



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:43 PM UTC

PDB ID : 3I7K / pdb_00003i7k
Title : Crystal Structure of DDB1 in Complex with the H-Box Motif of WHX
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

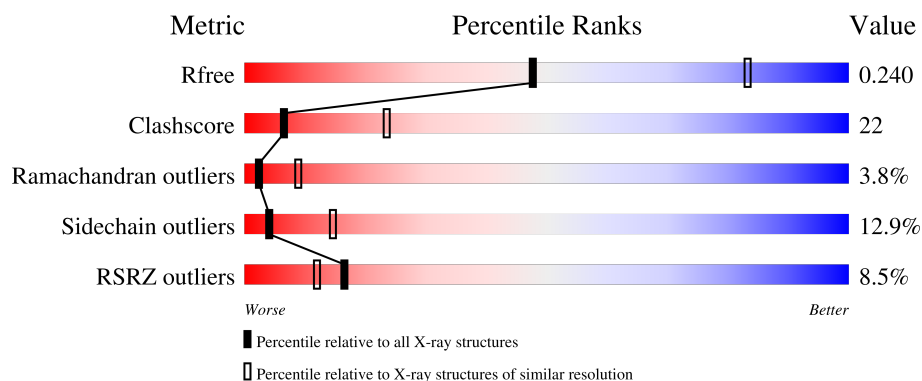
1 Overall quality at a glance

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	8% 54% 34% 9% ...
2	B	14	7% 57% 43%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8843 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

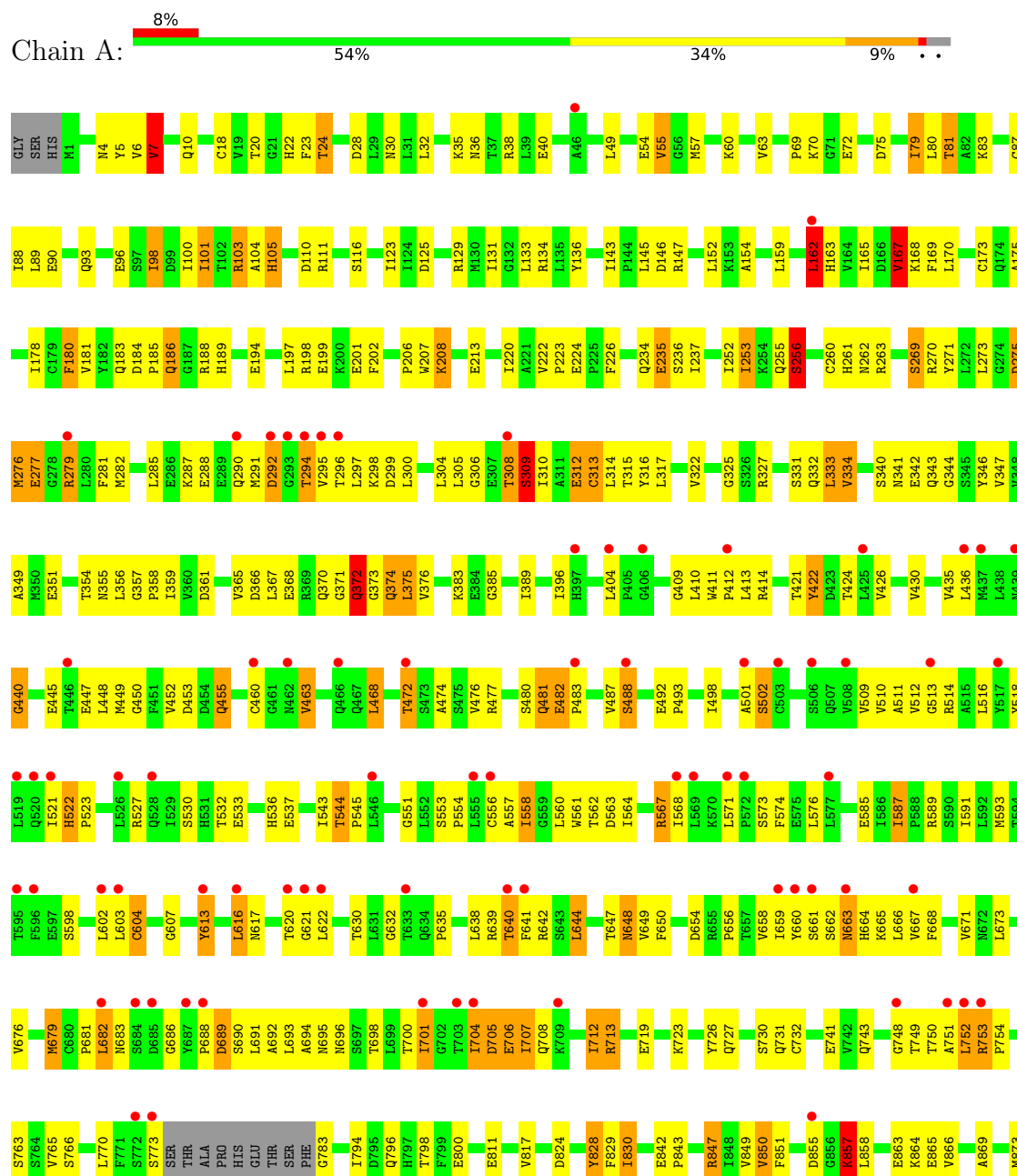
- Molecule 2 is a protein called X protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	14	Total	C	N	O	S	0	0	0
			117	74	23	19	1			

3 Residue-property plots

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





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.08Å 132.22Å 184.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.03 – 2.80 46.03 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.0 (46.03-2.80) 94.0 (46.03-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.230 , 0.271 0.233 , 0.240	Depositor DCC
R_{free} test set	1927 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	55.8	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 64.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8843	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 3.94% 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	0.80	5/8885 (0.1%)	1.18	38/12034 (0.3%)
2	B	0.85	0/121	1.90	3/162 (1.9%)
All	All	0.81	5/9006 (0.1%)	1.19	41/12196 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	899	VAL	CA-CB	7.39	1.63	1.54
1	A	850	VAL	CA-CB	-6.29	1.46	1.54
1	A	851	PHE	CA-C	-5.32	1.46	1.52
1	A	830	ILE	CA-C	-5.32	1.46	1.52
1	A	850	VAL	C-O	-5.06	1.18	1.24

