Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2023 – 04:14 PM EDT

PDB ID	:	3I89
Title	:	Crystal Structure of DDB1 in Complex with the H-Box Motif of WDR22
Authors	:	Li, T.; Robert, E.I.; Breugel, P.C.V.; Strubin, M.; Zheng, N.
Deposited on	:	2009-07-09
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:

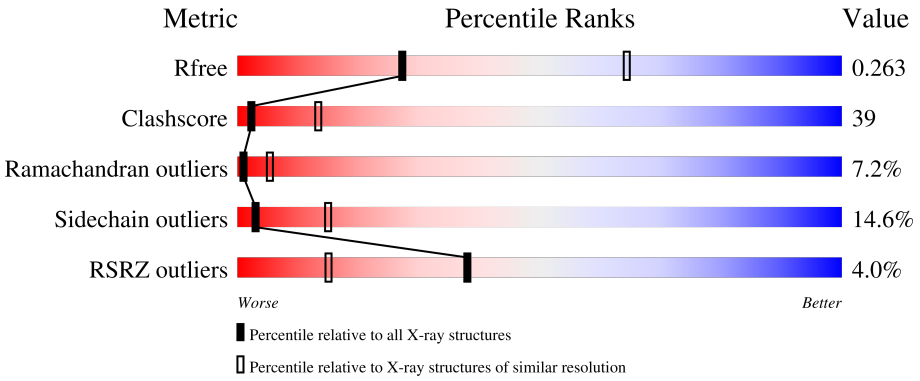
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 <=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	4% 42% 43% 11% . .
2	B	13	23% 15% 46% 31% 8%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8821 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 22.

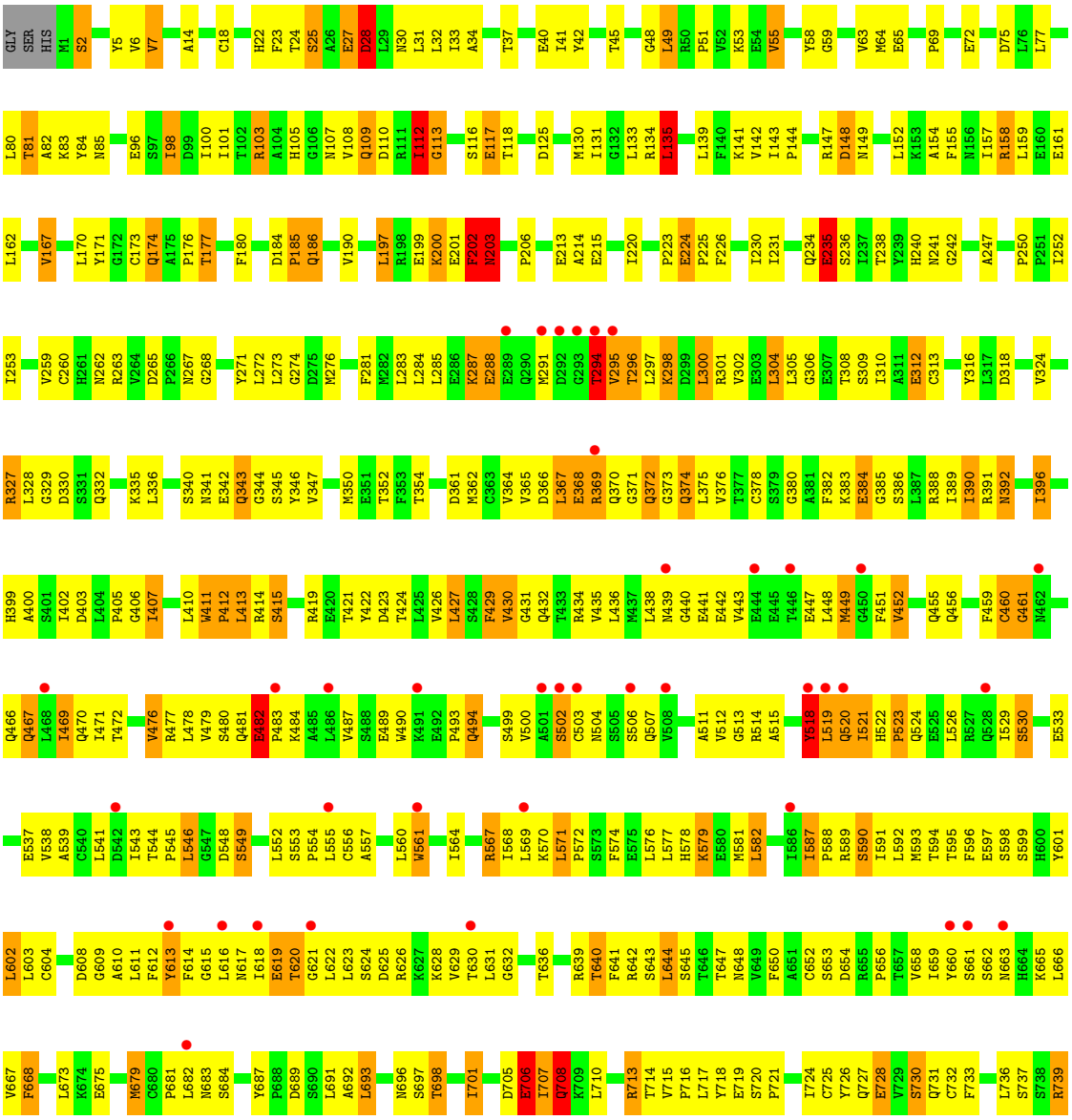
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	13	Total	C	N	O	0	0	0
			95	60	19	16			

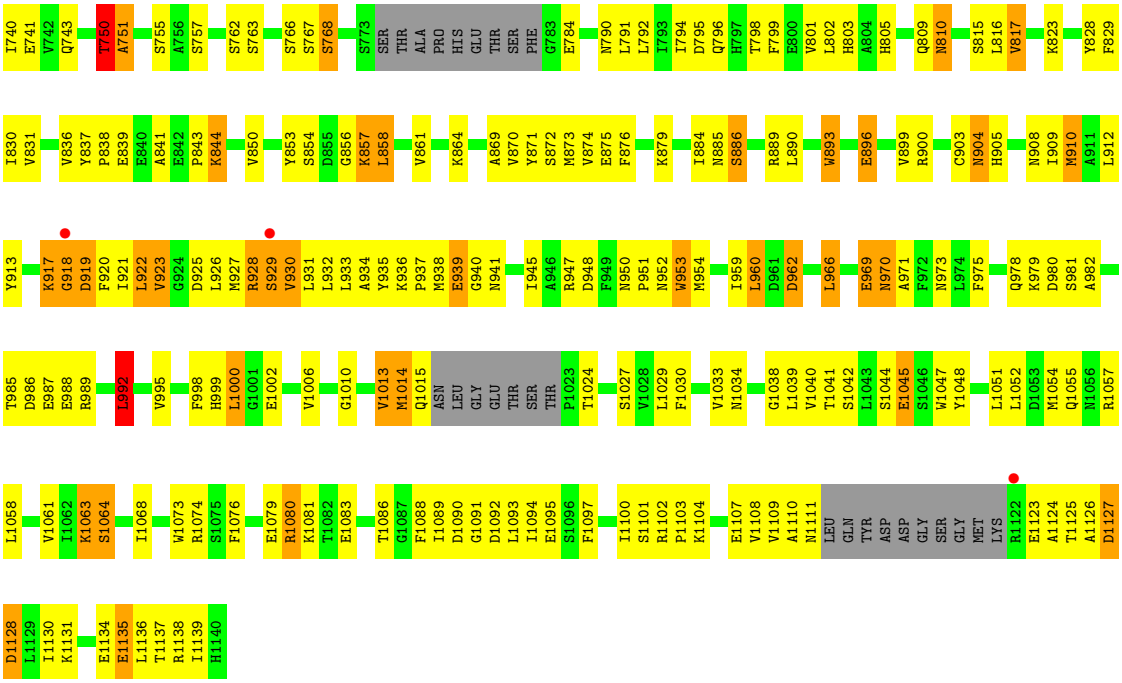
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

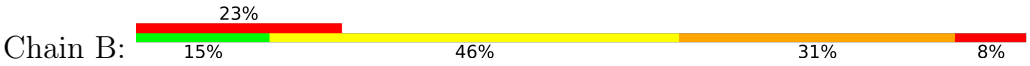
• Molecule 1: DNA damage-binding protein 1

Chain A:





• Molecule 2: WD repeat-containing protein 22



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	63.29Å 133.67Å 184.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.22 – 3.00 45.24 – 2.90	Depositor EDS
% Data completeness (in resolution range)	94.7 (45.22-3.00) 92.1 (45.24-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.83 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.251 , 0.304 0.260 , 0.263	Depositor DCC
R_{free} test set	1590 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å^2)	69.7	Xtriage
Anisotropy	0.338	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 57.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	8821	wwPDB-VP
Average B, all atoms (Å^2)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.73	7/8885 (0.1%)	0.81	10/12034 (0.1%)
2	B	1.44	1/96 (1.0%)	1.32	1/127 (0.8%)
All	All	0.74	8/8981 (0.1%)	0.82	11/12161 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1135	GLU	CD-OE1	19.79	1.47	1.25
1	A	939	GLU	CD-OE2	15.23	1.42	1.25
1	A	939	GLU	CD-OE1	11.23	1.38	1.25
2	B	16	GLY	CA-C	9.19	1.66	1.51
1	A	384	GLU	CD-OE1	6.18	1.32	1.25
1	A	725	CYS	CB-SG	-6.02	1.72	1.82
1	A	384	GLU	CD-OE2	5.52	1.31	1.25
1	A	928	ARG	C-N	-5.47	1.21	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	561	TRP	N-CA-C	7.92	132.38	111.00
2	B	16	GLY	CA-C-O	-6.43	109.02	120.60
1	A	203	ASN	N-CA-C	-6.41	93.69	111.00
1	A	330	ASP	CB-CG-OD1	6.34	124.01	118.30
1	A	992	LEU	CA-CB-CG	6.27	129.73	115.30
1	A	1135	GLU	OE1-CD-OE2	5.81	130.28	123.30
1	A	202	PHE	N-CA-C	-5.78	95.40	111.00
1	A	135	LEU	CA-CB-CG	5.42	127.75	115.30
1	A	928	ARG	CB-CA-C	5.32	121.04	110.40
1	A	693	LEU	CA-CB-CG	5.21	127.28	115.30
1	A	167	VAL	CB-CA-C	-5.19	101.53	111.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	661	0
2	B	95	0	95	32	0
All	All	8821	0	8800	683	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 39.

