



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:44 AM UTC

PDB ID : 3I7N / pdb_00003i7n
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

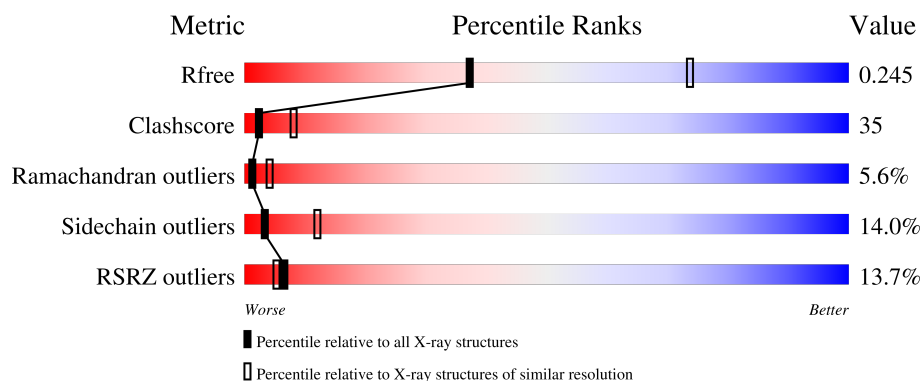
1 Overall quality at a glance

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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 of 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	13% 55% 32% 8% • •
2	B	13	8% 54% 15% 15% 15%

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

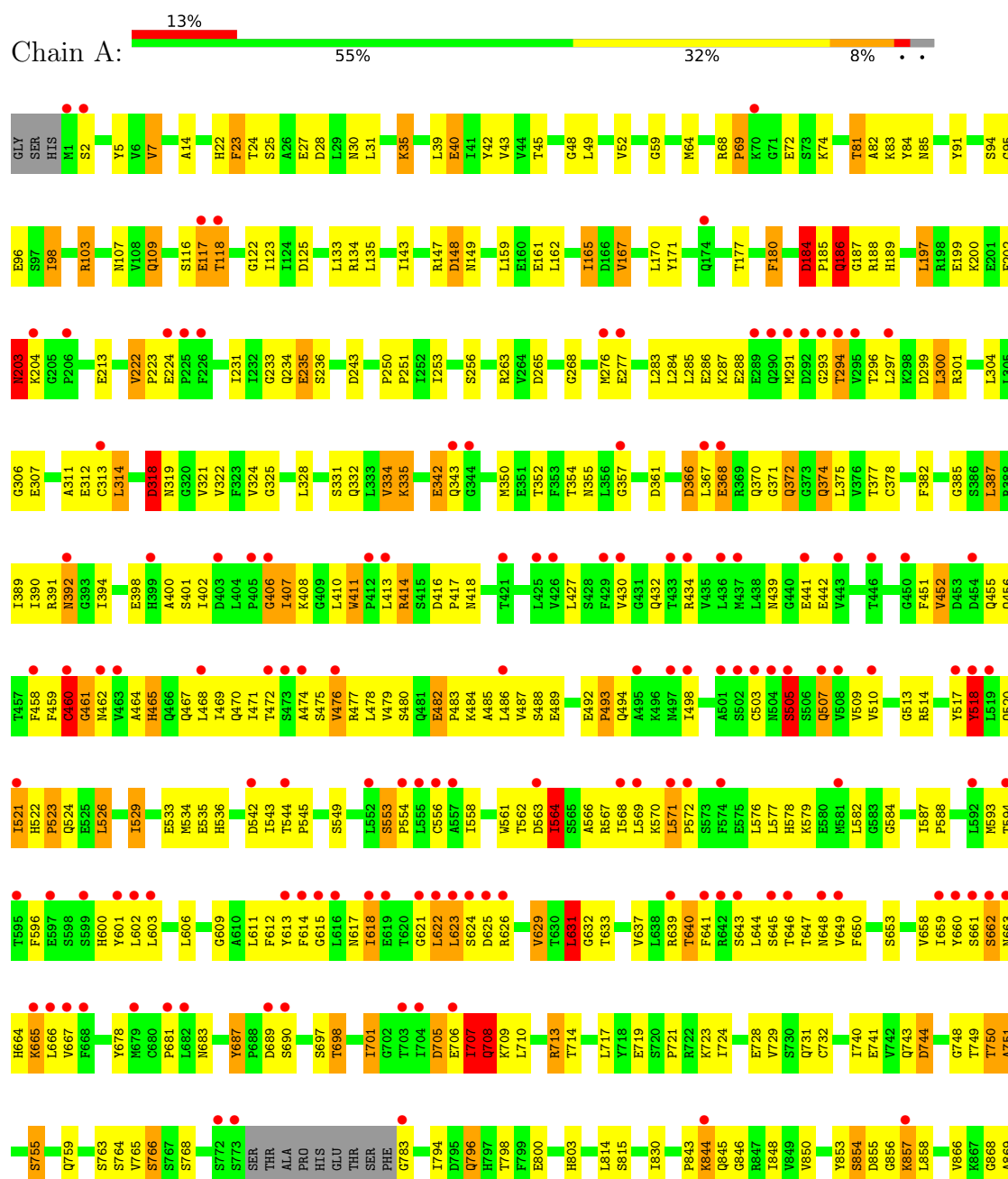
- Molecule 2 is a protein called WD and tetratricopeptide repeats protein 1.

