Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:15 PM GMT

PDB ID	:	1ST6
Title	:	Crystal structure of a cytoskeletal protein
Authors	:	Bakolitsa, C.; Liddington, R.C.
Deposited on	:	2004-03-25
Resolution	:	3.10 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:

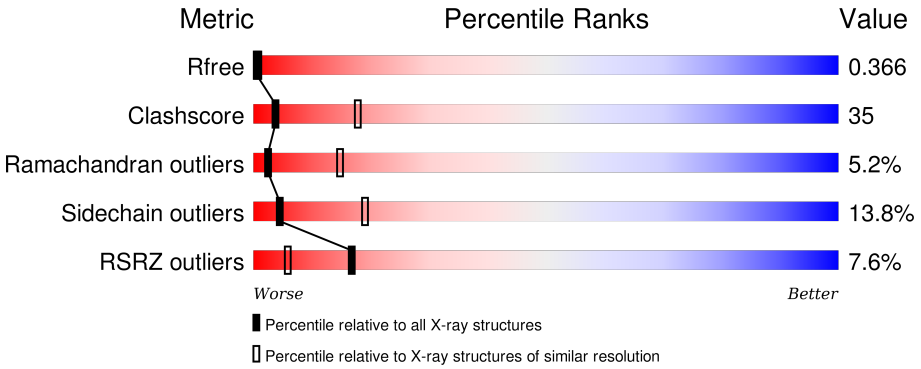
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.10 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	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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	1069	7% 52% 35% 7%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 8058 atoms, of which 3 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 Vinculin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	1049	8058	4978	3	1460	1568	49	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

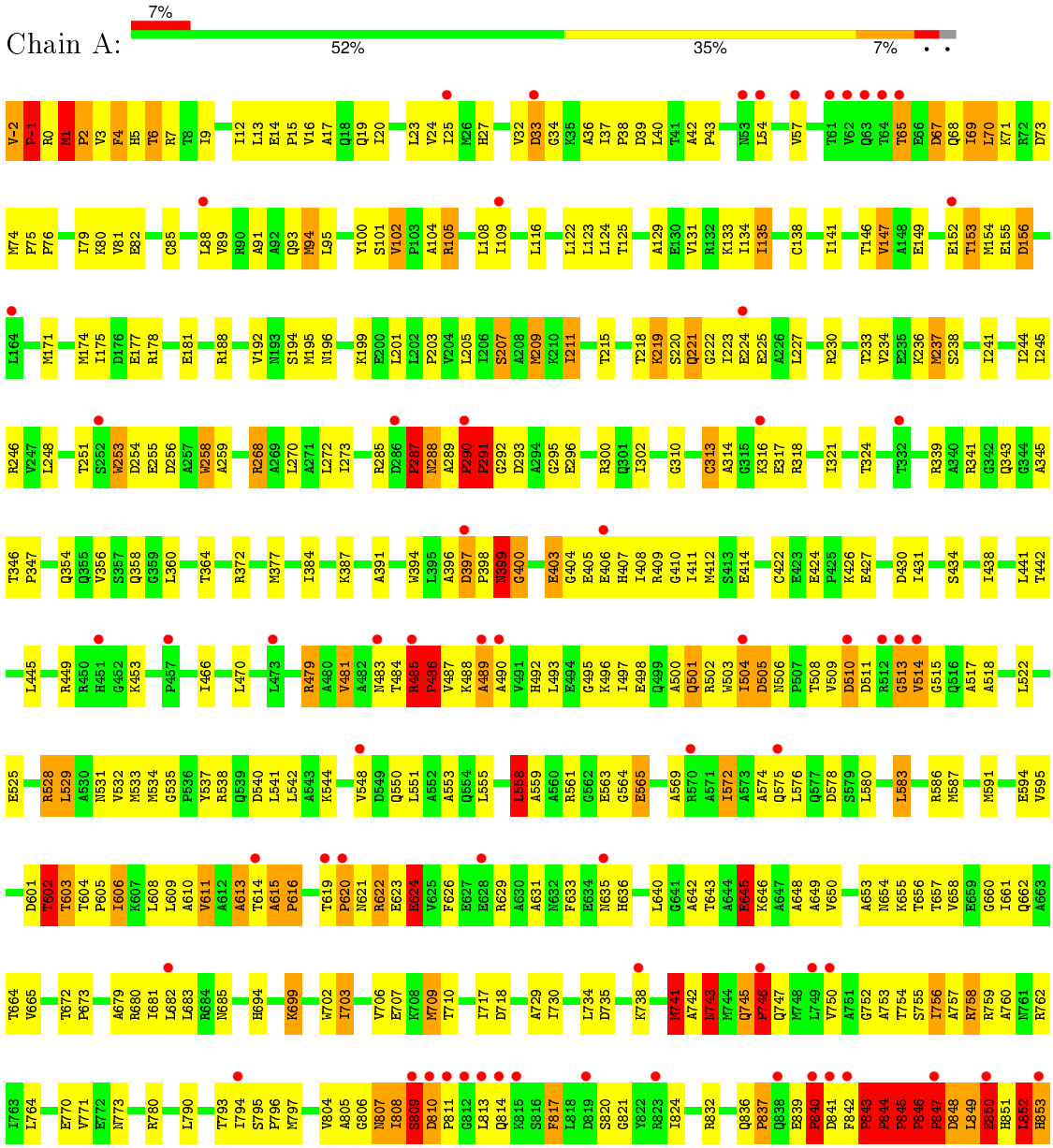
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	VAL	-	CLONING ARTIFACT	UNP P12003
A	-1	PRO	-	CLONING ARTIFACT	UNP P12003
A	0	ARG	-	CLONING ARTIFACT	UNP P12003
A	1	MET	-	INITIATING METHIONINE	UNP P12003

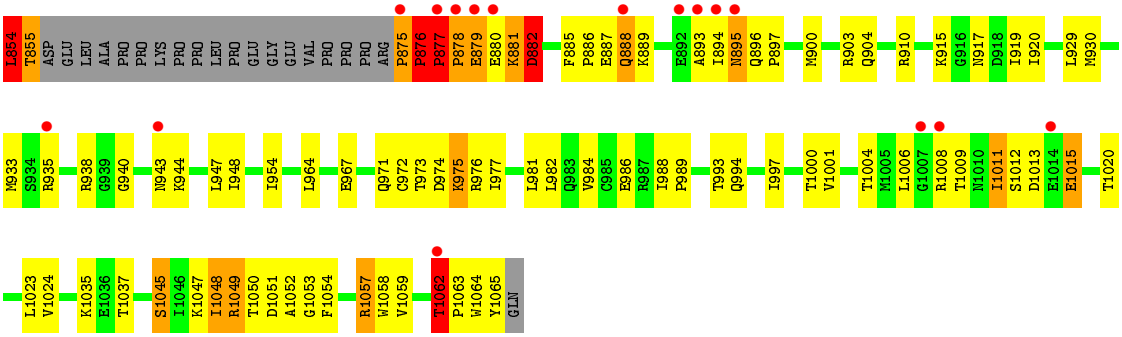
3 Residue-property plots (i)

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: Vinculin

Chain A:




L854 T855 ASP GLU LEU ALA PRO PRO LYS PRO PRO LEU PRO GLU GLY GLU VAL PRO PRO PRO ARG P875 P876 P877 P878 E879 E880 K881 D882 F885 P886 E887 Q888 K889 E892 A893 I894 N895 Q896 P897 N900 A903 Q904 A910 K915 G916 N917 D918 I919 I920 L929 N930
N933 S934 R935 R938 G939 G940 N943 N944 L947 I948 I954 L964 E967 Q971 C972 T973 D974 K975 R976 I977 L981 I982 Q983 V984 C985 E986 R987 I988 P989 T993 Q994 I997 T1000 V1001 T1004 M1005 L1006 G1007 R1008 T1009 N1010 I1011 S1012 D1013 E1014 E1015 T1020
L1023 V1024 K1035 E1036 T1037 S1045 I1046 K1047 I1048 R1049 T1050 D1051 A1052 G1053 F1054 R1057 W1058 V1059 T1062 P1063 W1064 Y1065 GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	56.02Å 126.95Å 351.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.96 – 3.10 46.96 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.96-3.10) 99.5 (46.96-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.41 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.316 , 0.357 0.320 , 0.366	Depositor DCC
R_{free} test set	1134 reflections (4.85%)	DCC
Wilson B-factor (Å^2)	102.2	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 97.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Outliers	0 of 25732 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	8058	wwPDB-VP
Average B, all atoms (Å^2)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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	0.83	20/8154 (0.2%)	1.06	51/11006 (0.5%)

