



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 06:11 PM EDT

PDB ID : 3I8C / pdb_00003i8c
Title : Crystal Structure of DDB1 in Complex with the H-Box Motif of WDR21A
Authors : Li, T.; Robert, E.I.; Breugel, P.C.V.; Strubin, M.; Zheng, N.
Deposited on : 2009-07-09
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

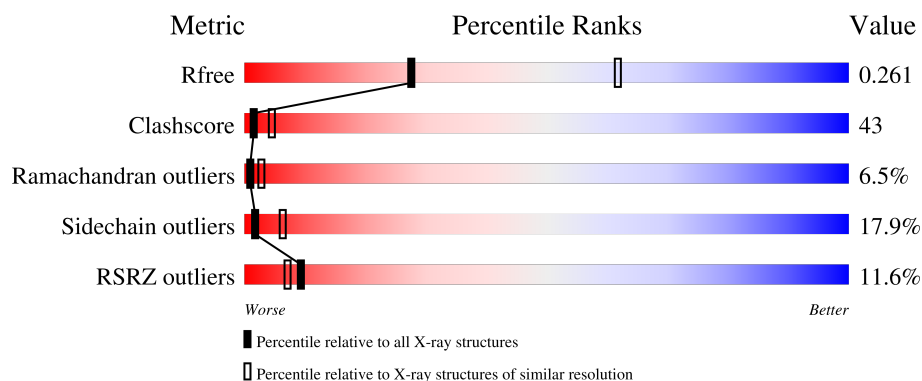
1 Overall quality at a glance

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	11% 40% 42% 13% • •
2	B	13	8% 8% 62% 31%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8825 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

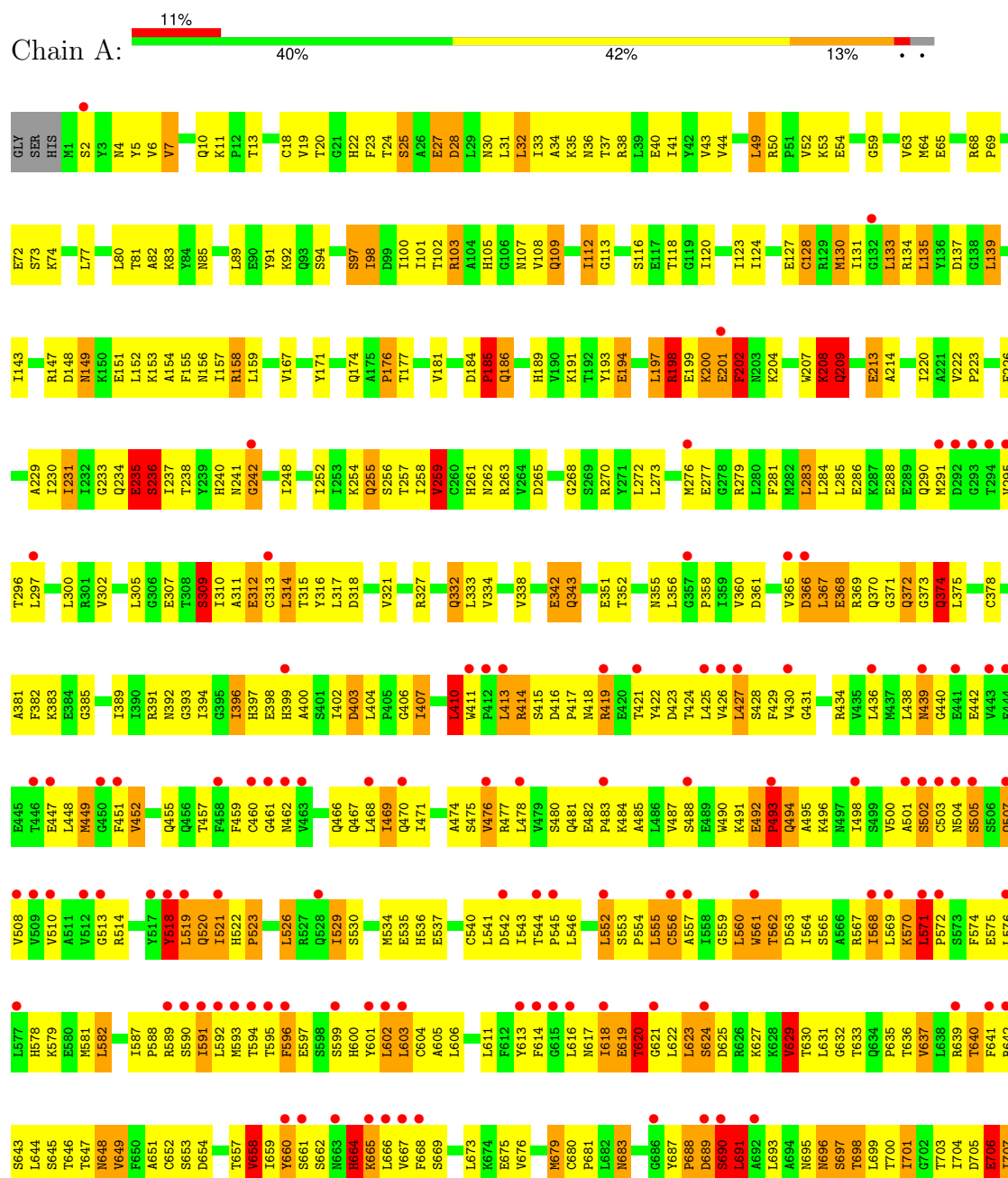
- Molecule 2 is a protein called WD repeat-containing protein 21A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	13	Total	C	N	O	S	0	0	0
			99	61	19	18	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	64.11Å 134.47Å 183.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.88 – 2.80 45.88 – 2.80	Depositor EDS
% Data completeness (in resolution range)	80.9 (45.88-2.80) 80.9 (45.88-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.251 , 0.308 0.262 , 0.261	Depositor DCC
R_{free} test set	1662 reflections (3.53%)	wwPDB-VP
Wilson B-factor (Å ²)	62.8	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 64.3	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	8825	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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	0.98	14/8885 (0.2%)	1.24	64/12034 (0.5%)
2	B	1.72	0/99	2.28	4/129 (3.1%)
All	All	0.99	14/8984 (0.2%)	1.25	68/12163 (0.6%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	697	SER	C-O	-11.71	1.11	1.23
1	A	919	ASP	N-CA	-11.57	1.31	1.46
1	A	202	PHE	C-O	11.03	1.37	1.24
1	A	950	ASN	C-O	-9.54	1.14	1.24
1	A	899	VAL	CA-CB	8.83	1.63	1.53
1	A	194	GLU	C-O	-8.45	1.12	1.23
1	A	925	ASP	N-CA	8.22	1.56	1.46
1	A	924	GLY	N-CA	7.51	1.53	1.45
1	A	918	GLY	C-N	-7.51	1.23	1.33
1	A	725	CYS	CB-SG	-5.54	1.62	1.81
1	A	697	SER	CB-OG	-5.35	1.31	1.42
1	A	658	VAL	CA-CB	-5.21	1.48	1.54
1	A	930	VAL	N-CA	-5.15	1.40	1.46
1	A	209	GLN	CA-C	-5.03	1.46	1.52

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	186	GLN	N-CA-CB	-13.62	87.52	110.41
2	B	132	SER	N-CA-C	-12.86	96.69	112.38
1	A	918	GLY	O-C-N	-12.84	106.01	122.70
1	A	514	ARG	N-CA-C	-12.80	97.08	113.72
1	A	494	GLN	N-CA-CB	-12.53	84.61	110.67
1	A	918	GLY	CA-C-N	12.51	145.43	121.54
1	A	918	GLY	C-N-CA	12.51	145.43	121.54
1	A	514	ARG	N-CA-CB	-12.30	92.56	110.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	924	GLY	N-CA-C	9.87	124.10	111.37
2	B	132	SER	CA-C-N	-9.31	105.16	120.71
2	B	132	SER	C-N-CA	-9.31	105.16	120.71
1	A	697	SER	CA-C-O	-9.06	110.94	120.09
1	A	494	GLN	N-CA-C	8.93	125.69	113.37
1	A	763	SER	N-CA-C	8.84	121.95	108.52
1	A	1110	ALA	N-CA-C	-8.80	102.95	114.31
1	A	493	PRO	CB-CA-C	8.49	125.57	111.56
1	A	213	GLU	N-CA-C	8.25	121.57	110.35
1	A	185	PRO	N-CA-C	8.17	129.31	112.47
1	A	374	GLN	N-CA-C	-7.94	97.32	109.95
1	A	947	ARG	N-CA-C	7.93	118.73	108.34
1	A	1066	GLY	N-CA-C	-7.75	102.38	115.62
1	A	945	ILE	N-CA-C	7.63	118.40	110.62
1	A	556	CYS	N-CA-C	7.61	119.24	108.74
1	A	130	MET	N-CA-C	7.46	118.08	108.24
1	A	185	PRO	CB-CA-C	7.44	123.83	111.56
2	B	127	SER	N-CA-C	-7.33	102.46	111.33
1	A	108	VAL	N-CA-C	7.04	118.91	112.29
1	A	194	GLU	O-C-N	-7.03	114.77	122.79
1	A	690	SER	N-CA-CB	6.87	121.25	109.10
1	A	1090	ASP	N-CA-CB	6.74	120.93	110.21
1	A	35	LYS	CA-C-N	-6.72	113.44	121.90
1	A	35	LYS	C-N-CA	-6.72	113.44	121.90
1	A	969	GLU	N-CA-C	6.70	119.51	108.99
1	A	648	ASN	N-CA-C	6.45	120.16	109.96
1	A	928	ARG	N-CA-C	6.34	120.62	112.12
1	A	398	GLU	N-CA-C	6.20	118.27	108.67
1	A	553	SER	CA-C-N	6.16	127.54	119.84
1	A	553	SER	C-N-CA	6.16	127.54	119.84
1	A	691	LEU	N-CA-C	-6.13	97.75	110.80
1	A	697	SER	O-C-N	5.97	129.71	123.62
1	A	745	THR	N-CA-C	-5.97	105.83	114.12
1	A	926	LEU	N-CA-C	5.92	117.60	111.03
1	A	660	TYR	CB-CA-C	-5.86	108.62	117.07
1	A	1091	GLY	N-CA-C	-5.74	105.72	113.24
1	A	1089	ILE	CA-C-N	-5.73	114.80	122.42
1	A	1089	ILE	C-N-CA	-5.73	114.80	122.42
1	A	236	SER	N-CA-C	5.69	117.92	108.99
1	A	697	SER	CA-CB-OG	5.69	122.47	111.10
1	A	492	GLU	O-C-N	5.60	126.39	121.18
1	A	309	SER	N-CA-C	-5.60	102.99	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	649	VAL	N-CA-C	5.59	115.91	107.80
1	A	664	HIS	N-CA-C	-5.51	99.07	110.80
1	A	716	PRO	CB-CA-C	-5.49	105.58	111.56
1	A	50	ARG	CA-C-N	5.43	125.34	119.85
1	A	50	ARG	C-N-CA	5.43	125.34	119.85
1	A	49	LEU	N-CA-C	5.41	117.57	108.96
1	A	925	ASP	N-CA-C	5.34	122.17	110.80
1	A	1123	GLU	N-CA-C	5.31	115.14	108.45
1	A	36	ASN	N-CA-C	-5.31	103.43	111.34
1	A	229	ALA	N-CA-C	5.29	118.04	109.06
1	A	139	LEU	N-CA-C	5.17	118.16	110.14
1	A	1061	VAL	N-CA-C	5.11	115.83	110.62
1	A	332	GLN	N-CA-C	5.09	116.81	109.07
1	A	1006	VAL	N-CA-C	5.06	115.20	108.27
1	A	198	ARG	N-CA-C	-5.04	105.06	111.11
1	A	571	LEU	CA-C-N	-5.03	114.56	119.64
1	A	571	LEU	C-N-CA	-5.03	114.56	119.64
1	A	725	CYS	N-CA-C	5.00	117.22	108.76

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	8705	732	0
2	B	99	0	102	40	0
All	All	8825	0	8807	758	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 43.

