Full wwPDB X-ray Structure Validation Report (i)

Aug 27, 2020 – 01:53 PM BST

PDB ID	:	6T1W
Title	:	Structure of E. coli BamA in complex with lipoprotein RcsF
Authors	:	Letoquart, J.; Remaut, H.; Collet, J.F.
Deposited on	:	2019-10-07
Resolution	:	3.79 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 (i) symbol.

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

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13
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)	:	2.13

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.79 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	Percentile Ranks	Value
Rfree		0.360
Clashscore		12
Ramachandran outliers		0.7%
Sidechain outliers		8.0%
RSRZ outliers		9.1%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
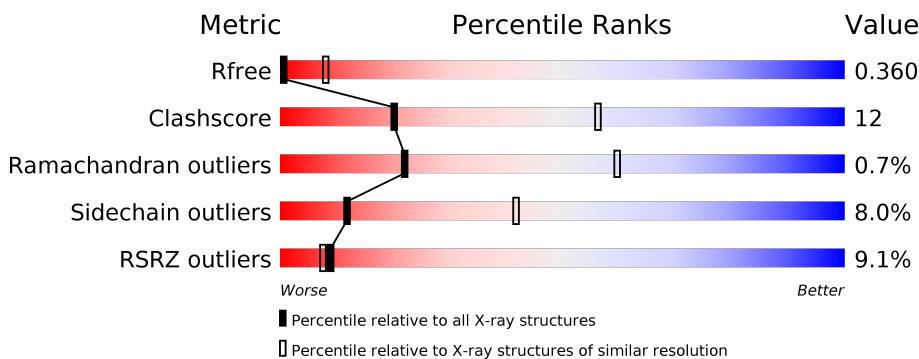
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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 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	810	7% — 66% / 25% / • 6%
1	B	810	4% — 43% / 13% • 42%
2	C	134	15% — 46% / 13% • 40%
2	D	134	14% — 49% / 11% 40%
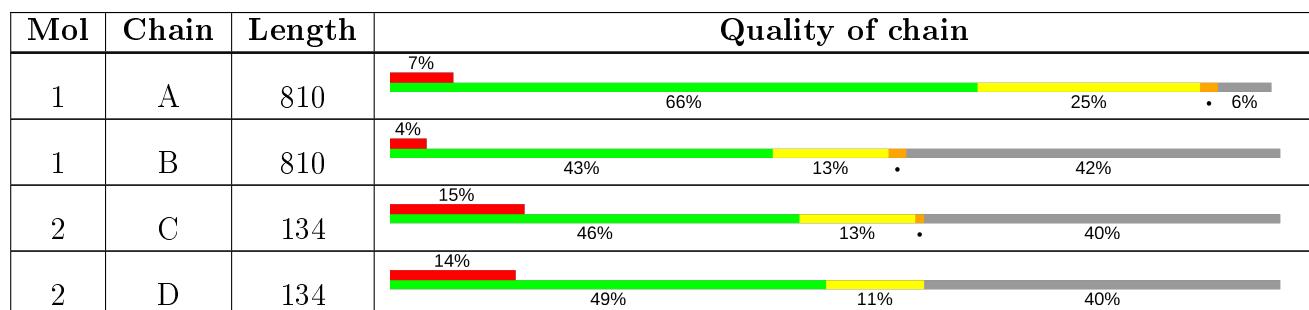
2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10838 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 Outer membrane protein assembly factor BamA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	761	Total 5991	C 3780	N 1004	O 1191	S 16	0	0	0
1	B	466	Total 3661	C 2318	N 595	O 736	S 12	0	0	0

- Molecule 2 is a protein called Outer membrane lipoprotein RcsF.

| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	80	Total 589	C 358	N 107	O 118	S 6	0	0	0
2	D	81	Total 597	C 364	N 108	O 119	S 6	0	0	0