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

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	-1	PRO	N-CD	23.26	1.80	1.47
1	A	-1	PRO	N-CA	15.96	1.74	1.47
1	A	613	ALA	CA-CB	-12.15	1.26	1.52
1	A	645	GLU	CB-CG	11.13	1.73	1.52
1	A	-1	PRO	CA-CB	-10.99	1.31	1.53
1	A	875	PRO	N-CD	9.59	1.61	1.47
1	A	875	PRO	CA-C	-8.01	1.36	1.52
1	A	645	GLU	CG-CD	7.87	1.63	1.51
1	A	718	ASP	CB-CG	7.59	1.67	1.51
1	A	291	PRO	CA-C	-7.23	1.38	1.52
1	A	853	HIS	CB-CG	6.77	1.62	1.50
1	A	-2	VAL	C-N	6.50	1.46	1.34
1	A	203	PRO	CA-C	-5.65	1.41	1.52
1	A	836	GLN	C-N	5.56	1.44	1.34
1	A	293	ASP	CB-CG	-5.46	1.40	1.51
1	A	1015	GLU	CD-OE2	-5.44	1.19	1.25
1	A	253	TRP	CB-CG	5.37	1.59	1.50
1	A	-1	PRO	CA-C	5.26	1.63	1.52
1	A	850	GLU	CB-CG	5.18	1.61	1.52
1	A	611	VAL	CA-CB	5.11	1.65	1.54

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	-2	VAL	C-N-CD	-29.51	55.68	120.60
1	A	-1	PRO	CA-N-CD	-19.13	84.71	111.50
1	A	-1	PRO	N-CA-CB	17.13	123.86	103.30
1	A	843	PRO	CA-N-CD	-10.52	96.77	111.50
1	A	-2	VAL	O-C-N	10.46	140.97	121.10
1	A	565	GLU	N-CA-C	-9.80	84.53	111.00
1	A	845	PRO	CA-N-CD	-9.12	98.72	111.50
1	A	1	MET	C-N-CD	-8.93	100.96	120.60
1	A	485	ARG	N-CA-C	8.88	134.97	111.00
1	A	854	LEU	CB-CA-C	-8.83	93.43	110.20
1	A	645	GLU	N-CA-CB	8.73	126.31	110.60
1	A	844	PRO	CA-N-CD	-8.58	99.49	111.50
1	A	-1	PRO	N-CA-C	-8.51	89.99	112.10
1	A	289	ALA	N-CA-C	-8.37	88.41	111.00
1	A	486	PRO	CA-N-CD	-8.29	99.89	111.50
1	A	291	PRO	N-CA-C	8.28	133.63	112.10
1	A	809	SER	N-CA-C	8.22	133.19	111.00
1	A	847	PRO	CA-N-CD	-8.12	100.13	111.50
1	A	485	ARG	C-N-CD	-8.10	102.77	120.60
1	A	876	PRO	N-CA-C	8.10	133.17	112.10
1	A	513	GLY	N-CA-C	-8.09	92.88	113.10
1	A	852	LEU	C-N-CA	-7.99	101.73	121.70
1	A	2	PRO	CA-N-CD	-7.98	100.33	111.50
1	A	293	ASP	CB-CG-OD1	-7.90	111.19	118.30
1	A	564	GLY	C-N-CA	7.79	141.17	121.70
1	A	875	PRO	CA-N-CD	-7.50	101.00	111.50
1	A	807	ASN	N-CA-CB	-7.42	97.23	110.60
1	A	611	VAL	C-N-CA	-7.31	103.42	121.70
1	A	-2	VAL	CA-C-N	-6.75	98.21	117.10
1	A	806	GLY	N-CA-C	-6.59	96.63	113.10
1	A	877	PRO	N-CA-C	6.42	128.78	112.10
1	A	489	ALA	N-CA-C	6.38	128.21	111.00
1	A	602	THR	C-N-CA	6.33	137.53	121.70
1	A	611	VAL	N-CA-CB	6.31	125.39	111.50
1	A	849	LEU	C-N-CA	6.08	136.91	121.70
1	A	290	PRO	N-CA-C	6.01	127.72	112.10
1	A	487	VAL	N-CA-C	-5.94	94.95	111.00
1	A	718	ASP	CB-CG-OD1	5.89	123.60	118.30
1	A	875	PRO	N-CA-C	5.76	127.07	112.10
1	A	718	ASP	N-CA-CB	5.71	120.88	110.60
1	A	203	PRO	CA-N-CD	-5.67	103.57	111.50
1	A	603	THR	N-CA-C	5.65	126.25	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	840	PRO	CA-N-CD	-5.60	103.65	111.50
1	A	293	ASP	N-CA-CB	5.59	120.67	110.60
1	A	291	PRO	CA-N-CD	-5.45	103.86	111.50
1	A	293	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	564	GLY	CA-C-N	-5.30	105.54	117.20
1	A	1015	GLU	OE1-CD-OE2	-5.25	117.00	123.30
1	A	741	MET	N-CA-C	5.13	124.86	111.00
1	A	291	PRO	CA-C-N	-5.11	105.98	116.20
1	A	837	PRO	CA-N-CD	-5.04	104.44	111.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	MET	Mainchain

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	8055	3	8219	573	1
All	All	8055	3	8219	573	1

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 35.

All (573) 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:613:ALA:HB3	1:A:683:LEU:CD1	1.35	1.49
1:A:-1:PRO:N	1:A:-1:PRO:CA	1.74	1.49
1:A:74:MET:SD	1:A:74:MET:CE	2.04	1.45
1:A:391:ALA:CB	1:A:407:HIS:HB3	1.54	1.37
1:A:613:ALA:CB	1:A:683:LEU:HD13	1.54	1.36
1:A:149:GLU:HG3	1:A:230:ARG:CZ	1.56	1.33