All (683) 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:368:GLU:CG	1:A:370:GLN:HE21	1.50	1.24
2:B:18:LEU:HD23	2:B:18:LEU:O	1.37	1.18
1:A:613:TYR:HD1	1:A:614:PHE:N	1.40	1.17
1:A:459:PHE:CE2	1:A:503:CYS:HB3	1.78	1.15
1:A:909:ILE:HG12	1:A:927:MET:HE3	1.21	1.15
1:A:615:GLY:H	1:A:624:SER:CB	1.61	1.14
1:A:482:GLU:HB2	1:A:483:PRO:HD3	1.13	1.13
1:A:621:GLY:C	1:A:622:LEU:HD12	1.70	1.12
1:A:504:ASN:HD21	1:A:545:PRO:CD	1.63	1.11
1:A:630:THR:HG23	1:A:631:LEU:H	1.05	1.10
1:A:157:ILE:HD13	1:A:201:GLU:O	1.51	1.09
2:B:18:LEU:HD23	2:B:18:LEU:C	1.66	1.08
2:B:23:LEU:HD13	2:B:23:LEU:N	1.62	1.08
1:A:614:PHE:HB3	1:A:624:SER:OG	1.54	1.07
1:A:713:ARG:CG	1:A:713:ARG:HH11	1.67	1.07
1:A:642:ARG:HH22	1:A:683:ASN:HB2	1.01	1.07
1:A:112:ILE:HG22	1:A:113:GLY:H	1.17	1.06
1:A:368:GLU:HG3	1:A:370:GLN:NE2	1.70	1.06
1:A:482:GLU:HB2	1:A:483:PRO:CD	1.88	1.04
1:A:368:GLU:HG3	1:A:370:GLN:HE21	0.88	1.03
1:A:909:ILE:HG12	1:A:927:MET:CE	1.86	1.03
1:A:400:ALA:H	1:A:701:ILE:HD11	1.17	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:929:SER:O	1:A:930:VAL:HG22	1.61	1.00
1:A:611:LEU:HB3	1:A:629:VAL:CG2	1.91	1.00
1:A:537:GLU:O	1:A:561:TRP:HD1	1.45	1.00
1:A:504:ASN:HD21	1:A:545:PRO:HD2	1.22	0.99
1:A:929:SER:O	1:A:930:VAL:HG13	1.61	0.99
1:A:613:TYR:CD1	1:A:613:TYR:C	2.30	0.98
1:A:613:TYR:CD1	1:A:614:PHE:N	2.30	0.98
1:A:1024:THR:HB	1:A:1041:THR:HG21	1.45	0.97
1:A:641:PHE:HA	1:A:681:PRO:HG3	1.43	0.97
2:B:23:LEU:HD13	2:B:23:LEU:H	1.21	0.96
1:A:642:ARG:NH2	1:A:683:ASN:HB2	1.80	0.95
1:A:98:ILE:HD13	1:A:98:ILE:H	1.32	0.95
1:A:870:VAL:HG11	1:A:873:MET:CE	1.96	0.94
1:A:614:PHE:CE1	1:A:626:ARG:HA	2.03	0.93
1:A:81:THR:HG22	1:A:83:LYS:H	1.32	0.93
2:B:23:LEU:N	2:B:23:LEU:CD1	2.29	0.93
1:A:713:ARG:HH11	1:A:713:ARG:HG2	1.33	0.92
1:A:368:GLU:CG	1:A:370:GLN:NE2	2.29	0.91
1:A:23:PHE:H	1:A:30:ASN:ND2	1.68	0.91
1:A:630:THR:HG23	1:A:631:LEU:N	1.84	0.91
1:A:1024:THR:HB	1:A:1041:THR:CG2	2.00	0.91
1:A:1125:THR:HG22	1:A:1126:ALA:H	1.34	0.91
1:A:560:LEU:HD12	1:A:567:ARG:NH1	1.86	0.91
1:A:364:VAL:O	1:A:365:VAL:HG23	1.70	0.90
1:A:1125:THR:HG22	1:A:1126:ALA:N	1.87	0.90
1:A:385:GLY:HA3	1:A:719:GLU:O	1.71	0.89
1:A:642:ARG:HH22	1:A:683:ASN:CB	1.86	0.89
1:A:611:LEU:HB3	1:A:629:VAL:HG21	1.54	0.89
1:A:197:LEU:HD23	1:A:197:LEU:H	1.36	0.89
1:A:662:SER:HB3	1:A:665:LYS:HB2	1.53	0.88
1:A:23:PHE:H	1:A:30:ASN:HD22	1.22	0.87
1:A:112:ILE:HD12	1:A:112:ILE:N	1.90	0.87
1:A:480:SER:HB2	1:A:484:LYS:H	1.40	0.86
1:A:611:LEU:HD23	1:A:612:PHE:N	1.90	0.86
1:A:170:LEU:HD12	1:A:177:THR:HG22	1.57	0.86
1:A:612:PHE:CE2	1:A:628:LYS:HB2	2.11	0.85
1:A:614:PHE:CB	1:A:624:SER:OG	2.23	0.85
1:A:184:ASP:HB2	1:A:185:PRO:HD2	1.58	0.85
1:A:614:PHE:CD1	1:A:625:ASP:O	2.30	0.85
1:A:2:SER:CB	1:A:995:VAL:HG23	2.07	0.84
1:A:2:SER:HB3	1:A:995:VAL:HG23	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:611:LEU:HD23	1:A:612:PHE:O	1.76	0.84
1:A:107:ASN:OD1	1:A:109:GLN:HG2	1.78	0.84
1:A:184:ASP:HB2	1:A:185:PRO:CD	2.08	0.84
1:A:611:LEU:HD23	1:A:612:PHE:C	1.97	0.84
1:A:1014:MET:SD	1:A:1015:GLN:HG2	2.18	0.84
1:A:641:PHE:CZ	1:A:648:ASN:HB2	2.12	0.83
1:A:644:LEU:HG	1:A:645:SER:H	1.43	0.83
1:A:400:ALA:N	1:A:701:ILE:HD11	1.93	0.83
1:A:504:ASN:HD21	1:A:545:PRO:HD3	1.39	0.83
1:A:1127:ASP:O	1:A:1130:ILE:HG22	1.78	0.83
1:A:611:LEU:CB	1:A:629:VAL:CG2	2.57	0.83
1:A:98:ILE:H	1:A:98:ILE:CD1	1.91	0.82
1:A:611:LEU:H	1:A:629:VAL:CG2	1.92	0.82
1:A:620:THR:OG1	1:A:622:LEU:HD13	1.80	0.82
1:A:630:THR:CG2	1:A:631:LEU:H	1.89	0.82
1:A:571:LEU:HB3	1:A:572:PRO:HD3	1.60	0.82
1:A:609:GLY:O	1:A:631:LEU:HB2	1.79	0.82
1:A:368:GLU:HG2	1:A:370:GLN:CG	2.08	0.81
1:A:537:GLU:O	1:A:561:TRP:CD1	2.33	0.81
1:A:364:VAL:O	1:A:365:VAL:CG2	2.28	0.81
1:A:561:TRP:CZ3	1:A:587:ILE:HD12	2.14	0.81
2:B:18:LEU:C	2:B:18:LEU:CD2	2.48	0.81
1:A:614:PHE:HB3	1:A:624:SER:HG	1.45	0.81
1:A:170:LEU:HD12	1:A:177:THR:CG2	2.11	0.80
1:A:561:TRP:CZ3	1:A:587:ILE:CD1	2.64	0.80
1:A:614:PHE:HE1	1:A:626:ARG:HA	1.44	0.80
1:A:611:LEU:HB3	1:A:629:VAL:HG22	1.63	0.80
1:A:929:SER:O	1:A:930:VAL:CG1	2.30	0.80
1:A:368:GLU:HG2	1:A:370:GLN:HG3	1.61	0.80
1:A:929:SER:C	1:A:930:VAL:HG22	2.03	0.79
1:A:727:GLN:HB2	1:A:829:PHE:CE1	2.17	0.79
1:A:81:THR:CG2	1:A:83:LYS:H	1.96	0.79
1:A:396:ILE:CD1	1:A:673:LEU:HD21	2.13	0.79
1:A:929:SER:O	1:A:930:VAL:CG2	2.30	0.79
1:A:507:GLN:HE22	1:A:553:SER:HB2	1.46	0.79
1:A:112:ILE:HG22	1:A:113:GLY:N	1.97	0.78
1:A:1033:VAL:HG11	2:B:24:HIS:CB	2.14	0.78
1:A:238:THR:HG22	1:A:247:ALA:HB2	1.64	0.78
1:A:610:ALA:CB	1:A:628:LYS:CE	2.61	0.78
1:A:504:ASN:ND2	1:A:545:PRO:CD	2.46	0.78
1:A:507:GLN:HE22	1:A:553:SER:CB	1.96	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:614:PHE:CE1	1:A:625:ASP:O	2.37	0.77
1:A:713:ARG:HH11	1:A:713:ARG:HG3	1.47	0.77
2:B:23:LEU:O	2:B:24:HIS:HB3	1.82	0.77
1:A:610:ALA:CB	1:A:628:LYS:HE2	2.15	0.77
1:A:870:VAL:HG11	1:A:873:MET:HE3	1.66	0.77
1:A:250:PRO:HB2	1:A:252:ILE:HG22	1.65	0.76
1:A:1051:LEU:HD22	1:A:1094:ILE:HD12	1.66	0.76
1:A:185:PRO:HB2	1:A:186:GLN:OE1	1.84	0.76
1:A:328:LEU:O	1:A:380:GLY:HA2	1.86	0.76
1:A:1024:THR:CB	1:A:1041:THR:HG21	2.16	0.76
1:A:14:ALA:HB1	1:A:327:ARG:HB3	1.66	0.75
1:A:614:PHE:HE1	1:A:626:ARG:CA	1.99	0.75
1:A:1125:THR:HB	1:A:1128:ASP:HB2	1.66	0.75
1:A:342:GLU:O	1:A:343:GLN:HB3	1.85	0.75
1:A:610:ALA:HB3	1:A:628:LYS:HE3	1.67	0.75
1:A:611:LEU:H	1:A:629:VAL:HG23	1.50	0.75
1:A:396:ILE:HD12	1:A:673:LEU:HD21	1.68	0.75
1:A:476:VAL:HG13	1:A:490:TRP:HB3	1.67	0.75
1:A:412:PRO:O	1:A:413:LEU:HB2	1.87	0.74
1:A:143:ILE:HG12	1:A:154:ALA:HB2	1.69	0.74
1:A:514:ARG:O	1:A:533:GLU:HA	1.87	0.74
1:A:342:GLU:O	1:A:343:GLN:CB	2.35	0.74
1:A:701:ILE:N	1:A:701:ILE:HD13	2.02	0.74
1:A:117:GLU:OE1	1:A:117:GLU:HA	1.87	0.74
1:A:504:ASN:ND2	1:A:545:PRO:HD3	2.01	0.74
1:A:482:GLU:CB	1:A:483:PRO:HD3	2.08	0.73
1:A:615:GLY:N	1:A:624:SER:CB	2.46	0.73
1:A:1033:VAL:HG11	2:B:24:HIS:HB2	1.69	0.73
1:A:701:ILE:HD13	1:A:701:ILE:H	1.54	0.73
1:A:272:LEU:O	1:A:273:LEU:HD23	1.88	0.72
1:A:936:LYS:C	1:A:938:MET:H	1.91	0.72
1:A:112:ILE:HD12	1:A:112:ILE:H	1.51	0.72
1:A:304:LEU:HD12	1:A:305:LEU:N	2.05	0.72
1:A:537:GLU:HB3	1:A:561:TRP:CD1	2.25	0.72
1:A:844:LYS:H	1:A:844:LYS:HD3	1.55	0.72
1:A:762:SER:O	1:A:763:SER:HB3	1.89	0.72
1:A:928:ARG:O	1:A:929:SER:HB3	1.89	0.72
1:A:1090:ASP:HB2	1:A:1092:ASP:HB2	1.71	0.72
1:A:69:PRO:HD2	1:A:72:GLU:HG3	1.70	0.72
1:A:713:ARG:CG	1:A:713:ARG:NH1	2.40	0.72
1:A:1134:GLU:C	1:A:1136:LEU:H	1.93	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:20:GLN:HA	2:B:23:LEU:HD22	1.72	0.71
1:A:615:GLY:H	1:A:624:SER:HB2	1.55	0.71
1:A:854:SER:HB2	1:A:857:LYS:HG3	1.72	0.71
1:A:63:VAL:HB	1:A:80:LEU:HB3	1.72	0.71
1:A:366:ASP:O	1:A:369:ARG:N	2.23	0.71
1:A:917:LYS:O	1:A:919:ASP:N	2.24	0.71
1:A:167:VAL:HG13	1:A:180:PHE:HB3	1.73	0.71
1:A:610:ALA:CB	1:A:628:LYS:HE3	2.21	0.71
1:A:304:LEU:HD12	1:A:305:LEU:H	1.55	0.71
1:A:611:LEU:CA	1:A:629:VAL:HG22	2.21	0.70
1:A:719:GLU:OE2	1:A:755:SER:HB3	1.90	0.70
1:A:621:GLY:O	1:A:622:LEU:HD12	1.91	0.70
1:A:546:LEU:HD11	1:A:593:MET:SD	2.31	0.70
1:A:871:TYR:OH	2:B:14:VAL:HG21	1.91	0.70
1:A:611:LEU:CB	1:A:629:VAL:HG22	2.21	0.70
2:B:18:LEU:O	2:B:18:LEU:CD2	2.30	0.70
1:A:388:ARG:HD3	1:A:714:THR:OG1	1.92	0.70
1:A:537:GLU:C	1:A:561:TRP:HD1	1.95	0.70
1:A:1000:LEU:HD13	1:A:1002:GLU:HB2	1.72	0.70
1:A:459:PHE:CD2	1:A:503:CYS:HB3	2.26	0.70
1:A:691:LEU:O	1:A:701:ILE:HA	1.93	0.69
1:A:238:THR:HG22	1:A:247:ALA:CB	2.21	0.69
1:A:49:LEU:O	1:A:51:PRO:HD3	1.91	0.69
1:A:520:GLN:NE2	1:A:529:ILE:HD11	2.08	0.69
