Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2023 – 02:30 PM EDT

PDB ID	:	3I8C
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:

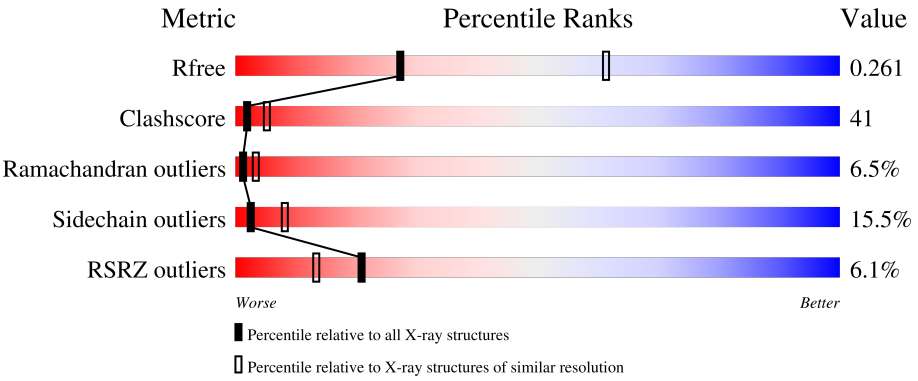
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1143	6% 43% 42% 12%
2	B	13	15% 8% 69% 23%

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	1114	8726	5529	1472	1677	48	0	0	0

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.

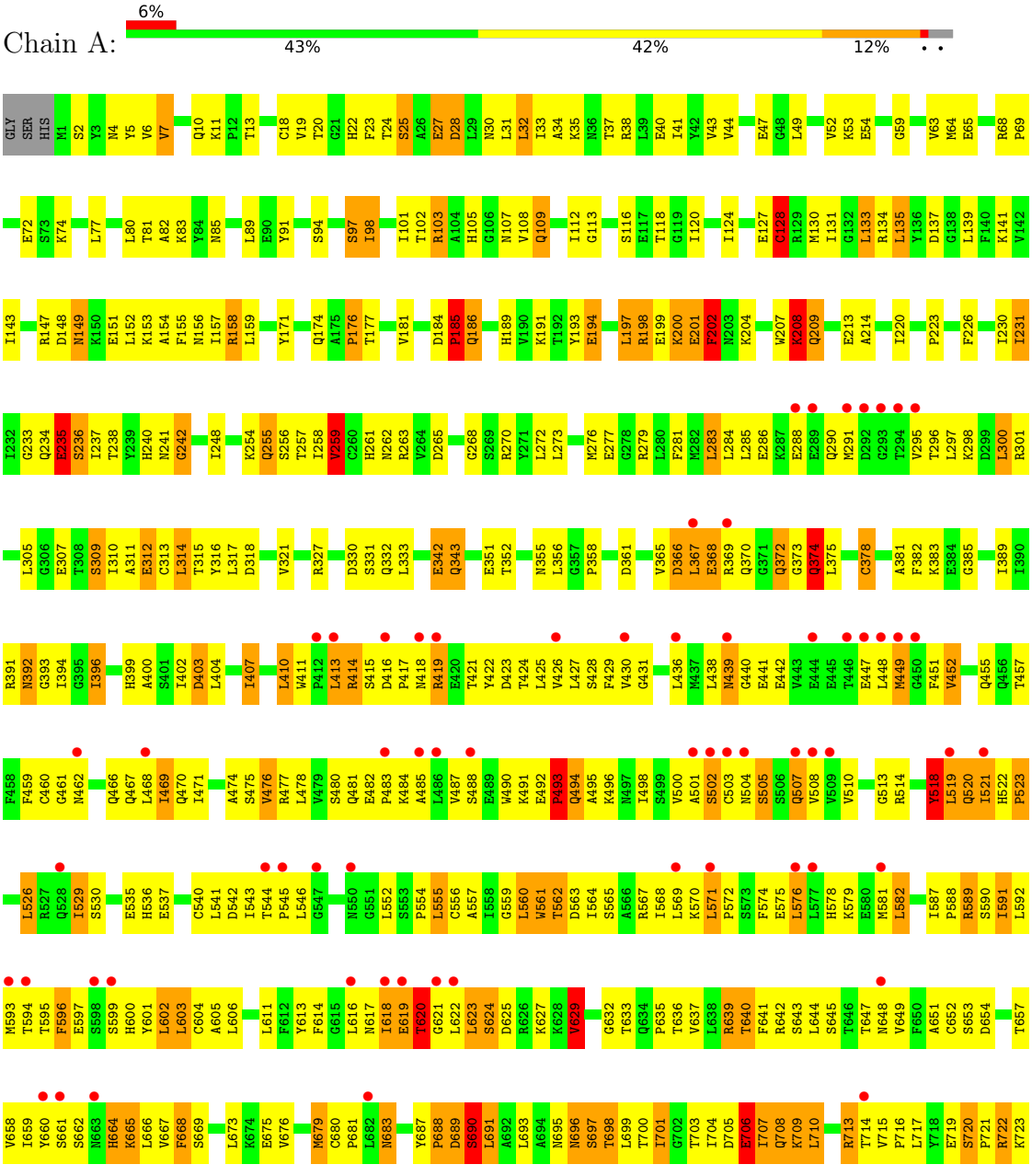
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	13	99	61	19	18	1	0	0	0