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	290	GLN	N-CA-C	-29.76	84.38	108.78
1	A	290	GLN	CB-CA-C	23.43	150.81	117.07
1	A	291	MET	N-CA-C	-19.63	68.99	110.80
1	A	309	SER	N-CA-CB	-16.88	84.28	111.62
1	A	291	MET	CB-CA-C	-15.40	79.78	110.42
2	B	98	MET	N-CA-CB	-14.41	84.72	110.37
1	A	308	THR	CB-CA-C	11.75	133.80	110.42
1	A	514	ARG	N-CA-CB	-11.66	93.38	110.53
2	B	98	MET	N-CA-C	10.97	134.06	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	514	ARG	N-CA-C	-9.66	101.62	113.50
1	A	292	ASP	N-CA-C	9.64	131.33	110.80
1	A	865	GLU	N-CA-C	-8.64	96.58	110.32
1	A	829	PHE	N-CA-C	-8.13	95.27	108.52
2	B	90	TRP	N-CA-C	-7.39	103.30	111.36
1	A	309	SER	N-CA-C	-7.16	98.48	109.14
1	A	857	LYS	N-CA-C	7.03	118.44	108.74
1	A	275	ASP	N-CA-C	6.96	119.72	110.53
1	A	279	ARG	N-CA-C	-6.55	99.85	110.20
1	A	648	ASN	N-CA-C	6.45	119.72	109.65
1	A	558	ILE	N-CA-C	6.41	116.82	108.35
1	A	1110	ALA	N-CA-C	-6.15	107.61	114.62
1	A	828	TYR	N-CA-C	-6.12	100.22	109.95
1	A	180	PHE	N-CA-C	6.04	118.31	108.76
1	A	167	VAL	CB-CA-C	-5.99	100.34	110.71
1	A	949	PHE	N-CA-C	-5.82	100.69	109.60
1	A	712	ILE	N-CA-C	5.80	116.50	107.28
1	A	184	ASP	CA-C-N	-5.73	113.88	119.78
1	A	184	ASP	C-N-CA	-5.73	113.88	119.78
1	A	404	LEU	CA-C-N	5.60	126.84	119.84
1	A	404	LEU	C-N-CA	5.60	126.84	119.84
1	A	829	PHE	CB-CA-C	-5.45	101.25	110.19
1	A	1053	ASP	N-CA-C	-5.41	105.08	110.97
1	A	903	CYS	N-CA-C	5.27	119.19	112.34
1	A	7	VAL	CB-CA-C	-5.27	102.71	110.82
1	A	682	LEU	N-CA-C	5.23	114.74	107.73
1	A	55	VAL	N-CA-C	5.14	116.12	108.46
1	A	884	ILE	CB-CA-C	-5.12	104.87	111.53
1	A	96	GLU	N-CA-C	-5.10	106.75	113.17
1	A	260	CYS	N-CA-C	5.04	116.47	108.96
1	A	1109	VAL	N-CA-C	5.03	114.81	107.37
1	A	88	ILE	CB-CA-C	-5.01	103.21	110.63

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	312	GLU	Peptide
1	A	522	HIS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8726	0	8706	381	0
2	B	117	0	107	3	0
All	All	8843	0	8813	384	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 22.

