Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:22 AM GMT

PDB ID	:	3I7L
Title	:	Crystal Structure of DDB1 in Complex with the H-Box Motif of DDB2
Authors	:	Li, T.; Robert, E.I.; Breugel, P.C.V.; Strubin, M.; Zheng, N.
Deposited on	:	2009-07-08
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

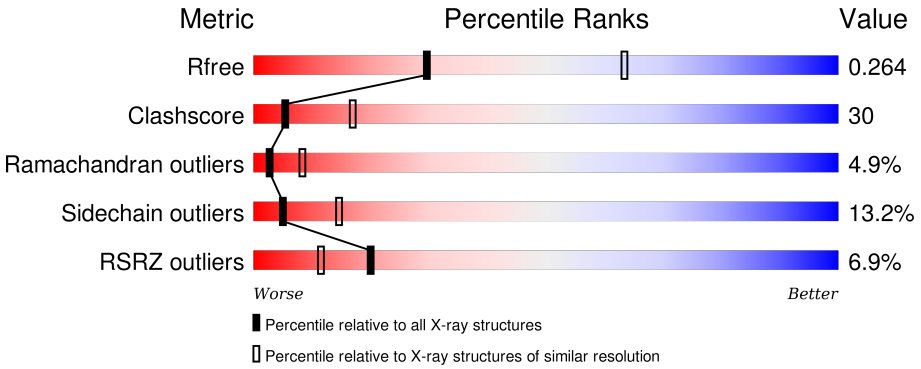
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	7%, 52%, 35%, 9%
2	B	14	86%, 7%, 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8840 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 DNA damage-binding protein 2.

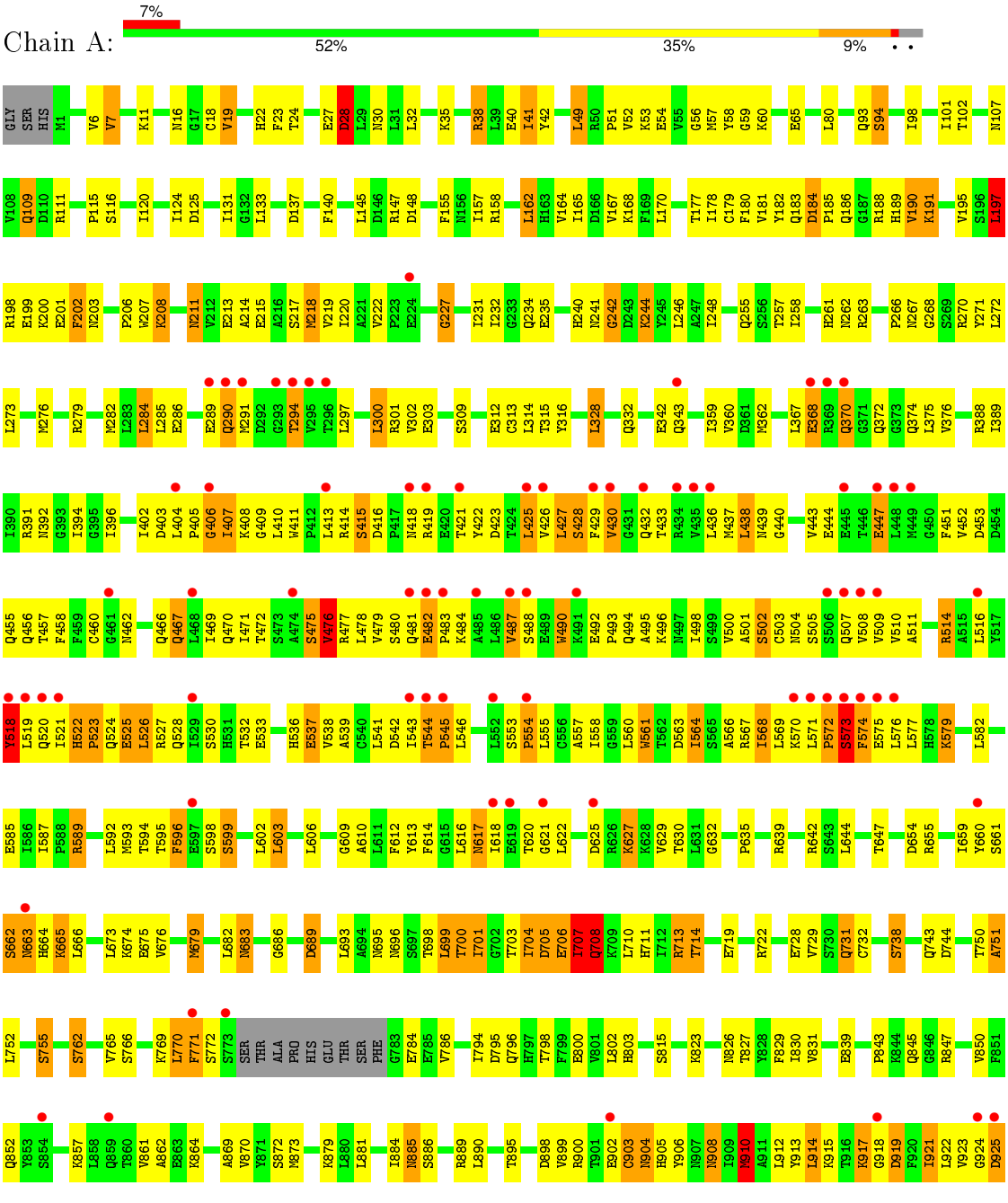
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	14	114	70	26	18	0	0	0

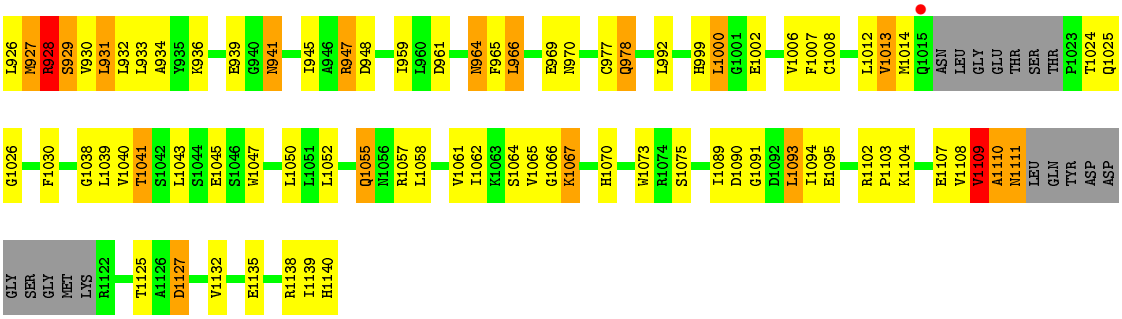
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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

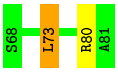
Chain A:





- Molecule 2: DNA damage-binding protein 2

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	63.78Å 134.15Å 182.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.74 – 2.80 48.71 – 2.79	Depositor EDS
% Data completeness (in resolution range)	96.0 (48.74-2.80) 95.6 (48.71-2.79)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	12.40 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.247 , 0.289 0.252 , 0.264	Depositor DCC
R_{free} test set	1954 reflections (5.43%)	DCC
Wilson B-factor (Å^2)	62.8	Xtriage
Anisotropy	0.342	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 61.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 39364 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	8840	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 3.92% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.73	4/8885 (0.0%)	0.87	22/12034 (0.2%)
2	B	0.69	0/115	0.80	0/151
All	All	0.72	4/9000 (0.0%)	0.87	22/12185 (0.2%)

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	1	0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	453	ASP	CG-OD1	15.53	1.61	1.25
1	A	453	ASP	CG-OD2	14.28	1.58	1.25
1	A	1008	CYS	CB-SG	-6.68	1.70	1.82
1	A	642	ARG	CZ-NH2	6.59	1.41	1.33

