



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:53 PM UTC

PDB ID : 3I8E / pdb_00003i8e
Title : Crystal Structure of DDB1 in Complex with the H-Box Motif of WDR42A
Authors : Li, T.; Robert, E.I.; Breugel, P.C.V.; Strubin, M.; Zheng, N.
Deposited on : 2009-07-09
Resolution : 3.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

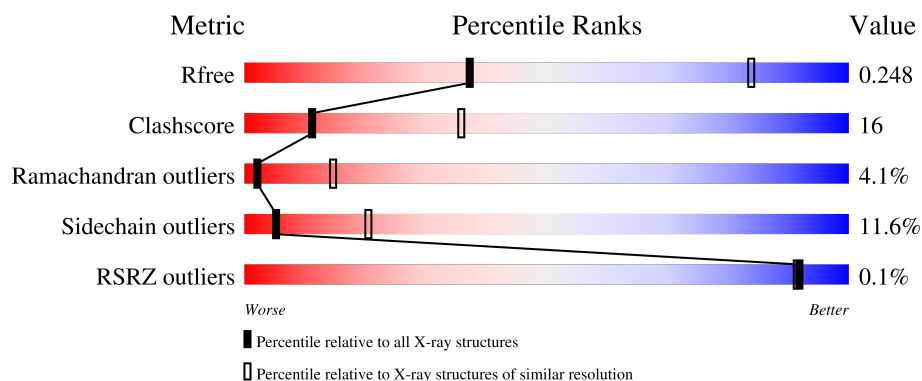
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	
1	B	1143	
2	C	13	
2	D	13	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 17652 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			
1	B	1114	Total	C	N	O	S	0	0	0
			8726	5529	1472	1677	48			

There are 12 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
B	-2	GLY	-	expression tag	UNP Q16531
B	-1	SER	-	expression tag	UNP Q16531
B	0	HIS	-	expression tag	UNP Q16531
B	422	TYR	ASP	SEE REMARK 999	UNP Q16531
B	898	ASP	GLU	SEE REMARK 999	UNP Q16531
B	899	VAL	LEU	SEE REMARK 999	UNP Q16531

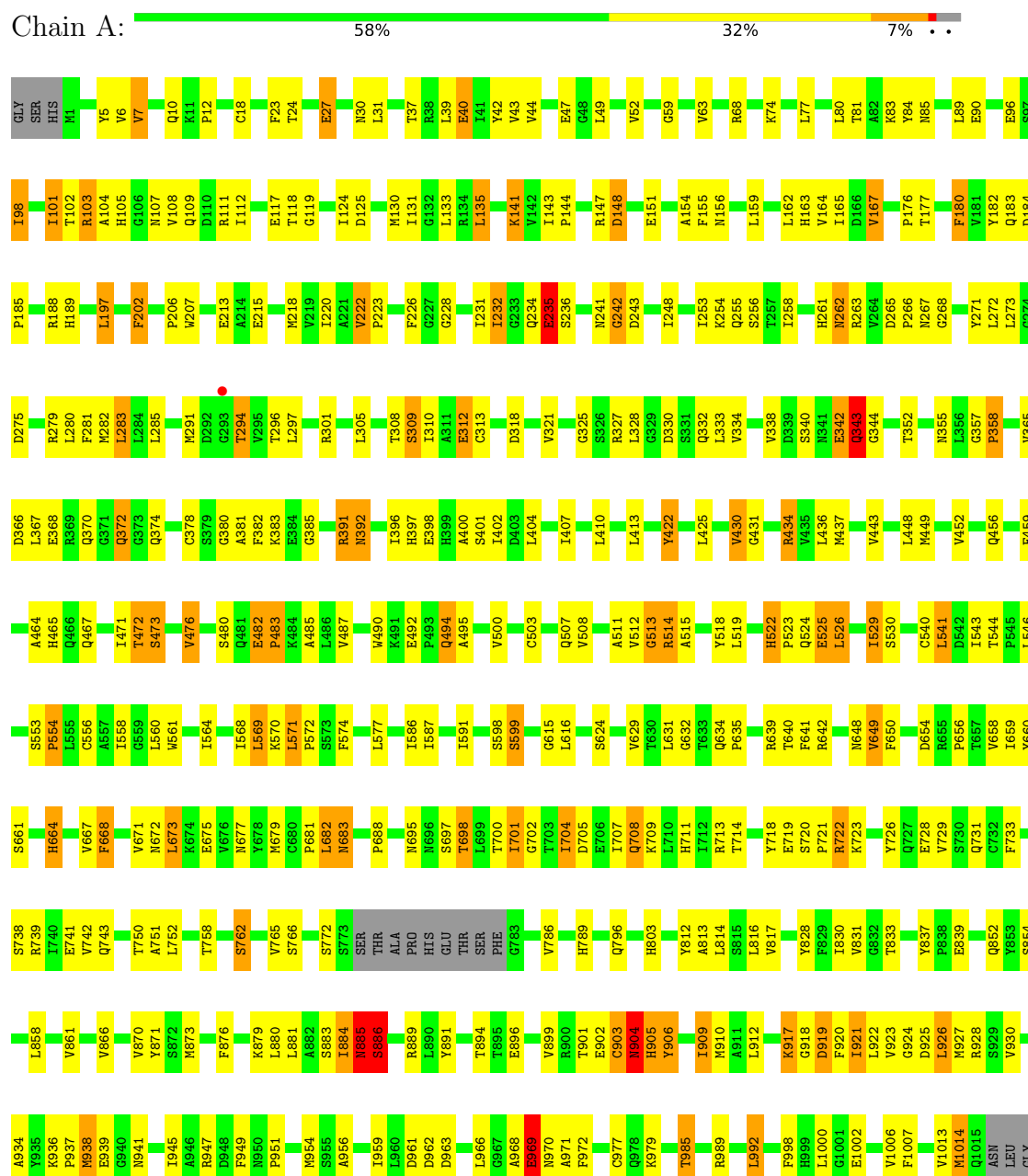
- Molecule 2 is a protein called WD repeat-containing protein 42A.

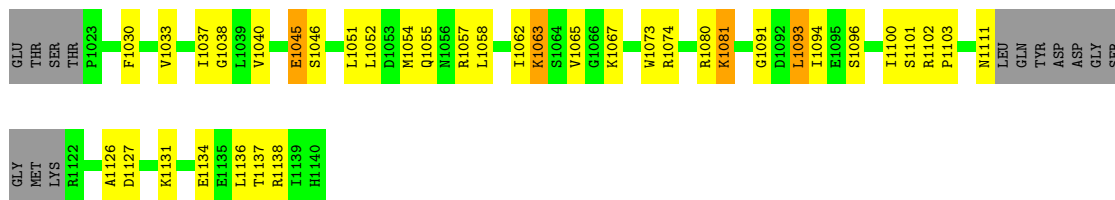
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	13	Total	C	N	O	0	0	0
			100	61	20	19			
2	D	13	Total	C	N	O	0	0	0
			100	61	20	19			

3 Residue-property plots

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

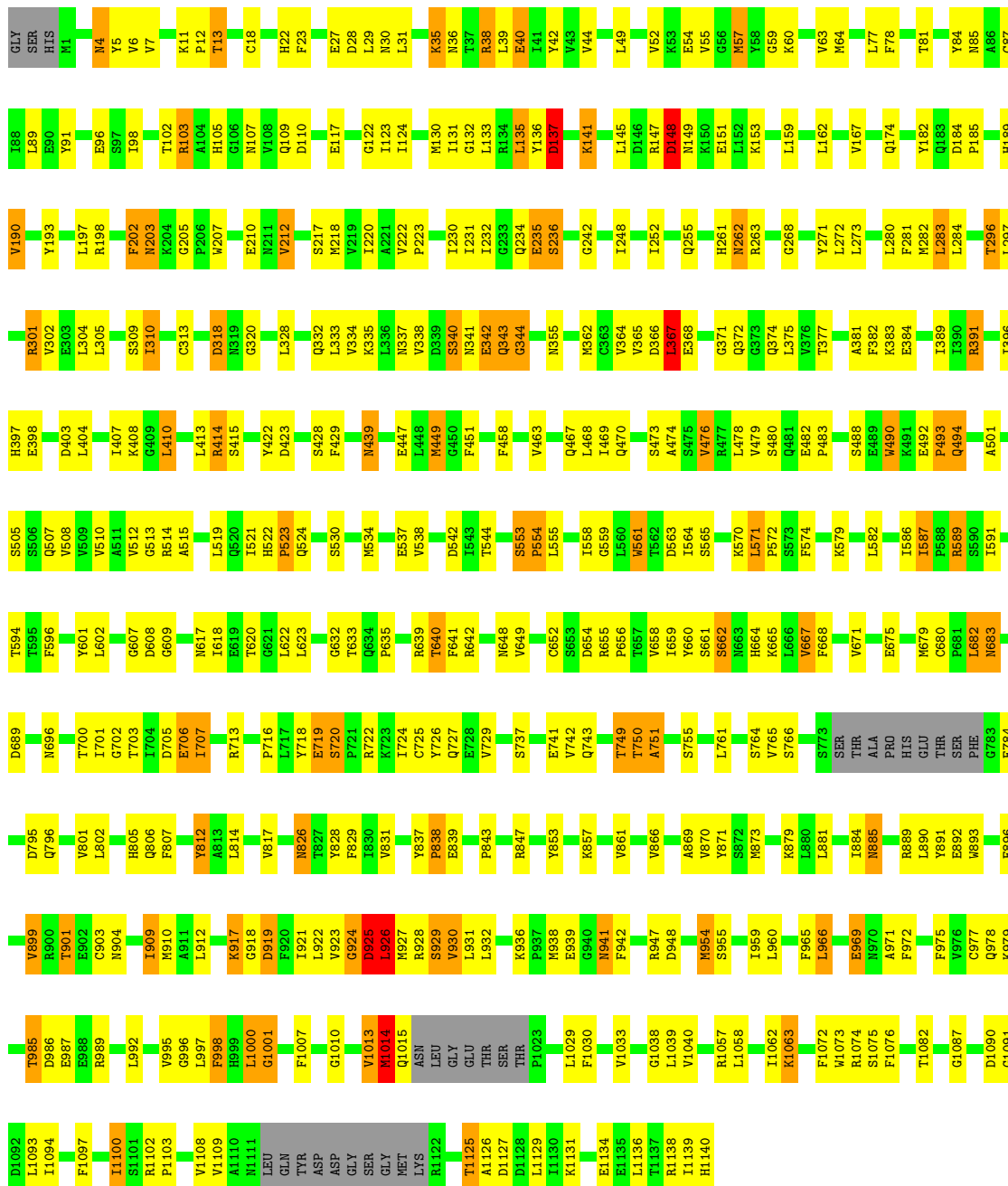
• Molecule 1: DNA damage-binding protein 1