All (384) 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:907:ASN:HB2	1:A:942:PHE:CZ	1.77	1.19
1:A:22:HIS:HD2	1:A:28:ASP:O	1.38	1.04
1:A:587:ILE:HD13	1:A:587:ILE:H	1.23	1.04
1:A:750:THR:HG22	1:A:751:ALA:N	1.71	1.03
1:A:750:THR:HG22	1:A:751:ALA:H	0.90	1.03
1:A:907:ASN:HB2	1:A:942:PHE:CE2	1.99	0.97
1:A:522:HIS:HB2	1:A:527:ARG:HH12	1.28	0.94
1:A:753:ARG:HG3	1:A:754:PRO:HD2	1.50	0.93
1:A:907:ASN:CB	1:A:942:PHE:CZ	2.52	0.93
1:A:413:LEU:HB3	1:A:424:THR:HB	1.54	0.90
1:A:907:ASN:HA	1:A:942:PHE:HZ	1.37	0.90
1:A:277:GLU:OE1	1:A:279:ARG:NH1	2.05	0.89
1:A:1051:LEU:HD22	1:A:1094:ILE:HD13	1.54	0.87
1:A:22:HIS:CD2	1:A:28:ASP:O	2.28	0.85
1:A:921:ILE:HG22	1:A:922:LEU:H	1.41	0.85
1:A:589:ARG:HG3	1:A:635:PRO:HB2	1.59	0.84
1:A:282:MET:HB2	1:A:305:LEU:HD21	1.61	0.82
1:A:750:THR:CG2	1:A:751:ALA:H	1.75	0.82
1:A:753:ARG:CG	1:A:754:PRO:HD2	2.09	0.81
1:A:907:ASN:CA	1:A:942:PHE:HZ	1.94	0.81
1:A:1061:VAL:HG21	1:A:1108:VAL:HG22	1.63	0.80
1:A:587:ILE:H	1:A:587:ILE:CD1	1.95	0.79
1:A:262:ASN:ND2	1:A:316:TYR:H	1.81	0.79
1:A:482:GLU:HB3	1:A:483:PRO:HD3	1.65	0.78
1:A:910:MET:O	1:A:910:MET:HG3	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:731:GLN:O	1:A:796:GLN:HG2	1.85	0.77
1:A:24:THR:H	1:A:30:ASN:HD21	1.30	0.77
1:A:480:SER:HB3	1:A:483:PRO:HD2	1.66	0.77
1:A:522:HIS:HB2	1:A:527:ARG:NH1	1.99	0.77
1:A:110:ASP:HB2	1:A:136:TYR:CE1	2.20	0.76
1:A:185:PRO:O	1:A:186:GLN:HB2	1.84	0.76
1:A:752:LEU:O	1:A:753:ARG:HB2	1.85	0.76
1:A:864:LYS:HE2	1:A:899:VAL:O	1.86	0.76
2:B:94:ARG:HA	2:B:97:GLY:O	1.87	0.75
1:A:907:ASN:HD21	1:A:909:ILE:HG13	1.50	0.74
1:A:285:LEU:HD22	1:A:300:LEU:HD22	1.69	0.74
1:A:383:LYS:HB3	1:A:753:ARG:NH2	2.03	0.73
1:A:1026:GLY:O	1:A:1041:THR:HG23	1.88	0.73
1:A:1032:THR:HB	1:A:1036:MET:H	1.53	0.73
1:A:613:TYR:H	1:A:613:TYR:HD2	1.34	0.73
1:A:752:LEU:C	1:A:752:LEU:HD12	2.13	0.73
1:A:752:LEU:O	1:A:753:ARG:CB	2.37	0.73
1:A:83:LYS:NZ	1:A:1077:HIS:HB3	2.03	0.73
1:A:1123:GLU:O	1:A:1124:ALA:HB3	1.89	0.72
1:A:562:THR:O	1:A:564:ILE:HD12	1.90	0.72
1:A:731:GLN:HA	1:A:796:GLN:HE21	1.54	0.71
1:A:1125:THR:HB	1:A:1128:ASP:HB2	1.73	0.71
1:A:770:LEU:HD12	1:A:847:ARG:HD2	1.72	0.70
1:A:309:SER:HB3	1:A:332:GLN:OE1	1.93	0.69
1:A:55:VAL:HG11	1:A:100:ILE:HD12	1.72	0.69
1:A:522:HIS:CB	1:A:527:ARG:HH12	2.03	0.69
1:A:396:ILE:HD11	1:A:673:LEU:HD11	1.75	0.69
1:A:919:ASP:CG	1:A:920:PHE:H	2.01	0.69
1:A:1125:THR:HG22	1:A:1127:ASP:H	1.57	0.68
1:A:676:VAL:HG21	1:A:693:LEU:HD23	1.75	0.68
1:A:894:THR:HG22	1:A:896:GLU:H	1.57	0.68
1:A:907:ASN:CA	1:A:942:PHE:CZ	2.75	0.68
1:A:1032:THR:HG22	1:A:1034:ASN:H	1.59	0.67
1:A:1122:ARG:C	1:A:1123:GLU:CD	2.63	0.66
1:A:375:LEU:HD12	1:A:376:VAL:N	2.11	0.66
1:A:502:SER:HB3	1:A:509:VAL:O	1.95	0.66
1:A:468:LEU:HD21	1:A:481:GLN:HG2	1.77	0.66
1:A:24:THR:CG2	1:A:28:ASP:OD2	2.44	0.66
1:A:308:THR:HG22	1:A:347:VAL:HG11	1.76	0.66
1:A:1122:ARG:C	1:A:1123:GLU:OE1	2.39	0.65
1:A:1110:ALA:C	1:A:1111:ASN:HD22	2.05	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1123:GLU:OE1	1:A:1123:GLU:N	2.30	0.65
1:A:396:ILE:CD1	1:A:673:LEU:HD11	2.27	0.65
1:A:770:LEU:HG	1:A:863:GLU:OE1	1.97	0.64
1:A:1030:PHE:CZ	1:A:1038:GLY:HA3	2.32	0.64
1:A:731:GLN:C	1:A:796:GLN:HG2	2.22	0.63
1:A:411:TRP:HB3	1:A:460:CYS:O	1.99	0.63
1:A:308:THR:CG2	1:A:347:VAL:HG11	2.28	0.62
1:A:24:THR:H	1:A:30:ASN:ND2	1.97	0.62
1:A:285:LEU:HD13	1:A:297:LEU:HD11	1.80	0.62
1:A:907:ASN:OD1	1:A:909:ILE:HB	2.00	0.62
1:A:72:GLU:OE2	1:A:103:ARG:NH2	2.27	0.62
1:A:185:PRO:O	1:A:186:GLN:CB	2.48	0.61
1:A:726:TYR:OH	1:A:796:GLN:NE2	2.33	0.61
1:A:55:VAL:HG11	1:A:100:ILE:CD1	2.29	0.61
1:A:270:ARG:HB3	1:A:282:MET:HE2	1.83	0.61
1:A:1030:PHE:O	1:A:1037:ILE:HA	1.99	0.61
1:A:263:ARG:HG2	1:A:263:ARG:HH11	1.65	0.61
1:A:342:GLU:C	1:A:344:GLY:H	2.09	0.60
1:A:921:ILE:HG22	1:A:922:LEU:N	2.14	0.60
1:A:167:VAL:HG13	1:A:180:PHE:HB3	1.84	0.60
1:A:917:LYS:HD2	1:A:921:ILE:HD12	1.83	0.60
1:A:925:ASP:C	1:A:925:ASP:OD1	2.44	0.60
1:A:263:ARG:HB2	1:A:271:TYR:CE2	2.37	0.60
1:A:798:THR:OG1	1:A:800:GLU:HG2	2.01	0.60
1:A:409:GLY:O	1:A:410:LEU:HD23	2.01	0.60
1:A:389:ILE:HD12	1:A:389:ILE:N	2.17	0.60
1:A:1032:THR:HG22	1:A:1034:ASN:N	2.17	0.59
1:A:879:LYS:HB3	1:A:891:TYR:O	2.02	0.59
1:A:985:THR:HG22	1:A:989:ARG:HD3	1.84	0.59
1:A:1057:ARG:HD3	1:A:1108:VAL:O	2.03	0.59
1:A:370:GLN:HB2	1:A:372:GLN:HG3	1.84	0.59
1:A:660:TYR:HB2	1:A:667:VAL:HB	1.83	0.59
1:A:23:PHE:H	1:A:30:ASN:ND2	1.99	0.59
1:A:24:THR:HG21	1:A:28:ASP:OD2	2.02	0.59
1:A:38:ARG:HD2	1:A:54:GLU:OE1	2.03	0.59
1:A:1125:THR:HG22	1:A:1126:ALA:N	2.18	0.59
1:A:587:ILE:HD13	1:A:587:ILE:N	2.07	0.58
1:A:917:LYS:O	1:A:919:ASP:N	2.37	0.58
1:A:90:GLU:HB3	1:A:101:ILE:CG2	2.34	0.58
1:A:752:LEU:C	1:A:752:LEU:CD1	2.75	0.58
1:A:315:THR:HG22	1:A:317:LEU:HD23	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:PHE:HZ	1:A:287:LYS:HG2	1.67	0.58
1:A:1055:GLN:HE21	1:A:1089:ILE:HG23	1.68	0.58
1:A:917:LYS:HG2	1:A:959:ILE:HG21	1.86	0.58
1:A:1050:LEU:O	1:A:1053:ASP:HB3	2.03	0.58
1:A:662:SER:OG	1:A:663:ASN:N	2.37	0.57
1:A:732:CYS:HB2	1:A:794:ILE:O	2.02	0.57
1:A:1055:GLN:HE22	1:A:1089:ILE:HA	1.69	0.57
1:A:659:ILE:HG12	1:A:668:PHE:CE1	2.39	0.57
1:A:960:LEU:HD21	1:A:966:LEU:HB2	1.86	0.57
1:A:365:VAL:O	1:A:374:GLN:HB2	2.03	0.57
1:A:312:GLU:HG3	1:A:327:ARG:HD3	1.86	0.57
1:A:676:VAL:CG2	1:A:693:LEU:HD23	2.35	0.57
1:A:953:TRP:HB2	1:A:970:ASN:HB2	1.86	0.57
1:A:642:ARG:HA	1:A:647:THR:HB	1.85	0.57
1:A:705:ASP:O	1:A:706:GLU:O	2.22	0.57
1:A:1123:GLU:O	1:A:1124:ALA:CB	2.52	0.57
1:A:90:GLU:HB3	1:A:101:ILE:HG22	1.87	0.56
1:A:741:GLU:HB3	1:A:749:THR:HB	1.87	0.56
1:A:926:LEU:HB3	1:A:931:LEU:HD11	1.86	0.56
1:A:234:GLN:O	1:A:236:SER:N	2.38	0.56
1:A:558:ILE:HG23	1:A:567:ARG:HG2	1.87	0.56
