



Full wwPDB X-ray Structure Validation Report ⓘ

May 12, 2020 – 11:45 pm BST

PDB ID : 3I8E
Title : Crystal Structure of DDB1 in Complex with the H-Box Motif of WDR42A
Authors : Li, T.; Robert, E.I.; Breugel, P.C.V.; Strubin, M.; Zheng, N.
Deposited on : 2009-07-09
Resolution : 3.40 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

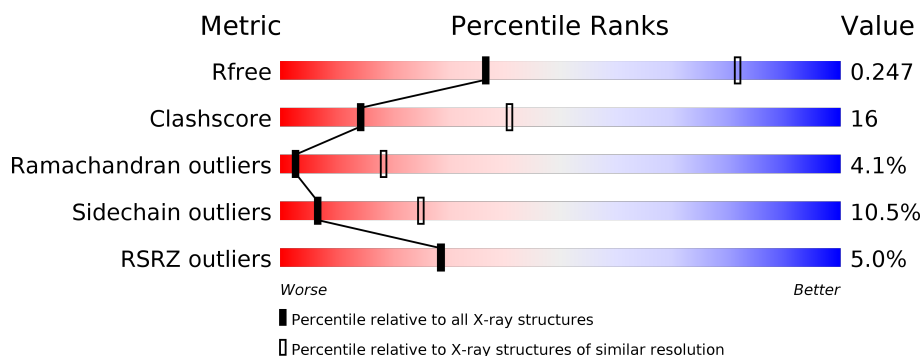
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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>4%</div> <div>61% 30% 6%</div> </div>
1	B	1143	<div> <div>4%</div> <div>61% 30% 6%</div> </div>
2	C	13	<div> <div>23%</div> <div>77% 23%</div> </div>
2	D	13	<div> <div>69%</div> <div>46% 46% 8%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 17652 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			
1	B	1114	Total	C	N	O	S	0	0	0
			8726	5529	1472	1677	48			

There are 12 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
B	-2	GLY	-	EXPRESSION TAG	UNP Q16531
B	-1	SER	-	EXPRESSION TAG	UNP Q16531
B	0	HIS	-	EXPRESSION TAG	UNP Q16531
B	422	TYR	ASP	SEE REMARK 999	UNP Q16531
B	898	ASP	GLU	SEE REMARK 999	UNP Q16531
B	899	VAL	LEU	SEE REMARK 999	UNP Q16531

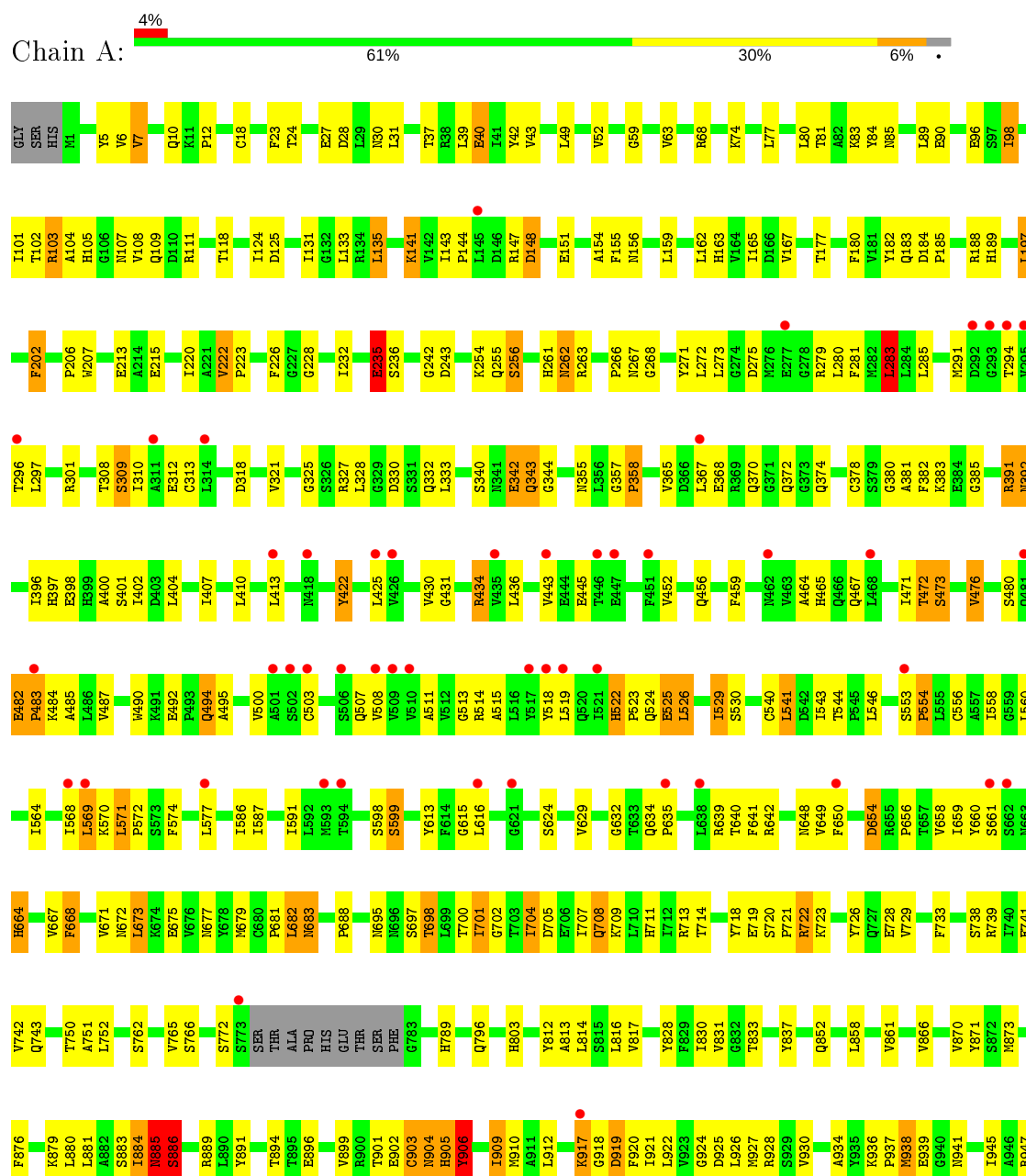
- Molecule 2 is a protein called WD repeat-containing protein 42A.

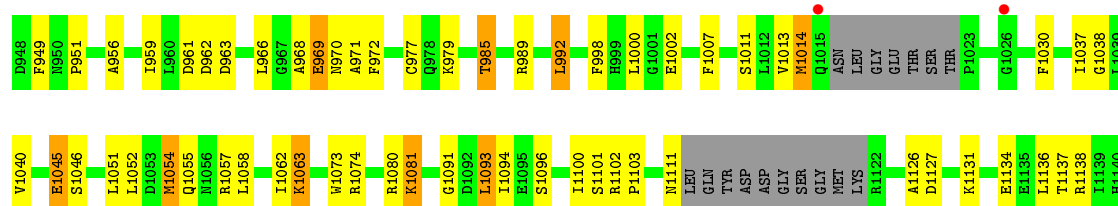
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	13	Total	C	N	O	0	0	0
			100	61	20	19			
2	D	13	Total	C	N	O	0	0	0
			100	61	20	19			

3 Residue-property plots

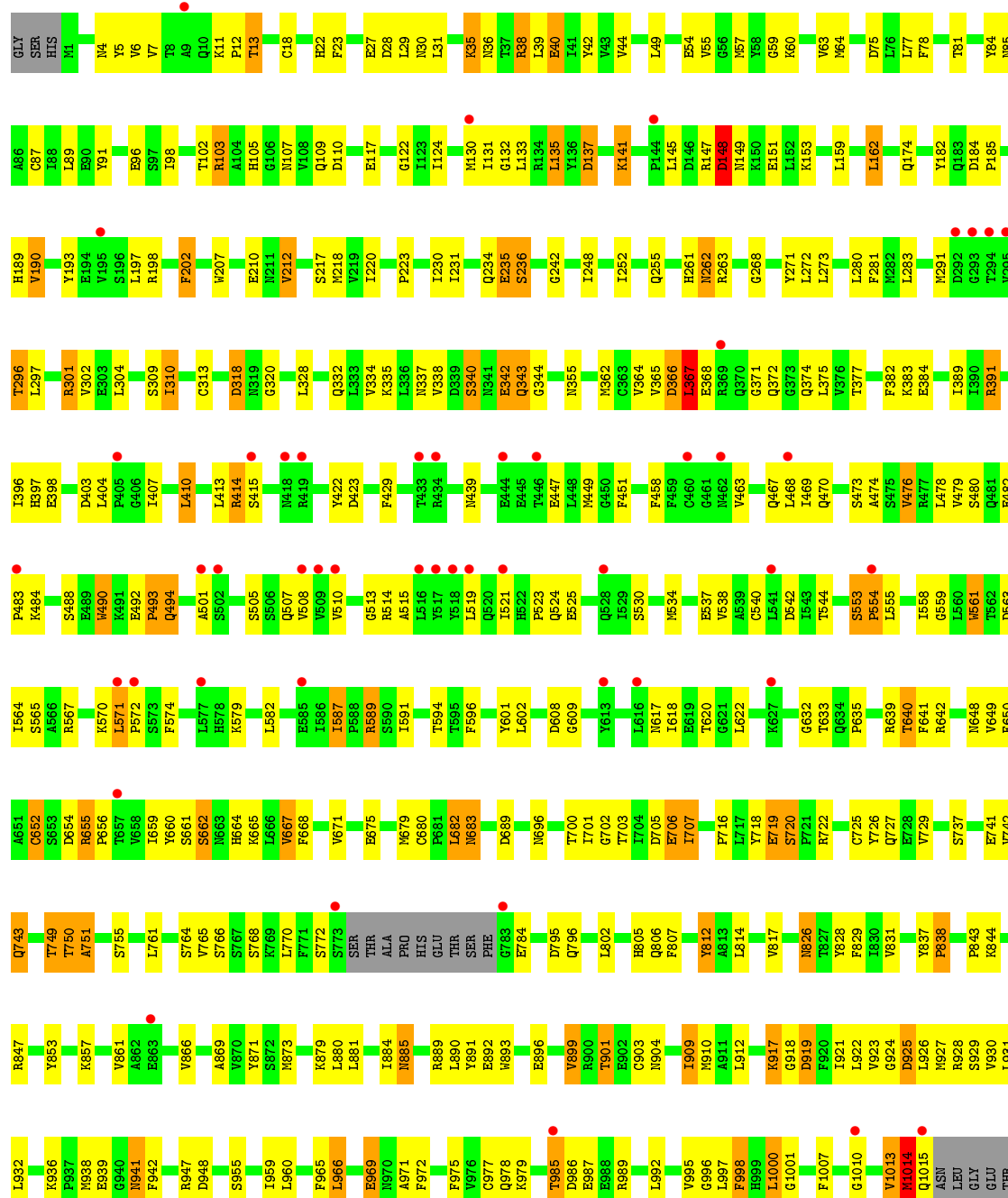
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