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	573	SER	N-CA-CB	-19.51	81.24	110.50
1	A	290	GLN	CB-CA-C	16.40	143.19	110.40
1	A	453	ASP	CB-CG-OD1	-13.42	106.22	118.30
1	A	514	ARG	N-CA-CB	-11.02	90.76	110.60
1	A	290	GLN	N-CA-C	-9.98	84.05	111.00
1	A	829	PHE	CB-CA-C	-8.41	93.57	110.40
1	A	291	MET	N-CA-C	-8.02	89.34	111.00
1	A	902	GLU	CB-CA-C	7.06	124.52	110.40
1	A	928	ARG	N-CA-C	-6.70	92.92	111.00
1	A	453	ASP	OD1-CG-OD2	6.68	135.99	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	294	THR	N-CA-CB	-6.30	98.33	110.30
1	A	573	SER	N-CA-C	6.05	127.34	111.00
1	A	291	MET	N-CA-CB	-5.97	99.85	110.60
1	A	603	LEU	CA-CB-CG	5.93	128.94	115.30
1	A	407	ILE	N-CA-C	-5.91	95.05	111.00
1	A	917	LYS	O-C-N	5.67	132.83	123.20
1	A	203	ASN	N-CA-C	-5.62	95.84	111.00
1	A	903	CYS	N-CA-C	-5.60	95.87	111.00
1	A	197	LEU	CA-CB-CG	5.55	128.06	115.30
1	A	314	LEU	CA-CB-CG	5.47	127.89	115.30
1	A	1109	VAL	N-CA-C	-5.29	96.71	111.00
1	A	1109	VAL	N-CA-CB	-5.20	100.06	111.50

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	902	GLU	CA

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	8706	528	0
2	B	114	0	122	6	0
All	All	8840	0	8828	528	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 30.