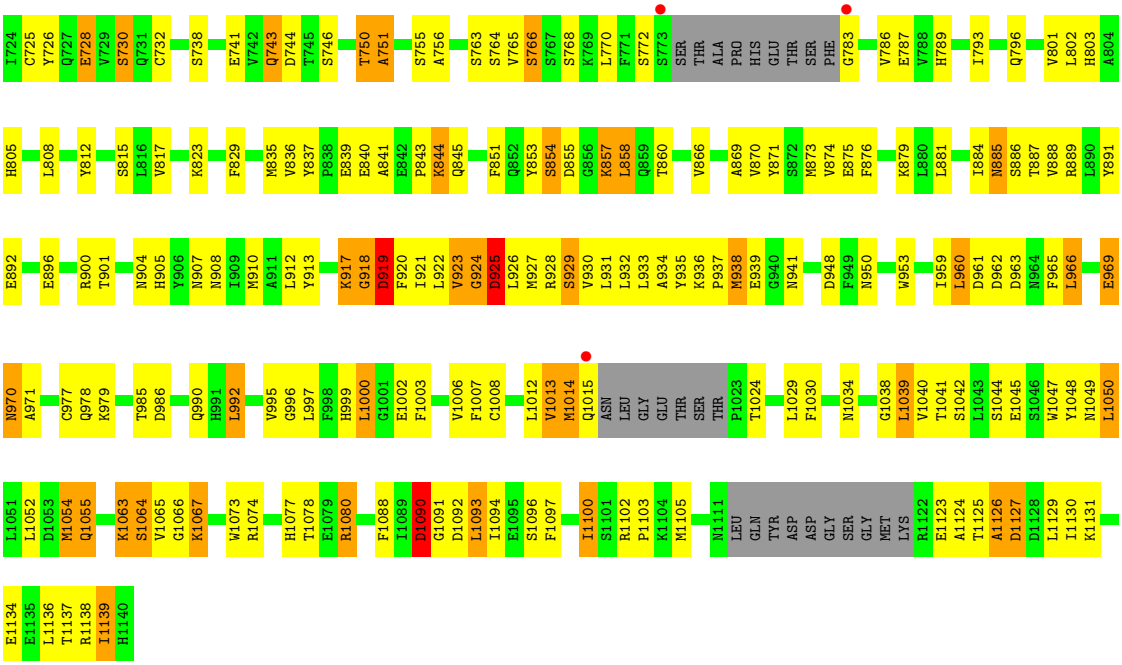
3 Residue-property plots (i)

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

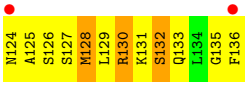
Chain A:





• Molecule 2: WD repeat-containing protein 21A

Chain B:



4 Data and refinement statistics (i)

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 45.26 – 2.65	Depositor EDS
% Data completeness (in resolution range)	80.9 (45.88-2.80) 71.2 (45.26-2.65)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (4.75%)	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]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	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.*