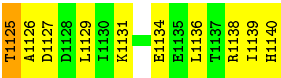
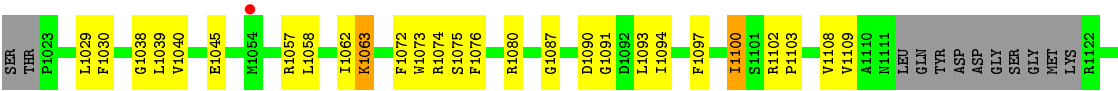
- Molecule 1: DNA damage-binding protein 1



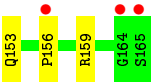
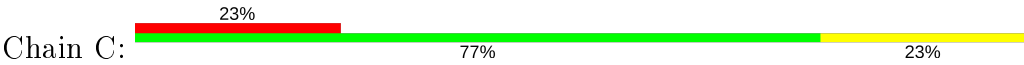


• Molecule 1: DNA damage-binding protein 1

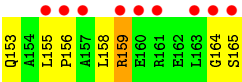




• Molecule 2: WD repeat-containing protein 42A



• Molecule 2: WD repeat-containing protein 42A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.14Å 133.81Å 184.00Å 90.00° 90.45° 90.00°	Depositor
Resolution (Å)	49.15 – 3.40 49.12 – 3.18	Depositor EDS
% Data completeness (in resolution range)	87.3 (49.15-3.40) 81.7 (49.12-3.18)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.260 , 0.338 0.249 , 0.247	Depositor DCC
R_{free} test set	2192 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å ²)	71.6	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 29.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.407 for h,-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	17652	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.45	1/8885 (0.0%)	0.65	2/12034 (0.0%)
1	B	0.46	2/8885 (0.0%)	0.67	4/12034 (0.0%)
2	C	0.44	0/100	0.63	0/133
2	D	0.39	0/100	0.62	0/133
All	All	0.45	3/17970 (0.0%)	0.66	6/24334 (0.0%)

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
1	B	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	367	LEU	C-O	7.37	1.37	1.23
1	B	1013	VAL	CA-C	-7.04	1.34	1.52
1	A	342	GLU	C-N	7.03	1.50	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1013	VAL	CB-CA-C	-16.00	81.00	111.40
1	B	1014	MET	N-CA-CB	-14.77	84.01	110.60
1	B	1013	VAL	N-CA-C	13.43	147.25	111.00
1	A	992	LEU	CA-CB-CG	5.10	127.03	115.30
1	B	162	LEU	CA-CB-CG	5.05	126.92	115.30
1	A	283	LEU	CA-CB-CG	5.02	126.84	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	886	SER	Mainchain
1	B	367	LEU	Mainchain

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	272	0
1	B	8726	0	8706	271	0
2	C	100	0	103	7	0
2	D	100	0	103	8	0
All	All	17652	0	17618	547	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 16.

