



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:45 PM UTC

PDB ID : 3I7P / pdb_00003i7p
Title : Crystal Structure of DDB1 in Complex with the H-Box Motif of WDR40A
Authors : Li, T.; Robert, E.I.; Breugel, P.C.V.; Strubin, M.; Zheng, N.
Deposited on : 2009-07-08
Resolution : 3.00 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

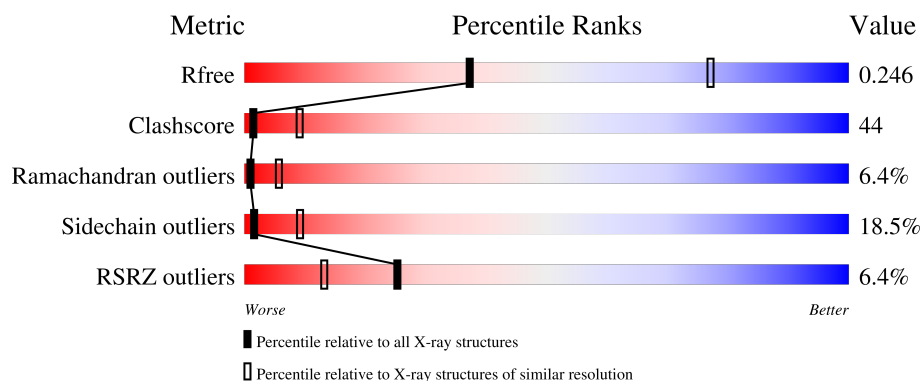
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	6% 38% 42% 15% • •
2	B	13	38% 62%

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

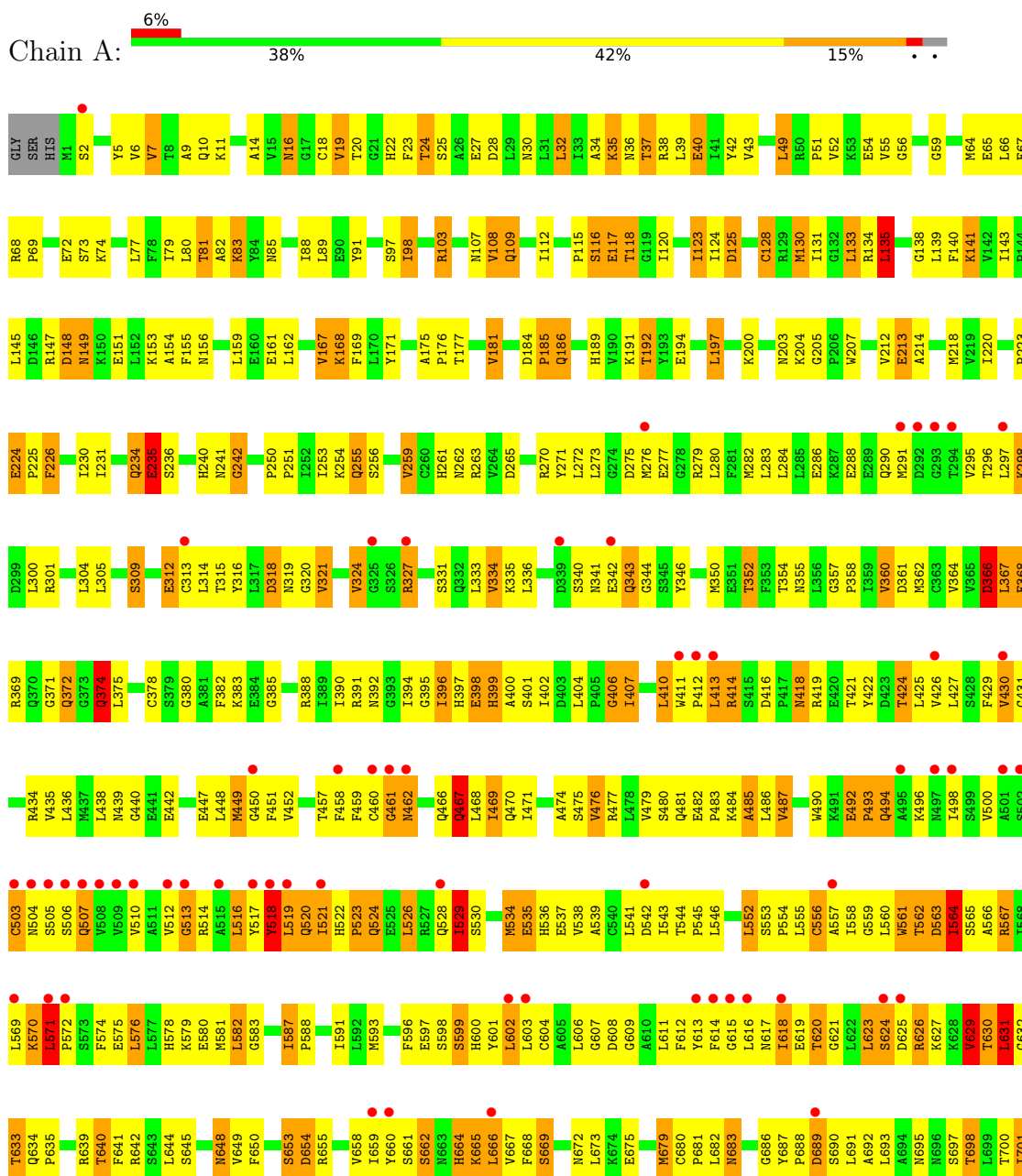
- Molecule 2 is a protein called WD repeat-containing protein 40A.

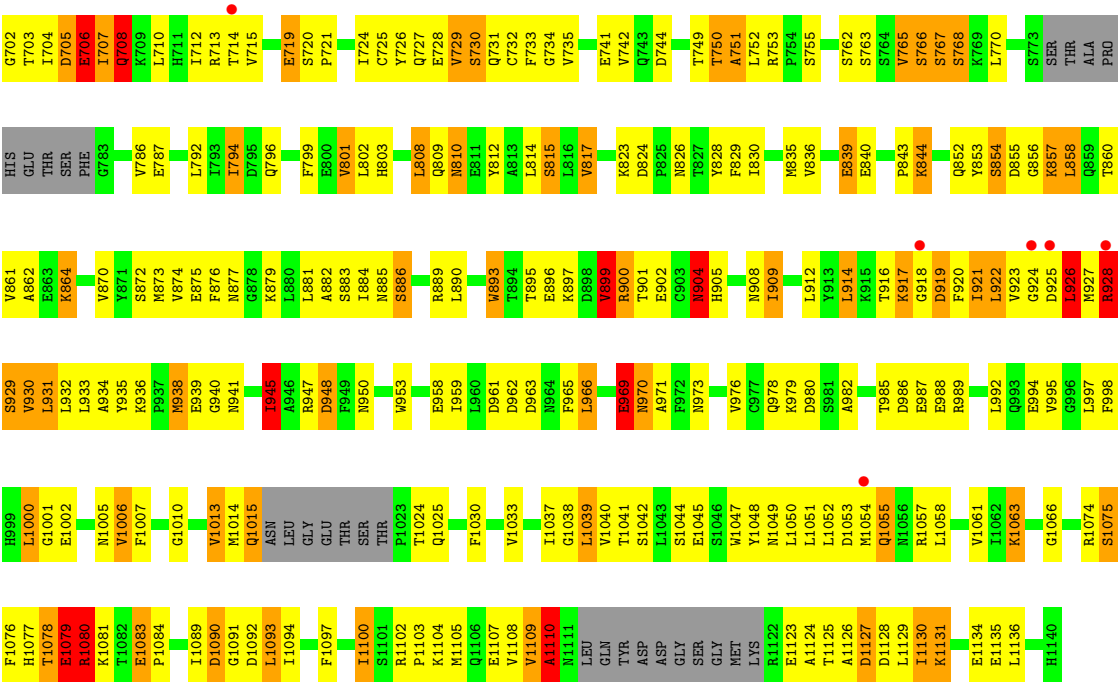
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	13	Total	C	N	O	0	0	0
			116	76	21	19			

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





● Molecule 2: WD repeat-containing protein 40A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.60Å 132.52Å 183.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.79 – 3.00 45.79 – 3.00	Depositor EDS
% Data completeness (in resolution range)	87.0 (45.79-3.00) 87.0 (45.79-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.32 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.240 , 0.301 0.251 , 0.246	Depositor DCC
R_{free} test set	1410 reflections (4.32%)	wwPDB-VP
Wilson B-factor (Å ²)	66.8	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 61.3	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	0.90	EDS
Total number of atoms	8842	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% 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	1.02	6/8885 (0.1%)	1.29	83/12034 (0.7%)
2	B	1.57	1/117 (0.9%)	1.25	2/156 (1.3%)
All	All	1.02	7/9002 (0.1%)	1.29	85/12190 (0.7%)

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

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

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	924	GLY	N-CA	9.59	1.54	1.45
1	A	899	VAL	CA-CB	9.23	1.65	1.54
1	A	925	ASP	N-CA	7.65	1.56	1.46
2	B	52	ASN	C-O	-5.82	1.19	1.23
1	A	1078	THR	CA-C	-5.30	1.46	1.52
1	A	930	VAL	C-O	-5.05	1.19	1.24
1	A	725	CYS	CB-SG	-5.01	1.64	1.81

