Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 02:21 PM EDT

PDB ID	:	5AZ4
Title	:	Crystal structure of a 79KDa fragment of FlgE, the hook protein from Campylobacter jejuni
Authors	:	Samatey, F.A.; Kido, Y.
Deposited on	:	2015-09-25
Resolution	:	2.45 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

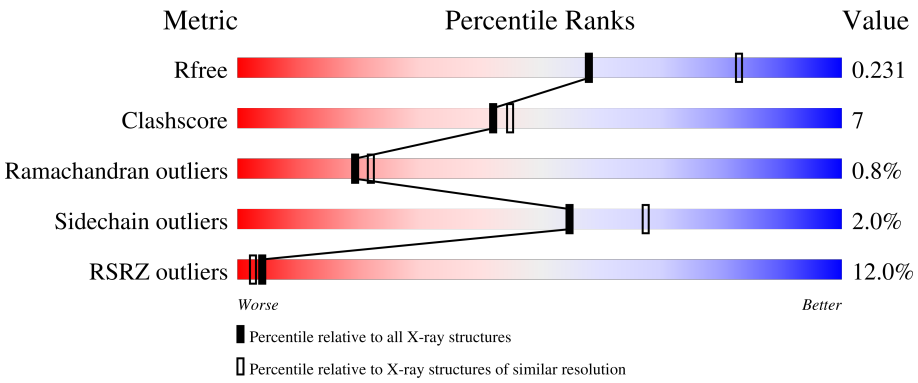
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.45 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	741	5% 86% 12% •
1	B	741	7% 82% 14% • •
1	C	741	18% 82% 15% • •
1	D	741	18% 78% 19% • •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 23180 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 Flagellar hook subunit protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	726	5428	3348	949	1123	8	0	0	0
1	B	726	5428	3348	949	1123	8	0	0	0
1	C	726	5428	3348	949	1123	8	0	0	0
1	D	726	5428	3348	949	1123	8	0	0	0

- Molecule 2 is water.

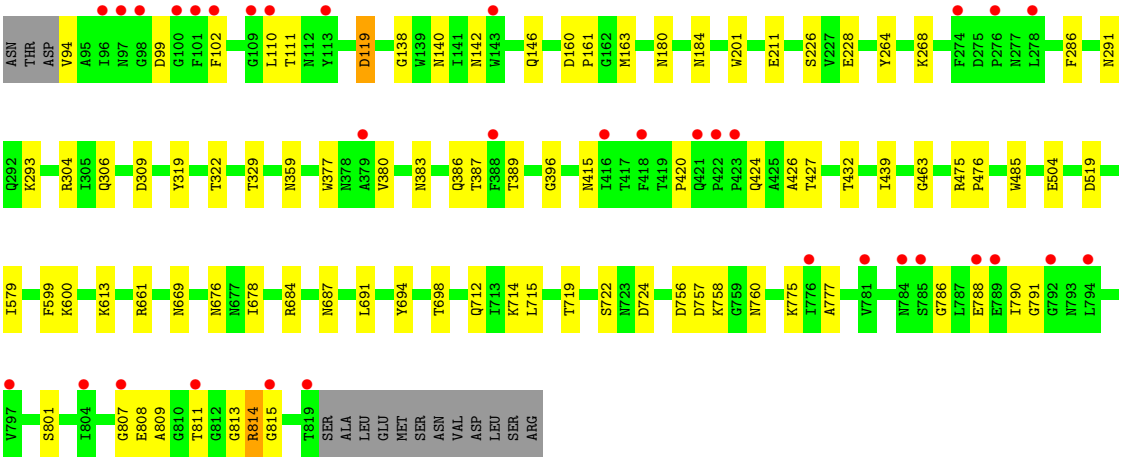
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	372	372	372	0	0
2	B	417	417	417	0	0
2	C	388	388	388	0	0
2	D	291	291	291	0	0

3 Residue-property plots (i)

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

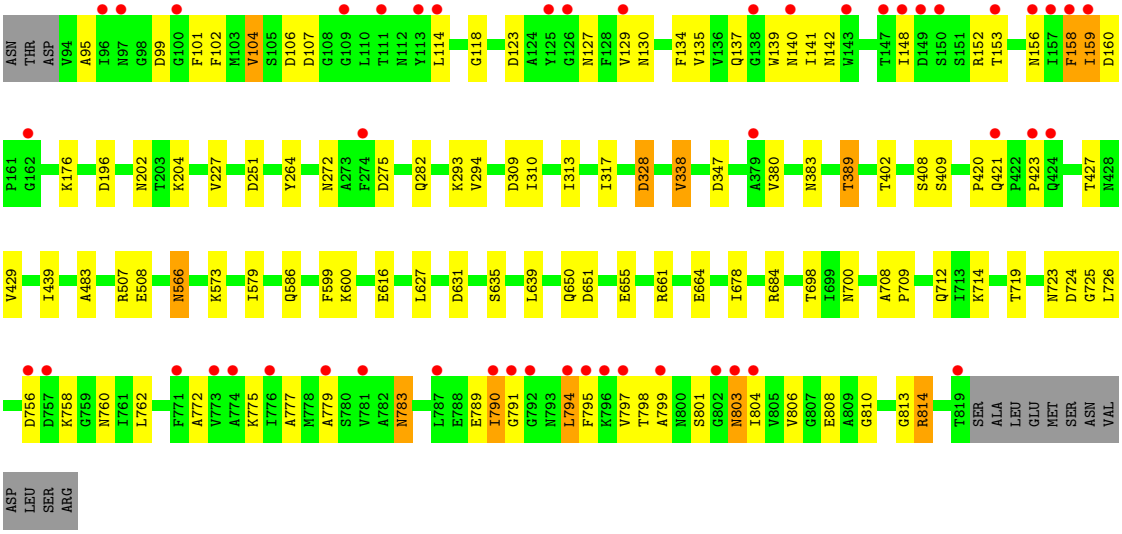
• Molecule 1: Flagellar hook subunit protein

Chain A:



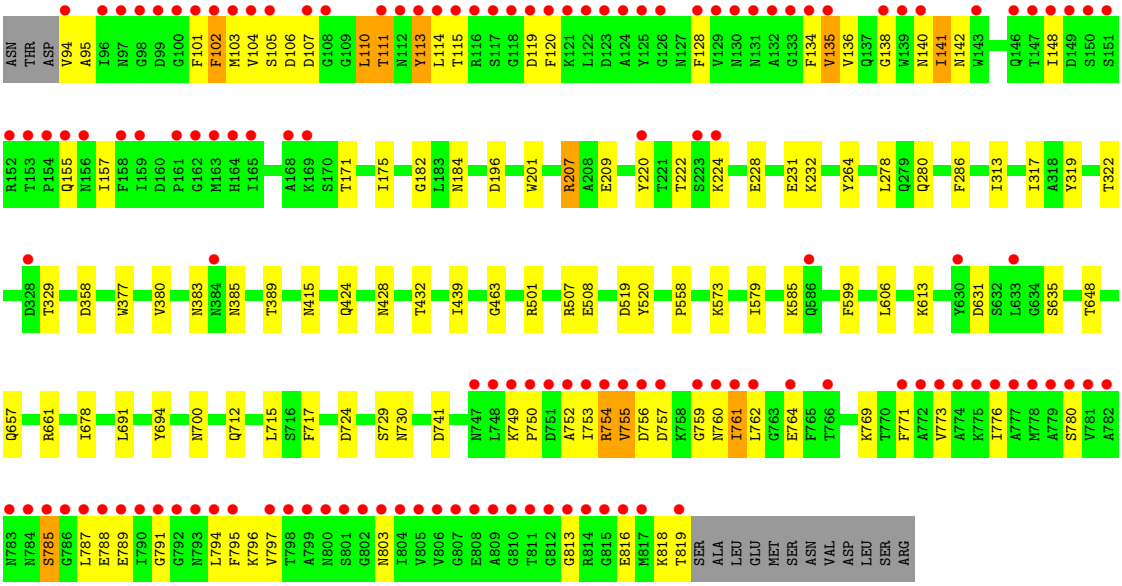
• Molecule 1: Flagellar hook subunit protein

Chain B:



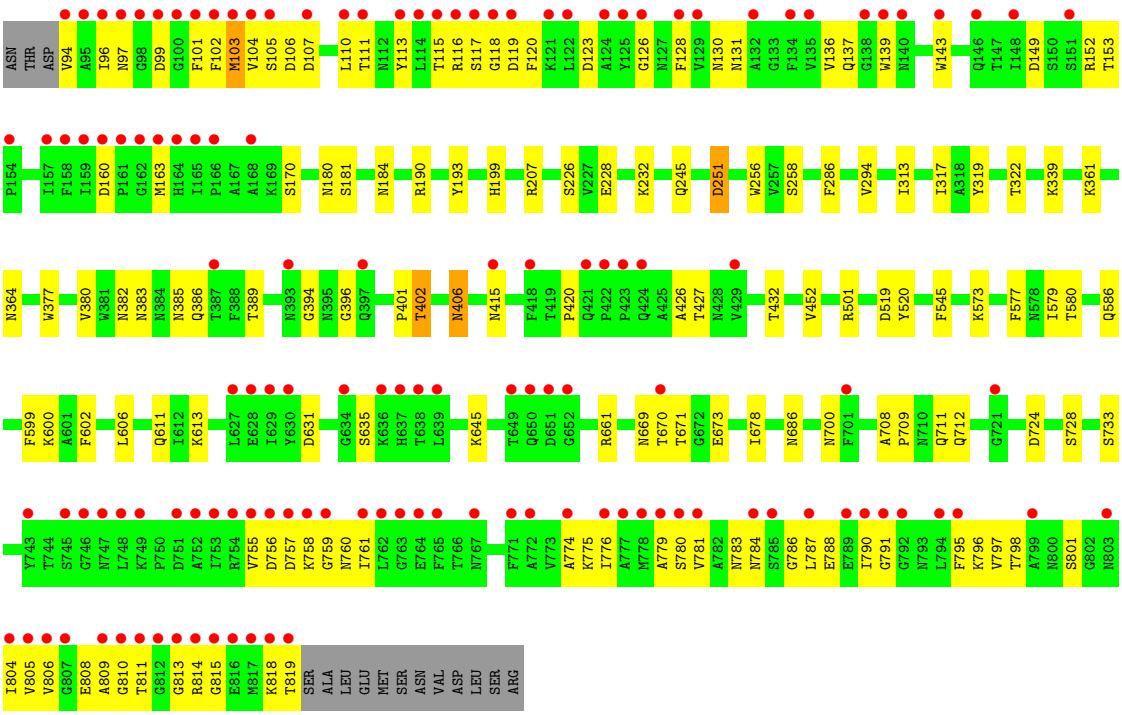
• Molecule 1: Flagellar hook subunit protein

Chain C:



- Molecule 1: Flagellar hook subunit protein

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	75.46Å 173.54Å 147.09Å 90.00° 102.66° 90.00°	Depositor
Resolution (Å)	24.96 – 2.45 41.01 – 2.45	Depositor EDS
% Data completeness (in resolution range)	98.7 (24.96-2.45) 94.3 (41.01-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.21 (at 2.45Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.202 , 0.229 0.202 , 0.231	Depositor DCC
R_{free} test set	7994 reflections (5.99%)	wwPDB-VP
Wilson B-factor (Å^2)	38.8	Xtriage
Anisotropy	0.384	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 55.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	23180	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.27	0/5527	0.47	0/7533
1	B	0.25	0/5527	0.43	0/7533
1	C	0.28	0/5527	0.49	0/7533
1	D	0.28	0/5527	0.49	0/7533
All	All	0.27	0/22108	0.47	0/30132

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5428	0	5168	52	0
1	B	5428	0	5168	65	0
1	C	5428	0	5168	79	1
1	D	5428	0	5168	101	1
2	A	372	0	0	8	0
2	B	417	0	0	7	0
2	C	388	0	0	9	0
2	D	291	0	0	13	0
All	All	23180	0	20672	292	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 7.