All (547) 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:1014:MET:SD	1:B:1015:GLN:HG2	1.79	1.23
1:B:1014:MET:CG	1:B:1015:GLN:H	1.58	1.12
1:B:1014:MET:SD	1:B:1015:GLN:N	2.30	1.04
1:B:706:GLU:O	1:B:707:ILE:HG13	1.57	1.04
1:A:1063:LYS:H	1:A:1063:LYS:HD3	1.18	1.03
1:A:81:THR:HB	1:A:85:ASN:HB2	1.40	1.01
1:A:707:ILE:HG22	1:A:708:GLN:H	1.26	1.00
1:B:1014:MET:HG3	1:B:1015:GLN:H	1.22	1.00
1:B:639:ARG:HD3	1:B:640:THR:H	1.33	0.93
1:B:482:GLU:HB2	1:B:483:PRO:HD3	1.51	0.93
1:B:660:TYR:HB2	1:B:707:ILE:HG21	1.50	0.93
1:B:843:PRO:HG2	1:B:869:ALA:HB2	1.51	0.92
1:B:1063:LYS:H	1:B:1063:LYS:HD3	1.34	0.92
1:B:1014:MET:CG	1:B:1015:GLN:N	2.30	0.90
1:A:222:VAL:HG12	1:A:223:PRO:HD2	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:PHE:H	1:B:30:ASN:ND2	1.73	0.84
1:B:660:TYR:HB3	1:B:667:VAL:HB	1.60	0.84
1:A:184:ASP:HB2	1:A:185:PRO:HD2	1.60	0.84
2:D:153:GLN:HB2	2:D:156:PRO:HD2	1.60	0.82
1:B:1014:MET:SD	1:B:1015:GLN:CG	2.66	0.82
1:A:81:THR:CB	1:A:85:ASN:HB2	2.09	0.82
1:B:530:SER:HB2	1:B:574:PHE:HE1	1.44	0.82
1:B:391:ARG:HH11	1:B:391:ARG:HG3	1.46	0.81
1:A:541:LEU:HD23	1:A:558:ILE:HG21	1.61	0.81
1:A:884:ILE:HD12	1:A:884:ILE:N	1.96	0.81
1:A:507:GLN:HE22	1:A:553:SER:HB3	1.45	0.80
1:A:1080:ARG:O	1:A:1081:LYS:HB3	1.82	0.79
1:B:81:THR:HG22	1:B:85:ASN:H	1.47	0.79
1:A:391:ARG:HH11	1:A:391:ARG:HG3	1.49	0.78
1:A:615:GLY:H	1:A:624:SER:HB2	1.48	0.78
1:B:941:ASN:HD22	1:B:942:PHE:H	1.28	0.78
1:B:998:PHE:CE1	1:B:1074:ARG:HD2	2.19	0.77
1:B:1014:MET:HG3	1:B:1015:GLN:N	1.98	0.77
1:A:905:HIS:O	1:A:906:TYR:HB2	1.84	0.76
1:A:934:ALA:HB2	1:A:945:ILE:HD11	1.68	0.76
1:B:335:LYS:HG3	1:B:337:ASN:HD21	1.50	0.75
1:A:98:ILE:H	1:A:98:ILE:HD13	1.53	0.74
1:A:884:ILE:O	1:A:885:ASN:CB	2.36	0.73
1:B:301:ARG:HG2	1:B:302:VAL:N	2.04	0.73
1:A:883:SER:C	1:A:884:ILE:HD12	2.10	0.72
1:A:59:GLY:HA2	1:A:1073:TRP:CZ3	2.25	0.72
1:A:741:GLU:CG	1:A:750:THR:O	2.38	0.71
1:B:397:HIS:O	1:B:702:GLY:HA3	1.90	0.71
1:B:889:ARG:HG3	1:B:904:ASN:OD1	1.90	0.71
1:B:750:THR:O	1:B:751:ALA:HB2	1.91	0.71
1:B:881:LEU:HD21	1:B:922:LEU:HD21	1.72	0.71
1:A:81:THR:HG22	1:A:83:LYS:H	1.55	0.71
1:A:629:VAL:HG21	1:A:668:PHE:HE2	1.55	0.71
1:B:335:LYS:HG3	1:B:337:ASN:ND2	2.06	0.71
1:A:396:ILE:HG21	1:A:673:LEU:HD11	1.73	0.70
1:B:743:GLN:HB3	1:B:784:GLU:HB2	1.72	0.70
1:A:812:TYR:HB3	2:C:159:ARG:HH22	1.55	0.70
1:A:885:ASN:O	1:A:886:SER:CB	2.36	0.70
1:B:893:TRP:HZ3	1:B:899:VAL:HG22	1.57	0.70
1:A:434:ARG:HH11	1:A:434:ARG:HG2	1.57	0.70
1:A:23:PHE:H	1:A:30:ASN:ND2	1.89	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:570:LYS:HD3	1:A:571:LEU:H	1.57	0.70
1:B:36:ASN:OD1	1:B:60:LYS:HG2	1.92	0.70
1:A:397:HIS:O	1:A:702:GLY:HA3	1.92	0.70
1:A:884:ILE:O	1:A:884:ILE:HG22	1.90	0.69
1:B:538:VAL:HG13	1:B:558:ILE:HD11	1.75	0.69
1:B:110:ASP:OD1	1:B:141:LYS:HE2	1.93	0.69
1:B:1063:LYS:HD3	1:B:1063:LYS:N	2.06	0.69
1:B:917:LYS:O	1:B:919:ASP:N	2.26	0.69
1:A:903:CYS:O	1:A:904:ASN:HB3	1.93	0.68
1:B:909:ILE:HG21	1:B:927:MET:HG2	1.75	0.68
1:B:978:GLN:HE21	1:B:995:VAL:HG11	1.58	0.68
1:A:482:GLU:HB2	1:A:483:PRO:HD3	1.76	0.68
1:B:309:SER:H	1:B:332:GLN:NE2	1.92	0.68
2:C:153:GLN:HB2	2:C:156:PRO:HD2	1.74	0.68
1:A:654:ASP:HA	1:A:675:GLU:HG3	1.77	0.67
1:B:660:TYR:HB2	1:B:707:ILE:CG2	2.24	0.67
1:A:476:VAL:HG13	1:A:490:TRP:HB3	1.75	0.67
1:A:529:ILE:HG22	1:A:530:SER:H	1.60	0.67
1:A:707:ILE:HG22	1:A:708:GLN:N	2.04	0.67
1:B:1102:ARG:N	1:B:1103:PRO:HD2	2.08	0.67
1:A:726:TYR:CE2	1:A:728:GLU:HB2	2.30	0.67
1:B:743:GLN:HG2	1:B:784:GLU:H	1.59	0.67
1:A:697:SER:O	1:A:698:THR:HB	1.94	0.67
1:B:23:PHE:H	1:B:30:ASN:HD22	1.41	0.67
1:B:871:TYR:HE1	1:B:885:ASN:OD1	1.78	0.66
1:B:639:ARG:HD3	1:B:640:THR:N	2.07	0.66
1:B:923:VAL:HA	1:B:931:LEU:O	1.94	0.66
1:B:23:PHE:CE2	1:B:91:TYR:HB2	2.30	0.66
1:A:765:VAL:HG22	1:A:766:SER:H	1.61	0.65
1:B:133:LEU:HD23	1:B:135:LEU:HD21	1.78	0.65
1:A:18:CYS:N	1:A:313:CYS:SG	2.70	0.65
1:A:385:GLY:HA3	1:A:719:GLU:O	1.95	0.65
1:A:529:ILE:HG22	1:A:530:SER:N	2.12	0.65
1:B:103:ARG:HB3	1:B:103:ARG:HH11	1.61	0.65
1:A:813:ALA:HA	1:A:833:THR:HG22	1.78	0.65
1:B:594:THR:HG21	1:B:649:VAL:HG21	1.78	0.65
1:B:1057:ARG:HD2	1:B:1108:VAL:O	1.97	0.65
1:B:596:PHE:HE2	1:B:648:ASN:HA	1.61	0.65
1:A:884:ILE:O	1:A:885:ASN:HB2	1.95	0.65
1:A:881:LEU:HD21	1:A:922:LEU:HD21	1.79	0.64
1:A:500:VAL:HG11	1:A:540:CYS:HA	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:713:ARG:HG2	1:A:713:ARG:HH11	1.61	0.64
1:A:374:GLN:HE22	1:A:391:ARG:HB2	1.63	0.64
1:B:571:LEU:HB3	1:B:572:PRO:HD3	1.80	0.64
1:A:103:ARG:HB3	1:A:103:ARG:HH11	1.62	0.64
1:A:1030:PHE:CE2	1:A:1038:GLY:HA3	2.33	0.63
1:A:6:VAL:HG12	1:A:1040:VAL:HG22	1.79	0.63
1:B:81:THR:HG22	1:B:85:ASN:N	2.13	0.63
1:B:410:LEU:HD13	1:B:680:CYS:SG	2.38	0.63
1:A:382:PHE:H	1:A:720:SER:HB3	1.64	0.63
1:A:814:LEU:HD23	2:C:159:ARG:HH21	1.64	0.63
1:B:22:HIS:CD2	1:B:28:ASP:O	2.51	0.63
1:B:340:SER:HB3	1:B:344:GLY:HA2	1.80	0.63
1:B:941:ASN:HD22	1:B:942:PHE:N	1.95	0.63
1:B:1063:LYS:H	1:B:1063:LYS:CD	2.06	0.63
1:A:556:CYS:HB3	1:A:569:LEU:HD12	1.81	0.62
1:A:828:TYR:HE2	1:A:861:VAL:HG21	1.64	0.62
1:A:541:LEU:HD23	1:A:558:ILE:CG2	2.29	0.62
1:B:648:ASN:ND2	1:B:660:TYR:HD1	1.97	0.62
1:B:530:SER:HB2	1:B:574:PHE:CE1	2.30	0.62
1:A:741:GLU:HG2	1:A:750:THR:O	1.99	0.62
1:A:1013:VAL:O	1:A:1014:MET:HG3	2.00	0.61
1:A:648:ASN:HB3	1:A:659:ILE:O	1.99	0.61
1:B:342:GLU:O	1:B:343:GLN:HB2	2.01	0.61
1:B:750:THR:O	1:B:751:ALA:CB	2.48	0.61
1:A:1030:PHE:CZ	1:A:1038:GLY:HA3	2.35	0.61
1:A:507:GLN:NE2	1:A:553:SER:HB3	2.14	0.61
1:A:1102:ARG:N	1:A:1103:PRO:HD2	2.14	0.61
1:A:23:PHE:H	1:A:30:ASN:HD22	1.47	0.61
1:A:90:GLU:HB3	1:A:101:ILE:HG22	1.81	0.61
1:A:1063:LYS:CD	1:A:1063:LYS:H	2.02	0.61
1:A:905:HIS:CG	1:A:906:TYR:H	2.19	0.61
1:B:507:GLN:HE22	1:B:553:SER:HB3	1.63	0.60
1:A:884:ILE:CD1	1:A:884:ILE:N	2.64	0.60
1:B:301:ARG:HG2	1:B:302:VAL:H	1.65	0.60
1:A:107:ASN:OD1	1:A:109:GLN:HG2	2.01	0.60
1:A:642:ARG:HH22	1:A:683:ASN:HB2	1.67	0.60
1:A:998:PHE:CZ	1:A:1074:ARG:HD2	2.37	0.59
1:B:1014:MET:C	1:B:1014:MET:SD	2.77	0.59
1:B:997:LEU:HB3	1:B:1076:PHE:CD1	2.37	0.59
1:B:81:THR:CG2	1:B:85:ASN:H	2.15	0.59
1:B:59:GLY:HA2	1:B:1073:TRP:CZ3	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:570:LYS:HG2	1:B:571:LEU:H	1.67	0.59
1:B:719:GLU:HG2	1:B:755:SER:HB3	1.84	0.59
1:B:463:VAL:HG12	1:B:505:SER:HA	1.85	0.59
1:A:368:GLU:CB	1:A:370:GLN:HE21	2.15	0.59
1:B:741:GLU:HG2	1:B:751:ALA:HA	1.83	0.59
1:B:5:TYR:OH	1:B:1091:GLY:HA3	2.03	0.58
1:A:871:TYR:HE1	1:A:885:ASN:HA	1.68	0.58
1:B:1014:MET:CE	1:B:1015:GLN:CG	2.80	0.58
1:B:184:ASP:HB2	1:B:185:PRO:CD	2.33	0.58
1:A:368:GLU:HB3	1:A:370:GLN:HE21	1.68	0.58
1:B:467:GLN:NE2	1:B:524:GLN:HA	2.18	0.58
1:B:889:ARG:HD2	1:B:891:TYR:CE1	2.39	0.58
1:A:750:THR:OG1	1:A:751:ALA:N	2.30	0.58
1:B:765:VAL:HG23	1:B:806:GLN:HB3	1.85	0.58
1:B:997:LEU:O	1:B:998:PHE:HB2	2.02	0.58
1:A:814:LEU:CD2	2:C:159:ARG:HH21	2.18	0.57
1:B:310:ILE:HG21	1:B:328:LEU:HD12	1.87	0.57
1:B:296:THR:OG1	1:B:297:LEU:N	2.38	0.57
1:A:508:VAL:HB	1:A:519:LEU:HB2	1.86	0.57
1:B:124:ILE:HG12	1:B:131:ILE:HG12	1.86	0.57
1:A:649:VAL:HB	1:A:659:ILE:HB	1.87	0.57
1:B:131:ILE:HG13	1:B:145:LEU:HD12	1.87	0.57
1:A:522:HIS:HB3	1:A:523:PRO:CD	2.35	0.56
1:B:415:SER:H	1:B:423:ASP:HB3	1.71	0.56
1:B:184:ASP:HB2	1:B:185:PRO:HD2	1.87	0.56
1:A:639:ARG:HG3	1:A:640:THR:N	2.21	0.56
1:B:263:ARG:HD3	1:B:268:GLY:HA2	1.88	0.56
1:B:130:MET:HA	1:B:145:LEU:H	1.70	0.56
1:B:234:GLN:O	1:B:235:GLU:HG2	2.06	0.56
1:A:24:THR:H	1:A:30:ASN:ND2	2.04	0.56
1:A:370:GLN:HB2	1:A:372:GLN:HE21	1.71	0.56
1:B:726:TYR:OH	1:B:796:GLN:NE2	2.34	0.56
1:B:1029:LEU:HD23	1:B:1039:LEU:HD13	1.86	0.56
1:A:309:SER:H	1:A:332:GLN:NE2	2.04	0.55
1:A:641:PHE:CZ	1:A:648:ASN:HB2	2.41	0.55
1:A:936:LYS:C	1:A:938:MET:H	2.09	0.55
1:A:571:LEU:HB3	1:A:572:PRO:HD3	1.87	0.55
1:A:998:PHE:CE1	1:A:1074:ARG:HD2	2.42	0.55
1:B:719:GLU:OE1	1:B:737:SER:HB2	2.06	0.55
1:B:656:PRO:HB2	1:B:671:VAL:HB	1.86	0.55
1:B:559:GLY:HA2	1:B:565:SER:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:648:ASN:HB3	1:B:659:ILE:O	2.07	0.55
1:B:1007:PHE:CD2	1:B:1030:PHE:HB3	2.42	0.55
1:B:367:LEU:HB2	1:B:374:GLN:HG3	1.89	0.55
1:A:889:ARG:HD2	1:A:891:TYR:CZ	2.42	0.55