All (758) 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:921:ILE:CG2	1:A:932:LEU:HD11	1.42	1.49
1:A:368:GLU:CG	1:A:370:GLN:HE21	1.38	1.34
1:A:658:VAL:HG11	1:A:660:TYR:CE2	1.64	1.30
2:B:125:ALA:CA	2:B:128:MET:HB2	1.67	1.23
1:A:413:LEU:HD23	1:A:424:THR:CB	1.69	1.22
1:A:589:ARG:HD3	1:A:589:ARG:O	1.36	1.21
1:A:199:GLU:HG2	1:A:201:GLU:HG2	1.22	1.19
1:A:413:LEU:CD2	1:A:424:THR:HB	1.71	1.18
1:A:413:LEU:HD23	1:A:424:THR:CG2	1.75	1.17
1:A:660:TYR:CE1	1:A:707:ILE:HG22	1.78	1.17
1:A:889:ARG:HD2	1:A:891:TYR:CZ	1.80	1.17
1:A:542:ASP:CB	1:A:592:LEU:HD23	1.76	1.16
1:A:503:CYS:CA	1:A:543:ILE:HD11	1.78	1.14
1:A:589:ARG:NH1	1:A:637:VAL:HG13	1.63	1.13
1:A:503:CYS:HA	1:A:543:ILE:CD1	1.77	1.12
2:B:125:ALA:HA	2:B:128:MET:CB	1.78	1.13
1:A:595:THR:HG22	1:A:596:PHE:H	0.96	1.12
1:A:706:GLU:O	1:A:707:ILE:HG23	1.47	1.12
1:A:595:THR:HG23	1:A:599:SER:O	1.49	1.11
2:B:125:ALA:HA	2:B:128:MET:HB2	1.26	1.11
1:A:812:TYR:HD2	1:A:836:VAL:HG21	1.17	1.10
1:A:368:GLU:HG3	1:A:370:GLN:HE21	1.04	1.10
1:A:368:GLU:HG3	1:A:370:GLN:NE2	1.68	1.08
1:A:591:ILE:HD13	1:A:604:CYS:HB2	1.34	1.07
1:A:921:ILE:HG22	1:A:932:LEU:HD11	1.08	1.05
1:A:658:VAL:CG1	1:A:660:TYR:CE2	2.38	1.05
1:A:921:ILE:HG22	1:A:932:LEU:CD1	1.87	1.05
1:A:199:GLU:HG2	1:A:201:GLU:CG	1.86	1.04
1:A:413:LEU:HD23	1:A:424:THR:HB	1.27	1.03
1:A:654:ASP:HA	1:A:675:GLU:HG3	1.38	1.03
1:A:542:ASP:HB2	1:A:592:LEU:CD2	1.88	1.02
1:A:413:LEU:O	1:A:422:TYR:HB3	1.59	1.02
1:A:922:LEU:O	1:A:932:LEU:HD12	1.59	1.02
1:A:198:ARG:HG2	1:A:198:ARG:HH11	1.25	1.02
1:A:414:ARG:HA	1:A:422:TYR:HA	1.41	1.01
1:A:595:THR:HG22	1:A:596:PHE:N	1.74	1.01
1:A:1063:LYS:H	1:A:1063:LYS:HD3	1.25	1.01
1:A:81:THR:HG22	1:A:83:LYS:H	1.20	1.00
1:A:591:ILE:HD12	1:A:603:LEU:O	1.59	1.00
1:A:921:ILE:CG2	1:A:932:LEU:CD1	2.39	1.00
1:A:707:ILE:HG13	1:A:708:GLN:H	1.23	1.00
1:A:413:LEU:CD2	1:A:424:THR:CG2	2.40	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:ARG:HG2	1:A:414:ARG:HH11	1.22	0.99
1:A:660:TYR:CZ	1:A:707:ILE:HG22	1.97	0.99
1:A:482:GLU:HB2	1:A:483:PRO:HD3	1.41	0.99
1:A:413:LEU:HB3	1:A:424:THR:O	1.62	0.99
2:B:125:ALA:O	2:B:129:LEU:HG	1.60	0.99
1:A:812:TYR:CD2	1:A:836:VAL:HG21	1.98	0.98
1:A:368:GLU:CG	1:A:370:GLN:NE2	2.23	0.97
1:A:929:SER:O	1:A:930:VAL:HG13	1.65	0.97
1:A:197:LEU:HD23	1:A:197:LEU:H	1.26	0.97
1:A:593:MET:O	1:A:594:THR:HG23	1.65	0.96
2:B:125:ALA:C	2:B:128:MET:HB2	1.89	0.96
1:A:1127:ASP:O	1:A:1130:ILE:HG22	1.65	0.95
1:A:706:GLU:O	1:A:707:ILE:CG2	2.15	0.95
1:A:542:ASP:CG	1:A:592:LEU:HD22	1.91	0.95
1:A:1014:MET:SD	1:A:1015:GLN:HG2	2.06	0.95
1:A:542:ASP:HB2	1:A:592:LEU:HD23	0.96	0.94
1:A:595:THR:CG2	1:A:596:PHE:H	1.79	0.94
1:A:540:CYS:SG	1:A:591:ILE:HG22	2.08	0.94
1:A:639:ARG:HG3	1:A:640:THR:H	1.33	0.94
1:A:660:TYR:CE1	1:A:707:ILE:CG2	2.51	0.93
1:A:589:ARG:HD3	1:A:589:ARG:C	1.93	0.93
1:A:921:ILE:HG23	1:A:932:LEU:HD11	1.49	0.93
1:A:413:LEU:HD23	1:A:424:THR:HG22	1.51	0.93
1:A:889:ARG:HH11	1:A:901:THR:CG2	1.82	0.92
1:A:722:ARG:NH1	2:B:130:ARG:CD	2.32	0.92
1:A:589:ARG:CZ	1:A:637:VAL:HG13	1.99	0.92
1:A:714:THR:O	1:A:715:VAL:HG23	1.70	0.92
1:A:199:GLU:HG3	1:A:201:GLU:OE2	1.70	0.92
1:A:368:GLU:HG2	1:A:370:GLN:HE21	1.33	0.91
1:A:690:SER:O	1:A:691:LEU:HD23	1.69	0.91
1:A:402:ILE:O	1:A:698:THR:HA	1.71	0.91
1:A:658:VAL:HG11	1:A:660:TYR:CZ	2.05	0.91
1:A:713:ARG:CG	1:A:713:ARG:HH11	1.84	0.90
1:A:923:VAL:HA	1:A:931:LEU:O	1.72	0.90
1:A:841:ALA:O	2:B:124:ASN:HA	1.72	0.89
1:A:414:ARG:NH1	1:A:422:TYR:CE2	2.41	0.89
1:A:503:CYS:HA	1:A:543:ILE:HD11	0.91	0.89
1:A:889:ARG:NH1	1:A:901:THR:CG2	2.36	0.89
2:B:124:ASN:C	2:B:126:SER:H	1.80	0.89
1:A:98:ILE:HD13	1:A:98:ILE:H	1.38	0.88
1:A:812:TYR:HE2	1:A:836:VAL:HG11	1.38	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ARG:HH11	1:A:198:ARG:CG	1.86	0.88
1:A:662:SER:HB3	1:A:665:LYS:HB2	1.56	0.88
1:A:416:ASP:OD1	1:A:417:PRO:HD2	1.74	0.87
1:A:658:VAL:CG1	1:A:660:TYR:CD2	2.57	0.87
1:A:542:ASP:CB	1:A:592:LEU:CD2	2.49	0.87
1:A:571:LEU:HB3	1:A:572:PRO:HD3	1.55	0.87
1:A:707:ILE:HG13	1:A:708:GLN:N	1.90	0.86
1:A:542:ASP:CG	1:A:592:LEU:CD2	2.49	0.86
1:A:722:ARG:HH12	2:B:130:ARG:NE	1.74	0.86
1:A:413:LEU:CG	1:A:424:THR:HB	2.06	0.86
1:A:889:ARG:NH1	1:A:901:THR:HG21	1.91	0.86
1:A:199:GLU:CG	1:A:201:GLU:CD	2.49	0.86
1:A:414:ARG:HH11	1:A:414:ARG:CG	1.89	0.86
1:A:438:LEU:HD23	1:A:442:GLU:O	1.76	0.86
1:A:722:ARG:NH1	2:B:130:ARG:HD2	1.91	0.85
1:A:1041:THR:HG22	1:A:1042:SER:H	1.41	0.85
1:A:542:ASP:OD1	1:A:592:LEU:HD22	1.77	0.85
1:A:469:ILE:CD1	1:A:471:ILE:HG13	2.07	0.85
1:A:414:ARG:HG2	1:A:414:ARG:NH1	1.83	0.84
1:A:889:ARG:HD2	1:A:891:TYR:CE1	2.13	0.84
1:A:199:GLU:HG3	1:A:201:GLU:CD	2.02	0.84
1:A:480:SER:HB3	1:A:483:PRO:HD2	1.58	0.84
1:A:413:LEU:CD2	1:A:424:THR:CB	2.39	0.84
1:A:413:LEU:C	1:A:422:TYR:HB3	2.02	0.83
1:A:414:ARG:NH1	1:A:422:TYR:HE2	1.75	0.83
1:A:593:MET:O	1:A:594:THR:CG2	2.27	0.83
1:A:6:VAL:HG12	1:A:1040:VAL:HG22	1.60	0.82
1:A:107:ASN:OD1	1:A:109:GLN:HG2	1.78	0.82
1:A:866:VAL:HG11	1:A:884:ILE:HD13	1.60	0.82
1:A:722:ARG:HH12	2:B:130:ARG:CD	1.91	0.81
1:A:869:ALA:HB3	1:A:885:ASN:HD21	1.46	0.81
1:A:658:VAL:HG11	1:A:660:TYR:CD2	2.14	0.81
2:B:125:ALA:CA	2:B:128:MET:CB	2.45	0.81
1:A:394:ILE:CD1	1:A:660:TYR:HE2	1.93	0.80
1:A:394:ILE:HD13	1:A:660:TYR:CE2	2.16	0.79
1:A:928:ARG:O	1:A:929:SER:HB2	1.81	0.79
1:A:614:PHE:HB3	1:A:624:SER:OG	1.82	0.79
1:A:960:LEU:HD21	1:A:966:LEU:HB2	1.63	0.79
1:A:714:THR:O	1:A:715:VAL:CG2	2.30	0.79
1:A:23:PHE:H	1:A:30:ASN:HD22	1.29	0.79
1:A:385:GLY:HA3	1:A:719:GLU:O	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:TRP:CH2	1:A:459:PHE:HA	2.18	0.79
1:A:690:SER:O	1:A:691:LEU:CD2	2.31	0.79
1:A:708:GLN:O	1:A:710:LEU:N	2.16	0.79
2:B:125:ALA:C	2:B:128:MET:CB	2.56	0.79
1:A:255:GLN:HB3	1:A:279:ARG:NH2	1.97	0.79
1:A:415:SER:CB	1:A:423:ASP:OD1	2.32	0.78
1:A:589:ARG:HH12	1:A:637:VAL:HG13	1.49	0.78
1:A:98:ILE:HD13	1:A:98:ILE:N	1.99	0.78
1:A:415:SER:HB2	1:A:423:ASP:OD1	1.83	0.78
1:A:500:VAL:HG12	1:A:500:VAL:O	1.81	0.78
1:A:921:ILE:C	1:A:922:LEU:HD12	2.08	0.78
1:A:209:GLN:HG2	1:A:209:GLN:O	1.84	0.78
1:A:812:TYR:CD2	2:B:130:ARG:NH2	2.50	0.78
1:A:938:MET:HG2	1:A:939:GLU:N	1.99	0.78
1:A:503:CYS:HB2	1:A:507:GLN:O	1.82	0.78
1:A:595:THR:O	1:A:596:PHE:CD1	2.37	0.78
1:A:889:ARG:CD	1:A:891:TYR:CZ	2.65	0.77
1:A:157:ILE:HD13	1:A:201:GLU:O	1.83	0.77
1:A:469:ILE:HD11	1:A:471:ILE:CG1	2.14	0.77
1:A:312:GLU:HG3	1:A:327:ARG:HG2	1.66	0.77
1:A:1030:PHE:CZ	1:A:1038:GLY:HA3	2.19	0.77
1:A:199:GLU:CG	1:A:201:GLU:CG	2.63	0.77
1:A:504:ASN:HD22	1:A:545:PRO:HD3	1.46	0.77
1:A:936:LYS:C	1:A:938:MET:H	1.93	0.77
1:A:591:ILE:HD13	1:A:604:CYS:CB	2.12	0.76
1:A:5:TYR:CE2	1:A:7:VAL:HG22	2.19	0.76
1:A:889:ARG:HH11	1:A:901:THR:HG23	1.50	0.76
1:A:616:LEU:HG	1:A:617:ASN:H	1.50	0.76
1:A:414:ARG:HH12	1:A:422:TYR:HE2	1.31	0.76
1:A:411:TRP:CZ2	1:A:459:PHE:HA	2.21	0.76
1:A:112:ILE:HD12	1:A:112:ILE:N	2.02	0.75
1:A:620:THR:OG1	1:A:622:LEU:HD13	1.85	0.75
1:A:658:VAL:HG12	1:A:660:TYR:CD2	2.22	0.75
1:A:922:LEU:O	1:A:932:LEU:CD1	2.35	0.75
1:A:706:GLU:C	1:A:707:ILE:HG23	2.12	0.75
1:A:708:GLN:O	1:A:709:LYS:C	2.29	0.74
1:A:938:MET:CG	1:A:939:GLU:H	2.00	0.74
1:A:1066:GLY:O	1:A:1067:LYS:HB2	1.86	0.74
1:A:507:GLN:HE22	1:A:552:LEU:HA	1.52	0.74
1:A:812:TYR:CD2	1:A:836:VAL:CG2	2.69	0.74
1:A:929:SER:O	1:A:930:VAL:CG1	2.35	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:641:PHE:CZ	1:A:648:ASN:HB2	2.23	0.74
1:A:1024:THR:HB	1:A:1041:THR:HG21	1.70	0.74
1:A:812:TYR:CE2	1:A:836:VAL:HG11	2.22	0.74
1:A:480:SER:CB	1:A:483:PRO:HD2	2.17	0.73
1:A:570:LYS:HG2	1:A:571:LEU:H	1.53	0.73
1:A:416:ASP:OD1	1:A:417:PRO:CD	2.36	0.73
1:A:518:TYR:HD2	1:A:518:TYR:C	1.96	0.73
1:A:719:GLU:OE2	1:A:755:SER:HB3	1.87	0.73
1:A:500:VAL:HG12	1:A:541:LEU:HD12	1.70	0.73
1:A:587:ILE:HB	1:A:588:PRO:HD2	1.68	0.73
1:A:368:GLU:HG2	1:A:370:GLN:HG3	1.69	0.73
1:A:410:LEU:HD12	1:A:680:CYS:SG	2.29	0.73
1:A:413:LEU:O	1:A:422:TYR:CB	2.36	0.73
1:A:613:TYR:CZ	1:A:627:LYS:HB2	2.25	0.72
1:A:127:GLU:O	1:A:128:CYS:HB2	1.89	0.72
1:A:81:THR:HG22	1:A:83:LYS:N	2.01	0.71
1:A:614:PHE:HD2	1:A:624:SER:HG	1.36	0.71
1:A:623:LEU:CD2	1:A:624:SER:H	2.03	0.71
1:A:570:LYS:NZ	1:A:572:PRO:HD2	2.05	0.71
2:B:131:LYS:C	2:B:133:GLN:N	2.41	0.71
1:A:482:GLU:HB2	1:A:483:PRO:CD	2.19	0.71
1:A:1041:THR:HG22	1:A:1042:SER:N	2.05	0.71
1:A:589:ARG:C	1:A:589:ARG:CD	2.64	0.70