[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	0.77	12/8885 (0.1%)	0.91	20/12034 (0.2%)
2	B	1.30	0/99	1.39	2/129 (1.6%)
All	All	0.78	12/8984 (0.1%)	0.91	22/12163 (0.2%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	725	CYS	CB-SG	-11.35	1.62	1.82
1	A	697	SER	CB-OG	-8.31	1.31	1.42
1	A	202	PHE	C-O	7.64	1.37	1.23
1	A	919	ASP	N-CA	-7.54	1.31	1.46
1	A	697	SER	C-O	-6.33	1.11	1.23
1	A	194	GLU	C-O	-5.77	1.12	1.23
1	A	128	CYS	CB-SG	-5.76	1.72	1.81
1	A	977	CYS	CB-SG	-5.63	1.72	1.81
1	A	378	CYS	CB-SG	-5.50	1.72	1.81
1	A	925	ASP	N-CA	5.22	1.56	1.46
1	A	913	TYR	CE1-CZ	5.14	1.45	1.38
1	A	924	GLY	N-CA	5.05	1.53	1.46

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	494	GLN	N-CA-CB	-14.44	84.61	110.60
1	A	186	GLN	N-CA-CB	-12.82	87.52	110.60
1	A	330	ASP	CB-CG-OD1	11.68	128.81	118.30
1	A	918	GLY	O-C-N	-10.43	106.01	122.70
1	A	514	ARG	N-CA-CB	-10.02	92.56	110.60
1	A	918	GLY	C-N-CA	9.49	145.43	121.70
1	A	690	SER	N-CA-CB	7.17	121.25	110.50
1	A	330	ASP	CB-CG-OD2	-7.12	111.89	118.30
1	A	918	GLY	CA-C-N	6.91	132.40	117.20
1	A	185	PRO	N-CA-C	6.62	129.31	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	132	SER	C-N-CA	-6.61	105.16	121.70
1	A	1090	ASP	N-CA-CB	5.74	120.93	110.60
1	A	960	LEU	CB-CG-CD1	-5.64	101.41	111.00
1	A	494	GLN	N-CA-C	5.44	125.69	111.00
1	A	493	PRO	CB-CA-C	5.43	125.57	112.00
2	B	132	SER	N-CA-C	-5.30	96.69	111.00
1	A	576	LEU	CA-CB-CG	5.25	127.37	115.30
1	A	300	LEU	CA-CB-CG	5.24	127.34	115.30
1	A	514	ARG	N-CA-C	-5.16	97.08	111.00
1	A	722	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	374	GLN	N-CA-C	-5.07	97.32	111.00
1	A	725	CYS	CA-CB-SG	-5.06	104.89	114.00

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	703	0
2	B	99	0	102	41	0
All	All	8825	0	8807	730	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 41.