All (292) 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:D:758:LYS:O	1:D:775:LYS:NZ	2.09	0.85
1:C:757:ASP:HA	1:C:816:GLU:HB3	1.59	0.82
1:D:117:SER:OG	1:D:119:ASP:OD1	2.01	0.79
1:B:137:GLN:NE2	1:B:156:ASN:OD1	2.19	0.74
1:D:779:ALA:HA	1:D:806:VAL:HA	1.70	0.74
1:A:712:GLN:NE2	1:D:686:ASN:OD1	2.21	0.73
1:C:141:ILE:HG12	1:C:148:ILE:HG12	1.70	0.73
1:C:95:ALA:HB2	1:C:754:ARG:HH22	1.55	0.72
1:D:119:ASP:OD2	1:D:131:ASN:ND2	2.22	0.72
1:B:655:GLU:HG3	1:B:684:ARG:HG2	1.72	0.71
1:B:650:GLN:NE2	2:B:908:HOH:O	2.24	0.71
1:B:798:THR:H	1:B:801:SER:HB3	1.56	0.71
1:D:787:LEU:HD12	1:D:788:GLU:H	1.56	0.70
1:C:754:ARG:O	1:C:762:LEU:N	2.26	0.68
1:D:797:VAL:HG11	1:D:804:ILE:HD11	1.73	0.68
1:B:483:ALA:O	2:B:901:HOH:O	2.11	0.68
1:B:664:GLU:OE1	2:B:902:HOH:O	2.12	0.67
1:C:141:ILE:HD11	1:C:773:VAL:HA	1.77	0.67
1:A:684:ARG:NH2	2:A:910:HOH:O	2.26	0.67
1:D:780:SER:N	1:D:805:VAL:O	2.22	0.67
1:C:138:GLY:O	1:C:155:GLN:N	2.21	0.67
1:B:130:ASN:HD21	1:B:134:PHE:HB2	1.58	0.66
1:B:803:ASN:OD1	1:B:803:ASN:N	2.29	0.66
1:B:328:ASP:N	1:B:328:ASP:OD1	2.28	0.65
1:C:729:SER:OG	2:C:902:HOH:O	2.14	0.65
1:C:519:ASP:OD1	2:C:901:HOH:O	2.13	0.65
1:D:245:GLN:OE1	2:D:901:HOH:O	2.14	0.65
1:A:758:LYS:O	1:A:775:LYS:NZ	2.22	0.65
1:C:224:LYS:NZ	2:C:911:HOH:O	2.30	0.65
1:B:176:LYS:NZ	1:B:723:ASN:O	2.30	0.65
1:B:655:GLU:OE2	1:B:684:ARG:NH1	2.29	0.64
1:C:104:VAL:HG23	1:C:136:VAL:HG13	1.78	0.64
1:D:104:VAL:HG23	1:D:137:GLN:HB2	1.80	0.64
1:D:733:SER:O	2:D:903:HOH:O	2.15	0.64
1:B:579:ILE:O	1:B:600:LYS:NZ	2.30	0.64
1:B:700:ASN:OD1	1:B:712:GLN:NE2	2.30	0.64
1:D:611:GLN:OE1	2:D:902:HOH:O	2.15	0.64
1:B:758:LYS:O	1:B:775:LYS:NZ	2.30	0.63
1:A:226:SER:OG	1:A:228:GLU:OE2	2.16	0.63
1:A:788:GLU:N	1:A:788:GLU:OE1	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:798:THR:OG1	1:B:799:ALA:N	2.30	0.63
1:D:787:LEU:HD21	1:D:795:PHE:HB3	1.80	0.62
1:B:783:ASN:ND2	1:B:801:SER:O	2.28	0.62
1:D:119:ASP:OD1	1:D:119:ASP:N	2.32	0.62
1:A:291:ASN:OD1	1:B:99:ASP:HB2	1.99	0.62
1:D:251:ASP:OD2	2:D:905:HOH:O	2.16	0.61
1:A:790:ILE:HG13	1:A:791:GLY:H	1.65	0.61
1:B:227:VAL:O	1:B:661:ARG:NH1	2.31	0.61
1:B:421:GLN:HB3	1:B:423:PRO:HG2	1.83	0.61
1:D:579:ILE:O	1:D:600:LYS:NZ	2.32	0.61
1:C:749:LYS:HG3	1:C:752:ALA:HB3	1.83	0.60
1:C:415:ASN:HB2	1:C:432:THR:HB	1.84	0.60
1:B:293:LYS:HD3	1:B:309:ASP:HA	1.84	0.60
1:B:698:THR:HG22	1:B:714:LYS:HA	1.84	0.59
1:B:275:ASP:O	1:B:282:GLN:NE2	2.33	0.59
1:C:140:ASN:ND2	1:C:155:GLN:OE1	2.36	0.59
1:D:670:THR:HG23	1:D:671:THR:HG23	1.84	0.59
1:D:94:VAL:HA	1:D:120:PHE:H	1.67	0.58
1:D:180:ASN:ND2	1:D:184:ASN:O	2.36	0.58
1:C:753:ILE:HD11	1:C:761:ILE:HD11	1.85	0.58
1:C:101:PHE:HB3	1:C:102:PHE:HD2	1.68	0.58
1:A:383:ASN:O	1:A:386:GLN:NE2	2.35	0.58
1:A:519:ASP:OD1	2:A:901:HOH:O	2.17	0.58
1:C:136:VAL:O	1:C:157:ILE:HG12	2.04	0.58
1:D:102:PHE:CD1	1:D:116:ARG:HA	2.39	0.57
1:D:102:PHE:HB3	1:D:115:THR:O	2.05	0.57
1:A:814:ARG:NH2	2:A:924:HOH:O	2.33	0.57
1:D:319:TYR:O	1:D:322:THR:OG1	2.20	0.57
1:C:385:ASN:ND2	2:C:923:HOH:O	2.35	0.57
1:C:759:GLY:O	1:C:776:ILE:N	2.30	0.57
1:A:268:LYS:NZ	2:A:936:HOH:O	2.37	0.56
1:C:113:TYR:HE1	1:C:134:PHE:CE2	2.22	0.56
1:D:415:ASN:HB2	1:D:432:THR:HB	1.86	0.56
1:D:519:ASP:OD1	2:D:904:HOH:O	2.18	0.56
1:A:579:ILE:O	1:A:600:LYS:NZ	2.39	0.56
1:D:761:ILE:HD12	1:D:774:ALA:HB3	1.87	0.56
1:C:700:ASN:OD1	1:C:712:GLN:NE2	2.39	0.55
1:D:94:VAL:N	1:D:819:THR:O	2.39	0.55
1:C:787:LEU:HD12	1:C:788:GLU:H	1.70	0.55
1:D:96:ILE:HA	1:D:118:GLY:HA3	1.89	0.55
1:D:190:ARG:NH2	2:D:938:HOH:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:669:ASN:ND2	1:D:673:GLU:O	2.28	0.55
1:B:159:ILE:HG12	1:B:160:ASP:H	1.72	0.54
1:B:789:GLU:HG3	1:B:795:PHE:HE1	1.72	0.54
1:B:566:ASN:ND2	2:B:934:HOH:O	2.41	0.54
1:C:501:ARG:NH2	2:C:930:HOH:O	2.37	0.53
1:B:264:TYR:HB2	1:B:439:ILE:HG13	1.89	0.53
1:D:286:PHE:HB3	1:D:377:TRP:CD1	2.44	0.53
1:C:428:ASN:ND2	2:C:912:HOH:O	2.30	0.53
1:D:139:TRP:NE1	1:D:152:ARG:O	2.30	0.53
1:D:501:ARG:NH1	2:D:913:HOH:O	2.33	0.53
1:D:380:VAL:HB	1:D:389:THR:HG23	1.90	0.53
1:C:107:ASP:HB2	1:C:134:PHE:CZ	2.44	0.53
1:C:232:LYS:HZ2	1:C:657:GLN:CD	2.11	0.52
1:B:579:ILE:HG13	1:B:599:PHE:O	2.09	0.52
1:A:786:GLY:O	1:A:801:SER:HB3	2.10	0.52
1:D:143:TRP:HH2	1:D:163:MET:SD	2.31	0.52
1:B:380:VAL:HB	1:B:389:THR:HG22	1.92	0.52