1:A:766:SER:HB3	1:A:808:LEU:HD23	1.71	0.70
1:A:230:ILE:C	1:A:231:ILE:HD12	2.17	0.70
1:A:504:ASN:HD22	1:A:545:PRO:CD	2.02	0.70
1:A:394:ILE:CD1	1:A:660:TYR:CE2	2.73	0.70
1:A:812:TYR:HE2	1:A:836:VAL:CG1	2.04	0.70
1:A:713:ARG:HH11	1:A:713:ARG:HG3	1.55	0.70
1:A:518:TYR:C	1:A:518:TYR:CD2	2.70	0.70
1:A:1048:TYR:CE2	1:A:1052:LEU:HD12	2.27	0.70
1:A:184:ASP:HB2	1:A:185:PRO:HD2	1.73	0.69
2:B:124:ASN:C	2:B:126:SER:N	2.50	0.69
1:A:69:PRO:HD2	1:A:72:GLU:HG3	1.74	0.69
1:A:143:ILE:HG12	1:A:154:ALA:HB2	1.74	0.69
1:A:614:PHE:CB	1:A:624:SER:OG	2.41	0.69
1:A:1125:THR:HG22	1:A:1126:ALA:H	1.58	0.69
1:A:413:LEU:HG	1:A:424:THR:HB	1.74	0.69
1:A:938:MET:HG2	1:A:939:GLU:H	1.55	0.69
1:A:466:GLN:HB3	1:A:481:GLN:HB2	1.73	0.68
1:A:617:ASN:CB	1:A:620:THR:HG23	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:VAL:CG1	1:A:541:LEU:HD12	2.23	0.68
1:A:593:MET:C	1:A:594:THR:HG23	2.19	0.68
1:A:1039:LEU:HD21	1:A:1139:ILE:HG22	1.73	0.68
1:A:920:PHE:HB3	1:A:935:TYR:HB3	1.76	0.68
1:A:197:LEU:H	1:A:197:LEU:CD2	2.05	0.67
1:A:418:ASN:OD1	1:A:419:ARG:N	2.28	0.67
1:A:1007:PHE:O	1:A:1008:CYS:HB3	1.93	0.67
1:A:2:SER:HB2	1:A:995:VAL:HG23	1.77	0.67
1:A:366:ASP:O	1:A:367:LEU:C	2.37	0.66
1:A:469:ILE:HD11	1:A:471:ILE:HG12	1.77	0.66
1:A:112:ILE:HD12	1:A:112:ILE:H	1.60	0.66
1:A:591:ILE:O	1:A:591:ILE:HG23	1.95	0.66
1:A:595:THR:O	1:A:596:PHE:CG	2.49	0.66
1:A:812:TYR:CG	2:B:130:ARG:NH2	2.62	0.66
1:A:475:SER:HB2	1:A:490:TRP:O	1.95	0.66
1:A:713:ARG:HH11	1:A:713:ARG:HG2	1.61	0.66
1:A:24:THR:H	1:A:30:ASN:HD21	1.42	0.65
1:A:714:THR:C	1:A:715:VAL:HG23	2.20	0.65
1:A:765:VAL:HG22	1:A:766:SER:N	2.12	0.65
2:B:125:ALA:HA	2:B:128:MET:CG	2.27	0.65
1:A:5:TYR:HE2	1:A:7:VAL:CG2	2.10	0.65
1:A:368:GLU:OE2	1:A:372:GLN:NE2	2.29	0.65
1:A:960:LEU:CD2	1:A:966:LEU:HB2	2.25	0.65
1:A:396:ILE:HD11	1:A:673:LEU:HD21	1.78	0.65
1:A:288:GLU:HB3	1:A:296:THR:HG23	1.77	0.65
1:A:469:ILE:HD11	1:A:471:ILE:HG13	1.73	0.65
1:A:475:SER:HB3	1:A:491:LYS:HD2	1.78	0.65
1:A:492:GLU:O	1:A:493:PRO:C	2.38	0.65
1:A:659:ILE:HA	1:A:667:VAL:O	1.97	0.65
1:A:24:THR:H	1:A:30:ASN:ND2	1.94	0.64
1:A:449:MET:HG3	1:A:484:LYS:HG3	1.80	0.64
1:A:662:SER:HB3	1:A:665:LYS:CB	2.26	0.64
1:A:504:ASN:CG	1:A:505:SER:H	2.04	0.64
1:A:5:TYR:HE2	1:A:7:VAL:HG22	1.62	0.64
1:A:38:ARG:NH1	1:A:54:GLU:OE2	2.30	0.64
1:A:199:GLU:HG2	1:A:201:GLU:CD	2.20	0.64
1:A:199:GLU:CG	1:A:201:GLU:OE2	2.42	0.64
1:A:199:GLU:OE2	1:A:199:GLU:N	2.29	0.64
1:A:540:CYS:SG	1:A:591:ILE:CG2	2.84	0.64
1:A:478:LEU:HD11	1:A:521:ILE:CG2	2.28	0.64
1:A:642:ARG:NH2	1:A:683:ASN:HB2	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:660:TYR:CD1	1:A:707:ILE:HG21	2.32	0.64
1:A:829:PHE:O	1:A:851:PHE:HB2	1.97	0.64
1:A:504:ASN:ND2	1:A:545:PRO:HD3	2.13	0.64
1:A:1125:THR:HG22	1:A:1126:ALA:N	2.12	0.64
1:A:155:PHE:CZ	1:A:200:LYS:HG3	2.33	0.63
1:A:591:ILE:CD1	1:A:604:CYS:HB2	2.20	0.63
1:A:644:LEU:HG	1:A:645:SER:H	1.63	0.63
1:A:438:LEU:C	1:A:440:GLY:H	2.07	0.63
1:A:617:ASN:HB2	1:A:620:THR:HG23	1.81	0.63
1:A:948:ASP:HB2	1:A:992:LEU:HD11	1.81	0.63
1:A:68:ARG:NH1	1:A:74:LYS:HA	2.13	0.63
1:A:366:ASP:OD1	1:A:373:GLY:HA2	1.97	0.63
1:A:1090:ASP:HB2	1:A:1092:ASP:HB2	1.81	0.63
1:A:542:ASP:CB	1:A:592:LEU:HA	2.28	0.63
1:A:570:LYS:HZ1	1:A:572:PRO:HD2	1.62	0.63
1:A:812:TYR:CE2	1:A:836:VAL:HB	2.33	0.63
1:A:372:GLN:NE2	1:A:372:GLN:O	2.32	0.63
1:A:639:ARG:CG	1:A:640:THR:H	2.10	0.63
1:A:766:SER:HB3	1:A:808:LEU:CD2	2.29	0.62
1:A:870:VAL:HG11	1:A:873:MET:HE3	1.81	0.62
1:A:812:TYR:CE2	1:A:836:VAL:CG1	2.81	0.62
1:A:116:SER:OG	1:A:134:ARG:CZ	2.47	0.62
1:A:969:GLU:O	1:A:971:ALA:N	2.32	0.62
1:A:22:HIS:CD2	1:A:28:ASP:O	2.52	0.62
1:A:415:SER:HB3	1:A:423:ASP:OD1	1.98	0.62
1:A:660:TYR:CD1	1:A:707:ILE:CG2	2.82	0.62
1:A:197:LEU:HD23	1:A:197:LEU:N	2.05	0.62
1:A:571:LEU:CB	1:A:572:PRO:HD3	2.27	0.62
2:B:125:ALA:O	2:B:129:LEU:N	2.33	0.62
1:A:478:LEU:HD11	1:A:521:ILE:HG21	1.81	0.62
1:A:396:ILE:CD1	1:A:673:LEU:HD21	2.30	0.61
1:A:679:MET:SD	1:A:679:MET:C	2.83	0.61
1:A:1123:GLU:HG2	1:A:1124:ALA:H	1.65	0.61
1:A:948:ASP:HB2	1:A:992:LEU:CD1	2.31	0.61
1:A:660:TYR:HB2	1:A:667:VAL:HB	1.81	0.61
1:A:198:ARG:CG	1:A:198:ARG:NH1	2.54	0.61
1:A:542:ASP:OD2	1:A:593:MET:N	2.27	0.61
1:A:518:TYR:HD2	1:A:519:LEU:N	1.97	0.61
1:A:708:GLN:C	1:A:710:LEU:N	2.55	0.61
1:A:928:ARG:O	1:A:929:SER:CB	2.46	0.61
1:A:38:ARG:HD2	1:A:54:GLU:OE1	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1063:LYS:HD3	1:A:1063:LYS:N	2.03	0.60
2:B:126:SER:OG	2:B:127:SER:N	2.30	0.60
1:A:365:VAL:O	1:A:367:LEU:N	2.31	0.60
1:A:368:GLU:H	1:A:368:GLU:CD	2.07	0.60
1:A:764:SER:HB2	1:A:805:HIS:ND1	2.17	0.60
1:A:929:SER:C	1:A:930:VAL:HG13	2.25	0.60
1:A:248:ILE:O	1:A:248:ILE:HG13	2.01	0.60
1:A:413:LEU:CD2	1:A:424:THR:HG21	2.31	0.60
1:A:689:ASP:OD2	1:A:689:ASP:C	2.42	0.60
1:A:1048:TYR:HE2	1:A:1052:LEU:HD12	1.65	0.60
1:A:394:ILE:HG21	1:A:660:TYR:OH	2.02	0.60
1:A:889:ARG:HH12	1:A:901:THR:HG21	1.66	0.60
1:A:1102:ARG:N	1:A:1103:PRO:HD2	2.16	0.60
1:A:394:ILE:HD13	1:A:660:TYR:OH	2.02	0.60
1:A:714:THR:HG22	1:A:716:PRO:HD3	1.84	0.60
2:B:131:LYS:O	2:B:132:SER:C	2.43	0.60
1:A:98:ILE:N	1:A:98:ILE:CD1	2.64	0.60
1:A:812:TYR:CE2	1:A:836:VAL:CB	2.85	0.60
1:A:1064:SER:OG	1:A:1065:VAL:N	2.30	0.60
1:A:116:SER:HB2	1:A:137:ASP:OD1	2.01	0.59
1:A:262:ASN:ND2	1:A:316:TYR:H	1.99	0.59
1:A:632:GLY:HA3	1:A:653:SER:OG	2.02	0.59
1:A:1136:LEU:C	1:A:1138:ARG:H	2.10	0.59
1:A:231:ILE:HD12	1:A:231:ILE:N	2.16	0.59
1:A:679:MET:SD	1:A:679:MET:O	2.60	0.59
1:A:939:GLU:HG3	1:A:941:ASN:HB2	1.84	0.59
1:A:68:ARG:HH11	1:A:74:LYS:HA	1.68	0.59
1:A:410:LEU:CD1	1:A:680:CYS:SG	2.90	0.59
1:A:411:TRP:O	1:A:425:LEU:HD12	2.02	0.59
1:A:484:LYS:HG3	1:A:484:LYS:O	2.03	0.59
1:A:41:ILE:HD12	1:A:53:LYS:HB3	1.85	0.59
1:A:503:CYS:HB3	1:A:508:VAL:HA	1.85	0.59
1:A:713:ARG:CG	1:A:713:ARG:NH1	2.54	0.59
1:A:25:SER:HB2	1:A:27:GLU:O	2.03	0.58
1:A:1078:THR:C	1:A:1080:ARG:H	2.11	0.58
1:A:690:SER:O	1:A:691:LEU:CG	2.51	0.58
1:A:1091:GLY:HA2	1:A:1094:ILE:HB	1.85	0.58
1:A:424:THR:HA	1:A:436:LEU:O	2.03	0.58
1:A:928:ARG:O	1:A:950:ASN:O	2.20	0.58
1:A:394:ILE:HD13	1:A:660:TYR:CZ	2.38	0.58
1:A:402:ILE:HG22	1:A:404:LEU:HG	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:ARG:O	1:A:358:PRO:HD3	2.03	0.58
1:A:639:ARG:HG3	1:A:640:THR:N	2.09	0.58
1:A:889:ARG:HD2	1:A:891:TYR:OH	2.03	0.58
1:A:283:LEU:HD21	1:A:300:LEU:HD12	1.85	0.57
1:A:413:LEU:CD2	1:A:424:THR:HG22	2.22	0.57
1:A:439:ASN:HB2	1:A:442:GLU:HB3	1.86	0.57
1:A:480:SER:OG	1:A:487:VAL:HG21	2.03	0.57
1:A:562:THR:HG22	1:A:563:ASP:N	2.16	0.57
1:A:743:GLN:HG2	1:A:783:GLY:N	2.20	0.57
1:A:1055:GLN:HG2	1:A:1093:LEU:HD12	1.84	0.57
1:A:2:SER:HB2	1:A:995:VAL:CG2	2.35	0.57
1:A:839:GLU:CD	1:A:839:GLU:H	2.10	0.57
1:A:43:VAL:HG23	1:A:52:VAL:HG21	1.85	0.57
1:A:699:LEU:HG	1:A:700:THR:N	2.19	0.57
1:A:750:THR:O	1:A:751:ALA:HB2	2.04	0.57
1:A:18:CYS:N	1:A:313:CYS:SG	2.78	0.57
1:A:309:SER:H	1:A:332:GLN:NE2	2.03	0.57
1:A:480:SER:HB2	1:A:484:LYS:H	1.70	0.57
1:A:844:LYS:HE2	1:A:845:GLN:HG2	1.85	0.57
1:A:789:HIS:CD2	1:A:812:TYR:HD1	2.23	0.56
1:A:932:LEU:HD22	1:A:965:PHE:CZ	2.41	0.56
1:A:1039:LEU:HD21	1:A:1139:ILE:CG2	2.36	0.56
2:B:129:LEU:O	2:B:133:GLN:HG3	2.04	0.56
1:A:688:PRO:O	1:A:690:SER:N	2.39	0.56
1:A:1066:GLY:O	1:A:1067:LYS:CB	2.53	0.56
1:A:268:GLY:O	1:A:285:LEU:HD12	2.06	0.56
1:A:263:ARG:HG2	1:A:263:ARG:HH11	1.69	0.56
1:A:413:LEU:HD21	1:A:424:THR:HG21	1.87	0.56
1:A:741:GLU:HG2	1:A:751:ALA:HA	1.88	0.56
1:A:342:GLU:O	1:A:343:GLN:CB	2.53	0.56
1:A:413:LEU:HD21	1:A:424:THR:CG2	2.32	0.56
1:A:623:LEU:HD23	1:A:624:SER:H	1.70	0.56
1:A:135:LEU:N	1:A:135:LEU:HD22	2.20	0.56
1:A:707:ILE:O	1:A:708:GLN:C	2.49	0.56
1:A:131:ILE:HG22	1:A:133:LEU:HD13	1.88	0.56
1:A:870:VAL:HG11	1:A:873:MET:CE	2.35	0.56
1:A:415:SER:HB3	1:A:423:ASP:CG	2.31	0.55
1:A:589:ARG:O	1:A:589:ARG:CD	2.31	0.55
1:A:687:TYR:N	1:A:688:PRO:HD3	2.20	0.55
1:A:596:PHE:HE2	1:A:648:ASN:HA	1.71	0.55
1:A:1097:PHE:O	1:A:1100:ILE:HB	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ARG:HG2	1:A:284:LEU:HD23	1.87	0.55
1:A:400:ALA:HB3	1:A:701:ILE:HD11	1.88	0.55
2:B:127:SER:OG	2:B:131:LYS:NZ	2.30	0.55
1:A:77:LEU:HB3	1:A:89:LEU:HB2	1.89	0.55
1:A:879:LYS:HB3	1:A:891:TYR:O	2.06	0.55
1:A:367:LEU:HB2	1:A:368:GLU:OE1	2.06	0.55
1:A:763:SER:HA	1:A:803:HIS:CE1	2.42	0.55
1:A:368:GLU:HG2	1:A:370:GLN:NE2	2.09	0.55