2:B:15:VAL:O	2:B:16:GLY:C	2.31	0.69
1:A:284:LEU:O	1:A:300:LEU:HA	1.93	0.68
1:A:611:LEU:CD2	1:A:612:PHE:O	2.41	0.68
1:A:931:LEU:HD12	1:A:931:LEU:N	2.09	0.68
1:A:623:LEU:HG	1:A:624:SER:N	2.09	0.68
1:A:909:ILE:CG1	1:A:927:MET:CE	2.68	0.68
1:A:948:ASP:HB2	1:A:992:LEU:CD1	2.24	0.68
1:A:382:PHE:H	1:A:720:SER:HB3	1.58	0.67
1:A:513:GLY:O	1:A:538:VAL:HG23	1.93	0.67
1:A:530:SER:HB2	1:A:574:PHE:HE1	1.59	0.67
1:A:312:GLU:HG3	1:A:327:ARG:HG3	1.77	0.67
1:A:931:LEU:HG	1:A:947:ARG:HB3	1.74	0.67
1:A:713:ARG:HG2	1:A:713:ARG:NH1	2.04	0.67
2:B:23:LEU:O	2:B:24:HIS:CB	2.42	0.67
1:A:5:TYR:CE2	1:A:7:VAL:HG22	2.30	0.67
1:A:133:LEU:HD23	1:A:135:LEU:HD21	1.77	0.67
1:A:81:THR:CG2	1:A:82:ALA:N	2.58	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:ASP:CB	1:A:185:PRO:HD2	2.25	0.66
1:A:622:LEU:HD12	1:A:622:LEU:N	2.10	0.66
1:A:452:VAL:HB	1:A:455:GLN:HB2	1.76	0.66
1:A:202:PHE:O	1:A:203:ASN:ND2	2.30	0.65
1:A:518:TYR:HD2	1:A:519:LEU:N	1.94	0.65
1:A:953:TRP:HB2	1:A:970:ASN:HB2	1.77	0.65
1:A:1123:GLU:HG2	1:A:1124:ALA:H	1.62	0.65
1:A:24:THR:H	1:A:30:ASN:HD21	1.45	0.65
1:A:611:LEU:N	1:A:629:VAL:CG2	2.59	0.65
1:A:296:THR:OG1	1:A:297:LEU:N	2.29	0.65
1:A:366:ASP:O	1:A:367:LEU:C	2.34	0.65
1:A:587:ILE:HB	1:A:588:PRO:HD2	1.79	0.65
1:A:614:PHE:CA	1:A:624:SER:OG	2.45	0.65
1:A:615:GLY:H	1:A:624:SER:HB3	1.59	0.64
1:A:978:GLN:O	1:A:992:LEU:HB2	1.97	0.64
1:A:294:THR:HG22	1:A:295:VAL:HG22	1.80	0.64
1:A:556:CYS:N	1:A:569:LEU:O	2.29	0.64
1:A:186:GLN:OE1	1:A:186:GLN:N	2.30	0.64
1:A:936:LYS:O	1:A:940:GLY:HA2	1.96	0.64
2:B:20:GLN:C	2:B:22:GLY:H	2.00	0.64
1:A:112:ILE:CG2	1:A:113:GLY:H	1.98	0.64
1:A:391:ARG:HD2	1:A:392:ASN:O	1.97	0.64
1:A:478:LEU:HD13	1:A:526:LEU:HD21	1.79	0.63
1:A:920:PHE:O	1:A:934:ALA:HA	1.97	0.63
1:A:1136:LEU:HD23	1:A:1139:ILE:HD12	1.80	0.63
1:A:197:LEU:HD23	1:A:197:LEU:N	2.09	0.63
1:A:1002:GLU:OE2	1:A:1034:ASN:HB2	1.98	0.63
2:B:20:GLN:C	2:B:22:GLY:N	2.52	0.63
1:A:613:TYR:HD1	1:A:614:PHE:CA	2.11	0.63
1:A:701:ILE:N	1:A:701:ILE:CD1	2.61	0.63
1:A:1091:GLY:HA2	1:A:1094:ILE:HB	1.80	0.63
1:A:112:ILE:H	1:A:112:ILE:CD1	2.10	0.63
1:A:424:THR:HA	1:A:436:LEU:O	1.98	0.63
1:A:184:ASP:O	1:A:185:PRO:C	2.37	0.62
1:A:364:VAL:C	1:A:365:VAL:HG23	2.19	0.62
1:A:81:THR:HG23	1:A:82:ALA:N	2.14	0.62
1:A:98:ILE:CD1	1:A:98:ILE:N	2.58	0.62
1:A:530:SER:HB2	1:A:574:PHE:CE1	2.34	0.62
1:A:273:LEU:HB2	1:A:281:PHE:HB2	1.81	0.62
1:A:556:CYS:SG	1:A:557:ALA:N	2.68	0.62
1:A:982:ALA:HB1	1:A:988:GLU:OE1	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:874:VAL:HG22	1:A:875:GLU:O	1.98	0.62
2:B:14:VAL:O	2:B:18:LEU:CB	2.48	0.62
1:A:828:TYR:HE2	1:A:861:VAL:HG21	1.64	0.62
1:A:265:ASP:O	1:A:268:GLY:N	2.33	0.62
1:A:929:SER:O	1:A:930:VAL:CB	2.46	0.61
1:A:909:ILE:HG21	1:A:927:MET:HG2	1.82	0.61
1:A:1057:ARG:HH12	1:A:1110:ALA:H	1.48	0.61
1:A:611:LEU:H	1:A:629:VAL:HG22	1.65	0.61
1:A:617:ASN:HB2	1:A:621:GLY:H	1.66	0.61
1:A:741:GLU:HG2	1:A:751:ALA:HA	1.83	0.61
1:A:480:SER:CB	1:A:483:PRO:HD2	2.31	0.61
2:B:14:VAL:O	2:B:18:LEU:HB3	2.01	0.61
1:A:220:ILE:HB	1:A:230:ILE:HB	1.81	0.61
1:A:378:CYS:HB3	1:A:721:PRO:HB2	1.82	0.61
1:A:1134:GLU:O	1:A:1136:LEU:N	2.34	0.60
1:A:81:THR:HG22	1:A:83:LYS:N	2.09	0.60
1:A:367:LEU:HB2	1:A:368:GLU:OE1	2.01	0.60
1:A:679:MET:SD	1:A:679:MET:C	2.80	0.60
2:B:22:GLY:O	2:B:23:LEU:C	2.39	0.60
1:A:856:GLY:H	1:A:857:LYS:HG2	1.66	0.60
1:A:287:LYS:O	1:A:288:GLU:HB2	2.00	0.60
1:A:449:MET:HG3	1:A:484:LYS:O	2.02	0.60
1:A:726:TYR:CE2	1:A:728:GLU:HB2	2.37	0.60
1:A:18:CYS:N	1:A:313:CYS:SG	2.75	0.60
1:A:611:LEU:CD2	1:A:612:PHE:C	2.69	0.60
1:A:654:ASP:HA	1:A:675:GLU:HG3	1.83	0.60
1:A:345:SER:C	1:A:347:VAL:H	2.04	0.60
1:A:639:ARG:HG3	1:A:640:THR:N	2.18	0.59
1:A:480:SER:HB3	1:A:483:PRO:HD2	1.85	0.59
1:A:560:LEU:HD12	1:A:567:ARG:HH11	1.67	0.59
1:A:613:TYR:CD1	1:A:614:PHE:CA	2.84	0.59
1:A:623:LEU:HG	1:A:624:SER:H	1.66	0.59
1:A:917:LYS:HZ2	1:A:921:ILE:HD12	1.66	0.59
1:A:921:ILE:C	1:A:922:LEU:HD12	2.22	0.59
1:A:923:VAL:HG11	1:A:959:ILE:HD11	1.84	0.59
1:A:969:GLU:O	1:A:971:ALA:N	2.36	0.59
1:A:262:ASN:ND2	1:A:316:TYR:H	2.01	0.59
1:A:414:ARG:HA	1:A:422:TYR:HA	1.85	0.59
1:A:184:ASP:CB	1:A:185:PRO:CD	2.74	0.59
1:A:928:ARG:O	1:A:929:SER:CB	2.50	0.59
1:A:828:TYR:CE2	1:A:861:VAL:HG21	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:611:LEU:N	1:A:629:VAL:HG22	2.17	0.58
1:A:844:LYS:HD3	1:A:844:LYS:N	2.17	0.58
1:A:1057:ARG:HH22	1:A:1111:ASN:C	2.05	0.58
1:A:84:TYR:CE2	1:A:135:LEU:HD12	2.38	0.58
1:A:611:LEU:CB	1:A:629:VAL:HG21	2.28	0.58
1:A:186:GLN:CD	1:A:186:GLN:H	2.07	0.58
1:A:5:TYR:HE2	1:A:7:VAL:CG2	2.17	0.58
1:A:6:VAL:HG12	1:A:1040:VAL:HG22	1.84	0.58
1:A:157:ILE:HG22	1:A:158:ARG:N	2.17	0.58
1:A:885:ASN:O	1:A:886:SER:HB2	2.03	0.58
1:A:571:LEU:CB	1:A:572:PRO:HD3	2.32	0.57
1:A:616:LEU:HG	1:A:617:ASN:N	2.19	0.57
1:A:312:GLU:HG3	1:A:327:ARG:CG	2.34	0.57
1:A:500:VAL:HG11	1:A:541:LEU:HD12	1.86	0.57
1:A:1125:THR:CG2	1:A:1126:ALA:N	2.58	0.57
1:A:836:VAL:HG22	2:B:15:VAL:HG21	1.86	0.57
1:A:539:ALA:HA	1:A:561:TRP:NE1	2.19	0.57
1:A:368:GLU:HG2	1:A:370:GLN:HE21	1.57	0.57
1:A:504:ASN:ND2	1:A:545:PRO:HD2	2.06	0.57
1:A:918:GLY:O	1:A:919:ASP:O	2.23	0.57
1:A:197:LEU:H	1:A:197:LEU:CD2	2.14	0.57
1:A:803:HIS:HD2	1:A:858:LEU:HG	1.70	0.57
1:A:365:VAL:HG12	1:A:367:LEU:H	1.70	0.57
1:A:452:VAL:HG22	1:A:477:ARG:HH11	1.70	0.57
1:A:24:THR:H	1:A:30:ASN:ND2	2.04	0.56
1:A:659:ILE:HG12	1:A:668:PHE:CE1	2.41	0.56
1:A:660:TYR:CG	1:A:707:ILE:HG23	2.40	0.56
1:A:828:TYR:CD2	1:A:850:VAL:CG1	2.87	0.56
1:A:364:VAL:HG12	1:A:365:VAL:N	2.20	0.56
1:A:609:GLY:HA3	1:A:632:GLY:O	2.05	0.56
1:A:909:ILE:HG22	1:A:925:ASP:OD2	2.04	0.56
1:A:591:ILE:HD12	1:A:604:CYS:HB2	1.85	0.56
1:A:611:LEU:O	1:A:629:VAL:HG22	2.06	0.56
1:A:727:GLN:HB2	1:A:829:PHE:HE1	1.66	0.56
1:A:366:ASP:OD1	1:A:372:GLN:O	2.24	0.56
1:A:22:HIS:CD2	1:A:28:ASP:O	2.59	0.56
1:A:708:GLN:CD	1:A:710:LEU:O	2.44	0.56
1:A:641:PHE:HB3	1:A:679:MET:HE3	1.87	0.56
1:A:870:VAL:CG1	1:A:873:MET:HE3	2.34	0.56
1:A:876:PHE:CZ	1:A:922:LEU:HD11	2.40	0.56
1:A:938:MET:HG2	1:A:939:GLU:N	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1127:ASP:N	1:A:1127:ASP:OD1	2.37	0.56
1:A:925:ASP:OD2	1:A:926:LEU:N	2.39	0.56
1:A:537:GLU:CB	1:A:561:TRP:CD1	2.89	0.55
1:A:978:GLN:HE21	1:A:995:VAL:HG21	1.70	0.55
1:A:611:LEU:HD23	1:A:612:PHE:H	1.69	0.55
1:A:438:LEU:C	1:A:440:GLY:H	2.09	0.55
1:A:2:SER:HB2	1:A:995:VAL:HG23	1.88	0.55
1:A:33:ILE:HD12	1:A:42:TYR:CE1	2.41	0.55
1:A:998:PHE:CZ	1:A:1074:ARG:HD2	2.41	0.55
1:A:658:VAL:CG1	1:A:659:ILE:N	2.70	0.55
1:A:954:MET:O	2:B:21:ARG:NH2	2.40	0.55
1:A:2:SER:CB	1:A:995:VAL:CG2	2.82	0.55
1:A:55:VAL:HG21	1:A:100:ILE:HD13	1.89	0.55
1:A:108:VAL:O	1:A:141:LYS:NZ	2.40	0.55
1:A:427:LEU:HD13	1:A:429:PHE:CD2	2.42	0.54
2:B:15:VAL:O	2:B:18:LEU:N	2.40	0.54
1:A:53:LYS:HE2	1:A:98:ILE:HG12	1.89	0.54
1:A:364:VAL:HG21	1:A:1010:GLY:HA3	1.89	0.54
1:A:480:SER:OG	1:A:487:VAL:HG21	2.06	0.54
1:A:484:LYS:O	1:A:484:LYS:HG3	2.07	0.54
1:A:512:VAL:HB	1:A:515:ALA:HB3	1.89	0.54
1:A:343:GLN:O	1:A:343:GLN:HG2	2.08	0.54
1:A:22:HIS:HD2	1:A:28:ASP:O	1.90	0.54
1:A:459:PHE:CE2	1:A:503:CYS:CB	2.72	0.54
1:A:660:TYR:CD1	1:A:707:ILE:HG23	2.42	0.54
1:A:938:MET:CG	1:A:939:GLU:H	2.19	0.54
1:A:402:ILE:HD11	1:A:443:VAL:HG21	1.90	0.54
1:A:561:TRP:HZ3	1:A:587:ILE:HD12	1.71	0.54
1:A:1024:THR:HB	1:A:1041:THR:HG22	1.85	0.54
1:A:429:PHE:O	1:A:431:GLY:N	2.39	0.53
1:A:644:LEU:HG	1:A:645:SER:N	2.18	0.53
1:A:614:PHE:CE1	1:A:625:ASP:C	2.82	0.53
1:A:929:SER:C	1:A:930:VAL:CG2	2.74	0.53
1:A:936:LYS:C	1:A:938:MET:N	2.60	0.53