1:A:613:TYR:N	1:A:613:TYR:CD2	2.73	0.56
1:A:888:VAL:HB	1:A:907:ASN:OD1	2.05	0.56
1:A:691:LEU:O	1:A:701:ILE:HA	2.06	0.56
1:A:1102:ARG:NH2	1:A:1126:ALA:HB1	2.19	0.56
1:A:341:ASN:OD1	1:A:342:GLU:O	2.24	0.56
1:A:811:GLU:OE1	1:A:847:ARG:NH1	2.38	0.56
1:A:322:VAL:HB	1:A:334:VAL:HG12	1.88	0.56
1:A:660:TYR:CE1	1:A:707:ILE:HA	2.40	0.56
1:A:312:GLU:HG3	1:A:327:ARG:HB2	1.88	0.56
1:A:7:VAL:HG13	1:A:1091:GLY:HA3	1.88	0.55
1:A:907:ASN:HD21	1:A:909:ILE:CG1	2.19	0.55
1:A:270:ARG:HB3	1:A:282:MET:CE	2.36	0.55
1:A:607:GLY:HA2	1:A:635:PRO:HB3	1.88	0.55
1:A:926:LEU:HG	1:A:927:MET:N	2.21	0.55
1:A:1048:TYR:O	1:A:1052:LEU:HB2	2.07	0.55
1:A:617:ASN:HB2	1:A:620:THR:H	1.72	0.55
1:A:170:LEU:HD13	1:A:207:TRP:CH2	2.42	0.55
1:A:313:CYS:HB3	1:A:325:GLY:HA3	1.89	0.54
1:A:613:TYR:HD2	1:A:613:TYR:N	2.02	0.54
1:A:468:LEU:CD2	1:A:481:GLN:HG2	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:LEU:HB2	1:A:374:GLN:HG3	1.89	0.54
1:A:1047:TRP:HZ3	1:A:1132:VAL:HG13	1.72	0.54
1:A:375:LEU:HD12	1:A:376:VAL:H	1.71	0.54
1:A:591:ILE:HG13	1:A:604:CYS:HB2	1.90	0.53
1:A:917:LYS:HG3	1:A:959:ILE:HD13	1.91	0.53
1:A:220:ILE:HG12	1:A:261:HIS:CE1	2.43	0.53
1:A:511:ALA:HB2	1:A:516:LEU:HD23	1.90	0.53
1:A:206:PRO:O	1:A:207:TRP:HB3	2.09	0.53
1:A:573:SER:O	1:A:574:PHE:HB2	2.08	0.53
1:A:396:ILE:HG22	1:A:704:ILE:HG12	1.89	0.53
1:A:6:VAL:HG22	1:A:1040:VAL:HG22	1.91	0.53
1:A:22:HIS:O	1:A:75:ASP:HB2	2.08	0.53
1:A:385:GLY:HA3	1:A:719:GLU:O	2.09	0.53
1:A:1039:LEU:HD21	1:A:1139:ILE:HG23	1.89	0.53
1:A:935:TYR:CD1	1:A:941:ASN:O	2.61	0.53
1:A:498:ILE:HG23	1:A:510:VAL:HB	1.91	0.53
1:A:1045:GLU:HG2	1:A:1046:SER:N	2.23	0.53
1:A:24:THR:HG22	1:A:28:ASP:OD2	2.09	0.53
1:A:372:GLN:OE1	1:A:373:GLY:N	2.40	0.53
1:A:383:LYS:CB	1:A:753:ARG:NH2	2.72	0.53
1:A:543:ILE:O	1:A:543:ILE:HD12	2.10	0.53
1:A:1136:LEU:O	1:A:1139:ILE:HB	2.08	0.53
1:A:129:ARG:NH2	1:A:197:LEU:HD21	2.24	0.52
1:A:277:GLU:CD	1:A:279:ARG:HH12	2.10	0.52
1:A:532:THR:HG22	1:A:533:GLU:N	2.24	0.52
1:A:492:GLU:HG3	1:A:512:VAL:HG21	1.92	0.52
1:A:907:ASN:HA	1:A:942:PHE:CZ	2.29	0.52
1:A:235:GLU:HA	1:A:253:ILE:HG22	1.91	0.52
1:A:426:VAL:HG21	1:A:460:CYS:SG	2.50	0.52
1:A:894:THR:HG22	1:A:896:GLU:N	2.25	0.52
1:A:226:PHE:CD2	1:A:297:LEU:HD12	2.45	0.51
1:A:5:TYR:OH	1:A:1091:GLY:HA2	2.11	0.51
1:A:472:THR:HG23	1:A:474:ALA:H	1.74	0.51
1:A:18:CYS:N	1:A:313:CYS:SG	2.84	0.51
1:A:110:ASP:HB2	1:A:136:TYR:HE1	1.73	0.51
1:A:727:GLN:HE21	1:A:730:SER:HB2	1.75	0.51
1:A:824:ASP:OD2	1:A:828:TYR:OH	2.23	0.51
1:A:1006:VAL:O	1:A:1030:PHE:HA	2.11	0.51
1:A:864:LYS:CE	1:A:899:VAL:O	2.56	0.51
1:A:543:ILE:HG21	1:A:571:LEU:HD11	1.92	0.51
1:A:928:ARG:HE	1:A:928:ARG:HA	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:CYS:HA	1:A:32:LEU:O	2.11	0.50
1:A:928:ARG:HD3	1:A:953:TRP:HA	1.92	0.50
1:A:881:LEU:HD21	1:A:922:LEU:HD21	1.93	0.50
1:A:923:VAL:HG21	1:A:959:ILE:HG13	1.92	0.50
1:A:93:GLN:HG3	1:A:98:ILE:HG22	1.94	0.50
1:A:482:GLU:CB	1:A:483:PRO:HD3	2.39	0.50
1:A:83:LYS:HZ1	1:A:1077:HIS:HB3	1.77	0.50
1:A:163:HIS:CD2	1:A:183:GLN:HB3	2.47	0.50
1:A:4:ASN:ND2	1:A:976:VAL:HG21	2.27	0.50
1:A:199:GLU:HG3	1:A:201:GLU:HG3	1.94	0.50
1:A:1102:ARG:NH2	1:A:1126:ALA:CB	2.75	0.50
1:A:501:ALA:O	1:A:502:SER:HB2	2.11	0.50
1:A:936:LYS:HG3	1:A:943:GLU:HB2	1.92	0.50
1:A:706:GLU:HG3	1:A:707:ILE:N	2.27	0.50
1:A:340:SER:HB3	1:A:346:TYR:CZ	2.47	0.49
1:A:1097:PHE:HE2	1:A:1130:ILE:HA	1.77	0.49
1:A:536:HIS:HB2	1:A:560:LEU:HD13	1.93	0.49
1:A:942:PHE:O	1:A:942:PHE:CD1	2.64	0.49
1:A:984:THR:O	1:A:986:ASP:N	2.45	0.49
1:A:1054:MET:O	1:A:1058:LEU:HB2	2.12	0.49
1:A:304:LEU:HD12	1:A:306:GLY:H	1.78	0.49
1:A:564:ILE:CD1	1:A:585:GLU:HA	2.41	0.49
1:A:679:MET:HA	1:A:692:ALA:O	2.12	0.49
1:A:104:ALA:O	1:A:105:HIS:HB3	2.11	0.49
1:A:294:THR:HG22	1:A:295:VAL:H	1.78	0.49
1:A:656:PRO:HB2	1:A:671:VAL:HB	1.94	0.49
1:A:811:GLU:OE2	1:A:847:ARG:NH1	2.41	0.49
1:A:10:GLN:O	1:A:1036:MET:O	2.30	0.49
1:A:452:VAL:HG13	1:A:477:ARG:CZ	2.43	0.49
1:A:49:LEU:HD13	1:A:333:LEU:HD21	1.95	0.49
1:A:741:GLU:CB	1:A:749:THR:HB	2.43	0.49
1:A:1080:ARG:HG2	1:A:1081:LYS:HG2	1.93	0.49
1:A:213:GLU:OE1	1:A:234:GLN:O	2.31	0.48
1:A:753:ARG:CG	1:A:754:PRO:CD	2.86	0.48
1:A:985:THR:HA	1:A:989:ARG:HB2	1.95	0.48
1:A:893:TRP:CE3	1:A:899:VAL:HG13	2.47	0.48
1:A:226:PHE:CZ	1:A:287:LYS:HG2	2.47	0.48
1:A:288:GLU:HG3	1:A:298:LYS:HD3	1.95	0.48
1:A:811:GLU:CD	1:A:847:ARG:HH11	2.22	0.48
1:A:743:GLN:HB3	1:A:783:GLY:N	2.28	0.48
1:A:811:GLU:CD	1:A:847:ARG:NH1	2.72	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:GLU:CG	1:A:327:ARG:HD3	2.44	0.48
1:A:888:VAL:HB	1:A:907:ASN:CG	2.38	0.48
1:A:1002:GLU:HB3	1:A:1032:THR:HG23	1.95	0.48
1:A:731:GLN:HA	1:A:796:GLN:NE2	2.24	0.47
1:A:949:PHE:O	1:A:950:ASN:HB3	2.14	0.47
1:A:83:LYS:NZ	1:A:1077:HIS:CB	2.76	0.47
1:A:87:CYS:SG	1:A:89:LEU:HD21	2.55	0.47
1:A:255:GLN:O	1:A:256:SER:C	2.57	0.47
1:A:518:TYR:HB3	1:A:530:SER:HB2	1.96	0.47
1:A:173:CYS:C	1:A:175:ALA:H	2.23	0.47
1:A:660:TYR:CG	1:A:707:ILE:HG23	2.50	0.47
1:A:288:GLU:CG	1:A:298:LYS:HB2	2.45	0.47
1:A:923:VAL:CG2	1:A:959:ILE:HG13	2.45	0.47
1:A:1047:TRP:CZ3	1:A:1132:VAL:HG13	2.50	0.47
1:A:57:MET:HE2	1:A:79:ILE:HG21	1.96	0.47
1:A:440:GLY:O	1:A:686:GLY:HA3	2.14	0.47
2:B:93:ASN:O	2:B:97:GLY:O	2.33	0.47
1:A:864:LYS:HB2	1:A:899:VAL:HG23	1.97	0.47
1:A:679:MET:O	1:A:679:MET:SD	2.72	0.47
1:A:131:ILE:HG22	1:A:133:LEU:CD1	2.45	0.46
1:A:926:LEU:CB	1:A:931:LEU:HD11	2.45	0.46
1:A:502:SER:OG	1:A:543:ILE:HG13	2.15	0.46
1:A:817:VAL:HG12	1:A:830:ILE:HB	1.98	0.46
1:A:1125:THR:CG2	1:A:1126:ALA:N	2.79	0.46
1:A:69:PRO:HD2	1:A:72:GLU:HG3	1.98	0.46
1:A:143:ILE:HG12	1:A:154:ALA:HB2	1.98	0.46
1:A:518:TYR:HB2	1:A:574:PHE:CZ	2.51	0.46
1:A:1030:PHE:CE2	1:A:1038:GLY:HA3	2.50	0.46
