	1:A:966:LEU:HB2	1.97	0.46
1:A:267:ASN:ND2	1:A:269:SER:HB3	2.30	0.45
1:A:1030:PHE:CZ	1:A:1038:GLY:HA3	2.51	0.45
1:A:719:GLU:OE2	1:A:755:SER:CB	2.64	0.45
1:A:268:GLY:O	1:A:285:LEU:HD12	2.17	0.45
1:A:406:GLY:O	1:A:407:ILE:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:ASP:HA	1:A:417:PRO:HD3	1.78	0.45
1:A:895:THR:C	1:A:897:LYS:H	2.19	0.45
1:A:1011:SER:HG	1:A:1013:VAL:HG22	1.80	0.45
1:A:605:ALA:HB1	1:A:636:THR:HB	1.97	0.45
1:A:706:GLU:CG	1:A:707:ILE:N	2.61	0.45
1:A:766:SER:HB3	1:A:808:LEU:CD2	2.47	0.45
1:A:107:ASN:OD1	1:A:109:GLN:CG	2.59	0.45
1:A:116:SER:HB2	1:A:137:ASP:OD1	2.15	0.45
1:A:165:ILE:HG21	1:A:217:SER:HA	1.98	0.45
1:A:600:HIS:CD2	1:A:618:ILE:HG12	2.52	0.45
1:A:382:PHE:H	1:A:720:SER:HB3	1.80	0.45
1:A:24:THR:HA	1:A:91:TYR:HD2	1.82	0.45
1:A:400:ALA:N	1:A:701:ILE:HD11	2.32	0.45
1:A:469:ILE:CD1	1:A:471:ILE:HG13	2.47	0.45
1:A:1039:LEU:HD21	1:A:1139:ILE:HG22	1.99	0.45
1:A:24:THR:H	1:A:30:ASN:ND2	2.13	0.45
1:A:438:LEU:CD2	1:A:442:GLU:O	2.65	0.45
1:A:1097:PHE:HA	1:A:1100:ILE:HD12	1.99	0.44
1:A:744:ASP:HB2	1:A:748:GLY:O	2.17	0.44
1:A:923:VAL:CG1	1:A:959:ILE:HD11	2.47	0.44
1:A:1041:THR:CG2	1:A:1042:SER:N	2.79	0.44
1:A:844:LYS:HG2	1:A:845:GLN:HG3	1.99	0.44
1:A:98:ILE:N	1:A:98:ILE:HD13	2.32	0.44
1:A:105:HIS:CA	1:A:152:LEU:HD12	2.47	0.44
1:A:609:GLY:HA3	1:A:632:GLY:O	2.17	0.44
1:A:81:THR:CG2	1:A:85:ASN:H	2.29	0.44
1:A:402:ILE:O	1:A:698:THR:HA	2.16	0.44
1:A:808:LEU:HG	1:A:811:GLU:OE1	2.17	0.44
1:A:889:ARG:HG2	1:A:904:ASN:HB3	1.99	0.44
1:A:556:CYS:SG	1:A:557:ALA:N	2.90	0.44
1:A:504:ASN:ND2	1:A:507:GLN:HB2	2.32	0.44
1:A:578:HIS:CG	1:A:579:LYS:N	2.86	0.44
1:A:709:LYS:NZ	1:A:1140:HIS:O	2.32	0.44
1:A:429:PHE:O	1:A:431:GLY:N	2.51	0.44
1:A:40:GLU:HB3	1:A:42:TYR:CE1	2.52	0.44
1:A:713:ARG:HG2	1:A:713:ARG:HH11	1.83	0.44
1:A:305:LEU:HD13	1:A:336:LEU:HD22	1.99	0.43
1:A:45:THR:N	1:A:48:GLY:O	2.46	0.43
1:A:665:LYS:HB3	1:A:666:LEU:H	1.61	0.43
1:A:84:TYR:HB2	1:A:109:GLN:HB3	2.00	0.43
1:A:884:ILE:C	1:A:886:SER:N	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:920:PHE:HB3	1:A:935:TYR:CB	2.31	0.43
1:A:1109:VAL:HG21	1:A:1125:THR:O	2.18	0.43
1:A:611:LEU:HD23	1:A:612:PHE:C	2.39	0.43