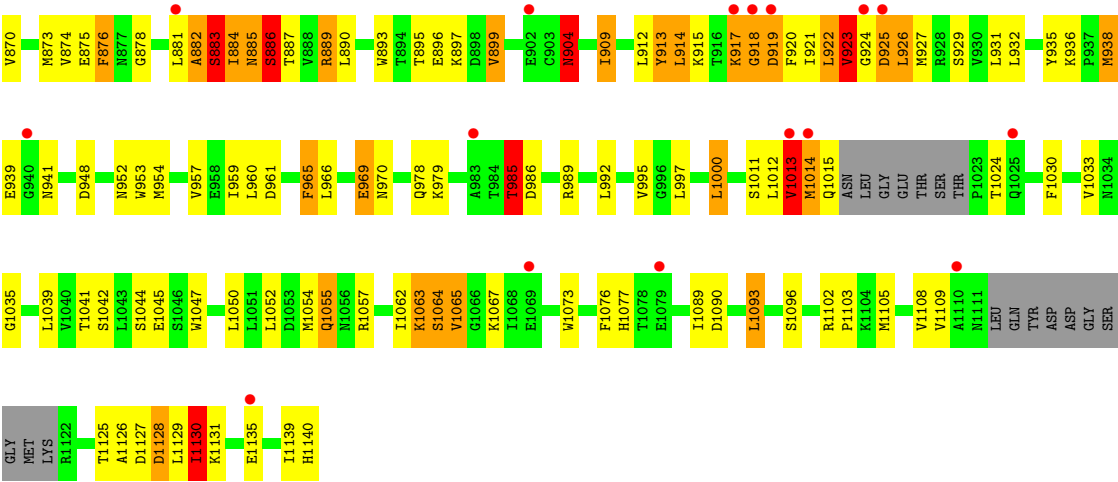
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	13	Total	C	N	O	0	0	0
			116	70	25	21			

3 Residue-property plots [i](#)

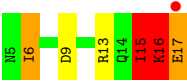
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 2: WD and tetratricopeptide repeats 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 (Not available) , 0.245	Depositor DCC
R_{free} test set	1972 reflections (4.99%)	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 , 59.6	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	0.97	10/8885 (0.1%)	1.29	69/12034 (0.6%)
2	B	1.57	2/115 (1.7%)	1.86	4/150 (2.7%)
All	All	0.98	12/9000 (0.1%)	1.30	73/12184 (0.6%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	899	VAL	CA-CB	10.43	1.65	1.53
1	A	925	ASP	N-CA	8.81	1.58	1.46
1	A	924	GLY	N-CA	8.48	1.54	1.45
1	A	912	LEU	CA-C	-8.03	1.42	1.52
2	B	13	ARG	CZ-NH2	6.42	1.41	1.33
1	A	913	TYR	N-CA	6.18	1.53	1.45
2	B	16	LYS	N-CA	6.06	1.54	1.46
1	A	848	ILE	CA-CB	-5.43	1.48	1.54
1	A	914	LEU	C-O	5.43	1.30	1.23
1	A	882	ALA	CA-CB	-5.34	1.44	1.53
1	A	385	GLY	N-CA	5.08	1.52	1.45
1	A	143	ILE	CA-CB	-5.05	1.48	1.53