1:A:530:SER:HB3	1:A:574:PHE:HE1	1.72	0.55
1:A:366:ASP:O	1:A:369:ARG:N	2.39	0.55
1:A:272:LEU:O	1:A:273:LEU:HD23	2.08	0.54
1:A:429:PHE:O	1:A:431:GLY:N	2.40	0.54
1:A:714:THR:HG22	1:A:715:VAL:N	2.22	0.54
1:A:787:GLU:HB2	1:A:812:TYR:HE1	1.72	0.54
1:A:133:LEU:HB3	1:A:135:LEU:HD21	1.89	0.54
1:A:611:LEU:HB3	1:A:629:VAL:HG23	1.90	0.54
1:A:917:LYS:HG2	1:A:959:ILE:HG21	1.88	0.54
1:A:200:LYS:HZ2	1:A:200:LYS:CB	2.20	0.54
1:A:579:LYS:NZ	1:A:581:MET:SD	2.79	0.54
1:A:936:LYS:O	1:A:938:MET:N	2.39	0.54
1:A:886:SER:HB2	1:A:908:ASN:O	2.08	0.54
1:A:23:PHE:H	1:A:30:ASN:ND2	2.03	0.54
1:A:368:GLU:HG2	1:A:370:GLN:CG	2.37	0.54
1:A:80:LEU:HD23	1:A:120:ILE:HG21	1.90	0.54
1:A:213:GLU:CD	1:A:233:GLY:HA3	2.33	0.54
1:A:910:MET:HE2	1:A:912:LEU:HD21	1.90	0.54
1:A:241:ASN:OD1	1:A:242:GLY:N	2.41	0.54
1:A:614:PHE:CD2	1:A:624:SER:OG	2.61	0.54
1:A:556:CYS:SG	1:A:557:ALA:N	2.80	0.54
1:A:599:SER:HB2	1:A:664:HIS:HE1	1.73	0.54
1:A:614:PHE:HD2	1:A:624:SER:OG	1.91	0.54
1:A:381:ALA:HA	1:A:720:SER:HB3	1.89	0.53
1:A:571:LEU:HB3	1:A:572:PRO:CD	2.34	0.53
1:A:587:ILE:HB	1:A:588:PRO:CD	2.37	0.53
1:A:869:ALA:HB3	1:A:885:ASN:ND2	2.19	0.53
1:A:198:ARG:HG2	1:A:198:ARG:NH1	2.08	0.53
1:A:276:MET:O	1:A:276:MET:SD	2.66	0.53
1:A:932:LEU:C	1:A:933:LEU:HD12	2.33	0.53
1:A:969:GLU:OE2	1:A:971:ALA:HB3	2.08	0.53
1:A:578:HIS:NE2	1:A:623:LEU:HG	2.23	0.53
1:A:555:LEU:HB2	1:A:569:LEU:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:HIS:CG	1:A:579:LYS:N	2.77	0.53
1:A:1002:GLU:OE2	1:A:1034:ASN:HB2	2.08	0.53
1:A:1090:ASP:OD2	1:A:1090:ASP:N	2.39	0.53
1:A:560:LEU:N	1:A:560:LEU:HD23	2.24	0.53
1:A:700:THR:C	1:A:701:ILE:HD13	2.33	0.53
1:A:713:ARG:CG	1:A:714:THR:H	2.22	0.53
2:B:125:ALA:O	2:B:128:MET:CB	2.56	0.53
1:A:403:ASP:OD2	1:A:403:ASP:N	2.41	0.53
1:A:112:ILE:HG22	1:A:113:GLY:N	2.24	0.53
1:A:200:LYS:HZ2	1:A:200:LYS:HB2	1.73	0.53
1:A:231:ILE:N	1:A:231:ILE:CD1	2.72	0.53
1:A:713:ARG:HG2	1:A:713:ARG:NH1	2.22	0.53
1:A:59:GLY:HA2	1:A:1073:TRP:CZ3	2.44	0.52
1:A:537:GLU:O	1:A:561:TRP:HB2	2.09	0.52
1:A:840:GLU:O	2:B:124:ASN:OD1	2.27	0.52
1:A:1078:THR:O	1:A:1080:ARG:N	2.36	0.52
1:A:1003:PHE:C	1:A:1003:PHE:CD2	2.87	0.52
1:A:234:GLN:O	1:A:236:SER:N	2.42	0.52
1:A:498:ILE:HG23	1:A:510:VAL:HB	1.91	0.52
1:A:399:HIS:HB3	1:A:687:TYR:HE1	1.74	0.52
1:A:413:LEU:O	1:A:422:TYR:CA	2.58	0.52
1:A:596:PHE:CE2	1:A:648:ASN:HA	2.44	0.52
1:A:258:ILE:HG22	1:A:259:VAL:N	2.24	0.52
1:A:529:ILE:HG22	1:A:530:SER:N	2.25	0.52
1:A:590:SER:HB3	1:A:605:ALA:HB3	1.92	0.52
1:A:492:GLU:OE1	1:A:496:LYS:HB2	2.09	0.52
1:A:611:LEU:C	1:A:611:LEU:HD23	2.35	0.52
1:A:476:VAL:HG13	1:A:490:TRP:HB3	1.92	0.51
1:A:690:SER:O	1:A:691:LEU:HG	2.09	0.51
1:A:750:THR:O	1:A:751:ALA:CB	2.57	0.51
1:A:368:GLU:OE1	1:A:368:GLU:N	2.30	0.51
1:A:112:ILE:H	1:A:112:ILE:CD1	2.23	0.51
1:A:478:LEU:HD23	1:A:487:VAL:HG12	1.92	0.51
1:A:620:THR:OG1	1:A:621:GLY:N	2.43	0.51
1:A:689:ASP:O	1:A:703:THR:HG22	2.11	0.51
1:A:697:SER:O	1:A:698:THR:CB	2.57	0.51
1:A:1000:LEU:HD13	1:A:1002:GLU:HB2	1.93	0.51
1:A:102:THR:OG1	1:A:1065:VAL:O	2.26	0.51
1:A:124:ILE:HG12	1:A:131:ILE:HG12	1.93	0.51
1:A:10:GLN:HG2	1:A:356:LEU:HD12	1.93	0.51
1:A:237:ILE:HG22	1:A:238:THR:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:996:GLY:O	1:A:997:LEU:HD23	2.11	0.51
1:A:881:LEU:HD21	1:A:922:LEU:CD2	2.40	0.51
1:A:133:LEU:HB3	1:A:135:LEU:CD2	2.41	0.51
1:A:411:TRP:CH2	1:A:459:PHE:CA	2.91	0.51
1:A:953:TRP:HB2	1:A:970:ASN:HB2	1.91	0.51
1:A:265:ASP:O	1:A:268:GLY:N	2.44	0.51
1:A:452:VAL:HG22	1:A:477:ARG:HH11	1.75	0.51
1:A:504:ASN:CG	1:A:505:SER:N	2.68	0.51
1:A:595:THR:HA	1:A:601:TYR:HD1	1.76	0.51
1:A:23:PHE:CE2	1:A:91:TYR:HB2	2.45	0.50
1:A:844:LYS:HD3	1:A:844:LYS:N	2.25	0.50
1:A:501:ALA:O	1:A:502:SER:HB3	2.11	0.50
1:A:262:ASN:HD21	1:A:316:TYR:H	1.58	0.50
1:A:667:VAL:HG12	1:A:668:PHE:N	2.26	0.50
1:A:707:ILE:CG1	1:A:708:GLN:H	2.10	0.50
1:A:920:PHE:O	1:A:934:ALA:HA	2.11	0.50
1:A:2:SER:CB	1:A:995:VAL:HG23	2.40	0.50
1:A:365:VAL:CG1	1:A:726:TYR:CE2	2.94	0.50
1:A:789:HIS:NE2	1:A:812:TYR:CD1	2.80	0.50
1:A:589:ARG:NH2	1:A:637:VAL:HG13	2.27	0.50
1:A:636:THR:HA	1:A:652:CYS:O	2.11	0.50
1:A:643:SER:OG	1:A:644:LEU:N	2.44	0.50
1:A:707:ILE:O	1:A:708:GLN:O	2.30	0.50
1:A:176:PRO:O	1:A:194:GLU:HA	2.12	0.50
1:A:705:ASP:O	1:A:706:GLU:O	2.29	0.50
1:A:22:HIS:HD2	1:A:28:ASP:O	1.93	0.50
1:A:570:LYS:HG2	1:A:571:LEU:N	2.24	0.50
1:A:588:PRO:HA	1:A:606:LEU:HA	1.93	0.50
2:B:124:ASN:O	2:B:125:ALA:HB3	2.12	0.50
1:A:654:ASP:HA	1:A:675:GLU:CG	2.27	0.50
1:A:905:HIS:HD2	1:A:908:ASN:HD21	1.59	0.50
2:B:131:LYS:C	2:B:133:GLN:H	2.18	0.49
2:B:135:GLY:O	2:B:136:PHE:O	2.30	0.49
1:A:640:THR:HA	1:A:648:ASN:O	2.12	0.49
1:A:744:ASP:HB3	1:A:746:SER:H	1.75	0.49
1:A:155:PHE:CE1	1:A:200:LYS:HG3	2.46	0.49
1:A:378:CYS:HB3	1:A:721:PRO:HG2	1.93	0.49
1:A:105:HIS:CD2	1:A:1067:LYS:HB2	2.47	0.49
1:A:197:LEU:CD2	1:A:197:LEU:N	2.72	0.49
1:A:207:TRP:O	1:A:208:LYS:O	2.30	0.49
1:A:416:ASP:OD1	1:A:417:PRO:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:689:ASP:OD2	1:A:689:ASP:O	2.30	0.49
1:A:812:TYR:CE2	2:B:130:ARG:NH2	2.81	0.49
1:A:870:VAL:CG1	1:A:873:MET:HE3	2.43	0.49
1:A:879:LYS:HD3	1:A:892:GLU:HG2	1.94	0.49
1:A:905:HIS:CE1	1:A:907:ASN:HB3	2.47	0.49
1:A:1125:THR:CG2	1:A:1126:ALA:H	2.20	0.49
1:A:257:THR:HG22	1:A:258:ILE:O	2.12	0.49
1:A:843:PRO:HG2	1:A:869:ALA:HB2	1.95	0.49
1:A:209:GLN:O	1:A:209:GLN:CG	2.46	0.49
1:A:374:GLN:OE1	1:A:391:ARG:HG3	2.13	0.49
1:A:1013:VAL:O	1:A:1014:MET:HG3	2.13	0.49
1:A:63:VAL:HB	1:A:80:LEU:HB3	1.94	0.49
1:A:309:SER:H	1:A:332:GLN:HE22	1.59	0.49
1:A:1078:THR:C	1:A:1080:ARG:N	2.69	0.49
1:A:687:TYR:H	1:A:688:PRO:HD3	1.78	0.48
1:A:1136:LEU:C	1:A:1138:ARG:N	2.67	0.48
1:A:171:TYR:CG	1:A:223:PRO:HA	2.48	0.48
1:A:296:THR:OG1	1:A:297:LEU:N	2.47	0.48
1:A:520:GLN:NE2	1:A:529:ILE:HD11	2.27	0.48
1:A:1041:THR:CG2	1:A:1042:SER:H	2.19	0.48
1:A:194:GLU:O	1:A:202:PHE:O	2.31	0.48
1:A:365:VAL:HG13	1:A:726:TYR:CE2	2.48	0.48
1:A:451:PHE:HA	1:A:470:GLN:OE1	2.13	0.48
1:A:921:ILE:O	1:A:922:LEU:HD12	2.13	0.48
1:A:602:LEU:HD23	1:A:614:PHE:HB2	1.95	0.48
1:A:722:ARG:NH1	2:B:130:ARG:HD3	2.26	0.48
1:A:921:ILE:HG21	1:A:932:LEU:HD11	1.71	0.48
1:A:687:TYR:N	1:A:688:PRO:CD	2.76	0.48
1:A:691:LEU:O	1:A:701:ILE:HA	2.14	0.48
1:A:559:GLY:C	1:A:560:LEU:HD23	2.38	0.48
1:A:644:LEU:HG	1:A:645:SER:N	2.28	0.48
1:A:812:TYR:CD2	1:A:836:VAL:CB	2.96	0.48
1:A:37:THR:HG22	1:A:59:GLY:O	2.14	0.48
1:A:966:LEU:HD13	1:A:1007:PHE:CE2	2.49	0.48
1:A:31:LEU:HD21	1:A:33:ILE:HD11	1.96	0.47
1:A:452:VAL:HB	1:A:455:GLN:HB2	1.96	0.47
1:A:20:THR:HB	1:A:315:THR:CG2	2.44	0.47
1:A:855:ASP:HB2	1:A:857:LYS:HE2	1.95	0.47
1:A:926:LEU:HG	1:A:927:MET:N	2.28	0.47
1:A:155:PHE:CG	1:A:200:LYS:HG2	2.49	0.47
1:A:375:LEU:HB2	1:A:1012:LEU:HD21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:641:PHE:HA	1:A:681:PRO:HG3	1.96	0.47
1:A:922:LEU:C	1:A:923:VAL:HG12	2.39	0.47
1:A:522:HIS:O	1:A:523:PRO:C	2.58	0.47
1:A:155:PHE:CE1	1:A:200:LYS:CG	2.98	0.47
1:A:342:GLU:H	1:A:342:GLU:CD	2.23	0.47
1:A:478:LEU:CD1	1:A:521:ILE:CG2	2.92	0.47
1:A:836:VAL:HG13	2:B:124:ASN:ND2	2.30	0.47
1:A:889:ARG:NH1	1:A:901:THR:OG1	2.48	0.47
2:B:125:ALA:O	2:B:128:MET:HB3	2.14	0.47
1:A:494:GLN:O	1:A:495:ALA:HB3	2.15	0.47
1:A:191:LYS:NZ	1:A:193:TYR:OH	2.48	0.47
1:A:5:TYR:CE2	1:A:7:VAL:CG2	2.88	0.47
1:A:34:ALA:HB2	1:A:64:MET:CE	2.45	0.47
1:A:392:ASN:HD22	1:A:393:GLY:N	2.13	0.47
1:A:237:ILE:CG2	1:A:238:THR:N	2.79	0.46
1:A:404:LEU:HB2	1:A:407:ILE:HD11	1.96	0.46
1:A:756:ALA:HB1	1:A:801:VAL:HG21	1.97	0.46
1:A:836:VAL:HG13	2:B:124:ASN:HD22	1.80	0.46
1:A:1014:MET:SD	1:A:1015:GLN:N	2.88	0.46
2:B:129:LEU:O	2:B:133:GLN:N	2.48	0.46
1:A:917:LYS:O	1:A:919:ASP:N	2.48	0.46
1:A:411:TRP:CE3	1:A:460:CYS:HB2	2.50	0.46
1:A:502:SER:O	1:A:503:CYS:HB3	2.15	0.46
2:B:135:GLY:O	2:B:136:PHE:C	2.54	0.46
1:A:112:ILE:N	1:A:112:ILE:CD1	2.72	0.46
1:A:1063:LYS:C	1:A:1064:SER:O	2.54	0.46
1:A:139:LEU:HD22	1:A:156:ASN:HB3	1.97	0.46
1:A:478:LEU:HD13	1:A:526:LEU:HD21	1.97	0.46
1:A:679:MET:HE2	1:A:680:CYS:HA	1.97	0.46
1:A:954:MET:HE1	1:A:975:PHE:CE2	2.51	0.46
1:A:1130:ILE:O	1:A:1134:GLU:HG3	2.16	0.46
1:A:235:GLU:HG2	1:A:254:LYS:NZ	2.30	0.46
1:A:866:VAL:HG11	1:A:884:ILE:CD1	2.38	0.46
1:A:342:GLU:O	1:A:343:GLN:HB2	2.14	0.46
1:A:667:VAL:HG12	1:A:668:PHE:H	1.81	0.46
1:A:103:ARG:HH11	1:A:103:ARG:HB3	1.80	0.46
1:A:695:ASN:O	1:A:696:ASN:C	2.59	0.46