3 Residue-property plots ⓘ

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

- Molecule 1: Outer membrane protein assembly factor BamA
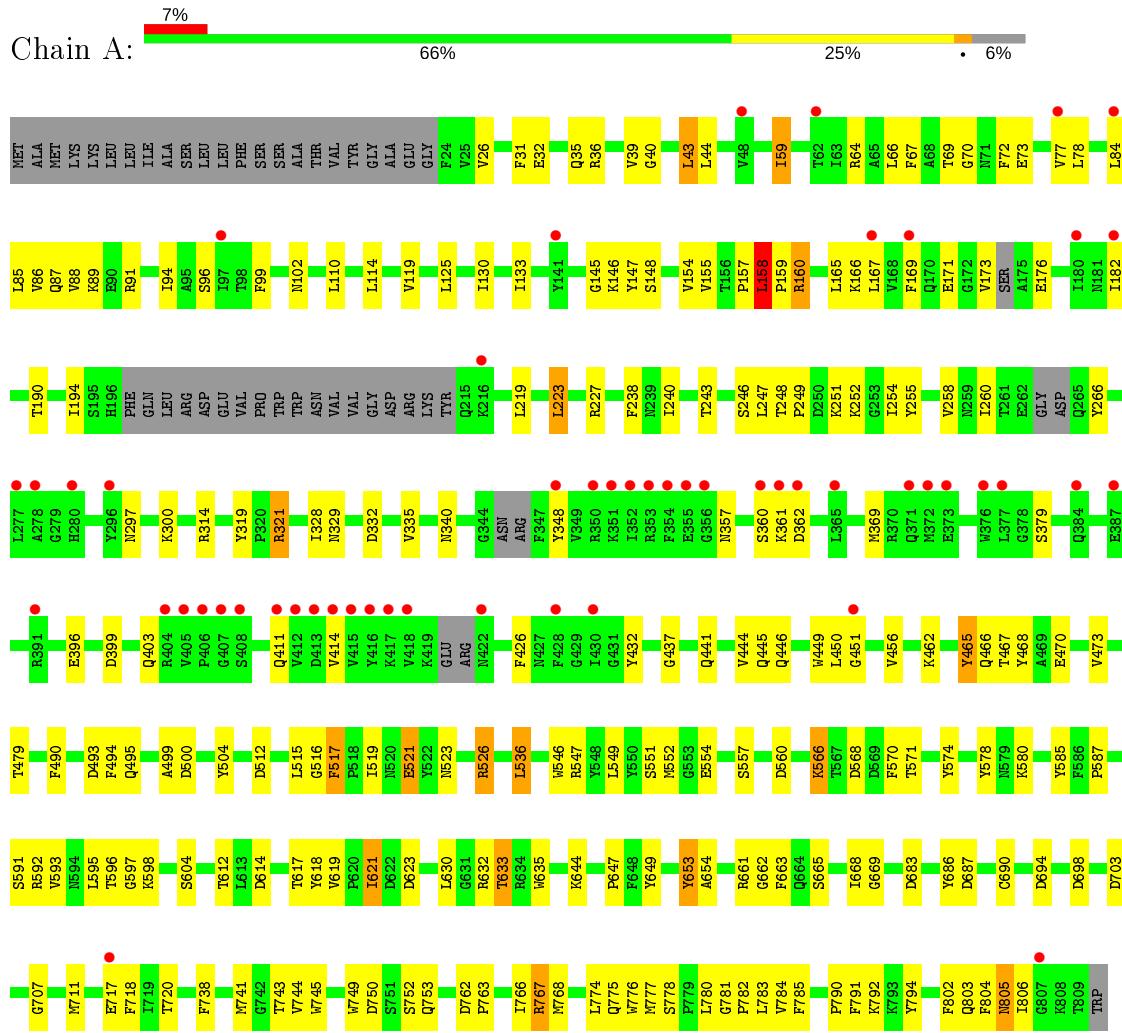
- Molecule 1: Outer membrane protein assembly factor BamA
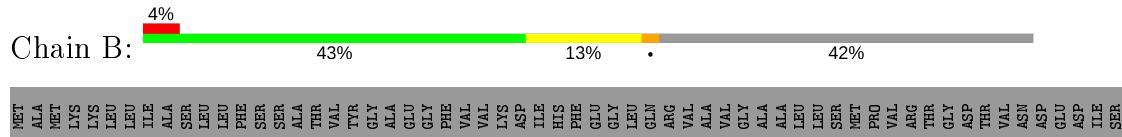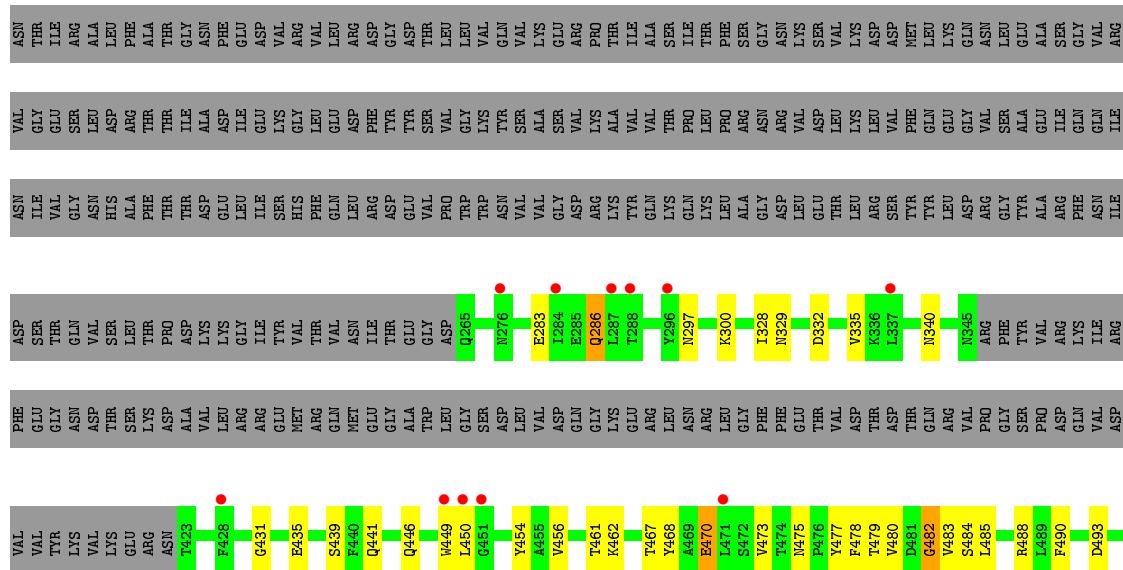
• Molecule 2: Outer membrane lipoprotein RcsF

Chain C:

15%

46%   13%   •   40%

• Molecule 2: Outer membrane lipoprotein RcsF

Chain D:

14%

49%   11%   40%
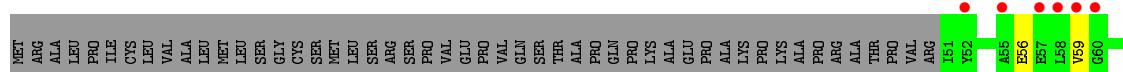
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	158.84Å 142.53Å 116.42Å 90.00° 102.61° 90.00°	Depositor
Resolution (Å)	48.58 – 3.79 48.58 – 3.79	Depositor EDS
% Data completeness (in resolution range)	73.4 (48.58-3.79) 73.4 (48.58-3.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.43 (at 3.77Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.281 , 0.317 0.313 , 0.360	Depositor DCC
R_{free} test set	973 reflections (5.26%)	wwPDB-VP
Wilson B-factor (Å^2)	161.7	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 185.7	EDS
L-test for twinning[2]	$<|L|> = 0.45$, $<L^2> = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	10838	wwPDB-VP
Average B, all atoms (Å^2)	193.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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	0.53	0/6122	0.74	1/8297 (0.0%)
1	B	0.46	0/3762	0.72	2/5114 (0.0%)
2	C	0.54	0/597	0.68	0/807
2	D	0.47	0/605	0.68	0/818
All	All	0.50	0/11086	0.73	3/15036 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	521	GLU	N-CA-CB	5.22	119.99	110.60
1	B	735	THR	CB-CA-C	-5.15	97.68	111.60
1	B	732	SER	CB-CA-C	-5.10	100.41	110.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5991	0	5715	178	1
1	B	3661	0	3383	76	0
2	C	589	0	579	15	0
2	D	597	0	590	17	0
All	All	10838	0	10267	263	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 12.