• Molecule 1: DNA damage-binding protein 1

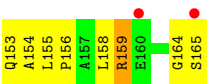
Chain B: 60% 31% 7% ..



• Molecule 2: WD repeat-containing protein 42A



● Molecule 2: WD repeat-containing protein 42A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.14Å 133.81Å 184.00Å 90.00° 90.45° 90.00°	Depositor
Resolution (Å)	49.15 – 3.40 49.15 – 3.40	Depositor EDS
% Data completeness (in resolution range)	87.3 (49.15-3.40) 85.4 (49.15-3.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.260 , 0.338 0.249 , 0.248	Depositor DCC
R_{free} test set	2192 reflections (4.21%)	wwPDB-VP
Wilson B-factor (Å ²)	71.6	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 39.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.407 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17652	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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	0.62	4/8885 (0.0%)	0.91	13/12034 (0.1%)
1	B	0.62	8/8885 (0.1%)	1.00	23/12034 (0.2%)
2	C	0.60	0/100	0.80	0/133
2	D	0.55	0/100	0.72	0/133
All	All	0.62	12/17970 (0.1%)	0.95	36/24334 (0.1%)

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

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

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1013	VAL	CA-C	-14.44	1.34	1.52
1	A	342	GLU	C-N	11.80	1.50	1.33
1	B	367	LEU	C-O	10.62	1.37	1.24
1	A	885	ASN	CA-C	-8.18	1.41	1.52
1	B	1013	VAL	CA-CB	-7.56	1.46	1.54
1	B	924	GLY	N-CA	6.64	1.51	1.45
1	A	343	GLN	C-N	6.24	1.40	1.33
1	A	514	ARG	N-CA	-6.08	1.38	1.46
1	B	1014	MET	CA-C	-5.62	1.45	1.52
1	B	203	ASN	C-N	-5.27	1.26	1.33
1	B	925	ASP	N-CA	5.25	1.52	1.46
1	B	1014	MET	N-CA	-5.07	1.39	1.46

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1013	VAL	N-CA-C	35.21	147.25	113.10
1	B	1013	VAL	CB-CA-C	-27.21	81.00	110.93
1	B	1014	MET	N-CA-CB	-15.67	84.01	110.49
1	B	924	GLY	N-CA-C	7.57	122.09	110.88
1	B	222	VAL	CA-C-N	7.16	128.79	119.84
1	B	222	VAL	C-N-CA	7.16	128.79	119.84
1	A	854	SER	N-CA-C	6.62	114.21	108.78
1	A	969	GLU	N-CA-C	6.58	119.21	108.55
1	A	513	GLY	CA-C-N	6.52	133.99	121.54
1	A	513	GLY	C-N-CA	6.52	133.99	121.54
1	A	561	TRP	N-CA-C	6.49	119.61	111.24
1	A	312	GLU	N-CA-C	-6.39	106.01	113.88
1	B	713	ARG	N-CA-C	6.30	117.94	111.14
1	B	344	GLY	CA-C-N	-6.25	114.45	122.77
1	B	344	GLY	C-N-CA	-6.25	114.45	122.77
1	A	265	ASP	CA-C-N	5.88	125.35	119.24
1	A	265	ASP	C-N-CA	5.88	125.35	119.24
1	A	923	VAL	N-CA-C	5.68	115.81	107.75
1	B	205	GLY	CA-C-N	5.60	126.83	119.84
1	B	205	GLY	C-N-CA	5.60	126.83	119.84
1	B	929	SER	CB-CA-C	-5.53	110.18	116.54
1	B	341	ASN	CA-C-N	5.45	128.57	120.95
1	B	341	ASN	C-N-CA	5.45	128.57	120.95
1	B	930	VAL	N-CA-C	5.38	116.66	108.80
1	B	439	ASN	N-CA-C	-5.37	107.28	112.97
1	A	513	GLY	O-C-N	-5.35	115.75	122.70
1	B	926	LEU	N-CA-C	5.33	118.12	111.24
1	B	1014	MET	N-CA-C	5.31	122.11	110.80
1	B	1001	GLY	N-CA-C	-5.27	107.77	115.72
1	B	724	ILE	N-CA-C	5.25	115.93	108.42
1	A	180	PHE	N-CA-C	5.21	117.00	109.07
1	B	344	GLY	O-C-N	5.14	129.38	122.70
1	A	904	ASN	N-CA-C	5.11	121.69	110.80
1	A	1006	VAL	N-CA-C	5.11	116.01	108.45
1	B	954	MET	N-CA-C	5.05	117.22	110.35
1	B	4	ASN	N-CA-C	5.03	117.44	109.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	886	SER	Mainchain
1	B	367	LEU	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8726	0	8706	288	0
1	B	8726	0	8706	282	0
2	C	100	0	103	7	0
2	D	100	0	103	9	0
All	All	17652	0	17618	574	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 16.