1:A:694:TYR:OH	1:A:715:LEU:O	2.19	0.52
1:B:141:ILE:HA	1:B:148:ILE:HG12	1.91	0.52
1:D:586:GLN:N	1:D:586:GLN:OE1	2.43	0.52
1:A:415:ASN:HB3	1:A:432:THR:HB	1.92	0.51
1:B:408:SER:OG	1:B:409:SER:N	2.43	0.51
1:D:788:GLU:OE1	1:D:788:GLU:N	2.43	0.51
1:B:724:ASP:OD1	1:B:724:ASP:N	2.43	0.51
1:A:811:THR:O	1:A:814:ARG:NE	2.31	0.51
1:C:579:ILE:HG13	1:C:599:PHE:O	2.10	0.51
1:C:606:LEU:HD13	1:C:613:LYS:HG2	1.91	0.51
1:D:103:MET:HG3	1:D:136:VAL:HG13	1.91	0.51
1:C:128:PHE:H	1:C:157:ILE:HD12	1.76	0.51
1:B:616:GLU:OE1	2:B:903:HOH:O	2.19	0.50
1:C:105:SER:HB3	1:C:134:PHE:CD2	2.46	0.50
1:C:286:PHE:HB3	1:C:377:TRP:CD1	2.46	0.50
1:D:645:LYS:NZ	2:D:942:HOH:O	2.40	0.50
1:D:790:ILE:HG13	1:D:791:GLY:H	1.76	0.50
1:A:99:ASP:OD1	1:A:99:ASP:N	2.41	0.49
1:B:148:ILE:HD11	1:B:772:ALA:O	2.12	0.49
1:C:796:LYS:NZ	1:C:797:VAL:O	2.42	0.49
1:A:387:THR:HG21	1:B:101:PHE:HZ	1.76	0.49
1:D:160:ASP:HB3	1:D:163:MET:SD	2.52	0.49
1:D:170:SER:O	1:D:711:GLN:NE2	2.35	0.49
1:A:286:PHE:HB3	1:A:377:TRP:CD1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:769:LYS:HD3	1:C:771:PHE:HE2	1.78	0.49
1:D:226:SER:OG	1:D:228:GLU:OE2	2.31	0.49
1:D:579:ILE:HG13	1:D:599:PHE:O	2.12	0.49
1:A:160:ASP:HB3	1:A:163:MET:HB2	1.94	0.49
1:C:358:ASP:OD2	1:C:585:LYS:NZ	2.44	0.49
1:D:394:GLY:HA3	1:D:401:PRO:O	2.13	0.49
1:B:313:ILE:O	1:B:317:ILE:HG12	2.12	0.49
1:D:809:ALA:HA	1:D:814:ARG:HD2	1.93	0.49
1:D:102:PHE:CE1	1:D:116:ARG:HG3	2.48	0.48
1:D:123:ASP:OD1	1:D:126:GLY:N	2.45	0.48
1:B:272:ASN:ND2	2:B:947:HOH:O	2.45	0.48
1:D:199:HIS:NE2	2:D:926:HOH:O	2.35	0.48
1:D:756:ASP:OD1	1:D:760:ASN:N	2.41	0.48
1:B:95:ALA:O	1:B:118:GLY:HA3	2.13	0.48
1:B:114:LEU:HD11	1:B:804:ILE:HD11	1.94	0.48
1:A:712:GLN:OE1	2:A:902:HOH:O	2.20	0.48
1:B:420:PRO:HD3	1:B:427:THR:HG23	1.96	0.48
1:C:380:VAL:HB	1:C:389:THR:HG23	1.96	0.48
1:C:694:TYR:OH	1:C:715:LEU:O	2.22	0.48
1:C:114:LEU:HD21	1:C:780:SER:HA	1.96	0.48
1:D:117:SER:OG	1:D:130:ASN:HB2	2.14	0.48
1:D:420:PRO:HD2	1:D:426:ALA:HA	1.94	0.48
1:B:114:LEU:O	1:B:794:LEU:HA	2.14	0.48
1:C:103:MET:N	1:C:115:THR:O	2.47	0.48
1:D:520:TYR:CG	1:D:573:LYS:HD2	2.49	0.48
1:A:293:LYS:HD3	1:A:309:ASP:HA	1.96	0.47
1:B:106:ASP:OD1	1:B:107:ASP:N	2.47	0.47
1:D:96:ILE:HG22	1:D:97:ASN:H	1.79	0.47
1:A:698:THR:HG22	1:A:714:LYS:HA	1.96	0.47
1:D:606:LEU:HD13	1:D:613:LYS:HG2	1.96	0.47
1:A:661:ARG:HG2	1:A:678:ILE:HG12	1.96	0.47
1:B:631:ASP:OD2	1:B:635:SER:HB2	2.14	0.47
1:C:228:GLU:HB3	2:C:924:HOH:O	2.15	0.47
1:B:756:ASP:OD1	1:B:760:ASN:N	2.47	0.47
1:C:207:ARG:NH1	1:C:209:GLU:OE2	2.39	0.47
1:C:264:TYR:HB2	1:C:439:ILE:HG13	1.96	0.47
1:C:319:TYR:O	1:C:322:THR:OG1	2.22	0.47
1:A:201:TRP:CD2	1:A:463:GLY:HA2	2.49	0.47
1:C:755:VAL:HA	1:C:761:ILE:HA	1.97	0.47
1:A:119:ASP:N	1:A:119:ASP:OD1	2.48	0.47
1:B:129:VAL:HG12	1:B:135:VAL:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:ILE:HG13	1:C:157:ILE:O	2.15	0.46
1:B:294:VAL:HG23	1:B:310:ILE:HB	1.98	0.46
1:D:545:PHE:HB3	1:D:602:PHE:HZ	1.80	0.46
1:A:319:TYR:O	1:A:322:THR:OG1	2.24	0.46
1:C:787:LEU:HG	1:C:795:PHE:CD1	2.51	0.46
1:B:708:ALA:HA	1:B:709:PRO:HD3	1.82	0.46
1:B:810:GLY:N	1:B:814:ARG:O	2.30	0.46
1:C:631:ASP:OD1	1:C:635:SER:N	2.41	0.46
1:D:396:GLY:HA2	1:D:402:THR:HG22	1.98	0.46
1:C:113:TYR:HE1	1:C:134:PHE:HE2	1.62	0.46
1:C:182:GLY:HA3	1:C:730:ASN:OD1	2.16	0.46
1:C:135:VAL:HG23	1:C:157:ILE:HD11	1.97	0.46
1:C:791:GLY:HA3	1:C:794:LEU:HB2	1.98	0.46
1:C:755:VAL:HB	1:C:761:ILE:HA	1.98	0.45
1:D:143:TRP:CH2	1:D:163:MET:SD	3.08	0.45
1:D:787:LEU:HD11	1:D:796:LYS:H	1.82	0.45
1:A:304:ARG:NH2	1:A:306:GLN:OE1	2.50	0.45
1:D:382:ASN:OD1	1:D:385:ASN:N	2.38	0.45
1:A:579:ILE:HG13	1:A:599:PHE:O	2.17	0.45
1:D:97:ASN:ND2	1:D:99:ASP:O	2.50	0.45
1:D:758:LYS:HD2	1:D:810:GLY:HA3	1.99	0.45
1:B:661:ARG:HG2	1:B:678:ILE:HG12	1.99	0.45
1:D:106:ASP:OD1	1:D:107:ASP:N	2.49	0.45
1:D:120:PHE:HB3	1:D:128:PHE:CZ	2.51	0.45
1:D:775:LYS:HE3	1:D:808:GLU:OE1	2.17	0.45
1:D:787:LEU:HD12	1:D:788:GLU:N	2.28	0.45
1:A:475:ARG:HG3	1:A:485:TRP:CD1	2.51	0.45
1:C:171:THR:OG1	1:C:741:ASP:OD2	2.23	0.45
1:C:94:VAL:O	1:C:818:LYS:NZ	2.36	0.45
1:C:724:ASP:OD1	1:C:724:ASP:N	2.50	0.45
1:D:94:VAL:HA	1:D:120:PHE:N	2.31	0.45
1:D:102:PHE:CZ	1:D:116:ARG:HG3	2.52	0.45
2:C:928:HOH:O	1:D:207:ARG:HD3	2.17	0.44
1:D:631:ASP:OD1	1:D:635:SER:N	2.45	0.44