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:845:PRO:O	1:A:847:PRO:HD3	1.29	1.25
1:A:613:ALA:CB	1:A:683:LEU:CG	2.17	1.23
1:A:613:ALA:CB	1:A:683:LEU:CD1	2.14	1.21
1:A:613:ALA:HB1	1:A:683:LEU:CD2	1.72	1.20
1:A:613:ALA:CB	1:A:683:LEU:HD22	1.71	1.20
1:A:0:ARG:O	1:A:1:MET:HG2	1.42	1.18
1:A:613:ALA:CB	1:A:683:LEU:HB3	1.73	1.18
1:A:268:ARG:NH2	1:A:645:GLU:OE1	1.73	1.18
1:A:138:CYS:HA	1:A:141:ILE:HD12	1.17	1.16
1:A:613:ALA:CB	1:A:683:LEU:CD2	2.27	1.12
1:A:149:GLU:HG3	1:A:230:ARG:NH1	1.64	1.12
1:A:391:ALA:HB2	1:A:407:HIS:HB3	1.19	1.11
1:A:613:ALA:HB1	1:A:683:LEU:HD22	1.23	1.11
1:A:613:ALA:CB	1:A:683:LEU:CB	2.30	1.10
1:A:504:ILE:HG13	1:A:576:LEU:HD23	1.35	1.09
1:A:490:ALA:HB1	1:A:496:LYS:HE2	1.20	1.09
1:A:845:PRO:O	1:A:847:PRO:CD	2.02	1.08
1:A:1045:SER:O	1:A:1048:ILE:HD11	1.52	1.07
1:A:613:ALA:HB2	1:A:683:LEU:HB3	1.32	1.07
1:A:613:ALA:HB3	1:A:683:LEU:CG	1.83	1.06
1:A:387:LYS:HB2	1:A:411:ILE:HD11	1.08	1.05
1:A:314:ALA:HA	1:A:485:ARG:HG2	1.35	1.05
1:A:391:ALA:HB1	1:A:407:HIS:HB3	1.35	1.04
1:A:699:LYS:O	1:A:703:ILE:HD13	1.58	1.03
1:A:504:ILE:HG13	1:A:576:LEU:CD2	1.89	1.02
1:A:851:HIS:O	1:A:852:LEU:CD1	2.09	1.00
1:A:752:GLY:O	1:A:756:ILE:HD13	1.62	0.99
1:A:559:ALA:HB2	1:A:563:GLU:O	1.63	0.98
1:A:613:ALA:C	1:A:683:LEU:HD22	1.84	0.98
1:A:756:ILE:HG13	1:A:797:MET:HE3	1.45	0.97
1:A:0:ARG:O	1:A:1:MET:CG	2.11	0.97
1:A:391:ALA:CB	1:A:407:HIS:CB	2.43	0.97
1:A:613:ALA:HB1	1:A:683:LEU:CB	1.93	0.97
1:A:149:GLU:CG	1:A:230:ARG:CZ	2.42	0.95
1:A:613:ALA:HB1	1:A:683:LEU:CG	1.92	0.95
1:A:605:PRO:HB3	1:A:633:PHE:HD1	1.26	0.95
1:A:605:PRO:CB	1:A:633:PHE:HD1	1.80	0.95
1:A:285:ARG:O	1:A:287:PRO:HD3	1.68	0.94
1:A:741:MET:CE	1:A:817:PHE:CE2	2.51	0.94
1:A:74:MET:HE2	1:A:122:LEU:CD1	1.99	0.93
1:A:653:ALA:O	1:A:657:THR:HB	1.68	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:ALA:CA	1:A:485:ARG:HG2	1.98	0.93
1:A:741:MET:SD	1:A:817:PHE:HE2	1.91	0.92
1:A:844:PRO:C	1:A:846:PRO:HD2	1.90	0.92
1:A:753:ALA:HA	1:A:756:ILE:HD11	1.52	0.92
1:A:741:MET:SD	1:A:817:PHE:CE2	2.63	0.91
1:A:606:ILE:H	1:A:606:ILE:HD13	1.34	0.91
1:A:851:HIS:O	1:A:852:LEU:HD12	1.68	0.91
1:A:738:LYS:HZ2	1:A:817:PHE:HE1	0.91	0.90
1:A:116:LEU:HD13	1:A:1001:VAL:HG22	1.51	0.90
1:A:149:GLU:HG3	1:A:230:ARG:NH2	1.85	0.89
1:A:613:ALA:HB3	1:A:683:LEU:HD13	0.88	0.88
1:A:973:THR:HG21	1:A:1049:ARG:CG	2.04	0.88
1:A:591:MET:SD	1:A:717:ILE:HG13	2.14	0.87
1:A:514:VAL:HB	1:A:517:ALA:HB3	1.57	0.87
1:A:525:GLU:O	1:A:529:LEU:HG	1.74	0.87
1:A:611:VAL:O	1:A:615:ALA:HB3	1.74	0.87
1:A:795:SER:HB3	1:A:796:PRO:HD3	1.58	0.86
1:A:613:ALA:HB1	1:A:683:LEU:HB3	1.54	0.86
1:A:-2:VAL:HG12	1:A:-1:PRO:N	1.91	0.85
1:A:-2:VAL:CG1	1:A:-1:PRO:N	2.39	0.85
1:A:391:ALA:HB2	1:A:407:HIS:CB	2.03	0.85
1:A:603:THR:HA	1:A:606:ILE:HD11	1.59	0.85
1:A:734:LEU:HB3	1:A:738:LYS:HE2	1.60	0.84
1:A:973:THR:CG2	1:A:1049:ARG:HG3	2.07	0.84
1:A:605:PRO:HB3	1:A:633:PHE:CD1	2.12	0.84
1:A:74:MET:CE	1:A:122:LEU:CD1	2.55	0.84
1:A:504:ILE:HG23	1:A:505:ASP:N	1.94	0.83
1:A:314:ALA:HA	1:A:485:ARG:CG	2.08	0.83
1:A:851:HIS:O	1:A:852:LEU:HD13	1.76	0.83
1:A:387:LYS:CB	1:A:411:ILE:HD11	2.02	0.82
1:A:528:ARG:CG	1:A:529:LEU:HD23	2.08	0.82
1:A:529:LEU:HD23	1:A:529:LEU:N	1.94	0.81
1:A:285:ARG:O	1:A:287:PRO:CD	2.29	0.81
1:A:971:GLN:HA	1:A:1049:ARG:HH21	1.44	0.80
1:A:734:LEU:HD22	1:A:738:LYS:HZ3	1.46	0.79
1:A:738:LYS:O	1:A:741:MET:HB2	1.81	0.79
1:A:138:CYS:HA	1:A:141:ILE:CD1	2.07	0.79
1:A:613:ALA:CA	1:A:683:LEU:HD22	2.12	0.79
1:A:74:MET:CE	1:A:122:LEU:HD11	2.14	0.78
1:A:974:ASP:OD2	1:A:976:ARG:HG2	1.84	0.78
1:A:504:ILE:CG1	1:A:576:LEU:HD23	2.12	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:896:GLN:N	1:A:897:PRO:HD3	1.99	0.78
1:A:613:ALA:O	1:A:683:LEU:HD22	1.84	0.78
1:A:407:HIS:O	1:A:411:ILE:HG12	1.83	0.77
1:A:756:ILE:CG1	1:A:797:MET:HE3	2.12	0.77
1:A:971:GLN:HA	1:A:1049:ARG:NH2	2.00	0.77
1:A:756:ILE:HG13	1:A:797:MET:CE	2.15	0.77
1:A:-1:PRO:N	1:A:-1:PRO:C	2.38	0.76
1:A:138:CYS:CA	1:A:141:ILE:HD12	2.09	0.76
1:A:976:ARG:HG3	1:A:977:ILE:N	2.01	0.76
1:A:314:ALA:HB3	1:A:317:GLU:HB3	1.67	0.76
1:A:756:ILE:CG1	1:A:797:MET:CE	2.64	0.76
1:A:504:ILE:HG23	1:A:505:ASP:H	1.51	0.75
1:A:408:ILE:O	1:A:412:MET:HG3	1.86	0.75
1:A:738:LYS:NZ	1:A:817:PHE:HE1	1.80	0.75
1:A:742:ALA:O	1:A:745:GLN:NE2	2.20	0.75
1:A:391:ALA:HB1	1:A:407:HIS:CB	2.11	0.75
1:A:605:PRO:CB	1:A:633:PHE:CD1	2.67	0.74
1:A:808:ILE:N	1:A:813:LEU:HD11	2.02	0.74
1:A:74:MET:CE	1:A:122:LEU:HD12	2.18	0.74
1:A:9:ILE:HD12	1:A:123:LEU:HB3	1.69	0.74
1:A:141:ILE:HD13	1:A:171:MET:SD	2.28	0.74
1:A:74:MET:HE2	1:A:122:LEU:HD12	1.69	0.74
1:A:408:ILE:HG22	1:A:412:MET:SD	2.29	0.73
1:A:741:MET:HE3	1:A:817:PHE:CE2	2.22	0.73
1:A:614:THR:O	1:A:616:PRO:CD	2.37	0.73
1:A:149:GLU:CG	1:A:230:ARG:NH2	2.51	0.73
1:A:613:ALA:HB3	1:A:683:LEU:CD2	2.09	0.73
1:A:69:ILE:H	1:A:69:ILE:HD13	1.52	0.73
1:A:973:THR:HG21	1:A:1049:ARG:HG3	1.65	0.73
1:A:853:HIS:O	1:A:854:LEU:HG	1.89	0.72
1:A:845:PRO:N	1:A:846:PRO:HD2	2.04	0.72
1:A:808:ILE:O	1:A:813:LEU:HG	1.89	0.72
1:A:702:TRP:HE3	1:A:703:ILE:HD12	1.55	0.72
1:A:255:GLU:O	1:A:258:TRP:CE3	2.42	0.72
1:A:196:ASN:HA	1:A:199:LYS:HD3	1.72	0.72
1:A:559:ALA:CB	1:A:563:GLU:O	2.38	0.72
1:A:993:THR:O	1:A:997:ILE:HD13	1.89	0.72
1:A:490:ALA:CB	1:A:496:LYS:HE2	2.11	0.71
1:A:845:PRO:N	1:A:846:PRO:CD	2.53	0.71
1:A:528:ARG:HG3	1:A:529:LEU:HD23	1.72	0.71
1:A:613:ALA:HB2	1:A:683:LEU:HD13	1.65	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:GLU:O	1:A:410:GLY:HA3	1.91	0.71
1:A:503:TRP:CD1	1:A:515:GLY:HA3	2.26	0.71
1:A:729:ALA:HB3	1:A:759:ARG:HH22	1.55	0.70
1:A:747:GLN:HE22	1:A:750:VAL:HG21	1.55	0.70
1:A:109:ILE:HD11	1:A:1004:THR:HA	1.73	0.70
1:A:9:ILE:CD1	1:A:123:LEU:HD22	2.21	0.70
1:A:528:ARG:HG3	1:A:529:LEU:CD2	2.22	0.70
1:A:734:LEU:HD22	1:A:738:LYS:NZ	2.06	0.69
1:A:404:GLY:HA2	1:A:407:HIS:HD2	1.57	0.69
1:A:227:LEU:HD22	1:A:230:ARG:HH22	1.56	0.69
1:A:528:ARG:HG2	1:A:529:LEU:HD23	1.75	0.69
1:A:653:ALA:HB3	1:A:658:VAL:HG23	1.73	0.69
1:A:614:THR:O	1:A:616:PRO:HD3	1.93	0.69
1:A:853:HIS:O	1:A:854:LEU:CG	2.41	0.68
1:A:504:ILE:HG12	1:A:555:LEU:HD13	1.74	0.68
1:A:756:ILE:HB	1:A:797:MET:CE	2.23	0.68
1:A:608:LEU:HB3	1:A:629:ARG:HD3	1.75	0.68