All (574) 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:B:1014:MET:SD	1:B:1015:GLN:HG2	1.79	1.23
1:B:1014:MET:CG	1:B:1015:GLN:H	1.58	1.12
1:B:1014:MET:SD	1:B:1015:GLN:N	2.30	1.04
1:B:706:GLU:O	1:B:707:ILE:HG13	1.57	1.04
1:A:1063:LYS:H	1:A:1063:LYS:HD3	1.18	1.03
1:A:81:THR:HB	1:A:85:ASN:HB2	1.40	1.01
1:A:707:ILE:HG22	1:A:708:GLN:H	1.26	1.00
1:B:1014:MET:HG3	1:B:1015:GLN:H	1.22	1.00
1:B:639:ARG:HD3	1:B:640:THR:H	1.33	0.93
1:B:482:GLU:HB2	1:B:483:PRO:HD3	1.51	0.93
1:B:660:TYR:HB2	1:B:707:ILE:HG21	1.50	0.93
1:B:843:PRO:HG2	1:B:869:ALA:HB2	1.51	0.92
1:B:1063:LYS:H	1:B:1063:LYS:HD3	1.34	0.92
1:B:1014:MET:CG	1:B:1015:GLN:N	2.30	0.90
1:B:910:MET:HE2	1:B:926:LEU:HD22	1.53	0.90
1:A:222:VAL:HG12	1:A:223:PRO:HD2	1.55	0.88
1:B:23:PHE:H	1:B:30:ASN:ND2	1.73	0.84
1:B:660:TYR:HB3	1:B:667:VAL:HB	1.60	0.84
1:A:184:ASP:HB2	1:A:185:PRO:HD2	1.60	0.84
1:A:910:MET:HE2	1:A:926:LEU:HD22	1.61	0.82
2:D:153:GLN:HB2	2:D:156:PRO:HD2	1.60	0.82
1:B:1014:MET:SD	1:B:1015:GLN:CG	2.66	0.82
1:A:81:THR:CB	1:A:85:ASN:HB2	2.09	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:530:SER:HB2	1:B:574:PHE:HE1	1.44	0.82
1:B:391:ARG:HG3	1:B:391:ARG:HH11	1.46	0.81
1:A:541:LEU:HD23	1:A:558:ILE:HG21	1.61	0.81
1:A:884:ILE:N	1:A:884:ILE:HD12	1.96	0.81
1:A:507:GLN:HE22	1:A:553:SER:HB3	1.45	0.80
1:A:1080:ARG:O	1:A:1081:LYS:HB3	1.82	0.79
1:B:81:THR:HG22	1:B:85:ASN:H	1.47	0.79
1:A:391:ARG:HG3	1:A:391:ARG:HH11	1.49	0.78
1:A:615:GLY:H	1:A:624:SER:HB2	1.48	0.78
1:B:941:ASN:HD22	1:B:942:PHE:H	1.28	0.78
1:B:998:PHE:CE1	1:B:1074:ARG:HD2	2.19	0.77
1:A:883:SER:C	1:A:884:ILE:HD12	2.10	0.77
1:B:282:MET:HE2	1:B:305:LEU:HD11	1.65	0.77
1:B:1014:MET:HG3	1:B:1015:GLN:N	1.98	0.77
1:A:905:HIS:O	1:A:906:TYR:HB2	1.84	0.76
1:A:934:ALA:HB2	1:A:945:ILE:HD11	1.68	0.76
1:B:335:LYS:HG3	1:B:337:ASN:HD21	1.50	0.75
1:A:98:ILE:HD13	1:A:98:ILE:H	1.53	0.74
1:A:884:ILE:O	1:A:885:ASN:CB	2.36	0.73
1:B:301:ARG:HG2	1:B:302:VAL:N	2.04	0.73
1:A:59:GLY:HA2	1:A:1073:TRP:CZ3	2.25	0.72
1:A:741:GLU:CG	1:A:750:THR:O	2.38	0.71
1:B:397:HIS:O	1:B:702:GLY:HA3	1.90	0.71
1:B:889:ARG:HG3	1:B:904:ASN:OD1	1.90	0.71
1:B:750:THR:O	1:B:751:ALA:HB2	1.91	0.71
1:B:881:LEU:HD21	1:B:922:LEU:HD21	1.72	0.71
1:A:81:THR:HG22	1:A:83:LYS:H	1.55	0.71
1:A:629:VAL:HG21	1:A:668:PHE:HE2	1.55	0.71
1:B:335:LYS:HG3	1:B:337:ASN:ND2	2.06	0.71
1:A:396:ILE:HG21	1:A:673:LEU:HD11	1.73	0.70
1:B:743:GLN:HB3	1:B:784:GLU:HB2	1.72	0.70
1:A:812:TYR:HB3	2:C:159:ARG:HH22	1.55	0.70
1:A:885:ASN:O	1:A:886:SER:CB	2.36	0.70
1:B:893:TRP:HZ3	1:B:899:VAL:HG22	1.57	0.70
1:A:434:ARG:HG2	1:A:434:ARG:HH11	1.57	0.70
1:A:23:PHE:H	1:A:30:ASN:ND2	1.89	0.70
1:A:570:LYS:HD3	1:A:571:LEU:H	1.57	0.70
1:B:36:ASN:OD1	1:B:60:LYS:HG2	1.92	0.70
1:A:397:HIS:O	1:A:702:GLY:HA3	1.92	0.70
1:A:884:ILE:O	1:A:884:ILE:HG22	1.90	0.69
1:B:538:VAL:HG13	1:B:558:ILE:HD11	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:ASP:OD1	1:B:141:LYS:HE2	1.93	0.69
1:B:917:LYS:O	1:B:919:ASP:N	2.26	0.69
1:B:1063:LYS:HD3	1:B:1063:LYS:N	2.06	0.69
1:A:903:CYS:O	1:A:904:ASN:HB3	1.93	0.68
1:B:909:ILE:HG21	1:B:927:MET:HG2	1.75	0.68
1:B:978:GLN:HE21	1:B:995:VAL:HG11	1.58	0.68
1:A:482:GLU:HB2	1:A:483:PRO:HD3	1.76	0.68
1:B:309:SER:H	1:B:332:GLN:NE2	1.92	0.68
2:C:153:GLN:HB2	2:C:156:PRO:HD2	1.74	0.68
1:A:654:ASP:HA	1:A:675:GLU:HG3	1.77	0.67
1:B:660:TYR:HB2	1:B:707:ILE:CG2	2.24	0.67
1:A:476:VAL:HG13	1:A:490:TRP:HB3	1.75	0.67
1:A:529:ILE:HG22	1:A:530:SER:H	1.60	0.67
1:A:707:ILE:HG22	1:A:708:GLN:N	2.04	0.67
1:B:1102:ARG:N	1:B:1103:PRO:HD2	2.08	0.67
1:A:726:TYR:CE2	1:A:728:GLU:HB2	2.30	0.67
1:B:743:GLN:HG2	1:B:784:GLU:H	1.59	0.67
1:A:697:SER:O	1:A:698:THR:HB	1.94	0.67
1:B:23:PHE:H	1:B:30:ASN:HD22	1.41	0.67
1:B:871:TYR:HE1	1:B:885:ASN:OD1	1.78	0.66
1:B:639:ARG:HD3	1:B:640:THR:N	2.07	0.66
1:B:923:VAL:HA	1:B:931:LEU:O	1.94	0.66
1:B:23:PHE:CE2	1:B:91:TYR:HB2	2.30	0.66
1:A:765:VAL:HG22	1:A:766:SER:H	1.61	0.65
1:B:133:LEU:HD23	1:B:135:LEU:HD21	1.78	0.65
1:A:18:CYS:N	1:A:313:CYS:SG	2.70	0.65
1:A:385:GLY:HA3	1:A:719:GLU:O	1.95	0.65
1:A:529:ILE:HG22	1:A:530:SER:N	2.12	0.65
1:B:103:ARG:HH11	1:B:103:ARG:HB3	1.61	0.65
1:A:813:ALA:HA	1:A:833:THR:HG22	1.78	0.65
1:B:594:THR:HG21	1:B:649:VAL:HG21	1.78	0.65
1:B:596:PHE:HE2	1:B:648:ASN:HA	1.61	0.65
1:B:1057:ARG:HD2	1:B:1108:VAL:O	1.97	0.65
1:A:884:ILE:O	1:A:885:ASN:HB2	1.95	0.65
1:A:881:LEU:HD21	1:A:922:LEU:HD21	1.79	0.64
1:B:1014:MET:SD	1:B:1014:MET:C	2.77	0.64
1:A:500:VAL:HG11	1:A:540:CYS:HA	1.78	0.64
1:A:713:ARG:HH11	1:A:713:ARG:HG2	1.61	0.64
1:A:374:GLN:HE22	1:A:391:ARG:HB2	1.63	0.64
1:B:571:LEU:HB3	1:B:572:PRO:HD3	1.80	0.64
1:A:103:ARG:HH11	1:A:103:ARG:HB3	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:910:MET:HE3	1:B:912:LEU:HD21	1.80	0.64
1:A:1030:PHE:CE2	1:A:1038:GLY:HA3	2.33	0.63
1:A:6:VAL:HG12	1:A:1040:VAL:HG22	1.79	0.63
1:B:81:THR:HG22	1:B:85:ASN:N	2.13	0.63
1:B:410:LEU:HD13	1:B:680:CYS:SG	2.38	0.63
1:A:382:PHE:H	1:A:720:SER:HB3	1.64	0.63
1:A:814:LEU:HD23	2:C:159:ARG:HH21	1.64	0.63
1:B:22:HIS:CD2	1:B:28:ASP:O	2.51	0.63
1:B:340:SER:HB3	1:B:344:GLY:HA2	1.80	0.63
1:B:941:ASN:HD22	1:B:942:PHE:N	1.95	0.63
1:B:1063:LYS:H	1:B:1063:LYS:CD	2.06	0.63
1:A:556:CYS:HB3	1:A:569:LEU:HD12	1.81	0.62
1:A:828:TYR:HE2	1:A:861:VAL:HG21	1.64	0.62
1:A:541:LEU:HD23	1:A:558:ILE:CG2	2.29	0.62
1:B:648:ASN:ND2	1:B:660:TYR:HD1	1.97	0.62
1:B:530:SER:HB2	1:B:574:PHE:CE1	2.30	0.62
1:A:741:GLU:HG2	1:A:750:THR:O	1.99	0.62
1:A:648:ASN:HB3	1:A:659:ILE:O	1.99	0.61
1:A:1013:VAL:O	1:A:1014:MET:HG3	2.00	0.61
1:B:342:GLU:O	1:B:343:GLN:HB2	2.01	0.61
1:B:870:VAL:HG11	1:B:873:MET:HE3	1.82	0.61
1:B:750:THR:O	1:B:751:ALA:CB	2.48	0.61
1:A:507:GLN:NE2	1:A:553:SER:HB3	2.14	0.61
1:A:1030:PHE:CZ	1:A:1038:GLY:HA3	2.35	0.61
1:A:23:PHE:H	1:A:30:ASN:HD22	1.47	0.61
1:A:1102:ARG:N	1:A:1103:PRO:HD2	2.14	0.61
1:A:90:GLU:HB3	1:A:101:ILE:HG22	1.81	0.61
1:A:905:HIS:CG	1:A:906:TYR:H	2.19	0.61
1:A:1063:LYS:H	1:A:1063:LYS:CD	2.02	0.61
1:A:910:MET:HE3	1:A:912:LEU:HD21	1.83	0.60
1:B:507:GLN:HE22	1:B:553:SER:HB3	1.63	0.60
1:A:936:LYS:C	1:A:938:MET:H	2.09	0.60
1:A:884:ILE:N	1:A:884:ILE:CD1	2.64	0.60
1:B:301:ARG:HG2	1:B:302:VAL:H	1.65	0.60
1:A:107:ASN:OD1	1:A:109:GLN:HG2	2.01	0.60
1:A:642:ARG:HH22	1:A:683:ASN:HB2	1.67	0.60
1:A:998:PHE:CZ	1:A:1074:ARG:HD2	2.37	0.59
1:B:997:LEU:HB3	1:B:1076:PHE:CD1	2.37	0.59
1:B:81:THR:CG2	1:B:85:ASN:H	2.15	0.59