1:C:141:ILE:HG22	1:C:142:ASN:C	2.38	0.44
1:D:661:ARG:HG2	1:D:678:ILE:HG12	1.98	0.44
1:A:613:LYS:NZ	2:A:913:HOH:O	2.28	0.44
1:C:184:ASN:ND2	2:C:955:HOH:O	2.49	0.44
1:D:452:VAL:N	2:D:963:HOH:O	2.50	0.44
1:A:807:GLY:HA3	1:A:814:ARG:NH1	2.32	0.44
1:C:94:VAL:HA	1:C:120:PHE:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ASN:ND2	2:A:964:HOH:O	2.51	0.44
1:A:138:GLY:HA2	1:A:777:ALA:HB2	2.00	0.44
1:B:106:ASP:HB3	1:B:137:GLN:NE2	2.33	0.44
1:D:313:ILE:O	1:D:317:ILE:HG12	2.18	0.44
1:C:119:ASP:OD1	1:C:119:ASP:N	2.47	0.43
1:C:196:ASP:N	1:C:231:GLU:OE2	2.40	0.43
1:B:202:ASN:OD1	1:B:204:LYS:HG2	2.17	0.43
1:C:749:LYS:HA	1:C:750:PRO:HD3	1.78	0.43
1:D:105:SER:O	1:D:113:TYR:N	2.47	0.43
1:D:755:VAL:HG22	1:D:761:ILE:HG12	2.01	0.43
1:A:211:GLU:HB2	1:A:504:GLU:HG2	1.98	0.43
1:A:691:LEU:HD21	1:A:694:TYR:HD1	1.83	0.43
1:B:123:ASP:OD2	1:B:127:ASN:HB2	2.18	0.43
1:C:818:LYS:HG2	1:C:819:THR:H	1.81	0.43
1:B:176:LYS:HD2	1:B:725:GLY:O	2.18	0.43
1:B:627:LEU:HB2	1:B:639:LEU:HB2	2.01	0.43
1:B:507:ARG:NH2	1:B:508:GLU:OE1	2.50	0.43
1:C:201:TRP:CE2	1:C:463:GLY:HA2	2.54	0.43
1:C:757:ASP:OD1	1:C:757:ASP:N	2.51	0.43
1:A:142:ASN:O	1:A:146:GLN:N	2.51	0.43
1:C:756:ASP:OD1	1:C:760:ASN:HB2	2.18	0.43
1:D:420:PRO:HD2	1:D:427:THR:H	1.82	0.43
1:C:507:ARG:NH2	1:C:508:GLU:OE1	2.52	0.43
1:D:798:THR:H	1:D:801:SER:HB3	1.84	0.43
1:A:809:ALA:HB1	1:A:815:GLY:HA2	2.01	0.43
1:B:142:ASN:OD1	2:B:904:HOH:O	2.21	0.43
1:C:313:ILE:O	1:C:317:ILE:HG12	2.19	0.42
1:A:264:TYR:HB2	1:A:439:ILE:HG13	2.01	0.42
1:C:631:ASP:OD2	1:C:635:SER:HB2	2.18	0.42
1:C:661:ARG:HG2	1:C:678:ILE:HG12	2.01	0.42
1:A:669:ASN:O	1:A:676:ASN:HA	2.20	0.42
1:A:756:ASP:OD2	1:A:760:ASN:HB2	2.19	0.42
1:C:110:LEU:HB2	1:C:111:THR:H	1.57	0.42
1:A:359:ASN:ND2	2:A:942:HOH:O	2.41	0.42
1:B:338:VAL:HG12	1:B:347:ASP:HB2	2.02	0.42
1:C:115:THR:HG22	1:C:794:LEU:HG	2.02	0.42
1:D:294:VAL:HG12	1:D:377:TRP:CZ2	2.54	0.42
1:D:364:ASN:OD1	2:D:906:HOH:O	2.21	0.42
1:D:700:ASN:OD1	1:D:712:GLN:NE2	2.53	0.42
1:D:724:ASP:OD1	1:D:724:ASP:N	2.49	0.42
1:A:475:ARG:HA	1:A:476:PRO:HD3	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:558:PRO:O	1:D:207:ARG:NH2	2.52	0.42
1:A:724:ASP:OD1	1:A:724:ASP:N	2.49	0.42
1:C:106:ASP:O	1:C:135:VAL:HG13	2.20	0.42
1:D:258:SER:O	1:D:577:PHE:HA	2.20	0.42
1:D:818:LYS:HG2	1:D:819:THR:H	1.85	0.42
1:B:130:ASN:ND2	1:B:134:PHE:HB2	2.31	0.42
1:B:402:THR:HG22	1:B:427:THR:O	2.20	0.42
1:B:779:ALA:HB2	1:B:806:VAL:HG23	2.02	0.42
1:C:278:LEU:HG	1:C:280:GLN:HG2	2.02	0.41
1:B:139:TRP:CZ3	1:B:777:ALA:HA	2.55	0.41
1:B:775:LYS:HD3	1:B:808:GLU:HG2	2.03	0.41
1:D:193:TYR:CE2	1:D:232:LYS:HD3	2.55	0.41
1:D:256:TRP:HB2	1:D:580:THR:OG1	2.20	0.41
1:D:759:GLY:O	1:D:776:ILE:HG12	2.20	0.41
1:D:96:ILE:HG22	1:D:97:ASN:N	2.36	0.41
1:D:149:ASP:OD2	1:D:152:ARG:HG2	2.20	0.41
1:D:708:ALA:HA	1:D:709:PRO:HD3	1.91	0.41
1:D:787:LEU:CD2	1:D:795:PHE:HB3	2.48	0.41
1:A:420:PRO:HD2	1:A:426:ALA:HA	2.01	0.41
1:C:788:GLU:OE1	1:C:788:GLU:N	2.53	0.41
1:C:175:ILE:HG22	1:C:717:PHE:CD1	2.56	0.41
1:C:752:ALA:HB1	1:C:764:GLU:OE1	2.20	0.41
1:D:406:ASN:O	1:D:406:ASN:ND2	2.45	0.41
1:A:180:ASN:ND2	1:A:184:ASN:O	2.54	0.41
1:B:104:VAL:HG21	1:B:779:ALA:HB3	2.02	0.41
1:B:140:ASN:HB3	1:B:158:PHE:CD2	2.56	0.41
1:A:380:VAL:HB	1:A:389:THR:HG23	2.03	0.41
1:A:757:ASP:N	1:A:757:ASP:OD1	2.51	0.41
1:C:220:TYR:CZ	1:C:222:THR:HG22	2.55	0.41
1:A:396:GLY:HA2	1:A:427:THR:O	2.20	0.41
1:A:687:ASN:O	1:B:586:GLN:HG3	2.20	0.41
1:A:722:SER:OG	1:A:724:ASP:OD1	2.26	0.41
1:C:106:ASP:OD1	1:C:107:ASP:N	2.54	0.41
1:D:101:PHE:CZ	1:D:779:ALA:O	2.74	0.41
1:D:339:LYS:HG2	2:D:1137:HOH:O	2.21	0.41
1:D:787:LEU:HD11	1:D:796:LYS:N	2.35	0.41
1:D:811:THR:O	1:D:814:ARG:NE	2.54	0.41
1:D:104:VAL:HA	1:D:113:TYR:O	2.21	0.41
1:D:152:ARG:HA	1:D:152:ARG:HH11	1.86	0.41
1:C:520:TYR:CG	1:C:573:LYS:HD2	2.56	0.40
1:C:691:LEU:HD21	1:C:694:TYR:HD1	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:361:LYS:O	2:D:907:HOH:O	2.22	0.40
1:D:383:ASN:O	1:D:386:GLN:NE2	2.48	0.40
1:A:160:ASP:HA	1:A:161:PRO:HD3	1.84	0.40
1:B:158:PHE:CG	1:B:159:ILE:N	2.90	0.40
1:D:181:SER:HB3	1:D:728:SER:OG	2.21	0.40
1:D:757:ASP:HB2	1:D:815:GLY:HA2	2.04	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:C:785:SER:N	1:D:783:ASN:O[2_454]	2.08	0.12