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	561	TRP	N-CA-C	35.50	156.59	112.92
1	A	342	GLU	N-CA-C	27.22	147.72	112.34
1	A	561	TRP	CB-CA-C	-20.17	76.47	110.56
1	A	343	GLN	N-CA-C	-16.91	92.50	114.31
1	A	367	LEU	N-CA-C	-14.71	89.05	111.56
1	A	564	ILE	N-CA-C	-13.20	86.95	107.15
1	A	343	GLN	N-CA-CB	-12.42	94.38	110.90
1	A	562	THR	N-CA-CB	-11.95	93.12	110.81
1	A	714	THR	N-CA-C	11.86	127.75	109.96
2	B	13	ARG	NE-CZ-NH1	-10.59	110.91	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	924	GLY	N-CA-C	10.40	126.40	111.00
1	A	187	GLY	N-CA-C	10.35	131.51	112.77
1	A	714	THR	N-CA-CB	-8.88	96.62	109.85
1	A	925	ASP	N-CA-C	8.69	121.89	108.07
1	A	387	LEU	N-CA-C	-8.52	96.40	109.95
1	A	514	ARG	N-CA-C	-8.52	102.44	113.17
1	A	564	ILE	N-CA-CB	-8.44	102.04	111.66
1	A	374	GLN	N-CA-C	-7.92	98.80	110.52
1	A	664	HIS	N-CA-C	-7.75	102.08	114.09
1	A	926	LEU	N-CA-C	7.28	120.63	111.24
1	A	342	GLU	CB-CA-C	-7.02	94.45	110.18
1	A	556	CYS	N-CA-C	6.95	119.50	109.14
1	A	914	LEU	CA-C-O	-6.95	113.55	121.40
1	A	923	VAL	CA-C-O	-6.94	114.44	120.96
1	A	367	LEU	N-CA-CB	-6.63	99.80	110.14
1	A	633	THR	N-CA-C	-6.51	105.49	113.50
1	A	83	LYS	N-CA-C	-6.37	105.80	112.93
1	A	1035	GLY	N-CA-C	-6.27	105.97	115.00
1	A	553	SER	CA-C-N	6.23	127.63	119.84
1	A	553	SER	C-N-CA	6.23	127.63	119.84
1	A	1128	ASP	N-CA-C	-6.18	104.65	111.82
2	B	15	ILE	CA-C-N	6.11	133.22	121.54
2	B	15	ILE	C-N-CA	6.11	133.22	121.54
1	A	889	ARG	N-CA-C	6.04	118.60	109.41
1	A	915	LYS	N-CA-C	-6.02	99.99	108.96
1	A	884	ILE	N-CA-C	5.88	117.12	107.24
1	A	969	GLU	N-CA-C	5.86	117.97	109.07
1	A	413	LEU	N-CA-C	5.83	117.11	107.20
1	A	1013	VAL	N-CA-C	5.79	121.39	109.34
2	B	13	ARG	NE-CZ-NH2	5.76	124.39	119.20
1	A	265	ASP	CA-C-N	5.76	126.15	119.47
1	A	265	ASP	C-N-CA	5.76	126.15	119.47
1	A	759	GLN	N-CA-C	-5.75	105.85	112.92
1	A	887	THR	N-CA-C	-5.62	100.72	109.72
1	A	1062	ILE	N-CA-C	5.61	116.81	108.23
1	A	594	THR	N-CA-C	5.54	115.60	108.34
1	A	938	MET	N-CA-C	-5.53	99.33	108.12
1	A	923	VAL	N-CA-C	5.53	115.13	108.06
1	A	398	GLU	N-CA-C	5.52	117.70	109.25
1	A	125	ASP	CA-C-N	5.48	124.94	119.24
1	A	125	ASP	C-N-CA	5.48	124.94	119.24
1	A	184	ASP	C-N-CD	-5.41	102.84	125.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1077	HIS	N-CA-C	5.39	118.18	108.48
1	A	577	LEU	CA-C-O	5.39	121.06	117.94
1	A	904	ASN	N-CA-C	5.36	117.92	108.75
1	A	878	GLY	N-CA-C	-5.35	107.94	115.32
1	A	649	VAL	N-CA-C	5.32	115.76	107.99
1	A	180	PHE	N-CA-C	5.32	117.48	109.23
1	A	1064	SER	N-CA-C	-5.29	101.91	110.32
1	A	23	PHE	N-CA-C	-5.25	107.25	113.97
1	A	165	ILE	N-CA-C	5.21	115.88	110.82
1	A	1089	ILE	CA-C-N	-5.20	114.24	121.99
1	A	1089	ILE	C-N-CA	-5.20	114.24	121.99
1	A	411	TRP	CA-C-N	5.20	126.33	119.84
1	A	411	TRP	C-N-CA	5.20	126.33	119.84
1	A	965	PHE	N-CA-C	5.19	116.97	108.52
1	A	732	CYS	N-CA-C	5.18	115.89	108.74
1	A	939	GLU	N-CA-C	-5.08	106.92	113.02
1	A	1090	ASP	N-CA-CB	5.05	118.01	109.94
1	A	899	VAL	N-CA-CB	5.04	117.51	111.31
1	A	122	GLY	CA-C-N	-5.01	115.81	122.77
1	A	122	GLY	C-N-CA	-5.01	115.81	122.77
1	A	577	LEU	CB-CA-C	-5.00	109.86	117.07

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	310	0
2	B	116	0	126	3	0
All	All	8842	0	8832	312	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 35.