1:A:726:TYR:CE2	1:A:728:GLU:HB2	2.50	0.45
1:A:888:VAL:O	1:A:904:ASN:HA	2.15	0.45
1:A:20:THR:HB	1:A:315:THR:HG21	1.97	0.45
1:A:438:LEU:C	1:A:440:GLY:N	2.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:ASN:O	1:A:242:GLY:C	2.59	0.45
1:A:651:ALA:HB3	1:A:657:THR:HB	1.97	0.45
1:A:235:GLU:HB3	1:A:254:LYS:CG	2.46	0.45
1:A:394:ILE:HD11	1:A:669:SER:HB2	1.97	0.45
1:A:649:VAL:HB	1:A:659:ILE:HB	1.97	0.45
1:A:835:MET:O	1:A:843:PRO:HB3	2.16	0.45
1:A:871:TYR:CZ	1:A:910:MET:HE3	2.52	0.45
1:A:1077:HIS:C	1:A:1077:HIS:CD2	2.93	0.45
1:A:94:SER:N	1:A:97:SER:O	2.49	0.45
1:A:155:PHE:HE1	1:A:157:ILE:HD11	1.81	0.45
1:A:741:GLU:HG2	1:A:751:ALA:CA	2.47	0.45
1:A:396:ILE:HD13	1:A:396:ILE:O	2.16	0.45
1:A:722:ARG:HH12	2:B:130:ARG:CZ	2.28	0.45
2:B:129:LEU:O	2:B:130:ARG:C	2.58	0.45
1:A:105:HIS:HA	1:A:152:LEU:HD12	1.97	0.45
1:A:367:LEU:HD11	1:A:389:ILE:HG21	1.97	0.45
1:A:428:SER:HB2	1:A:457:THR:O	2.17	0.45
1:A:1049:ASN:O	1:A:1050:LEU:C	2.60	0.45
1:A:542:ASP:HB2	1:A:592:LEU:HA	1.97	0.45
1:A:999:HIS:O	1:A:1074:ARG:NH1	2.45	0.45
1:A:1070:HIS:CD2	1:A:1070:HIS:C	2.95	0.45
1:A:40:GLU:HG3	1:A:54:GLU:HG2	1.99	0.45
1:A:848:ILE:HG12	1:A:873:MET:HE1	1.99	0.45
1:A:10:GLN:NE2	1:A:11:LYS:O	2.46	0.44
1:A:151:GLU:HB2	1:A:153:LYS:HE2	1.99	0.44
1:A:361:ASP:OD1	1:A:723:LYS:HD2	2.17	0.44
1:A:414:ARG:HB3	1:A:421:THR:O	2.17	0.44
1:A:600:HIS:CD2	1:A:618:ILE:HG12	2.52	0.44
1:A:706:GLU:HB3	1:A:707:ILE:H	1.62	0.44
1:A:81:THR:CG2	1:A:82:ALA:N	2.79	0.44
1:A:149:ASN:OD1	1:A:153:LYS:N	2.47	0.44
1:A:535:GLU:HB3	1:A:536:HIS:CD2	2.52	0.44
1:A:590:SER:O	1:A:591:ILE:HB	2.17	0.44
1:A:642:ARG:HH22	1:A:683:ASN:CG	2.25	0.44
1:A:787:GLU:HB2	1:A:812:TYR:CE1	2.51	0.44
1:A:1134:GLU:C	1:A:1136:LEU:N	2.76	0.44
1:A:220:ILE:HB	1:A:230:ILE:HB	1.98	0.44
1:A:595:THR:C	1:A:596:PHE:CD1	2.95	0.44
1:A:699:LEU:HG	1:A:700:THR:H	1.82	0.44
1:A:765:VAL:CG2	1:A:766:SER:N	2.79	0.44
1:A:938:MET:CG	1:A:939:GLU:N	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1044:SER:OG	1:A:1047:TRP:HB2	2.18	0.44
1:A:969:GLU:O	1:A:970:ASN:C	2.61	0.44
1:A:273:LEU:HB2	1:A:281:PHE:HB2	2.00	0.44
1:A:413:LEU:HD22	1:A:426:VAL:HG23	2.00	0.44
1:A:530:SER:CB	1:A:574:PHE:HE1	2.31	0.44
1:A:623:LEU:HD22	1:A:624:SER:H	1.81	0.44
1:A:687:TYR:O	1:A:688:PRO:O	2.36	0.44
1:A:765:VAL:HG22	1:A:766:SER:H	1.83	0.44
1:A:1096:SER:O	1:A:1097:PHE:C	2.61	0.44
1:A:596:PHE:HZ	1:A:649:VAL:HG23	1.82	0.44
1:A:793:ILE:O	1:A:802:LEU:N	2.47	0.44
1:A:853:TYR:HA	1:A:857:LYS:O	2.18	0.44
1:A:925:ASP:OD2	1:A:926:LEU:N	2.51	0.44
1:A:255:GLN:HB3	1:A:279:ARG:HH22	1.77	0.43
1:A:181:VAL:HA	1:A:189:HIS:O	2.18	0.43
1:A:226:PHE:CD2	1:A:297:LEU:HD11	2.52	0.43
1:A:258:ILE:HG22	1:A:259:VAL:H	1.83	0.43
1:A:263:ARG:HG2	1:A:263:ARG:NH1	2.32	0.43
1:A:427:LEU:HD12	1:A:427:LEU:O	2.18	0.43
1:A:504:ASN:HD22	1:A:545:PRO:CG	2.32	0.43
1:A:589:ARG:NH2	1:A:637:VAL:CG1	2.81	0.43
1:A:661:SER:HA	1:A:666:LEU:HA	1.99	0.43
2:B:125:ALA:HA	2:B:128:MET:HB3	1.88	0.43
1:A:24:THR:HG23	1:A:91:TYR:CE2	2.53	0.43
1:A:207:TRP:C	1:A:208:LYS:O	2.58	0.43
1:A:469:ILE:HD12	1:A:471:ILE:HG13	1.96	0.43
1:A:714:THR:C	1:A:715:VAL:CG2	2.86	0.43
1:A:961:ASP:O	1:A:963:ASP:N	2.51	0.43
1:A:258:ILE:CG2	1:A:259:VAL:N	2.81	0.43
1:A:589:ARG:HH12	1:A:637:VAL:CG1	2.23	0.43
1:A:691:LEU:HD12	1:A:704:ILE:HD11	1.99	0.43
1:A:589:ARG:CZ	1:A:637:VAL:CG1	2.86	0.43
1:A:18:CYS:HA	1:A:32:LEU:O	2.18	0.43
1:A:44:VAL:HG13	1:A:317:LEU:HD13	2.01	0.43
1:A:630:THR:O	1:A:631:LEU:C	2.61	0.43
1:A:869:ALA:HB3	1:A:871:TYR:CE1	2.54	0.43
1:A:921:ILE:HA	1:A:933:LEU:O	2.18	0.43
1:A:1014:MET:O	1:A:1015:GLN:C	2.61	0.43
1:A:1134:GLU:C	1:A:1136:LEU:H	2.25	0.43
1:A:197:LEU:O	1:A:198:ARG:C	2.62	0.43
1:A:594:THR:O	1:A:601:TYR:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:936:LYS:C	1:A:938:MET:N	2.63	0.43
1:A:65:GLU:O	1:A:77:LEU:HD12	2.18	0.43
1:A:391:ARG:HD2	1:A:392:ASN:O	2.19	0.43
1:A:568:ILE:C	1:A:569:LEU:HD12	2.44	0.43
1:A:714:THR:CG2	1:A:715:VAL:N	2.81	0.43
1:A:803:HIS:CD2	1:A:858:LEU:HB2	2.53	0.43
1:A:1101:SER:C	1:A:1103:PRO:HD2	2.44	0.43
1:A:416:ASP:HA	1:A:417:PRO:HD3	1.73	0.42
1:A:960:LEU:O	1:A:961:ASP:HB3	2.19	0.42
1:A:563:ASP:OD1	1:A:563:ASP:C	2.62	0.42
1:A:1136:LEU:O	1:A:1138:ARG:N	2.52	0.42
1:A:207:TRP:O	1:A:208:LYS:C	2.62	0.42
1:A:234:GLN:C	1:A:235:GLU:HG3	2.43	0.42
1:A:507:GLN:NE2	1:A:552:LEU:HA	2.27	0.42
1:A:537:GLU:HB3	1:A:561:TRP:CD1	2.54	0.42
1:A:24:THR:HA	1:A:91:TYR:CD2	2.54	0.42
1:A:726:TYR:OH	1:A:796:GLN:NE2	2.48	0.42
1:A:746:SER:C	1:A:748:GLY:H	2.27	0.42
1:A:1102:ARG:HA	1:A:1105:MET:HB3	2.01	0.42
1:A:4:ASN:O	1:A:1088:PHE:HA	2.20	0.42
1:A:582:LEU:H	1:A:582:LEU:HG	1.58	0.42
1:A:986:ASP:O	1:A:990:GLN:HB2	2.19	0.42
1:A:571:LEU:CB	1:A:572:PRO:CD	2.95	0.42
1:A:1054:MET:HE3	1:A:1054:MET:HB3	1.75	0.42
1:A:155:PHE:CD1	1:A:200:LYS:HG2	2.54	0.42
1:A:504:ASN:OD1	1:A:505:SER:N	2.53	0.42
1:A:520:GLN:CD	1:A:529:ILE:HD11	2.45	0.42
1:A:717:LEU:HD23	1:A:717:LEU:HA	1.82	0.42
1:A:256:SER:CB	1:A:277:GLU:HG2	2.50	0.42
1:A:371:GLY:O	1:A:1014:MET:HE3	2.20	0.42
1:A:480:SER:CB	1:A:484:LYS:H	2.32	0.42
1:A:520:GLN:HB2	1:A:522:HIS:CD2	2.55	0.42
1:A:534:MET:O	1:A:535:GLU:C	2.62	0.42
1:A:886:SER:O	1:A:887:THR:OG1	2.34	0.42
1:A:200:LYS:HD3	1:A:200:LYS:N	2.34	0.42
1:A:309:SER:N	1:A:332:GLN:HE22	2.18	0.42
1:A:406:GLY:O	1:A:407:ILE:C	2.61	0.42
1:A:613:TYR:O	1:A:625:ASP:O	2.38	0.42
1:A:700:THR:HA	1:A:701:ILE:HD13	2.02	0.42
1:A:722:ARG:CZ	2:B:130:ARG:HD2	2.47	0.42
1:A:876:PHE:CZ	1:A:920:PHE:HA	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:GLU:CB	1:A:483:PRO:HD3	2.28	0.42
1:A:570:LYS:HZ3	1:A:572:PRO:HD2	1.79	0.42
1:A:700:THR:CA	1:A:701:ILE:HD13	2.50	0.42
1:A:926:LEU:O	1:A:953:TRP:HA	2.20	0.42
1:A:127:GLU:O	1:A:128:CYS:CB	2.64	0.41
1:A:255:GLN:CB	1:A:279:ARG:NH2	2.77	0.41
2:B:124:ASN:O	2:B:126:SER:N	2.52	0.41
1:A:80:LEU:HD12	1:A:85:ASN:O	2.19	0.41
1:A:220:ILE:HG12	1:A:261:HIS:CE1	2.55	0.41
1:A:311:ALA:HB1	1:A:314:LEU:HD13	2.01	0.41
1:A:730:SER:HB2	1:A:732:CYS:SG	2.61	0.41
1:A:837:TYR:CD1	1:A:837:TYR:N	2.88	0.41
1:A:32:LEU:HD12	1:A:32:LEU:HA	1.88	0.41
1:A:415:SER:O	1:A:416:ASP:HB2	2.19	0.41
1:A:593:MET:C	1:A:594:THR:CG2	2.85	0.41
1:A:690:SER:C	1:A:691:LEU:HD23	2.43	0.41
1:A:411:TRP:CH2	1:A:459:PHE:N	2.89	0.41
1:A:924:GLY:O	1:A:925:ASP:HB2	2.21	0.41
1:A:13:THR:HB	1:A:355:ASN:HA	2.01	0.41
1:A:157:ILE:HG22	1:A:158:ARG:N	2.36	0.41
1:A:258:ILE:CG2	1:A:259:VAL:H	2.34	0.41
1:A:503:CYS:CA	1:A:543:ILE:CD1	2.63	0.41
1:A:1074:ARG:HD3	1:A:1074:ARG:HA	1.72	0.41
1:A:365:VAL:HG21	1:A:726:TYR:CG	2.55	0.41
1:A:764:SER:OG	1:A:803:HIS:NE2	2.45	0.41
1:A:231:ILE:HD13	1:A:240:HIS:HD2	1.86	0.41
1:A:469:ILE:HD13	1:A:471:ILE:N	2.36	0.41
1:A:500:VAL:HG11	1:A:541:LEU:HD12	2.00	0.41
1:A:570:LYS:CG	1:A:571:LEU:H	2.26	0.41
1:A:19:VAL:HG12	1:A:32:LEU:CB	2.51	0.41
1:A:226:PHE:HD2	1:A:297:LEU:HD11	1.86	0.41
1:A:365:VAL:HG21	1:A:726:TYR:CB	2.51	0.41
1:A:365:VAL:HG11	1:A:726:TYR:CE2	2.56	0.41
1:A:874:VAL:HG22	1:A:875:GLU:N	2.35	0.41
1:A:197:LEU:O	1:A:200:LYS:CD	2.69	0.41
1:A:234:GLN:C	1:A:236:SER:H	2.29	0.41
1:A:382:PHE:H	1:A:720:SER:HB3	1.86	0.41
1:A:614:PHE:CA	1:A:624:SER:OG	2.68	0.41
1:A:619:GLU:H	1:A:619:GLU:HG2	1.75	0.41
1:A:713:ARG:CG	1:A:714:THR:N	2.84	0.41
1:A:912:LEU:HD23	1:A:912:LEU:HA	1.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:963:ASP:O	1:A:978:GLN:HA	2.21	0.41
1:A:1029:LEU:HD23	1:A:1039:LEU:HB2	2.03	0.41
1:A:1093:LEU:O	1:A:1094:ILE:C	2.63	0.40
1:A:490:TRP:NE1	1:A:519:LEU:HD22	2.36	0.40
1:A:939:GLU:O	1:A:940:GLY:C	2.64	0.40
1:A:1047:TRP:O	1:A:1048:TYR:C	2.65	0.40
1:A:770:LEU:HD23	1:A:770:LEU:HA	1.90	0.40
1:A:1024:THR:HB	1:A:1041:THR:CG2	2.45	0.40
1:A:197:LEU:O	1:A:200:LYS:HD2	2.21	0.40
1:A:496:LYS:HB2	1:A:496:LYS:HE3	1.77	0.40
1:A:676:VAL:HG11	1:A:693:LEU:HD23	2.02	0.40
1:A:763:SER:CA	1:A:803:HIS:CE1	3.04	0.40
1:A:789:HIS:CD2	1:A:812:TYR:CD1	3.07	0.40
1:A:854:SER:HB2	1:A:855:ASP:H	1.60	0.40
1:A:213:GLU:OE1	1:A:233:GLY:HA3	2.22	0.40
1:A:658:VAL:HG12	1:A:660:TYR:CE2	2.40	0.40
1:A:789:HIS:NE2	1:A:812:TYR:HD1	2.19	0.40
1:A:922:LEU:HD12	1:A:922:LEU:N	2.36	0.40
1:A:1090:ASP:C	1:A:1092:ASP:N	2.78	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1106/1143 (97%)	881 (80%)	152 (14%)	73 (7%)	1	3
2	B	11/13 (85%)	9 (82%)	2 (18%)	0	100	100
All	All	1117/1156 (97%)	890 (80%)	154 (14%)	73 (6%)	1	3