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1080	ARG	N-CA-CB	-18.29	79.57	110.49
1	A	186	GLN	N-CA-CB	-15.39	83.34	110.42
1	A	367	LEU	N-CA-CB	-14.19	89.16	110.16
1	A	561	TRP	N-CA-C	12.06	126.80	111.24
1	A	514	ARG	N-CA-C	-11.10	99.85	113.50
1	A	1080	ARG	N-CA-C	10.68	133.54	110.80
1	A	374	GLN	N-CA-C	-8.77	97.48	110.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1066	GLY	N-CA-C	-8.64	103.25	115.43
1	A	945	ILE	N-CA-C	8.55	118.63	110.42
1	A	556	CYS	N-CA-C	8.49	119.84	108.38
1	A	185	PRO	CB-CA-C	8.25	125.17	111.56
1	A	664	HIS	N-CA-C	-8.03	100.26	113.50
1	A	1089	ILE	CA-C-N	-7.89	111.93	122.42
1	A	1089	ILE	C-N-CA	-7.89	111.93	122.42
1	A	309	SER	N-CA-C	-7.81	100.46	110.53
1	A	185	PRO	N-CA-C	7.80	128.54	112.47
1	A	1078	THR	N-CA-C	-7.47	96.77	109.24
1	A	360	VAL	N-CA-C	-7.39	105.91	112.12
1	A	969	GLU	N-CA-C	7.20	120.02	109.07
1	A	366	ASP	CA-C-N	7.05	130.30	120.29
1	A	366	ASP	C-N-CA	7.05	130.30	120.29
1	A	924	GLY	N-CA-C	6.95	123.94	111.01
1	A	1083	GLU	CA-C-N	-6.77	113.54	120.85
1	A	1083	GLU	C-N-CA	-6.77	113.54	120.85
1	A	854	SER	N-CA-C	6.75	115.23	108.75
1	A	649	VAL	N-CA-C	6.74	117.34	107.37
1	A	553	SER	CA-C-N	6.67	128.17	119.84
1	A	553	SER	C-N-CA	6.67	128.17	119.84
1	A	398	GLU	N-CA-C	6.63	119.67	107.99
1	A	882	ALA	N-CA-C	6.63	118.47	107.20
2	B	50	LEU	N-CA-C	-6.59	104.18	111.36
1	A	648	ASN	N-CA-C	6.58	119.92	109.65
1	A	1090	ASP	N-CA-CB	6.54	120.61	110.21
1	A	712	ILE	CB-CA-C	-6.47	101.51	110.96
1	A	367	LEU	N-CA-C	-6.35	104.44	111.36
1	A	854	SER	CB-CA-C	-6.29	107.28	116.53
1	A	1110	ALA	N-CA-C	-6.21	97.57	110.80
1	A	899	VAL	N-CA-CB	6.21	117.90	110.95
1	A	207	TRP	N-CA-C	6.12	118.47	108.55
1	A	83	LYS	N-CA-C	-6.06	104.25	112.26
1	A	904	ASN	N-CA-C	5.93	118.12	108.76
1	A	1013	VAL	N-CA-C	5.92	116.04	108.82
1	A	368	GLU	N-CA-C	-5.91	106.03	113.18
1	A	36	ASN	N-CA-C	-5.90	105.17	112.72
1	A	938	MET	N-CA-C	-5.90	98.24	110.80
1	A	702	GLY	N-CA-C	5.88	119.34	110.18
1	A	563	ASP	N-CA-C	-5.85	105.80	113.17
1	A	213	GLU	N-CA-C	5.81	118.69	110.50
1	A	116	SER	N-CA-C	5.78	118.25	109.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	9	ALA	N-CA-C	-5.77	106.41	113.50
1	A	719	GLU	N-CA-C	-5.73	100.84	108.34
1	A	37	THR	N-CA-C	-5.72	104.04	111.71
1	A	397	HIS	N-CA-C	5.69	117.58	108.41
1	A	486	LEU	N-CA-C	5.69	122.92	110.80
1	A	753	ARG	CA-C-N	-5.69	114.07	119.76
1	A	753	ARG	C-N-CA	-5.69	114.07	119.76
1	A	416	ASP	CA-C-N	5.66	126.91	119.84
1	A	416	ASP	C-N-CA	5.66	126.91	119.84
1	A	571	LEU	CA-C-N	-5.65	113.85	119.56
1	A	571	LEU	C-N-CA	-5.65	113.85	119.56
1	A	854	SER	CA-C-O	5.64	121.88	118.33
1	A	900	ARG	N-CA-C	5.59	118.21	108.76
1	A	135	LEU	N-CA-C	-5.56	106.17	113.12
1	A	562	THR	N-CA-C	-5.56	106.66	113.50
1	A	352	THR	CA-C-N	-5.54	114.90	122.93
1	A	352	THR	C-N-CA	-5.54	114.90	122.93
1	A	1053	ASP	N-CA-C	-5.46	105.01	110.97
2	B	46	LEU	N-CA-C	-5.46	106.62	113.28
1	A	108	VAL	N-CA-C	5.44	120.65	109.34
1	A	725	CYS	CA-CB-SG	-5.42	101.92	114.40
1	A	925	ASP	N-CA-C	5.41	122.32	110.80
1	A	16	ASN	N-CA-C	-5.31	106.97	113.50
1	A	295	VAL	N-CA-C	5.24	116.00	108.93
1	A	35	LYS	CA-C-N	-5.13	113.23	122.46
1	A	35	LYS	C-N-CA	-5.13	113.23	122.46
1	A	181	VAL	N-CA-C	-5.11	103.01	109.80
1	A	926	LEU	N-CA-C	5.10	116.53	111.07
1	A	1001	GLY	N-CA-C	-5.08	108.05	115.72
1	A	399	HIS	N-CA-C	5.08	116.66	111.03
1	A	924	GLY	CA-C-O	-5.07	116.82	122.14
1	A	1005	ASN	N-CA-C	5.07	117.92	111.69
1	A	767	SER	N-CA-C	-5.06	105.95	112.68
1	A	948	ASP	N-CA-C	-5.03	101.50	109.76
1	A	334	VAL	N-CA-C	5.01	115.86	108.45
1	A	467	GLN	N-CA-C	5.00	116.67	109.07

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	PRO	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	730	0
2	B	116	0	124	57	0
All	All	8842	0	8830	774	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 44.