All (730) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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
2:B:125:ALA:C	2:B:128:MET:HB2	1.89	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:542:ASP:CG	1:A:592:LEU:HD22	1.91	0.90
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
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
1:A:198:ARG:HH11	1:A:198:ARG:CG	1.86	0.88
1:A:589:ARG:HD3	1:A:589:ARG:C	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:707:ILE:HG13	1:A:708:GLN:N	1.90	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: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: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
2:B:124:ASN:C	2:B:126:SER:H	1.80	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:542:ASP:CG	1:A:592:LEU:CD2	2.49	0.81
1:A:722:ARG:HH12	2:B:130:ARG:CD	1.91	0.81
1:A:199:GLU:CG	1:A:201:GLU:CD	2.49	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:199:GLU:HG3	1:A:201:GLU:CD	2.02	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:413:LEU:C	1:A:422:TYR:HB3	2.02	0.79
1:A:385:GLY:HA3	1:A:719:GLU:O	1.83	0.79
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
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
2:B:125:ALA:C	2:B:128:MET:CB	2.56	0.74
1:A:480:SER:CB	1:A:483:PRO:HD2	2.17	0.73
1:A:921:ILE:C	1:A:922:LEU:HD12	2.08	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:482:GLU:HB2	1:A:483:PRO:CD	2.19	0.71
1:A:936:LYS:C	1:A:938:MET:H	1.93	0.71
1:A:1041:THR:HG22	1:A:1042:SER:N	2.05	0.71
1:A:766:SER:HB3	1:A:808:LEU:HD23	1.71	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:706:GLU:C	1:A:707:ILE:HG23	2.12	0.70
1:A:713:ARG:HH11	1:A:713:ARG:HG3	1.55	0.70
1:A:708:GLN:O	1:A:709:LYS:C	2.29	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
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
1:A:518:TYR:HD2	1:A:518:TYR:C	1.96	0.68
1:A:500:VAL:CG1	1:A:541:LEU:HD12	2.23	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:199:GLU:CG	1:A:201:GLU:OE2	2.42	0.67
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:469:ILE:HD11	1:A:471:ILE:HG12	1.77	0.66
2:B:131:LYS:C	2:B:133:GLN:N	2.41	0.66
1:A:112:ILE:HD12	1:A:112:ILE:H	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:230:ILE:C	1:A:231:ILE:HD12	2.17	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: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:518:TYR:C	1:A:518:TYR:CD2	2.70	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:659:ILE:HA	1:A:667:VAL:O	1.97	0.65
1:A:589:ARG:C	1:A:589:ARG:CD	2.64	0.64
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: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: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
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:593:MET:C	1:A:594:THR:HG23	2.19	0.63
1:A:644:LEU:HG	1:A:645:SER:H	1.63	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
2:B:124:ASN:C	2:B:126:SER:N	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:366:ASP:O	1:A:367:LEU:C	2.37	0.62
1:A:209:GLN:O	1:A:209:GLN:CG	2.46	0.62
1:A:396:ILE:CD1	1:A:673:LEU:HD21	2.30	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: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
1:A:714:THR:C	1:A:715:VAL:HG23	2.20	0.60
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:764:SER:HB2	1:A:805:HIS:ND1	2.17	0.60
1:A:639:ARG:HG3	1:A:640:THR:N	2.09	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:492:GLU:O	1:A:493:PRO:C	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:714:THR:HG22	1:A:716:PRO:HD3	1.84	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:231:ILE:HD12	1:A:231:ILE:N	2.16	0.59
1:A:679:MET:O	1:A:679:MET:SD	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: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:562:THR:HG22	1:A:563:ASP:N	2.16	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:438:LEU:C	1:A:440:GLY:H	2.07	0.58
1:A:402:ILE:HG22	1:A:404:LEU:HG	1.85	0.58
1:A:327:ARG:O	1:A:358:PRO:HD3	2.03	0.58
1:A:504:ASN:CG	1:A:505:SER:H	2.04	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: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: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:679:MET:SD	1:A:679:MET:C	2.83	0.57
1:A:18:CYS:N	1:A:313:CYS:SG	2.78	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:689:ASP:OD2	1:A:689:ASP:C	2.42	0.56
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:708:GLN:C	1:A:710:LEU:N	2.55	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:368:GLU:H	1:A:368:GLU:CD	2.07	0.56
1:A:929:SER:C	1:A:930:VAL:HG13	2.25	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: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
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
2:B:131:LYS:O	2:B:132:SER:C	2.43	0.55
1:A:570:LYS:HZ1	1:A:572:PRO:HD2	1.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:199:GLU:HG2	1:A:201:GLU:CD	2.20	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:1078:THR:C	1:A:1080:ARG:H	2.11	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: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:839:GLU:CD	1:A:839:GLU:H	2.10	0.53
1:A:555:LEU:HB2	1:A:569:LEU:O	2.07	0.53
1:A:578:HIS:CG	1:A:579:LYS:N	2.77	0.53
1:A:614:PHE:HD2	1:A:624:SER:HG	1.55	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:713:ARG:CG	1:A:714:THR:H	2.22	0.53