All (263) 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:566:LYS:O	1:A:566:LYS:HD2	1.31	1.22
1:A:462:LYS:CD	1:A:467:THR:HG22	1.76	1.15
1:B:488:ARG:NH1	2:D:81:SER:HA	1.60	1.14
1:A:462:LYS:HD3	1:A:467:THR:HG22	1.15	1.11
1:A:158:LEU:HB3	1:A:159:PRO:HD2	1.35	1.09
1:A:632:ARG:HD3	2:C:116:PRO:HB3	1.33	1.06
1:A:462:LYS:HD3	1:A:467:THR:CG2	1.85	1.04
1:A:566:LYS:O	1:A:566:LYS:CD	2.05	1.03
1:A:219:LEU:O	1:A:219:LEU:HD12	1.58	1.03
1:A:146:LYS:HE2	1:A:173:VAL:HG22	1.45	0.99
1:B:632:ARG:HD2	2:D:116:PRO:HB3	1.41	0.98
1:B:479:THR:HG22	1:B:480:VAL:H	1.28	0.98
1:A:157:PRO:O	1:A:158:LEU:HD22	1.61	0.97
1:A:783:LEU:HD13	1:A:806:ILE:HG13	1.45	0.96
1:A:157:PRO:C	1:A:158:LEU:HD23	1.86	0.95
1:A:110:LEU:HD21	1:A:169:PHE:CZ	2.02	0.93
1:A:632:ARG:HD3	2:C:116:PRO:CB	1.97	0.93
1:A:40:GLY:HA2	1:A:43:LEU:HD23	1.50	0.91
1:A:557:SER:HB3	1:A:560:ASP:OD1	1.70	0.91
1:A:158:LEU:HB3	1:A:159:PRO:CD	2.01	0.89
1:B:462:LYS:HD3	1:B:467:THR:HB	1.52	0.89
1:A:157:PRO:C	1:A:158:LEU:CD2	2.43	0.87
1:A:157:PRO:O	1:A:158:LEU:CD2	2.24	0.86
1:B:488:ARG:HH12	2:D:81:SER:HA	1.40	0.86
1:B:479:THR:CG2	1:B:480:VAL:H	1.89	0.85
1:B:488:ARG:HH11	2:D:81:SER:HA	1.40	0.83
1:B:479:THR:HG22	1:B:480:VAL:N	1.92	0.83
2:C:90:LYS:HE2	2:C:94:ILE:HD11	1.63	0.80
1:A:146:LYS:HE2	1:A:173:VAL:CG2	2.13	0.79
1:A:219:LEU:CD1	1:A:223:LEU:HD23	2.12	0.79
1:A:750:ASP:OD2	1:A:753:GLN:HB2	1.84	0.78
1:A:125:LEU:CD2	1:A:165:LEU:HD12	2.13	0.78
2:D:90:LYS:HE2	2:D:94:ILE:HD11	1.64	0.78
1:A:219:LEU:HD13	1:A:223:LEU:HD23	1.67	0.77
1:A:155:VAL:O	1:A:155:VAL:HG12	1.86	0.76
1:A:462:LYS:CD	1:A:467:THR:CG2	2.55	0.75
1:A:783:LEU:HD12	1:A:784:VAL:H	1.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:LYS:HD2	1:A:467:THR:HG22	1.69	0.75
1:A:632:ARG:NH2	1:A:661:ARG:NH1	2.37	0.73
1:A:467:THR:OG1	1:A:493:ASP:HB3	1.90	0.71
1:B:441:GLN:HE21	1:B:461:THR:HG23	1.55	0.71
1:A:465:TYR:HD1	1:A:466:GLN:H	1.37	0.71
1:A:767:ARG:HD2	1:A:794:TYR:HD2	1.56	0.70
1:B:478:PHE:HB3	1:B:483:VAL:HG13	1.73	0.70
1:A:630:LEU:HB3	1:A:717:GLU:HB2	1.74	0.69
1:A:73:GLU:HG3	1:A:91:ARG:HA	1.75	0.68
2:C:95:ASN:O	2:C:99:MET:HG2	1.93	0.68
1:B:770:ALA:HB3	1:B:791:PHE:CE1	2.28	0.68
1:A:450:LEU:HG	1:A:450:LEU:O	1.94	0.67
1:A:125:LEU:CD2	1:A:165:LEU:CD1	2.72	0.67
1:A:154:VAL:HB	1:A:166:LYS:HB3	1.75	0.67
1:A:99:PHE:HE1	1:A:167:LEU:HD12	1.59	0.67
1:B:630:LEU:HB3	1:B:717:GLU:HB2	1.77	0.66
1:A:247:LEU:HD21	1:A:254:ILE:HG12	1.77	0.66
1:A:247:LEU:CD2	1:A:254:ILE:HG12	2.25	0.66
1:A:536:LEU:HD11	1:A:649:TYR:CE1	2.30	0.66
1:A:77:VAL:O	1:A:78:LEU:HD23	1.96	0.65
1:A:125:LEU:HD22	1:A:165:LEU:HD12	1.78	0.65
1:A:805:ASN:HB3	2:C:113:SER:CB	2.27	0.65
1:B:450:LEU:O	1:B:450:LEU:HG	1.97	0.65
1:A:125:LEU:HD22	1:A:165:LEU:CD1	2.27	0.65
1:B:738:PHE:CE2	1:B:773:ALA:HB2	2.33	0.64
1:A:805:ASN:HB3	2:C:113:SER:HB2	1.79	0.64
1:B:475:ASN:H	1:B:485:LEU:HB3	1.62	0.64
1:B:479:THR:CG2	1:B:480:VAL:N	2.57	0.64
1:A:632:ARG:NH2	1:A:717:GLU:OE1	2.31	0.64
1:B:468:TYR:HE1	1:B:490:PHE:HB2	1.63	0.63
1:A:227:ARG:HG2	1:A:238:PHE:HE2	1.64	0.63
1:A:246:SER:O	1:A:247:LEU:HD23	2.00	0.61
1:A:102:ASN:HA	1:A:171:GLU:OE2	2.00	0.61
1:A:574:TYR:CZ	1:A:597:GLY:HA3	2.36	0.60
1:B:488:ARG:HH12	2:D:81:SER:CA	2.13	0.60
1:B:766:ILE:HG21	1:B:768:MET:CE	2.31	0.60
1:A:99:PHE:CE1	1:A:167:LEU:HD12	2.38	0.59
1:A:176:GLU:O	1:A:254:ILE:HB	2.02	0.59
1:B:488:ARG:HH11	2:D:82:PRO:HD3	1.68	0.58
1:A:711:MET:HG3	1:A:744:VAL:HG22	1.84	0.58
1:B:439:SER:HB2	1:B:441:GLN:HE22	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:520:ASN:HB3	1:B:523:ASN:HD22	1.67	0.57
1:B:571:THR:HG21	1:B:598:LYS:HD3	1.85	0.57
1:A:519:ILE:HD11	1:B:627:TRP:CZ3	2.39	0.57
1:A:557:SER:HB3	1:A:560:ASP:CG	2.24	0.57
1:A:571:THR:HG21	1:A:598:LYS:HD3	1.85	0.57
1:B:591:SER:HB3	1:B:617:THR:HG23	1.85	0.57
1:B:782:PRO:HG2	2:D:111:VAL:O	2.05	0.57
1:B:743:THR:OG1	1:B:766:ILE:HA	2.06	0.56
1:B:766:ILE:HG21	1:B:768:MET:HE2	1.86	0.56