1:B:193:TYR:HD2	1:B:202:PHE:HB3	1.72	0.55
1:B:220:ILE:HB	1:B:230:ILE:HB	1.87	0.55
1:B:35:LYS:NZ	1:B:40:GLU:OE1	2.33	0.55
1:A:59:GLY:HA3	1:A:81:THR:HG23	1.89	0.54
1:B:742:VAL:O	1:B:749:THR:HG22	2.07	0.54
1:A:273:LEU:HB2	1:A:281:PHE:HB2	1.89	0.54
1:A:104:ALA:O	1:A:105:HIS:HB3	2.06	0.54
1:B:182:TYR:CZ	1:B:189:HIS:HB2	2.43	0.54
1:B:273:LEU:HB2	1:B:281:PHE:HB2	1.88	0.54
1:B:480:SER:HB3	1:B:483:PRO:HD2	1.88	0.54
1:B:492:GLU:O	1:B:494:GLN:N	2.32	0.54
1:A:568:ILE:HD12	1:A:616:LEU:HD13	1.88	0.54
1:B:936:LYS:HB3	1:B:938:MET:HB3	1.89	0.54
1:B:366:ASP:O	1:B:368:GLU:N	2.41	0.54
1:A:926:LEU:HG	1:A:927:MET:N	2.22	0.54
1:A:271:TYR:HB2	1:A:283:LEU:HB3	1.88	0.54
1:A:642:ARG:NH2	1:A:683:ASN:HB2	2.22	0.54
1:B:1014:MET:CE	1:B:1015:GLN:HG3	2.38	0.54
1:B:563:ASP:HB3	1:B:565:SER:HB3	1.90	0.54
1:B:77:LEU:HB3	1:B:89:LEU:HB2	1.90	0.53
1:B:977:CYS:HB3	1:B:992:LEU:HD13	1.89	0.53
1:A:629:VAL:HG21	1:A:668:PHE:CE2	2.40	0.53
1:B:660:TYR:CG	1:B:661:SER:N	2.76	0.53
1:B:1013:VAL:HG23	1:B:1014:MET:N	2.23	0.53
1:B:682:LEU:O	1:B:683:ASN:HB2	2.07	0.53
1:A:726:TYR:OH	1:A:796:GLN:NE2	2.42	0.53
1:A:396:ILE:O	1:A:396:ILE:HD12	2.08	0.53
1:A:741:GLU:CD	1:A:750:THR:O	2.47	0.53
1:B:476:VAL:HG13	1:B:490:TRP:HB2	1.91	0.53
1:A:1091:GLY:HA2	1:A:1094:ILE:HB	1.90	0.53
1:A:365:VAL:HG21	1:A:733:PHE:HE2	1.73	0.53
1:B:107:ASN:OD1	1:B:109:GLN:HG2	2.09	0.53
1:B:570:LYS:NZ	1:B:572:PRO:HD2	2.23	0.53
1:A:77:LEU:HD23	1:A:89:LEU:HD12	1.92	0.52
1:A:24:THR:H	1:A:30:ASN:HD21	1.57	0.52
1:A:105:HIS:O	1:A:151:GLU:HA	2.10	0.52
1:A:530:SER:HB2	1:A:574:PHE:HE1	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1091:GLY:HA2	1:B:1094:ILE:HB	1.90	0.52
1:B:234:GLN:O	1:B:236:SER:N	2.42	0.52
1:B:5:TYR:CZ	1:B:1091:GLY:HA3	2.44	0.52
1:B:133:LEU:HD23	1:B:135:LEU:CD2	2.38	0.52
1:B:261:HIS:O	1:B:262:ASN:HB2	2.10	0.52
1:A:124:ILE:HG12	1:A:131:ILE:HG12	1.92	0.52
1:B:722:ARG:HG3	1:B:722:ARG:HH11	1.75	0.52
1:B:22:HIS:HD2	1:B:28:ASP:O	1.93	0.51
1:B:383:LYS:HE3	1:B:384:GLU:OE2	2.09	0.51
1:A:480:SER:HB2	1:A:483:PRO:HD2	1.92	0.51
1:B:149:ASN:OD1	1:B:153:LYS:N	2.43	0.51
1:A:273:LEU:HD11	1:A:283:LEU:HB2	1.92	0.51
1:B:263:ARG:HB2	1:B:271:TYR:CE2	2.45	0.51
1:A:707:ILE:CG2	1:A:708:GLN:H	2.07	0.51
1:A:939:GLU:HG3	1:A:941:ASN:HB2	1.92	0.51
1:A:682:LEU:O	1:A:683:ASN:HB2	2.11	0.51
1:B:826:ASN:N	1:B:826:ASN:OD1	2.43	0.51
1:A:235:GLU:HB3	1:A:254:LYS:HG3	1.93	0.51
1:A:660:TYR:CD2	1:A:707:ILE:HG12	2.46	0.51
1:B:869:ALA:O	1:B:884:ILE:HA	2.11	0.51
1:A:1051:LEU:O	1:A:1055:GLN:HB2	2.11	0.50
1:A:1136:LEU:C	1:A:1138:ARG:H	2.14	0.50
1:A:133:LEU:HD23	1:A:135:LEU:HD21	1.92	0.50
1:A:852:GLN:HB2	1:A:861:VAL:HG21	1.93	0.50
1:A:977:CYS:HB3	1:A:992:LEU:HD13	1.93	0.50
1:A:830:ILE:HD13	1:A:880:LEU:HD13	1.94	0.50
1:A:910:MET:HE2	1:A:926:LEU:HD22	1.93	0.50
1:A:313:CYS:HB3	1:A:325:GLY:HA3	1.93	0.50
1:A:40:GLU:HB3	1:A:42:TYR:CE1	2.45	0.50
1:A:378:CYS:HB3	1:A:721:PRO:HG2	1.92	0.50
1:A:881:LEU:HD21	1:A:922:LEU:CD2	2.42	0.50
1:B:537:GLU:O	1:B:561:TRP:HB2	2.11	0.50
1:B:975:PHE:HA	1:B:996:GLY:O	2.11	0.50
1:A:814:LEU:HD23	2:C:159:ARG:NH2	2.26	0.50
1:A:197:LEU:H	1:A:197:LEU:HD23	1.77	0.50
1:A:658:VAL:HG23	1:A:671:VAL:HG21	1.94	0.50
1:B:23:PHE:CE1	1:B:77:LEU:HB2	2.47	0.50
1:A:383:LYS:HA	1:A:718:TYR:O	2.12	0.50
1:B:648:ASN:HD21	1:B:660:TYR:HD1	1.59	0.50
1:B:992:LEU:O	1:B:992:LEU:HD12	2.12	0.50
1:A:402:ILE:HG12	1:A:443:VAL:HG21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:ARG:HD3	1:A:268:GLY:HA2	1.94	0.49
1:A:400:ALA:HB3	1:A:701:ILE:HD11	1.94	0.49
1:A:280:LEU:HD13	1:A:308:THR:HG21	1.94	0.49
1:B:655:ARG:HH12	1:B:1138:ARG:HD3	1.77	0.49
1:A:37:THR:HG22	1:A:59:GLY:O	2.12	0.49
1:B:807:PHE:CZ	1:B:831:VAL:HG11	2.48	0.49
1:A:901:THR:HG22	1:A:902:GLU:N	2.27	0.49
1:A:938:MET:HG2	1:A:939:GLU:N	2.27	0.49
1:B:413:LEU:O	1:B:422:TYR:HB3	2.12	0.49
1:B:197:LEU:H	1:B:197:LEU:HD23	1.78	0.49
1:B:271:TYR:HB2	1:B:283:LEU:HB3	1.94	0.49
1:B:480:SER:CB	1:B:483:PRO:HD2	2.43	0.49
1:B:476:VAL:HG13	1:B:490:TRP:CB	2.42	0.49
1:B:889:ARG:HD3	1:B:901:THR:HG23	1.94	0.49
1:B:513:GLY:C	1:B:515:ALA:H	2.16	0.49
1:A:816:LEU:HD13	1:A:831:VAL:HG22	1.95	0.49
1:B:364:VAL:HG21	1:B:1010:GLY:HA3	1.95	0.49
1:A:431:GLY:HA2	1:A:456:GLN:HB2	1.95	0.48
1:B:609:GLY:HA3	1:B:632:GLY:O	2.13	0.48
1:A:1045:GLU:HG2	1:A:1046:SER:N	2.28	0.48
1:B:1030:PHE:CZ	1:B:1038:GLY:HA3	2.48	0.48
1:B:234:GLN:C	1:B:236:SER:H	2.17	0.48
1:B:414:ARG:HA	1:B:423:ASP:H	1.79	0.48
1:A:108:VAL:HG11	1:A:143:ILE:HD11	1.96	0.48
1:A:434:ARG:HG2	1:A:434:ARG:NH1	2.26	0.48
1:A:828:TYR:CE2	1:A:861:VAL:HG21	2.47	0.48
1:A:382:PHE:O	1:A:719:GLU:O	2.31	0.48
1:A:634:GLN:HG2	1:A:654:ASP:HB3	1.95	0.48
1:B:193:TYR:CD2	1:B:202:PHE:HB3	2.48	0.48
1:A:167:VAL:HG13	1:A:180:PHE:HB3	1.95	0.48
1:B:11:LYS:NZ	1:B:38:ARG:HH21	2.12	0.48
1:A:742:VAL:HG13	1:A:752:LEU:HD21	1.95	0.48
1:A:143:ILE:HG12	1:A:154:ALA:HB2	1.95	0.48
1:B:63:VAL:HG11	1:B:122:GLY:HA3	1.96	0.48
1:A:812:TYR:CB	2:C:159:ARG:HH22	2.26	0.48
1:A:261:HIS:O	1:A:262:ASN:HB2	2.13	0.48
1:A:873:MET:HE2	1:A:880:LEU:HD21	1.95	0.48
1:A:222:VAL:HG23	1:A:228:GLY:O	2.14	0.48
1:A:1093:LEU:O	1:A:1096:SER:HB3	2.13	0.47
1:A:507:GLN:HG3	1:A:518:TYR:HE1	1.79	0.47
1:A:969:GLU:O	1:A:971:ALA:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:164:GLY:O	2:D:165:SER:C	2.51	0.47
1:A:570:LYS:HD3	1:A:571:LEU:N	2.27	0.47
1:A:1063:LYS:N	1:A:1063:LYS:HD3	2.03	0.47
1:A:598:SER:O	1:A:599:SER:CB	2.62	0.47
1:A:708:GLN:HE21	1:A:711:HIS:HA	1.79	0.47
1:A:255:GLN:HB2	1:A:279:ARG:HH22	1.79	0.47
1:B:391:ARG:HG3	1:B:391:ARG:NH1	2.22	0.47
1:B:391:ARG:CG	1:B:391:ARG:HH11	2.23	0.47
1:A:1131:LYS:O	1:A:1134:GLU:HB2	2.15	0.47
1:B:596:PHE:HD1	1:B:601:TYR:CE1	2.32	0.47
1:A:197:LEU:H	1:A:197:LEU:CD2	2.27	0.47
1:A:985:THR:HB	1:A:989:ARG:HB2	1.97	0.47
1:A:634:GLN:HB3	1:A:635:PRO:HD2	1.97	0.47
1:A:912:LEU:HG	1:A:926:LEU:HB2	1.95	0.47
1:A:947:ARG:HG3	1:A:949:PHE:CE1	2.50	0.47
1:B:1109:VAL:HG11	1:B:1125:THR:O	2.14	0.47
1:B:11:LYS:HB3	1:B:12:PRO:HD2	1.97	0.47
1:A:413:LEU:O	1:A:422:TYR:HB3	2.15	0.47
1:A:885:ASN:O	1:A:886:SER:HB3	2.15	0.47
1:A:972:PHE:HB3	1:A:1002:GLU:N	2.30	0.47
1:B:795:ASP:HB2	1:B:802:LEU:HD21	1.96	0.47
1:A:530:SER:HB2	1:A:574:PHE:CE1	2.50	0.47
1:A:683:ASN:HA	1:A:688:PRO:HA	1.96	0.47
1:B:18:CYS:N	1:B:313:CYS:SG	2.88	0.47
1:B:727:GLN:HB2	1:B:829:PHE:CE1	2.50	0.47
1:A:404:LEU:HB2	1:A:407:ILE:HD11	1.97	0.47
1:A:909:ILE:HG21	1:A:927:MET:HG2	1.95	0.47
1:A:917:LYS:HB2	1:A:959:ILE:HD13	1.97	0.47
1:B:1129:LEU:C	1:B:1131:LYS:H	2.18	0.47
1:A:327:ARG:O	1:A:358:PRO:HD3	2.14	0.46
1:A:365:VAL:HG12	1:A:367:LEU:HG	1.95	0.46
1:A:876:PHE:CZ	1:A:920:PHE:HA	2.50	0.46
1:B:272:LEU:HD22	1:B:280:LEU:HD11	1.97	0.46
1:B:617:ASN:HD22	1:B:620:THR:HG1	1.63	0.46
1:B:764:SER:O	1:B:805:HIS:HA	2.15	0.46
1:A:340:SER:HB3	1:A:344:GLY:HA2	1.96	0.46
1:B:375:LEU:O	1:B:389:ILE:HA	2.16	0.46
2:D:153:GLN:HB2	2:D:156:PRO:CD	2.40	0.46
1:A:490:TRP:HB2	1:A:526:LEU:HG	1.97	0.46
1:A:1100:ILE:HG22	1:A:1101:SER:O	2.15	0.46
1:A:522:HIS:HB3	1:A:523:PRO:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:ASP:OD1	1:B:148:ASP:N	2.48	0.46
1:B:542:ASP:HB2	1:B:591:ILE:HG23	1.97	0.46
1:B:828:TYR:HE2	1:B:861:VAL:HG21	1.80	0.46
1:A:494:GLN:O	1:A:495:ALA:HB3	2.15	0.46
1:A:522:HIS:HB2	1:A:525:GLU:OE1	2.15	0.46
1:B:716:PRO:HB2	1:B:718:TYR:CZ	2.51	0.46
1:A:961:ASP:O	1:A:963:ASP:N	2.49	0.46
1:B:190:VAL:HG13	1:B:210:GLU:HB2	1.97	0.46
1:B:252:ILE:HD11	1:B:304:LEU:HD22	1.98	0.46
1:B:60:LYS:HE2	1:B:972:PHE:CE1	2.51	0.46
1:A:206:PRO:HB2	1:A:207:TRP:CE3	2.51	0.46
1:B:594:THR:O	1:B:601:TYR:HD1	1.99	0.46
1:A:80:LEU:HA	1:A:85:ASN:O	2.16	0.46
1:A:909:ILE:HD12	1:A:928:ARG:HD3	1.98	0.46
1:B:60:LYS:NZ	1:B:1001:GLY:O	2.40	0.46
1:B:81:THR:HG22	1:B:85:ASN:HB2	1.98	0.46
1:A:956:ALA:HB3	1:A:968:ALA:HB3	1.98	0.46
1:B:1134:GLU:C	1:B:1136:LEU:H	2.19	0.46
1:A:328:LEU:HD23	1:A:381:ALA:HB3	1.96	0.45
1:A:1074:ARG:HD3	1:A:1074:ARG:HA	1.72	0.45
1:A:641:PHE:HD2	1:A:650:PHE:HB2	1.81	0.45
1:B:662:SER:HB3	1:B:665:LYS:HB2	1.98	0.45
1:B:382:PHE:H	1:B:720:SER:HB3	1.81	0.45
1:A:391:ARG:HH11	1:A:391:ARG:CG	2.26	0.45
1:A:43:VAL:HG23	1:A:52:VAL:HG21	1.98	0.45