All (312) 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:623:LEU:HD23	1:A:624:SER:N	1.36	1.37
1:A:881:LEU:CD2	1:A:890:LEU:CD1	2.21	1.19
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: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:HD23	1:A:631:LEU:H	1.16	1.02
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: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: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: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:68:ARG:HH11	1:A:74:LYS:CA	1.82	0.91
1:A:623:LEU:CD2	1:A:624:SER:N	2.31	0.91
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
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:870:VAL:HG11	1:A:873:MET:HE3	1.57	0.86
1:A:389:ILE:HD13	1:A:713:ARG:HD3	1.59	0.85
1:A:844:LYS:H	1:A:844:LYS:HD3	1.41	0.84
1:A:184:ASP:OD1	1:A:189:HIS:HE1	1.60	0.83
1:A:1125:THR:HB	1:A:1128:ASP:HB2	1.59	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:623:LEU:HD23	1:A:623:LEU:C	2.04	0.82
1:A:623:LEU:HD23	1:A:624:SER:H	1.37	0.82
1:A:631:LEU:HD23	1:A:631:LEU:N	1.95	0.81
1:A:571:LEU:HB3	1:A:572:PRO:HD3	1.62	0.81
1:A:23:PHE:H	1:A:30:ASN:HD22	1.28	0.81
1:A:708:GLN:CG	1:A:710:LEU:O	2.29	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:706:GLU:HG3	1:A:707:ILE:H	1.46	0.80
1:A:469:ILE:HD11	1:A:471:ILE:CG1	2.13	0.78
1:A:614:PHE:CE2	1:A:626:ARG:HG3	2.12	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: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:853:TYR:HA	1:A:857:LYS:O	1.87	0.75
1:A:1063:LYS:H	1:A:1063:LYS:HD3	1.51	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:480:SER:CB	1:A:483:PRO:HD2	2.16	0.74
1:A:197:LEU:CD2	1:A:197:LEU:H	1.99	0.74
1:A:1125:THR:HG22	1:A:1126:ALA:N	2.01	0.73
1:A:59:GLY:HA2	1:A:1073:TRP:CZ3	2.23	0.73
1:A:662:SER:HB3	1:A:665:LYS:HB2	1.71	0.72
1:A:116:SER:OG	1:A:134:ARG:CZ	2.37	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:1057:ARG:HD2	1:A:1108:VAL:O	1.91	0.71
1:A:921:ILE:C	1:A:922:LEU:HD12	2.16	0.71
1:A:165:ILE:HG12	1:A:188:ARG:HH21	1.55	0.70
1:A:641:PHE:CZ	1:A:648:ASN:HB2	2.26	0.70
1:A:570:LYS:HZ1	1:A:572:PRO:HD2	1.55	0.70
1:A:184:ASP:OD1	1:A:189:HIS:CE1	2.44	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:536:HIS:CD2	1:A:563:ASP:OD2	2.45	0.69
1:A:876:PHE:CB	1:A:881:LEU:HD11	2.22	0.69
1:A:1065:VAL:C	1:A:1067:LYS:H	1.99	0.69
1:A:743:GLN:HG2	1:A:783:GLY:N	2.09	0.68
1:A:536:HIS:CD2	1:A:563:ASP:CG	2.72	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:876:PHE:CZ	1:A:920:PHE:HA	2.30	0.66
1:A:1024:THR:HB	1:A:1041:THR:CG2	2.23	0.65
1:A:660:TYR:CG	1:A:707:ILE:HG12	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:830:ILE:HG12	1:A:850:VAL:HG22	1.79	0.65
1:A:1014:MET:HG3	1:A:1015:GLN:N	2.10	0.64
1:A:596:PHE:HD1	1:A:601:TYR:CE1	2.16	0.64
1:A:882:ALA:O	1:A:914:LEU:HD11	1.98	0.64
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:234:GLN:C	1:A:235:GLU:HG3	2.22	0.63
1:A:498:ILE:HG23	1:A:510:VAL:HB	1.78	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:477:ARG:HH21	1:A:486:LEU:HD13	1.63	0.62
1:A:641:PHE:HA	1:A:681:PRO:HG3	1.81	0.62
1:A:926:LEU:O	1:A:953:TRP:HA	1.99	0.62
1:A:68:ARG:HD3	1:A:74:LYS:C	2.25	0.62
1:A:570:LYS:HG2	1:A:571:LEU:N	2.13	0.62
1:A:1055:GLN:HG2	1:A:1093:LEU:HD12	1.82	0.61
1:A:322:VAL:HB	1:A:334:VAL:HG12	1.82	0.61
1:A:509:VAL:HG12	1:A:509:VAL:O	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:919:ASP:CG	1:A:920:PHE:H	2.09	0.61
1:A:929:SER:HB3	1:A:952:ASN:HB2	1.82	0.61
1:A:103:ARG:HB3	1:A:103:ARG:NH1	2.13	0.60