1:A:931:LEU:N	1:A:931:LEU:CD1	2.72	0.53
1:A:31:LEU:HD21	1:A:33:ILE:HD11	1.89	0.53
1:A:384:GLU:OE1	1:A:384:GLU:HA	2.08	0.53
1:A:611:LEU:N	1:A:629:VAL:HG23	2.22	0.53
1:A:2:SER:HB3	1:A:995:VAL:CG2	2.37	0.53
1:A:593:MET:HA	1:A:601:TYR:O	2.09	0.53
1:A:947:ARG:O	1:A:992:LEU:HD12	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:985:THR:HG22	1:A:989:ARG:HH21	1.72	0.53
1:A:155:PHE:CE1	1:A:200:LYS:HB3	2.44	0.53
1:A:661:SER:HA	1:A:666:LEU:HA	1.90	0.53
1:A:843:PRO:HG2	1:A:869:ALA:HB2	1.89	0.53
1:A:853:TYR:HA	1:A:857:LYS:O	2.08	0.53
1:A:197:LEU:N	1:A:197:LEU:CD2	2.70	0.53
1:A:368:GLU:HG2	1:A:370:GLN:NE2	2.18	0.53
1:A:1102:ARG:N	1:A:1103:PRO:HD2	2.24	0.53
1:A:611:LEU:O	1:A:629:VAL:N	2.41	0.53
1:A:622:LEU:N	1:A:622:LEU:CD1	2.72	0.53
1:A:658:VAL:HG12	1:A:659:ILE:N	2.23	0.53
1:A:876:PHE:CZ	1:A:920:PHE:HA	2.43	0.53
1:A:2:SER:HB2	1:A:995:VAL:CG2	2.39	0.52
1:A:1057:ARG:NH1	1:A:1110:ALA:H	2.06	0.52
1:A:1101:SER:OG	1:A:1104:LYS:HG2	2.09	0.52
1:A:598:SER:O	1:A:599:SER:HB2	2.09	0.52
1:A:610:ALA:HB1	1:A:628:LYS:CE	2.38	0.52
1:A:809:GLN:O	1:A:810:ASN:HB2	2.09	0.52
1:A:615:GLY:N	1:A:624:SER:OG	2.40	0.52
1:A:909:ILE:HG21	1:A:927:MET:CG	2.38	0.52
1:A:930:VAL:C	1:A:931:LEU:HD12	2.29	0.52
1:A:5:TYR:HE2	1:A:7:VAL:HG22	1.75	0.52
1:A:411:TRP:CE2	1:A:459:PHE:HA	2.44	0.52
1:A:185:PRO:O	1:A:186:GLN:C	2.48	0.52
1:A:403:ASP:HA	1:A:698:THR:HA	1.92	0.52
1:A:948:ASP:HB2	1:A:992:LEU:HD12	1.90	0.52
1:A:65:GLU:O	1:A:77:LEU:HD12	2.09	0.52
1:A:611:LEU:C	1:A:629:VAL:HG22	2.30	0.52
1:A:399:HIS:CB	1:A:687:TYR:HE1	2.23	0.52
1:A:654:ASP:O	1:A:656:PRO:HD3	2.09	0.52
1:A:938:MET:HG2	1:A:939:GLU:H	1.75	0.52
1:A:612:PHE:HB3	1:A:614:PHE:CE2	2.45	0.52
1:A:231:ILE:HD13	1:A:240:HIS:HD2	1.73	0.51
1:A:909:ILE:CG1	1:A:927:MET:HE3	2.15	0.51
2:B:20:GLN:O	2:B:20:GLN:HG3	1.93	0.51
1:A:40:GLU:HB3	1:A:42:TYR:CE1	2.45	0.51
1:A:234:GLN:O	1:A:236:SER:N	2.42	0.51
1:A:368:GLU:H	1:A:368:GLU:CD	2.13	0.51
1:A:469:ILE:HD11	1:A:471:ILE:HG12	1.92	0.51
1:A:660:TYR:HB2	1:A:667:VAL:HB	1.93	0.51
1:A:876:PHE:HZ	1:A:920:PHE:HA	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:GLY:O	1:A:285:LEU:HD12	2.10	0.51
1:A:905:HIS:HD2	1:A:908:ASN:ND2	2.09	0.51
1:A:623:LEU:CG	1:A:624:SER:N	2.74	0.51
1:A:570:LYS:NZ	1:A:572:PRO:HD2	2.26	0.51
1:A:922:LEU:HD12	1:A:922:LEU:N	2.26	0.51
1:A:83:LYS:NZ	1:A:1073:TRP:O	2.42	0.51
1:A:518:TYR:C	1:A:518:TYR:CD2	2.85	0.51
1:A:931:LEU:HG	1:A:947:ARG:CB	2.41	0.51
1:A:141:LYS:HD2	1:A:154:ALA:HB3	1.93	0.50
1:A:1030:PHE:CZ	1:A:1038:GLY:HA3	2.46	0.50
1:A:623:LEU:CG	1:A:624:SER:H	2.24	0.50
1:A:25:SER:HB2	1:A:27:GLU:O	2.11	0.50
1:A:610:ALA:HB1	1:A:629:VAL:O	2.11	0.50
1:A:697:SER:O	1:A:698:THR:CB	2.59	0.50
1:A:224:GLU:CB	1:A:225:PRO:HD3	2.42	0.50
1:A:185:PRO:O	1:A:186:GLN:O	2.30	0.50
1:A:659:ILE:HG12	1:A:668:PHE:HE1	1.75	0.50
1:A:727:GLN:HB2	1:A:829:PHE:CZ	2.45	0.50
1:A:37:THR:HG22	1:A:59:GLY:O	2.11	0.50
1:A:879:LYS:HB2	1:A:890:LEU:HD11	1.93	0.50
1:A:912:LEU:HG	1:A:926:LEU:HB2	1.93	0.50
1:A:84:TYR:CD2	1:A:135:LEU:HD12	2.47	0.50
1:A:617:ASN:C	1:A:619:GLU:H	2.15	0.50
1:A:909:ILE:CG1	1:A:927:MET:HE2	2.39	0.50
1:A:81:THR:HB	1:A:85:ASN:HB2	1.93	0.50
1:A:117:GLU:OE1	1:A:117:GLU:CA	2.59	0.50
1:A:276:MET:O	1:A:310:ILE:HD12	2.11	0.50
1:A:570:LYS:HG2	1:A:571:LEU:H	1.77	0.50
1:A:389:ILE:HB	1:A:713:ARG:HB3	1.94	0.49
1:A:706:GLU:HG2	1:A:708:GLN:OE1	2.12	0.49
1:A:1048:TYR:CE2	1:A:1052:LEU:HD12	2.47	0.49
1:A:1063:LYS:H	1:A:1063:LYS:HD3	1.76	0.49
1:A:142:VAL:O	1:A:144:PRO:HD3	2.11	0.49
1:A:912:LEU:HB3	1:A:913:TYR:CE1	2.47	0.49
1:A:1058:LEU:HD11	1:A:1097:PHE:HB2	1.93	0.49
1:A:421:THR:HB	1:A:684:SER:HA	1.92	0.49
1:A:973:ASN:OD1	1:A:999:HIS:ND1	2.44	0.49
1:A:459:PHE:CE2	1:A:461:GLY:N	2.77	0.49
1:A:611:LEU:HB2	1:A:631:LEU:CD1	2.42	0.49
1:A:922:LEU:N	1:A:922:LEU:CD1	2.75	0.49
1:A:985:THR:CG2	1:A:989:ARG:HH21	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:ILE:HG21	1:A:201:GLU:O	2.13	0.49
1:A:998:PHE:HB2	1:A:1088:PHE:CD1	2.47	0.49
1:A:260:CYS:SG	1:A:274:GLY:HA3	2.52	0.49
1:A:340:SER:HB2	1:A:344:GLY:HA2	1.94	0.49
1:A:368:GLU:O	1:A:369:ARG:C	2.50	0.49
1:A:438:LEU:HD23	1:A:442:GLU:O	2.12	0.49
1:A:476:VAL:HG11	1:A:519:LEU:HD11	1.95	0.49
1:A:500:VAL:HB	1:A:511:ALA:HB3	1.95	0.49
1:A:368:GLU:OE1	1:A:368:GLU:N	2.30	0.48
1:A:620:THR:OG1	1:A:622:LEU:CD1	2.58	0.48
1:A:917:LYS:NZ	1:A:921:ILE:HD12	2.28	0.48
1:A:374:GLN:OE1	1:A:391:ARG:HG3	2.13	0.48
1:A:817:VAL:HG23	1:A:830:ILE:HB	1.95	0.48
1:A:375:LEU:HB3	1:A:390:ILE:HG13	1.94	0.48
1:A:449:MET:HG3	1:A:484:LYS:HG3	1.96	0.48
1:A:727:GLN:HG2	1:A:730:SER:OG	2.13	0.48
1:A:739:ARG:HD3	1:A:757:SER:OG	2.14	0.48
1:A:69:PRO:O	1:A:72:GLU:HB2	2.14	0.48
1:A:466:GLN:O	1:A:481:GLN:HG2	2.14	0.48
1:A:5:TYR:CE2	1:A:7:VAL:CG2	2.94	0.48
1:A:304:LEU:HD12	1:A:306:GLY:H	1.78	0.48
1:A:213:GLU:OE1	1:A:236:SER:HB3	2.14	0.48
1:A:932:LEU:O	1:A:933:LEU:HD12	2.13	0.48
2:B:24:HIS:O	2:B:24:HIS:ND1	2.47	0.48
1:A:365:VAL:HG21	1:A:733:PHE:HE2	1.78	0.47
1:A:467:GLN:HE22	1:A:524:GLN:HG2	1.77	0.47
1:A:611:LEU:HD23	1:A:612:PHE:CA	2.44	0.47
1:A:1044:SER:O	1:A:1047:TRP:N	2.47	0.47
1:A:614:PHE:CD1	1:A:625:ASP:C	2.88	0.47
1:A:705:ASP:O	1:A:706:GLU:O	2.32	0.47
1:A:611:LEU:CA	1:A:629:VAL:CG2	2.89	0.47
1:A:740:ILE:O	1:A:741:GLU:HG3	2.15	0.47
1:A:288:GLU:OE1	1:A:298:LYS:HB2	2.14	0.47
1:A:329:GLY:HA3	1:A:384:GLU:HB3	1.97	0.47
1:A:426:VAL:HB	1:A:460:CYS:SG	2.54	0.47
1:A:500:VAL:CG1	1:A:541:LEU:HD12	2.45	0.47
1:A:518:TYR:HD2	1:A:518:TYR:C	2.16	0.47
1:A:587:ILE:HD13	1:A:587:ILE:H	1.78	0.47
1:A:952:ASN:HB3	1:A:969:GLU:HG3	1.96	0.47
1:A:1033:VAL:CG1	2:B:24:HIS:CB	2.91	0.47
1:A:263:ARG:HB2	1:A:271:TYR:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:SER:HB2	1:A:423:ASP:OD2	2.14	0.47
1:A:643:SER:OG	1:A:647:THR:HA	2.13	0.47
1:A:889:ARG:CG	1:A:904:ASN:HB3	2.44	0.47
1:A:1091:GLY:O	1:A:1095:GLU:N	2.35	0.47
1:A:40:GLU:HB3	1:A:42:TYR:HE1	1.78	0.47
1:A:252:ILE:HG23	1:A:253:ILE:HG23	1.96	0.47
1:A:365:VAL:CG1	1:A:367:LEU:HD23	2.45	0.47
1:A:376:VAL:HG13	1:A:389:ILE:HG13	1.96	0.47
1:A:406:GLY:O	1:A:407:ILE:C	2.53	0.47
1:A:1063:LYS:H	1:A:1063:LYS:CD	2.27	0.47
1:A:81:THR:HG23	1:A:82:ALA:H	1.77	0.47
1:A:692:ALA:C	1:A:693:LEU:HD12	2.35	0.47
1:A:938:MET:CG	1:A:939:GLU:N	2.78	0.47
1:A:411:TRP:CZ2	1:A:459:PHE:HA	2.50	0.47
1:A:724:ILE:HG23	1:A:724:ILE:O	2.15	0.47
1:A:730:SER:HB2	1:A:732:CYS:SG	2.55	0.47
1:A:365:VAL:HG21	1:A:733:PHE:CE2	2.50	0.47
1:A:447:GLU:O	1:A:448:LEU:HD12	2.15	0.47
1:A:713:ARG:HG3	1:A:713:ARG:NH1	2.18	0.47
1:A:224:GLU:O	1:A:226:PHE:N	2.49	0.46
1:A:345:SER:O	1:A:347:VAL:N	2.48	0.46
1:A:452:VAL:CB	1:A:455:GLN:HB2	2.43	0.46
1:A:905:HIS:ND1	1:A:933:LEU:HD21	2.30	0.46
1:A:58:TYR:HB3	1:A:1073:TRP:HB2	1.97	0.46
1:A:504:ASN:C	1:A:506:SER:H	2.18	0.46
1:A:116:SER:OG	1:A:134:ARG:CZ	2.64	0.46
1:A:936:LYS:O	1:A:940:GLY:CA	2.63	0.46
1:A:234:GLN:C	1:A:236:SER:H	2.18	0.46
1:A:791:LEU:HD12	1:A:792:LEU:H	1.80	0.46
1:A:870:VAL:HG11	1:A:873:MET:HE2	1.91	0.46
1:A:539:ALA:HA	1:A:561:TRP:HE1	1.80	0.46
1:A:592:LEU:O	1:A:602:LEU:HA	2.15	0.46
1:A:715:VAL:HG21	1:A:799:PHE:HB3	1.97	0.46
1:A:838:PRO:HD2	1:A:839:GLU:OE2	2.16	0.46
1:A:884:ILE:CD1	1:A:889:ARG:HB2	2.45	0.46
1:A:920:PHE:HB3	1:A:935:TYR:HB3	1.97	0.46
1:A:1033:VAL:HG11	2:B:24:HIS:CG	2.51	0.46
1:A:1054:MET:O	1:A:1054:MET:HG3	2.16	0.46
1:A:184:ASP:HB2	1:A:185:PRO:HD3	1.91	0.46
1:A:213:GLU:HG3	1:A:215:GLU:H	1.81	0.46
1:A:432:GLN:O	1:A:456:GLN:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:560:LEU:HD12	1:A:567:ARG:CZ	2.46	0.46