All (774) 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:578:HIS:NE2	1:A:623:LEU:HB2	1.39	1.35
1:A:597:GLU:HB2	1:A:664:HIS:NE2	1.47	1.30
2:B:47:VAL:O	2:B:51:LYS:HG3	1.39	1.23
1:A:927:MET:O	1:A:928:ARG:HD3	1.38	1.23
2:B:51:LYS:HA	2:B:54:GLU:CG	1.73	1.19
2:B:50:LEU:O	2:B:54:GLU:HG2	1.44	1.17
1:A:578:HIS:CD2	1:A:623:LEU:HB2	1.77	1.17
1:A:469:ILE:HD11	1:A:471:ILE:HG13	1.25	1.14
1:A:98:ILE:HD13	1:A:98:ILE:H	1.16	1.10
1:A:1125:THR:HG22	1:A:1126:ALA:H	1.01	1.09
1:A:367:LEU:HD12	1:A:374:GLN:HG3	1.24	1.09
1:A:620:THR:HG23	1:A:621:GLY:H	1.20	1.07
2:B:51:LYS:HA	2:B:54:GLU:HG3	1.12	1.07
1:A:631:LEU:N	1:A:631:LEU:HD23	1.70	1.06
1:A:507:GLN:HE22	1:A:552:LEU:HA	1.20	1.05
2:B:45:SER:HB2	2:B:47:VAL:HG22	1.33	1.05
2:B:49:TYR:O	2:B:53:ARG:HG3	1.55	1.05
1:A:1024:THR:HB	1:A:1041:THR:HG21	1.34	1.04
1:A:410:LEU:HD12	1:A:680:CYS:SG	1.98	1.02
1:A:367:LEU:HD12	1:A:374:GLN:CG	1.89	1.02
1:A:641:PHE:HA	1:A:681:PRO:HG3	1.42	1.01
1:A:578:HIS:NE2	1:A:623:LEU:CB	2.22	1.01
1:A:870:VAL:HG11	1:A:873:MET:CE	1.89	1.01
1:A:1014:MET:SD	1:A:1015:GLN:HG2	2.00	1.01
1:A:400:ALA:H	1:A:701:ILE:HD11	1.22	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ARG:HD2	1:A:54:GLU:OE1	1.60	0.99
1:A:1033:VAL:HG11	2:B:56:ARG:HB2	1.45	0.99
1:A:578:HIS:CE1	1:A:623:LEU:HD12	1.96	0.98
1:A:665:LYS:O	1:A:666:LEU:HG	1.63	0.98
1:A:98:ILE:H	1:A:98:ILE:CD1	1.76	0.98
1:A:597:GLU:CB	1:A:664:HIS:NE2	2.25	0.98
2:B:51:LYS:CA	2:B:54:GLU:CG	2.41	0.97
1:A:578:HIS:NE2	1:A:623:LEU:HD12	1.80	0.96
1:A:597:GLU:HB2	1:A:664:HIS:CD2	2.00	0.96
1:A:616:LEU:HG	1:A:617:ASN:H	1.28	0.95
1:A:928:ARG:O	1:A:928:ARG:HG2	1.65	0.95
1:A:175:ALA:HB3	1:A:194:GLU:HG2	1.48	0.95
1:A:812:TYR:HD1	2:B:51:LYS:NZ	1.63	0.95
1:A:870:VAL:HG11	1:A:873:MET:HE3	1.48	0.94
2:B:51:LYS:CA	2:B:54:GLU:HG2	1.98	0.94
2:B:56:ARG:NH1	2:B:57:LEU:HB2	1.83	0.94
1:A:24:THR:H	1:A:30:ASN:HD21	1.14	0.94
1:A:614:PHE:HE2	1:A:625:ASP:O	1.50	0.94
1:A:644:LEU:HG	1:A:645:SER:H	1.29	0.93
1:A:870:VAL:CG1	1:A:873:MET:HE3	2.00	0.92
1:A:812:TYR:HD1	2:B:51:LYS:HZ3	1.14	0.92
1:A:378:CYS:HB3	1:A:721:PRO:HB2	1.51	0.92
1:A:614:PHE:HD2	1:A:624:SER:HG	1.18	0.92
1:A:367:LEU:CD1	1:A:374:GLN:HG3	1.99	0.91
1:A:1033:VAL:CG1	2:B:56:ARG:HB2	1.99	0.90
2:B:51:LYS:O	2:B:54:GLU:HB2	1.72	0.90
1:A:530:SER:HB3	1:A:574:PHE:HE1	1.36	0.90
1:A:1125:THR:HG22	1:A:1126:ALA:N	1.85	0.90
2:B:57:LEU:O	2:B:57:LEU:HD23	1.72	0.90
1:A:1125:THR:CG2	1:A:1126:ALA:H	1.84	0.89
1:A:133:LEU:HB3	1:A:135:LEU:CD2	2.03	0.89
1:A:1024:THR:HB	1:A:1041:THR:CG2	2.02	0.89
1:A:518:TYR:HD2	1:A:519:LEU:N	1.70	0.88
1:A:414:ARG:HG2	1:A:414:ARG:HH11	1.39	0.88
1:A:931:LEU:HD12	1:A:931:LEU:N	1.88	0.88
1:A:516:LEU:HD11	1:A:534:MET:SD	2.14	0.87
1:A:475:SER:HB2	1:A:490:TRP:O	1.74	0.87
1:A:978:GLN:HE21	1:A:995:VAL:HG21	1.38	0.87
1:A:1075:SER:OG	1:A:1084:PRO:HA	1.74	0.86
1:A:23:PHE:H	1:A:30:ASN:HD22	1.20	0.86
1:A:642:ARG:NH2	1:A:683:ASN:HB2	1.91	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:614:PHE:CE2	1:A:625:ASP:O	2.28	0.85
1:A:620:THR:HG23	1:A:621:GLY:N	1.91	0.84
1:A:11:LYS:HE2	1:A:38:ARG:HE	1.39	0.84
1:A:410:LEU:HD12	1:A:680:CYS:HG	1.37	0.83
1:A:597:GLU:CB	1:A:664:HIS:CD2	2.61	0.83
2:B:50:LEU:C	2:B:54:GLU:HG2	2.04	0.82
1:A:469:ILE:CD1	1:A:471:ILE:HG13	2.07	0.82
1:A:399:HIS:HB2	1:A:701:ILE:HG12	1.62	0.81
1:A:382:PHE:H	1:A:720:SER:HB3	1.46	0.81
1:A:1080:ARG:O	1:A:1080:ARG:HG3	1.78	0.81
1:A:623:LEU:C	1:A:623:LEU:HD23	2.04	0.81
1:A:81:THR:HG22	1:A:83:LYS:H	1.45	0.81
2:B:57:LEU:HD23	2:B:57:LEU:C	2.04	0.81
1:A:98:ILE:HD13	1:A:98:ILE:N	1.97	0.80
1:A:6:VAL:HG12	1:A:1040:VAL:HG22	1.62	0.80
1:A:131:ILE:HG13	1:A:145:LEU:HD11	1.63	0.80
2:B:45:SER:CB	2:B:47:VAL:HG22	2.12	0.80
1:A:1063:LYS:H	1:A:1063:LYS:HD3	1.46	0.79
1:A:928:ARG:O	1:A:928:ARG:CG	2.30	0.79
1:A:107:ASN:OD1	1:A:109:GLN:HG2	1.82	0.79
1:A:587:ILE:HB	1:A:588:PRO:HD2	1.63	0.79
1:A:98:ILE:CD1	1:A:98:ILE:N	2.42	0.78
1:A:662:SER:HB3	1:A:665:LYS:HB2	1.65	0.78
1:A:731:GLN:O	1:A:796:GLN:HG2	1.84	0.78
1:A:578:HIS:CE1	1:A:623:LEU:CD1	2.67	0.78
1:A:342:GLU:O	1:A:343:GLN:HB3	1.83	0.78
1:A:231:ILE:HD13	1:A:240:HIS:CD2	2.18	0.78
1:A:1024:THR:CB	1:A:1041:THR:HG21	2.14	0.78
1:A:181:VAL:HG13	1:A:212:VAL:HG21	1.66	0.78
1:A:630:THR:HG21	1:A:1134:GLU:OE1	1.82	0.78
1:A:139:LEU:HD22	1:A:156:ASN:HB3	1.66	0.77
1:A:194:GLU:HB2	1:A:203:ASN:HB2	1.64	0.77
1:A:81:THR:CG2	1:A:83:LYS:H	1.97	0.77
1:A:24:THR:H	1:A:30:ASN:ND2	1.83	0.77
1:A:1090:ASP:HB2	1:A:1092:ASP:HB2	1.65	0.77
2:B:50:LEU:O	2:B:54:GLU:CG	2.29	0.77
1:A:578:HIS:NE2	1:A:623:LEU:CD1	2.47	0.77
1:A:561:TRP:O	1:A:564:ILE:HD12	1.85	0.77
1:A:1105:MET:SD	1:A:1130:ILE:HD12	2.25	0.77
1:A:854:SER:HB2	1:A:857:LYS:HG2	1.67	0.76
1:A:400:ALA:N	1:A:701:ILE:HD11	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:THR:HB	1:A:85:ASN:HB2	1.67	0.76
1:A:133:LEU:HB3	1:A:135:LEU:HD21	1.65	0.76
1:A:513:GLY:O	1:A:538:VAL:HG23	1.85	0.76
1:A:523:PRO:O	1:A:524:GLN:HB2	1.85	0.76
2:B:55:VAL:O	2:B:56:ARG:CB	2.34	0.76
1:A:388:ARG:HD3	1:A:714:THR:OG1	1.86	0.75
1:A:922:LEU:O	1:A:932:LEU:HD12	1.87	0.75
1:A:927:MET:O	1:A:928:ARG:CD	2.30	0.74
1:A:68:ARG:NH1	1:A:74:LYS:HA	2.02	0.74
1:A:324:VAL:HG12	1:A:324:VAL:O	1.87	0.74
1:A:410:LEU:CD1	1:A:680:CYS:SG	2.75	0.74
1:A:1078:THR:O	1:A:1079:GLU:C	2.30	0.74
1:A:288:GLU:HB3	1:A:296:THR:HG23	1.70	0.74
1:A:449:MET:O	1:A:479:VAL:HG21	1.86	0.74
1:A:812:TYR:CD1	2:B:51:LYS:NZ	2.53	0.74
1:A:11:LYS:HE2	1:A:38:ARG:NE	2.03	0.74
1:A:480:SER:HB3	1:A:483:PRO:HD2	1.70	0.74
1:A:661:SER:HA	1:A:666:LEU:HA	1.70	0.74
1:A:484:LYS:O	1:A:485:ALA:HB2	1.87	0.74
1:A:617:ASN:HB3	1:A:620:THR:HG22	1.69	0.73
2:B:51:LYS:C	2:B:54:GLU:HG2	2.13	0.73
1:A:930:VAL:C	1:A:931:LEU:HD12	2.13	0.73
1:A:116:SER:OG	1:A:134:ARG:CZ	2.37	0.73
1:A:130:MET:HA	1:A:145:LEU:HD12	1.69	0.73
1:A:482:GLU:HB2	1:A:483:PRO:HD3	1.69	0.73
1:A:213:GLU:OE1	1:A:236:SER:HB3	1.89	0.73
1:A:507:GLN:NE2	1:A:552:LEU:HA	2.00	0.73
2:B:52:ASN:C	2:B:54:GLU:N	2.45	0.73
1:A:480:SER:HB2	1:A:484:LYS:H	1.52	0.72
1:A:418:ASN:HD22	1:A:419:ARG:H	1.37	0.72
1:A:438:LEU:HD23	1:A:442:GLU:O	1.90	0.72
1:A:256:SER:HB3	1:A:275:ASP:OD2	1.90	0.72
1:A:400:ALA:H	1:A:701:ILE:CD1	2.00	0.72
1:A:518:TYR:HD2	1:A:518:TYR:C	1.97	0.72
1:A:701:ILE:N	1:A:701:ILE:HD13	2.05	0.72
1:A:22:HIS:CD2	1:A:28:ASP:O	2.43	0.71
1:A:364:VAL:HG22	1:A:375:LEU:CD1	2.19	0.71
1:A:591:ILE:HD12	1:A:604:CYS:HB2	1.71	0.71
1:A:687:TYR:O	1:A:690:SER:HB2	1.91	0.71
1:A:414:ARG:HA	1:A:422:TYR:HA	1.72	0.71
1:A:117:GLU:OE1	1:A:117:GLU:HA	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:LEU:HD13	1:A:429:PHE:HD2	1.55	0.71
1:A:641:PHE:HA	1:A:681:PRO:CG	2.18	0.71
1:A:312:GLU:HG3	1:A:327:ARG:HG3	1.72	0.70
1:A:571:LEU:HB3	1:A:572:PRO:HD3	1.72	0.70
1:A:870:VAL:HG11	1:A:873:MET:HE1	1.73	0.70
1:A:927:MET:O	1:A:928:ARG:HB3	1.90	0.70
1:A:312:GLU:HG3	1:A:327:ARG:CG	2.21	0.70
1:A:16:ASN:ND2	1:A:35:LYS:O	2.23	0.70
1:A:37:THR:HG22	1:A:59:GLY:O	1.92	0.70
2:B:51:LYS:C	2:B:54:GLU:CG	2.65	0.70
1:A:1033:VAL:HG11	2:B:56:ARG:CB	2.22	0.70
1:A:394:ILE:HD11	1:A:669:SER:HB2	1.74	0.70
1:A:620:THR:CG2	1:A:621:GLY:H	2.02	0.70
1:A:366:ASP:HB3	1:A:372:GLN:O	1.92	0.69
1:A:654:ASP:HA	1:A:675:GLU:CG	2.21	0.69
1:A:835:MET:O	1:A:843:PRO:HB3	1.92	0.69
1:A:1048:TYR:CE2	1:A:1052:LEU:HD12	2.25	0.69
1:A:374:GLN:OE1	1:A:391:ARG:HG3	1.93	0.69
1:A:364:VAL:HG22	1:A:375:LEU:HD12	1.75	0.69
1:A:5:TYR:CE2	1:A:7:VAL:HG22	2.27	0.69
1:A:103:ARG:HH11	1:A:103:ARG:HB3	1.56	0.69
1:A:642:ARG:HH21	1:A:683:ASN:HB2	1.56	0.69
1:A:272:LEU:O	1:A:273:LEU:HD23	1.93	0.68
1:A:426:VAL:HG22	1:A:435:VAL:HG13	1.76	0.68
2:B:56:ARG:HH12	2:B:57:LEU:HB2	1.57	0.68
1:A:427:LEU:HD13	1:A:429:PHE:CD2	2.29	0.68
1:A:342:GLU:O	1:A:343:GLN:CB	2.41	0.68
1:A:874:VAL:HG22	1:A:875:GLU:N	2.08	0.68
1:A:691:LEU:O	1:A:701:ILE:HA	1.93	0.68
1:A:931:LEU:N	1:A:931:LEU:CD1	2.56	0.68
1:A:414:ARG:HG2	1:A:414:ARG:NH1	2.04	0.68
1:A:853:TYR:HA	1:A:857:LYS:O	1.94	0.68
1:A:263:ARG:HA	1:A:271:TYR:CD2	2.29	0.68
1:A:969:GLU:O	1:A:971:ALA:N	2.26	0.68
1:A:355:ASN:OD1	1:A:357:GLY:N	2.27	0.68
1:A:518:TYR:C	1:A:518:TYR:CD2	2.71	0.67
1:A:241:ASN:O	1:A:242:GLY:C	2.37	0.67
1:A:197:LEU:HD23	1:A:197:LEU:H	1.58	0.67
1:A:905:HIS:HD2	1:A:908:ASN:HD21	1.43	0.67
1:A:642:ARG:NH2	1:A:683:ASN:CB	2.58	0.67
1:A:613:TYR:CZ	1:A:627:LYS:HB2	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:55:VAL:O	2:B:56:ARG:HB2	1.95	0.67
1:A:542:ASP:O	1:A:593:MET:HE3	1.95	0.67
1:A:570:LYS:NZ	1:A:572:PRO:HD2	2.10	0.67
1:A:923:VAL:HA	1:A:931:LEU:O	1.95	0.67