1:A:623:LEU:CD2	1:A:623:LEU:C	2.71	0.60
1:A:335:LYS:HB2	1:A:350:MET:SD	2.40	0.60
1:A:708:GLN:HG3	1:A:710:LEU:C	2.25	0.60
1:A:5:TYR:CE2	1:A:7:VAL:HG22	2.37	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:922:LEU:HD12	1:A:922:LEU:N	2.18	0.58
1:A:1127:ASP:O	1:A:1130:ILE:HG22	2.03	0.58
1:A:492:GLU:O	1:A:494:GLN:N	2.34	0.58
1:A:701:ILE:HD13	1:A:701:ILE:H	1.66	0.58
1:A:1093:LEU:O	1:A:1096:SER:HB3	2.04	0.58
1:A:375:LEU:HB2	1:A:1012:LEU:HD21	1.85	0.58
1:A:427:LEU:HD12	1:A:427:LEU:O	2.04	0.58
1:A:475:SER:HA	1:A:498:ILE:HD12	1.85	0.58
1:A:617:ASN:HB2	1:A:621:GLY:HA2	1.84	0.58
1:A:492:GLU:C	1:A:494:GLN:H	2.11	0.58
1:A:1139:ILE:HG22	1:A:1139:ILE:O	2.04	0.58
1:A:1125:THR:CB	1:A:1128:ASP:HB2	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:TYR:C	1:A:518:TYR:CD2	2.83	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:507:GLN:HE22	1:A:553:SER:N	2.01	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:1011:SER:HG	1:A:1013:VAL:CG2	2.19	0.56
1:A:844:LYS:H	1:A:844:LYS:CD	2.17	0.56
1:A:884:ILE:C	1:A:886:SER:H	2.13	0.56
1:A:961:ASP:OD2	1:A:961:ASP:C	2.49	0.56
1:A:660:TYR:CD1	1:A:707:ILE:CG2	2.83	0.55
1:A:451:PHE:CD1	1:A:479:VAL:HG21	2.41	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: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:639:ARG:HG3	1:A:640:THR:N	2.22	0.54
1:A:1044:SER:OG	1:A:1047:TRP:HB2	2.08	0.54
1:A:165:ILE:HG12	1:A:188:ARG:NH2	2.21	0.54
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
1:A:366:ASP:OD1	1:A:366:ASP:N	2.30	0.53
1:A:708:GLN:CD	1:A:710:LEU:O	2.51	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:876:PHE:HB2	1:A:881:LEU:HD12	1.84	0.53
1:A:185:PRO:O	1:A:186:GLN:HG2	2.05	0.53
1:A:1063:LYS:H	1:A:1063:LYS:CD	2.21	0.53
1:A:469:ILE:HG12	1:A:470:GLN:N	2.24	0.52
1:A:596:PHE:CE2	1:A:648:ASN:HA	2.45	0.52
1:A:701:ILE:N	1:A:701:ILE:CD1	2.73	0.52
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1054:MET:SD	1:A:1129:LEU:HD12	2.51	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: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
1:A:895:THR:C	1:A:897:LYS:H	2.19	0.51
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:328:LEU:HD21	2:B:15:ILE:HG23	1.92	0.50
1:A:707:ILE:O	1:A:708:GLN:O	2.29	0.50
1:A:378:CYS:HB3	1:A:721:PRO:HB2	1.94	0.50
1:A:406:GLY:O	1:A:407:ILE:C	2.55	0.50
1:A:617:ASN:CB	1:A:621:GLY:CA	2.84	0.50
1:A:876:PHE:HZ	1:A:920:PHE:HA	1.75	0.50
1:A:885:ASN:O	1:A:886:SER:HB2	2.11	0.50
1:A:1033:VAL:O	1:A:1033:VAL:CG1	2.60	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:874:VAL:CG2	1:A:875:GLU:N	2.75	0.49
1:A:276:MET:O	1:A:276:MET:SD	2.70	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:81:THR:HG23	1:A:82:ALA:N	2.28	0.49
1:A:521:ILE:HD13	1:A:526:LEU:CD2	2.42	0.49
1:A:639:ARG:HG3	1:A:640:THR:H	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: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:535:GLU:HB3	1:A:536:HIS:CD2	2.48	0.48
1:A:843:PRO:CG	1:A:869:ALA:HB2	2.38	0.48
1:A:43:VAL:HG23	1:A:52:VAL:HG21	1.96	0.48
1:A:997:LEU:HB3	1:A:1076:PHE:CD1	2.49	0.48
1:A:1033:VAL:O	1:A:1033:VAL:HG12	2.13	0.48
1:A:615:GLY:N	1:A:624:SER:OG	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:558:ILE:O	1:A:566:ALA:HA	2.15	0.47
1:A:741:GLU:HB3	1:A:749:THR:HB	1.97	0.47
1:A:611:LEU:HD23	1:A:612:PHE:C	2.39	0.47
1:A:744:ASP:N	1:A:748:GLY:O	2.37	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:588:PRO:HA	1:A:606:LEU:HD23	1.96	0.46
1:A:909:ILE:HG22	1:A:925:ASP:CG	2.40	0.46