1:A:1013:VAL:O	1:A:1014:MET:HG3	2.16	0.46
1:A:582:LEU:H	1:A:582:LEU:HG	1.45	0.46
1:A:267:ASN:ND2	1:A:287:LYS:NZ	2.64	0.46
1:A:923:VAL:CG1	1:A:959:ILE:HD11	2.46	0.46
1:A:335:LYS:HB2	1:A:350:MET:SD	2.56	0.46
1:A:451:PHE:CE2	1:A:470:GLN:HB2	2.51	0.46
1:A:611:LEU:HB2	1:A:631:LEU:HD12	1.98	0.46
1:A:364:VAL:CG1	1:A:365:VAL:N	2.78	0.45
1:A:459:PHE:CD2	1:A:460:CYS:N	2.84	0.45
1:A:641:PHE:HB3	1:A:679:MET:CE	2.44	0.45
1:A:707:ILE:O	1:A:708:GLN:O	2.33	0.45
1:A:716:PRO:HB2	1:A:718:TYR:CE1	2.52	0.45
1:A:1136:LEU:O	1:A:1137:THR:C	2.53	0.45
1:A:893:TRP:HA	1:A:893:TRP:CE3	2.50	0.45
1:A:170:LEU:HD12	1:A:177:THR:HG21	1.96	0.45
1:A:427:LEU:HD11	1:A:434:ARG:HB2	1.97	0.45
1:A:731:GLN:HA	1:A:796:GLN:NE2	2.32	0.45
1:A:595:THR:HG22	1:A:596:PHE:N	2.31	0.45
1:A:610:ALA:HB3	1:A:628:LYS:CE	2.34	0.45
1:A:740:ILE:HG22	1:A:741:GLU:N	2.32	0.45
1:A:1064:SER:OG	1:A:1068:ILE:N	2.50	0.45
1:A:365:VAL:HG12	1:A:367:LEU:HD23	1.99	0.45
1:A:816:LEU:CD1	1:A:831:VAL:HG22	2.46	0.45
1:A:987:GLU:C	1:A:989:ARG:H	2.20	0.45
1:A:45:THR:N	1:A:48:GLY:O	2.48	0.45
1:A:609:GLY:O	1:A:630:THR:O	2.34	0.45
1:A:419:ARG:HD3	1:A:421:THR:OG1	2.17	0.45
1:A:919:ASP:CG	1:A:920:PHE:H	2.20	0.45
1:A:105:HIS:HA	1:A:152:LEU:HD12	1.99	0.44
1:A:717:LEU:HD23	1:A:717:LEU:HA	1.80	0.44
1:A:230:ILE:C	1:A:231:ILE:HD12	2.37	0.44
1:A:561:TRP:HZ3	1:A:587:ILE:CD1	2.26	0.44
1:A:909:ILE:HG12	1:A:927:MET:HE2	1.84	0.44
1:A:610:ALA:HB2	1:A:628:LYS:HE2	1.99	0.44
1:A:794:ILE:HG23	1:A:799:PHE:HA	1.98	0.44
1:A:1027:SER:OG	1:A:1039:LEU:HD11	2.18	0.44
1:A:1051:LEU:HB2	1:A:1089:ILE:HD13	1.99	0.44
1:A:1064:SER:HG	1:A:1068:ILE:N	2.15	0.44
1:A:578:HIS:CG	1:A:579:LYS:N	2.85	0.44
1:A:624:SER:O	1:A:625:ASP:OD1	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:PHE:O	1:A:203:ASN:CB	2.66	0.44
1:A:234:GLN:O	1:A:235:GLU:CD	2.56	0.44
1:A:803:HIS:CD2	1:A:858:LEU:HB2	2.53	0.44
1:A:815:SER:HB3	1:A:872:SER:HA	1.99	0.44
1:A:1079:GLU:O	1:A:1080:ARG:HB3	2.18	0.44
1:A:1134:GLU:C	1:A:1136:LEU:N	2.58	0.44
1:A:98:ILE:HD13	1:A:98:ILE:N	2.12	0.44
1:A:288:GLU:HB3	1:A:296:THR:HG23	1.99	0.44
1:A:424:THR:CG2	1:A:435:VAL:HG12	2.48	0.44
1:A:479:VAL:HG12	1:A:480:SER:N	2.33	0.44
1:A:570:LYS:HG2	1:A:571:LEU:N	2.33	0.44
1:A:613:TYR:CE2	1:A:666:LEU:HD12	2.53	0.44
1:A:736:LEU:HD23	1:A:736:LEU:HA	1.82	0.44
1:A:795:ASP:HB3	1:A:798:THR:OG1	2.18	0.44
1:A:366:ASP:OD1	1:A:373:GLY:HA2	2.18	0.44
1:A:614:PHE:HA	1:A:624:SER:OG	2.17	0.44
1:A:910:MET:CE	2:B:14:VAL:HG11	2.48	0.44
1:A:1111:ASN:OD1	1:A:1111:ASN:N	2.51	0.44
1:A:361:ASP:OD2	1:A:362:MET:N	2.50	0.43
1:A:590:SER:O	1:A:604:CYS:HA	2.18	0.43
1:A:110:ASP:OD1	1:A:141:LYS:NZ	2.43	0.43
1:A:512:VAL:HG12	1:A:512:VAL:O	2.18	0.43
1:A:571:LEU:HB3	1:A:572:PRO:CD	2.42	0.43
1:A:636:THR:HA	1:A:652:CYS:O	2.17	0.43
1:A:903:CYS:C	1:A:904:ASN:HD22	2.22	0.43
1:A:5:TYR:OH	1:A:1091:GLY:HA3	2.18	0.43
1:A:31:LEU:CD2	1:A:33:ILE:HD11	2.48	0.43
1:A:610:ALA:HB1	1:A:628:LYS:HE2	1.92	0.43
1:A:679:MET:HA	1:A:692:ALA:O	2.19	0.43
1:A:345:SER:C	1:A:347:VAL:N	2.70	0.43
1:A:451:PHE:CD1	1:A:479:VAL:HG21	2.53	0.43
1:A:871:TYR:OH	2:B:14:VAL:CG2	2.62	0.43
1:A:731:GLN:HA	1:A:796:GLN:HE21	1.83	0.43
1:A:841:ALA:O	2:B:13:SER:HA	2.18	0.43
1:A:342:GLU:OE1	1:A:342:GLU:HA	2.18	0.43
1:A:367:LEU:O	1:A:369:ARG:N	2.51	0.43
1:A:399:HIS:HB3	1:A:687:TYR:HE1	1.84	0.43
1:A:1139:ILE:O	1:A:1139:ILE:CG2	2.66	0.43
1:A:611:LEU:O	1:A:628:LYS:HA	2.19	0.43
1:A:630:THR:O	1:A:631:LEU:HB2	2.19	0.43
1:A:905:HIS:CD2	1:A:908:ASN:ND2	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1102:ARG:NH2	1:A:1127:ASP:OD2	2.52	0.43
1:A:241:ASN:O	1:A:242:GLY:C	2.58	0.42
1:A:522:HIS:O	1:A:523:PRO:C	2.56	0.42
1:A:608:ASP:OD2	1:A:609:GLY:N	2.52	0.42
1:A:569:LEU:HG	1:A:576:LEU:HA	2.01	0.42
1:A:641:PHE:CD2	1:A:650:PHE:HB2	2.54	0.42
1:A:1061:VAL:HG21	1:A:1108:VAL:HG22	2.00	0.42
1:A:507:GLN:HE22	1:A:553:SER:HB3	1.82	0.42
1:A:719:GLU:OE2	1:A:755:SER:CB	2.62	0.42
1:A:72:GLU:OE1	1:A:103:ARG:NH2	2.53	0.42
1:A:912:LEU:CB	1:A:913:TYR:CE1	3.02	0.42
1:A:975:PHE:CD1	1:A:975:PHE:C	2.92	0.42
1:A:1051:LEU:CB	1:A:1089:ILE:HD13	2.50	0.42
1:A:22:HIS:O	1:A:75:ASP:HB2	2.19	0.42
1:A:767:SER:O	1:A:768:SER:O	2.37	0.42
1:A:953:TRP:N	1:A:953:TRP:CD1	2.86	0.42
1:A:384:GLU:OE1	1:A:384:GLU:CA	2.65	0.42
1:A:403:ASP:OD2	1:A:403:ASP:N	2.45	0.42
1:A:131:ILE:HG22	1:A:133:LEU:HD13	2.02	0.42
1:A:231:ILE:HD13	1:A:240:HIS:CD2	2.53	0.42
1:A:399:HIS:HB2	1:A:687:TYR:HE1	1.83	0.42
1:A:305:LEU:HD13	1:A:336:LEU:HD22	2.02	0.42
1:A:309:SER:H	1:A:332:GLN:NE2	2.18	0.42
1:A:987:GLU:C	1:A:989:ARG:N	2.73	0.42
2:B:14:VAL:O	2:B:18:LEU:HB2	2.19	0.42
1:A:308:THR:HB	1:A:324:VAL:HG11	2.01	0.42
1:A:482:GLU:CB	1:A:483:PRO:CD	2.73	0.42
1:A:850:VAL:HG12	1:A:861:VAL:HB	2.02	0.42
1:A:896:GLU:H	1:A:896:GLU:HG3	1.60	0.42
1:A:265:ASP:HB3	1:A:267:ASN:OD1	2.20	0.41
1:A:34:ALA:HB2	1:A:64:MET:HE2	2.03	0.41
1:A:109:GLN:HE21	1:A:109:GLN:HB2	1.64	0.41
1:A:561:TRP:CZ3	1:A:587:ILE:HD11	2.51	0.41
1:A:1013:VAL:HB	1:A:1014:MET:H	1.68	0.41
1:A:438:LEU:C	1:A:440:GLY:N	2.74	0.41
1:A:499:SER:OG	1:A:511:ALA:O	2.28	0.41
1:A:614:PHE:CZ	1:A:626:ARG:HA	2.52	0.41
1:A:750:THR:O	1:A:751:ALA:HB2	2.20	0.41
1:A:917:LYS:O	1:A:918:GLY:C	2.58	0.41
1:A:1107:GLU:C	1:A:1109:VAL:N	2.74	0.41
1:A:41:ILE:HD12	1:A:53:LYS:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:TYR:CG	1:A:223:PRO:HA	2.55	0.41
1:A:396:ILE:HD13	1:A:396:ILE:O	2.20	0.41
1:A:570:LYS:CG	1:A:571:LEU:H	2.33	0.41
1:A:740:ILE:O	1:A:741:GLU:CG	2.68	0.41
1:A:889:ARG:HG3	1:A:904:ASN:HB3	2.03	0.41
1:A:174:GLN:H	1:A:174:GLN:HG2	1.54	0.41
1:A:512:VAL:O	1:A:512:VAL:CG1	2.69	0.41
1:A:449:MET:O	1:A:479:VAL:HG21	2.20	0.41
1:A:471:ILE:HG23	1:A:476:VAL:HB	2.01	0.41
1:A:503:CYS:HG	1:A:504:ASN:N	2.19	0.41
1:A:610:ALA:CB	1:A:629:VAL:O	2.69	0.41
1:A:642:ARG:NH2	1:A:682:LEU:O	2.54	0.41
1:A:503:CYS:SG	1:A:504:ASN:N	2.94	0.41
1:A:568:ILE:HB	1:A:577:LEU:HB2	2.03	0.41
1:A:927:MET:O	1:A:928:ARG:HG3	2.20	0.41
1:A:84:TYR:HE2	1:A:135:LEU:HD12	1.82	0.41
1:A:407:ILE:HG21	1:A:410:LEU:HD23	2.02	0.41
2:B:21:ARG:O	2:B:21:ARG:HG3	2.20	0.41
1:A:366:ASP:O	1:A:368:GLU:N	2.54	0.41
1:A:493:PRO:O	1:A:494:GLN:CB	2.68	0.41
1:A:549:SER:HB2	1:A:552:LEU:O	2.21	0.41
2:B:23:LEU:H	2:B:23:LEU:CD1	1.98	0.41
1:A:173:CYS:SG	1:A:177:THR:HB	2.61	0.40
1:A:451:PHE:HA	1:A:470:GLN:OE1	2.20	0.40
1:A:603:LEU:HA	1:A:613:TYR:HA	2.03	0.40
1:A:805:HIS:HB2	1:A:858:LEU:HD12	2.03	0.40
1:A:926:LEU:HG	1:A:927:MET:N	2.36	0.40
1:A:980:ASP:O	1:A:989:ARG:NH1	2.54	0.40
1:A:1041:THR:HG22	1:A:1042:SER:N	2.36	0.40
1:A:1081:LYS:HG3	1:A:1083:GLU:OE1	2.22	0.40
1:A:642:ARG:HH12	1:A:683:ASN:ND2	2.18	0.40
1:A:837:TYR:HB3	1:A:839:GLU:OE2	2.21	0.40
1:A:659:ILE:HA	1:A:667:VAL:O	2.21	0.40
1:A:743:GLN:HB3	1:A:784:GLU:HB2	2.02	0.40
1:A:960:LEU:HD21	1:A:966:LEU:HB2	2.02	0.40
1:A:1052:LEU:O	1:A:1055:GLN:HB2	2.21	0.40
1:A:1076:PHE:C	1:A:1076:PHE:CD2	2.95	0.40
1:A:157:ILE:CG2	1:A:158:ARG:N	2.82	0.40
1:A:161:GLU:N	1:A:161:GLU:CD	2.75	0.40
1:A:932:LEU:C	1:A:933:LEU:HD12	2.42	0.40
1:A:939:GLU:HG3	1:A:941:ASN:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:978:GLN:NE2	1:A:995:VAL:HG21	2.33	0.40
1:A:614:PHE:HE1	1:A:626:ARG:N	2.19	0.40
1:A:617:ASN:C	1:A:619:GLU:N	2.74	0.40
1:A:739:ARG:NH1	1:A:790:ASN:HD21	2.20	0.40
1:A:1091:GLY:O	1:A:1092:ASP:C	2.59	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%)	867 (78%)	162 (15%)	77 (7%)	1	6
2	B	11/13 (85%)	5 (46%)	3 (27%)	3 (27%)	0	0
All	All	1117/1156 (97%)	872 (78%)	165 (15%)	80 (7%)	1	5