1:B:641:PHE:CZ	1:B:648:ASN:HB2	2.52	0.45
1:B:929:SER:OG	1:B:948:ASP:HB3	2.16	0.45
1:A:144:PRO:HG3	1:A:155:PHE:HE2	1.81	0.45
1:A:165:ILE:N	1:A:165:ILE:HD12	2.31	0.45
1:B:36:ASN:HD21	1:B:60:LYS:NZ	2.13	0.45
1:B:912:LEU:HG	1:B:926:LEU:HB2	1.98	0.45
1:B:997:LEU:O	1:B:998:PHE:CB	2.64	0.45
1:B:493:PRO:O	1:B:494:GLN:HG3	2.17	0.45
1:B:1097:PHE:O	1:B:1100:ILE:HG13	2.16	0.45
1:B:642:ARG:HH22	1:B:683:ASN:HD22	1.63	0.45
1:A:889:ARG:HG3	1:A:904:ASN:HB3	1.98	0.45
1:A:925:ASP:CG	1:A:926:LEU:H	2.20	0.45
1:B:133:LEU:CD2	1:B:135:LEU:HD21	2.45	0.45
1:B:39:LEU:HB3	1:B:55:VAL:HG23	1.98	0.45
1:A:503:CYS:HA	1:A:543:ILE:HD11	1.98	0.45
1:A:1057:ARG:HH22	1:A:1111:ASN:H	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:594:THR:HG21	1:B:649:VAL:CG2	2.44	0.45
1:B:650:PHE:HE2	1:B:652:CYS:HG	1.62	0.45
1:B:722:ARG:CZ	2:D:159:ARG:HG2	2.47	0.45
1:A:226:PHE:HE1	1:A:267:ASN:O	2.00	0.45
1:A:296:THR:OG1	1:A:297:LEU:N	2.48	0.45
1:A:63:VAL:HB	1:A:80:LEU:HB3	1.98	0.45
1:B:132:GLY:O	1:B:133:LEU:HD12	2.17	0.45
1:B:404:LEU:HB2	1:B:407:ILE:HD11	1.98	0.45
1:B:81:THR:CG2	1:B:85:ASN:HB2	2.47	0.45
1:A:464:ALA:O	1:A:465:HIS:HB2	2.17	0.44
1:A:68:ARG:HH11	1:A:74:LYS:HA	1.82	0.44
1:A:894:THR:OG1	1:A:896:GLU:HB2	2.17	0.44
1:B:1129:LEU:C	1:B:1131:LYS:N	2.69	0.44
1:B:659:ILE:HA	1:B:667:VAL:O	2.17	0.44
1:A:886:SER:O	1:A:886:SER:OG	2.30	0.44
1:B:960:LEU:HD21	1:B:966:LEU:HD12	2.00	0.44
1:B:917:LYS:HB2	1:B:959:ILE:HG21	1.99	0.44
1:A:59:GLY:HA2	1:A:1073:TRP:CE3	2.52	0.44
1:A:391:ARG:NH1	1:A:391:ARG:HG3	2.25	0.44
1:A:492:GLU:OE1	1:A:494:GLN:HB2	2.17	0.44
1:A:677:ASN:HB2	1:A:695:ASN:HA	1.98	0.44
1:A:762:SER:O	1:A:803:HIS:HA	2.18	0.44
1:B:4:ASN:HB2	1:B:1087:GLY:O	2.17	0.44
1:B:890:LEU:HB3	1:B:903:CYS:SG	2.57	0.44
1:B:924:GLY:O	1:B:925:ASP:HB2	2.17	0.44
1:B:912:LEU:HD22	2:D:158:LEU:HD11	1.99	0.44
1:A:333:LEU:HA	1:A:333:LEU:HD12	1.88	0.44
1:B:570:LYS:HZ3	1:B:572:PRO:HD2	1.83	0.44
1:A:31:LEU:HB3	1:A:42:TYR:HB2	1.99	0.44
1:A:905:HIS:CG	1:A:906:TYR:N	2.84	0.44
1:B:207:TRP:CG	1:B:242:GLY:HA3	2.53	0.44
1:B:909:ILE:HD13	1:B:928:ARG:HD3	2.00	0.44
1:A:765:VAL:HG22	1:A:766:SER:N	2.31	0.44
1:B:320:GLY:O	1:B:335:LYS:HA	2.18	0.44
1:B:451:PHE:HA	1:B:470:GLN:OE1	2.18	0.43
1:B:501:ALA:HA	1:B:510:VAL:HG12	1.99	0.43
1:B:812:TYR:CD2	1:B:812:TYR:N	2.85	0.43
1:A:487:VAL:HG12	1:A:524:GLN:O	2.18	0.43
1:A:77:LEU:HB3	1:A:89:LEU:HB2	1.98	0.43
1:B:928:ARG:NH2	1:B:947:ARG:HH12	2.16	0.43
1:A:342:GLU:O	1:A:343:GLN:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:GLN:HA	1:A:480:SER:HA	1.98	0.43
1:A:639:ARG:HG3	1:A:640:THR:H	1.82	0.43
1:B:768:SER:HG	1:B:770:LEU:HG	1.84	0.43
1:B:87:CYS:HA	1:B:105:HIS:HA	2.01	0.43
1:A:374:GLN:NE2	1:A:391:ARG:HB2	2.29	0.43
1:B:212:VAL:HG11	1:B:231:ILE:HG21	1.99	0.43
1:B:765:VAL:HG22	1:B:766:SER:H	1.83	0.43
1:B:78:PHE:CD1	1:B:131:ILE:HD13	2.53	0.43
1:A:12:PRO:HG3	1:A:1002:GLU:OE1	2.18	0.43
1:A:667:VAL:HG12	1:A:668:PHE:N	2.34	0.43
1:A:722:ARG:O	1:A:723:LYS:HG2	2.19	0.43
1:B:31:LEU:HD23	1:B:49:LEU:HD21	2.00	0.43
1:A:330:ASP:HA	1:A:355:ASN:HB3	2.01	0.43
1:A:459:PHE:CE2	1:A:503:CYS:HB3	2.54	0.43
1:A:879:LYS:HB3	1:A:891:TYR:O	2.19	0.43
1:A:936:LYS:C	1:A:938:MET:N	2.71	0.43
1:B:929:SER:OG	1:B:930:VAL:N	2.51	0.43
1:A:472:THR:O	1:A:473:SER:C	2.56	0.43
1:A:382:PHE:N	1:A:720:SER:HB3	2.33	0.43
1:A:40:GLU:HB3	1:A:42:TYR:HE1	1.83	0.43
1:B:396:ILE:HD12	1:B:396:ILE:O	2.18	0.43
1:B:507:GLN:NE2	1:B:553:SER:HB3	2.31	0.43
1:B:553:SER:HA	1:B:554:PRO:HD3	1.89	0.43
1:B:59:GLY:HA3	1:B:81:THR:OG1	2.18	0.43
1:B:654:ASP:HA	1:B:675:GLU:HG3	2.01	0.43
1:A:513:GLY:C	1:A:515:ALA:H	2.22	0.43
1:B:969:GLU:OE2	1:B:971:ALA:HB3	2.19	0.43
1:A:10:GLN:HB3	1:A:1037:ILE:HB	2.01	0.43
1:A:1054:MET:HE3	1:A:1094:ILE:HG23	2.01	0.43
1:A:656:PRO:HB2	1:A:671:VAL:HB	2.01	0.43
1:A:873:MET:HA	1:A:881:LEU:O	2.19	0.43
1:B:362:MET:HB3	1:B:377:THR:HG22	2.00	0.43
1:B:978:GLN:NE2	1:B:995:VAL:HG11	2.28	0.43
1:A:263:ARG:HB2	1:A:271:TYR:CE2	2.54	0.42
1:B:5:TYR:CE2	1:B:7:VAL:HG23	2.54	0.42
1:B:837:TYR:HA	1:B:838:PRO:HD3	1.91	0.42
1:B:853:TYR:HA	1:B:857:LYS:O	2.19	0.42
1:B:889:ARG:HD2	1:B:891:TYR:CZ	2.55	0.42
1:B:924:GLY:O	1:B:925:ASP:CB	2.67	0.42
1:A:392:ASN:HD21	1:A:709:LYS:HE3	1.84	0.42
1:A:697:SER:O	1:A:698:THR:CB	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:870:VAL:HG11	1:A:873:MET:HE3	2.01	0.42
1:B:40:GLU:HB3	1:B:42:TYR:CE1	2.55	0.42
1:B:716:PRO:HB2	1:B:718:TYR:CE1	2.53	0.42
1:A:133:LEU:HB2	1:A:141:LYS:HB3	2.02	0.42
1:A:165:ILE:HG12	1:A:188:ARG:HH21	1.83	0.42
1:A:182:TYR:CZ	1:A:189:HIS:HB2	2.53	0.42
1:A:641:PHE:HA	1:A:681:PRO:HG3	2.02	0.42
1:B:458:PHE:HE2	1:B:473:SER:HA	1.85	0.42
1:B:909:ILE:HG21	1:B:927:MET:CG	2.45	0.42
1:B:722:ARG:HH12	2:D:159:ARG:HH11	1.67	0.42
1:B:722:ARG:NH1	2:D:159:ARG:HH11	2.16	0.42
1:A:471:ILE:HG23	1:A:476:VAL:HB	2.02	0.42
1:A:658:VAL:HG23	1:A:671:VAL:CG2	2.49	0.42
1:B:1000:LEU:HD11	1:B:1030:PHE:CE1	2.55	0.42
1:B:812:TYR:N	1:B:812:TYR:HD2	2.17	0.42
1:B:6:VAL:HG23	1:B:1090:ASP:HA	2.01	0.42
1:B:910:MET:CE	1:B:926:LEU:HD22	2.50	0.42
1:A:425:LEU:O	1:A:436:LEU:HB2	2.19	0.42
1:B:507:GLN:HE22	1:B:553:SER:N	2.18	0.42
1:B:985:THR:HB	1:B:989:ARG:HB2	2.02	0.42
1:A:261:HIS:HA	1:A:272:LEU:O	2.19	0.42
1:A:632:GLY:HA3	1:A:654:ASP:OD1	2.19	0.42
1:A:698:THR:O	1:A:698:THR:HG22	2.20	0.42
1:B:478:LEU:HD22	1:B:488:SER:HB3	2.01	0.42
1:B:893:TRP:CZ3	1:B:899:VAL:HG22	2.46	0.42
1:A:511:ALA:HA	1:A:515:ALA:O	2.20	0.42
1:B:13:THR:HB	1:B:355:ASN:HA	2.01	0.42
1:B:463:VAL:HG11	1:B:521:ILE:HD12	2.02	0.42
1:A:328:LEU:O	1:A:380:GLY:HA2	2.20	0.42
1:A:519:LEU:HD13	1:A:526:LEU:HD11	2.02	0.42
1:A:704:ILE:HA	1:A:704:ILE:HD13	1.83	0.42
1:B:608:ASP:OD2	1:B:608:ASP:N	2.53	0.42
1:B:932:LEU:HD13	1:B:965:PHE:CZ	2.55	0.42
1:A:266:PRO:C	1:A:268:GLY:H	2.23	0.41
1:A:947:ARG:HE	1:A:947:ARG:HB2	1.60	0.41
1:B:468:LEU:HB2	1:B:479:VAL:HB	2.01	0.41
1:B:6:VAL:HG12	1:B:1040:VAL:HG22	2.02	0.41
1:A:1007:PHE:CD2	1:A:1030:PHE:HB3	2.55	0.41
1:A:5:TYR:CZ	1:A:1091:GLY:HA3	2.55	0.41
1:A:553:SER:HA	1:A:554:PRO:HD3	1.91	0.41
1:A:924:GLY:HA2	1:A:930:VAL:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:ARG:CG	1:B:302:VAL:N	2.79	0.41
1:B:564:ILE:O	1:B:582:LEU:HB2	2.20	0.41
1:A:972:PHE:HB3	1:A:1002:GLU:H	1.84	0.41
1:A:220:ILE:HD12	1:A:232:ILE:HD11	2.02	0.41
1:B:873:MET:HE2	1:B:880:LEU:HD21	2.01	0.41
1:B:1058:LEU:HD22	1:B:1062:ILE:HD12	2.02	0.41
1:B:1072:PHE:O	1:B:1075:SER:HB2	2.20	0.41
1:A:5:TYR:CE1	1:A:1091:GLY:HA3	2.55	0.41
1:A:789:HIS:CE1	2:C:159:ARG:HH12	2.38	0.41
1:B:301:ARG:HB3	1:B:301:ARG:HE	1.73	0.41
1:A:342:GLU:OE1	1:A:342:GLU:HA	2.20	0.41
1:B:6:VAL:CG1	1:B:1040:VAL:HG22	2.51	0.41
1:A:84:TYR:CB	1:A:109:GLN:HB3	2.51	0.41
1:B:508:VAL:HB	1:B:519:LEU:HB2	2.03	0.41
1:B:761:LEU:HD12	1:B:802:LEU:HA	2.03	0.41
1:B:879:LYS:HD3	1:B:892:GLU:HG2	2.01	0.41
1:B:871:TYR:CE1	1:B:885:ASN:OD1	2.66	0.41
1:A:1058:LEU:HD22	1:A:1062:ILE:HD11	2.02	0.41
1:A:141:LYS:HE2	1:A:156:ASN:HD21	1.85	0.41
1:A:177:THR:HG21	1:A:206:PRO:HD3	2.02	0.41
1:A:910:MET:CE	1:A:926:LEU:HD22	2.50	0.41
1:B:81:THR:O	1:B:84:TYR:N	2.47	0.41
1:B:60:LYS:HE2	1:B:972:PHE:CD1	2.56	0.41
1:B:561:TRP:CE3	1:B:587:ILE:HG21	2.56	0.41
1:B:589:ARG:HG3	1:B:635:PRO:HB3	2.03	0.41
1:A:202:PHE:HA	1:A:202:PHE:HD2	1.80	0.40
1:A:917:LYS:O	1:A:919:ASP:N	2.54	0.40
1:B:29:LEU:HD23	1:B:44:VAL:HG21	2.03	0.40
1:A:256:SER:HB3	1:A:275:ASP:OD2	2.21	0.40
1:A:367:LEU:CD2	1:A:796:GLN:HB2	2.52	0.40
1:A:213:GLU:HG3	1:A:215:GLU:H	1.87	0.40
1:B:217:SER:O	1:B:218:MET:HG2	2.21	0.40
1:B:365:VAL:HG12	1:B:367:LEU:H	1.86	0.40
1:B:64:MET:HG3	1:B:77:LEU:HD11	2.02	0.40
1:B:5:TYR:CE2	1:B:7:VAL:CG2	3.04	0.40
1:B:812:TYR:HD1	2:D:159:ARG:CZ	2.33	0.40
1:B:939:GLU:HG3	1:B:941:ASN:HB2	2.02	0.40
1:A:5:TYR:CE2	1:A:7:VAL:HG22	2.57	0.40
1:B:1039:LEU:HD22	1:B:1140:HIS:HB3	2.03	0.40
1:B:38:ARG:HD2	1:B:38:ARG:HA	1.72	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	1106/1143 (97%)	921 (83%)	134 (12%)	51 (5%)	2	15
1	B	1106/1143 (97%)	906 (82%)	161 (15%)	39 (4%)	3	21
2	C	11/13 (85%)	9 (82%)	2 (18%)	0	100	100
2	D	11/13 (85%)	10 (91%)	0	1 (9%)	1	4
All	All	2234/2312 (97%)	1846 (83%)	297 (13%)	91 (4%)	3	18