1:A:159:LEU:HD23	1:A:161:GLU:H	1.80	0.46
1:A:39:LEU:CD1	1:A:64:MET:SD	3.04	0.46
1:A:623:LEU:HD23	1:A:624:SER:C	2.40	0.46
1:A:706:GLU:CG	1:A:707:ILE:H	2.14	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:355:ASN:ND2	1:A:357:GLY:HA2	2.31	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:522:HIS:O	1:A:523:PRO:C	2.59	0.46
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:416:ASP:HA	1:A:417:PRO:HD3	1.78	0.45
1:A:948:ASP:OD1	1:A:948:ASP:C	2.57	0.45
1:A:107:ASN:OD1	1:A:109:GLN:CG	2.59	0.45
1:A:568:ILE:C	1:A:569:LEU:HD12	2.41	0.45
1:A:600:HIS:CD2	1:A:618:ILE:HG12	2.52	0.45
1:A:24:THR:HA	1:A:91:TYR:HD2	1.82	0.45
1:A:611:LEU:HD23	1:A:611:LEU:C	2.42	0.45
1:A:400:ALA:N	1:A:701:ILE:HD11	2.32	0.45
1:A:24:THR:H	1:A:30:ASN:ND2	2.13	0.45
1:A:1039:LEU:HD21	1:A:1139:ILE:HG22	1.99	0.45
1:A:98:ILE:HD13	1:A:98:ILE:N	2.32	0.44
1:A:563:ASP:CG	1:A:563:ASP:O	2.60	0.44
1:A:1041:THR:CG2	1:A:1042:SER:N	2.79	0.44
1:A:81:THR:CG2	1:A:85:ASN:H	2.29	0.44
1:A:609:GLY:HA3	1:A:632:GLY:O	2.17	0.44
1:A:250:PRO:O	1:A:251:PRO:C	2.60	0.44
1:A:402:ILE:O	1:A:698:THR:HA	2.16	0.44
1:A:707:ILE:O	1:A:708:GLN:C	2.60	0.44
1:A:889:ARG:HG2	1:A:904:ASN:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1076:PHE:C	1:A:1076:PHE:CD2	2.96	0.44
1:A:213:GLU:CD	1:A:233:GLY:HA3	2.42	0.44
1:A:534:MET:O	1:A:535:GLU:C	2.59	0.44
1:A:578:HIS:CG	1:A:579:LYS:N	2.86	0.44
1:A:355:ASN:C	1:A:357:GLY:N	2.75	0.44
1:A:45:THR:N	1:A:48:GLY:O	2.46	0.43
1:A:84:TYR:HB2	1:A:109:GLN:HB3	2.00	0.43
1:A:650:PHE:C	1:A:650:PHE:CD2	2.96	0.43
1:A:665:LYS:HB3	1:A:666:LEU:H	1.61	0.43
1:A:920:PHE:HB3	1:A:935:TYR:CB	2.31	0.43
1:A:856:GLY:H	1:A:857:LYS:HG2	1.83	0.43
1:A:1109:VAL:HG21	1:A:1125:THR:O	2.18	0.43
1:A:709:LYS:NZ	1:A:1140:HIS:O	2.32	0.43
1:A:868:GLY:HA3	1:A:884:ILE:HG22	2.00	0.43
1:A:713:ARG:CG	1:A:713:ARG:NH1	2.79	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:596:PHE:CD1	1:A:601:TYR:CE1	3.02	0.43
1:A:697:SER:O	1:A:698:THR:OG1	2.31	0.43
1:A:118:THR:HG22	1:A:118:THR:O	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:728:GLU:O	1:A:729:VAL:C	2.62	0.42
1:A:1000:LEU:HD11	1:A:1030:PHE:CE1	2.54	0.42
1:A:392:ASN:HD21	1:A:709:LYS:HE3	1.84	0.42
1:A:368:GLU:H	1:A:368:GLU:HG2	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:NH1	1:A:414:ARG:HG2	2.35	0.42
1:A:1102:ARG:HA	1:A:1105:MET:HB3	2.02	0.42
1:A:14:ALA:O	1:A:35:LYS:HD2	2.20	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:542:ASP:O	1:A:593:MET:HE3	2.20	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:492:GLU:C	1:A:494:GLN:N	2.77	0.41
1:A:936:LYS:HB2	1:A:938:MET:HE2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:VAL:H	1:A:222:VAL:HG23	1.62	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: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:520:GLN:CD	1:A:529:ILE:HD11	2.46	0.41
1:A:660:TYR:HB3	1:A:661:SER:H	1.58	0.41
1:A:917:LYS:O	1:A:918:GLY:C	2.64	0.41
1:A:1125:THR:CG2	1:A:1126:ALA:N	2.68	0.41
1:A:171:TYR:CD1	1:A:223:PRO:HA	2.56	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:846:GLY:C	1:A:866:VAL:HG22	2.46	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:913:TYR:C	1:A:914:LEU:HG	2.46	0.40
1:A:40:GLU:HB3	1:A:42:TYR:HE1	1.85	0.40
1:A:311:ALA:HB1	1:A:314:LEU:HD13	2.03	0.40
1:A:763:SER:C	1:A:803:HIS:CE1	2.99	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%)	1 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	11/13 (85%)	10 (91%)	0	1 (9%)	0	1
All	All	1117/1156 (97%)	906 (81%)	149 (13%)	62 (6%)	1	4