1:A:468:TYR:HE1	1:A:490:PHE:HB2	1.71	0.56
1:A:357:ASN:HD21	1:A:362:ASP:CG	2.09	0.56
1:A:591:SER:HB3	1:A:617:THR:HG23	1.87	0.55
1:A:782:PRO:HD3	2:C:110:GLU:HB3	1.89	0.55
1:A:445:GLN:HE21	2:C:86:PRO:HG2	1.71	0.55
1:B:467:THR:HG22	1:B:493:ASP:HB3	1.90	0.54
1:B:522:TYR:HE1	1:B:578:TYR:CE2	2.26	0.54
2:D:69:VAL:HG21	2:D:96:ALA:HB2	1.89	0.54
1:A:155:VAL:HG22	1:A:165:LEU:HG	1.88	0.54
1:A:465:TYR:HD2	1:A:499:ALA:HA	1.72	0.54
2:C:69:VAL:HG21	2:C:96:ALA:HB2	1.89	0.54
1:A:632:ARG:HH22	1:A:661:ARG:NH1	2.04	0.54
1:A:147:TYR:HE2	1:A:254:ILE:HD11	1.73	0.53
1:A:247:LEU:HD23	1:A:254:ILE:HA	1.89	0.53
1:A:632:ARG:NH2	1:A:661:ARG:HH12	2.07	0.53
1:B:531:TYR:CD1	1:B:570:PHE:HD1	2.27	0.53
1:A:432:TYR:HA	1:A:437:GLY:O	2.08	0.53
1:A:775:GLN:HA	1:A:783:LEU:O	2.08	0.53
1:A:662:GLY:O	1:A:790:PRO:HG3	2.09	0.53
1:A:190:THR:O	1:A:194:ILE:HG12	2.09	0.53
1:A:85:LEU:HG	1:A:86:VAL:N	2.23	0.52
1:A:768:MET:HB2	1:A:791:PHE:CE2	2.44	0.52
1:A:70:GLY:HA2	1:A:91:ARG:HH21	1.74	0.52
1:A:632:ARG:HH22	1:A:661:ARG:CZ	2.23	0.52
1:A:158:LEU:N	1:A:158:LEU:HD23	2.23	0.52
1:A:547:ARG:HH22	1:A:749:TRP:HE3	1.58	0.52
1:A:783:LEU:HD21	1:A:785:PHE:HE1	1.75	0.52
1:A:778:SER:OG	1:A:780:LEU:HD12	2.09	0.52
1:A:248:THR:HB	1:A:249:PRO:HD2	1.92	0.51
1:A:653:TYR:CD2	1:A:707:GLY:HA3	2.45	0.51
1:A:632:ARG:CD	2:C:116:PRO:HB3	2.23	0.51
1:A:319:TYR:HB3	1:A:321:ARG:HH11	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:668:ILE:HG23	1:B:767:ARG:HD3	1.92	0.51
1:B:785:PHE:CD1	1:B:785:PHE:O	2.63	0.51
1:A:32:GLU:HG3	1:A:85:LEU:HD11	1.91	0.51
1:B:738:PHE:HE2	1:B:773:ALA:HB2	1.75	0.51
1:B:732:SER:HB2	1:B:777:MET:HB2	1.92	0.51
1:A:227:ARG:HG3	1:A:240:ILE:HD12	1.92	0.51
1:A:158:LEU:CB	1:A:159:PRO:CD	2.85	0.51
1:B:478:PHE:HB2	1:B:485:LEU:HB2	1.93	0.50
1:A:566:LYS:CD	1:A:566:LYS:C	2.79	0.50
1:B:659:THR:O	1:B:740:ASP:OD2	2.29	0.50
1:A:69:THR:HG21	1:A:72:PHE:CE1	2.47	0.50
1:A:99:PHE:HD1	1:A:167:LEU:HB2	1.77	0.50
1:B:456:VAL:HG12	1:B:473:VAL:HG22	1.94	0.50
1:A:99:PHE:CG	1:A:110:LEU:HD23	2.46	0.49
1:A:72:PHE:CD2	1:A:88:VAL:HB	2.48	0.49
1:A:114:LEU:HB3	1:A:119:VAL:HG13	1.94	0.49
1:A:711:MET:CG	1:A:744:VAL:HG22	2.42	0.49
1:B:784:VAL:CG2	1:B:805:ASN:HB3	2.43	0.49
1:A:176:GLU:OE1	1:A:252:LYS:HB2	2.13	0.49
1:A:456:VAL:HG12	1:A:473:VAL:HG22	1.95	0.49
1:A:711:MET:HB2	1:A:744:VAL:HG13	1.94	0.49
1:B:470:GLU:OE2	2:D:82:PRO:HG3	2.13	0.49
1:A:148:SER:N	1:A:251:LYS:HB3	2.27	0.49
1:A:782:PRO:HG3	2:C:111:VAL:O	2.13	0.49
1:A:446:GLN:HB3	1:A:449:TRP:HB2	1.95	0.48
1:A:621:ILE:CD1	1:A:718:PHE:HE1	2.25	0.48
1:B:446:GLN:HB3	1:B:449:TRP:HB2	1.93	0.48
1:A:40:GLY:HA2	1:A:43:LEU:CD2	2.35	0.48
1:A:767:ARG:HD2	1:A:794:TYR:CD2	2.44	0.48
1:A:803:GLN:O	1:A:804:PHE:HB3	2.13	0.48
1:A:774:LEU:O	1:A:784:VAL:HA	2.13	0.48
1:A:158:LEU:CD2	1:A:158:LEU:N	2.72	0.48
1:A:66:LEU:O	1:A:69:THR:HG22	2.14	0.48
1:B:283:GLU:O	1:B:286:GLN:NE2	2.47	0.48
1:B:653:TYR:CD2	1:B:707:GLY:HA3	2.48	0.48
1:A:536:LEU:HD21	1:A:649:TYR:CD1	2.48	0.48
1:B:717:GLU:HG2	1:B:738:PHE:HB3	1.96	0.47
2:C:105:LEU:HB2	2:C:129:LEU:HD11	1.95	0.47
1:A:552:MET:HA	1:A:644:LYS:HE2	1.96	0.47
1:A:110:LEU:HD21	1:A:169:PHE:HZ	1.72	0.47
1:A:745:TRP:CE2	1:A:763:PRO:HB3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:592:ARG:HH12	2:D:121:GLN:NE2	2.12	0.47
2:D:105:LEU:HB2	2:D:129:LEU:HD11	1.96	0.47
1:A:504:TYR:OH	1:A:649:TYR:HA	2.14	0.47
1:A:776:TRP:HD1	1:A:777:MET:H	1.63	0.47
1:B:475:ASN:O	1:B:484:SER:HA	2.13	0.47
1:A:94:ILE:HD11	1:A:125:LEU:HB2	1.97	0.47
1:B:621:ILE:CD1	1:B:718:PHE:HE1	2.27	0.47
1:A:361:LYS:HG2	1:A:451:GLY:HA3	1.96	0.46
1:A:426:PHE:HD1	1:A:444:VAL:HG23	1.79	0.46
1:A:570:PHE:H	1:A:604:SER:HB3	1.79	0.46
1:B:552:MET:HA	1:B:644:LYS:HE2	1.96	0.46
1:B:576:TRP:HE1	1:B:578:TYR:HD1	1.62	0.46
1:A:781:GLY:HA2	2:C:110:GLU:CD	2.36	0.46
1:A:783:LEU:HD13	1:A:806:ILE:CG1	2.32	0.46
1:A:158:LEU:CB	1:A:159:PRO:HD2	2.25	0.46
1:A:246:SER:HB2	1:A:255:TYR:HB2	1.96	0.46