1:A:234:GLN:OE1	1:A:234:GLN:HA	2.16	0.46
1:A:688:PRO:O	1:A:689:ASP:C	2.59	0.46
1:A:36:ASN:HD21	1:A:60:LYS:HG2	1.79	0.46
1:A:700:THR:C	1:A:701:ILE:HD13	2.41	0.46
1:A:455:GLN:HE21	1:A:455:GLN:HA	1.80	0.46
1:A:616:LEU:HD12	1:A:622:LEU:O	2.16	0.46
1:A:954:MET:HE1	1:A:967:GLY:HA3	1.97	0.46
1:A:750:THR:CG2	1:A:751:ALA:N	2.45	0.46
1:A:910:MET:O	1:A:925:ASP:O	2.33	0.46
1:A:1107:GLU:C	1:A:1109:VAL:N	2.71	0.46
1:A:919:ASP:HB3	1:A:921:ILE:HG13	1.98	0.46
1:A:679:MET:HB2	1:A:693:LEU:HG	1.98	0.45
1:A:1000:LEU:HD13	1:A:1002:GLU:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:ILE:HG13	1:A:1035:GLY:HA2	1.98	0.45
1:A:662:SER:HB3	1:A:665:LYS:HB3	1.97	0.45
1:A:288:GLU:HG3	1:A:298:LYS:HB2	1.99	0.45
1:A:690:SER:OG	1:A:691:LEU:N	2.50	0.45
1:A:948:ASP:C	1:A:949:PHE:O	2.57	0.45
1:A:183:GLN:HG3	1:A:188:ARG:HG2	1.98	0.45
1:A:424:THR:HG23	1:A:436:LEU:O	2.17	0.45
1:A:450:GLY:C	1:A:477:ARG:HH21	2.25	0.45
1:A:553:SER:HA	1:A:554:PRO:HD3	1.80	0.45
1:A:706:GLU:C	1:A:707:ILE:HG13	2.42	0.45
1:A:857:LYS:HB2	1:A:857:LYS:NZ	2.32	0.45
1:A:1045:GLU:CG	1:A:1046:SER:N	2.79	0.45
1:A:81:THR:HG22	1:A:83:LYS:H	1.81	0.44
1:A:919:ASP:CG	1:A:920:PHE:N	2.72	0.44
1:A:1032:THR:HG22	1:A:1033:VAL:N	2.31	0.44
1:A:383:LYS:CB	1:A:753:ARG:HH21	2.30	0.44
1:A:830:ILE:HG22	1:A:873:MET:HE1	1.99	0.44
2:B:94:ARG:CA	2:B:97:GLY:O	2.63	0.44
1:A:355:ASN:CG	1:A:357:GLY:H	2.26	0.44
1:A:275:ASP:HB3	1:A:277:GLU:H	1.82	0.44
1:A:1127:ASP:O	1:A:1130:ILE:HG22	2.18	0.44
1:A:23:PHE:H	1:A:30:ASN:HD22	1.64	0.44
1:A:358:PRO:HA	1:A:1033:VAL:O	2.17	0.44
1:A:917:LYS:C	1:A:919:ASP:N	2.75	0.44
1:A:598:SER:HB2	1:A:664:HIS:NE2	2.33	0.43
1:A:692:ALA:HA	1:A:700:THR:O	2.17	0.43
1:A:921:ILE:CG2	1:A:932:LEU:HD11	2.47	0.43
1:A:383:LYS:HB3	1:A:753:ARG:HH21	1.82	0.43
1:A:69:PRO:O	1:A:72:GLU:HB2	2.19	0.43
1:A:695:ASN:OD1	1:A:698:THR:N	2.51	0.43
1:A:81:THR:HG22	1:A:83:LYS:N	2.33	0.43
1:A:920:PHE:O	1:A:934:ALA:HA	2.18	0.43
1:A:694:ALA:HA	1:A:698:THR:O	2.19	0.43
1:A:997:LEU:O	1:A:998:PHE:HB2	2.19	0.43
1:A:925:ASP:OD1	1:A:926:LEU:N	2.52	0.42
1:A:1044:SER:O	1:A:1045:GLU:C	2.62	0.42
1:A:123:ILE:HD12	1:A:169:PHE:CD1	2.54	0.42
1:A:563:ASP:O	1:A:564:ILE:C	2.63	0.42
1:A:660:TYR:HB3	1:A:661:SER:H	1.56	0.42
1:A:57:MET:HE3	1:A:57:MET:HB3	1.94	0.42
1:A:134:ARG:HD2	1:A:134:ARG:C	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:ARG:HB2	1:A:422:TYR:HA	2.00	0.42
1:A:639:ARG:HG3	1:A:640:THR:N	2.34	0.42
1:A:893:TRP:HE3	1:A:899:VAL:HG13	1.84	0.42
1:A:269:SER:HB3	1:A:287:LYS:HE2	2.01	0.42
1:A:276:MET:O	1:A:310:ILE:HD13	2.19	0.42
1:A:864:LYS:HB2	1:A:899:VAL:CG2	2.50	0.42
1:A:690:SER:O	1:A:691:LEU:HD23	2.20	0.42
1:A:1057:ARG:O	1:A:1061:VAL:HG23	2.18	0.42
1:A:38:ARG:NH1	1:A:54:GLU:OE2	2.52	0.42
1:A:411:TRP:HB2	1:A:460:CYS:HB3	2.01	0.42
1:A:869:ALA:H	1:A:885:ASN:HB2	1.85	0.42
1:A:162:LEU:N	1:A:162:LEU:HD12	2.34	0.42
1:A:194:GLU:O	1:A:202:PHE:O	2.38	0.42
1:A:1110:ALA:C	1:A:1111:ASN:ND2	2.76	0.42
1:A:222:VAL:HA	1:A:223:PRO:HD3	1.85	0.42
1:A:368:GLU:O	1:A:370:GLN:HG3	2.20	0.42
1:A:93:GLN:HG3	1:A:98:ILE:CG2	2.50	0.41
1:A:332:GLN:HB2	1:A:351:GLU:O	2.20	0.41
1:A:389:ILE:HD13	1:A:713:ARG:HB3	2.02	0.41
1:A:828:TYR:HB3	1:A:850:VAL:HG13	2.02	0.41
1:A:926:LEU:HG	1:A:927:MET:H	1.84	0.41
1:A:40:GLU:HG2	1:A:54:GLU:HG2	2.02	0.41
1:A:294:THR:HG22	1:A:295:VAL:HG22	2.02	0.41
1:A:557:ALA:HB2	1:A:593:MET:HE3	2.03	0.41
1:A:648:ASN:HB3	1:A:649:VAL:H	1.74	0.41
1:A:887:THR:HA	1:A:907:ASN:O	2.20	0.41
1:A:237:ILE:HD11	1:A:253:ILE:HD11	2.02	0.41
1:A:312:GLU:CG	1:A:327:ARG:HB2	2.50	0.41
1:A:367:LEU:HD23	1:A:367:LEU:HA	1.81	0.41
1:A:516:LEU:HB3	1:A:574:PHE:HE1	1.83	0.41
1:A:909:ILE:HA	1:A:926:LEU:HD13	2.01	0.41
1:A:1063:LYS:H	1:A:1063:LYS:HG2	1.69	0.41
1:A:361:ASP:OD2	1:A:723:LYS:HA	2.19	0.41
1:A:1048:TYR:CE2	1:A:1052:LEU:HD12	2.55	0.41
1:A:5:TYR:CE2	1:A:7:VAL:HG22	2.56	0.41
1:A:640:THR:O	1:A:681:PRO:HG3	2.21	0.41
1:A:966:LEU:HD13	1:A:1007:PHE:CE2	2.56	0.41
1:A:977:CYS:HB3	1:A:992:LEU:HD13	2.03	0.41
1:A:1126:ALA:O	1:A:1130:ILE:HB	2.21	0.41
1:A:5:TYR:OH	1:A:1091:GLY:CA	2.69	0.41
1:A:63:VAL:HB	1:A:80:LEU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:VAL:HA	1:A:189:HIS:O	2.21	0.41
1:A:422:TYR:CD1	1:A:422:TYR:N	2.89	0.41
1:A:492:GLU:O	1:A:493:PRO:C	2.63	0.41
1:A:571:LEU:HD23	1:A:574:PHE:CE2	2.55	0.41
1:A:658:VAL:HG23	1:A:671:VAL:CG2	2.51	0.41
1:A:706:GLU:HG3	1:A:707:ILE:H	1.86	0.41
1:A:920:PHE:HB3	1:A:935:TYR:HB3	2.02	0.41
1:A:1089:ILE:HG23	1:A:1094:ILE:HD12	2.03	0.41
1:A:273:LEU:HB2	1:A:281:PHE:HB2	2.03	0.41
1:A:333:LEU:HD12	1:A:333:LEU:HA	1.82	0.41
1:A:1032:THR:OG1	1:A:1036:MET:HB3	2.21	0.41
1:A:593:MET:HE2	1:A:602:LEU:HD22	2.03	0.40
1:A:641:PHE:CE2	1:A:650:PHE:HB2	2.56	0.40
1:A:661:SER:HA	1:A:665:LYS:O	2.20	0.40
1:A:270:ARG:CB	1:A:282:MET:HE2	2.51	0.40
1:A:487:VAL:O	1:A:488:SER:HB3	2.21	0.40
1:A:532:THR:CG2	1:A:533:GLU:N	2.84	0.40
1:A:544:THR:HA	1:A:545:PRO:HD2	1.91	0.40
1:A:842:GLU:HA	1:A:843:PRO:HD3	1.94	0.40
1:A:1089:ILE:CG2	1:A:1094:ILE:HD12	2.50	0.40
1:A:334:VAL:HG23	1:A:349:ALA:HA	2.04	0.40
1:A:411:TRP:HA	1:A:412:PRO:HD3	1.97	0.40
1:A:545:PRO:HG3	1:A:551:GLY:H	1.86	0.40
1:A:632:GLY:HA3	1:A:654:ASP:OD1	2.22	0.40
1:A:558:ILE:HG23	1:A:567:ARG:CG	2.51	0.40
1:A:111:ARG:HD2	1:A:111:ARG:HA	1.86	0.40
1:A:356:LEU:HD21	1:A:712:ILE:HD13	2.04	0.40
1:A:906:TYR:O	1:A:942:PHE:CZ	2.75	0.40
1:A:912:LEU:HD13	1:A:913:TYR:CZ	2.57	0.40
1:A:1101:SER:HB2	1:A:1103:PRO:HD2	2.03	0.40
1:A:1104:LYS:O	1:A:1108:VAL:HG23	2.22	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%)	918 (83%)	145 (13%)	43 (4%)	2	8
2	B	12/14 (86%)	11 (92%)	1 (8%)	0	100	100
All	All	1118/1157 (97%)	929 (83%)	146 (13%)	43 (4%)	2	9