1:A:1136:LEU:C	1:A:1138:ARG:H	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:570:LYS:HZ3	1:A:572:PRO:HD2	1.72	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: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: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:707:ILE:O	1:A:708:GLN:C	2.49	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
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:415:SER:HB3	1:A:423:ASP:CG	2.31	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:595:THR:CG2	1:A:596:PHE:N	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:870:VAL:HG11	1:A:873:MET:HE3	1.94	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:936:LYS:C	1:A:938:MET:N	2.63	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: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:213:GLU:CD	1:A:233:GLY:HA3	2.33	0.49
1:A:416:ASP:OD1	1:A:417:PRO:N	2.45	0.49
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: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:374:GLN:OE1	1:A:391:ARG:HG3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:700:THR:C	1:A:701:ILE:HD13	2.33	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:687:TYR:H	1:A:688:PRO:HD3	1.78	0.48
1:A:932:LEU:C	1:A:933:LEU:HD12	2.33	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: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:1003:PHE:C	1:A:1003:PHE:CD2	2.87	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:1136:LEU:C	1:A:1138:ARG:N	2.67	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
1:A:641:PHE:HA	1:A:681:PRO:HG3	1.96	0.47
1:A:611:LEU:C	1:A:611:LEU:HD23	2.35	0.47
1:A:155:PHE:CE1	1:A:200:LYS:CG	2.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:112:ILE:N	1:A:112:ILE:CD1	2.72	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: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: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: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
2:B:131:LYS:C	2:B:133:GLN:H	2.18	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:81:THR:CG2	1:A:82:ALA:N	2.79	0.45
1:A:396:ILE:HD13	1:A:396:ILE:O	2.16	0.45
1:A:504:ASN:CG	1:A:505:SER:N	2.68	0.45
1:A:722:ARG:HH12	2:B:130:ARG:CZ	2.28	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:542:ASP:HB2	1:A:592:LEU:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:999:HIS:O	1:A:1074:ARG:NH1	2.45	0.45
1:A:40:GLU:HG3	1:A:54:GLU:HG2	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: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:787:GLU:HB2	1:A:812:TYR:CE1	2.51	0.44
1:A:220:ILE:HB	1:A:230:ILE:HB	1.98	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
1:A:1044:SER:OG	1:A:1047:TRP:HB2	2.18	0.44
1:A:559:GLY:C	1:A:560:LEU:HD23	2.38	0.44
1:A:1063:LYS:C	1:A:1064:SER:O	2.54	0.44
1:A:1078:THR:C	1:A:1080:ARG:N	2.69	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: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:614:PHE:HB3	1:A:624:SER:HG	1.76	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:258:ILE:CG2	1:A:259:VAL:N	2.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:922:LEU:C	1:A:923:VAL:HG12	2.39	0.43
1:A:469:ILE:HD12	1:A:471:ILE:HG13	1.96	0.43
1:A:961:ASP:O	1:A:963:ASP:N	2.51	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:570:LYS:HZ3	1:A:572:PRO:CD	2.32	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: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:594:THR:O	1:A:601:TYR:N	2.52	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: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: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:1136:LEU:O	1:A:1138:ARG:N	2.52	0.42
1:A:507:GLN:NE2	1:A:552:LEU:HA	2.27	0.42
1:A:522:HIS:O	1:A:523:PRO:C	2.58	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:342:GLU:H	1:A:342:GLU:CD	2.23	0.42
1:A:726:TYR:OH	1:A:796:GLN:NE2	2.48	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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:482:GLU:CB	1:A:483:PRO:HD3	2.28	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
2:B:135:GLY:O	2:B:136:PHE:C	2.54	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: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:695:ASN:O	1:A:696:ASN:C	2.59	0.41
1:A:19:VAL:HG12	1:A:32:LEU:CB	2.51	0.41
1:A:108:VAL:O	1:A:141:LYS:NZ	2.39	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:438:LEU:C	1:A:440:GLY:N	2.74	0.41
1:A:874:VAL:HG22	1:A:875:GLU:N	2.35	0.41
1:A:34:ALA:HB2	1:A:64:MET:HE2	2.03	0.41
1:A:197:LEU:O	1:A:200:LYS:CD	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:TRP:C	1:A:208:LYS:O	2.58	0.41
1:A:241:ASN:O	1:A:242:GLY:C	2.59	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
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
2:B:126:SER:C	2:B:128:MET:N	2.72	0.41
1:A:1054:MET:HE3	1:A:1054:MET:HB3	1.76	0.40
1:A:490:TRP:NE1	1:A:519:LEU:HD22	2.36	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:1077:HIS:CD2	1:A:1077:HIS:C	2.93	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
2:B:129:LEU:O	2:B:130:ARG:C	2.58	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:1049:ASN:O	1:A:1050:LEU:C	2.60	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%)	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