1:B:613:LEU:HB2	1:B:635:TRP:HB2	1.97	0.46
1:A:717:GLU:HG2	1:A:738:PHE:HB3	1.96	0.46
1:A:743:THR:OG1	1:A:766:ILE:HA	2.15	0.46
1:A:462:LYS:HD3	1:A:467:THR:HG21	1.91	0.45
1:A:783:LEU:CD1	1:A:784:VAL:H	2.25	0.45
1:A:551:SER:HB3	1:A:644:LYS:HA	1.99	0.45
1:B:587:PRO:HG2	1:B:618:TYR:CZ	2.52	0.45
1:A:125:LEU:HD21	1:A:165:LEU:CD1	2.46	0.45
1:A:587:PRO:HG2	1:A:618:TYR:CZ	2.52	0.45
1:A:26:VAL:HG21	1:A:84:LEU:HD22	1.98	0.45
1:B:570:PHE:H	1:B:604:SER:HB3	1.81	0.45
1:B:435:GLU:OE1	1:B:805:ASN:HB2	2.17	0.45
1:A:247:LEU:CD2	1:A:254:ILE:CG1	2.95	0.45
1:A:59:ILE:HD13	1:A:78:LEU:CD2	2.47	0.44
1:B:518:PRO:HG2	2:D:90:LYS:HE3	1.99	0.44
1:A:182:ILE:CG2	1:A:260:ILE:HD12	2.47	0.44
1:A:148:SER:O	1:A:251:LYS:CE	2.65	0.44
1:A:465:TYR:O	1:A:495:GLN:NE2	2.50	0.44
1:B:515:LEU:O	1:B:515:LEU:HD12	2.18	0.44
1:B:488:ARG:HH11	2:D:82:PRO:CD	2.30	0.44
2:D:56:GLU:HA	2:D:59:VAL:HG23	1.99	0.44
1:A:72:PHE:CD1	1:A:72:PHE:N	2.84	0.44
1:A:523:ASN:ND2	1:A:578:TYR:HD2	2.16	0.44
1:A:238:PHE:CE1	1:A:260:ILE:HG23	2.52	0.44
1:A:515:LEU:HB3	1:A:517:PHE:HE1	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:632:ARG:HH21	1:A:661:ARG:HH12	1.65	0.44
1:A:647:PRO:HB3	1:A:649:TYR:CE1	2.52	0.44
1:B:467:THR:CG2	1:B:493:ASP:HB3	2.48	0.44
1:A:147:TYR:H	1:A:251:LYS:HB2	1.83	0.43
1:A:219:LEU:CD1	1:A:219:LEU:O	2.48	0.43
1:A:783:LEU:HD12	1:A:805:ASN:O	2.19	0.43
1:A:593:VAL:HA	1:A:614:ASP:O	2.17	0.43
1:A:663:PHE:CG	1:A:668:ILE:HD11	2.53	0.43
1:A:297:ASN:HB3	1:A:300:LYS:HD2	2.01	0.43
1:A:77:VAL:O	1:A:78:LEU:CD2	2.64	0.43
1:B:617:THR:O	1:B:630:LEU:HD12	2.19	0.43
1:B:297:ASN:HB3	1:B:300:LYS:HD2	2.01	0.43
1:A:546:TRP:HA	1:A:549:LEU:HD12	2.00	0.43
1:A:762:ASP:HA	1:A:763:PRO:HD3	1.93	0.43
1:A:632:ARG:HH21	1:A:661:ARG:NH1	2.15	0.43
1:A:130:ILE:HA	1:A:133:ILE:HD12	2.01	0.43
1:A:328:ILE:HA	1:A:335:VAL:HG22	2.01	0.43
1:A:266:TYR:OH	1:A:328:ILE:HG23	2.17	0.43
1:A:654:ALA:HB3	1:A:668:ILE:HB	2.01	0.43
1:A:669:GLY:H	1:A:767:ARG:NH2	2.17	0.43
1:A:784:VAL:O	1:A:804:PHE:CB	2.67	0.43
1:A:73:GLU:N	1:A:89:LYS:O	2.51	0.42
1:B:647:PRO:HB3	1:B:649:TYR:CE1	2.54	0.42
1:A:148:SER:O	1:A:251:LYS:HE3	2.20	0.42
1:B:286:GLN:HB3	1:B:286:GLN:HE21	1.61	0.42
2:C:56:GLU:HA	2:C:59:VAL:HG23	2.01	0.42
1:A:348:TYR:HB2	1:A:411:GLN:HG2	2.02	0.42
1:B:551:SER:HB3	1:B:644:LYS:HA	2.00	0.42
1:B:477:TYR:HB2	1:B:482:GLY:HA2	2.01	0.42
1:B:654:ALA:HB3	1:B:668:ILE:HB	2.01	0.42
1:A:243:THR:HG22	1:A:258:VAL:HG23	2.02	0.42
1:A:86:VAL:HG12	1:A:88:VAL:HG12	2.00	0.42
1:B:477:TYR:CG	1:B:477:TYR:O	2.73	0.42
1:B:454:TYR:CD1	1:B:475:ASN:HB2	2.55	0.42
1:A:426:PHE:CD1	1:A:444:VAL:HG23	2.54	0.42
1:A:741:MET:HA	1:A:767:ARG:O	2.19	0.42
1:B:632:ARG:HD2	2:D:116:PRO:CB	2.31	0.42
1:A:783:LEU:HG	1:A:784:VAL:N	2.34	0.41
1:B:431:GLY:HA3	1:B:806:ILE:O	2.20	0.41
1:B:729:TYR:HA	1:B:729:TYR:HD1	1.79	0.41
1:B:766:ILE:HG21	1:B:768:MET:HE3	1.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:GLY:HA2	1:A:526:ARG:HA	2.03	0.41
1:A:72:PHE:HD2	1:A:88:VAL:HB	1.84	0.41
1:A:147:TYR:HB2	1:A:251:LYS:HA	2.02	0.41
1:A:40:GLY:O	1:A:43:LEU:HG	2.21	0.41
1:A:785:PHE:CD2	1:A:802:PHE:CE2	3.09	0.41
1:B:741:MET:SD	1:B:768:MET:CE	3.08	0.41
1:A:633:THR:HG1	1:A:635:TRP:HE1	1.67	0.41
1:A:85:LEU:HD21	1:A:87:GLN:HG2	2.03	0.41
1:B:776:TRP:HD1	1:B:777:MET:N	2.19	0.41
1:B:592:ARG:HH22	2:D:121:GLN:HE22	1.68	0.41
1:A:595:LEU:HD23	1:A:596:THR:N	2.36	0.41
1:A:617:THR:O	1:A:630:LEU:HD12	2.21	0.41
1:A:85:LEU:HD23	1:A:87:GLN:HG3	2.02	0.41
1:B:535:SER:HB2	1:B:566:LYS:HG2	2.03	0.41
1:A:314:ARG:HA	1:A:379:SER:HB3	2.02	0.40
1:B:767:ARG:N	1:B:767:ARG:HD2	2.36	0.40
2:C:91:ARG:HA	2:C:94:ILE:HD12	2.03	0.40
1:A:783:LEU:CG	1:A:784:VAL:N	2.84	0.40
1:A:31:PHE:CE2	1:A:39:VAL:HG13	2.56	0.40
1:A:784:VAL:O	1:A:804:PHE:HB2	2.21	0.40
1:B:328:ILE:HA	1:B:335:VAL:HG22	2.03	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:160:ARG:O	1:A:698:ASP:OD2[4_446]	2.17	0.03