1:A:1078:THR:OG1	1:A:1080:ARG:HG2	1.95	0.67
1:A:159:LEU:HD23	1:A:161:GLU:H	1.60	0.67
1:A:341:ASN:HB2	1:A:342:GLU:OE1	1.94	0.66
1:A:385:GLY:HA3	1:A:719:GLU:O	1.95	0.66
1:A:419:ARG:HD3	1:A:421:THR:OG1	1.94	0.66
1:A:644:LEU:CG	1:A:645:SER:H	2.07	0.66
1:A:81:THR:CG2	1:A:82:ALA:N	2.58	0.66
1:A:367:LEU:HD12	1:A:374:GLN:CD	2.20	0.66
1:A:539:ALA:HB3	1:A:559:GLY:O	1.96	0.66
1:A:561:TRP:O	1:A:564:ILE:CD1	2.43	0.66
1:A:978:GLN:NE2	1:A:995:VAL:HG21	2.08	0.66
2:B:48:TYR:O	2:B:52:ASN:HB2	1.95	0.66
2:B:51:LYS:CA	2:B:54:GLU:HG3	2.03	0.66
1:A:921:ILE:C	1:A:922:LEU:HD12	2.21	0.66
1:A:602:LEU:HD23	1:A:614:PHE:HB2	1.78	0.65
1:A:427:LEU:HD12	1:A:427:LEU:O	1.96	0.65
1:A:1044:SER:OG	1:A:1047:TRP:HB2	1.95	0.65
1:A:366:ASP:OD1	1:A:366:ASP:N	2.29	0.65
1:A:642:ARG:HH22	1:A:683:ASN:CG	2.04	0.65
1:A:803:HIS:CD2	1:A:858:LEU:HB2	2.32	0.65
1:A:920:PHE:O	1:A:934:ALA:HA	1.96	0.65
1:A:364:VAL:HG21	1:A:1010:GLY:HA3	1.79	0.65
1:A:382:PHE:N	1:A:720:SER:HB3	2.11	0.65
1:A:1123:GLU:HG2	1:A:1124:ALA:H	1.62	0.65
1:A:5:TYR:CE2	1:A:7:VAL:CG2	2.80	0.65
1:A:480:SER:OG	1:A:487:VAL:HG21	1.96	0.65
1:A:469:ILE:HD11	1:A:471:ILE:CG1	2.15	0.65
1:A:653:SER:HB3	1:A:655:ARG:H	1.62	0.65
1:A:578:HIS:NE2	1:A:623:LEU:CG	2.59	0.64
1:A:234:GLN:O	1:A:236:SER:N	2.30	0.64
1:A:695:ASN:OD1	1:A:698:THR:HB	1.97	0.64
1:A:714:THR:HG22	1:A:715:VAL:N	2.13	0.64
1:A:1000:LEU:HD13	1:A:1002:GLU:HB2	1.79	0.64
1:A:1030:PHE:CZ	1:A:1038:GLY:HA3	2.32	0.64
1:A:530:SER:CB	1:A:574:PHE:HE1	2.10	0.64
1:A:623:LEU:C	1:A:623:LEU:CD2	2.71	0.64
1:A:726:TYR:OH	1:A:796:GLN:NE2	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:928:ARG:O	1:A:928:ARG:NE	2.30	0.64
1:A:1102:ARG:N	1:A:1103:PRO:HD2	2.13	0.64
1:A:18:CYS:N	1:A:313:CYS:SG	2.71	0.64
1:A:133:LEU:HB3	1:A:135:LEU:HD22	1.77	0.64
1:A:305:LEU:HD13	1:A:336:LEU:HD22	1.79	0.64
1:A:578:HIS:CE1	1:A:623:LEU:HB2	2.28	0.64
2:B:57:LEU:C	2:B:57:LEU:CD2	2.71	0.64
1:A:920:PHE:HB3	1:A:935:TYR:HB3	1.78	0.64
1:A:1033:VAL:HG13	2:B:55:VAL:O	1.99	0.63
1:A:476:VAL:HG13	1:A:490:TRP:HB3	1.78	0.63
1:A:396:ILE:HD12	1:A:673:LEU:HD21	1.81	0.63
1:A:342:GLU:OE1	1:A:342:GLU:N	2.30	0.63
1:A:372:GLN:O	1:A:372:GLN:NE2	2.32	0.63
1:A:598:SER:N	1:A:664:HIS:NE2	2.46	0.63
1:A:234:GLN:OE1	1:A:234:GLN:HA	1.99	0.63
1:A:615:GLY:H	1:A:624:SER:CB	2.12	0.63
1:A:641:PHE:CZ	1:A:648:ASN:HB2	2.34	0.63
1:A:471:ILE:HG12	1:A:476:VAL:HB	1.79	0.63
1:A:24:THR:N	1:A:30:ASN:HD21	1.90	0.63
1:A:985:THR:HG21	1:A:989:ARG:HH21	1.63	0.63
1:A:939:GLU:HG3	1:A:941:ASN:HB2	1.79	0.62
1:A:520:GLN:NE2	1:A:529:ILE:HD11	2.14	0.62
1:A:659:ILE:HA	1:A:667:VAL:O	1.99	0.62
1:A:741:GLU:HB3	1:A:749:THR:HB	1.80	0.62
1:A:763:SER:C	1:A:803:HIS:HE1	2.06	0.62
1:A:1050:LEU:HD22	1:A:1054:MET:HE2	1.80	0.62
1:A:500:VAL:CG1	1:A:541:LEU:HD12	2.30	0.62
1:A:750:THR:O	1:A:751:ALA:CB	2.48	0.62
1:A:5:TYR:HE2	1:A:7:VAL:CG2	2.12	0.62
1:A:231:ILE:HD13	1:A:240:HIS:HD2	1.63	0.62
1:A:1055:GLN:HG2	1:A:1093:LEU:HD12	1.81	0.62
1:A:367:LEU:HB2	1:A:368:GLU:OE1	2.00	0.62
2:B:52:ASN:O	2:B:54:GLU:N	2.33	0.62
1:A:276:MET:O	1:A:276:MET:SD	2.58	0.61
1:A:615:GLY:H	1:A:624:SER:HB3	1.65	0.61
1:A:81:THR:HG22	1:A:83:LYS:N	2.14	0.61
1:A:368:GLU:OE1	1:A:368:GLU:N	2.30	0.61
1:A:654:ASP:HA	1:A:675:GLU:HG3	1.81	0.61
1:A:593:MET:HA	1:A:601:TYR:O	2.01	0.61
1:A:34:ALA:HB2	1:A:64:MET:CE	2.31	0.61
1:A:81:THR:HG23	1:A:82:ALA:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:936:LYS:C	1:A:938:MET:H	2.09	0.61
2:B:56:ARG:O	2:B:57:LEU:C	2.43	0.61
1:A:518:TYR:CD2	1:A:519:LEU:N	2.61	0.61
1:A:750:THR:O	1:A:751:ALA:HB2	2.01	0.60
2:B:52:ASN:C	2:B:54:GLU:H	2.07	0.60
1:A:265:ASP:OD2	1:A:270:ARG:NE	2.33	0.60
1:A:484:LYS:O	1:A:484:LYS:HG3	2.00	0.60
1:A:69:PRO:HD2	1:A:72:GLU:HG3	1.81	0.60
1:A:1025:GLN:O	1:A:1041:THR:HG23	2.01	0.60
1:A:367:LEU:CD1	1:A:374:GLN:CG	2.71	0.60
1:A:520:GLN:CD	1:A:529:ILE:HD11	2.27	0.60
1:A:1077:HIS:C	1:A:1077:HIS:CD2	2.80	0.60
1:A:642:ARG:HH22	1:A:683:ASN:CB	2.14	0.60
1:A:340:SER:HB2	1:A:344:GLY:C	2.27	0.60
1:A:459:PHE:HE2	1:A:461:GLY:CA	2.15	0.60
1:A:660:TYR:HB2	1:A:667:VAL:HB	1.84	0.60
1:A:493:PRO:O	1:A:494:GLN:HG2	2.00	0.60
1:A:927:MET:O	1:A:928:ARG:CB	2.49	0.60
1:A:985:THR:HB	1:A:989:ARG:HE	1.67	0.60
1:A:1033:VAL:HG13	2:B:56:ARG:HB2	1.83	0.60
1:A:480:SER:CB	1:A:483:PRO:HD2	2.32	0.59
1:A:623:LEU:HD23	1:A:624:SER:N	2.17	0.59
1:A:1013:VAL:O	1:A:1014:MET:HG3	2.02	0.59
1:A:139:LEU:HD22	1:A:156:ASN:CB	2.31	0.59
1:A:396:ILE:CD1	1:A:673:LEU:HD21	2.32	0.59
1:A:1109:VAL:HG12	1:A:1110:ALA:H	1.67	0.59
1:A:492:GLU:OE1	1:A:494:GLN:HB2	2.02	0.59
1:A:1127:ASP:N	1:A:1127:ASP:OD1	2.35	0.59
2:B:55:VAL:HG23	2:B:56:ARG:N	2.18	0.59
1:A:20:THR:HB	1:A:315:THR:HG21	1.84	0.59
1:A:107:ASN:OD1	1:A:109:GLN:CG	2.50	0.59
1:A:534:MET:O	1:A:535:GLU:C	2.45	0.59
1:A:600:HIS:CD2	1:A:618:ILE:HG12	2.38	0.59
1:A:49:LEU:O	1:A:51:PRO:HD3	2.02	0.59
1:A:516:LEU:CD2	1:A:538:VAL:HG21	2.32	0.59
1:A:874:VAL:CG2	1:A:875:GLU:N	2.66	0.59
1:A:883:SER:H	1:A:914:LEU:HD11	1.67	0.59
1:A:1061:VAL:HG13	1:A:1104:LYS:HD2	1.84	0.59
1:A:484:LYS:O	1:A:485:ALA:CB	2.51	0.59
1:A:490:TRP:CD1	1:A:519:LEU:HD13	2.37	0.59
1:A:625:ASP:O	1:A:626:ARG:HB2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:563:ASP:CG	1:A:565:SER:HB3	2.28	0.59
1:A:609:GLY:HA2	1:A:632:GLY:O	2.03	0.58
1:A:705:ASP:O	1:A:706:GLU:O	2.21	0.58
1:A:936:LYS:O	1:A:938:MET:N	2.28	0.58
1:A:1127:ASP:HA	1:A:1130:ILE:HG22	1.86	0.58
1:A:226:PHE:HB3	1:A:297:LEU:HD11	1.85	0.58
1:A:288:GLU:OE1	1:A:298:LYS:HE3	2.04	0.58
1:A:844:LYS:H	1:A:844:LYS:HD3	1.69	0.58
1:A:23:PHE:N	1:A:30:ASN:HD22	1.95	0.58
1:A:429:PHE:O	1:A:431:GLY:N	2.35	0.58
1:A:327:ARG:O	1:A:358:PRO:HD3	2.03	0.58
1:A:870:VAL:CG1	1:A:873:MET:CE	2.66	0.58
1:A:719:GLU:OE2	1:A:755:SER:HB3	2.03	0.58
1:A:726:TYR:HB2	1:A:733:PHE:HE2	1.69	0.58
1:A:203:ASN:O	1:A:204:LYS:C	2.47	0.57
1:A:570:LYS:HZ1	1:A:572:PRO:HD2	1.67	0.57
1:A:538:VAL:HG13	1:A:558:ILE:HD11	1.86	0.57
1:A:679:MET:HA	1:A:692:ALA:O	2.03	0.57
2:B:52:ASN:O	2:B:53:ARG:C	2.43	0.57
1:A:617:ASN:CB	1:A:620:THR:HG22	2.34	0.57
1:A:609:GLY:CA	1:A:632:GLY:O	2.52	0.57
1:A:1051:LEU:HD23	1:A:1054:MET:HE3	1.86	0.57
1:A:889:ARG:HG3	1:A:904:ASN:HB3	1.85	0.57
1:A:130:MET:HE3	1:A:176:PRO:HB3	1.87	0.57
1:A:713:ARG:NH1	1:A:799:PHE:CD1	2.71	0.57
1:A:220:ILE:HB	1:A:230:ILE:HB	1.86	0.57
1:A:614:PHE:CD2	1:A:624:SER:OG	2.57	0.57
1:A:43:VAL:HG23	1:A:52:VAL:HG21	1.87	0.57
1:A:256:SER:CB	1:A:277:GLU:HG2	2.34	0.57
1:A:378:CYS:HB3	1:A:721:PRO:CB	2.31	0.57
1:A:480:SER:HB2	1:A:483:PRO:HB2	1.87	0.57
1:A:742:VAL:HG13	1:A:752:LEU:HD21	1.86	0.57
1:A:467:GLN:HE22	1:A:524:GLN:HA	1.69	0.57
1:A:639:ARG:HG3	1:A:640:THR:N	2.20	0.57
1:A:1050:LEU:HD21	1:A:1129:LEU:HD11	1.85	0.57
1:A:250:PRO:HG2	1:A:253:ILE:HG12	1.86	0.56
1:A:632:GLY:O	1:A:633:THR:C	2.48	0.56
1:A:679:MET:SD	1:A:679:MET:C	2.89	0.56
1:A:741:GLU:HG2	1:A:751:ALA:N	2.20	0.56
1:A:881:LEU:HD21	1:A:922:LEU:CD2	2.35	0.56
1:A:870:VAL:HG12	1:A:873:MET:HE3	1.84	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:877:ASN:C	1:A:879:LYS:H	2.13	0.56
1:A:184:ASP:HB2	1:A:185:PRO:CD	2.36	0.56
1:A:410:LEU:HD13	1:A:425:LEU:HD21	1.88	0.56
1:A:482:GLU:HB2	1:A:483:PRO:CD	2.35	0.56
1:A:707:ILE:O	1:A:708:GLN:O	2.24	0.56
1:A:138:GLY:O	1:A:159:LEU:N	2.39	0.56
1:A:235:GLU:HG2	1:A:254:LYS:NZ	2.20	0.56
1:A:616:LEU:CG	1:A:617:ASN:H	2.06	0.56
1:A:378:CYS:SG	1:A:724:ILE:HB	2.45	0.56
1:A:457:THR:HG22	1:A:459:PHE:H	1.70	0.56
1:A:1052:LEU:HD23	1:A:1052:LEU:O	2.06	0.56
1:A:665:LYS:O	1:A:666:LEU:CG	2.47	0.55
1:A:836:VAL:HG11	2:B:47:VAL:HG21	1.88	0.55
1:A:460:CYS:O	1:A:461:GLY:O	2.24	0.55
1:A:482:GLU:CB	1:A:483:PRO:HD3	2.37	0.55
1:A:889:ARG:HD3	1:A:901:THR:HG23	1.89	0.55
1:A:22:HIS:HD2	1:A:28:ASP:O	1.88	0.55
1:A:558:ILE:O	1:A:566:ALA:HA	2.06	0.55
1:A:644:LEU:HG	1:A:645:SER:N	2.12	0.55
1:A:688:PRO:O	1:A:689:ASP:C	2.50	0.55
1:A:559:GLY:HA2	1:A:565:SER:O	2.06	0.55
1:A:23:PHE:H	1:A:30:ASN:ND2	1.97	0.55
1:A:556:CYS:SG	1:A:557:ALA:N	2.79	0.55
1:A:578:HIS:CG	1:A:579:LYS:N	2.75	0.55
1:A:658:VAL:HG11	1:A:660:TYR:CD1	2.41	0.55
1:A:690:SER:OG	1:A:701:ILE:HB	2.06	0.55
1:A:660:TYR:CD1	1:A:707:ILE:HG23	2.43	0.54
1:A:263:ARG:HB2	1:A:271:TYR:CE2	2.41	0.54
1:A:564:ILE:HG22	1:A:564:ILE:O	2.06	0.54
1:A:602:LEU:CD2	1:A:614:PHE:HB2	2.36	0.54
1:A:614:PHE:HD2	1:A:624:SER:OG	1.85	0.54
1:A:412:PRO:O	1:A:413:LEU:HB2	2.07	0.54
1:A:765:VAL:HG13	1:A:766:SER:O	2.07	0.54
1:A:318:ASP:HB3	1:A:319:ASN:ND2	2.23	0.54
1:A:535:GLU:HB3	1:A:536:HIS:CD2	2.43	0.54
1:A:701:ILE:CD1	1:A:701:ILE:N	2.71	0.54