All (528) 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:509:VAL:CG1	1:A:571:LEU:HD11	1.32	1.57
1:A:570:LYS:HB3	1:A:573:SER:CB	1.47	1.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:VAL:HG11	1:A:571:LEU:CD1	1.48	1.42
1:A:570:LYS:HB3	1:A:573:SER:OG	1.30	1.22
1:A:616:LEU:HG	1:A:617:ASN:H	1.04	1.20
1:A:543:ILE:HG21	1:A:571:LEU:HD13	1.24	1.15
1:A:570:LYS:CB	1:A:573:SER:CB	2.25	1.14
1:A:1057:ARG:HB3	1:A:1108:VAL:CG1	1.77	1.14
1:A:912:LEU:HD11	1:A:926:LEU:HD22	1.14	1.10
1:A:912:LEU:CD1	1:A:926:LEU:HD22	1.80	1.10
1:A:170:LEU:CD2	1:A:179:CYS:HB2	1.80	1.10
1:A:571:LEU:HA	1:A:572:PRO:C	1.70	1.06
1:A:537:GLU:O	1:A:561:TRP:HB2	1.54	1.04
1:A:912:LEU:HD11	1:A:926:LEU:CD2	1.87	1.04
1:A:695:ASN:HD21	1:A:698:THR:HB	1.21	1.03
1:A:427:LEU:N	1:A:427:LEU:HD12	1.68	1.02
1:A:571:LEU:HA	1:A:572:PRO:O	1.57	1.02
1:A:170:LEU:HD21	1:A:179:CYS:HB2	1.04	1.01
1:A:490:TRP:HD1	1:A:526:LEU:HD22	1.25	1.00
1:A:1057:ARG:HB3	1:A:1108:VAL:HG13	1.39	1.00
1:A:570:LYS:C	1:A:573:SER:HB3	1.83	0.98
1:A:170:LEU:HD21	1:A:179:CYS:CB	1.94	0.97
1:A:570:LYS:CB	1:A:573:SER:HB3	1.93	0.95
1:A:131:ILE:HG13	1:A:145:LEU:HD11	1.48	0.95
1:A:576:LEU:C	1:A:577:LEU:HD12	1.86	0.95
1:A:931:LEU:C	1:A:931:LEU:HD12	1.86	0.95
1:A:532:THR:HG22	1:A:533:GLU:H	1.30	0.95
1:A:570:LYS:HB3	1:A:573:SER:HB3	1.48	0.94
1:A:616:LEU:HG	1:A:617:ASN:N	1.84	0.92
1:A:1057:ARG:CB	1:A:1108:VAL:CG1	2.46	0.92
1:A:328:LEU:HD21	2:B:80:ARG:NH2	1.85	0.91
1:A:931:LEU:HD12	1:A:932:LEU:N	1.85	0.90
1:A:487:VAL:HG11	1:A:524:GLN:HB3	1.53	0.90
1:A:309:SER:H	1:A:332:GLN:NE2	1.68	0.90
1:A:910:MET:HE1	2:B:73:LEU:HD11	1.55	0.89
1:A:396:ILE:HG12	1:A:673:LEU:HD11	1.54	0.89
1:A:1057:ARG:CB	1:A:1108:VAL:HG13	2.02	0.88
1:A:864:LYS:HD3	1:A:899:VAL:HG23	1.56	0.87
1:A:576:LEU:HD13	1:A:577:LEU:N	1.90	0.87
1:A:522:HIS:HB3	1:A:523:PRO:HD2	1.57	0.86
1:A:546:LEU:HD22	1:A:618:ILE:HG21	1.56	0.86
1:A:427:LEU:N	1:A:427:LEU:CD1	2.38	0.85
1:A:23:PHE:H	1:A:30:ASN:ND2	1.74	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:VAL:HG12	1:A:571:LEU:HD11	1.58	0.83
1:A:490:TRP:CD1	1:A:526:LEU:HD22	2.13	0.83
1:A:522:HIS:HB3	1:A:523:PRO:CD	2.08	0.83
1:A:503:CYS:SG	1:A:504:ASN:N	2.52	0.83
1:A:492:GLU:HB2	1:A:496:LYS:O	1.79	0.82
1:A:617:ASN:HD21	1:A:621:GLY:H	1.27	0.82
1:A:930:VAL:HG13	1:A:931:LEU:N	1.93	0.82
1:A:923:VAL:HG12	1:A:924:GLY:N	1.95	0.82
1:A:1026:GLY:O	1:A:1041:THR:HG23	1.78	0.81
1:A:1057:ARG:HB3	1:A:1108:VAL:HG11	1.60	0.81
1:A:22:HIS:HD2	1:A:28:ASP:O	1.63	0.81
1:A:427:LEU:HD12	1:A:427:LEU:H	1.43	0.81
1:A:654:ASP:HA	1:A:675:GLU:HG3	1.61	0.81
1:A:309:SER:H	1:A:332:GLN:HE22	1.23	0.80
1:A:509:VAL:CG1	1:A:571:LEU:CD1	2.25	0.80
1:A:425:LEU:O	1:A:427:LEU:HD12	1.82	0.79
1:A:185:PRO:O	1:A:186:GLN:HB2	1.81	0.79
1:A:1057:ARG:CB	1:A:1108:VAL:HG11	2.11	0.79
1:A:568:ILE:HG22	1:A:568:ILE:O	1.81	0.79
1:A:500:VAL:HG12	1:A:541:LEU:HD12	1.66	0.78
1:A:425:LEU:O	1:A:427:LEU:CD1	2.32	0.78
1:A:570:LYS:HB3	1:A:573:SER:HG	1.47	0.78
1:A:575:GLU:HG3	1:A:577:LEU:HD11	1.64	0.77
1:A:402:ILE:HG12	1:A:443:VAL:HG21	1.65	0.77
1:A:571:LEU:C	1:A:571:LEU:HD23	2.04	0.77
1:A:964:ASN:HD21	1:A:978:GLN:HE21	1.32	0.77
1:A:912:LEU:CG	1:A:926:LEU:HD22	2.15	0.77
1:A:573:SER:O	1:A:574:PHE:HB2	1.84	0.77
1:A:924:GLY:O	1:A:925:ASP:HB2	1.84	0.76
1:A:101:ILE:HD12	1:A:102:THR:H	1.50	0.76
1:A:879:LYS:HE3	1:A:890:LEU:HD21	1.66	0.76
1:A:570:LYS:CG	1:A:573:SER:HB2	2.16	0.76
1:A:427:LEU:CD1	1:A:427:LEU:H	1.97	0.76
1:A:910:MET:CE	2:B:73:LEU:HD11	2.16	0.75
1:A:1095:GLU:OE2	1:A:1140:HIS:HE1	1.68	0.75
1:A:655:ARG:HH12	1:A:1138:ARG:HD3	1.50	0.75
1:A:910:MET:O	1:A:926:LEU:HB3	1.85	0.74
1:A:576:LEU:C	1:A:576:LEU:HD13	2.07	0.74
1:A:948:ASP:HB2	1:A:992:LEU:HD11	1.69	0.74
1:A:368:GLU:O	1:A:370:GLN:HG3	1.88	0.74
1:A:573:SER:O	1:A:574:PHE:CB	2.35	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:GLU:OE2	1:A:215:GLU:HB2	1.88	0.74
1:A:571:LEU:CA	1:A:572:PRO:C	2.52	0.73
1:A:539:ALA:HB2	1:A:561:TRP:CD1	2.23	0.73
1:A:23:PHE:H	1:A:30:ASN:HD22	1.35	0.73
1:A:413:LEU:O	1:A:422:TYR:HB3	1.88	0.73
1:A:570:LYS:CA	1:A:573:SER:HB3	2.20	0.72
1:A:570:LYS:CG	1:A:573:SER:CB	2.68	0.72
1:A:695:ASN:ND2	1:A:698:THR:HB	2.02	0.72
1:A:185:PRO:O	1:A:186:GLN:CB	2.38	0.72
1:A:415:SER:HB2	1:A:423:ASP:OD2	1.90	0.72
1:A:570:LYS:CB	1:A:573:SER:OG	2.25	0.72
1:A:930:VAL:CG1	1:A:931:LEU:N	2.53	0.72
1:A:359:ILE:HG21	1:A:362:MET:HE3	1.72	0.71
1:A:124:ILE:HG12	1:A:131:ILE:HG12	1.72	0.71
1:A:507:GLN:HB3	1:A:509:VAL:HG23	1.71	0.71
1:A:427:LEU:HD11	1:A:436:LEU:HD11	1.70	0.71
1:A:1108:VAL:O	1:A:1108:VAL:HG12	1.90	0.71
1:A:268:GLY:O	1:A:285:LEU:HD22	1.90	0.71
1:A:881:LEU:CD2	1:A:922:LEU:HD22	2.21	0.71
1:A:569:LEU:HD13	1:A:574:PHE:O	1.91	0.70
1:A:722:ARG:HE	1:A:738:SER:HB3	1.57	0.70
1:A:926:LEU:C	1:A:928:ARG:H	1.95	0.70
1:A:107:ASN:OD1	1:A:109:GLN:HB3	1.93	0.69
1:A:924:GLY:O	1:A:925:ASP:CB	2.40	0.69
1:A:869:ALA:H	1:A:885:ASN:HD22	1.38	0.69
1:A:467:GLN:HE22	1:A:521:ILE:HG22	1.58	0.69
1:A:869:ALA:H	1:A:885:ASN:ND2	1.91	0.68
1:A:977:CYS:HB3	1:A:992:LEU:HD13	1.76	0.68
1:A:923:VAL:HG12	1:A:924:GLY:H	1.56	0.67
1:A:409:GLY:O	1:A:427:LEU:HB3	1.95	0.67
1:A:532:THR:HG22	1:A:533:GLU:N	2.08	0.67
1:A:197:LEU:H	1:A:197:LEU:HD23	1.58	0.67
1:A:507:GLN:NE2	1:A:509:VAL:HG21	2.09	0.67
1:A:246:LEU:HD12	1:A:297:LEU:HD23	1.76	0.67
1:A:262:ASN:ND2	1:A:316:TYR:H	1.93	0.67
1:A:743:GLN:HB2	1:A:784:GLU:HB2	1.76	0.67
1:A:577:LEU:N	1:A:577:LEU:HD12	2.09	0.67
1:A:41:ILE:HG13	1:A:53:LYS:O	1.94	0.67
1:A:543:ILE:HG21	1:A:571:LEU:CD1	2.16	0.67
1:A:912:LEU:HG	1:A:926:LEU:HB2	1.76	0.66
1:A:931:LEU:C	1:A:931:LEU:CD1	2.62	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:LEU:CD2	2:B:80:ARG:NH2	2.59	0.66
1:A:568:ILE:C	1:A:569:LEU:HD23	2.16	0.66
1:A:109:GLN:HG2	1:A:109:GLN:O	1.94	0.66
1:A:910:MET:O	1:A:926:LEU:CB	2.44	0.66
1:A:617:ASN:ND2	1:A:621:GLY:H	1.93	0.66
1:A:414:ARG:HA	1:A:422:TYR:HB3	1.78	0.66