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	208	LYS
1	A	235	GLU
1	A	256	SER
1	A	689	ASP
1	A	706	GLU
1	A	753	ARG
1	A	918	GLY
1	A	986	ASP
1	A	1045	GLU
1	A	186	GLN
1	A	371	GLY
1	A	463	VAL
1	A	502	SER
1	A	513	GLY
1	A	644	LEU
1	A	683	ASN
1	A	707	ILE
1	A	748	GLY
1	A	894	THR
1	A	970	ASN
1	A	985	THR
1	A	987	GLU
1	A	162	LEU
1	A	855	ASP
1	A	1103	PRO
1	A	35	LYS
1	A	372	GLN
1	A	430	VAL
1	A	621	GLY
1	A	696	ASN
1	A	919	ASP
1	A	950	ASN
1	A	998	PHE

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Mol	Chain	Res	Type
1	A	1124	ALA
1	A	343	GLN
1	A	366	ASP
1	A	523	PRO
1	A	1014	MET
1	A	1037	ILE
1	A	105	HIS
1	A	440	GLY
1	A	488	SER
1	A	1065	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	977/1001 (98%)	850 (87%)	127 (13%)	4	14
2	B	12/12 (100%)	11 (92%)	1 (8%)	10	32
All	All	989/1013 (98%)	861 (87%)	128 (13%)	4	14