1:A:683:ASN:CG	1:A:683:ASN:O	2.49	0.54
1:A:714:THR:CG2	1:A:715:VAL:N	2.70	0.54
1:A:719:GLU:OE2	1:A:755:SER:CB	2.56	0.54
1:A:917:LYS:O	1:A:919:ASP:N	2.41	0.54
1:A:171:TYR:CD1	1:A:223:PRO:HA	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:HIS:O	1:A:524:GLN:N	2.41	0.54
1:A:528:GLN:O	1:A:529:ILE:HG12	2.08	0.53
1:A:726:TYR:HB2	1:A:733:PHE:CE2	2.43	0.53
1:A:803:HIS:CD2	1:A:858:LEU:CB	2.91	0.53
1:A:876:PHE:CZ	1:A:920:PHE:HA	2.43	0.53
1:A:226:PHE:N	1:A:226:PHE:CD1	2.76	0.53
1:A:414:ARG:NH1	1:A:422:TYR:CE2	2.76	0.53
1:A:817:VAL:HG22	1:A:830:ILE:HB	1.89	0.53
1:A:969:GLU:OE2	1:A:971:ALA:HB3	2.07	0.53
1:A:609:GLY:N	1:A:633:THR:O	2.41	0.53
1:A:658:VAL:CG1	1:A:659:ILE:N	2.69	0.53
1:A:697:SER:O	1:A:698:THR:OG1	2.24	0.53
1:A:982:ALA:O	1:A:985:THR:HG22	2.08	0.53
1:A:141:LYS:HE2	1:A:156:ASN:HD21	1.72	0.53
1:A:617:ASN:CB	1:A:620:THR:CG2	2.87	0.53
1:A:1006:VAL:O	1:A:1030:PHE:HA	2.08	0.53
1:A:68:ARG:HH11	1:A:74:LYS:HA	1.71	0.53
1:A:498:ILE:HG23	1:A:510:VAL:HB	1.91	0.53
1:A:987:GLU:C	1:A:989:ARG:H	2.16	0.53
1:A:563:ASP:C	1:A:563:ASP:OD1	2.49	0.53
1:A:578:HIS:CE1	1:A:579:LYS:O	2.62	0.53
1:A:421:THR:HG22	1:A:683:ASN:O	2.07	0.53
1:A:500:VAL:HG12	1:A:541:LEU:HD12	1.91	0.53
1:A:928:ARG:HA	1:A:929:SER:HB2	1.91	0.52
1:A:969:GLU:OE1	1:A:973:ASN:HB2	2.09	0.52
1:A:135:LEU:HD22	1:A:135:LEU:N	2.23	0.52
1:A:424:THR:HA	1:A:436:LEU:O	2.08	0.52
1:A:826:ASN:ND2	1:A:852:GLN:NE2	2.58	0.52
1:A:936:LYS:C	1:A:938:MET:N	2.67	0.52
1:A:335:LYS:HB2	1:A:350:MET:SD	2.49	0.52
1:A:563:ASP:O	1:A:564:ILE:C	2.53	0.52
1:A:296:THR:OG1	1:A:297:LEU:N	2.40	0.52
1:A:691:LEU:HD12	1:A:704:ILE:HD11	1.91	0.52
1:A:917:LYS:HG2	1:A:959:ILE:HG21	1.92	0.52
1:A:277:GLU:HA	1:A:277:GLU:OE1	2.09	0.52
1:A:1041:THR:HG22	1:A:1042:SER:O	2.10	0.52
1:A:234:GLN:C	1:A:236:SER:H	2.18	0.52
1:A:1091:GLY:HA2	1:A:1094:ILE:HB	1.91	0.52
1:A:707:ILE:HG22	1:A:708:GLN:N	2.24	0.52
1:A:571:LEU:CB	1:A:572:PRO:HD3	2.40	0.52
1:A:467:GLN:OE1	1:A:521:ILE:HG22	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:569:LEU:HG	1:A:576:LEU:HA	1.90	0.51
1:A:606:LEU:HB2	1:A:608:ASP:OD2	2.10	0.51
1:A:763:SER:C	1:A:803:HIS:CE1	2.88	0.51
1:A:997:LEU:HD22	1:A:1076:PHE:CD1	2.45	0.51
1:A:38:ARG:NH1	1:A:56:GLY:CA	2.74	0.51
1:A:466:GLN:HB3	1:A:481:GLN:HB2	1.92	0.51
1:A:654:ASP:HA	1:A:675:GLU:HG2	1.91	0.51
1:A:542:ASP:O	1:A:556:CYS:SG	2.68	0.51
1:A:546:LEU:HD11	1:A:593:MET:SD	2.50	0.51
1:A:698:THR:HG22	1:A:700:THR:HG23	1.90	0.51
1:A:839:GLU:HG2	1:A:840:GLU:H	1.76	0.51
1:A:404:LEU:HB2	1:A:407:ILE:HD11	1.93	0.51
1:A:355:ASN:OD1	1:A:357:GLY:CA	2.59	0.51
1:A:394:ILE:CD1	1:A:669:SER:HB2	2.40	0.51
1:A:459:PHE:CE2	1:A:461:GLY:CA	2.94	0.51
1:A:133:LEU:HD23	1:A:135:LEU:HD21	1.93	0.50
1:A:341:ASN:O	1:A:342:GLU:C	2.54	0.50
1:A:490:TRP:NE1	1:A:519:LEU:HD22	2.27	0.50
1:A:250:PRO:O	1:A:251:PRO:C	2.53	0.50
1:A:262:ASN:ND2	1:A:316:TYR:H	2.09	0.50
1:A:475:SER:CB	1:A:490:TRP:O	2.53	0.50
1:A:596:PHE:CE2	1:A:648:ASN:HA	2.46	0.50
1:A:890:LEU:O	1:A:890:LEU:HG	2.10	0.50
1:A:38:ARG:CD	1:A:54:GLU:OE1	2.49	0.50
1:A:391:ARG:HD2	1:A:392:ASN:O	2.11	0.50
1:A:457:THR:OG1	1:A:470:GLN:NE2	2.37	0.50
1:A:682:LEU:O	1:A:683:ASN:HB2	2.12	0.50
1:A:966:LEU:HD13	1:A:1007:PHE:CE2	2.47	0.50
1:A:630:THR:C	1:A:631:LEU:O	2.54	0.50
1:A:633:THR:OG1	1:A:634:GLN:N	2.43	0.50
1:A:151:GLU:HB2	1:A:153:LYS:HE2	1.93	0.50
1:A:630:THR:O	1:A:631:LEU:O	2.29	0.50
1:A:763:SER:HA	1:A:803:HIS:CE1	2.46	0.50
1:A:492:GLU:HG3	1:A:512:VAL:HG21	1.94	0.50
1:A:537:GLU:HB3	1:A:561:TRP:CD1	2.47	0.50
1:A:1033:VAL:CG1	2:B:56:ARG:CB	2.81	0.50
1:A:355:ASN:CG	1:A:357:GLY:HA2	2.37	0.50
1:A:487:VAL:HG12	1:A:524:GLN:O	2.12	0.50
1:A:530:SER:HB3	1:A:574:PHE:CE1	2.28	0.50
1:A:1078:THR:O	1:A:1079:GLU:O	2.29	0.49
1:A:355:ASN:OD1	1:A:357:GLY:HA2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:929:SER:HB2	1:A:950:ASN:O	2.12	0.49
2:B:51:LYS:N	2:B:54:GLU:HG2	2.26	0.49
1:A:141:LYS:HE2	1:A:156:ASN:ND2	2.27	0.49
1:A:459:PHE:HE2	1:A:461:GLY:HA3	1.77	0.49
1:A:564:ILE:CD1	1:A:564:ILE:N	2.76	0.49
1:A:763:SER:CA	1:A:803:HIS:CE1	2.96	0.49
1:A:5:TYR:CZ	1:A:1091:GLY:HA3	2.48	0.49
1:A:255:GLN:HB3	1:A:279:ARG:NH2	2.27	0.49
1:A:321:VAL:CG1	1:A:350:MET:HE1	2.42	0.49
1:A:563:ASP:O	1:A:564:ILE:O	2.30	0.49
1:A:181:VAL:HG13	1:A:212:VAL:CG2	2.40	0.49
1:A:611:LEU:C	1:A:611:LEU:HD23	2.37	0.49
1:A:414:ARG:HH12	1:A:422:TYR:HE2	1.61	0.49
1:A:658:VAL:HG11	1:A:660:TYR:CE1	2.47	0.49
1:A:23:PHE:N	1:A:30:ASN:ND2	2.60	0.49
1:A:395:GLY:HA2	1:A:672:ASN:HB2	1.94	0.49
1:A:632:GLY:O	1:A:634:GLN:O	2.31	0.49
1:A:917:LYS:CG	1:A:959:ILE:HG21	2.43	0.49
1:A:616:LEU:HG	1:A:617:ASN:N	2.11	0.48
1:A:538:VAL:HA	1:A:560:LEU:HD22	1.95	0.48
1:A:926:LEU:O	1:A:953:TRP:HA	2.12	0.48
1:A:458:PHE:O	1:A:459:PHE:HB2	2.13	0.48
1:A:563:ASP:OD1	1:A:564:ILE:N	2.46	0.48
1:A:932:LEU:HD12	1:A:932:LEU:HA	1.57	0.48
1:A:220:ILE:HG12	1:A:261:HIS:CE1	2.47	0.48
1:A:358:PRO:HD2	1:A:380:GLY:HA2	1.95	0.48
1:A:426:VAL:HB	1:A:460:CYS:SG	2.54	0.48
1:A:1054:MET:O	1:A:1058:LEU:HB2	2.13	0.48
1:A:304:LEU:HD12	1:A:305:LEU:N	2.27	0.48
1:A:1129:LEU:C	1:A:1131:LYS:H	2.21	0.48
1:A:731:GLN:C	1:A:796:GLN:HG2	2.39	0.48
1:A:905:HIS:CD2	1:A:908:ASN:HD21	2.28	0.48
1:A:65:GLU:O	1:A:77:LEU:HD12	2.13	0.48
1:A:1041:THR:HG22	1:A:1042:SER:N	2.28	0.48
1:A:5:TYR:OH	1:A:1091:GLY:HA3	2.13	0.48
1:A:305:LEU:CD1	1:A:336:LEU:HD22	2.43	0.48
1:A:368:GLU:O	1:A:369:ARG:HB3	2.13	0.48
1:A:23:PHE:CD1	1:A:66:LEU:HD21	2.49	0.48
1:A:598:SER:O	1:A:599:SER:HB2	2.13	0.48
1:A:731:GLN:HA	1:A:796:GLN:HE21	1.79	0.48
1:A:927:MET:O	1:A:927:MET:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:VAL:C	2:B:49:TYR:H	2.21	0.48
1:A:123:ILE:HG13	1:A:169:PHE:CE1	2.49	0.47
1:A:125:ASP:OD2	1:A:128:CYS:N	2.47	0.47
1:A:762:SER:O	1:A:763:SER:HB3	2.14	0.47
1:A:24:THR:HB	1:A:30:ASN:HD21	1.78	0.47
1:A:116:SER:OG	1:A:134:ARG:NE	2.47	0.47
1:A:449:MET:HG2	1:A:484:LYS:HD2	1.95	0.47
1:A:698:THR:CG2	1:A:700:THR:HG23	2.44	0.47
1:A:371:GLY:O	1:A:1014:MET:HE3	2.14	0.47
1:A:449:MET:CG	1:A:484:LYS:HD2	2.43	0.47
1:A:235:GLU:HG2	1:A:254:LYS:HZ3	1.79	0.47
1:A:631:LEU:N	1:A:631:LEU:CD2	2.44	0.47
1:A:109:GLN:HE21	1:A:109:GLN:HB2	1.46	0.47
1:A:728:GLU:O	1:A:731:GLN:N	2.30	0.47
1:A:24:THR:N	1:A:30:ASN:ND2	2.57	0.47
1:A:81:THR:HG23	1:A:82:ALA:H	1.77	0.47
1:A:112:ILE:HD12	1:A:112:ILE:N	2.29	0.47
1:A:235:GLU:HB3	1:A:254:LYS:HB2	1.97	0.47
1:A:414:ARG:HH11	1:A:414:ARG:CG	2.20	0.47
1:A:580:GLU:CG	1:A:582:LEU:HD23	2.44	0.47
1:A:600:HIS:CE1	1:A:618:ILE:HG23	2.50	0.47
1:A:642:ARG:HH22	1:A:683:ASN:ND2	2.13	0.47
1:A:697:SER:O	1:A:698:THR:CB	2.62	0.47
1:A:921:ILE:HA	1:A:933:LEU:O	2.15	0.47
1:A:1049:ASN:O	1:A:1050:LEU:C	2.58	0.47
1:A:1131:LYS:O	1:A:1131:LYS:HG2	2.15	0.47
1:A:263:ARG:HB2	1:A:271:TYR:HE2	1.78	0.47
1:A:969:GLU:C	1:A:971:ALA:H	2.21	0.47
1:A:1048:TYR:HE2	1:A:1052:LEU:HD12	1.75	0.47
1:A:117:GLU:OE1	1:A:117:GLU:CA	2.61	0.47
1:A:438:LEU:C	1:A:440:GLY:H	2.23	0.47
1:A:530:SER:CB	1:A:574:PHE:CE1	2.95	0.47
1:A:690:SER:O	1:A:691:LEU:HD23	2.15	0.47
1:A:130:MET:CA	1:A:145:LEU:HD12	2.41	0.46
1:A:632:GLY:HA3	1:A:653:SER:HB3	1.95	0.46
1:A:828:TYR:CE2	1:A:861:VAL:HG11	2.50	0.46
1:A:938:MET:CG	1:A:939:GLU:H	2.28	0.46
1:A:953:TRP:HB2	1:A:970:ASN:HB2	1.96	0.46
1:A:579:LYS:NZ	1:A:581:MET:SD	2.83	0.46
1:A:6:VAL:HG21	1:A:998:PHE:CE2	2.50	0.46
1:A:500:VAL:HG11	1:A:541:LEU:HD12	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:881:LEU:HD21	1:A:922:LEU:HD23	1.97	0.46
1:A:902:GLU:OE2	1:A:935:TYR:OH	2.29	0.46
1:A:682:LEU:HB3	1:A:690:SER:HB3	1.98	0.46
1:A:1125:THR:HB	1:A:1128:ASP:HB2	1.97	0.46
1:A:38:ARG:NH1	1:A:56:GLY:HA3	2.29	0.46
1:A:658:VAL:HG12	1:A:659:ILE:N	2.28	0.46
1:A:40:GLU:HG3	1:A:54:GLU:HG2	1.98	0.46
1:A:641:PHE:CD2	1:A:650:PHE:HB2	2.51	0.46
1:A:1057:ARG:HD2	1:A:1108:VAL:O	2.16	0.46
1:A:80:LEU:HG	1:A:81:THR:O	2.15	0.46
1:A:459:PHE:CE2	1:A:461:GLY:N	2.84	0.46
1:A:580:GLU:HG3	1:A:582:LEU:HD23	1.98	0.46
1:A:881:LEU:CD2	1:A:922:LEU:CD2	2.93	0.46
1:A:1097:PHE:O	1:A:1100:ILE:HB	2.15	0.46
2:B:56:ARG:HH11	2:B:57:LEU:H	1.64	0.46
1:A:131:ILE:HG22	1:A:133:LEU:HD13	1.98	0.46
1:A:133:LEU:CB	1:A:135:LEU:HD21	2.42	0.46
1:A:234:GLN:C	1:A:235:GLU:HG3	2.40	0.46
1:A:611:LEU:HD23	1:A:612:PHE:C	2.41	0.46
1:A:874:VAL:CG2	1:A:875:GLU:H	2.28	0.46
1:A:961:ASP:O	1:A:963:ASP:N	2.49	0.46
1:A:67:PHE:HD1	1:A:128:CYS:SG	2.38	0.46
1:A:5:TYR:HE2	1:A:7:VAL:HG21	1.79	0.45
1:A:564:ILE:HG21	1:A:583:GLY:O	2.15	0.45
1:A:155:PHE:HB3	1:A:200:LYS:HE3	1.97	0.45
1:A:355:ASN:ND2	1:A:357:GLY:HA2	2.30	0.45