1:A:856:GLY:H	1:A:857:LYS:HG2	1.83	0.43
1:A:958:GLU:HG3	1:A:959:ILE:N	2.33	0.43
1:A:199:GLU:OE1	1:A:199:GLU:HA	2.18	0.43
1:A:391:ARG:HD2	1:A:392:ASN:O	2.18	0.43
1:A:396:ILE:HD11	1:A:673:LEU:HD21	1.99	0.43
1:A:762:SER:O	1:A:763:SER:HB3	2.17	0.43
1:A:936:LYS:C	1:A:938:MET:N	2.71	0.43
1:A:272:LEU:O	1:A:273:LEU:HD23	2.18	0.43
1:A:546:LEU:HD11	1:A:593:MET:SD	2.57	0.43
1:A:868:GLY:HA3	1:A:884:ILE:HG22	2.00	0.43
2:B:16:LYS:CG	2:B:17:GLU:N	2.78	0.43
1:A:148:ASP:HB2	1:A:149:ASN:H	1.43	0.43
1:A:480:SER:OG	1:A:487:VAL:HG21	2.18	0.43
1:A:619:GLU:OE1	1:A:619:GLU:HA	2.18	0.43
1:A:713:ARG:NH1	1:A:713:ARG:CG	2.79	0.43
1:A:1065:VAL:HG12	1:A:1066:GLY:N	2.34	0.43
1:A:108:VAL:HG11	1:A:143:ILE:HD11	2.01	0.43
1:A:223:PRO:HG3	1:A:263:ARG:HE	1.84	0.43
1:A:284:LEU:O	1:A:300:LEU:HA	2.19	0.43
1:A:706:GLU:O	1:A:707:ILE:CG1	2.55	0.43
1:A:764:SER:OG	1:A:803:HIS:NE2	2.44	0.43
1:A:1051:LEU:HB2	1:A:1089:ILE:HD13	2.01	0.43
1:A:455:GLN:HE21	1:A:455:GLN:HA	1.83	0.43
1:A:569:LEU:HG	1:A:576:LEU:HA	2.01	0.43
1:A:596:PHE:CD1	1:A:601:TYR:CE1	3.02	0.43
1:A:636:THR:HA	1:A:652:CYS:O	2.19	0.43
1:A:697:SER:O	1:A:698:THR:OG1	2.31	0.43
1:A:118:THR:O	1:A:118:THR:HG22	2.19	0.42
1:A:222:VAL:HG12	1:A:223:PRO:HD2	2.00	0.42
1:A:288:GLU:HB3	1:A:296:THR:HG22	1.96	0.42
1:A:464:ALA:O	1:A:465:HIS:HB2	2.19	0.42
1:A:807:PHE:CZ	1:A:831:VAL:HG11	2.53	0.42
1:A:1000:LEU:HD11	1:A:1030:PHE:CE1	2.54	0.42
1:A:2:SER:HB2	1:A:995:VAL:CG2	2.50	0.42
1:A:512:VAL:HB	1:A:515:ALA:HB3	2.01	0.42
1:A:1051:LEU:CB	1:A:1089:ILE:HD13	2.49	0.42
1:A:455:GLN:HE21	1:A:455:GLN:CA	2.32	0.42
1:A:687:TYR:O	1:A:690:SER:CB	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:ASN:HD21	1:A:709:LYS:HE3	1.84	0.42
1:A:928:ARG:CZ	1:A:947:ARG:NH2	2.83	0.42
1:A:1041:THR:CG2	1:A:1042:SER:H	2.31	0.42
1:A:368:GLU:HG2	1:A:368:GLU:H	1.61	0.42
1:A:705:ASP:HB3	1:A:706:GLU:H	1.62	0.42
1:A:368:GLU:HG3	1:A:370:GLN:HE21	1.83	0.42
1:A:414:ARG:HG2	1:A:414:ARG:NH1	2.35	0.42
2:B:15:ILE:CG2	2:B:15:ILE:O	2.68	0.42
1:A:38:ARG:NH1	1:A:56:GLY:N	2.68	0.42
1:A:623:LEU:HD23	1:A:624:SER:O	2.19	0.42
1:A:1102:ARG:HA	1:A:1105:MET:HB3	2.02	0.42