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	20	THR
1	A	24	THR
1	A	70	LYS
1	A	79	ILE
1	A	81	THR
1	A	98	ILE
1	A	101	ILE
1	A	103	ARG
1	A	116	SER
1	A	125	ASP
1	A	145	LEU
1	A	146	ASP

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Mol	Chain	Res	Type
1	A	147	ARG
1	A	152	LEU
1	A	159	LEU
1	A	162	LEU
1	A	165	ILE
1	A	167	VAL
1	A	168	LYS
1	A	178	ILE
1	A	198	ARG
1	A	208	LYS
1	A	224	GLU
1	A	252	ILE
1	A	253	ILE
1	A	256	SER
1	A	269	SER
1	A	276	MET
1	A	277	GLU
1	A	292	ASP
1	A	294	THR
1	A	296	THR
1	A	299	ASP
1	A	309	SER
1	A	313	CYS
1	A	314	LEU
1	A	331	SER
1	A	333	LEU
1	A	334	VAL
1	A	354	THR
1	A	372	GLN
1	A	374	GLN
1	A	375	LEU
1	A	421	THR
1	A	422	TYR
1	A	435	VAL
1	A	445	GLU
1	A	447	GLU
1	A	448	LEU
1	A	449	MET
1	A	453	ASP
1	A	455	GLN
1	A	463	VAL
1	A	468	LEU