1:A:741:GLU:HG2	1:A:750:THR:C	2.41	0.45
1:A:394:ILE:HD11	1:A:669:SER:CB	2.45	0.45
1:A:411:TRP:HB2	1:A:460:CYS:HB2	1.98	0.45
1:A:280:LEU:HD12	1:A:280:LEU:HA	1.69	0.45
1:A:732:CYS:HB2	1:A:794:ILE:O	2.15	0.45
1:A:148:ASP:HB2	1:A:149:ASN:H	1.47	0.45
1:A:167:VAL:O	1:A:168:LYS:HG2	2.16	0.45
1:A:490:TRP:CE2	1:A:519:LEU:HD22	2.52	0.45
1:A:660:TYR:HB3	1:A:661:SER:H	1.60	0.45
1:A:978:GLN:HE21	1:A:995:VAL:CG2	2.21	0.45
1:A:414:ARG:NH1	1:A:422:TYR:HE2	2.14	0.45
1:A:402:ILE:O	1:A:698:THR:HA	2.16	0.45
1:A:520:GLN:O	1:A:526:LEU:HA	2.16	0.45
1:A:14:ALA:HB1	1:A:327:ARG:HB3	1.98	0.45
1:A:630:THR:HG21	1:A:1134:GLU:CD	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:879:LYS:HD2	1:A:890:LEU:HD21	1.98	0.45
1:A:1081:LYS:HE3	1:A:1083:GLU:HG2	1.98	0.45
1:A:20:THR:HB	1:A:315:THR:CG2	2.47	0.45
1:A:226:PHE:N	1:A:226:PHE:HD1	2.14	0.44
1:A:282:MET:HG3	1:A:284:LEU:HG	1.99	0.44
1:A:1079:GLU:O	1:A:1081:LYS:N	2.50	0.44
2:B:45:SER:OG	2:B:48:TYR:CE2	2.69	0.44
1:A:81:THR:CB	1:A:85:ASN:HB2	2.43	0.44
1:A:226:PHE:HD1	1:A:226:PHE:H	1.65	0.44
1:A:597:GLU:HB3	1:A:664:HIS:CD2	2.51	0.44
1:A:742:VAL:O	1:A:749:THR:HG22	2.17	0.44
1:A:1033:VAL:HG11	2:B:56:ARG:CG	2.47	0.44
2:B:51:LYS:C	2:B:54:GLU:HB2	2.40	0.44
1:A:520:GLN:HB2	1:A:522:HIS:HD2	1.82	0.44
1:A:641:PHE:HB3	1:A:679:MET:CE	2.47	0.44
1:A:817:VAL:CG1	1:A:873:MET:HG3	2.48	0.44
1:A:939:GLU:CG	1:A:941:ASN:HB2	2.47	0.44
1:A:1090:ASP:OD2	1:A:1090:ASP:N	2.49	0.44
1:A:587:ILE:HB	1:A:588:PRO:CD	2.43	0.44
1:A:934:ALA:HB2	1:A:945:ILE:CD1	2.47	0.44
1:A:1074:ARG:HD3	1:A:1074:ARG:HA	1.70	0.44
1:A:438:LEU:HD23	1:A:442:GLU:C	2.42	0.44
1:A:609:GLY:HA3	1:A:632:GLY:O	2.17	0.44
1:A:1109:VAL:HG12	1:A:1110:ALA:N	2.31	0.44
1:A:124:ILE:HG12	1:A:131:ILE:HG12	1.99	0.44
1:A:826:ASN:ND2	1:A:852:GLN:HE22	2.15	0.44
1:A:912:LEU:HG	1:A:926:LEU:HB2	1.99	0.44
1:A:958:GLU:HG3	1:A:959:ILE:N	2.33	0.44
1:A:1055:GLN:HE21	1:A:1055:GLN:HB3	1.52	0.44
1:A:462:ASN:HD22	1:A:462:ASN:HA	1.68	0.44
1:A:579:LYS:HE3	1:A:580:GLU:O	2.17	0.44
1:A:985:THR:CG2	1:A:989:ARG:HH21	2.31	0.44
2:B:54:GLU:HA	2:B:54:GLU:OE1	2.18	0.44
1:A:35:LYS:HB2	1:A:38:ARG:HB2	1.99	0.44
1:A:786:VAL:HG22	1:A:787:GLU:H	1.83	0.44
1:A:1109:VAL:HG21	1:A:1125:THR:O	2.17	0.44
1:A:108:VAL:HG11	1:A:143:ILE:HD11	1.99	0.44
1:A:411:TRP:CZ2	1:A:459:PHE:HA	2.53	0.44
1:A:482:GLU:CB	1:A:483:PRO:CD	2.96	0.44
1:A:734:GLY:C	1:A:735:VAL:HG23	2.43	0.44
1:A:1041:THR:CG2	1:A:1042:SER:N	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:LEU:C	1:A:422:TYR:HB3	2.42	0.43
1:A:223:PRO:C	1:A:225:PRO:HD2	2.43	0.43
1:A:591:ILE:HD11	1:A:602:LEU:HD11	2.00	0.43
1:A:141:LYS:HD2	1:A:154:ALA:HB3	1.99	0.43
1:A:388:ARG:CD	1:A:714:THR:OG1	2.59	0.43
1:A:742:VAL:C	1:A:749:THR:HG22	2.43	0.43
1:A:241:ASN:OD1	1:A:242:GLY:N	2.51	0.43
1:A:948:ASP:OD2	1:A:994:GLU:HG2	2.19	0.43
1:A:1127:ASP:CA	1:A:1130:ILE:HG22	2.47	0.43
1:A:23:PHE:CE2	1:A:91:TYR:HB2	2.53	0.43
1:A:629:VAL:HG11	1:A:668:PHE:HE2	1.83	0.43
1:A:665:LYS:C	1:A:666:LEU:HG	2.39	0.43
1:A:809:GLN:O	1:A:810:ASN:HB2	2.19	0.43
1:A:451:PHE:HA	1:A:470:GLN:OE1	2.19	0.43
1:A:563:ASP:OD2	1:A:567:ARG:NH1	2.52	0.43
1:A:965:PHE:O	1:A:976:VAL:HA	2.18	0.43
1:A:159:LEU:HD22	1:A:161:GLU:O	2.18	0.43
1:A:192:THR:HB	1:A:205:GLY:HA3	2.01	0.43
1:A:398:GLU:O	1:A:398:GLU:HG3	2.19	0.43
1:A:407:ILE:HG21	1:A:410:LEU:HD23	2.00	0.43
1:A:1078:THR:O	1:A:1078:THR:OG1	2.31	0.43
1:A:117:GLU:O	1:A:118:THR:CB	2.66	0.43
1:A:520:GLN:HB2	1:A:522:HIS:CD2	2.54	0.43
1:A:706:GLU:C	1:A:707:ILE:HG13	2.43	0.43
1:A:836:VAL:CG1	2:B:47:VAL:HG21	2.48	0.43
1:A:877:ASN:C	1:A:879:LYS:N	2.70	0.43
1:A:133:LEU:HB2	1:A:141:LYS:HB3	2.01	0.43
1:A:570:LYS:HB2	1:A:575:GLU:HG2	2.01	0.43
1:A:617:ASN:HB2	1:A:621:GLY:H	1.83	0.43
1:A:623:LEU:HD23	1:A:624:SER:C	2.44	0.43
1:A:836:VAL:CG1	2:B:48:TYR:CE2	3.01	0.43
2:B:56:ARG:HH11	2:B:57:LEU:N	2.17	0.43
1:A:450:GLY:HA2	1:A:477:ARG:NH2	2.34	0.42
1:A:459:PHE:CD2	1:A:460:CYS:N	2.87	0.42
1:A:538:VAL:CG1	1:A:558:ILE:HD11	2.49	0.42
1:A:679:MET:HB2	1:A:693:LEU:HG	2.00	0.42
1:A:932:LEU:HD22	1:A:965:PHE:CE1	2.54	0.42
1:A:171:TYR:CG	1:A:223:PRO:HA	2.54	0.42
1:A:701:ILE:HD13	1:A:701:ILE:H	1.82	0.42
1:A:932:LEU:O	1:A:933:LEU:HD12	2.18	0.42
1:A:39:LEU:HD11	1:A:64:MET:SD	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:PHE:HB2	1:A:159:LEU:HD12	2.02	0.42
1:A:406:GLY:O	1:A:407:ILE:C	2.62	0.42
1:A:546:LEU:HD22	1:A:600:HIS:ND1	2.33	0.42
1:A:644:LEU:CG	1:A:645:SER:N	2.79	0.42
1:A:707:ILE:O	1:A:708:GLN:C	2.63	0.42
1:A:320:GLY:HA3	1:A:335:LYS:HE3	2.00	0.42
1:A:459:PHE:CD2	1:A:461:GLY:N	2.83	0.42
2:B:47:VAL:HG23	2:B:48:TYR:N	2.33	0.42
1:A:118:THR:HG22	1:A:118:THR:O	2.20	0.42
1:A:460:CYS:O	1:A:461:GLY:C	2.63	0.42
1:A:815:SER:HB3	1:A:872:SER:HA	2.02	0.42
1:A:861:VAL:HG12	1:A:861:VAL:O	2.19	0.42
1:A:938:MET:C	1:A:940:GLY:H	2.27	0.42
2:B:46:LEU:O	2:B:50:LEU:HG	2.18	0.42
1:A:2:SER:CB	1:A:995:VAL:HG23	2.50	0.42
1:A:504:ASN:ND2	1:A:545:PRO:HD3	2.34	0.42
1:A:580:GLU:OE1	1:A:623:LEU:HD11	2.19	0.42
1:A:616:LEU:CG	1:A:617:ASN:N	2.80	0.42
2:B:55:VAL:CG2	2:B:56:ARG:N	2.82	0.42
1:A:534:MET:HE3	1:A:534:MET:HB3	1.75	0.42
1:A:987:GLU:C	1:A:989:ARG:N	2.78	0.42
2:B:45:SER:OG	2:B:48:TYR:HE2	2.03	0.42
1:A:181:VAL:HA	1:A:189:HIS:O	2.20	0.42
1:A:611:LEU:HD23	1:A:612:PHE:N	2.35	0.42
1:A:639:ARG:CG	1:A:640:THR:N	2.83	0.42
1:A:88:ILE:O	1:A:89:LEU:HD23	2.20	0.42
1:A:727:GLN:HB2	1:A:829:PHE:CE1	2.55	0.42
1:A:808:LEU:HD23	1:A:808:LEU:HA	1.92	0.42
1:A:864:LYS:HD3	1:A:899:VAL:HG23	2.01	0.42
1:A:928:ARG:HA	1:A:929:SER:CB	2.48	0.42
2:B:51:LYS:O	2:B:54:GLU:CB	2.55	0.42
2:B:55:VAL:O	2:B:56:ARG:HB3	2.14	0.42
1:A:706:GLU:O	1:A:707:ILE:HG13	2.19	0.41
2:B:55:VAL:HG23	2:B:56:ARG:H	1.85	0.41
1:A:80:LEU:HD23	1:A:120:ILE:HG21	2.03	0.41
1:A:367:LEU:CG	1:A:374:GLN:HG3	2.48	0.41
1:A:449:MET:O	1:A:479:VAL:CG2	2.62	0.41
1:A:980:ASP:HB3	1:A:988:GLU:O	2.20	0.41
1:A:1102:ARG:O	1:A:1105:MET:HB3	2.20	0.41
1:A:413:LEU:H	1:A:422:TYR:HB3	1.85	0.41
1:A:620:THR:CG2	1:A:621:GLY:N	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:742:VAL:CG1	1:A:752:LEU:HD21	2.51	0.41
1:A:932:LEU:HD22	1:A:965:PHE:HE1	1.85	0.41
1:A:1134:GLU:C	1:A:1136:LEU:N	2.78	0.41
1:A:19:VAL:HG12	1:A:32:LEU:HB2	2.03	0.41
1:A:138:GLY:O	1:A:159:LEU:CB	2.69	0.41
1:A:396:ILE:HD12	1:A:673:LEU:HD11	2.02	0.41
1:A:504:ASN:CG	1:A:545:PRO:HD3	2.46	0.41
1:A:555:LEU:HD23	1:A:555:LEU:H	1.85	0.41
1:A:692:ALA:C	1:A:693:LEU:HD12	2.45	0.41
1:A:361:ASP:OD2	1:A:362:MET:N	2.54	0.41
1:A:660:TYR:CE2	1:A:707:ILE:HG12	2.56	0.41
1:A:879:LYS:HB2	1:A:890:LEU:HD11	2.03	0.41
1:A:686:GLY:O	1:A:687:TYR:CG	2.74	0.41
1:A:792:LEU:HA	1:A:792:LEU:HD23	1.74	0.41
1:A:824:ASP:OD2	1:A:893:TRP:NE1	2.49	0.41
1:A:876:PHE:HZ	1:A:920:PHE:HA	1.83	0.41
1:A:893:TRP:HA	1:A:893:TRP:CE3	2.55	0.41
1:A:600:HIS:CE1	1:A:618:ILE:CG2	3.03	0.41
1:A:660:TYR:CE1	1:A:707:ILE:HA	2.55	0.41
1:A:10:GLN:HB3	1:A:1037:ILE:HB	2.03	0.41
1:A:34:ALA:N	1:A:64:MET:HE1	2.36	0.41
1:A:650:PHE:C	1:A:650:PHE:CD2	2.99	0.41
1:A:884:ILE:HD12	1:A:889:ARG:HB2	2.03	0.41
1:A:1100:ILE:O	1:A:1105:MET:CE	2.69	0.41
1:A:40:GLU:HB3	1:A:42:TYR:CE1	2.56	0.41
1:A:340:SER:HB3	1:A:346:TYR:CZ	2.55	0.41
1:A:570:LYS:HZ3	1:A:572:PRO:HD2	1.85	0.41
1:A:607:GLY:HA2	1:A:635:PRO:HB3	2.02	0.41
1:A:708:GLN:CD	1:A:710:LEU:O	2.63	0.41
1:A:730:SER:HB2	1:A:732:CYS:SG	2.61	0.41
1:A:879:LYS:CB	1:A:890:LEU:HD11	2.51	0.41
1:A:909:ILE:HG21	1:A:927:MET:HG2	2.03	0.41
1:A:912:LEU:HD23	1:A:912:LEU:HA	1.80	0.41
1:A:928:ARG:O	1:A:928:ARG:CD	2.68	0.41
1:A:953:TRP:N	1:A:953:TRP:CD1	2.88	0.41
1:A:961:ASP:OD2	1:A:961:ASP:C	2.64	0.41
1:A:1039:LEU:HD12	1:A:1040:VAL:N	2.36	0.41
1:A:1129:LEU:C	1:A:1131:LYS:N	2.79	0.41
2:B:47:VAL:C	2:B:49:TYR:N	2.78	0.41
1:A:895:THR:C	1:A:897:LYS:H	2.28	0.41
1:A:24:THR:HG22	1:A:28:ASP:OD2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:767:SER:OG	1:A:768:SER:N	2.54	0.40
1:A:155:PHE:CB	1:A:200:LYS:HE3	2.52	0.40
1:A:169:PHE:HA	1:A:177:THR:O	2.21	0.40
1:A:1024:THR:CG2	1:A:1041:THR:HG21	2.50	0.40
1:A:38:ARG:NH1	1:A:56:GLY:N	2.69	0.40
1:A:399:HIS:HB3	1:A:687:TYR:HE1	1.86	0.40
1:A:726:TYR:CE1	1:A:796:GLN:NE2	2.89	0.40
1:A:1123:GLU:HG2	1:A:1124:ALA:N	2.32	0.40
1:A:2:SER:HB3	1:A:995:VAL:HG23	2.03	0.40
1:A:342:GLU:N	1:A:342:GLU:CD	2.79	0.40
1:A:410:LEU:HD22	1:A:425:LEU:HD21	2.04	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%)	869 (79%)	167 (15%)	70 (6%)	1	6
2	B	11/13 (85%)	7 (64%)	2 (18%)	2 (18%)	0	0
All	All	1117/1156 (97%)	876 (78%)	169 (15%)	72 (6%)	1	6