1:A:434:SER:O	1:A:438:ILE:HD13	1.92	0.68
1:A:0:ARG:C	1:A:1:MET:HG2	2.13	0.68
1:A:971:GLN:OE1	1:A:1049:ARG:NH2	2.24	0.68
1:A:354:GLN:O	1:A:358:GLN:HG2	1.94	0.68
1:A:558:LEU:HD23	1:A:559:ALA:N	2.08	0.68
1:A:797:MET:HG3	1:A:824:ILE:HD11	1.76	0.68
1:A:131:VAL:O	1:A:135:ILE:HD13	1.93	0.68
1:A:753:ALA:HA	1:A:756:ILE:CD1	2.23	0.68
1:A:569:ALA:HA	1:A:572:ILE:HD11	1.76	0.68
1:A:205:LEU:O	1:A:209:MET:HG3	1.93	0.68
1:A:318:ARG:HA	1:A:321:ILE:HD12	1.76	0.67
1:A:9:ILE:HG22	1:A:9:ILE:O	1.94	0.67
1:A:747:GLN:NE2	1:A:750:VAL:HG21	2.08	0.67
1:A:314:ALA:CB	1:A:317:GLU:HB3	2.24	0.67
1:A:808:ILE:O	1:A:813:LEU:CD1	2.43	0.67
1:A:149:GLU:O	1:A:149:GLU:HG2	1.94	0.67
1:A:3:VAL:C	1:A:4:PHE:HD2	1.98	0.67
1:A:973:THR:HG21	1:A:1049:ARG:HG2	1.75	0.67
1:A:384:ILE:HD11	1:A:414:GLU:HB3	1.77	0.67
1:A:407:HIS:O	1:A:411:ILE:CG1	2.42	0.67
1:A:738:LYS:HA	1:A:741:MET:HG3	1.77	0.67
1:A:569:ALA:HA	1:A:572:ILE:CD1	2.25	0.67
1:A:525:GLU:HA	1:A:528:ARG:HD3	1.76	0.66
1:A:591:MET:HE1	1:A:717:ILE:HD11	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:PHE:CD2	1:A:4:PHE:N	2.63	0.66
1:A:258:TRP:CZ2	1:A:486:PRO:HG3	2.30	0.66
1:A:930:MET:HA	1:A:930:MET:CE	2.26	0.65
1:A:533:MET:CE	1:A:537:TYR:CD2	2.79	0.65
1:A:730:ILE:HD11	1:A:759:ARG:HB3	1.78	0.65
1:A:141:ILE:HD13	1:A:171:MET:CE	2.27	0.65
1:A:9:ILE:HD12	1:A:123:LEU:HD22	1.79	0.65
1:A:853:HIS:CG	1:A:854:LEU:H	2.15	0.65
1:A:514:VAL:HB	1:A:517:ALA:CB	2.26	0.64
1:A:427:GLU:O	1:A:431:ILE:HG12	1.97	0.64
1:A:504:ILE:CG2	1:A:505:ASP:N	2.60	0.64
1:A:976:ARG:CG	1:A:977:ILE:N	2.60	0.64
1:A:255:GLU:O	1:A:258:TRP:HE3	1.78	0.64
1:A:973:THR:CG2	1:A:1049:ARG:CG	2.69	0.64
1:A:1020:THR:O	1:A:1024:VAL:HG23	1.97	0.64
1:A:645:GLU:O	1:A:645:GLU:HG3	1.96	0.64
1:A:88:LEU:HD22	1:A:108:LEU:HD12	1.79	0.64
1:A:756:ILE:HD12	1:A:797:MET:SD	2.38	0.64
1:A:503:TRP:HD1	1:A:515:GLY:HA3	1.63	0.64
1:A:404:GLY:HA2	1:A:407:HIS:CD2	2.33	0.64
1:A:504:ILE:CG2	1:A:505:ASP:H	2.11	0.64
1:A:149:GLU:CD	1:A:230:ARG:NH2	2.50	0.64
1:A:583:LEU:O	1:A:587:MET:HG3	1.97	0.63
1:A:12:ILE:HD11	1:A:54:LEU:HD11	1.80	0.63
1:A:610:ALA:O	1:A:614:THR:CB	2.46	0.63
1:A:881:LYS:HZ1	1:A:915:LYS:HE2	1.63	0.63
1:A:196:ASN:HA	1:A:199:LYS:CD	2.28	0.63
1:A:881:LYS:O	1:A:882:ASP:HB2	1.98	0.63
1:A:201:LEU:HD13	1:A:237:MET:HG2	1.80	0.63
1:A:220:SER:O	1:A:223:ILE:HG13	1.98	0.63
1:A:207:SER:O	1:A:694:HIS:HD2	1.81	0.62
1:A:1048:ILE:HD12	1:A:1048:ILE:H	1.65	0.62
1:A:614:THR:O	1:A:616:PRO:HD2	2.00	0.62
1:A:887:GLU:O	1:A:888:GLN:HB2	2.00	0.62
1:A:555:LEU:HG	1:A:572:ILE:HD12	1.81	0.62
1:A:756:ILE:CB	1:A:797:MET:CE	2.77	0.62
1:A:3:VAL:HB	1:A:124:LEU:HD21	1.81	0.61
1:A:605:PRO:HB2	1:A:633:PHE:CD1	2.36	0.61
1:A:509:VAL:HG12	1:A:510:ASP:N	2.15	0.61
1:A:853:HIS:O	1:A:854:LEU:CB	2.48	0.61
1:A:273:ILE:HG23	1:A:302:ILE:HG23	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:606:ILE:CD1	1:A:606:ILE:H	2.06	0.61
1:A:225:GLU:HB3	1:A:681:ILE:HD11	1.83	0.61
1:A:734:LEU:O	1:A:738:LYS:HG2	2.01	0.61
1:A:511:ASP:OD2	1:A:900:MET:SD	2.59	0.61
1:A:548:VAL:HG21	1:A:583:LEU:HD12	1.82	0.61
1:A:238:SER:HA	1:A:241:ILE:HD12	1.83	0.61
1:A:1011:ILE:O	1:A:1011:ILE:HG13	2.00	0.61
1:A:237:MET:O	1:A:241:ILE:HG13	2.00	0.60
1:A:492:HIS:O	1:A:496:LYS:HG3	2.01	0.60
1:A:504:ILE:HG13	1:A:576:LEU:HD21	1.83	0.60
1:A:756:ILE:HB	1:A:797:MET:HE3	1.82	0.60
1:A:23:LEU:HD21	1:A:40:LEU:HD11	1.84	0.60
1:A:291:PRO:O	1:A:296:GLU:HG3	2.01	0.60
1:A:650:VAL:O	1:A:650:VAL:HG12	2.02	0.60
1:A:4:PHE:N	1:A:4:PHE:HD2	2.00	0.60
1:A:225:GLU:CB	1:A:681:ILE:HD11	2.32	0.60
1:A:479:ARG:HG2	1:A:483:ASN:HB2	1.84	0.59
1:A:227:LEU:CD2	1:A:230:ARG:HH22	2.15	0.59
1:A:976:ARG:CG	1:A:977:ILE:H	2.15	0.59
1:A:422:CYS:SG	1:A:484:THR:HG21	2.43	0.59
1:A:74:MET:N	1:A:75:PRO:CD	2.66	0.59
1:A:610:ALA:O	1:A:614:THR:HB	2.02	0.59
1:A:947:LEU:O	1:A:947:LEU:HD23	2.02	0.59
1:A:653:ALA:HB3	1:A:658:VAL:CG2	2.33	0.59
1:A:513:GLY:O	1:A:514:VAL:HG13	2.02	0.59
1:A:15:PRO:O	1:A:19:GLN:HG2	2.02	0.59
1:A:24:VAL:CG1	1:A:948:ILE:HD11	2.33	0.59
1:A:74:MET:HE1	1:A:122:LEU:HD11	1.85	0.59
1:A:893:ALA:HB1	1:A:894:ILE:HD12	1.85	0.58
1:A:408:ILE:O	1:A:412:MET:N	2.31	0.58
1:A:258:TRP:CE2	1:A:486:PRO:HG3	2.38	0.58
1:A:929:LEU:HD13	1:A:954:ILE:HG13	1.85	0.58
1:A:645:GLU:O	1:A:648:ALA:N	2.34	0.58
1:A:679:ALA:O	1:A:683:LEU:HB2	2.03	0.58
1:A:702:TRP:O	1:A:706:VAL:HG23	2.04	0.58
1:A:85:CYS:O	1:A:89:VAL:HG23	2.03	0.58
1:A:79:ILE:HG22	1:A:80:LYS:N	2.19	0.58
1:A:756:ILE:CB	1:A:797:MET:HE1	2.34	0.58
1:A:339:ARG:O	1:A:343:GLN:HA	2.04	0.58
1:A:851:HIS:C	1:A:852:LEU:HD13	2.24	0.57
1:A:741:MET:CE	1:A:817:PHE:HE2	2.01	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:613:ALA:HB2	1:A:683:LEU:CB	2.09	0.57
1:A:532:VAL:HG12	1:A:532:VAL:O	2.04	0.57
1:A:756:ILE:CB	1:A:797:MET:HE3	2.34	0.57
1:A:153:THR:HG23	1:A:155:GLU:H	1.70	0.57
1:A:844:PRO:C	1:A:846:PRO:CD	2.69	0.57
1:A:149:GLU:CG	1:A:230:ARG:NH1	2.55	0.56
1:A:895:ASN:C	1:A:897:PRO:HD3	2.25	0.56
1:A:528:ARG:CG	1:A:529:LEU:CD2	2.78	0.56
1:A:804:VAL:HA	1:A:813:LEU:HD22	1.87	0.56
1:A:397:ASP:N	1:A:398:PRO:HD3	2.21	0.56
1:A:529:LEU:N	1:A:529:LEU:CD2	2.64	0.56
1:A:68:GLN:OE1	1:A:71:LYS:HD2	2.05	0.56
1:A:606:ILE:N	1:A:606:ILE:HD13	2.13	0.56
1:A:645:GLU:O	1:A:646:LYS:C	2.44	0.56
1:A:734:LEU:HD21	1:A:756:ILE:HG21	1.88	0.56
1:A:752:GLY:O	1:A:756:ILE:CD1	2.46	0.56
1:A:795:SER:CB	1:A:796:PRO:HD3	2.34	0.56
1:A:69:ILE:N	1:A:69:ILE:HD13	2.18	0.56
1:A:23:LEU:HD22	1:A:108:LEU:HD11	1.87	0.56
1:A:809:SER:HB3	1:A:811:PRO:HD2	1.88	0.56
1:A:314:ALA:C	1:A:485:ARG:HG2	2.27	0.55
1:A:147:VAL:O	1:A:147:VAL:HG13	2.07	0.55
1:A:74:MET:HG2	1:A:125:THR:HG21	1.87	0.55
1:A:694:HIS:O	1:A:694:HIS:ND1	2.39	0.55
1:A:572:ILE:HA	1:A:575:GLN:HG2	1.89	0.55
1:A:310:GLY:O	1:A:313:CYS:HB2	2.06	0.55
1:A:604:THR:HB	1:A:605:PRO:HD3	1.88	0.55
1:A:219:LYS:N	1:A:219:LYS:CD	2.70	0.55
1:A:976:ARG:HG3	1:A:977:ILE:H	1.72	0.55
1:A:619:THR:H	1:A:620:PRO:CD	2.20	0.55
1:A:591:MET:CE	1:A:717:ILE:HD11	2.37	0.55
1:A:894:ILE:HG22	1:A:895:ASN:N	2.22	0.55
1:A:603:THR:CA	1:A:606:ILE:HD11	2.34	0.54
1:A:610:ALA:O	1:A:614:THR:OG1	2.23	0.54
1:A:601:ASP:O	1:A:603:THR:N	2.40	0.54
1:A:500:ALA:HB2	1:A:518:ALA:HB3	1.88	0.54
1:A:1062:THR:HG1	1:A:1064:TRP:HD1	1.53	0.54
1:A:645:GLU:OE2	1:A:649:ALA:HB2	2.08	0.54