1:A:117:GLU:O	1:A:118:THR:CB	2.67	0.42
1:A:909:ILE:HG22	1:A:925:ASP:CG	2.40	0.42
1:A:14:ALA:O	1:A:35:LYS:HD2	2.20	0.42
1:A:410:LEU:HD12	1:A:680:CYS:SG	2.60	0.42
1:A:883:SER:HB3	1:A:914:LEU:HD11	2.00	0.42
1:A:235:GLU:HA	1:A:253:ILE:HG13	2.02	0.41
1:A:854:SER:HB2	1:A:857:LYS:CG	2.40	0.41
1:A:929:SER:HA	1:A:954:MET:SD	2.59	0.41
1:A:948:ASP:OD1	1:A:948:ASP:C	2.57	0.41
1:A:270:ARG:HG2	1:A:284:LEU:HD23	2.02	0.41
1:A:364:VAL:HG22	1:A:375:LEU:CD1	2.48	0.41
1:A:623:LEU:HD23	1:A:624:SER:C	2.40	0.41
1:A:399:HIS:HB3	1:A:687:TYR:HE1	1.85	0.41
1:A:925:ASP:OD2	1:A:926:LEU:N	2.53	0.41
1:A:222:VAL:HG23	1:A:222:VAL:H	1.62	0.41
1:A:839:GLU:HG2	1:A:840:GLU:N	2.35	0.41
1:A:925:ASP:O	1:A:954:MET:HG2	2.20	0.41
1:A:35:LYS:HB2	1:A:38:ARG:HB2	2.01	0.41
1:A:643:SER:OG	1:A:647:THR:HA	2.20	0.41
1:A:644:LEU:HG	1:A:645:SER:H	1.86	0.41
1:A:646:THR:O	1:A:648:ASN:ND2	2.54	0.41
1:A:812:TYR:N	1:A:812:TYR:CD2	2.88	0.41
1:A:256:SER:CB	1:A:277:GLU:HG2	2.51	0.41
1:A:478:LEU:CD2	1:A:488:SER:HB3	2.50	0.41
1:A:660:TYR:CE1	1:A:707:ILE:HA	2.55	0.41
1:A:798:THR:OG1	1:A:800:GLU:HG3	2.21	0.41
1:A:861:VAL:O	1:A:861:VAL:HG12	2.20	0.41
1:A:522:HIS:O	1:A:523:PRO:C	2.59	0.41
1:A:660:TYR:HB3	1:A:661:SER:H	1.58	0.41
1:A:1125:THR:CG2	1:A:1126:ALA:N	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:TYR:CD1	1:A:223:PRO:HA	2.56	0.40
1:A:267:ASN:HD21	1:A:269:SER:HB3	1.86	0.40
1:A:377:THR:O	1:A:387:LEU:HA	2.21	0.40
1:A:387:LEU:HG	1:A:717:LEU:HD11	2.02	0.40
1:A:487:VAL:HG12	1:A:524:GLN:O	2.21	0.40
1:A:766:SER:HB3	1:A:808:LEU:HD21	2.03	0.40
1:A:197:LEU:N	1:A:197:LEU:CD2	2.74	0.40
1:A:394:ILE:HD11	1:A:707:ILE:O	2.21	0.40
1:A:492:GLU:HA	1:A:493:PRO:HD3	1.91	0.40
1:A:523:PRO:O	1:A:524:GLN:HB2	2.21	0.40
1:A:311:ALA:HB1	1:A:314:LEU:HD13	2.03	0.40
1:A:368:GLU:HG3	1:A:370:GLN:NE2	2.37	0.40
1:A:40:GLU:HB3	1:A:42:TYR:HE1	1.85	0.40
1:A:568:ILE:C	1:A:569:LEU:HD12	2.41	0.40
2:B:10:LEU:O	2:B:14:GLN:HG3	2.22	0.40
1:A:925:ASP:O	1:A:954:MET:CG	2.69	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	1106/1143 (97%)	896 (81%)	149 (14%)	61 (6%)	2	5
2	B	11/13 (85%)	10 (91%)	0	1 (9%)	1	1
All	All	1117/1156 (97%)	906 (81%)	149 (13%)	62 (6%)	2	5