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	749/810 (92%)	685 (92%)	61 (8%)	3 (0%)	34	70
1	B	462/810 (57%)	419 (91%)	41 (9%)	2 (0%)	34	70
2	C	78/134 (58%)	70 (90%)	6 (8%)	2 (3%)	5	36
2	D	79/134 (59%)	70 (89%)	7 (9%)	2 (2%)	5	36
All	All	1368/1888 (72%)	1244 (91%)	115 (8%)	9 (1%)	22	60

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	145	GLY
1	A	160	ARG
2	C	100	LYS
2	C	117	GLY
2	D	100	LYS
1	A	158	LEU
1	B	519	ILE
2	D	117	GLY
1	B	482	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	646/688 (94%)	591 (92%)	55 (8%)	10	40
1	B	389/688 (56%)	352 (90%)	37 (10%)	8	34
2	C	66/111 (60%)	65 (98%)	1 (2%)	65	81
2	D	67/111 (60%)	67 (100%)	0	100	100
All	All	1168/1598 (73%)	1075 (92%)	93 (8%)	12	42

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	36	ARG

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Mol	Chain	Res	Type
1	A	43	LEU
1	A	44	LEU
1	A	59	ILE
1	A	64	ARG
1	A	67	PHE
1	A	96	SER
1	A	158	LEU
1	A	223	LEU
1	A	321	ARG
1	A	329	ASN
1	A	332	ASP
1	A	340	ASN
1	A	360	SER
1	A	369	MET
1	A	396	GLU
1	A	399	ASP
1	A	403	GLN
1	A	414	VAL
1	A	441	GLN
1	A	465	TYR
1	A	470	GLU
1	A	479	THR
1	A	494	PHE
1	A	500	ASP
1	A	512	ASP
1	A	517	PHE
1	A	521	GLU
1	A	526	ARG
1	A	536	LEU
1	A	554	GLU
1	A	566	LYS
1	A	568	ASP
1	A	580	LYS
1	A	585	TYR
1	A	592	ARG
1	A	612	THR
1	A	619	VAL
1	A	621	ILE
1	A	623	ASP
1	A	633	THR
1	A	653	TYR
1	A	665	SER

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Mol	Chain	Res	Type
1	A	683	ASP
1	A	686	TYR
1	A	687	ASP
1	A	690	CYS
1	A	694	ASP
1	A	703	ASP
1	A	720	THR
1	A	752	SER
1	A	767	ARG
1	A	792	LYS
1	A	805	ASN
1	B	286	GLN
1	B	329	ASN
1	B	332	ASP
1	B	340	ASN
1	B	470	GLU
1	B	500	ASP
1	B	517	PHE
1	B	519	ILE
1	B	521	GLU
1	B	523	ASN
1	B	533	HIS
1	B	568	ASP
1	B	578	TYR
1	B	585	TYR
1	B	591	SER
1	B	592	ARG
1	B	595	LEU
1	B	619	VAL
1	B	621	ILE
1	B	623	ASP
1	B	632	ARG
1	B	633	THR
1	B	639	ASP
1	B	653	TYR
1	B	665	SER
1	B	683	ASP
1	B	686	TYR
1	B	687	ASP
1	B	690	CYS
1	B	694	ASP
1	B	720	THR