1:A:4:PHE:HD1	1:A:994:GLN:HG2	1.72	0.54
1:A:1057:ARG:HD3	1:A:1059:VAL:HG23	1.89	0.54
1:A:81:VAL:HG13	1:A:82:GLU:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:MET:O	1:A:175:ILE:HG12	2.06	0.54
1:A:503:TRP:HH2	1:A:511:ASP:HB3	1.71	0.54
1:A:153:THR:HG22	1:A:156:ASP:H	1.72	0.54
1:A:27:HIS:ND1	1:A:108:LEU:HD23	2.23	0.53
1:A:219:LYS:CD	1:A:219:LYS:H	2.20	0.53
1:A:509:VAL:O	1:A:510:ASP:HB2	2.07	0.53
1:A:273:ILE:HG23	1:A:302:ILE:HD12	1.89	0.53
1:A:893:ALA:C	1:A:894:ILE:HD12	2.29	0.53
1:A:207:SER:O	1:A:694:HIS:CD2	2.61	0.53
1:A:324:THR:O	1:A:324:THR:HG22	2.08	0.53
1:A:682:LEU:O	1:A:683:LEU:HG	2.08	0.53
1:A:233:THR:O	1:A:237:MET:HG3	2.08	0.53
1:A:729:ALA:HB3	1:A:759:ARG:NH2	2.23	0.53
1:A:738:LYS:HD2	1:A:817:PHE:CZ	2.43	0.53
1:A:591:MET:SD	1:A:717:ILE:CG1	2.92	0.53
1:A:9:ILE:HG23	1:A:123:LEU:HD13	1.90	0.53
1:A:3:VAL:HG13	1:A:251:THR:HG23	1.90	0.53
1:A:5:HIS:CD2	1:A:6:THR:HG22	2.44	0.53
1:A:504:ILE:CD1	1:A:576:LEU:HD23	2.40	0.52
1:A:808:ILE:O	1:A:813:LEU:CG	2.54	0.52
1:A:67:ASP:CB	1:A:70:LEU:HD22	2.39	0.52
1:A:1023:LEU:O	1:A:1023:LEU:HG	2.09	0.52
1:A:735:ASP:HA	1:A:738:LYS:HG2	1.91	0.52
1:A:804:VAL:HG22	1:A:813:LEU:HD22	1.91	0.52
1:A:930:MET:CE	1:A:933:MET:SD	2.98	0.52
1:A:292:GLY:HA2	1:A:296:GLU:HB2	1.90	0.52
1:A:37:ILE:HG21	1:A:95:LEU:HD13	1.92	0.52
1:A:398:PRO:O	1:A:400:GLY:N	2.42	0.52
1:A:503:TRP:HH2	1:A:511:ASP:CB	2.23	0.52
1:A:32:VAL:HG23	1:A:33:ASP:OD1	2.10	0.51
1:A:804:VAL:HG12	1:A:804:VAL:O	2.10	0.51
1:A:920:ILE:HD11	1:A:1058:TRP:CZ3	2.46	0.51
1:A:896:GLN:N	1:A:897:PRO:CD	2.73	0.51
1:A:854:LEU:O	1:A:855:THR:O	2.29	0.51
1:A:73:ASP:C	1:A:76:PRO:HD2	2.31	0.51
1:A:756:ILE:CD1	1:A:797:MET:SD	2.99	0.51
1:A:729:ALA:CB	1:A:759:ARG:HH22	2.22	0.51
1:A:621:ASN:O	1:A:622:ARG:C	2.48	0.51
1:A:245:ILE:HA	1:A:248:LEU:HD12	1.93	0.51
1:A:13:LEU:O	1:A:16:VAL:HG12	2.11	0.50
1:A:551:LEU:HD13	1:A:575:GLN:HG3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:ILE:H	1:A:69:ILE:CD1	2.13	0.50
1:A:258:TRP:CZ2	1:A:486:PRO:CG	2.94	0.50
1:A:595:VAL:HG12	1:A:595:VAL:O	2.11	0.50
1:A:703:ILE:CD1	1:A:703:ILE:N	2.75	0.50
1:A:493:LEU:O	1:A:497:ILE:HG12	2.12	0.50
1:A:1049:ARG:O	1:A:1052:ALA:N	2.43	0.50
1:A:391:ALA:HA	1:A:407:HIS:CG	2.46	0.50
1:A:222:GLY:HA3	1:A:681:ILE:HG12	1.93	0.50
1:A:887:GLU:HG2	1:A:903:ARG:NH2	2.26	0.50
1:A:930:MET:HE1	1:A:933:MET:SD	2.52	0.49
1:A:538:ARG:HG3	1:A:542:LEU:HD12	1.94	0.49
1:A:636:HIS:O	1:A:640:LEU:HG	2.12	0.49
1:A:793:THR:CG2	1:A:824:ILE:HG12	2.42	0.49
1:A:808:ILE:H	1:A:813:LEU:HD11	1.73	0.49
1:A:754:THR:O	1:A:757:ALA:HB3	2.12	0.49
1:A:391:ALA:HB2	1:A:407:HIS:CG	2.47	0.49
1:A:646:LYS:O	1:A:650:VAL:HG23	2.11	0.49
1:A:94:MET:SD	1:A:104:ALA:HB2	2.52	0.49
1:A:74:MET:CG	1:A:125:THR:HG21	2.41	0.49
1:A:614:THR:C	1:A:616:PRO:HD3	2.32	0.49
1:A:135:ILE:CD1	1:A:135:ILE:N	2.75	0.49
1:A:9:ILE:O	1:A:9:ILE:CG2	2.60	0.49
1:A:754:THR:HG22	1:A:758:ARG:HE	1.77	0.49
1:A:1062:THR:HG22	1:A:1063:PRO:HD3	1.95	0.49
1:A:764:LEU:HD21	1:A:790:LEU:HB2	1.95	0.49
1:A:930:MET:HA	1:A:930:MET:HE2	1.93	0.49
1:A:619:THR:N	1:A:620:PRO:CD	2.76	0.49
1:A:760:ALA:CB	1:A:794:ILE:HD11	2.43	0.49
1:A:7:ARG:HB3	1:A:181:GLU:O	2.13	0.49
1:A:793:THR:HG21	1:A:824:ILE:HA	1.94	0.48
1:A:14:GLU:N	1:A:15:PRO:HD2	2.28	0.48
1:A:205:LEU:O	1:A:209:MET:CG	2.59	0.48
1:A:215:THR:HG21	1:A:223:ILE:HA	1.94	0.48
1:A:1062:THR:C	1:A:1064:TRP:H	2.16	0.48
1:A:1045:SER:C	1:A:1048:ILE:HD11	2.28	0.48
1:A:558:LEU:O	1:A:561:ARG:HG2	2.12	0.48
1:A:656:THR:CG2	1:A:656:THR:O	2.60	0.48
1:A:658:VAL:O	1:A:662:GLN:HG3	2.13	0.48
1:A:94:MET:HG2	1:A:95:LEU:N	2.28	0.48
1:A:134:ILE:N	1:A:134:ILE:HD12	2.29	0.48
1:A:24:VAL:HG12	1:A:948:ILE:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:PRO:N	1:A:76:PRO:CD	2.75	0.48
1:A:741:MET:SD	1:A:817:PHE:CZ	3.05	0.48
1:A:287:PRO:HB3	1:A:345:ALA:HB2	1.95	0.48
1:A:408:ILE:CG2	1:A:412:MET:SD	2.99	0.48
1:A:886:PRO:HB2	1:A:889:LYS:HE2	1.95	0.48
1:A:310:GLY:HA2	1:A:321:ILE:HD13	1.95	0.48
1:A:25:ILE:HG23	1:A:948:ILE:HD13	1.95	0.48
1:A:981:LEU:O	1:A:984:VAL:HG12	2.14	0.48
1:A:445:LEU:HD11	1:A:466:ILE:HD12	1.95	0.48
1:A:0:ARG:O	1:A:1:MET:SD	2.72	0.47
1:A:288:ASN:O	1:A:290:PRO:HD3	2.14	0.47
1:A:609:LEU:HD21	1:A:633:PHE:HB2	1.96	0.47
1:A:234:VAL:HG12	1:A:234:VAL:O	2.14	0.47
1:A:920:ILE:HD11	1:A:1058:TRP:CH2	2.49	0.47
1:A:661:ILE:O	1:A:664:THR:HB	2.14	0.47
1:A:408:ILE:HD12	1:A:408:ILE:N	2.30	0.47
1:A:808:ILE:H	1:A:813:LEU:HD21	1.79	0.47
1:A:67:ASP:OD2	1:A:69:ILE:HD11	2.15	0.47
1:A:710:THR:HG23	1:A:762:ARG:NH2	2.30	0.47
1:A:919:ILE:HD11	1:A:964:LEU:HB3	1.97	0.47
1:A:74:MET:CG	1:A:74:MET:CE	2.91	0.47
1:A:804:VAL:HG13	1:A:813:LEU:HD22	1.95	0.47
1:A:509:VAL:HG12	1:A:510:ASP:H	1.80	0.47
1:A:919:ILE:HG13	1:A:964:LEU:HD13	1.97	0.47
1:A:1054:PHE:C	1:A:1054:PHE:CD1	2.88	0.47
1:A:498:GLU:OE1	1:A:1035:LYS:NZ	2.43	0.46
1:A:346:THR:HB	1:A:347:PRO:HD2	1.96	0.46
1:A:141:ILE:CD1	1:A:171:MET:SD	3.01	0.46
1:A:555:LEU:CG	1:A:572:ILE:HD12	2.44	0.46
1:A:258:TRP:CG	1:A:259:ALA:N	2.83	0.46
1:A:572:ILE:O	1:A:576:LEU:HB3	2.15	0.46
1:A:746:PRO:O	1:A:747:GLN:HB2	2.14	0.46
1:A:133:LYS:HZ2	1:A:174:MET:HE2	1.81	0.46
1:A:314:ALA:HB1	1:A:485:ARG:NE	2.30	0.46
1:A:504:ILE:HD13	1:A:504:ILE:C	2.36	0.46
1:A:313:CYS:SG	1:A:321:ILE:HD13	2.56	0.46
1:A:1064:TRP:HA	1:A:1064:TRP:CE3	2.51	0.46
1:A:504:ILE:HG12	1:A:555:LEU:CD1	2.43	0.46
1:A:555:LEU:HD21	1:A:572:ILE:CD1	2.46	0.46
1:A:9:ILE:CD1	1:A:123:LEU:HB3	2.40	0.46
1:A:619:THR:H	1:A:620:PRO:HD3	1.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:-2:VAL:C	1:A:-1:PRO:CA	2.70	0.46
1:A:391:ALA:CB	1:A:407:HIS:CG	2.98	0.46
1:A:734:LEU:HB3	1:A:738:LYS:CE	2.41	0.46
1:A:853:HIS:CG	1:A:854:LEU:N	2.83	0.46
1:A:548:VAL:HG21	1:A:583:LEU:CD1	2.46	0.46
1:A:613:ALA:HB2	1:A:683:LEU:CD1	2.29	0.46
1:A:484:THR:OG1	1:A:485:ARG:N	2.49	0.46
1:A:609:LEU:HD11	1:A:633:PHE:CG	2.52	0.46
1:A:220:SER:O	1:A:222:GLY:N	2.49	0.45
1:A:134:ILE:HD12	1:A:134:ILE:H	1.80	0.45
1:A:1048:ILE:HG22	1:A:1052:ALA:CB	2.46	0.45
1:A:894:ILE:HD12	1:A:894:ILE:N	2.32	0.45
1:A:133:LYS:NZ	1:A:174:MET:HE2	2.32	0.45
1:A:1012:SER:HB2	1:A:1015:GLU:HB2	1.98	0.45
1:A:502:ARG:N	1:A:502:ARG:HD3	2.31	0.45
1:A:470:LEU:HD23	1:A:470:LEU:O	2.17	0.45