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	724/741 (98%)	701 (97%)	19 (3%)	4 (1%)	25	29
1	B	724/741 (98%)	681 (94%)	34 (5%)	9 (1%)	13	12
1	C	724/741 (98%)	699 (96%)	21 (3%)	4 (1%)	25	29
1	D	724/741 (98%)	699 (96%)	20 (3%)	5 (1%)	22	25
All	All	2896/2964 (98%)	2780 (96%)	94 (3%)	22 (1%)	19	22

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	159	ILE
1	C	102	PHE
1	C	785	SER
1	D	784	ASN

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Mol	Chain	Res	Type
1	A	111	THR
1	B	196	ASP
1	A	813	GLY
1	B	158	PHE
1	B	783	ASN
1	B	813	GLY
1	C	111	THR
1	A	102	PHE
1	A	119	ASP
1	B	790	ILE
1	D	111	THR
1	B	102	PHE
1	B	104	VAL
1	D	781	VAL
1	D	786	GLY
1	B	791	GLY
1	C	813	GLY
1	D	813	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	581/595 (98%)	574 (99%)	7 (1%)	71 81
1	B	581/595 (98%)	562 (97%)	19 (3%)	38 49
1	C	581/595 (98%)	567 (98%)	14 (2%)	49 61
1	D	581/595 (98%)	575 (99%)	6 (1%)	76 84
All	All	2324/2380 (98%)	2278 (98%)	46 (2%)	55 67

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	VAL
1	A	110	LEU
1	A	329	THR

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Mol	Chain	Res	Type
1	A	424	GLN
1	A	719	THR
1	A	808	GLU
1	A	814	ARG
1	B	152	ARG
1	B	153	THR
1	B	251	ASP
1	B	328	ASP
1	B	338	VAL
1	B	383	ASN
1	B	389	THR
1	B	429	VAL
1	B	566	ASN
1	B	573	LYS
1	B	651	ASP
1	B	719	THR
1	B	726	LEU
1	B	762	LEU
1	B	790	ILE
1	B	794	LEU
1	B	797	VAL
1	B	803	ASN
1	B	814	ARG
1	C	110	LEU
1	C	113	TYR
1	C	135	VAL
1	C	141	ILE
1	C	207	ARG
1	C	329	THR
1	C	383	ASN
1	C	424	GLN
1	C	648	THR
1	C	754	ARG
1	C	755	VAL
1	C	761	ILE
1	C	789	GLU
1	C	803	ASN
1	D	103	MET
1	D	110	LEU
1	D	153	THR
1	D	251	ASP
1	D	402	THR