1:B:59:GLY:HA2	1:B:1073:TRP:CZ3	2.37	0.59
1:B:570:LYS:HG2	1:B:571:LEU:H	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:719:GLU:HG2	1:B:755:SER:HB3	1.84	0.59
1:B:463:VAL:HG12	1:B:505:SER:HA	1.85	0.59
1:A:368:GLU:CB	1:A:370:GLN:HE21	2.15	0.59
1:B:741:GLU:HG2	1:B:751:ALA:HA	1.83	0.59
1:B:5:TYR:OH	1:B:1091:GLY:HA3	2.03	0.58
1:A:871:TYR:HE1	1:A:885:ASN:HA	1.68	0.58
1:B:1014:MET:CE	1:B:1015:GLN:CG	2.80	0.58
1:B:184:ASP:HB2	1:B:185:PRO:CD	2.33	0.58
1:A:368:GLU:HB3	1:A:370:GLN:HE21	1.68	0.58
1:B:467:GLN:NE2	1:B:524:GLN:HA	2.18	0.58
1:B:889:ARG:HD2	1:B:891:TYR:CE1	2.39	0.58
1:A:750:THR:OG1	1:A:751:ALA:N	2.30	0.58
1:B:765:VAL:HG23	1:B:806:GLN:HB3	1.85	0.58
1:B:997:LEU:O	1:B:998:PHE:HB2	2.02	0.58
1:A:741:GLU:CD	1:A:750:THR:O	2.47	0.57
1:A:814:LEU:CD2	2:C:159:ARG:HH21	2.18	0.57
1:B:310:ILE:HG21	1:B:328:LEU:HD12	1.87	0.57
1:B:938:MET:HE3	1:B:939:GLU:HG2	1.86	0.57
1:B:296:THR:OG1	1:B:297:LEU:N	2.38	0.57
1:A:508:VAL:HB	1:A:519:LEU:HB2	1.86	0.57
1:B:124:ILE:HG12	1:B:131:ILE:HG12	1.86	0.57
1:A:649:VAL:HB	1:A:659:ILE:HB	1.87	0.57
1:B:131:ILE:HG13	1:B:145:LEU:HD12	1.87	0.57
1:A:522:HIS:HB3	1:A:523:PRO:CD	2.35	0.56
1:B:415:SER:H	1:B:423:ASP:HB3	1.71	0.56
1:B:184:ASP:HB2	1:B:185:PRO:HD2	1.87	0.56
1:A:639:ARG:HG3	1:A:640:THR:N	2.21	0.56
1:B:263:ARG:HD3	1:B:268:GLY:HA2	1.88	0.56
1:B:130:MET:HA	1:B:145:LEU:H	1.70	0.56
1:B:234:GLN:O	1:B:235:GLU:HG2	2.06	0.56
1:A:24:THR:H	1:A:30:ASN:ND2	2.04	0.56
1:A:370:GLN:HB2	1:A:372:GLN:HE21	1.71	0.56
1:B:726:TYR:OH	1:B:796:GLN:NE2	2.34	0.56
1:B:1029:LEU:HD23	1:B:1039:LEU:HD13	1.86	0.56
1:A:309:SER:H	1:A:332:GLN:NE2	2.04	0.55
1:A:641:PHE:CZ	1:A:648:ASN:HB2	2.41	0.55
1:A:571:LEU:HB3	1:A:572:PRO:HD3	1.87	0.55
1:A:998:PHE:CE1	1:A:1074:ARG:HD2	2.42	0.55
1:B:719:GLU:OE1	1:B:737:SER:HB2	2.06	0.55
1:B:656:PRO:HB2	1:B:671:VAL:HB	1.86	0.55
1:B:559:GLY:HA2	1:B:565:SER:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1136:LEU:C	1:A:1138:ARG:H	2.14	0.55
1:B:648:ASN:HB3	1:B:659:ILE:O	2.07	0.55
1:B:367:LEU:HB2	1:B:374:GLN:HG3	1.89	0.55
1:B:1007:PHE:CD2	1:B:1030:PHE:HB3	2.42	0.55
1:A:889:ARG:HD2	1:A:891:TYR:CZ	2.42	0.55
1:B:35:LYS:NZ	1:B:40:GLU:OE1	2.33	0.55
1:B:193:TYR:HD2	1:B:202:PHE:HB3	1.72	0.55
1:B:220:ILE:HB	1:B:230:ILE:HB	1.87	0.55
1:A:59:GLY:HA3	1:A:81:THR:HG23	1.89	0.54
1:B:742:VAL:O	1:B:749:THR:HG22	2.07	0.54
1:A:273:LEU:HB2	1:A:281:PHE:HB2	1.89	0.54
1:A:104:ALA:O	1:A:105:HIS:HB3	2.06	0.54
1:B:182:TYR:CZ	1:B:189:HIS:HB2	2.43	0.54
1:B:273:LEU:HB2	1:B:281:PHE:HB2	1.88	0.54
1:B:480:SER:HB3	1:B:483:PRO:HD2	1.88	0.54
1:B:492:GLU:O	1:B:494:GLN:N	2.32	0.54
1:A:568:ILE:HD12	1:A:616:LEU:HD13	1.88	0.54
1:B:936:LYS:HB3	1:B:938:MET:HB3	1.89	0.54
1:B:366:ASP:O	1:B:368:GLU:N	2.41	0.54
1:A:926:LEU:HG	1:A:927:MET:N	2.22	0.54
1:A:271:TYR:HB2	1:A:283:LEU:HB3	1.88	0.54
1:A:642:ARG:NH2	1:A:683:ASN:HB2	2.22	0.54
1:B:563:ASP:HB3	1:B:565:SER:HB3	1.90	0.54
1:B:1014:MET:CE	1:B:1015:GLN:HG3	2.38	0.54
1:B:77:LEU:HB3	1:B:89:LEU:HB2	1.90	0.53
1:B:513:GLY:C	1:B:515:ALA:H	2.16	0.53
1:B:977:CYS:HB3	1:B:992:LEU:HD13	1.89	0.53
1:A:629:VAL:HG21	1:A:668:PHE:CE2	2.40	0.53
1:B:660:TYR:CG	1:B:661:SER:N	2.76	0.53
1:B:1013:VAL:HG23	1:B:1014:MET:N	2.23	0.53
1:B:234:GLN:C	1:B:236:SER:H	2.17	0.53
1:B:682:LEU:O	1:B:683:ASN:HB2	2.07	0.53
1:A:726:TYR:OH	1:A:796:GLN:NE2	2.42	0.53
1:A:396:ILE:HD12	1:A:396:ILE:O	2.08	0.53
1:B:476:VAL:HG13	1:B:490:TRP:HB2	1.91	0.53
1:A:365:VAL:HG21	1:A:733:PHE:HE2	1.73	0.53
1:A:1091:GLY:HA2	1:A:1094:ILE:HB	1.90	0.53
1:B:107:ASN:OD1	1:B:109:GLN:HG2	2.09	0.53
1:B:570:LYS:NZ	1:B:572:PRO:HD2	2.23	0.53
1:A:77:LEU:HD23	1:A:89:LEU:HD12	1.92	0.52
1:A:24:THR:H	1:A:30:ASN:HD21	1.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:164:GLY:O	2:D:165:SER:C	2.51	0.52
1:A:105:HIS:O	1:A:151:GLU:HA	2.10	0.52
1:A:530:SER:HB2	1:A:574:PHE:HE1	1.74	0.52
1:B:1091:GLY:HA2	1:B:1094:ILE:HB	1.90	0.52
1:B:234:GLN:O	1:B:236:SER:N	2.42	0.52
1:B:5:TYR:CZ	1:B:1091:GLY:HA3	2.44	0.52
1:B:133:LEU:HD23	1:B:135:LEU:CD2	2.38	0.52
1:B:261:HIS:O	1:B:262:ASN:HB2	2.10	0.52
1:A:124:ILE:HG12	1:A:131:ILE:HG12	1.92	0.52
1:B:722:ARG:HG3	1:B:722:ARG:HH11	1.75	0.52
1:B:22:HIS:HD2	1:B:28:ASP:O	1.93	0.51
1:B:383:LYS:HE3	1:B:384:GLU:OE2	2.09	0.51
1:A:480:SER:HB2	1:A:483:PRO:HD2	1.92	0.51
1:B:149:ASN:OD1	1:B:153:LYS:N	2.43	0.51
1:A:273:LEU:HD11	1:A:283:LEU:HB2	1.92	0.51
1:B:263:ARG:HB2	1:B:271:TYR:CE2	2.45	0.51
1:B:1129:LEU:C	1:B:1131:LYS:H	2.18	0.51
1:A:130:MET:HE3	1:A:176:PRO:HG2	1.93	0.51
1:A:707:ILE:CG2	1:A:708:GLN:H	2.07	0.51
1:A:939:GLU:HG3	1:A:941:ASN:HB2	1.92	0.51
1:A:682:LEU:O	1:A:683:ASN:HB2	2.11	0.51
1:B:826:ASN:OD1	1:B:826:ASN:N	2.43	0.51
1:A:235:GLU:HB3	1:A:254:LYS:HG3	1.93	0.51
1:A:660:TYR:CD2	1:A:707:ILE:HG12	2.46	0.51
1:B:869:ALA:O	1:B:884:ILE:HA	2.11	0.51
1:A:133:LEU:HD23	1:A:135:LEU:HD21	1.92	0.50
1:A:282:MET:HE2	1:A:305:LEU:HD11	1.92	0.50
1:A:852:GLN:HB2	1:A:861:VAL:HG21	1.93	0.50
1:A:870:VAL:HG11	1:A:873:MET:HE3	1.93	0.50
1:A:1051:LEU:O	1:A:1055:GLN:HB2	2.11	0.50
1:A:977:CYS:HB3	1:A:992:LEU:HD13	1.93	0.50
1:B:930:VAL:HG13	1:B:954:MET:HE2	1.94	0.50
1:A:830:ILE:HD13	1:A:880:LEU:HD13	1.94	0.50
1:B:1134:GLU:C	1:B:1136:LEU:H	2.19	0.50
1:A:313:CYS:HB3	1:A:325:GLY:HA3	1.93	0.50
1:A:40:GLU:HB3	1:A:42:TYR:CE1	2.45	0.50
1:A:378:CYS:HB3	1:A:721:PRO:HG2	1.92	0.50
1:A:814:LEU:HD23	2:C:159:ARG:NH2	2.26	0.50
1:A:881:LEU:HD21	1:A:922:LEU:CD2	2.42	0.50
1:B:537:GLU:O	1:B:561:TRP:HB2	2.11	0.50
1:B:975:PHE:HA	1:B:996:GLY:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:LEU:HD23	1:A:197:LEU:H	1.77	0.50
1:A:658:VAL:HG23	1:A:671:VAL:HG21	1.94	0.50
1:B:23:PHE:CE1	1:B:77:LEU:HB2	2.47	0.50
1:A:383:LYS:HA	1:A:718:TYR:O	2.12	0.50
1:B:648:ASN:HD21	1:B:660:TYR:HD1	1.59	0.50
1:B:992:LEU:O	1:B:992:LEU:HD12	2.12	0.50
1:A:402:ILE:HG12	1:A:443:VAL:HG21	1.94	0.50
1:A:263:ARG:HD3	1:A:268:GLY:HA2	1.94	0.49
1:A:400:ALA:HB3	1:A:701:ILE:HD11	1.94	0.49
1:A:925:ASP:CG	1:A:926:LEU:H	2.20	0.49
1:A:280:LEU:HD13	1:A:308:THR:HG21	1.94	0.49
1:B:655:ARG:HH12	1:B:1138:ARG:HD3	1.77	0.49
1:A:37:THR:HG22	1:A:59:GLY:O	2.12	0.49
1:B:807:PHE:CZ	1:B:831:VAL:HG11	2.48	0.49
1:A:901:THR:HG22	1:A:902:GLU:N	2.27	0.49
1:A:938:MET:HG2	1:A:939:GLU:N	2.27	0.49
1:B:413:LEU:O	1:B:422:TYR:HB3	2.12	0.49
1:B:197:LEU:H	1:B:197:LEU:HD23	1.78	0.49
1:B:271:TYR:HB2	1:B:283:LEU:HB3	1.94	0.49
1:B:480:SER:CB	1:B:483:PRO:HD2	2.43	0.49