All (73) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	ASP
1	A	208	LYS
1	A	214	ALA
1	A	235	GLU
1	A	291	MET
1	A	318	ASP
1	A	366	ASP
1	A	407	ILE
1	A	430	VAL
1	A	554	PRO
1	A	571	LEU
1	A	591	ILE
1	A	689	ASP
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	929	SER
1	A	970	ASN
1	A	1080	ARG
1	A	149	ASN
1	A	174	GLN
1	A	259	VAL
1	A	343	GLN
1	A	367	LEU
1	A	461	GLY
1	A	518	TYR
1	A	529	ILE
1	A	564	ILE
1	A	620	THR
1	A	624	SER
1	A	629	VAL
1	A	688	PRO
1	A	709	LYS
1	A	242	GLY
1	A	474	ALA
1	A	523	PRO
1	A	635	PRO
1	A	665	LYS

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Mol	Chain	Res	Type
1	A	683	ASN
1	A	860	THR
1	A	885	ASN
1	A	962	ASP
1	A	985	THR
1	A	1126	ALA
1	A	368	GLU
1	A	410	LEU
1	A	413	LEU
1	A	493	PRO
1	A	623	LEU
1	A	743	GLN
1	A	937	PRO
1	A	1067	LYS
1	A	1137	THR
1	A	128	CYS
1	A	176	PRO
1	A	439	ASN
1	A	485	ALA
1	A	502	SER
1	A	546	LEU
1	A	596	PHE
1	A	691	LEU
1	A	696	ASN
1	A	910	MET
1	A	925	ASP
1	A	1064	SER
1	A	664	HIS
1	A	513	GLY
1	A	185	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%)	802 (82%)	175 (18%)	2 6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	11/11 (100%)	9 (82%)	2 (18%)	2	6
All	All	988/1012 (98%)	811 (82%)	177 (18%)	2	6