1:A:1109:VAL:O	1:A:1111:ASN:N	2.28	0.66
1:A:414:ARG:HD2	1:A:416:ASP:O	1.95	0.66
1:A:1055:GLN:HG2	1:A:1093:LEU:HD12	1.76	0.65
1:A:509:VAL:HG11	1:A:571:LEU:CG	2.24	0.65
1:A:272:LEU:C	1:A:273:LEU:HD12	2.17	0.65
1:A:301:ARG:NH1	1:A:303:GLU:OE1	2.30	0.65
1:A:6:VAL:HG12	1:A:1040:VAL:HG22	1.78	0.65
1:A:731:GLN:NE2	1:A:796:GLN:HE22	1.95	0.65
1:A:923:VAL:CG1	1:A:924:GLY:H	2.10	0.65
1:A:1058:LEU:HD22	1:A:1062:ILE:CD1	2.27	0.65
1:A:923:VAL:CG1	1:A:924:GLY:N	2.59	0.65
1:A:362:MET:HG2	1:A:1006:VAL:HG11	1.79	0.65
1:A:199:GLU:HB3	1:A:201:GLU:OE2	1.96	0.64
1:A:476:VAL:HG11	1:A:508:VAL:HG11	1.79	0.64
1:A:521:ILE:HD13	1:A:525:GLU:O	1.98	0.64
1:A:731:GLN:NE2	1:A:796:GLN:NE2	2.45	0.64
1:A:170:LEU:CD2	1:A:179:CYS:CB	2.64	0.64
1:A:263:ARG:HB2	1:A:271:TYR:CE2	2.33	0.64
1:A:948:ASP:HB2	1:A:992:LEU:CD1	2.28	0.63
1:A:912:LEU:HD12	1:A:926:LEU:HD13	1.80	0.63
1:A:905:HIS:HE1	1:A:931:LEU:HD21	1.63	0.63
1:A:22:HIS:CD2	1:A:28:ASP:O	2.49	0.63
1:A:368:GLU:HB2	1:A:370:GLN:OE1	1.99	0.63
1:A:750:THR:O	1:A:751:ALA:CB	2.47	0.63
1:A:543:ILE:CG2	1:A:571:LEU:HD13	2.15	0.63
1:A:131:ILE:HG13	1:A:145:LEU:CD1	2.27	0.63
1:A:467:GLN:HG2	1:A:524:GLN:HG3	1.80	0.62
1:A:771:PHE:HE1	1:A:847:ARG:HD3	1.64	0.62
1:A:610:ALA:HA	1:A:630:THR:HA	1.79	0.62
1:A:1070:HIS:HE1	1:A:1090:ASP:OD2	1.81	0.62
1:A:826:ASN:ND2	1:A:852:GLN:HE21	1.98	0.62
1:A:167:VAL:HG22	1:A:180:PHE:CB	2.29	0.62
1:A:1024:THR:HB	1:A:1041:THR:HG21	1.81	0.62
1:A:482:GLU:HB3	1:A:483:PRO:HD3	1.79	0.62
1:A:917:LYS:O	1:A:919:ASP:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:TRP:HZ3	1:A:492:GLU:HG2	1.66	0.61
1:A:544:THR:O	1:A:546:LEU:HD12	2.00	0.61
1:A:24:THR:H	1:A:30:ASN:HD21	1.48	0.61
1:A:731:GLN:HE21	1:A:796:GLN:NE2	1.99	0.61
1:A:570:LYS:HB3	1:A:573:SER:HB2	1.71	0.61
1:A:522:HIS:HB2	1:A:527:ARG:NH1	2.16	0.61
1:A:719:GLU:OE2	1:A:755:SER:HB2	2.00	0.61
1:A:7:VAL:HG13	1:A:1091:GLY:HA3	1.82	0.61
1:A:272:LEU:O	1:A:273:LEU:HD12	2.00	0.61
1:A:815:SER:HB3	1:A:872:SER:HA	1.82	0.61
1:A:544:THR:HG22	1:A:545:PRO:HD2	1.82	0.60
1:A:181:VAL:HG22	1:A:190:VAL:HG13	1.84	0.60
1:A:905:HIS:CE1	1:A:931:LEU:HD21	2.35	0.60
1:A:227:GLY:O	1:A:241:ASN:ND2	2.35	0.60
1:A:116:SER:HB3	1:A:137:ASP:OD1	2.01	0.60
1:A:573:SER:O	1:A:574:PHE:CG	2.54	0.60
1:A:932:LEU:HD12	1:A:933:LEU:H	1.67	0.60
1:A:263:ARG:HA	1:A:271:TYR:CD2	2.37	0.60
1:A:613:TYR:CD2	1:A:666:LEU:HD12	2.36	0.60
1:A:570:LYS:HD3	1:A:573:SER:HB2	1.84	0.60
1:A:263:ARG:HH11	1:A:263:ARG:HG2	1.65	0.60
1:A:881:LEU:HD21	1:A:922:LEU:HD22	1.83	0.60
1:A:1058:LEU:HD22	1:A:1062:ILE:HD11	1.83	0.60
1:A:1000:LEU:HD13	1:A:1002:GLU:HB2	1.83	0.60
1:A:501:ALA:O	1:A:502:SER:HB2	2.02	0.60
1:A:490:TRP:HD1	1:A:526:LEU:CD2	2.09	0.59
1:A:558:ILE:O	1:A:566:ALA:HA	2.01	0.59
1:A:309:SER:N	1:A:332:GLN:HE22	1.97	0.59
1:A:389:ILE:HB	1:A:713:ARG:HB2	1.83	0.59
1:A:826:ASN:ND2	1:A:852:GLN:NE2	2.50	0.59
1:A:571:LEU:C	1:A:571:LEU:CD2	2.71	0.59
1:A:1057:ARG:HB2	1:A:1108:VAL:HG11	1.84	0.59
1:A:732:CYS:HB2	1:A:794:ILE:O	2.02	0.59
1:A:263:ARG:HB2	1:A:271:TYR:HE2	1.67	0.59
1:A:518:TYR:O	1:A:528:GLN:HA	2.03	0.58
1:A:195:VAL:HG22	1:A:202:PHE:HE2	1.68	0.58
1:A:750:THR:O	1:A:751:ALA:HB2	2.02	0.58
1:A:886:SER:HB2	1:A:908:ASN:O	2.02	0.58
1:A:167:VAL:HG13	1:A:178:ILE:HG23	1.85	0.58
1:A:360:VAL:HG21	1:A:722:ARG:HA	1.84	0.58
1:A:926:LEU:HD12	1:A:927:MET:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:927:MET:O	1:A:927:MET:HG2	1.95	0.58
1:A:490:TRP:HE1	1:A:519:LEU:HD22	1.68	0.58
1:A:467:GLN:HE22	1:A:521:ILE:CG2	2.15	0.58
1:A:522:HIS:O	1:A:524:GLN:N	2.36	0.57
1:A:1057:ARG:HD3	1:A:1108:VAL:HG13	1.84	0.57
1:A:850:VAL:HB	1:A:862:ALA:HB3	1.87	0.57
1:A:342:GLU:O	1:A:343:GLN:HB2	2.02	0.57
1:A:881:LEU:HD22	1:A:922:LEU:HD22	1.85	0.57
1:A:140:PHE:CD2	1:A:202:PHE:HZ	2.23	0.57
1:A:509:VAL:HG11	1:A:571:LEU:HD11	0.59	0.57
1:A:522:HIS:HB2	1:A:527:ARG:HH12	1.70	0.57
1:A:27:GLU:H	1:A:27:GLU:CD	2.07	0.57
1:A:124:ILE:CG1	1:A:131:ILE:HG12	2.34	0.57
1:A:570:LYS:CD	1:A:573:SER:HB2	2.36	0.56
1:A:167:VAL:HG22	1:A:180:PHE:HB3	1.86	0.56
1:A:182:TYR:OH	1:A:191:LYS:HE2	2.05	0.56
1:A:795:ASP:HB2	1:A:802:LEU:HD21	1.87	0.56
1:A:931:LEU:CD1	1:A:932:LEU:O	2.53	0.56
1:A:553:SER:O	1:A:571:LEU:O	2.24	0.56
1:A:178:ILE:HG22	1:A:179:CYS:N	2.20	0.56
1:A:514:ARG:HG3	1:A:514:ARG:HH11	1.71	0.56
1:A:11:LYS:NZ	1:A:38:ARG:NH1	2.53	0.56
1:A:410:LEU:HA	1:A:411:TRP:CE3	2.40	0.56
1:A:472:THR:HG21	1:A:477:ARG:HH11	1.71	0.56
1:A:910:MET:HE3	1:A:912:LEU:HD21	1.88	0.55
1:A:644:LEU:H	1:A:644:LEU:HD23	1.71	0.55
1:A:613:TYR:CE2	1:A:666:LEU:HD12	2.41	0.55
1:A:59:GLY:HA2	1:A:1073:TRP:CZ3	2.42	0.55
1:A:617:ASN:ND2	1:A:620:THR:HB	2.22	0.55
1:A:93:GLN:O	1:A:94:SER:C	2.43	0.55
1:A:255:GLN:HB2	1:A:279:ARG:HH12	1.71	0.55
1:A:660:TYR:OH	1:A:707:ILE:HA	2.05	0.55
1:A:472:THR:HG23	1:A:475:SER:H	1.71	0.55
1:A:532:THR:CG2	1:A:533:GLU:H	2.10	0.55
1:A:155:PHE:CE1	1:A:157:ILE:HD11	2.42	0.55
1:A:195:VAL:HG22	1:A:202:PHE:CE2	2.41	0.55
1:A:698:THR:HG22	1:A:699:LEU:N	2.21	0.55
1:A:102:THR:HG21	1:A:1066:GLY:O	2.06	0.55
1:A:910:MET:HB3	1:A:926:LEU:HD23	1.88	0.55
1:A:478:LEU:HD23	1:A:487:VAL:HB	1.88	0.55
1:A:460:CYS:O	1:A:460:CYS:SG	2.65	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:GLU:HG2	1:A:290:GLN:O	2.07	0.55
1:A:469:ILE:HD12	1:A:470:GLN:H	1.72	0.55
1:A:185:PRO:O	1:A:186:GLN:CD	2.45	0.54
1:A:1047:TRP:HZ3	1:A:1132:VAL:HG13	1.71	0.54
1:A:576:LEU:C	1:A:576:LEU:CD1	2.75	0.54
1:A:490:TRP:CD1	1:A:526:LEU:CD2	2.88	0.54
1:A:49:LEU:O	1:A:51:PRO:HD3	2.08	0.54
1:A:443:VAL:HG12	1:A:444:GLU:H	1.71	0.54
1:A:689:ASP:C	1:A:689:ASP:OD2	2.47	0.54
1:A:543:ILE:HD12	1:A:543:ILE:O	2.08	0.53
1:A:388:ARG:NH1	1:A:714:THR:HG23	2.22	0.53
1:A:1043:LEU:CD1	1:A:1089:ILE:HD12	2.38	0.53
1:A:577:LEU:N	1:A:577:LEU:CD1	2.72	0.53
1:A:452:VAL:HG23	1:A:455:GLN:HB2	1.91	0.53
1:A:698:THR:HG22	1:A:699:LEU:H	1.74	0.53
1:A:185:PRO:HB2	1:A:186:GLN:NE2	2.24	0.53