1:B:1129:LEU:C	1:B:1131:LYS:N	2.69	0.49
1:B:57:MET:HE2	1:B:57:MET:HB3	1.75	0.49
1:B:476:VAL:HG13	1:B:490:TRP:CB	2.42	0.49
1:B:889:ARG:HD3	1:B:901:THR:HG23	1.94	0.49
1:A:816:LEU:HD13	1:A:831:VAL:HG22	1.95	0.49
1:B:364:VAL:HG21	1:B:1010:GLY:HA3	1.95	0.49
1:A:431:GLY:HA2	1:A:456:GLN:HB2	1.95	0.48
1:B:609:GLY:HA3	1:B:632:GLY:O	2.13	0.48
1:A:1045:GLU:HG2	1:A:1046:SER:N	2.28	0.48
1:B:414:ARG:HA	1:B:423:ASP:H	1.79	0.48
1:B:1030:PHE:CZ	1:B:1038:GLY:HA3	2.48	0.48
1:A:108:VAL:HG11	1:A:143:ILE:HD11	1.96	0.48
1:A:434:ARG:HG2	1:A:434:ARG:NH1	2.26	0.48
1:A:828:TYR:CE2	1:A:861:VAL:HG21	2.47	0.48
1:A:382:PHE:O	1:A:719:GLU:O	2.31	0.48
1:A:634:GLN:HG2	1:A:654:ASP:HB3	1.95	0.48
1:B:193:TYR:CD2	1:B:202:PHE:HB3	2.48	0.48
1:A:167:VAL:HG13	1:A:180:PHE:HB3	1.95	0.48
1:B:11:LYS:NZ	1:B:38:ARG:HH21	2.12	0.48
1:A:742:VAL:HG13	1:A:752:LEU:HD21	1.95	0.48
1:A:143:ILE:HG12	1:A:154:ALA:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:812:TYR:CB	2:C:159:ARG:HH22	2.26	0.48
1:B:63:VAL:HG11	1:B:122:GLY:HA3	1.96	0.48
1:A:261:HIS:O	1:A:262:ASN:HB2	2.13	0.48
1:A:472:THR:O	1:A:473:SER:C	2.56	0.48
1:A:222:VAL:HG23	1:A:228:GLY:O	2.14	0.48
1:A:936:LYS:C	1:A:938:MET:N	2.71	0.48
1:A:507:GLN:HG3	1:A:518:TYR:HE1	1.79	0.47
1:A:969:GLU:O	1:A:971:ALA:N	2.47	0.47
1:A:1093:LEU:O	1:A:1096:SER:HB3	2.13	0.47
1:A:513:GLY:C	1:A:515:ALA:H	2.22	0.47
1:A:570:LYS:HD3	1:A:571:LEU:N	2.27	0.47
1:A:598:SER:O	1:A:599:SER:CB	2.62	0.47
1:A:708:GLN:HE21	1:A:711:HIS:HA	1.79	0.47
1:A:1063:LYS:HD3	1:A:1063:LYS:N	2.03	0.47
1:A:255:GLN:HB2	1:A:279:ARG:HH22	1.79	0.47
1:B:391:ARG:HG3	1:B:391:ARG:NH1	2.22	0.47
1:B:391:ARG:HH11	1:B:391:ARG:CG	2.23	0.47
1:A:1131:LYS:O	1:A:1134:GLU:HB2	2.15	0.47
1:B:596:PHE:HD1	1:B:601:TYR:CE1	2.32	0.47
1:A:197:LEU:H	1:A:197:LEU:CD2	2.27	0.47
1:A:985:THR:HB	1:A:989:ARG:HB2	1.97	0.47
1:A:413:LEU:O	1:A:422:TYR:HB3	2.15	0.47
1:A:634:GLN:HB3	1:A:635:PRO:HD2	1.97	0.47
1:A:912:LEU:HG	1:A:926:LEU:HB2	1.95	0.47
1:A:947:ARG:HG3	1:A:949:PHE:CE1	2.50	0.47
1:B:11:LYS:HB3	1:B:12:PRO:HD2	1.97	0.47
1:B:1109:VAL:HG11	1:B:1125:THR:O	2.14	0.47
1:A:885:ASN:O	1:A:886:SER:HB3	2.15	0.47
1:A:972:PHE:HB3	1:A:1002:GLU:N	2.30	0.47
1:B:795:ASP:HB2	1:B:802:LEU:HD21	1.96	0.47
1:A:530:SER:HB2	1:A:574:PHE:CE1	2.50	0.47
1:A:683:ASN:HA	1:A:688:PRO:HA	1.96	0.47
1:B:18:CYS:N	1:B:313:CYS:SG	2.88	0.47
1:B:727:GLN:HB2	1:B:829:PHE:CE1	2.50	0.47
1:A:404:LEU:HB2	1:A:407:ILE:HD11	1.97	0.47
1:A:909:ILE:HG21	1:A:927:MET:HG2	1.95	0.47
1:A:917:LYS:HB2	1:A:959:ILE:HD13	1.97	0.47
1:A:327:ARG:O	1:A:358:PRO:HD3	2.14	0.46
1:A:365:VAL:HG12	1:A:367:LEU:HG	1.95	0.46
1:A:876:PHE:CZ	1:A:920:PHE:HA	2.50	0.46
1:B:272:LEU:HD22	1:B:280:LEU:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:617:ASN:HD22	1:B:620:THR:HG1	1.63	0.46
1:B:764:SER:O	1:B:805:HIS:HA	2.15	0.46
1:A:266:PRO:C	1:A:268:GLY:H	2.23	0.46
1:A:340:SER:HB3	1:A:344:GLY:HA2	1.96	0.46
1:A:641:PHE:HB3	1:A:679:MET:HE1	1.96	0.46
1:B:375:LEU:O	1:B:389:ILE:HA	2.16	0.46
2:D:153:GLN:HB2	2:D:156:PRO:CD	2.40	0.46
1:A:490:TRP:HB2	1:A:526:LEU:HG	1.97	0.46
1:A:522:HIS:HB3	1:A:523:PRO:HD2	1.97	0.46
1:A:1100:ILE:HG22	1:A:1101:SER:O	2.15	0.46
1:B:148:ASP:OD1	1:B:148:ASP:N	2.48	0.46
1:B:542:ASP:HB2	1:B:591:ILE:HG23	1.97	0.46
1:B:828:TYR:HE2	1:B:861:VAL:HG21	1.80	0.46
1:A:494:GLN:O	1:A:495:ALA:HB3	2.15	0.46
1:A:522:HIS:HB2	1:A:525:GLU:OE1	2.15	0.46
1:B:716:PRO:HB2	1:B:718:TYR:CZ	2.51	0.46
1:A:961:ASP:O	1:A:963:ASP:N	2.49	0.46
1:B:190:VAL:HG13	1:B:210:GLU:HB2	1.97	0.46
1:B:60:LYS:HE2	1:B:972:PHE:CE1	2.51	0.46
1:B:252:ILE:HD11	1:B:304:LEU:HD22	1.98	0.46
1:A:206:PRO:HB2	1:A:207:TRP:CE3	2.51	0.46
1:B:594:THR:O	1:B:601:TYR:HD1	1.99	0.46
1:A:80:LEU:HA	1:A:85:ASN:O	2.16	0.46
1:A:909:ILE:HD12	1:A:928:ARG:HD3	1.98	0.46
1:B:60:LYS:NZ	1:B:1001:GLY:O	2.40	0.46
1:B:81:THR:HG22	1:B:85:ASN:HB2	1.98	0.46
1:A:956:ALA:HB3	1:A:968:ALA:HB3	1.98	0.46
1:A:328:LEU:HD23	1:A:381:ALA:HB3	1.96	0.45
1:A:641:PHE:HD2	1:A:650:PHE:HB2	1.81	0.45
1:A:1074:ARG:HA	1:A:1074:ARG:HD3	1.72	0.45
1:B:382:PHE:H	1:B:720:SER:HB3	1.81	0.45
1:B:662:SER:HB3	1:B:665:LYS:HB2	1.98	0.45
1:A:43:VAL:HG23	1:A:52:VAL:HG21	1.98	0.45
1:A:391:ARG:HH11	1:A:391:ARG:CG	2.26	0.45
1:B:641:PHE:CZ	1:B:648:ASN:HB2	2.52	0.45
1:B:929:SER:OG	1:B:948:ASP:HB3	2.16	0.45
1:A:144:PRO:HG3	1:A:155:PHE:HE2	1.81	0.45
1:A:165:ILE:HD12	1:A:165:ILE:N	2.31	0.45
1:B:36:ASN:HD21	1:B:60:LYS:NZ	2.13	0.45
1:B:912:LEU:HG	1:B:926:LEU:HB2	1.98	0.45
1:B:997:LEU:O	1:B:998:PHE:CB	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:493:PRO:O	1:B:494:GLN:HG3	2.17	0.45
1:B:642:ARG:HH22	1:B:683:ASN:HD22	1.63	0.45
1:B:1097:PHE:O	1:B:1100:ILE:HG13	2.16	0.45
1:A:889:ARG:HG3	1:A:904:ASN:HB3	1.98	0.45
1:B:39:LEU:HB3	1:B:55:VAL:HG23	1.98	0.45
1:B:133:LEU:CD2	1:B:135:LEU:HD21	2.45	0.45
1:A:503:CYS:HA	1:A:543:ILE:HD11	1.98	0.45
1:A:1057:ARG:HH22	1:A:1111:ASN:H	1.65	0.45
1:B:594:THR:HG21	1:B:649:VAL:CG2	2.44	0.45
1:B:722:ARG:CZ	2:D:159:ARG:HG2	2.47	0.45
1:A:63:VAL:HB	1:A:80:LEU:HB3	1.98	0.45
1:A:164:VAL:C	1:A:165:ILE:HD12	2.41	0.45
1:A:226:PHE:HE1	1:A:267:ASN:O	2.00	0.45
1:A:296:THR:OG1	1:A:297:LEU:N	2.48	0.45
1:B:81:THR:CG2	1:B:85:ASN:HB2	2.47	0.45
1:B:132:GLY:O	1:B:133:LEU:HD12	2.17	0.45
1:B:404:LEU:HB2	1:B:407:ILE:HD11	1.98	0.45
1:A:68:ARG:HH11	1:A:74:LYS:HA	1.82	0.44
1:A:464:ALA:O	1:A:465:HIS:HB2	2.17	0.44
1:A:27:GLU:CD	1:A:27:GLU:H	2.26	0.44
1:A:894:THR:OG1	1:A:896:GLU:HB2	2.17	0.44
1:B:659:ILE:HA	1:B:667:VAL:O	2.17	0.44
1:A:886:SER:O	1:A:886:SER:OG	2.30	0.44
1:B:936:LYS:C	1:B:938:MET:N	2.76	0.44
1:B:960:LEU:HD21	1:B:966:LEU:HD12	2.00	0.44
1:B:917:LYS:HB2	1:B:959:ILE:HG21	1.99	0.44
1:A:59:GLY:HA2	1:A:1073:TRP:CE3	2.52	0.44
1:A:391:ARG:HG3	1:A:391:ARG:NH1	2.25	0.44
1:A:492:GLU:OE1	1:A:494:GLN:HB2	2.17	0.44
1:A:677:ASN:HB2	1:A:695:ASN:HA	1.98	0.44
1:A:762:SER:O	1:A:803:HIS:HA	2.18	0.44
1:B:4:ASN:HB2	1:B:1087:GLY:O	2.17	0.44
1:B:890:LEU:HB3	1:B:903:CYS:SG	2.57	0.44
1:B:912:LEU:HD22	2:D:158:LEU:HD11	1.99	0.44
1:B:924:GLY:O	1:B:925:ASP:HB2	2.17	0.44
1:A:333:LEU:HD12	1:A:333:LEU:HA	1.88	0.44
1:B:570:LYS:HZ3	1:B:572:PRO:HD2	1.83	0.44
1:B:607:GLY:C	1:B:609:GLY:H	2.26	0.44
1:A:31:LEU:HB3	1:A:42:TYR:HB2	1.99	0.44
1:A:930:VAL:HG13	1:A:954:MET:HE2	1.99	0.44
1:B:207:TRP:CG	1:B:242:GLY:HA3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:909:ILE:HD13	1:B:928:ARG:HD3	2.00	0.44