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Mol	Chain	Res	Type
1	A	472	THR
1	A	476	VAL
1	A	481	GLN
1	A	482	GLU
1	A	521	ILE
1	A	537	GLU
1	A	544	THR
1	A	556	CYS
1	A	561	TRP
1	A	567	ARG
1	A	568	ILE
1	A	576	LEU
1	A	587	ILE
1	A	603	LEU
1	A	604	CYS
1	A	613	TYR
1	A	616	LEU
1	A	630	THR
1	A	638	LEU
1	A	640	THR
1	A	644	LEU
1	A	663	ASN
1	A	666	LEU
1	A	679	MET
1	A	682	LEU
1	A	701	ILE
1	A	704	ILE
1	A	705	ASP
1	A	708	GLN
1	A	713	ARG
1	A	752	LEU
1	A	763	SER
1	A	765	VAL
1	A	766	SER
1	A	773	SER
1	A	847	ARG
1	A	849	VAL
1	A	857	LYS
1	A	858	LEU
1	A	866	VAL
1	A	903	CYS
1	A	910	MET

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Mol	Chain	Res	Type
1	A	912	LEU
1	A	916	THR
1	A	923	VAL
1	A	931	LEU
1	A	936	LYS
1	A	944	GLU
1	A	957	VAL
1	A	966	LEU
1	A	969	GLU
1	A	970	ASN
1	A	981	SER
1	A	984	THR
1	A	990	GLN
1	A	992	LEU
1	A	993	GLN
1	A	994	GLU
1	A	1000	LEU
1	A	1006	VAL
1	A	1041	THR
1	A	1042	SER
1	A	1045	GLU
1	A	1050	LEU
1	A	1052	LEU
1	A	1058	LEU
1	A	1069	GLU
1	A	1081	LYS
1	A	1093	LEU
1	A	1102	ARG
1	A	1111	ASN
1	A	1139	ILE
2	B	88	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	16	ASN
1	A	22	HIS
1	A	30	ASN
1	A	36	ASN
1	A	105	HIS
1	A	156	ASN

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Mol	Chain	Res	Type
1	A	163	HIS
1	A	261	HIS
1	A	262	ASN
1	A	290	GLN
1	A	439	ASN
1	A	455	GLN
1	A	456	GLN
1	A	462	ASN
1	A	466	GLN
1	A	467	GLN
1	A	507	GLN
1	A	550	ASN
1	A	600	HIS
1	A	648	ASN
1	A	708	GLN
1	A	727	GLN
1	A	731	GLN
1	A	796	GLN
1	A	806	GLN
1	A	826	ASN
1	A	904	ASN
1	A	941	ASN
1	A	952	ASN
1	A	1034	ASN
1	A	1055	GLN
1	A	1070	HIS
1	A	1111	ASN
2	B	91	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 oligosaccharides 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%)	0.38	95 (8%) 16 12	11, 61, 144, 192	0
2	B	14/14 (100%)	0.40	1 (7%) 22 16	24, 35, 65, 68	0
All	All	1128/1157 (97%)	0.38	96 (8%) 16 12	11, 61, 142, 192	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	751	ALA	6.4
1	A	660	TYR	6.2
1	A	752	LEU	5.9
2	B	97	GLY	5.8
1	A	569	LEU	5.6
1	A	613	TYR	5.4
1	A	907	ASN	5.2
1	A	556	CYS	5.0
1	A	508	VAL	5.0
1	A	571	LEU	4.7
1	A	667	VAL	4.2
1	A	917	LYS	4.0
1	A	1023	PRO	3.9
1	A	918	GLY	3.8
1	A	519	LEU	3.8
1	A	982	ALA	3.7
1	A	926	LEU	3.7
1	A	621	GLY	3.6
1	A	472	THR	3.6
1	A	953	TRP	3.4
1	A	503	CYS	3.4
1	A	460	CYS	3.4
1	A	294	THR	3.2
1	A	925	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	308	THR	3.2
1	A	659	ILE	3.1
1	A	753	ARG	3.1
1	A	501	ALA	3.1
1	A	439	ASN	3.1
1	A	290	GLN	3.1
1	A	709	LYS	3.1
1	A	555	LEU	3.0
1	A	295	VAL	3.0
1	A	406	GLY	3.0
1	A	521	ILE	3.0
1	A	616	LEU	3.0
1	A	983	ALA	3.0
1	A	462	ASN	2.9
1	A	568	ILE	2.9
1	A	688	PRO	2.8
1	A	596	PHE	2.8
1	A	425	LEU	2.8
1	A	483	PRO	2.8
1	A	602	LEU	2.7
1	A	772	SER	2.7
1	A	773	SER	2.7
1	A	517	TYR	2.6
1	A	293	GLY	2.6
1	A	595	THR	2.6
1	A	404	LEU	2.6
1	A	603	LEU	2.6
1	A	703	THR	2.6
1	A	513	GLY	2.6
1	A	984	THR	2.6
1	A	46	ALA	2.6
1	A	641	PHE	2.6
1	A	661	SER	2.5
1	A	506	SER	2.5
1	A	528	GLN	2.5
1	A	279	ARG	2.5
1	A	466	GLN	2.4
1	A	620	THR	2.4
1	A	1125	THR	2.4
1	A	684	SER	2.4
1	A	1065	VAL	2.3
1	A	296	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	436	LEU	2.3
1	A	412	PRO	2.3
1	A	663	ASN	2.3
1	A	1109	VAL	2.3
1	A	622	LEU	2.3
1	A	855	ASP	2.3
1	A	520	GLN	2.2
1	A	704	ILE	2.2
1	A	989	ARG	2.2
1	A	577	LEU	2.2
1	A	682	LEU	2.2
1	A	526	LEU	2.2
1	A	292	ASP	2.2
1	A	1128	ASP	2.2
1	A	748	GLY	2.2
1	A	633	THR	2.2
1	A	162	LEU	2.2
1	A	546	LEU	2.2
1	A	919	ASP	2.1
1	A	397	HIS	2.1
1	A	685	ASP	2.1
1	A	701	ILE	2.1
1	A	437	MET	2.1
1	A	927	MET	2.1
1	A	572	PRO	2.1
1	A	920	PHE	2.1
1	A	446	THR	2.0
1	A	488	SER	2.0
1	A	640	THR	2.0
1	A	687	TYR	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 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.