All (91) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	514	ARG
1	A	599	SER
1	A	683	ASN
1	A	886	SER
1	A	904	ASN
1	A	906	TYR
1	A	918	GLY
1	A	970	ASN
1	B	148	ASP
1	B	223	PRO
1	B	367	LEU
1	B	662	SER
1	B	683	ASN
1	B	689	ASP
1	B	706	GLU
1	B	751	ALA
1	B	918	GLY
1	B	925	ASP
1	B	1014	MET
1	A	148	ASP
1	A	235	GLU
1	A	242	GLY

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Mol	Chain	Res	Type
1	A	310	ILE
1	A	554	PRO
1	A	664	HIS
1	A	705	ASP
1	A	903	CYS
1	A	938	MET
1	A	1081	LYS
1	A	1126	ALA
1	B	494	GLN
1	B	523	PRO
1	B	554	PRO
1	B	707	ILE
1	B	919	ASP
1	B	998	PHE
1	B	1126	ALA
1	A	163	HIS
1	A	343	GLN
1	A	422	TYR
1	A	473	SER
1	A	483	PRO
1	A	485	ALA
1	A	708	GLN
1	A	885	ASN
1	A	919	ASP
1	B	35	LYS
1	B	255	GLN
1	B	262	ASN
1	B	318	ASP
1	B	343	GLN
1	B	449	MET
1	B	474	ALA
1	B	514	ARG
1	A	357	GLY
1	A	672	ASN
1	A	698	THR
1	A	714	THR
1	A	905	HIS
1	A	962	ASP
1	A	1137	THR
1	B	235	GLU
1	B	571	LEU
1	B	664	HIS