All (80) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	185	PRO
1	A	186	GLN
1	A	202	PHE
1	A	203	ASN
1	A	224	GLU
1	A	235	GLU
1	A	291	MET
1	A	341	ASN
1	A	367	LEU
1	A	407	ILE
1	A	430	VAL
1	A	494	GLN
1	A	502	SER

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Mol	Chain	Res	Type
1	A	554	PRO
1	A	571	LEU
1	A	689	ASP
1	A	698	THR
1	A	706	GLU
1	A	708	GLN
1	A	751	ALA
1	A	768	SER
1	A	810	ASN
1	A	886	SER
1	A	918	GLY
1	A	919	ASP
1	A	930	VAL
1	A	950	ASN
1	A	951	PRO
1	A	970	ASN
1	A	1080	ARG
2	B	24	HIS
1	A	28	ASP
1	A	288	GLU
1	A	294	THR
1	A	343	GLN
1	A	346	TYR
1	A	368	GLU
1	A	369	ARG
1	A	413	LEU
1	A	518	TYR
1	A	523	PRO
1	A	644	LEU
1	A	864	LYS
1	A	929	SER
1	A	1135	GLU
2	B	15	VAL
1	A	176	PRO
1	A	296	THR
1	A	412	PRO
1	A	461	GLY
1	A	546	LEU
1	A	923	VAL
1	A	962	ASP
1	A	1138	ARG
1	A	149	ASN