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	203	ASN
1	A	291	MET

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Mol	Chain	Res	Type
1	A	294	THR
1	A	318	ASP
1	A	474	ALA
1	A	554	PRO
1	A	571	LEU
1	A	631	LEU
1	A	689	ASP
1	A	698	THR
1	A	751	ALA
1	A	768	SER
1	A	883	SER
1	A	886	SER
1	A	918	GLY
1	A	919	ASP
1	A	970	ASN
1	A	985	THR
1	A	1014	MET
1	A	1065	VAL
2	B	16	LYS
1	A	69	PRO
1	A	95	GLY
1	A	184	ASP
1	A	186	GLN
1	A	407	ILE
1	A	430	VAL
1	A	460	CYS
1	A	461	GLY
1	A	476	VAL
1	A	489	GLU
1	A	503	CYS
1	A	683	ASN
1	A	707	ILE
1	A	708	GLN
1	A	885	ASN
1	A	35	LYS
1	A	94	SER
1	A	148	ASP
1	A	287	LYS
1	A	485	ALA
1	A	493	PRO
1	A	505	SER
1	A	523	PRO

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Mol	Chain	Res	Type
1	A	665	LYS
1	A	705	ASP
1	A	371	GLY
1	A	517	TYR
1	A	518	TYR
1	A	876	PHE
1	A	118	THR
1	A	149	ASN
1	A	382	PHE
1	A	406	GLY
1	A	662	SER
1	A	1013	VAL
1	A	482	GLU
1	A	513	GLY
1	A	629	VAL
1	A	1130	ILE
1	A	545	PRO
1	A	687	TYR

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	977/1001 (98%)	846 (87%)	131 (13%)	4	12
2	B	13/13 (100%)	10 (77%)	3 (23%)	1	2
All	All	990/1014 (98%)	856 (86%)	134 (14%)	4	11

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	25	SER
1	A	27	GLU
1	A	31	LEU
1	A	49	LEU

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Mol	Chain	Res	Type
1	A	81	THR
1	A	96	GLU
1	A	98	ILE
1	A	103	ARG
1	A	109	GLN
1	A	147	ARG
1	A	148	ASP
1	A	162	LEU
1	A	167	VAL
1	A	184	ASP
1	A	186	GLN
1	A	197	LEU
1	A	202	PHE
1	A	203	ASN
1	A	204	LYS
1	A	222	VAL
1	A	224	GLU
1	A	235	GLU
1	A	236	SER
1	A	243	ASP
1	A	283	LEU
1	A	298	LYS
1	A	300	LEU
1	A	301	ARG
1	A	312	GLU
1	A	314	LEU
1	A	318	ASP
1	A	321	VAL
1	A	331	SER
1	A	334	VAL
1	A	335	LYS
1	A	342	GLU
1	A	354	THR
1	A	363	CYS
1	A	366	ASP
1	A	368	GLU
1	A	372	GLN
1	A	374	GLN
1	A	390	ILE
1	A	392	ASN
1	A	401	SER
1	A	403	ASP

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Mol	Chain	Res	Type
1	A	414	ARG
1	A	418	ASN
1	A	419	ARG
1	A	429	PHE
1	A	434	ARG
1	A	439	ASN
1	A	441	GLU
1	A	452	VAL
1	A	455	GLN
1	A	460	CYS
1	A	465	HIS
1	A	467	GLN
1	A	468	LEU
1	A	472	THR
1	A	476	VAL
1	A	505	SER
1	A	507	GLN
1	A	518	TYR
1	A	521	ILE
1	A	526	LEU
1	A	543	ILE
1	A	544	THR
1	A	549	SER
1	A	553	SER
1	A	555	LEU
1	A	564	ILE
1	A	567	ARG
1	A	582	LEU
1	A	587	ILE
1	A	589	ARG
1	A	602	LEU
1	A	603	LEU
1	A	613	TYR
1	A	629	VAL
1	A	631	LEU
1	A	653	SER
1	A	654	ASP
1	A	655	ARG
1	A	663	ASN
1	A	679	MET
1	A	701	ILE
1	A	708	GLN

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Mol	Chain	Res	Type
1	A	713	ARG
1	A	740	ILE
1	A	744	ASP
1	A	750	THR
1	A	755	SER
1	A	766	SER
1	A	796	GLN
1	A	815	SER
1	A	844	LYS
1	A	855	ASP
1	A	857	LYS
1	A	858	LEU
1	A	883	SER
1	A	886	SER
1	A	896	GLU
1	A	900	ARG
1	A	904	ASN
1	A	909	ILE
1	A	917	LYS
1	A	922	LEU
1	A	923	VAL
1	A	941	ASN
1	A	947	ARG
1	A	960	LEU
1	A	966	LEU
1	A	969	GLU
1	A	972	PHE
1	A	979	LYS
1	A	986	ASP
1	A	992	LEU
1	A	1000	LEU
1	A	1013	VAL
1	A	1045	GLU
1	A	1050	LEU
1	A	1052	LEU
1	A	1055	GLN
1	A	1063	LYS
1	A	1064	SER
1	A	1128	ASP
1	A	1130	ILE
1	A	1131	LYS
1	A	1135	GLU