All (177) 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	32	LEU
1	A	49	LEU
1	A	73	SER
1	A	92	LYS
1	A	97	SER
1	A	98	ILE
1	A	100	ILE
1	A	101	ILE
1	A	103	ARG
1	A	109	GLN
1	A	112	ILE
1	A	118	THR
1	A	123	ILE
1	A	130	MET
1	A	133	LEU
1	A	135	LEU
1	A	147	ARG
1	A	148	ASP
1	A	158	ARG
1	A	159	LEU
1	A	167	VAL
1	A	177	THR
1	A	186	GLN
1	A	197	LEU
1	A	198	ARG
1	A	200	LYS
1	A	201	GLU
1	A	202	PHE
1	A	204	LYS
1	A	208	LYS
1	A	209	GLN
1	A	222	VAL
1	A	231	ILE

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Mol	Chain	Res	Type
1	A	235	GLU
1	A	236	SER
1	A	252	ILE
1	A	255	GLN
1	A	259	VAL
1	A	283	LEU
1	A	286	GLU
1	A	290	GLN
1	A	295	VAL
1	A	302	VAL
1	A	305	LEU
1	A	307	GLU
1	A	309	SER
1	A	310	ILE
1	A	312	GLU
1	A	314	LEU
1	A	321	VAL
1	A	333	LEU
1	A	334	VAL
1	A	338	VAL
1	A	342	GLU
1	A	351	GLU
1	A	352	THR
1	A	360	VAL
1	A	372	GLN
1	A	374	GLN
1	A	383	LYS
1	A	396	ILE
1	A	397	HIS
1	A	403	ASP
1	A	410	LEU
1	A	414	ARG
1	A	419	ARG
1	A	427	LEU
1	A	434	ARG
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