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Mol	Chain	Res	Type
1	B	705	ASP
1	B	885	ASN
1	A	262	ASN
1	A	294	THR
1	A	318	ASP
1	A	430	VAL
1	A	494	GLN
1	A	529	ILE
1	A	577	LEU
1	A	772	SER
1	A	951	PRO
1	B	696	ASN
1	B	987	GLU
1	B	1125	THR
2	D	155	LEU
1	A	522	HIS
1	A	546	LEU
1	B	137	ASP
1	B	493	PRO
1	A	937	PRO
1	A	358	PRO
1	A	564	ILE
1	B	310	ILE
1	A	482	GLU
1	A	571	LEU
1	B	371	GLY
1	B	838	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	977/1001 (98%)	882 (90%)	95 (10%)	8	28
1	B	977/1001 (98%)	866 (89%)	111 (11%)	5	21
2	C	10/10 (100%)	10 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	10/10 (100%)	9 (90%)	1 (10%)	7	27
All	All	1974/2022 (98%)	1767 (90%)	207 (10%)	7	25

All (207) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	27	GLU
1	A	28	ASP
1	A	39	LEU
1	A	40	GLU
1	A	49	LEU
1	A	96	GLU
1	A	98	ILE
1	A	102	THR
1	A	103	ARG
1	A	111	ARG
1	A	118	THR
1	A	125	ASP
1	A	135	LEU
1	A	141	LYS
1	A	147	ARG
1	A	148	ASP
1	A	159	LEU
1	A	162	LEU
1	A	183	GLN
1	A	197	LEU
1	A	202	PHE
1	A	222	VAL
1	A	235	GLU
1	A	236	SER
1	A	243	ASP
1	A	256	SER
1	A	283	LEU
1	A	285	LEU
1	A	291	MET
1	A	301	ARG
1	A	309	SER
1	A	312	GLU
1	A	321	VAL
1	A	391	ARG
1	A	392	ASN

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Mol	Chain	Res	Type
1	A	398	GLU
1	A	401	SER
1	A	410	LEU
1	A	434	ARG
1	A	445	GLU
1	A	452	VAL
1	A	472	THR
1	A	476	VAL
1	A	484	LYS
1	A	525	GLU
1	A	526	LEU
1	A	541	LEU
1	A	544	THR
1	A	560	LEU
1	A	569	LEU
1	A	586	ILE
1	A	587	ILE
1	A	591	ILE
1	A	613	TYR
1	A	654	ASP
1	A	661	SER
1	A	664	HIS
1	A	668	PHE
1	A	673	LEU
1	A	679	MET
1	A	682	LEU
1	A	700	THR
1	A	701	ILE
1	A	704	ILE
1	A	722	ARG
1	A	729	VAL
1	A	738	SER
1	A	739	ARG
1	A	743	GLN
1	A	817	VAL
1	A	837	TYR
1	A	858	LEU
1	A	866	VAL
1	A	884	ILE
1	A	885	ASN
1	A	886	SER
1	A	899	VAL