1:A:522:HIS:CB	1:A:523:PRO:CD	2.85	0.53
1:A:16:ASN:OD1	1:A:35:LYS:O	2.26	0.53
1:A:1057:ARG:CG	1:A:1108:VAL:HG13	2.39	0.52
1:A:655:ARG:NH1	1:A:1138:ARG:HD3	2.23	0.52
1:A:165:ILE:HG21	1:A:217:SER:HA	1.91	0.52
1:A:843:PRO:HG2	1:A:869:ALA:HB2	1.92	0.52
1:A:57:MET:HG2	1:A:1065:VAL:HG21	1.90	0.52
1:A:570:LYS:HG2	1:A:573:SER:HB2	1.92	0.52
1:A:213:GLU:HG2	1:A:214:ALA:N	2.25	0.52
1:A:58:TYR:HB3	1:A:1073:TRP:HB2	1.92	0.52
1:A:695:ASN:HD21	1:A:698:THR:CB	2.08	0.52
1:A:569:LEU:HD22	1:A:575:GLU:O	2.09	0.52
1:A:262:ASN:HD21	1:A:316:TYR:H	1.56	0.52
1:A:181:VAL:HA	1:A:189:HIS:O	2.10	0.51
1:A:451:PHE:CD1	1:A:479:VAL:HG21	2.45	0.51
1:A:270:ARG:HG2	1:A:284:LEU:HD23	1.92	0.51
1:A:930:VAL:HG13	1:A:931:LEU:H	1.73	0.51
1:A:167:VAL:CG1	1:A:178:ILE:HG23	2.39	0.51
1:A:426:VAL:C	1:A:427:LEU:HD12	2.29	0.51
1:A:457:THR:HG21	1:A:460:CYS:HB2	1.93	0.51
1:A:870:VAL:HG11	1:A:873:MET:CE	2.40	0.51
1:A:826:ASN:HD22	1:A:852:GLN:HE21	1.57	0.51
1:A:182:TYR:HE2	1:A:191:LYS:HB2	1.76	0.51
1:A:498:ILE:HD13	1:A:510:VAL:HG11	1.92	0.51
1:A:18:CYS:N	1:A:313:CYS:SG	2.84	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:ALA:HA	1:A:510:VAL:HG12	1.91	0.51
1:A:765:VAL:HG12	1:A:766:SER:N	2.26	0.51
1:A:456:GLN:O	1:A:472:THR:HA	2.11	0.50
1:A:999:HIS:HB2	1:A:1075:SER:O	2.11	0.50
1:A:705:ASP:O	1:A:706:GLU:O	2.28	0.50
1:A:167:VAL:HG22	1:A:180:PHE:HB2	1.94	0.50
1:A:490:TRP:NE1	1:A:519:LEU:HD22	2.27	0.50
1:A:931:LEU:CD1	1:A:932:LEU:N	2.66	0.50
1:A:391:ARG:HB3	1:A:711:HIS:HB3	1.93	0.50
1:A:425:LEU:O	1:A:427:LEU:HD11	2.10	0.50
1:A:65:GLU:OE2	1:A:65:GLU:HA	2.10	0.50
1:A:719:GLU:OE2	1:A:755:SER:CB	2.60	0.50
1:A:38:ARG:HD3	1:A:54:GLU:OE1	2.11	0.50
1:A:451:PHE:HA	1:A:470:GLN:NE2	2.26	0.50
1:A:218:MET:HB3	1:A:232:ILE:HB	1.92	0.50
1:A:19:VAL:HG12	1:A:32:LEU:HB2	1.91	0.50
1:A:542:ASP:OD1	1:A:592:LEU:HD12	2.12	0.50
1:A:222:VAL:O	1:A:227:GLY:HA2	2.11	0.50
1:A:676:VAL:HG11	1:A:693:LEU:HD23	1.94	0.50
1:A:609:GLY:HA3	1:A:632:GLY:O	2.12	0.50
1:A:830:ILE:HG12	1:A:850:VAL:HG22	1.93	0.50
1:A:1047:TRP:CZ3	1:A:1132:VAL:HG13	2.47	0.50
1:A:1102:ARG:N	1:A:1103:PRO:HD2	2.27	0.50
1:A:1030:PHE:CZ	1:A:1038:GLY:HA3	2.46	0.50
1:A:178:ILE:CG2	1:A:179:CYS:N	2.75	0.49
1:A:731:GLN:HA	1:A:796:GLN:NE2	2.27	0.49
1:A:405:PRO:O	1:A:406:GLY:C	2.50	0.49
1:A:328:LEU:HD21	2:B:80:ARG:HH22	1.71	0.49
1:A:408:LYS:N	1:A:428:SER:O	2.45	0.49
1:A:889:ARG:HG3	1:A:904:ASN:HB3	1.94	0.49
1:A:558:ILE:CG2	1:A:567:ARG:HB2	2.43	0.49
1:A:537:GLU:O	1:A:561:TRP:CB	2.44	0.49
1:A:183:GLN:NE2	1:A:188:ARG:HE	2.11	0.49
1:A:478:LEU:HD13	1:A:521:ILE:HD12	1.95	0.49
1:A:24:THR:H	1:A:30:ASN:ND2	2.10	0.49
1:A:101:ILE:HD12	1:A:102:THR:N	2.25	0.49
1:A:498:ILE:HD13	1:A:510:VAL:HG21	1.95	0.49
1:A:563:ASP:OD2	1:A:567:ARG:NH2	2.46	0.48
1:A:514:ARG:HG2	1:A:536:HIS:O	2.13	0.48
1:A:662:SER:OG	1:A:663:ASN:N	2.46	0.48
1:A:884:ILE:O	1:A:885:ASN:C	2.51	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:614:PHE:HA	1:A:625:ASP:O	2.13	0.48
1:A:575:GLU:O	1:A:577:LEU:CD1	2.62	0.48
1:A:910:MET:HG2	1:A:912:LEU:HD21	1.95	0.48
1:A:414:ARG:HG3	1:A:422:TYR:HA	1.95	0.48
1:A:162:LEU:H	1:A:162:LEU:HD12	1.78	0.48
1:A:503:CYS:HA	1:A:543:ILE:HD11	1.95	0.48
1:A:518:TYR:C	1:A:518:TYR:CD2	2.87	0.48
1:A:184:ASP:HB2	1:A:185:PRO:HD2	1.95	0.48
1:A:936:LYS:NZ	1:A:939:GLU:HG3	2.28	0.48
1:A:467:GLN:HG2	1:A:524:GLN:CG	2.44	0.48
1:A:241:ASN:O	1:A:242:GLY:C	2.51	0.48
1:A:1030:PHE:CE2	1:A:1038:GLY:HA3	2.49	0.48
1:A:487:VAL:HG11	1:A:524:GLN:CB	2.34	0.48
1:A:933:LEU:HD12	1:A:934:ALA:N	2.28	0.48
1:A:699:LEU:HD12	1:A:700:THR:H	1.79	0.47
1:A:402:ILE:HD12	1:A:402:ILE:H	1.79	0.47
1:A:961:ASP:OD1	1:A:964:ASN:HB2	2.14	0.47
1:A:606:LEU:HD11	1:A:612:PHE:HE1	1.79	0.47
1:A:910:MET:HE2	1:A:926:LEU:CD2	2.44	0.47
1:A:926:LEU:C	1:A:928:ARG:N	2.66	0.47
1:A:913:TYR:O	1:A:924:GLY:HA2	2.15	0.47
1:A:852:GLN:HB2	1:A:861:VAL:HG21	1.97	0.47
1:A:616:LEU:CG	1:A:617:ASN:H	1.92	0.47
1:A:476:VAL:CG1	1:A:508:VAL:HG11	2.44	0.47
1:A:467:GLN:NE2	1:A:521:ILE:CG2	2.78	0.47
1:A:932:LEU:HD12	1:A:933:LEU:N	2.28	0.47
1:A:1095:GLU:OE2	1:A:1140:HIS:CE1	2.58	0.47
1:A:415:SER:CB	1:A:423:ASP:OD2	2.60	0.47
1:A:246:LEU:HD12	1:A:297:LEU:CD2	2.44	0.47
1:A:928:ARG:HG2	1:A:947:ARG:HE	1.80	0.47
1:A:241:ASN:OD1	1:A:242:GLY:N	2.48	0.47
1:A:602:LEU:O	1:A:613:TYR:HA	2.15	0.47
1:A:771:PHE:CE2	1:A:845:GLN:HB3	2.50	0.47
1:A:917:LYS:HE2	1:A:921:ILE:HG13	1.96	0.47
1:A:595:THR:O	1:A:647:THR:OG1	2.29	0.47
1:A:375:LEU:HB2	1:A:1012:LEU:HD21	1.96	0.47
1:A:568:ILE:O	1:A:569:LEU:HD23	2.15	0.46
1:A:1109:VAL:O	1:A:1110:ALA:C	2.53	0.46
1:A:164:VAL:HG11	1:A:167:VAL:CG2	2.45	0.46
1:A:538:VAL:HA	1:A:560:LEU:HD23	1.96	0.46
1:A:707:ILE:HG22	1:A:708:GLN:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:570:LYS:HG2	1:A:573:SER:CB	2.45	0.46
1:A:246:LEU:HD23	1:A:246:LEU:HA	1.74	0.46
1:A:507:GLN:HE21	1:A:509:VAL:CG2	2.29	0.46
1:A:912:LEU:CD1	1:A:926:LEU:CD2	2.66	0.46
1:A:926:LEU:HG	1:A:927:MET:N	2.30	0.46
1:A:1058:LEU:HD22	1:A:1062:ILE:HD12	1.95	0.46
1:A:864:LYS:NZ	1:A:899:VAL:O	2.42	0.46
1:A:406:GLY:O	1:A:429:PHE:CD2	2.69	0.46
1:A:520:GLN:HB2	1:A:527:ARG:O	2.15	0.46
1:A:1013:VAL:O	1:A:1014:MET:C	2.55	0.46
1:A:679:MET:C	1:A:679:MET:SD	2.94	0.46
1:A:571:LEU:CD2	1:A:571:LEU:O	2.64	0.46
1:A:490:TRP:HE1	1:A:519:LEU:CD2	2.27	0.46
1:A:492:GLU:O	1:A:494:GLN:N	2.48	0.46
1:A:1025:GLN:O	1:A:1041:THR:HG22	2.16	0.46
1:A:914:LEU:O	1:A:915:LYS:HD3	2.16	0.46
1:A:38:ARG:NH1	1:A:54:GLU:OE2	2.48	0.45
1:A:438:LEU:C	1:A:440:GLY:H	2.19	0.45
1:A:931:LEU:HD12	1:A:932:LEU:C	2.37	0.45
1:A:1057:ARG:HB3	1:A:1108:VAL:CG2	2.46	0.45
1:A:472:THR:HG21	1:A:477:ARG:NH1	2.31	0.45
1:A:370:GLN:HG3	1:A:370:GLN:H	1.47	0.45
1:A:927:MET:O	1:A:927:MET:CG	2.63	0.45
1:A:359:ILE:HG21	1:A:362:MET:CE	2.44	0.45
1:A:391:ARG:NH2	1:A:711:HIS:CD2	2.85	0.45
1:A:798:THR:OG1	1:A:800:GLU:HG2	2.16	0.45
1:A:568:ILE:HA	1:A:568:ILE:HD13	1.72	0.45