All (62) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
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
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%)	841 (86%)	136 (14%)	3	12
2	B	13/13 (100%)	10 (77%)	3 (23%)	1	3
All	All	990/1014 (98%)	851 (86%)	139 (14%)	3	12

All (139) 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	40	GLU
1	A	49	LEU
1	A	81	THR
1	A	96	GLU
1	A	98	ILE
1	A	103	ARG
1	A	109	GLN
1	A	117	GLU
1	A	123	ILE
1	A	147	ARG
1	A	148	ASP
1	A	162	LEU
1	A	167	VAL
1	A	186	GLN
1	A	197	LEU
1	A	203	ASN
1	A	204	LYS
1	A	222	VAL
1	A	224	GLU
1	A	231	ILE
1	A	235	GLU
1	A	236	SER
1	A	243	ASP
1	A	283	LEU
1	A	300	LEU
1	A	301	ARG
1	A	307	GLU
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	352	THR
1	A	354	THR
1	A	366	ASP
1	A	368	GLU

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Mol	Chain	Res	Type
1	A	372	GLN
1	A	390	ILE
1	A	392	ASN
1	A	401	SER
1	A	410	LEU
1	A	414	ARG
1	A	418	ASN
1	A	434	ARG
1	A	439	ASN
1	A	441	GLU
1	A	442	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	529	ILE
1	A	533	GLU
1	A	543	ILE
1	A	544	THR
1	A	549	SER
1	A	564	ILE
1	A	567	ARG
1	A	576	LEU
1	A	582	LEU
1	A	587	ILE
1	A	602	LEU
1	A	603	LEU
1	A	613	TYR
1	A	618	ILE
1	A	622	LEU
1	A	623	LEU
1	A	629	VAL
1	A	631	LEU

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Mol	Chain	Res	Type
1	A	637	VAL
1	A	640	THR
1	A	653	SER
1	A	663	ASN
1	A	701	ILE
1	A	707	ILE
1	A	708	GLN
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	794	ILE
1	A	796	GLN
1	A	814	LEU
1	A	815	SER
1	A	844	LYS
1	A	854	SER
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	904	ASN
1	A	909	ILE
1	A	917	LYS
1	A	922	LEU
1	A	923	VAL
1	A	941	ASN
1	A	957	VAL
1	A	960	LEU
1	A	966	LEU
1	A	969	GLU
1	A	979	LYS
1	A	985	THR
1	A	986	ASP
1	A	992	LEU
1	A	1000	LEU
1	A	1013	VAL
1	A	1045	GLU

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Mol	Chain	Res	Type
1	A	1050	LEU
1	A	1052	LEU
1	A	1055	GLN
1	A	1063	LYS
1	A	1064	SER
1	A	1093	LEU
1	A	1130	ILE
1	A	1131	LYS
1	A	1135	GLU
2	B	6	ILE
2	B	15	ILE
2	B	17	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	30	ASN
1	A	109	GLN
1	A	156	ASN
1	A	189	HIS
1	A	203	ASN
1	A	240	HIS
1	A	261	HIS
1	A	332	GLN
1	A	370	GLN
1	A	374	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	462	ASN
1	A	494	GLN
1	A	497	ASN
1	A	507	GLN
1	A	531	HIS
1	A	536	HIS
1	A	617	ASN
1	A	727	GLN
1	A	759	GLN

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Mol	Chain	Res	Type
1	A	790	ASN
1	A	796	GLN
1	A	797	HIS
1	A	809	GLN
1	A	810	ASN
1	A	905	HIS
1	A	907	ASN
1	A	941	ASN
1	A	950	ASN
1	A	978	GLN
1	A	991	HIS
1	A	1055	GLN
1	A	1056	ASN
1	A	1070	HIS
1	A	1106	GLN
1	A	1140	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 oligosaccharides 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 ⓘ

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%)	0.52	153 (13%) 6 5	9, 58, 151, 199	0
2	B	13/13 (100%)	0.38	1 (7%) 19 14	24, 31, 65, 135	0
All	All	1127/1156 (97%)	0.51	154 (13%) 6 5	9, 58, 150, 199	0