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Mol	Chain	Res	Type
1	A	482	GLU
1	A	750	THR
1	A	802	LEU
1	A	937	PRO
1	A	1045	GLU
1	A	118	THR
1	A	200	LYS
1	A	206	PRO
1	A	489	GLU
1	A	564	ILE
1	A	696	ASN
1	A	148	ASP
1	A	214	ALA
1	A	287	LYS
1	A	618	ILE
1	A	707	ILE
1	A	953	TRP
2	B	16	GLY
1	A	112	ILE
1	A	259	VAL
1	A	371	GLY
1	A	405	PRO
1	A	521	ILE
1	A	801	VAL
1	A	113	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	977/1001 (98%)	836 (86%)	141 (14%)	3 15
2	B	10/10 (100%)	7 (70%)	3 (30%)	0 1
All	All	987/1011 (98%)	843 (85%)	144 (15%)	3 15

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	7	VAL
1	A	25	SER
1	A	27	GLU
1	A	28	ASP
1	A	32	LEU
1	A	49	LEU
1	A	55	VAL
1	A	81	THR
1	A	96	GLU
1	A	98	ILE
1	A	101	ILE
1	A	103	ARG
1	A	109	GLN
1	A	112	ILE
1	A	117	GLU
1	A	125	ASP
1	A	130	MET
1	A	135	LEU
1	A	139	LEU
1	A	147	ARG
1	A	148	ASP
1	A	158	ARG
1	A	159	LEU
1	A	162	LEU
1	A	174	GLN
1	A	177	THR
1	A	190	VAL
1	A	197	LEU
1	A	199	GLU
1	A	235	GLU
1	A	283	LEU
1	A	294	THR
1	A	295	VAL
1	A	298	LYS
1	A	300	LEU
1	A	301	ARG
1	A	302	VAL
1	A	304	LEU
1	A	312	GLU
1	A	318	ASP
1	A	327	ARG
1	A	352	THR