1:A:300:ARG:HB3	1:A:531:ASN:HD21	1.80	0.45
1:A:555:LEU:HD21	1:A:572:ILE:HD11	1.98	0.45
1:A:820:SER:O	1:A:824:ILE:HG13	2.17	0.45
1:A:879:GLU:HG3	1:A:880:GLU:HG3	1.99	0.45
1:A:653:ALA:O	1:A:657:THR:CB	2.52	0.45
1:A:215:THR:HG22	1:A:215:THR:O	2.15	0.45
1:A:67:ASP:HB3	1:A:70:LEU:HD22	1.97	0.45
1:A:889:LYS:HD3	1:A:935:ARG:NH1	2.32	0.45
1:A:574:ALA:O	1:A:578:ASP:OD2	2.33	0.45
1:A:844:PRO:HA	1:A:846:PRO:HD2	1.99	0.45
1:A:23:LEU:CD2	1:A:40:LEU:HD11	2.47	0.45
1:A:553:ALA:C	1:A:555:LEU:H	2.20	0.45
1:A:682:LEU:O	1:A:683:LEU:CG	2.64	0.45
1:A:396:ALA:O	1:A:397:ASP:HB2	2.17	0.45
1:A:397:ASP:OD1	1:A:397:ASP:N	2.50	0.45
1:A:997:ILE:HD12	1:A:997:ILE:N	2.32	0.44
1:A:694:HIS:ND1	1:A:694:HIS:C	2.70	0.44
1:A:528:ARG:HH12	1:A:646:LYS:HZ2	1.63	0.44
1:A:356:VAL:O	1:A:360:LEU:HG	2.16	0.44
1:A:74:MET:N	1:A:75:PRO:HD2	2.32	0.44
1:A:853:HIS:O	1:A:854:LEU:HB2	2.17	0.44
1:A:14:GLU:HG2	1:A:993:THR:HG21	1.99	0.44
1:A:234:VAL:CG1	1:A:234:VAL:O	2.66	0.44
1:A:408:ILE:O	1:A:412:MET:CG	2.62	0.44
1:A:70:LEU:HD11	1:A:129:ALA:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ILE:HA	1:A:302:ILE:CD1	2.48	0.44
1:A:877:PRO:N	1:A:878:PRO:HD2	2.33	0.44
1:A:504:ILE:CG1	1:A:576:LEU:CD2	2.78	0.44
1:A:790:LEU:O	1:A:794:ILE:HG12	2.17	0.44
1:A:441:LEU:O	1:A:466:ILE:HD11	2.16	0.44
1:A:12:ILE:CD1	1:A:54:LEU:HD11	2.45	0.44
1:A:211:ILE:HD11	1:A:694:HIS:CB	2.48	0.44
1:A:314:ALA:HB1	1:A:485:ARG:CZ	2.48	0.44
1:A:314:ALA:CB	1:A:485:ARG:HD3	2.47	0.44
1:A:703:ILE:O	1:A:703:ILE:HG22	2.17	0.44
1:A:285:ARG:O	1:A:287:PRO:HD2	2.13	0.44
1:A:219:LYS:HB2	1:A:223:ILE:HD11	2.00	0.44
1:A:403:GLU:C	1:A:405:GLU:H	2.21	0.44
1:A:940:GLY:HA2	1:A:943:ASN:HB2	2.00	0.44
1:A:821:GLY:HA2	1:A:824:ILE:HD12	2.00	0.43
1:A:974:ASP:HB3	1:A:977:ILE:HG22	2.00	0.43
1:A:665:VAL:HG22	1:A:709:MET:CE	2.48	0.43
1:A:665:VAL:HG22	1:A:709:MET:HE2	2.00	0.43
1:A:843:PRO:N	1:A:844:PRO:HD2	2.33	0.43
1:A:971:GLN:CG	1:A:1053:GLY:H	2.32	0.43
1:A:509:VAL:CG1	1:A:510:ASP:N	2.81	0.43
1:A:848:ASP:O	1:A:850:GLU:HG3	2.18	0.43
1:A:1048:ILE:HG22	1:A:1052:ALA:HB2	2.00	0.43
1:A:793:THR:HG22	1:A:824:ILE:HG12	2.00	0.43
1:A:619:THR:HB	1:A:620:PRO:HD3	2.00	0.43
1:A:100:TYR:N	1:A:100:TYR:CD1	2.85	0.43
1:A:880:GLU:O	1:A:881:LYS:HB3	2.18	0.43
1:A:747:GLN:NE2	1:A:750:VAL:CG2	2.80	0.43
1:A:839:GLU:O	1:A:840:PRO:C	2.57	0.43
1:A:664:THR:CG2	1:A:709:MET:HG3	2.49	0.43
1:A:178:ARG:HA	1:A:178:ARG:HD2	1.87	0.43
1:A:643:THR:O	1:A:643:THR:HG22	2.18	0.43
1:A:755:SER:O	1:A:756:ILE:C	2.56	0.43
1:A:756:ILE:HG21	1:A:797:MET:HE1	1.99	0.43
1:A:887:GLU:O	1:A:888:GLN:CB	2.65	0.43
1:A:1037:THR:O	1:A:1037:THR:HG22	2.19	0.43
1:A:917:ASN:OD1	1:A:920:ILE:HG12	2.19	0.43
1:A:844:PRO:CA	1:A:846:PRO:HD2	2.48	0.42
1:A:195:MET:O	1:A:199:LYS:HG3	2.19	0.42
1:A:24:VAL:HG11	1:A:948:ILE:HD11	2.01	0.42
1:A:1062:THR:HB	1:A:1063:PRO:CD	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:645:GLU:O	1:A:648:ALA:HB3	2.19	0.42
1:A:982:LEU:O	1:A:986:GLU:HB2	2.20	0.42
1:A:34:GLY:O	1:A:36:ALA:N	2.52	0.42
1:A:215:THR:CG2	1:A:223:ILE:HG12	2.49	0.42
1:A:660:GLY:O	1:A:661:ILE:C	2.58	0.42
1:A:642:ALA:O	1:A:646:LYS:HG2	2.19	0.42
1:A:219:LYS:HD2	1:A:219:LYS:N	2.35	0.42
1:A:81:VAL:CG1	1:A:82:GLU:N	2.83	0.42
1:A:967:GLU:HB3	1:A:1054:PHE:CE2	2.55	0.42
1:A:102:VAL:O	1:A:105:ARG:HG2	2.20	0.42
1:A:843:PRO:C	1:A:845:PRO:HD2	2.40	0.42
1:A:738:LYS:HD2	1:A:817:PHE:HZ	1.85	0.42
1:A:9:ILE:HD12	1:A:123:LEU:CB	2.46	0.42
1:A:929:LEU:HB3	1:A:954:ILE:HD11	2.00	0.42
1:A:149:GLU:CB	1:A:230:ARG:CZ	2.97	0.42
1:A:894:ILE:CG2	1:A:895:ASN:N	2.82	0.42
1:A:682:LEU:O	1:A:683:LEU:HD23	2.20	0.42
1:A:741:MET:HE1	1:A:814:GLN:HA	2.02	0.42
1:A:741:MET:HE1	1:A:817:PHE:CE2	2.48	0.42
1:A:853:HIS:C	1:A:854:LEU:HG	2.40	0.42
1:A:503:TRP:CH2	1:A:511:ASP:HB3	2.53	0.42
1:A:194:SER:HB2	1:A:244:ILE:HD11	2.01	0.42
1:A:631:ALA:O	1:A:635:ASN:ND2	2.53	0.42
1:A:74:MET:HE2	1:A:122:LEU:HD11	1.77	0.42
1:A:1048:ILE:N	1:A:1048:ILE:HD12	2.32	0.42
1:A:501:GLN:HA	1:A:504:ILE:HG22	2.02	0.42
1:A:702:TRP:CE3	1:A:703:ILE:HD12	2.44	0.42
1:A:558:LEU:HD23	1:A:559:ALA:HB2	2.02	0.42
1:A:405:GLU:O	1:A:409:ARG:HB2	2.20	0.42
1:A:973:THR:O	1:A:973:THR:OG1	2.25	0.41
1:A:703:ILE:HG22	1:A:707:GLU:HG3	2.02	0.41
1:A:703:ILE:O	1:A:707:GLU:HG3	2.20	0.41
1:A:653:ALA:HB1	1:A:657:THR:HB	2.02	0.41
1:A:876:PRO:HA	1:A:877:PRO:HD3	1.62	0.41
1:A:522:LEU:HD13	1:A:580:LEU:HD22	2.02	0.41
1:A:845:PRO:O	1:A:847:PRO:HD2	2.06	0.41
1:A:396:ALA:O	1:A:397:ASP:CB	2.68	0.41
1:A:91:ALA:HA	1:A:94:MET:SD	2.60	0.41
1:A:852:LEU:HA	1:A:852:LEU:HD12	1.67	0.41
1:A:853:HIS:CE1	1:A:855:THR:OG1	2.72	0.41
1:A:930:MET:CE	1:A:933:MET:HB3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:GLU:HB2	1:A:230:ARG:NE	2.35	0.41
1:A:938:ARG:HD3	1:A:938:ARG:HA	1.92	0.41
1:A:773:ASN:O	1:A:773:ASN:CG	2.58	0.41
1:A:314:ALA:H	1:A:318:ARG:HB2	1.86	0.41
1:A:604:THR:N	1:A:605:PRO:CD	2.83	0.41
1:A:623:GLU:O	1:A:624:GLU:C	2.57	0.41
1:A:227:LEU:HD22	1:A:230:ARG:NH2	2.29	0.41
1:A:758:ARG:H	1:A:758:ARG:HG3	1.57	0.41
1:A:1049:ARG:O	1:A:1051:ASP:N	2.53	0.41
1:A:974:ASP:O	1:A:975:LYS:C	2.58	0.41
1:A:930:MET:HE3	1:A:933:MET:SD	2.60	0.41
1:A:771:VAL:HG13	1:A:780:ARG:HG3	2.01	0.41
1:A:672:THR:N	1:A:673:PRO:CD	2.84	0.41
1:A:755:SER:O	1:A:759:ARG:HG2	2.20	0.41
1:A:211:ILE:HD11	1:A:694:HIS:CG	2.56	0.41
1:A:377:MET:HB3	1:A:481:VAL:CG1	2.51	0.41
1:A:42:ALA:N	1:A:43:PRO:HD2	2.35	0.41
1:A:258:TRP:CD1	1:A:258:TRP:C	2.93	0.41
1:A:20:ILE:HD11	1:A:1000:THR:HG22	2.03	0.41
1:A:188:ARG:O	1:A:192:VAL:HG23	2.21	0.41
1:A:399:ASN:HA	1:A:399:ASN:HD22	1.71	0.40
1:A:194:SER:CB	1:A:244:ILE:HD11	2.51	0.40
1:A:540:ASP:O	1:A:544:LYS:HG2	2.21	0.40
1:A:572:ILE:O	1:A:576:LEU:CB	2.70	0.40
1:A:70:LEU:HA	1:A:70:LEU:HD12	1.78	0.40
1:A:16:VAL:CG1	1:A:17:ALA:N	2.83	0.40
1:A:760:ALA:HB1	1:A:794:ILE:HD11	2.04	0.40
1:A:988:ILE:N	1:A:989:PRO:CD	2.84	0.40
1:A:442:THR:O	1:A:442:THR:HG22	2.20	0.40
1:A:1045:SER:OG	1:A:1045:SER:O	2.40	0.40
1:A:65:THR:HG21	1:A:70:LEU:HD23	2.04	0.40
1:A:25:ILE:HG23	1:A:948:ILE:CD1	2.50	0.40
1:A:495:GLY:O	1:A:498:GLU:HG2	2.22	0.40
1:A:506:ASN:O	1:A:508:THR:N	2.54	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:MET:CE	1:A:743:ASN:CB[3_655]	1.99	0.21