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Mol	Chain	Res	Type
1	A	906	TYR
1	A	909	ILE
1	A	917	LYS
1	A	921	ILE
1	A	966	LEU
1	A	969	GLU
1	A	979	LYS
1	A	985	THR
1	A	1000	LEU
1	A	1011	SER
1	A	1014	MET
1	A	1045	GLU
1	A	1052	LEU
1	A	1054	MET
1	A	1063	LYS
1	A	1093	LEU
1	A	1127	ASP
1	B	13	THR
1	B	27	GLU
1	B	38	ARG
1	B	40	GLU
1	B	54	GLU
1	B	57	MET
1	B	75	ASP
1	B	96	GLU
1	B	98	ILE
1	B	102	THR
1	B	103	ARG
1	B	117	GLU
1	B	135	LEU
1	B	137	ASP
1	B	141	LYS
1	B	147	ARG
1	B	148	ASP
1	B	151	GLU
1	B	159	LEU
1	B	162	LEU
1	B	174	GLN
1	B	190	VAL
1	B	198	ARG
1	B	202	PHE
1	B	212	VAL

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Mol	Chain	Res	Type
1	B	236	SER
1	B	248	ILE
1	B	291	MET
1	B	296	THR
1	B	301	ARG
1	B	318	ASP
1	B	334	VAL
1	B	338	VAL
1	B	340	SER
1	B	342	GLU
1	B	366	ASP
1	B	372	GLN
1	B	391	ARG
1	B	398	GLU
1	B	403	ASP
1	B	410	LEU
1	B	414	ARG
1	B	429	PHE
1	B	439	ASN
1	B	447	GLU
1	B	469	ILE
1	B	476	VAL
1	B	484	LYS
1	B	490	TRP
1	B	525	GLU
1	B	534	MET
1	B	540	CYS
1	B	544	THR
1	B	553	SER
1	B	555	LEU
1	B	561	TRP
1	B	567	ARG
1	B	579	LYS
1	B	587	ILE
1	B	589	ARG
1	B	602	LEU
1	B	618	ILE
1	B	622	LEU
1	B	633	THR
1	B	640	THR
1	B	652	CYS
1	B	655	ARG

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Mol	Chain	Res	Type
1	B	667	VAL
1	B	668	PHE
1	B	679	MET
1	B	682	LEU
1	B	700	THR
1	B	701	ILE
1	B	703	THR
1	B	719	GLU
1	B	720	SER
1	B	725	CYS
1	B	729	VAL
1	B	743	GLN
1	B	749	THR
1	B	750	THR
1	B	772	SER
1	B	812	TYR
1	B	814	LEU
1	B	817	VAL
1	B	826	ASN
1	B	844	LYS
1	B	847	ARG
1	B	866	VAL
1	B	896	GLU
1	B	899	VAL
1	B	901	THR
1	B	909	ILE
1	B	917	LYS
1	B	921	ILE
1	B	941	ASN
1	B	955	SER
1	B	966	LEU
1	B	969	GLU
1	B	979	LYS
1	B	985	THR
1	B	986	ASP
1	B	1000	LEU
1	B	1014	MET
1	B	1045	GLU
1	B	1063	LYS
1	B	1080	ARG
1	B	1093	LEU
1	B	1100	ILE

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Mol	Chain	Res	Type
1	B	1127	ASP
1	B	1139	ILE
2	D	159	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	16	ASN
1	A	30	ASN
1	A	109	GLN
1	A	189	HIS
1	A	261	HIS
1	A	332	GLN
1	A	337	ASN
1	A	370	GLN
1	A	372	GLN
1	A	392	ASN
1	A	455	GLN
1	A	462	ASN
1	A	634	GLN
1	A	648	ASN
1	A	664	HIS
1	A	683	ASN
1	A	731	GLN
1	A	796	GLN
1	A	885	ASN
1	A	1059	ASN
1	A	1070	HIS
1	A	1077	HIS
1	B	4	ASN
1	B	22	HIS
1	B	30	ASN
1	B	262	ASN
1	B	267	ASN
1	B	332	GLN
1	B	337	ASN
1	B	392	ASN
1	B	456	GLN
1	B	467	GLN
1	B	507	GLN
1	B	617	ASN

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Mol	Chain	Res	Type
1	B	648	ASN
1	B	683	ASN
1	B	731	GLN
1	B	796	GLN
1	B	803	HIS
1	B	805	HIS
1	B	852	GLN
1	B	877	ASN
1	B	905	HIS
1	B	908	ASN
1	B	941	ASN
1	B	950	ASN
1	B	978	GLN
1	B	1056	ASN
1	B	1140	HIS

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, 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%)	0.14	51 (4%) 32 32	39, 68, 118, 134	0
1	B	1114/1143 (97%)	0.14	49 (4%) 34 34	42, 69, 120, 137	0
2	C	13/13 (100%)	1.02	3 (23%) 0 1	81, 84, 86, 86	0
2	D	13/13 (100%)	3.50	9 (69%) 0 0	100, 103, 104, 104	0
All	All	2254/2312 (97%)	0.17	112 (4%) 28 29	39, 68, 120, 137	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	508	VAL	11.6
1	A	293	GLY	10.4
1	B	508	VAL	10.1
2	D	165	SER	9.2
2	D	164	GLY	7.5
1	B	502	SER	7.4
1	B	294	THR	6.7
1	A	294	THR	6.4
2	D	160	GLU	6.1
1	B	444	GLU	5.8
1	A	616	LEU	5.8
1	B	510	VAL	5.4
1	B	571	LEU	5.3
1	B	528	GLN	5.2
1	A	519	LEU	5.1
1	B	293	GLY	4.9
1	B	509	VAL	4.9
1	A	509	VAL	4.8
1	A	517	TYR	4.6
1	B	483	PRO	4.2
1	B	462	ASN	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	518	TYR	4.1
1	A	481	GLN	4.1
1	A	447	GLU	4.0
1	A	506	SER	4.0
1	A	521	ILE	4.0
1	B	130	MET	3.9
1	A	295	VAL	3.9
1	B	519	LEU	3.9
2	D	156	PRO	3.8
1	B	446	THR	3.8
2	D	161	ARG	3.8
1	A	468	LEU	3.8
1	B	295	VAL	3.7
1	B	585	GLU	3.7
1	A	483	PRO	3.6
1	B	1015	GLN	3.6
1	B	577	LEU	3.6
1	A	292	ASP	3.6
1	A	367	LEU	3.4
1	A	773	SER	3.4
1	B	517	TYR	3.3
2	D	163	LEU	3.3
1	A	594	THR	3.3
1	B	460	CYS	3.2
1	A	426	VAL	3.2
1	A	425	LEU	3.2
1	A	413	LEU	3.2
1	B	516	LEU	3.2
1	B	521	ILE	3.1
1	B	613	TYR	3.0
1	B	518	TYR	3.0
2	D	159	ARG	3.0
2	C	164	GLY	2.9
1	A	443	VAL	2.9
1	B	405	PRO	2.9
1	A	501	ALA	2.8
1	B	144	PRO	2.8
1	B	195	VAL	2.8
1	B	541	LEU	2.8
1	A	446	THR	2.8
1	B	418	ASN	2.7
1	A	568	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	616	LEU	2.7
1	A	314	LEU	2.7
1	B	627	LYS	2.6
1	B	292	ASP	2.6
1	A	553	SER	2.6
1	B	773	SER	2.6
1	A	462	ASN	2.6
1	A	435	VAL	2.5
1	A	1026	GLY	2.5
2	C	156	PRO	2.5
1	A	661	SER	2.5
1	B	985	THR	2.4
1	A	510	VAL	2.4
1	B	501	ALA	2.4
1	B	369	ARG	2.4
1	B	572	PRO	2.4
1	A	1015	GLN	2.4
2	C	165	SER	2.4
1	A	502	SER	2.3
1	B	863	GLU	2.3
1	A	650	PHE	2.3
1	B	415	SER	2.3
1	A	418	ASN	2.2
1	A	635	PRO	2.2
1	B	468	LEU	2.2
1	B	434	ARG	2.2
1	B	783	GLY	2.2
1	A	451	PHE	2.2
1	B	419	ARG	2.2
1	A	593	MET	2.2
1	B	1010	GLY	2.2
1	A	503	CYS	2.2
1	A	145	LEU	2.2
1	B	554	PRO	2.1
1	A	621	GLY	2.1
1	A	569	LEU	2.1
1	A	638	LEU	2.1
1	A	311	ALA	2.1
1	B	9	ALA	2.1
2	D	157	ALA	2.1
1	A	296	THR	2.1
1	B	433	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	657	THR	2.0
1	A	577	LEU	2.0
1	A	277	GLU	2.0
1	A	917	LYS	2.0
2	D	155	LEU	2.0
1	A	662	SER	2.0
1	B	1054	MET	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.