1:A:155:PHE:HE1	1:A:157:ILE:HD11	1.80	0.45
1:A:1104:LYS:O	1:A:1107:GLU:HB2	2.16	0.45
1:A:231:ILE:HD12	1:A:240:HIS:CD2	2.53	0.44
1:A:1024:THR:HB	1:A:1041:THR:CG2	2.47	0.44
1:A:538:VAL:HG13	1:A:558:ILE:HD11	1.98	0.44
1:A:177:THR:HG21	1:A:206:PRO:HD3	1.99	0.44
1:A:197:LEU:H	1:A:197:LEU:CD2	2.25	0.44
1:A:707:ILE:O	1:A:708:GLN:O	2.35	0.44
1:A:598:SER:O	1:A:599:SER:CB	2.65	0.44
1:A:682:LEU:HG	1:A:683:ASN:H	1.81	0.44
1:A:507:GLN:OE1	1:A:553:SER:N	2.51	0.44
1:A:571:LEU:O	1:A:571:LEU:HD23	2.18	0.44
1:A:157:ILE:O	1:A:158:ARG:C	2.56	0.44
1:A:98:ILE:HD12	1:A:98:ILE:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:GLN:NE2	1:A:257:THR:OG1	2.50	0.44
1:A:1057:ARG:CD	1:A:1108:VAL:HG13	2.46	0.44
1:A:258:ILE:HD13	1:A:273:LEU:HD23	2.00	0.44
1:A:469:ILE:HG13	1:A:470:GLN:N	2.32	0.44
1:A:1066:GLY:O	1:A:1067:LYS:CB	2.66	0.44
1:A:542:ASP:HB3	1:A:557:ALA:HB3	2.00	0.44
1:A:564:ILE:HG22	1:A:582:LEU:HB2	2.00	0.44
1:A:168:LYS:NZ	1:A:219:VAL:O	2.33	0.44
1:A:1024:THR:CB	1:A:1041:THR:HG21	2.47	0.44
1:A:451:PHE:HA	1:A:470:GLN:HE22	1.83	0.44
1:A:504:ASN:CG	1:A:505:SER:H	2.21	0.44
1:A:889:ARG:CG	1:A:904:ASN:HB3	2.48	0.44
1:A:931:LEU:HD13	1:A:932:LEU:O	2.18	0.43
1:A:731:GLN:O	1:A:796:GLN:HB2	2.17	0.43
1:A:704:ILE:HG12	1:A:705:ASP:H	1.82	0.43
1:A:447:GLU:HG2	1:A:447:GLU:H	1.51	0.43
1:A:1057:ARG:HD3	1:A:1108:VAL:CG1	2.48	0.43
1:A:870:VAL:HG11	1:A:873:MET:HE2	2.00	0.43
1:A:211:ASN:N	1:A:211:ASN:HD22	2.13	0.43
1:A:518:TYR:OH	1:A:520:GLN:NE2	2.51	0.43
1:A:879:LYS:HE3	1:A:890:LEU:CD2	2.41	0.43
1:A:394:ILE:HD11	1:A:660:TYR:HE1	1.81	0.43
1:A:408:LYS:HE3	1:A:430:VAL:HA	2.00	0.43
1:A:886:SER:HB3	1:A:910:MET:H	1.84	0.43
1:A:928:ARG:HB3	1:A:929:SER:H	1.38	0.43
1:A:467:GLN:NE2	1:A:521:ILE:HG22	2.29	0.43
1:A:466:GLN:C	1:A:467:GLN:HG3	2.39	0.43
1:A:519:LEU:HD23	1:A:528:GLN:HB2	2.00	0.43
1:A:405:PRO:O	1:A:407:ILE:HG13	2.18	0.43
1:A:418:ASN:HB3	1:A:419:ARG:H	1.44	0.43
1:A:511:ALA:HB2	1:A:516:LEU:HD23	2.00	0.43
1:A:414:ARG:HG3	1:A:421:THR:O	2.19	0.43
1:A:57:MET:HG2	1:A:1065:VAL:CG2	2.48	0.43
1:A:568:ILE:O	1:A:577:LEU:HD13	2.19	0.43
1:A:1066:GLY:O	1:A:1067:LYS:HB2	2.19	0.43
1:A:155:PHE:CE1	1:A:200:LYS:HA	2.54	0.43
1:A:367:LEU:HA	1:A:367:LEU:HD23	1.87	0.43
1:A:475:SER:HB2	1:A:490:TRP:HB3	2.01	0.43
1:A:520:GLN:O	1:A:527:ARG:N	2.52	0.43
1:A:429:PHE:HB3	1:A:432:GLN:HB2	2.01	0.43
1:A:507:GLN:NE2	1:A:509:VAL:CG2	2.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:ALA:O	1:A:502:SER:CB	2.66	0.42
1:A:589:ARG:HE	1:A:635:PRO:HB2	1.84	0.42
1:A:520:GLN:CB	1:A:527:ARG:HB3	2.49	0.42
1:A:433:THR:OG1	1:A:456:GLN:HA	2.19	0.42
1:A:248:ILE:HG21	1:A:300:LEU:O	2.19	0.42
1:A:183:GLN:CD	1:A:188:ARG:HE	2.22	0.42
1:A:328:LEU:CD2	2:B:80:ARG:HH22	2.28	0.42
1:A:362:MET:HG2	1:A:1006:VAL:CG1	2.47	0.42
1:A:413:LEU:HD22	1:A:460:CYS:SG	2.60	0.42
1:A:414:ARG:NH2	1:A:462:ASN:OD1	2.52	0.42
1:A:731:GLN:HA	1:A:796:GLN:HE21	1.83	0.42
1:A:964:ASN:ND2	1:A:978:GLN:HG3	2.34	0.42
1:A:488:SER:OG	1:A:526:LEU:HD12	2.19	0.42
1:A:285:LEU:HD12	1:A:300:LEU:CD1	2.50	0.42
1:A:7:VAL:CG1	1:A:1091:GLY:HA3	2.49	0.42
1:A:458:PHE:CB	1:A:501:ALA:HB2	2.50	0.42
1:A:404:LEU:HA	1:A:405:PRO:HD3	1.87	0.42
1:A:282:MET:O	1:A:302:VAL:HA	2.19	0.42
1:A:543:ILE:HG22	1:A:555:LEU:O	2.19	0.42
1:A:520:GLN:HB2	1:A:527:ARG:HB3	2.01	0.42
1:A:700:THR:C	1:A:701:ILE:HD13	2.41	0.41
1:A:131:ILE:HG22	1:A:133:LEU:HD13	2.01	0.41
1:A:157:ILE:CG2	1:A:202:PHE:CD1	3.02	0.41
1:A:208:LYS:H	1:A:208:LYS:HG2	1.50	0.41
1:A:440:GLY:O	1:A:686:GLY:HA3	2.20	0.41
1:A:598:SER:O	1:A:599:SER:HB2	2.20	0.41
1:A:966:LEU:HD11	1:A:1007:PHE:CE2	2.55	0.41
1:A:576:LEU:HD21	1:A:579:LYS:HG2	2.02	0.41
1:A:178:ILE:HG21	1:A:178:ILE:HD13	1.79	0.41
1:A:525:GLU:HB2	1:A:526:LEU:H	1.54	0.41
1:A:80:LEU:HD23	1:A:120:ILE:HG21	2.01	0.41
1:A:553:SER:HA	1:A:554:PRO:HD3	1.89	0.41
1:A:284:LEU:CD1	1:A:303:GLU:HG2	2.50	0.41
1:A:507:GLN:HE22	1:A:543:ILE:HD13	1.85	0.41
1:A:926:LEU:CD1	1:A:927:MET:H	2.31	0.41
1:A:490:TRP:NE1	1:A:519:LEU:CD2	2.84	0.41
1:A:443:VAL:HG12	1:A:444:GLU:N	2.36	0.41
1:A:262:ASN:ND2	1:A:315:THR:HA	2.36	0.41
1:A:389:ILE:N	1:A:389:ILE:HD12	2.36	0.41
1:A:241:ASN:O	1:A:244:LYS:N	2.54	0.41
1:A:458:PHE:HB3	1:A:501:ALA:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:LYS:HD3	1:A:38:ARG:HD2	2.03	0.41
1:A:1061:VAL:HG12	1:A:1104:LYS:HD3	2.01	0.41
1:A:484:LYS:HD2	1:A:484:LYS:HA	1.91	0.41
1:A:220:ILE:HG12	1:A:261:HIS:CE1	2.56	0.41
1:A:910:MET:HE2	1:A:926:LEU:HD23	2.03	0.41
1:A:285:LEU:HD12	1:A:300:LEU:HD11	2.02	0.41
1:A:480:SER:HB3	1:A:483:PRO:HB2	2.03	0.41
1:A:830:ILE:HG22	1:A:831:VAL:N	2.36	0.41
1:A:689:ASP:O	1:A:703:THR:HG22	2.21	0.41
1:A:56:GLY:O	1:A:1065:VAL:HG21	2.21	0.41
1:A:765:VAL:HG12	1:A:766:SER:H	1.86	0.41
1:A:959:ILE:HG12	1:A:965:PHE:CD2	2.56	0.41
1:A:770:LEU:O	1:A:772:SER:N	2.53	0.41
1:A:1039:LEU:HD21	1:A:1139:ILE:HG22	2.03	0.41
1:A:570:LYS:HG2	1:A:571:LEU:N	2.36	0.41
1:A:573:SER:OG	1:A:574:PHE:N	2.54	0.41
1:A:912:LEU:HG	1:A:926:LEU:HD22	1.98	0.41
1:A:613:TYR:CE1	1:A:627:LYS:HB3	2.55	0.41
1:A:494:GLN:HB2	1:A:496:LYS:HE2	2.03	0.40
1:A:932:LEU:HA	1:A:932:LEU:HD12	1.62	0.40
1:A:941:ASN:HA	1:A:941:ASN:HD22	1.57	0.40
1:A:905:HIS:HE1	1:A:931:LEU:CD2	2.34	0.40
1:A:184:ASP:HB2	1:A:185:PRO:CD	2.51	0.40
1:A:1127:ASP:OD2	1:A:1127:ASP:N	2.43	0.40
1:A:140:PHE:CD2	1:A:202:PHE:CZ	3.07	0.40
1:A:661:SER:HA	1:A:665:LYS:O	2.21	0.40
1:A:926:LEU:CG	1:A:927:MET:N	2.84	0.40
1:A:926:LEU:O	1:A:928:ARG:N	2.32	0.40
1:A:947:ARG:HG3	1:A:948:ASP:N	2.37	0.40
1:A:170:LEU:CD1	1:A:207:TRP:CH2	3.05	0.40
1:A:467:GLN:HE21	1:A:478:LEU:HD11	1.85	0.40
1:A:923:VAL:HA	1:A:931:LEU:O	2.22	0.40
1:A:40:GLU:HB3	1:A:42:TYR:CE1	2.57	0.40
1:A:762:SER:O	1:A:803:HIS:HA	2.21	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%)	899 (81%)	153 (14%)	54 (5%)	3 8
2	B	12/14 (86%)	7 (58%)	4 (33%)	1 (8%)	1 2
All	All	1118/1157 (97%)	906 (81%)	157 (14%)	55 (5%)	3 8