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	1045/1069 (98%)	898 (86%)	93 (9%)	54 (5%)	2 15

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	-1	PRO
1	A	221	GLN
1	A	290	PRO
1	A	291	PRO
1	A	397	ASP
1	A	399	ASN
1	A	453	LYS
1	A	489	ALA
1	A	510	ASP
1	A	535	GLY
1	A	565	GLU
1	A	743	ASN
1	A	809	SER
1	A	810	ASP
1	A	850	GLU
1	A	882	ASP
1	A	1050	THR
1	A	426	LYS
1	A	837	PRO
1	A	841	ASP
1	A	854	LEU
1	A	881	LYS
1	A	895	ASN
1	A	1011	ILE
1	A	101	SER
1	A	288	ASN
1	A	394	TRP
1	A	400	GLY

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Mol	Chain	Res	Type
1	A	602	THR
1	A	615	ALA
1	A	622	ARG
1	A	846	PRO
1	A	878	PRO
1	A	879	GLU
1	A	888	GLN
1	A	975	LYS
1	A	33	ASP
1	A	39	ASP
1	A	287	PRO
1	A	558	LEU
1	A	616	PRO
1	A	624	GLU
1	A	1062	THR
1	A	295	GLY
1	A	654	ASN
1	A	842	PHE
1	A	745	GLN
1	A	746	PRO
1	A	805	ALA
1	A	877	PRO
1	A	38	PRO
1	A	485	ARG
1	A	620	PRO
1	A	840	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	861/879 (98%)	742 (86%)	119 (14%)	4 19