1:A:218:MET:HE1	1:A:261:HIS:HD2	1.83	0.44
1:A:234:GLN:C	1:A:235:GLU:HG3	2.43	0.44
1:A:765:VAL:HG22	1:A:766:SER:N	2.31	0.44
1:B:320:GLY:O	1:B:335:LYS:HA	2.18	0.44
1:B:451:PHE:HA	1:B:470:GLN:OE1	2.18	0.43
1:B:501:ALA:HA	1:B:510:VAL:HG12	1.99	0.43
1:B:812:TYR:N	1:B:812:TYR:CD2	2.85	0.43
1:A:77:LEU:HB3	1:A:89:LEU:HB2	1.98	0.43
1:A:487:VAL:HG12	1:A:524:GLN:O	2.18	0.43
1:B:910:MET:HE1	2:D:154:ALA:HB1	1.99	0.43
1:B:928:ARG:NH2	1:B:947:ARG:HH12	2.16	0.43
1:A:342:GLU:O	1:A:343:GLN:HB2	2.18	0.43
1:A:467:GLN:HA	1:A:480:SER:HA	1.98	0.43
1:A:639:ARG:HG3	1:A:640:THR:H	1.82	0.43
1:B:87:CYS:HA	1:B:105:HIS:HA	2.01	0.43
1:A:374:GLN:NE2	1:A:391:ARG:HB2	2.29	0.43
1:B:78:PHE:CD1	1:B:131:ILE:HD13	2.53	0.43
1:B:212:VAL:HG11	1:B:231:ILE:HG21	1.99	0.43
1:B:765:VAL:HG22	1:B:766:SER:H	1.83	0.43
1:A:12:PRO:HG3	1:A:1002:GLU:OE1	2.18	0.43
1:A:667:VAL:HG12	1:A:668:PHE:N	2.34	0.43
1:A:722:ARG:O	1:A:723:LYS:HG2	2.19	0.43
1:B:31:LEU:HD23	1:B:49:LEU:HD21	2.00	0.43
1:A:330:ASP:HA	1:A:355:ASN:HB3	2.01	0.43
1:A:459:PHE:CE2	1:A:503:CYS:HB3	2.54	0.43
1:A:879:LYS:HB3	1:A:891:TYR:O	2.19	0.43
1:B:929:SER:OG	1:B:930:VAL:N	2.51	0.43
1:A:382:PHE:N	1:A:720:SER:HB3	2.33	0.43
1:A:40:GLU:HB3	1:A:42:TYR:HE1	1.83	0.43
1:B:59:GLY:HA3	1:B:81:THR:OG1	2.18	0.43
1:B:396:ILE:HD12	1:B:396:ILE:O	2.18	0.43
1:B:408:LYS:C	1:B:428:SER:HB3	2.44	0.43
1:B:507:GLN:NE2	1:B:553:SER:HB3	2.31	0.43
1:B:553:SER:HA	1:B:554:PRO:HD3	1.89	0.43
1:B:654:ASP:HA	1:B:675:GLU:HG3	2.01	0.43
1:B:969:GLU:OE2	1:B:971:ALA:HB3	2.19	0.43
1:A:10:GLN:HB3	1:A:1037:ILE:HB	2.01	0.43
1:A:656:PRO:HB2	1:A:671:VAL:HB	2.01	0.43
1:A:873:MET:HA	1:A:881:LEU:O	2.19	0.43
1:B:362:MET:HB3	1:B:377:THR:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:978:GLN:NE2	1:B:995:VAL:HG11	2.28	0.43
1:A:263:ARG:HB2	1:A:271:TYR:CE2	2.54	0.42
1:B:5:TYR:CE2	1:B:7:VAL:HG23	2.54	0.42
1:B:837:TYR:HA	1:B:838:PRO:HD3	1.91	0.42
1:B:853:TYR:HA	1:B:857:LYS:O	2.19	0.42
1:B:889:ARG:HD2	1:B:891:TYR:CZ	2.55	0.42
1:B:924:GLY:O	1:B:925:ASP:CB	2.67	0.42
1:A:392:ASN:HD21	1:A:709:LYS:HE3	1.84	0.42
1:A:697:SER:O	1:A:698:THR:CB	2.66	0.42
1:B:40:GLU:HB3	1:B:42:TYR:CE1	2.55	0.42
1:B:716:PRO:HB2	1:B:718:TYR:CE1	2.53	0.42
1:A:133:LEU:HB2	1:A:141:LYS:HB3	2.02	0.42
1:A:165:ILE:HG12	1:A:188:ARG:HH21	1.83	0.42
1:A:182:TYR:CZ	1:A:189:HIS:HB2	2.53	0.42
1:A:641:PHE:HA	1:A:681:PRO:HG3	2.02	0.42
1:B:458:PHE:HE2	1:B:473:SER:HA	1.85	0.42
1:B:909:ILE:HG21	1:B:927:MET:CG	2.45	0.42
1:A:68:ARG:HD3	1:A:74:LYS:C	2.44	0.42
1:A:1065:VAL:C	1:A:1067:LYS:H	2.26	0.42
1:B:722:ARG:HH12	2:D:159:ARG:HH11	1.67	0.42
1:B:722:ARG:NH1	2:D:159:ARG:HH11	2.16	0.42
1:A:471:ILE:HG23	1:A:476:VAL:HB	2.02	0.42
1:A:658:VAL:HG23	1:A:671:VAL:CG2	2.49	0.42
1:B:812:TYR:N	1:B:812:TYR:HD2	2.17	0.42
1:B:1000:LEU:HD11	1:B:1030:PHE:CE1	2.55	0.42
1:B:6:VAL:HG23	1:B:1090:ASP:HA	2.01	0.42
1:A:425:LEU:O	1:A:436:LEU:HB2	2.19	0.42
1:B:507:GLN:HE22	1:B:553:SER:N	2.18	0.42
1:B:522:HIS:O	1:B:523:PRO:C	2.62	0.42
1:B:985:THR:HB	1:B:989:ARG:HB2	2.02	0.42
1:A:261:HIS:HA	1:A:272:LEU:O	2.19	0.42
1:A:632:GLY:HA3	1:A:654:ASP:OD1	2.19	0.42
1:A:698:THR:O	1:A:698:THR:HG22	2.20	0.42
1:B:478:LEU:HD22	1:B:488:SER:HB3	2.01	0.42
1:B:893:TRP:CZ3	1:B:899:VAL:HG22	2.46	0.42
1:A:117:GLU:C	1:A:119:GLY:H	2.27	0.42
1:A:511:ALA:HA	1:A:515:ALA:O	2.20	0.42
1:B:13:THR:HB	1:B:355:ASN:HA	2.01	0.42
1:B:463:VAL:HG11	1:B:521:ILE:HD12	2.02	0.42
1:A:328:LEU:O	1:A:380:GLY:HA2	2.20	0.42
1:A:437:MET:HE1	1:A:448:LEU:HD13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:LEU:HD13	1:A:526:LEU:HD11	2.02	0.42
1:A:704:ILE:HD13	1:A:704:ILE:HA	1.83	0.42
1:A:1136:LEU:C	1:A:1138:ARG:N	2.77	0.42
1:B:608:ASP:OD2	1:B:608:ASP:N	2.53	0.42
1:B:932:LEU:HD13	1:B:965:PHE:CZ	2.55	0.42
1:A:947:ARG:HE	1:A:947:ARG:HB2	1.60	0.41
1:B:6:VAL:HG12	1:B:1040:VAL:HG22	2.02	0.41
1:B:468:LEU:HB2	1:B:479:VAL:HB	2.01	0.41
1:A:5:TYR:CZ	1:A:1091:GLY:HA3	2.55	0.41
1:A:553:SER:HA	1:A:554:PRO:HD3	1.91	0.41
1:A:904:ASN:O	1:A:905:HIS:C	2.63	0.41
1:A:924:GLY:HA2	1:A:930:VAL:HG12	2.02	0.41
1:A:1007:PHE:CD2	1:A:1030:PHE:HB3	2.55	0.41
1:B:301:ARG:CG	1:B:302:VAL:N	2.79	0.41
1:B:564:ILE:O	1:B:582:LEU:HB2	2.20	0.41
1:A:220:ILE:HD12	1:A:232:ILE:HD11	2.02	0.41
1:A:241:ASN:O	1:A:242:GLY:C	2.62	0.41
1:A:972:PHE:HB3	1:A:1002:GLU:H	1.84	0.41
1:B:706:GLU:C	1:B:707:ILE:HG13	2.38	0.41
1:B:1058:LEU:HD22	1:B:1062:ILE:HD12	2.02	0.41
1:B:1072:PHE:O	1:B:1075:SER:HB2	2.20	0.41
1:A:5:TYR:CE1	1:A:1091:GLY:HA3	2.55	0.41
1:A:789:HIS:CE1	2:C:159:ARG:HH12	2.38	0.41
1:B:301:ARG:HE	1:B:301:ARG:HB3	1.73	0.41
1:A:47:GLU:C	1:A:47:GLU:CD	2.88	0.41
1:A:342:GLU:HA	1:A:342:GLU:OE1	2.20	0.41
1:B:6:VAL:CG1	1:B:1040:VAL:HG22	2.51	0.41
1:A:84:TYR:CB	1:A:109:GLN:HB3	2.51	0.41
1:A:141:LYS:HE2	1:A:156:ASN:HD21	1.85	0.41
1:A:177:THR:HG21	1:A:206:PRO:HD3	2.02	0.41
1:A:1058:LEU:HD22	1:A:1062:ILE:HD11	2.02	0.41
1:B:60:LYS:HE2	1:B:972:PHE:CD1	2.56	0.41
1:B:81:THR:O	1:B:84:TYR:N	2.47	0.41
1:B:508:VAL:HB	1:B:519:LEU:HB2	2.03	0.41
1:B:761:LEU:HD12	1:B:802:LEU:HA	2.03	0.41
1:B:871:TYR:CE1	1:B:885:ASN:OD1	2.66	0.41
1:B:879:LYS:HD3	1:B:892:GLU:HG2	2.01	0.41
1:B:381:ALA:O	1:B:382:PHE:C	2.63	0.41
1:B:561:TRP:CE3	1:B:587:ILE:HG21	2.56	0.41
1:B:589:ARG:HG3	1:B:635:PRO:HB3	2.03	0.41
1:A:905:HIS:CG	1:A:906:TYR:N	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:PHE:HD2	1:A:202:PHE:HA	1.80	0.40
1:A:917:LYS:O	1:A:919:ASP:N	2.54	0.40
1:A:921:ILE:C	1:A:922:LEU:HD12	2.47	0.40
1:B:29:LEU:HD23	1:B:44:VAL:HG21	2.03	0.40
1:B:136:TYR:O	1:B:137:ASP:C	2.63	0.40
1:A:256:SER:HB3	1:A:275:ASP:OD2	2.21	0.40
1:A:366:ASP:C	1:A:368:GLU:H	2.28	0.40
1:A:367:LEU:CD2	1:A:796:GLN:HB2	2.52	0.40
1:A:213:GLU:HG3	1:A:215:GLU:H	1.87	0.40
1:B:5:TYR:CE2	1:B:7:VAL:CG2	3.04	0.40
1:B:64:MET:HG3	1:B:77:LEU:HD11	2.02	0.40
1:B:217:SER:O	1:B:218:MET:HG2	2.21	0.40
1:B:365:VAL:HG12	1:B:367:LEU:H	1.86	0.40
1:B:812:TYR:HD1	2:D:159:ARG:CZ	2.33	0.40
1:B:939:GLU:HG3	1:B:941:ASN:HB2	2.02	0.40
1:A:5:TYR:CE2	1:A:7:VAL:HG22	2.57	0.40
1:B:38:ARG:HD2	1:B:38:ARG:HA	1.72	0.40
1:B:1039:LEU:HD22	1:B:1140:HIS:HB3	2.03	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%)	921 (83%)	134 (12%)	51 (5%)	2	12
1	B	1106/1143 (97%)	906 (82%)	161 (15%)	39 (4%)	3	16
2	C	11/13 (85%)	9 (82%)	2 (18%)	0	100	100
2	D	11/13 (85%)	10 (91%)	0	1 (9%)	0	3
All	All	2234/2312 (97%)	1846 (83%)	297 (13%)	91 (4%)	2	15