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	ASP
1	A	406	GLY
1	A	487	VAL
1	A	502	SER
1	A	518	TYR
1	A	522	HIS
1	A	554	PRO
1	A	572	PRO
1	A	573	SER
1	A	599	SER
1	A	683	ASN
1	A	706	GLU
1	A	708	GLN
1	A	751	ALA
1	A	918	GLY
1	A	919	ASP
1	A	925	ASP
1	A	927	MET
1	A	1110	ALA
1	A	94	SER
1	A	148	ASP
1	A	242	GLY
1	A	415	SER
1	A	430	VAL
1	A	475	SER

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Mol	Chain	Res	Type
1	A	495	ALA
1	A	574	PHE
1	A	617	ASN
1	A	663	ASN
1	A	689	ASP
1	A	707	ILE
1	A	771	PHE
1	A	910	MET
1	A	928	ARG
1	A	929	SER
1	A	970	ASN
1	A	1067	LYS
1	A	471	ILE
1	A	523	PRO
1	A	662	SER
1	A	770	LEU
1	A	885	ASN
1	A	147	ARG
1	A	493	PRO
1	A	545	PRO
1	A	596	PHE
1	A	674	LYS
1	A	696	ASN
1	A	476	VAL
2	B	73	LEU
1	A	184	ASP
1	A	227	GLY
1	A	115	PRO
1	A	266	PRO
1	A	564	ILE