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	PRO
1	A	4	PHE
1	A	6	THR
1	A	57	VAL
1	A	65	THR
1	A	67	ASP
1	A	69	ILE
1	A	70	LEU
1	A	93	GLN
1	A	94	MET
1	A	102	VAL
1	A	105	ARG
1	A	135	ILE
1	A	146	THR
1	A	147	VAL
1	A	152	GLU
1	A	153	THR
1	A	154	MET
1	A	156	ASP
1	A	177	GLU
1	A	207	SER
1	A	209	MET
1	A	211	ILE
1	A	218	THR
1	A	219	LYS
1	A	221	GLN
1	A	224	GLU
1	A	236	LYS
1	A	237	MET
1	A	246	ARG
1	A	253	TRP
1	A	254	ASP
1	A	256	ASP
1	A	258	TRP
1	A	268	ARG
1	A	270	LEU
1	A	272	LEU
1	A	287	PRO
1	A	290	PRO
1	A	291	PRO
1	A	313	CYS
1	A	316	LYS
1	A	341	ARG

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Mol	Chain	Res	Type
1	A	364	THR
1	A	372	ARG
1	A	399	ASN
1	A	403	GLU
1	A	424	GLU
1	A	430	ASP
1	A	449	ARG
1	A	479	ARG
1	A	481	VAL
1	A	486	PRO
1	A	488	LYS
1	A	501	GLN
1	A	504	ILE
1	A	505	ASP
1	A	514	VAL
1	A	528	ARG
1	A	529	LEU
1	A	541	LEU
1	A	550	GLN
1	A	558	LEU
1	A	572	ILE
1	A	583	LEU
1	A	586	ARG
1	A	594	GLU
1	A	602	THR
1	A	606	ILE
1	A	624	GLU
1	A	626	PHE
1	A	645	GLU
1	A	655	LYS
1	A	680	ARG
1	A	685	ASN
1	A	699	LYS
1	A	703	ILE
1	A	709	MET
1	A	741	MET
1	A	743	ASN
1	A	746	PRO
1	A	756	ILE
1	A	758	ARG
1	A	770	GLU
1	A	807	ASN

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Mol	Chain	Res	Type
1	A	808	ILE
1	A	810	ASP
1	A	817	PHE
1	A	832	ARG
1	A	840	PRO
1	A	843	PRO
1	A	844	PRO
1	A	845	PRO
1	A	846	PRO
1	A	847	PRO
1	A	848	ASP
1	A	849	LEU
1	A	850	GLU
1	A	852	LEU
1	A	855	THR
1	A	875	PRO
1	A	876	PRO
1	A	882	ASP
1	A	885	PHE
1	A	904	GLN
1	A	910	ARG
1	A	944	LYS
1	A	972	CYS
1	A	1006	LEU
1	A	1008	ARG
1	A	1009	THR
1	A	1013	ASP
1	A	1045	SER
1	A	1047	LYS
1	A	1048	ILE
1	A	1049	ARG
1	A	1057	ARG
1	A	1062	THR
1	A	1065	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	63	GLN
1	A	83	ASN
1	A	179	GLN

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Mol	Chain	Res	Type
1	A	185	GLN
1	A	221	GLN
1	A	399	ASN
1	A	407	HIS
1	A	474	GLN
1	A	478	ASN
1	A	499	GLN
1	A	531	ASN
1	A	575	GLN
1	A	577	GLN
1	A	635	ASN
1	A	694	HIS
1	A	700	ASN
1	A	747	GLN
1	A	814	GLN
1	A	1010	ASN
1	A	1028	GLN
1	A	1029	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 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	1049/1069 (98%)	0.43	80 (7%) 17 6	36, 125, 181, 205	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	892	GLU	12.1
1	A	893	ALA	9.7
1	A	510	ASP	9.1
1	A	895	ASN	8.6
1	A	894	ILE	7.5
1	A	879	GLU	6.6
1	A	815	LYS	5.9
1	A	811	PRO	5.5
1	A	809	SER	5.4
1	A	286	ASP	5.1
1	A	738	LYS	4.8
1	A	850	GLU	4.6
1	A	935	ARG	4.4
1	A	823	ARG	4.1
1	A	847	PRO	4.1
1	A	1008	ARG	4.0
1	A	749	LEU	3.9
1	A	810	ASP	3.8
1	A	397	ASP	3.8
1	A	875	PRO	3.8
1	A	814	GLN	3.7
1	A	483	ASN	3.7
1	A	25	ILE	3.7
1	A	614	THR	3.7
1	A	1014	GLU	3.7
1	A	812	GLY	3.5
1	A	620	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	88	LEU	3.4
1	A	514	VAL	3.4
1	A	877	PRO	3.4
1	A	635	ASN	3.4
1	A	63	GLN	3.3
1	A	682	LEU	3.3
1	A	490	ALA	3.3
1	A	485	ARG	3.3
1	A	513	GLY	3.3
1	A	53	ASN	3.2
1	A	504	ILE	3.0
1	A	575	GLN	3.0
1	A	813	LEU	2.9
1	A	880	GLU	2.9
1	A	62	VAL	2.9
1	A	512	ARG	2.9
1	A	619	THR	2.9
1	A	332	THR	2.8
1	A	406	GLU	2.8
1	A	819	ASP	2.8
1	A	489	ALA	2.8
1	A	451	HIS	2.8
1	A	61	THR	2.7
1	A	64	THR	2.7
1	A	65	THR	2.7
1	A	1007	GLY	2.7
1	A	838	GLN	2.7
1	A	1062	THR	2.6
1	A	570	ARG	2.6
1	A	840	PRO	2.5
1	A	842	PHE	2.5
1	A	878	PRO	2.5
1	A	888	GLN	2.4
1	A	290	PRO	2.4
1	A	57	VAL	2.4
1	A	224	GLU	2.4
1	A	841	ASP	2.4
1	A	794	ILE	2.3
1	A	164	LEU	2.3
1	A	548	VAL	2.3
1	A	750	VAL	2.3
1	A	316	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	152	GLU	2.3
1	A	628	GLU	2.2
1	A	943	ASN	2.2
1	A	109	ILE	2.2
1	A	853	HIS	2.2
1	A	473	LEU	2.1
1	A	54	LEU	2.1
1	A	457	PRO	2.1
1	A	252	SER	2.1
1	A	746	PRO	2.0
1	A	33	ASP	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.