All (91) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	514	ARG
1	A	599	SER
1	A	683	ASN
1	A	886	SER
1	A	904	ASN
1	A	906	TYR
1	A	918	GLY
1	A	970	ASN
1	B	148	ASP
1	B	223	PRO
1	B	367	LEU
1	B	662	SER
1	B	683	ASN
1	B	689	ASP
1	B	706	GLU
1	B	751	ALA
1	B	918	GLY
1	B	925	ASP
1	B	1014	MET
1	A	148	ASP
1	A	235	GLU
1	A	242	GLY
1	A	310	ILE
1	A	554	PRO
1	A	664	HIS
1	A	705	ASP
1	A	903	CYS
1	A	938	MET
1	A	1081	LYS
1	A	1126	ALA
1	B	494	GLN
1	B	523	PRO
1	B	554	PRO
1	B	707	ILE
1	B	919	ASP
1	B	998	PHE
1	B	1126	ALA
1	A	163	HIS
1	A	343	GLN
1	A	422	TYR
1	A	473	SER
1	A	483	PRO
1	A	485	ALA

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Mol	Chain	Res	Type
1	A	708	GLN
1	A	885	ASN
1	A	919	ASP
1	B	35	LYS
1	B	255	GLN
1	B	262	ASN
1	B	318	ASP
1	B	343	GLN
1	B	449	MET
1	B	474	ALA
1	B	514	ARG
1	A	357	GLY
1	A	672	ASN
1	A	698	THR
1	A	714	THR
1	A	905	HIS
1	A	962	ASP
1	A	1137	THR
1	B	235	GLU
1	B	571	LEU
1	B	664	HIS
1	B	705	ASP
1	B	885	ASN
1	A	262	ASN
1	A	294	THR
1	A	318	ASP
1	A	430	VAL
1	A	494	GLN
1	A	529	ILE
1	A	577	LEU
1	A	772	SER
1	A	951	PRO
1	B	696	ASN
1	B	987	GLU
1	B	1125	THR
2	D	155	LEU
1	A	522	HIS
1	A	546	LEU
1	B	137	ASP
1	B	493	PRO
1	A	937	PRO
1	A	358	PRO