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%)	846 (87%)	131 (13%)	5 14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	12/12 (100%)	12 (100%)	0	100 100
All	All	989/1013 (98%)	858 (87%)	131 (13%)	5 14

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	19	VAL
1	A	28	ASP
1	A	38	ARG
1	A	41	ILE
1	A	49	LEU
1	A	52	VAL
1	A	60	LYS
1	A	109	GLN
1	A	111	ARG
1	A	125	ASP
1	A	162	LEU
1	A	190	VAL
1	A	191	LYS
1	A	197	LEU
1	A	198	ARG
1	A	202	PHE
1	A	208	LYS
1	A	211	ASN
1	A	218	MET
1	A	235	GLU
1	A	244	LYS
1	A	267	ASN
1	A	276	MET
1	A	284	LEU
1	A	286	GLU
1	A	294	THR
1	A	300	LEU
1	A	312	GLU
1	A	328	LEU
1	A	368	GLU
1	A	370	GLN
1	A	372	GLN
1	A	374	GLN
1	A	376	VAL
1	A	392	ASN

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Mol	Chain	Res	Type
1	A	403	ASP
1	A	425	LEU
1	A	427	LEU
1	A	428	SER
1	A	437	MET
1	A	438	LEU
1	A	439	ASN
1	A	447	GLU
1	A	467	GLN
1	A	476	VAL
1	A	481	GLN
1	A	482	GLU
1	A	490	TRP
1	A	518	TYR
1	A	525	GLU
1	A	526	LEU
1	A	530	SER
1	A	537	GLU
1	A	544	THR
1	A	561	TRP
1	A	568	ILE
1	A	579	LYS
1	A	585	GLU
1	A	587	ILE
1	A	589	ARG
1	A	593	MET
1	A	594	THR
1	A	596	PHE
1	A	603	LEU
1	A	622	LEU
1	A	627	LYS
1	A	629	VAL
1	A	639	ARG
1	A	659	ILE
1	A	664	HIS
1	A	665	LYS
1	A	679	MET
1	A	699	LEU
1	A	700	THR
1	A	701	ILE
1	A	704	ILE
1	A	705	ASP

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Mol	Chain	Res	Type
1	A	707	ILE
1	A	708	GLN
1	A	710	LEU
1	A	713	ARG
1	A	714	THR
1	A	728	GLU
1	A	729	VAL
1	A	731	GLN
1	A	738	SER
1	A	744	ASP
1	A	752	LEU
1	A	755	SER
1	A	762	SER
1	A	769	LYS
1	A	786	VAL
1	A	823	LYS
1	A	827	THR
1	A	839	GLU
1	A	857	LYS
1	A	895	THR
1	A	898	ASP
1	A	900	ARG
1	A	903	CYS
1	A	904	ASN
1	A	906	TYR
1	A	908	ASN
1	A	910	MET
1	A	914	LEU
1	A	921	ILE
1	A	928	ARG
1	A	931	LEU
1	A	941	ASN
1	A	945	ILE
1	A	947	ARG
1	A	964	ASN
1	A	966	LEU
1	A	969	GLU
1	A	978	GLN
1	A	1000	LEU
1	A	1013	VAL
1	A	1041	THR
1	A	1045	GLU

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Mol	Chain	Res	Type
1	A	1050	LEU
1	A	1052	LEU
1	A	1055	GLN
1	A	1064	SER
1	A	1093	LEU
1	A	1094	ILE
1	A	1109	VAL
1	A	1111	ASN
1	A	1125	THR
1	A	1127	ASP
1	A	1135	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	16	ASN
1	A	22	HIS
1	A	30	ASN
1	A	183	GLN
1	A	186	GLN
1	A	211	ASN
1	A	234	GLN
1	A	240	HIS
1	A	262	ASN
1	A	267	ASN
1	A	332	GLN
1	A	372	GLN
1	A	418	ASN
1	A	455	GLN
1	A	456	GLN
1	A	467	GLN
1	A	504	ASN
1	A	520	GLN
1	A	524	GLN
1	A	578	HIS
1	A	617	ASN
1	A	695	ASN
1	A	711	HIS
1	A	727	GLN
1	A	731	GLN
1	A	759	GLN

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Mol	Chain	Res	Type
1	A	790	ASN
1	A	796	GLN
1	A	806	GLN
1	A	809	GLN
1	A	826	ASN
1	A	885	ASN
1	A	905	HIS
1	A	941	ASN
1	A	964	ASN
1	A	1005	ASN
1	A	1034	ASN
1	A	1055	GLN
1	A	1070	HIS
1	A	1111	ASN
1	A	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 carbohydrates 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%)	0.14	78 (7%) 19 11	21, 65, 156, 202	0
2	B	14/14 (100%)	-0.15	0 100 100	36, 53, 79, 109	0
All	All	1128/1157 (97%)	0.14	78 (6%) 20 11	21, 65, 155, 202	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	508	VAL	18.5
1	A	572	PRO	15.0
1	A	291	MET	13.7
1	A	294	THR	13.5
1	A	293	GLY	11.2
1	A	571	LEU	11.2
1	A	295	VAL	7.4
1	A	506	SER	7.4
1	A	521	ILE	7.2
1	A	574	PHE	6.8
1	A	483	PRO	6.5
1	A	436	LEU	6.3
1	A	552	LEU	6.3
1	A	507	GLN	6.1
1	A	573	SER	5.6
1	A	413	LEU	5.5
1	A	434	ARG	5.4
1	A	545	PRO	5.4
1	A	544	THR	5.4
1	A	474	ALA	5.2
1	A	925	ASP	5.1
1	A	621	GLY	5.0
1	A	491	LYS	4.9
1	A	519	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	425	LEU	4.4
1	A	660	TYR	4.3
1	A	918	GLY	4.2
1	A	419	ARG	3.9
1	A	435	VAL	3.7
1	A	518	TYR	3.7
1	A	485	ALA	3.5
1	A	421	THR	3.4
1	A	430	VAL	3.4
1	A	554	PRO	3.4
1	A	369	ARG	3.3
1	A	461	GLY	3.3
1	A	575	GLU	3.3
1	A	625	ASP	3.2
1	A	426	VAL	3.2
1	A	597	GLU	3.1
1	A	448	LEU	3.1
1	A	468	LEU	3.0
1	A	773	SER	3.0
1	A	859	GLN	2.9
1	A	570	LYS	2.9
1	A	488	SER	2.9
1	A	418	ASN	2.9
1	A	1015	GLN	2.8
1	A	368	GLU	2.7
1	A	447	GLU	2.7
1	A	296	THR	2.7
1	A	529	ILE	2.7
1	A	445	GLU	2.7
1	A	482	GLU	2.7
1	A	771	PHE	2.6
1	A	663	ASN	2.6
1	A	429	PHE	2.5
1	A	432	GLN	2.4
1	A	618	ILE	2.4
1	A	404	LEU	2.4
1	A	289	GLU	2.4
1	A	924	GLY	2.3
1	A	854	SER	2.3
1	A	406	GLY	2.3
1	A	370	GLN	2.3
1	A	290	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	902	GLU	2.3
1	A	487	VAL	2.3
1	A	516	LEU	2.3
1	A	576	LEU	2.2
1	A	520	GLN	2.2
1	A	509	VAL	2.2
1	A	619	GLU	2.2
1	A	449	MET	2.1
1	A	224	GLU	2.1
1	A	481	GLN	2.1
1	A	543	ILE	2.1
1	A	343	GLN	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates 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.