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Mol	Chain	Res	Type
1	D	406	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	292	GLN
1	A	533	GLN
1	C	140	ASN
1	C	712	GLN
1	D	712	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	726/741 (97%)	0.22	34 (4%)	31	29	29, 51, 98, 126	0
1	B	726/741 (97%)	0.40	49 (6%)	17	14	23, 47, 118, 150	0
1	C	726/741 (97%)	1.51	133 (18%)	1	0	25, 48, 249, 302	0
1	D	726/741 (97%)	1.06	133 (18%)	1	0	27, 63, 190, 248	0
All	All	2904/2964 (97%)	0.80	349 (12%)	4	2	23, 52, 192, 302	0

All (349) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	777	ALA	65.8
1	C	776	ILE	53.0
1	C	781	VAL	43.9
1	D	812	GLY	20.2
1	C	133	GLY	19.5
1	C	790	ILE	18.7
1	C	807	GLY	18.0
1	C	803	ASN	16.8
1	C	100	GLY	16.8
1	D	98	GLY	16.4
1	C	102	PHE	15.9
1	D	810	GLY	15.6
1	C	802	GLY	15.5
1	C	778	MET	15.3
1	D	811	THR	14.9
1	C	132	ALA	14.8
1	C	113	TYR	14.7
1	D	813	GLY	14.5
1	C	124	ALA	14.0
1	C	813	GLY	13.8
1	C	104	VAL	13.7

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Mol	Chain	Res	Type	RSRZ
1	D	809	ALA	13.5
1	C	789	GLU	13.2
1	C	794	LEU	13.1
1	C	752	ALA	12.9
1	C	806	VAL	12.6
1	C	750	PRO	12.5
1	C	138	GLY	12.4
1	C	129	VAL	12.4
1	C	814	ARG	12.2
1	C	148	ILE	11.8
1	C	98	GLY	11.4
1	A	100	GLY	11.2
1	D	650	GLN	11.1
1	C	792	GLY	10.9
1	C	139	TRP	10.8
1	C	130	ASN	10.7
1	C	101	PHE	10.5
1	B	819	THR	10.5
1	C	804	ILE	10.5
1	C	810	GLY	10.5
1	B	157	ILE	10.5
1	C	805	VAL	10.3
1	C	780	SER	10.1
1	B	803	ASN	10.0
1	C	122	LEU	10.0
1	D	159	ILE	9.4
1	C	787	LEU	9.4
1	C	751	ASP	9.3
1	D	815	GLY	9.3
1	C	135	VAL	9.1
1	D	746	GLY	9.1
1	C	819	THR	9.0
1	C	134	PHE	9.0
1	D	100	GLY	8.9
1	C	116	ARG	8.8
1	D	115	THR	8.7
1	C	159	ILE	8.5
1	D	158	PHE	8.5
1	D	819	THR	8.3
1	C	125	TYR	8.2
1	C	773	VAL	8.2
1	C	793	ASN	8.2

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Mol	Chain	Res	Type	RSRZ
1	C	99	ASP	8.2
1	C	791	GLY	8.2
1	C	782	ALA	8.0
1	C	762	LEU	8.0
1	C	161	PRO	8.0
1	C	146	GLN	8.0
1	C	115	THR	7.9
1	C	772	ALA	7.9
1	C	783	ASN	7.8
1	C	811	THR	7.8
1	C	150	SER	7.7
1	D	752	ALA	7.6
1	D	791	GLY	7.4
1	C	795	PHE	7.4
1	D	790	ILE	7.4
1	C	131	ASN	7.3
1	D	781	VAL	7.1
1	C	147	THR	7.0
1	D	99	ASP	7.0
1	D	113	TYR	6.9
1	C	809	ALA	6.8
1	D	424	GLN	6.8
1	C	114	LEU	6.8
1	C	112	ASN	6.8
1	D	784	ASN	6.8
1	D	163	MET	6.7
1	D	804	ILE	6.4
1	D	794	LEU	6.4
1	C	149	ASP	6.4
1	B	424	GLN	6.4
1	C	162	GLY	6.3
1	D	162	GLY	6.3
1	D	125	TYR	6.3
1	B	158	PHE	6.2
1	D	787	LEU	6.2
1	C	117	SER	6.1
1	A	819	THR	6.1
1	D	814	ARG	6.1
1	D	764	GLU	6.0
1	C	111	THR	6.0
1	C	756	ASP	6.0
1	C	817	MET	6.0

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Mol	Chain	Res	Type	RSRZ
1	C	755	VAL	6.0
1	D	97	ASN	5.9
1	C	788	GLU	5.9
1	B	113	TYR	5.9
1	D	122	LEU	5.8
1	B	148	ILE	5.8
1	C	784	ASN	5.8
1	C	154	PRO	5.8
1	C	759	GLY	5.8
1	C	121	LYS	5.8
1	D	165	ILE	5.7
1	C	94	VAL	5.7
1	D	772	ALA	5.6
1	D	168	ALA	5.6
1	D	423	PRO	5.5
1	D	777	ALA	5.5
1	D	101	PHE	5.4
1	C	118	GLY	5.4
1	D	135	VAL	5.4
1	D	94	VAL	5.3
1	D	164	HIS	5.3
1	B	797	VAL	5.3
1	C	151	SER	5.3
1	D	778	MET	5.3
1	D	748	LEU	5.2
1	D	629	ILE	5.1
1	D	780	SER	5.0
1	C	120	PHE	5.0
1	D	785	SER	5.0
1	B	109	GLY	5.0
1	D	128	PHE	5.0
1	C	103	MET	4.9
1	C	771	PHE	4.9
1	C	96	ILE	4.9
1	C	786	GLY	4.7
1	C	812	GLY	4.7
1	B	776	ILE	4.7
1	D	792	GLY	4.7
1	A	102	PHE	4.7
1	C	128	PHE	4.6
1	B	792	GLY	4.6
1	D	747	ASN	4.6