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Mol	Chain	Res	Type
2	B	6	ILE
2	B	15	ILE
2	B	17	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	30	ASN
1	A	109	GLN
1	A	189	HIS
1	A	203	ASN
1	A	240	HIS
1	A	262	ASN
1	A	332	GLN
1	A	370	GLN
1	A	372	GLN
1	A	392	ASN
1	A	399	HIS
1	A	418	ASN
1	A	439	ASN
1	A	455	GLN
1	A	456	GLN
1	A	504	ASN
1	A	507	GLN
1	A	520	GLN
1	A	531	HIS
1	A	536	HIS
1	A	617	ASN
1	A	727	GLN
1	A	796	GLN
1	A	809	GLN
1	A	810	ASN
1	A	905	HIS
1	A	907	ASN
1	A	941	ASN
1	A	978	GLN
1	A	991	HIS
1	A	1055	GLN
1	A	1056	ASN
1	A	1070	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	A	1114/1143 (97%)	0.15	82 (7%) 14 8	9, 58, 151, 199	0
2	B	13/13 (100%)	0.28	1 (7%) 13 7	24, 31, 65, 135	0
All	All	1127/1156 (97%)	0.15	83 (7%) 14 8	9, 58, 150, 199	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	508	VAL	12.6
1	A	294	THR	12.5
1	A	462	ASN	9.4
1	A	621	GLY	7.5
1	A	291	MET	7.4
1	A	293	GLY	6.6
1	A	519	LEU	6.4
1	A	483	PRO	5.6
1	A	902	GLU	5.3
1	A	616	LEU	5.1
1	A	292	ASP	5.1
1	A	660	TYR	5.0
1	A	290	GLN	4.9
1	A	626	ARG	4.9
1	A	619	GLU	4.5
1	A	289	GLU	4.4
1	A	545	PRO	4.4
1	A	571	LEU	4.4
1	A	405	PRO	4.3
1	A	425	LEU	4.3
1	A	521	ILE	4.1
1	A	618	ILE	4.0
1	A	663	ASN	4.0
1	A	682	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
2	B	17	GLU	3.9
1	A	599	SER	3.9
1	A	569	LEU	3.8
1	A	482	GLU	3.8
1	A	773	SER	3.7
1	A	295	VAL	3.6
1	A	661	SER	3.6
1	A	503	CYS	3.6
1	A	468	LEU	3.6
1	A	473	SER	3.5
1	A	648	ASN	3.5
1	A	450	GLY	3.5
1	A	486	LEU	3.4
1	A	297	LEU	3.3
1	A	421	THR	3.2
1	A	502	SER	3.2
1	A	504	ASN	3.1
1	A	624	SER	3.1
1	A	662	SER	3.1
1	A	117	GLU	3.0
1	A	478	LEU	2.9
1	A	369	ARG	2.9
1	A	518	TYR	2.9
1	A	481	GLN	2.9
1	A	924	GLY	2.9
1	A	419	ARG	2.8
1	A	594	THR	2.7
1	A	491	LYS	2.7
1	A	446	THR	2.7
1	A	507	GLN	2.7
1	A	413	LEU	2.7
1	A	1015	GLN	2.6
1	A	551	GLY	2.6
1	A	418	ASN	2.5
1	A	573	SER	2.5
1	A	528	GLN	2.5
1	A	416	ASP	2.5
1	A	684	SER	2.5
1	A	443	VAL	2.5
1	A	402	ILE	2.4
1	A	939	GLU	2.4
1	A	343	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	436	LEU	2.4
1	A	430	VAL	2.4
1	A	520	GLN	2.3
1	A	415	SER	2.3
1	A	439	ASN	2.3
1	A	460	CYS	2.3
1	A	447	GLU	2.2
1	A	881	LEU	2.2
1	A	665	LYS	2.2
1	A	422	TYR	2.1
1	A	918	GLY	2.1
1	A	572	PRO	2.1
1	A	620	THR	2.0
1	A	458	PHE	2.0
1	A	783	GLY	2.0
1	A	434	ARG	2.0
1	A	598	SER	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.