All (154) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	508	VAL	9.4
1	A	294	THR	6.8
1	A	462	ASN	6.5
1	A	519	LEU	5.7
1	A	924	GLY	5.7
1	A	616	LEU	5.5
2	B	17	GLU	5.5
1	A	502	SER	5.4
1	A	660	TYR	5.3
1	A	571	LEU	5.3
1	A	902	GLU	5.2
1	A	618	ILE	4.9
1	A	569	LEU	4.7
1	A	572	PRO	4.4
1	A	426	VAL	4.3
1	A	313	CYS	4.3
1	A	613	TYR	4.3
1	A	458	PHE	4.2
1	A	460	CYS	4.2
1	A	557	ALA	4.1
1	A	117	GLU	4.1
1	A	521	ILE	4.0
1	A	626	ARG	4.0
1	A	663	ASN	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	925	ASP	3.8
1	A	568	ILE	3.8
1	A	413	LEU	3.8
1	A	293	GLY	3.7
1	A	510	VAL	3.7
1	A	468	LEU	3.7
1	A	292	ASP	3.7
1	A	556	CYS	3.7
1	A	615	GLY	3.7
1	A	1079	GLU	3.6
1	A	290	GLN	3.5
1	A	357	GLY	3.5
1	A	773	SER	3.5
1	A	918	GLY	3.5
1	A	425	LEU	3.5
1	A	555	LEU	3.5
1	A	204	LYS	3.5
1	A	917	LYS	3.5
1	A	648	ASN	3.5
1	A	297	LEU	3.4
1	A	430	VAL	3.4
1	A	2	SER	3.4
1	A	599	SER	3.4
1	A	503	CYS	3.3
1	A	668	PHE	3.3
1	A	602	LEU	3.3
1	A	603	LEU	3.3
1	A	343	GLN	3.3
1	A	295	VAL	3.3
1	A	639	ARG	3.3
1	A	624	SER	3.3
1	A	542	ASP	3.3
1	A	291	MET	3.3
1	A	518	TYR	3.2
1	A	1014	MET	3.2
1	A	783	GLY	3.2
1	A	881	LEU	3.1
1	A	504	ASN	3.1
1	A	621	GLY	3.1
1	A	501	ALA	3.0
1	A	507	GLN	3.0
1	A	405	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	706	GLU	3.0
1	A	289	GLU	3.0
1	A	597	GLU	3.0
1	A	498	ILE	2.9
1	A	486	LEU	2.9
1	A	646	THR	2.8
1	A	437	MET	2.8
1	A	592	LEU	2.8
1	A	226	PHE	2.8
1	A	495	ALA	2.8
1	A	412	PRO	2.8
1	A	441	GLU	2.7
1	A	595	THR	2.7
1	A	473	SER	2.7
1	A	690	SER	2.7
1	A	563	ASP	2.7
1	A	642	ARG	2.7
1	A	433	THR	2.7
1	A	844	LYS	2.6
1	A	446	THR	2.6
1	A	276	MET	2.6
1	A	666	LEU	2.6
1	A	681	PRO	2.5
1	A	472	THR	2.5
1	A	594	THR	2.5
1	A	505	SER	2.5
1	A	476	VAL	2.5
1	A	574	PHE	2.5
1	A	474	ALA	2.5
1	A	703	THR	2.5
1	A	552	LEU	2.5
1	A	623	LEU	2.5
1	A	344	GLY	2.5
1	A	601	TYR	2.5
1	A	919	ASP	2.4
1	A	659	ILE	2.4
1	A	940	GLY	2.4
1	A	463	VAL	2.4
1	A	983	ALA	2.4
1	A	517	TYR	2.4
1	A	434	ARG	2.4
1	A	614	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	772	SER	2.4
1	A	225	PRO	2.4
1	A	857	LYS	2.3
1	A	667	VAL	2.3
1	A	497	ASN	2.3
1	A	689	ASP	2.3
1	A	367	LEU	2.3
1	A	704	ILE	2.3
1	A	1110	ALA	2.3
1	A	436	LEU	2.3
1	A	399	HIS	2.3
1	A	429	PHE	2.3
1	A	619	GLU	2.3
1	A	70	LYS	2.3
1	A	645	SER	2.3
1	A	661	SER	2.3
1	A	450	GLY	2.3
1	A	443	VAL	2.2
1	A	643	SER	2.2
1	A	682	LEU	2.2
1	A	421	THR	2.2
1	A	625	ASP	2.2
1	A	206	PRO	2.2
1	A	662	SER	2.2
1	A	665	LYS	2.2
1	A	622	LEU	2.2
1	A	1069	GLU	2.2
1	A	554	PRO	2.2
1	A	1025	GLN	2.1
1	A	641	PHE	2.1
1	A	368	GLU	2.1
1	A	392	ASN	2.1
1	A	1013	VAL	2.1
1	A	118	THR	2.1
1	A	174	GLN	2.1
1	A	1	MET	2.1
1	A	581	MET	2.1
1	A	406	GLY	2.1
1	A	403	ASP	2.1
1	A	454	ASP	2.1
1	A	224	GLU	2.1
1	A	1135	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	277	GLU	2.0
1	A	679	MET	2.0
1	A	649	VAL	2.0
1	A	544	THR	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 oligosaccharides 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.