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Mol	Chain	Res	Type
1	A	354	THR
1	A	372	GLN
1	A	374	GLN
1	A	383	LYS
1	A	386	SER
1	A	390	ILE
1	A	392	ASN
1	A	396	ILE
1	A	411	TRP
1	A	415	SER
1	A	427	LEU
1	A	429	PHE
1	A	430	VAL
1	A	439	ASN
1	A	441	GLU
1	A	449	MET
1	A	452	VAL
1	A	460	CYS
1	A	467	GLN
1	A	469	ILE
1	A	472	THR
1	A	476	VAL
1	A	482	GLU
1	A	502	SER
1	A	518	TYR
1	A	519	LEU
1	A	520	GLN
1	A	521	ILE
1	A	530	SER
1	A	543	ILE
1	A	544	THR
1	A	548	ASP
1	A	549	SER
1	A	555	LEU
1	A	567	ARG
1	A	579	LYS
1	A	581	MET
1	A	582	LEU
1	A	587	ILE
1	A	589	ARG
1	A	590	SER
1	A	594	THR

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Mol	Chain	Res	Type
1	A	597	GLU
1	A	602	LEU
1	A	613	TYR
1	A	619	GLU
1	A	620	THR
1	A	640	THR
1	A	653	SER
1	A	663	ASN
1	A	668	PHE
1	A	679	MET
1	A	701	ILE
1	A	706	GLU
1	A	708	GLN
1	A	713	ARG
1	A	728	GLU
1	A	730	SER
1	A	737	SER
1	A	739	ARG
1	A	750	THR
1	A	766	SER
1	A	817	VAL
1	A	823	LYS
1	A	844	LYS
1	A	857	LYS
1	A	858	LEU
1	A	893	TRP
1	A	896	GLU
1	A	899	VAL
1	A	900	ARG
1	A	904	ASN
1	A	910	MET
1	A	917	LYS
1	A	922	LEU
1	A	945	ILE
1	A	960	LEU
1	A	962	ASP
1	A	966	LEU
1	A	969	GLU
1	A	979	LYS
1	A	981	SER
1	A	986	ASP
1	A	992	LEU

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Mol	Chain	Res	Type
1	A	1000	LEU
1	A	1006	VAL
1	A	1013	VAL
1	A	1014	MET
1	A	1029	LEU
1	A	1045	GLU
1	A	1063	LYS
1	A	1064	SER
1	A	1086	THR
1	A	1093	LEU
1	A	1100	ILE
1	A	1127	ASP
1	A	1128	ASP
1	A	1131	LYS
2	B	19	SER
2	B	20	GLN
2	B	23	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	30	ASN
1	A	109	GLN
1	A	189	HIS
1	A	240	HIS
1	A	262	ASN
1	A	267	ASN
1	A	332	GLN
1	A	337	ASN
1	A	370	GLN
1	A	372	GLN
1	A	374	GLN
1	A	432	GLN
1	A	455	GLN
1	A	456	GLN
1	A	504	ASN
1	A	507	GLN
1	A	520	GLN
1	A	790	ASN
1	A	796	GLN
1	A	809	GLN

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Mol	Chain	Res	Type
1	A	905	HIS
1	A	908	ASN
1	A	941	ASN
1	A	978	GLN
1	A	1055	GLN
1	A	1056	ASN
1	A	1070	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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, 95^{th} 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%)	-0.05	42 (3%)	40	16	26, 76, 168, 216	0
2	B	13/13 (100%)	0.87	3 (23%)	0	0	38, 39, 42, 73	0
All	All	1127/1156 (97%)	-0.04	45 (3%)	38	15	26, 75, 168, 216	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	621	GLY	9.9
1	A	462	ASN	8.5
1	A	508	VAL	6.3
1	A	294	THR	6.2
1	A	503	CYS	6.0
1	A	519	LEU	5.7
1	A	502	SER	5.6
1	A	292	ASP	5.4
2	B	25	GLY	5.3
1	A	483	PRO	4.7
1	A	661	SER	4.2
1	A	450	GLY	4.0
1	A	616	LEU	3.8
1	A	486	LEU	3.4
1	A	369	ARG	3.4
1	A	682	LEU	3.3
2	B	24	HIS	3.3
2	B	17	PHE	3.1
1	A	444	GLU	2.7
1	A	528	GLN	2.7
1	A	1122	ARG	2.6
1	A	520	GLN	2.6
1	A	542	ASP	2.6
1	A	289	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	555	LEU	2.5
1	A	506	SER	2.4
1	A	439	ASN	2.4
1	A	446	THR	2.4
1	A	569	LEU	2.4
1	A	468	LEU	2.3
1	A	518	TYR	2.3
1	A	291	MET	2.3
1	A	929	SER	2.3
1	A	293	GLY	2.2
1	A	660	TYR	2.2
1	A	491	LYS	2.2
1	A	630	THR	2.2
1	A	618	ILE	2.1
1	A	561	TRP	2.1
1	A	613	TYR	2.1
1	A	663	ASN	2.1
1	A	918	GLY	2.1
1	A	501	ALA	2.1
1	A	295	VAL	2.0
1	A	586	ILE	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 monosaccharides 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.