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Mol	Chain	Res	Type
1	A	469	ILE
1	A	476	VAL
1	A	488	SER
1	A	505	SER
1	A	507	GLN
1	A	518	TYR
1	A	519	LEU
1	A	520	GLN
1	A	521	ILE
1	A	526	LEU
1	A	544	THR
1	A	552	LEU
1	A	555	LEU
1	A	560	LEU
1	A	561	TRP
1	A	562	THR
1	A	565	SER
1	A	567	ARG
1	A	568	ILE
1	A	570	LYS
1	A	575	GLU
1	A	576	LEU
1	A	582	LEU
1	A	597	GLU
1	A	602	LEU
1	A	603	LEU
1	A	618	ILE
1	A	619	GLU
1	A	620	THR
1	A	629	VAL
1	A	633	THR
1	A	637	VAL
1	A	640	THR
1	A	646	THR
1	A	647	THR
1	A	658	VAL
1	A	679	MET
1	A	690	SER
1	A	701	ILE
1	A	706	GLU
1	A	710	LEU
1	A	713	ARG

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Mol	Chain	Res	Type
1	A	720	SER
1	A	728	GLU
1	A	730	SER
1	A	738	SER
1	A	740	ILE
1	A	750	THR
1	A	766	SER
1	A	772	SER
1	A	786	VAL
1	A	815	SER
1	A	817	VAL
1	A	823	LYS
1	A	839	GLU
1	A	844	LYS
1	A	854	SER
1	A	857	LYS
1	A	858	LEU
1	A	870	VAL
1	A	896	GLU
1	A	900	ARG
1	A	909	ILE
1	A	912	LEU
1	A	916	THR
1	A	917	LYS
1	A	921	ILE
1	A	922	LEU
1	A	923	VAL
1	A	926	LEU
1	A	938	MET
1	A	957	VAL
1	A	960	LEU
1	A	966	LEU
1	A	969	GLU
1	A	979	LYS
1	A	990	GLN
1	A	992	LEU
1	A	1000	LEU
1	A	1006	VAL
1	A	1013	VAL
1	A	1014	MET
1	A	1039	LEU
1	A	1045	GLU

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Mol	Chain	Res	Type
1	A	1050	LEU
1	A	1055	GLN
1	A	1058	LEU
1	A	1063	LYS
1	A	1090	ASP
1	A	1093	LEU
1	A	1096	SER
1	A	1100	ILE
1	A	1108	VAL
1	A	1127	ASP
1	A	1129	LEU
1	A	1131	LYS
1	A	1139	ILE
2	B	128	MET
2	B	130	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	30	ASN
1	A	105	HIS
1	A	109	GLN
1	A	189	HIS
1	A	211	ASN
1	A	240	HIS
1	A	261	HIS
1	A	262	ASN
1	A	267	ASN
1	A	332	GLN
1	A	343	GLN
1	A	370	GLN
1	A	374	GLN
1	A	392	ASN
1	A	439	ASN
1	A	455	GLN
1	A	462	ASN
1	A	497	ASN
1	A	520	GLN
1	A	522	HIS
1	A	536	HIS
1	A	550	ASN

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Mol	Chain	Res	Type
1	A	600	HIS
1	A	648	ASN
1	A	677	ASN
1	A	727	GLN
1	A	759	GLN
1	A	790	ASN
1	A	796	GLN
1	A	809	GLN
1	A	845	GLN
1	A	852	GLN
1	A	885	ASN
1	A	905	HIS
1	A	907	ASN
1	A	908	ASN
1	A	941	ASN
1	A	950	ASN
1	A	978	GLN
1	A	990	GLN
1	A	1015	GLN
1	A	1049	ASN
1	A	1055	GLN
1	A	1056	ASN
1	A	1059	ASN
1	A	1070	HIS
1	A	1077	HIS
2	B	124	ASN

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%)	0.58	130 (11%) 9 7	17, 66, 159, 207	0
2	B	13/13 (100%)	1.40	1 (7%) 19 14	20, 21, 24, 32	0
All	All	1127/1156 (97%)	0.59	131 (11%) 9 7	17, 66, 158, 207	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	660	TYR	7.4
1	A	508	VAL	7.1
1	A	714	THR	6.2
1	A	519	LEU	4.9
1	A	571	LEU	4.5
1	A	502	SER	4.5
1	A	504	ASN	4.5
1	A	925	ASP	4.5
1	A	468	LEU	4.5
1	A	572	PRO	4.4
1	A	602	LEU	4.4
1	A	569	LEU	4.3
1	A	462	ASN	4.3
2	B	136	PHE	4.3
1	A	412	PRO	4.3
1	A	616	LEU	4.3
1	A	666	LEU	4.3
1	A	426	VAL	4.2
1	A	297	LEU	4.1
1	A	447	GLU	4.1
1	A	521	ILE	4.0
1	A	503	CYS	4.0
1	A	929	SER	4.0
1	A	2	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	889	ARG	3.7
1	A	463	VAL	3.7
1	A	510	VAL	3.6
1	A	518	TYR	3.6
1	A	513	GLY	3.5
1	A	601	TYR	3.5
1	A	460	CYS	3.5
1	A	458	PHE	3.5
1	A	425	LEU	3.5
1	A	603	LEU	3.5
1	A	501	ALA	3.4
1	A	291	MET	3.4
1	A	568	ILE	3.4
1	A	357	GLY	3.4
1	A	618	ILE	3.4
1	A	885	ASN	3.4
1	A	557	ALA	3.4
1	A	483	PRO	3.2
1	A	593	MET	3.2
1	A	430	VAL	3.2
1	A	708	GLN	3.1
1	A	132	GLY	3.1
1	A	594	THR	3.1
1	A	413	LEU	3.1
1	A	292	ASP	3.1
1	A	461	GLY	3.1
1	A	613	TYR	3.1
1	A	542	ASP	3.0
1	A	595	THR	3.0
1	A	615	GLY	2.8
1	A	505	SER	2.8
1	A	493	PRO	2.8
1	A	498	ILE	2.8
1	A	592	LEU	2.8
1	A	427	LEU	2.7
1	A	1067	LYS	2.7
1	A	294	THR	2.7
1	A	577	LEU	2.6
1	A	556	CYS	2.6
1	A	293	GLY	2.6
1	A	509	VAL	2.6
1	A	439	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	665	LYS	2.6
1	A	918	GLY	2.5
1	A	276	MET	2.5
1	A	476	VAL	2.5
1	A	590	SER	2.5
1	A	591	ILE	2.5
1	A	517	TYR	2.5
1	A	544	THR	2.5
1	A	478	LEU	2.5
1	A	924	GLY	2.5
1	A	1066	GLY	2.5
1	A	411	TRP	2.5
1	A	421	THR	2.5
1	A	917	LYS	2.5
1	A	576	LEU	2.4
1	A	589	ARG	2.4
1	A	295	VAL	2.4
1	A	450	GLY	2.4
1	A	624	SER	2.4
1	A	436	LEU	2.4
1	A	552	LEU	2.4
1	A	365	VAL	2.4
1	A	313	CYS	2.3
1	A	667	VAL	2.3
1	A	663	ASN	2.3
1	A	507	GLN	2.3
1	A	904	ASN	2.3
1	A	561	TRP	2.3
1	A	443	VAL	2.3
1	A	596	PHE	2.2
1	A	692	ALA	2.2
1	A	1124	ALA	2.2
1	A	844	LYS	2.2
1	A	419	ARG	2.2
1	A	1065	VAL	2.2
1	A	441	GLU	2.2
1	A	1045	GLU	2.2
1	A	639	ARG	2.2
1	A	903	CYS	2.2
1	A	686	GLY	2.2
1	A	444	GLU	2.2
1	A	512	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	614	PHE	2.2
1	A	854	SER	2.2
1	A	661	SER	2.1
1	A	981	SER	2.1
1	A	201	GLU	2.1
1	A	528	GLN	2.1
1	A	668	PHE	2.1
1	A	399	HIS	2.1
1	A	545	PRO	2.1
1	A	366	ASP	2.1
1	A	621	GLY	2.1
1	A	451	PHE	2.1
1	A	689	ASP	2.1
1	A	599	SER	2.1
1	A	690	SER	2.1
1	A	642	ARG	2.1
1	A	902	GLU	2.1
1	A	488	SER	2.0
1	A	773	SER	2.0
1	A	242	GLY	2.0
1	A	641	PHE	2.0
1	A	446	THR	2.0
1	A	470	GLN	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.