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Mol	Chain	Res	Type
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
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 (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%)	826 (84%)	151 (16%)	2 8
2	B	11/11 (100%)	9 (82%)	2 (18%)	1 5
All	All	988/1012 (98%)	835 (84%)	153 (16%)	2 8

All (153) 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	35	LYS
1	A	47	GLU
1	A	49	LEU
1	A	97	SER
1	A	98	ILE
1	A	101	ILE
1	A	103	ARG
1	A	109	GLN
1	A	118	THR
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	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

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Mol	Chain	Res	Type
1	A	204	LYS
1	A	208	LYS
1	A	209	GLN
1	A	231	ILE
1	A	235	GLU
1	A	236	SER
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	298	LYS
1	A	301	ARG
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	331	SER
1	A	333	LEU
1	A	342	GLU
1	A	351	GLU
1	A	352	THR
1	A	372	GLN
1	A	374	GLN
1	A	383	LYS
1	A	392	ASN
1	A	396	ILE
1	A	403	ASP
1	A	414	ARG
1	A	419	ARG
1	A	441	GLU
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	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	575	GLU
1	A	576	LEU
1	A	582	LEU
1	A	589	ARG
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	639	ARG
1	A	640	THR
1	A	647	THR
1	A	668	PHE
1	A	679	MET
1	A	690	SER
1	A	701	ILE
1	A	706	GLU
1	A	710	LEU
1	A	713	ARG
1	A	720	SER
1	A	728	GLU

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Mol	Chain	Res	Type
1	A	730	SER
1	A	738	SER
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	844	LYS
1	A	854	SER
1	A	857	LYS
1	A	858	LEU
1	A	896	GLU
1	A	900	ARG
1	A	917	LYS
1	A	923	VAL
1	A	938	MET
1	A	966	LEU
1	A	969	GLU
1	A	979	LYS
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
1	A	1050	LEU
1	A	1054	MET
1	A	1055	GLN
1	A	1063	LYS
1	A	1090	ASP
1	A	1093	LEU
1	A	1096	SER
1	A	1100	ILE
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 (37) 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	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	456	GLN
1	A	462	ASN
1	A	520	GLN
1	A	522	HIS
1	A	536	HIS
1	A	550	ASN
1	A	648	ASN
1	A	677	ASN
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	941	ASN
1	A	978	GLN
1	A	990	GLN
1	A	1055	GLN
1	A	1056	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 monosaccharides 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, 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%)	0.03	67 (6%) 21 14	17, 66, 159, 207	0
2	B	13/13 (100%)	0.17	2 (15%) 2 1	20, 21, 24, 32	0
All	All	1127/1156 (97%)	0.03	69 (6%) 21 13	17, 66, 158, 207	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	483	PRO	11.6
1	A	291	MET	11.1
1	A	462	ASN	6.7
1	A	621	GLY	6.2
1	A	545	PRO	6.1
1	A	569	LEU	6.1
1	A	294	THR	5.9
1	A	660	TYR	5.7
1	A	293	GLY	5.7
1	A	508	VAL	5.2
1	A	292	ASP	5.0
1	A	618	ILE	4.9
1	A	468	LEU	4.8
1	A	503	CYS	4.8
1	A	519	LEU	4.7
1	A	295	VAL	4.6
1	A	502	SER	4.3
1	A	504	ASN	4.1
1	A	616	LEU	4.0
1	A	289	GLU	3.8
1	A	447	GLU	3.8
1	A	571	LEU	3.7
1	A	430	VAL	3.5
1	A	661	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	528	GLN	3.4
1	A	576	LEU	3.4
1	A	547	GLY	3.4
1	A	288	GLU	3.4
1	A	439	ASN	3.3
1	A	619	GLU	3.2
1	A	501	ALA	3.1
1	A	436	LEU	3.1
1	A	773	SER	3.1
1	A	622	LEU	3.0
1	A	416	ASP	3.0
1	A	521	ILE	3.0
1	A	544	THR	3.0
1	A	419	ARG	2.9
1	A	598	SER	2.9
1	A	577	LEU	2.9
1	A	783	GLY	2.8
1	A	412	PRO	2.7
2	B	124	ASN	2.7
1	A	648	ASN	2.7
1	A	418	ASN	2.6
1	A	413	LEU	2.6
1	A	714	THR	2.6
1	A	593	MET	2.6
1	A	581	MET	2.6
1	A	594	THR	2.6
1	A	449	MET	2.6
1	A	369	ARG	2.5
2	B	136	PHE	2.5
1	A	509	VAL	2.5
1	A	682	LEU	2.4
1	A	599	SER	2.4
1	A	550	ASN	2.4
1	A	507	GLN	2.4
1	A	488	SER	2.4
1	A	1015	GLN	2.3
1	A	426	VAL	2.3
1	A	446	THR	2.3
1	A	444	GLU	2.3
1	A	486	LEU	2.3
1	A	450	GLY	2.3
1	A	663	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	485	ALA	2.1
1	A	367	LEU	2.1
1	A	448	LEU	2.1

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.