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Mol	Chain	Res	Type	RSRZ
1	D	107	ASP	4.6
1	C	108	GLY	4.6
1	C	97	ASN	4.6
1	C	785	SER	4.5
1	D	806	VAL	4.5
1	D	116	ARG	4.5
1	B	423	PRO	4.5
1	C	775	LYS	4.5
1	B	779	ALA	4.5
1	A	96	ILE	4.5
1	C	749	LYS	4.4
1	B	781	VAL	4.4
1	C	774	ALA	4.4
1	D	126	GLY	4.3
1	D	818	LYS	4.2
1	C	155	GLN	4.2
1	C	126	GLY	4.2
1	D	117	SER	4.2
1	B	159	ILE	4.1
1	D	121	LYS	4.1
1	D	102	PHE	4.1
1	D	803	ASN	4.1
1	D	110	LEU	4.0
1	D	103	MET	4.0
1	C	223	SER	4.0
1	D	757	ASP	4.0
1	B	421	GLN	4.0
1	D	161	PRO	4.0
1	A	792	GLY	4.0
1	B	125	TYR	3.9
1	B	794	LEU	3.9
1	A	110	LEU	3.9
1	B	804	ILE	3.9
1	D	96	ILE	3.9
1	D	95	ALA	3.9
1	D	776	ILE	3.8
1	C	143	TRP	3.8
1	D	140	ASN	3.8
1	B	802	GLY	3.8
1	B	799	ALA	3.7
1	D	649	THR	3.7
1	C	105	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	148	ILE	3.7
1	D	765	PHE	3.6
1	A	109	GLY	3.6
1	A	797	VAL	3.6
1	D	771	PHE	3.5
1	C	384	ASN	3.5
1	D	111	THR	3.5
1	C	766	THR	3.5
1	D	132	ALA	3.5
1	C	754	ARG	3.5
1	C	156	ASN	3.5
1	C	119	ASP	3.4
1	C	153	THR	3.4
1	D	807	GLY	3.4
1	A	276	PRO	3.4
1	B	162	GLY	3.4
1	D	754	ARG	3.4
1	D	795	PHE	3.3
1	A	423	PRO	3.3
1	C	764	GLU	3.3
1	D	651	ASP	3.3
1	A	98	GLY	3.3
1	B	100	GLY	3.3
1	D	129	VAL	3.3
1	D	779	ALA	3.2
1	D	755	VAL	3.2
1	C	760	ASN	3.2
1	A	815	GLY	3.2
1	D	639	LEU	3.2
1	C	168	ALA	3.2
1	D	114	LEU	3.2
1	C	761	ILE	3.1
1	B	111	THR	3.1
1	B	790	ILE	3.1
1	D	157	ILE	3.1
1	D	638	THR	3.1
1	C	815	GLY	3.1
1	B	379	ALA	3.1
1	C	152	ARG	3.1
1	A	788	GLU	3.1
1	D	774	ALA	3.1
1	C	123	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	795	PHE	3.1
1	D	763	GLY	3.1
1	B	114	LEU	3.1
1	D	160	ASP	3.0
1	A	379	ALA	3.0
1	D	143	TRP	3.0
1	B	274	PHE	3.0
1	B	138	GLY	3.0
1	D	762	LEU	3.0
1	A	785	SER	3.0
1	B	150	SER	3.0
1	D	630	TYR	3.0
1	C	586	GLN	3.0
1	D	134	PHE	2.9
1	B	796	LYS	2.9
1	C	816	GLU	2.9
1	C	757	ASP	2.9
1	D	636	LYS	2.9
1	B	143	TRP	2.9
1	D	139	TRP	2.9
1	D	421	GLN	2.9
1	D	637	HIS	2.9
1	C	328	ASP	2.8
1	B	126	GLY	2.8
1	B	129	VAL	2.8
1	D	816	GLU	2.8
1	B	147	THR	2.8
1	C	753	ILE	2.8
1	A	274	PHE	2.7
1	C	779	ALA	2.7
1	D	104	VAL	2.7
1	D	817	MET	2.7
1	D	397	GLN	2.6
1	B	791	GLY	2.6
1	D	627	LEU	2.6
1	B	773	VAL	2.6
1	D	119	ASP	2.6
1	C	158	PHE	2.6
1	C	163	MET	2.6
1	D	751	ASP	2.6
1	D	154	PRO	2.6
1	D	652	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	789	GLU	2.6
1	C	808	GLU	2.6
1	A	794	LEU	2.5
1	C	224	LYS	2.5
1	D	805	VAL	2.5
1	C	165	ILE	2.5
1	D	759	GLY	2.5
1	D	628	GLU	2.5
1	A	784	ASN	2.5
1	D	393	ASN	2.5
1	D	415	ASN	2.5
1	A	776	ILE	2.5
1	B	140	ASN	2.5
1	C	630	TYR	2.5
1	D	418	PHE	2.5
1	C	798	THR	2.5
1	C	169	LYS	2.4
1	A	418	PHE	2.4
1	A	422	PRO	2.4
1	A	278	LEU	2.4
1	D	151	SER	2.4
1	D	745	SER	2.4
1	A	416	ILE	2.4
1	B	156	ASN	2.4
1	A	97	ASN	2.4
1	C	140	ASN	2.4
1	C	747	ASN	2.4
1	D	761	ILE	2.4
1	D	767	ASN	2.4
1	D	789	GLU	2.4
1	A	101	PHE	2.4
1	C	748	LEU	2.3
1	A	811	THR	2.3
1	D	753	ILE	2.3
1	C	107	ASP	2.2
1	A	388	PHE	2.2
1	B	771	PHE	2.2
1	D	124	ALA	2.2
1	D	701	PHE	2.2
1	D	758	LYS	2.2
1	A	113	TYR	2.2
1	B	97	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	797	VAL	2.2
1	B	96	ILE	2.2
1	D	799	ALA	2.2
1	D	118	GLY	2.2
1	D	138	GLY	2.2
1	B	757	ASP	2.2
1	C	800	ASN	2.2
1	A	143	TRP	2.2
1	A	781	VAL	2.2
1	B	774	ALA	2.2
1	B	149	ASP	2.2
1	A	804	ILE	2.2
1	A	807	GLY	2.2
1	D	634	GLY	2.2
1	C	220	TYR	2.1
1	D	721	GLY	2.1
1	B	153	THR	2.1
1	C	164	HIS	2.1
1	C	799	ALA	2.1
1	D	429	VAL	2.1
1	D	749	LYS	2.1
1	A	421	GLN	2.1
1	D	146	GLN	2.1
1	C	633	LEU	2.1
1	D	387	THR	2.1
1	D	422	PRO	2.1
1	D	670	THR	2.1
1	B	756	ASP	2.1
1	D	743	TYR	2.1
1	B	787	LEU	2.1
1	C	801	SER	2.1
1	D	105	SER	2.1
1	D	166	PRO	2.0
1	D	756	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 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.