All (72) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	214	ALA
1	A	235	GLU
1	A	318	ASP
1	A	407	ILE
1	A	430	VAL
1	A	461	GLY
1	A	485	ALA

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Mol	Chain	Res	Type
1	A	487	VAL
1	A	494	GLN
1	A	523	PRO
1	A	554	PRO
1	A	571	LEU
1	A	624	SER
1	A	631	LEU
1	A	665	LYS
1	A	683	ASN
1	A	698	THR
1	A	706	GLU
1	A	707	ILE
1	A	708	GLN
1	A	751	ALA
1	A	768	SER
1	A	918	GLY
1	A	919	ASP
1	A	928	ARG
1	A	970	ASN
1	A	1079	GLU
1	A	1080	ARG
1	A	1110	ALA
2	B	56	ARG
1	A	118	THR
1	A	242	GLY
1	A	474	ALA
1	A	505	SER
1	A	517	TYR
1	A	524	GLN
1	A	529	ILE
1	A	626	ARG
1	A	729	VAL
1	A	801	VAL
1	A	802	LEU
1	A	808	LEU
1	A	860	THR
1	A	886	SER
1	A	962	ASP
1	A	149	ASN
1	A	291	MET
1	A	343	GLN
1	A	413	LEU

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Mol	Chain	Res	Type
1	A	535	GLU
1	A	564	ILE
1	A	599	SER
1	A	662	SER
1	A	689	ASP
1	A	856	GLY
1	A	1107	GLU
2	B	53	ARG
1	A	503	CYS
1	A	518	TYR
1	A	620	THR
1	A	666	LEU
1	A	862	ALA
1	A	1130	ILE
1	A	810	ASN
1	A	864	LYS
1	A	929	SER
1	A	224	GLU
1	A	259	VAL
1	A	629	VAL
1	A	406	GLY
1	A	513	GLY
1	A	493	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%)	797 (82%)	180 (18%)	1	9
2	B	13/13 (100%)	10 (77%)	3 (23%)	1	5
All	All	990/1014 (98%)	807 (82%)	183 (18%)	1	9