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Mol	Chain	Res	Type
1	B	729	TYR
1	B	749	TRP
1	B	762	ASP
1	B	774	LEU
1	B	785	PHE
1	B	795	ASP
2	C	95	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	357	ASN
1	A	448	ASN
1	A	466	GLN
1	A	492	ASN
1	A	495	GLN
1	A	561	GLN
1	A	731	ASN
1	A	748	ASN
1	A	775	GLN
1	B	286	GLN
1	B	441	GLN
1	B	523	ASN
1	B	731	ASN
2	C	121	GLN
2	D	121	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	761/810 (93%)	0.12	54 (7%)	16	12	49, 160, 295, 300	0
1	B	466/810 (57%)	0.17	33 (7%)	16	12	101, 227, 277, 300	0
2	C	80/134 (59%)	1.16	20 (25%)	0	0	102, 206, 283, 296	0
2	D	81/134 (60%)	1.40	19 (23%)	0	0	189, 254, 297, 300	0
All	All	1388/1888 (73%)	0.27	126 (9%)	9	7	49, 202, 293, 300	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	597	GLY	11.2
2	D	55	ALA	8.1
1	A	355	GLU	7.6
2	D	64	ARG	6.9
2	C	60	GLY	6.8
2	D	51	ILE	6.7
1	A	377	LEU	6.4
2	D	130	ASN	6.3
1	A	406	PRO	6.1
1	A	356	GLY	6.1
2	C	58	LEU	6.0
1	A	350	ARG	5.9
2	D	58	LEU	5.8
2	D	105	LEU	5.8
2	D	56	GLU	5.5
1	A	296	TYR	5.4
2	C	104	VAL	5.2
1	A	807	GLY	5.1
1	A	352	ILE	5.0
1	A	360	SER	4.9
2	D	131	ILE	4.8

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Mol	Chain	Res	Type	RSRZ
2	D	106	LEU	4.8
1	A	353	ARG	4.7
1	A	354	PHE	4.6
1	A	413	ASP	4.6
1	A	277	LEU	4.4
1	A	422	ASN	4.4
1	A	169	PHE	4.3
1	A	365	LEU	4.2
1	A	361	LYS	4.2
1	A	372	MET	4.1
1	B	685	ASP	4.1
1	A	278	ALA	4.0
1	A	411	GLN	3.9
1	A	391	ARG	3.9
1	B	287	LEU	3.9
1	A	376	TRP	3.9
1	A	405	VAL	3.9
2	C	100	LYS	3.8
2	C	121	GLN	3.7
2	D	52	TYR	3.7
1	B	284	ILE	3.7
1	B	296	TYR	3.6
1	B	783	LEU	3.6
2	C	72	ASP	3.6
2	C	59	VAL	3.6
1	B	596	THR	3.5
2	D	65	ASP	3.5
1	A	180	ILE	3.4
1	A	415	VAL	3.4
1	A	348	TYR	3.4
1	A	167	LEU	3.3
1	A	414	VAL	3.3
1	A	373	GLU	3.2
2	C	57	GLU	3.2
1	A	407	GLY	3.2
1	B	573	ASN	3.1
2	D	129	LEU	3.1
1	B	806	ILE	3.0
2	D	110	GLU	3.0
1	B	526	ARG	3.0
1	B	554	GLU	3.0
1	A	351	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	182	ILE	3.0
1	A	417	LYS	2.9
2	C	111	VAL	2.9
2	C	129	LEU	2.9
1	B	638	GLY	2.8
1	A	404	ARG	2.8
1	A	362	ASP	2.8
1	A	408	SER	2.8
1	B	775	GLN	2.7
1	A	428	PHE	2.7
2	D	67	GLY	2.7
1	A	371	GLN	2.7
1	B	288	THR	2.7
2	C	128	ALA	2.7
2	C	55	ALA	2.6
1	B	471	LEU	2.6
1	B	603	GLY	2.6
1	A	77	VAL	2.6
1	A	384	GLN	2.6
1	B	697	LYS	2.6
2	C	122	ALA	2.6
1	A	418	VAL	2.5
1	B	337	LEU	2.5
2	D	114	GLY	2.5
2	D	98	LYS	2.4
1	A	84	LEU	2.4
2	C	69	VAL	2.4
1	A	216	LYS	2.4
1	B	733	VAL	2.4
1	A	451	GLY	2.4
1	B	645	GLU	2.3
2	C	99	MET	2.3
1	A	412	VAL	2.3
2	C	52	TYR	2.3
2	C	65	ASP	2.3
1	A	48	VAL	2.3
1	B	450	LEU	2.3
1	B	610	LYS	2.3
1	B	276	ASN	2.2
1	A	387	GLU	2.2
1	A	430	ILE	2.2
1	A	416	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	527	ALA	2.1
1	B	428	PHE	2.1
1	B	600	THR	2.1
1	A	97	ILE	2.1
2	C	83	PRO	2.1
1	A	62	THR	2.1
2	C	123	VAL	2.1
2	D	102	ASN	2.1
1	A	280	HIS	2.1
1	B	575	GLY	2.1
1	B	807	GLY	2.1
2	C	116	PRO	2.1
1	B	451	GLY	2.1
1	B	608	TYR	2.0
1	B	643	GLY	2.0
1	B	602	PRO	2.0
2	D	116	PRO	2.0
1	A	141	TYR	2.0
2	D	53	THR	2.0
1	B	449	TRP	2.0
1	A	717	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.