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Mol	Chain	Res	Type
1	A	564	ILE
1	B	310	ILE
1	A	482	GLU
1	A	571	LEU
1	B	371	GLY
1	B	838	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%)	865 (88%)	112 (12%)	5	20
1	B	977/1001 (98%)	862 (88%)	115 (12%)	5	20
2	C	10/10 (100%)	10 (100%)	0	100	100
2	D	10/10 (100%)	9 (90%)	1 (10%)	7	26
All	All	1974/2022 (98%)	1746 (88%)	228 (12%)	5	20

All (228) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	27	GLU
1	A	39	LEU
1	A	40	GLU
1	A	44	VAL
1	A	49	LEU
1	A	96	GLU
1	A	98	ILE
1	A	101	ILE
1	A	102	THR
1	A	103	ARG
1	A	111	ARG
1	A	112	ILE
1	A	118	THR
1	A	125	ASP

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Mol	Chain	Res	Type
1	A	135	LEU
1	A	141	LYS
1	A	147	ARG
1	A	148	ASP
1	A	159	LEU
1	A	162	LEU
1	A	167	VAL
1	A	183	GLN
1	A	197	LEU
1	A	202	PHE
1	A	222	VAL
1	A	231	ILE
1	A	232	ILE
1	A	235	GLU
1	A	236	SER
1	A	243	ASP
1	A	248	ILE
1	A	253	ILE
1	A	258	ILE
1	A	283	LEU
1	A	285	LEU
1	A	291	MET
1	A	294	THR
1	A	301	ARG
1	A	309	SER
1	A	312	GLU
1	A	321	VAL
1	A	334	VAL
1	A	338	VAL
1	A	352	THR
1	A	372	GLN
1	A	391	ARG
1	A	392	ASN
1	A	398	GLU
1	A	401	SER
1	A	410	LEU
1	A	430	VAL
1	A	434	ARG
1	A	449	MET
1	A	452	VAL
1	A	472	THR
1	A	476	VAL

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Mol	Chain	Res	Type
1	A	512	VAL
1	A	525	GLU
1	A	526	LEU
1	A	541	LEU
1	A	544	THR
1	A	560	LEU
1	A	569	LEU
1	A	586	ILE
1	A	587	ILE
1	A	591	ILE
1	A	631	LEU
1	A	649	VAL
1	A	661	SER
1	A	664	HIS
1	A	668	PHE
1	A	673	LEU
1	A	682	LEU
1	A	700	THR
1	A	701	ILE
1	A	704	ILE
1	A	722	ARG
1	A	729	VAL
1	A	731	GLN
1	A	738	SER
1	A	739	ARG
1	A	743	GLN
1	A	758	THR
1	A	762	SER
1	A	786	VAL
1	A	817	VAL
1	A	837	TYR
1	A	839	GLU
1	A	858	LEU
1	A	866	VAL
1	A	884	ILE
1	A	886	SER
1	A	899	VAL
1	A	909	ILE
1	A	917	LYS
1	A	921	ILE
1	A	926	LEU
1	A	966	LEU

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Mol	Chain	Res	Type
1	A	969	GLU
1	A	979	LYS
1	A	985	THR
1	A	992	LEU
1	A	1000	LEU
1	A	1014	MET
1	A	1033	VAL
1	A	1045	GLU
1	A	1052	LEU
1	A	1054	MET
1	A	1063	LYS
1	A	1093	LEU
1	A	1127	ASP
1	B	13	THR
1	B	27	GLU
1	B	38	ARG
1	B	40	GLU
1	B	52	VAL
1	B	54	GLU
1	B	57	MET
1	B	96	GLU
1	B	98	ILE
1	B	102	THR
1	B	103	ARG
1	B	117	GLU
1	B	123	ILE
1	B	135	LEU
1	B	137	ASP
1	B	141	LYS
1	B	147	ARG
1	B	148	ASP
1	B	151	GLU
1	B	159	LEU
1	B	162	LEU
1	B	167	VAL
1	B	174	GLN
1	B	190	VAL
1	B	198	ARG
1	B	202	PHE
1	B	203	ASN
1	B	212	VAL
1	B	232	ILE

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Mol	Chain	Res	Type
1	B	236	SER
1	B	248	ILE
1	B	283	LEU
1	B	284	LEU
1	B	296	THR
1	B	301	ARG
1	B	318	ASP
1	B	333	LEU
1	B	334	VAL
1	B	338	VAL
1	B	340	SER
1	B	342	GLU
1	B	372	GLN
1	B	391	ARG
1	B	398	GLU
1	B	403	ASP
1	B	410	LEU
1	B	414	ARG
1	B	429	PHE
1	B	439	ASN
1	B	447	GLU
1	B	449	MET
1	B	469	ILE
1	B	476	VAL
1	B	490	TRP
1	B	512	VAL
1	B	534	MET
1	B	544	THR
1	B	553	SER
1	B	555	LEU
1	B	561	TRP
1	B	579	LYS
1	B	586	ILE
1	B	587	ILE
1	B	589	ARG
1	B	602	LEU
1	B	618	ILE
1	B	622	LEU
1	B	623	LEU
1	B	633	THR
1	B	640	THR
1	B	652	CYS

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Mol	Chain	Res	Type
1	B	658	VAL
1	B	667	VAL
1	B	668	PHE
1	B	679	MET
1	B	682	LEU
1	B	700	THR
1	B	701	ILE
1	B	703	THR
1	B	719	GLU
1	B	720	SER
1	B	725	CYS
1	B	729	VAL
1	B	749	THR
1	B	750	THR
1	B	801	VAL
1	B	812	TYR
1	B	814	LEU
1	B	817	VAL
1	B	826	ASN
1	B	839	GLU
1	B	847	ARG
1	B	866	VAL
1	B	896	GLU
1	B	899	VAL
1	B	901	THR
1	B	909	ILE
1	B	917	LYS
1	B	921	ILE
1	B	926	LEU
1	B	941	ASN
1	B	955	SER
1	B	966	LEU
1	B	969	GLU
1	B	979	LYS
1	B	985	THR
1	B	986	ASP
1	B	1000	LEU
1	B	1033	VAL
1	B	1063	LYS
1	B	1082	THR
1	B	1093	LEU
1	B	1100	ILE

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Mol	Chain	Res	Type
1	B	1127	ASP
1	B	1139	ILE
2	D	159	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	16	ASN
1	A	30	ASN
1	A	109	GLN
1	A	156	ASN
1	A	189	HIS
1	A	261	HIS
1	A	332	GLN
1	A	370	GLN
1	A	372	GLN
1	A	392	ASN
1	A	455	GLN
1	A	462	ASN
1	A	481	GLN
1	A	494	GLN
1	A	634	GLN
1	A	683	ASN
1	A	708	GLN
1	A	727	GLN
1	A	731	GLN
1	A	743	GLN
1	A	759	GLN
1	A	796	GLN
1	A	885	ASN
1	A	978	GLN
1	A	1055	GLN
1	A	1056	ASN
1	A	1059	ASN
1	A	1070	HIS
1	A	1106	GLN
1	B	4	ASN
1	B	22	HIS
1	B	30	ASN
1	B	36	ASN
1	B	156	ASN

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Mol	Chain	Res	Type
1	B	262	ASN
1	B	267	ASN
1	B	332	GLN
1	B	337	ASN
1	B	392	ASN
1	B	456	GLN
1	B	467	GLN
1	B	507	GLN
1	B	524	GLN
1	B	617	ASN
1	B	648	ASN
1	B	670	ASN
1	B	683	ASN
1	B	731	GLN
1	B	743	GLN
1	B	796	GLN
1	B	805	HIS
1	B	809	GLN
1	B	852	GLN
1	B	907	ASN
1	B	908	ASN
1	B	941	ASN
1	B	950	ASN
1	B	978	GLN
1	B	993	GLN
1	B	1056	ASN
1	B	1140	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-1.30	1 (0%) 92 91	39, 68, 118, 134	0
1	B	1114/1143 (97%)	-1.30	0 100 100	42, 69, 120, 137	0
2	C	13/13 (100%)	-0.65	0 100 100	81, 84, 86, 86	0
2	D	13/13 (100%)	0.22	2 (15%) 5 7	100, 103, 104, 104	0
All	All	2254/2312 (97%)	-1.28	3 (0%) 92 91	39, 68, 120, 137	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	160	GLU	3.5
1	A	293	GLY	3.3
2	D	165	SER	2.4

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.