All (183) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	19	VAL
1	A	24	THR
1	A	25	SER
1	A	27	GLU
1	A	32	LEU
1	A	40	GLU
1	A	49	LEU
1	A	55	VAL
1	A	73	SER
1	A	79	ILE
1	A	81	THR
1	A	97	SER
1	A	98	ILE
1	A	103	ARG
1	A	109	GLN
1	A	117	GLU
1	A	123	ILE
1	A	125	ASP
1	A	128	CYS
1	A	130	MET
1	A	133	LEU
1	A	135	LEU
1	A	141	LYS
1	A	147	ARG
1	A	148	ASP
1	A	162	LEU
1	A	167	VAL
1	A	168	LYS
1	A	186	GLN
1	A	191	LYS
1	A	192	THR
1	A	197	LEU
1	A	218	MET
1	A	224	GLU
1	A	226	PHE
1	A	234	GLN
1	A	235	GLU
1	A	255	GLN
1	A	259	VAL
1	A	283	LEU
1	A	286	GLU
1	A	290	GLN

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Mol	Chain	Res	Type
1	A	298	LYS
1	A	300	LEU
1	A	301	ARG
1	A	309	SER
1	A	312	GLU
1	A	314	LEU
1	A	321	VAL
1	A	324	VAL
1	A	327	ARG
1	A	331	SER
1	A	333	LEU
1	A	334	VAL
1	A	352	THR
1	A	354	THR
1	A	360	VAL
1	A	366	ASP
1	A	372	GLN
1	A	374	GLN
1	A	383	LYS
1	A	390	ILE
1	A	396	ILE
1	A	401	SER
1	A	410	LEU
1	A	414	ARG
1	A	418	ASN
1	A	424	THR
1	A	430	VAL
1	A	434	ARG
1	A	439	ASN
1	A	447	GLU
1	A	448	LEU
1	A	449	MET
1	A	452	VAL
1	A	462	ASN
1	A	467	GLN
1	A	468	LEU
1	A	469	ILE
1	A	476	VAL
1	A	492	GLU
1	A	496	LYS
1	A	503	CYS
1	A	506	SER

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Mol	Chain	Res	Type
1	A	507	GLN
1	A	516	LEU
1	A	518	TYR
1	A	519	LEU
1	A	520	GLN
1	A	521	ILE
1	A	526	LEU
1	A	529	ILE
1	A	534	MET
1	A	543	ILE
1	A	544	THR
1	A	552	LEU
1	A	562	THR
1	A	564	ILE
1	A	567	ARG
1	A	570	LYS
1	A	576	LEU
1	A	582	LEU
1	A	587	ILE
1	A	602	LEU
1	A	603	LEU
1	A	618	ILE
1	A	619	GLU
1	A	623	LEU
1	A	629	VAL
1	A	630	THR
1	A	631	LEU
1	A	633	THR
1	A	640	THR
1	A	653	SER
1	A	654	ASP
1	A	669	SER
1	A	679	MET
1	A	701	ILE
1	A	703	THR
1	A	705	ASP
1	A	706	GLU
1	A	708	GLN
1	A	729	VAL
1	A	730	SER
1	A	744	ASP
1	A	750	THR

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Mol	Chain	Res	Type
1	A	765	VAL
1	A	766	SER
1	A	770	LEU
1	A	794	ILE
1	A	801	VAL
1	A	814	LEU
1	A	815	SER
1	A	817	VAL
1	A	823	LYS
1	A	839	GLU
1	A	844	LYS
1	A	855	ASP
1	A	857	LYS
1	A	858	LEU
1	A	885	ASN
1	A	886	SER
1	A	893	TRP
1	A	896	GLU
1	A	899	VAL
1	A	900	ARG
1	A	904	ASN
1	A	909	ILE
1	A	914	LEU
1	A	916	THR
1	A	917	LYS
1	A	921	ILE
1	A	922	LEU
1	A	926	LEU
1	A	928	ARG
1	A	931	LEU
1	A	945	ILE
1	A	947	ARG
1	A	966	LEU
1	A	969	GLU
1	A	979	LYS
1	A	986	ASP
1	A	992	LEU
1	A	1000	LEU
1	A	1006	VAL
1	A	1015	GLN
1	A	1039	LEU
1	A	1045	GLU

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Mol	Chain	Res	Type
1	A	1055	GLN
1	A	1063	LYS
1	A	1075	SER
1	A	1079	GLU
1	A	1080	ARG
1	A	1093	LEU
1	A	1100	ILE
1	A	1109	VAL
1	A	1127	ASP
1	A	1131	LYS
1	A	1135	GLU
2	B	45	SER
2	B	49	TYR
2	B	57	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	22	HIS
1	A	30	ASN
1	A	105	HIS
1	A	109	GLN
1	A	189	HIS
1	A	240	HIS
1	A	261	HIS
1	A	267	ASN
1	A	319	ASN
1	A	372	GLN
1	A	374	GLN
1	A	399	HIS
1	A	418	ASN
1	A	439	ASN
1	A	462	ASN
1	A	497	ASN
1	A	504	ASN
1	A	520	GLN
1	A	522	HIS
1	A	617	ASN
1	A	670	ASN
1	A	708	GLN
1	A	727	GLN

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Mol	Chain	Res	Type
1	A	790	ASN
1	A	796	GLN
1	A	809	GLN
1	A	826	ASN
1	A	845	GLN
1	A	885	ASN
1	A	904	ASN
1	A	905	HIS
1	A	941	ASN
1	A	950	ASN
1	A	978	GLN
1	A	990	GLN
1	A	1015	GLN
1	A	1055	GLN
1	A	1056	ASN
1	A	1059	ASN
1	A	1070	HIS
1	A	1077	HIS
1	A	1106	GLN

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%)	0.28	67 (6%) 27 14	18, 68, 160, 208	0
2	B	13/13 (100%)	1.63	5 (38%) 1 1	30, 30, 32, 47	0
All	All	1127/1156 (97%)	0.29	72 (6%) 25 13	18, 67, 160, 208	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	508	VAL	6.3
1	A	462	ASN	6.2
1	A	616	LEU	5.8
1	A	602	LEU	4.5
1	A	504	ASN	4.5
1	A	519	LEU	4.5
1	A	505	SER	4.1
1	A	510	VAL	4.1
1	A	503	CYS	3.8
1	A	313	CYS	3.7
1	A	572	PRO	3.7
1	A	291	MET	3.6
1	A	461	GLY	3.4
1	A	502	SER	3.4
1	A	925	ASP	3.3
1	A	571	LEU	3.3
1	A	521	ILE	3.3
1	A	542	ASP	3.3
1	A	603	LEU	3.3
1	A	426	VAL	3.3
2	B	57	LEU	3.2
2	B	56	ARG	3.2
2	B	55	VAL	3.2
1	A	460	CYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	506	SER	3.0
1	A	297	LEU	3.0
1	A	2	SER	2.9
1	A	518	TYR	2.9
1	A	292	ASP	2.9
1	A	569	LEU	2.9
1	A	501	ALA	2.9
1	A	660	TYR	2.9
1	A	689	ASP	2.8
2	B	48	TYR	2.8
1	A	412	PRO	2.8
1	A	624	SER	2.8
1	A	342	GLU	2.8
1	A	659	ILE	2.7
1	A	714	THR	2.7
1	A	507	GLN	2.6
1	A	666	LEU	2.6
1	A	509	VAL	2.6
1	A	613	TYR	2.6
1	A	327	ARG	2.5
1	A	498	ILE	2.5
1	A	413	LEU	2.5
1	A	528	GLN	2.5
1	A	294	THR	2.5
1	A	458	PHE	2.4
1	A	513	GLY	2.3
1	A	918	GLY	2.3
1	A	495	ALA	2.3
1	A	325	GLY	2.3
1	A	512	VAL	2.3
1	A	615	GLY	2.3
1	A	517	TYR	2.3
1	A	276	MET	2.2
1	A	293	GLY	2.2
1	A	625	ASP	2.2
1	A	497	ASN	2.2
1	A	924	GLY	2.2
1	A	928	ARG	2.2
1	A	339	ASP	2.2
1	A	618	ILE	2.1
1	A	614	PHE	2.1
1	A	430	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	46	LEU	2.1
1	A	411	TRP	2.1
1	A	1054	MET	2.1
1	A	450	GLY	2.1
1	A	557	ALA	2.0
1	A	515	ALA	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.