



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:34 am GMT

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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

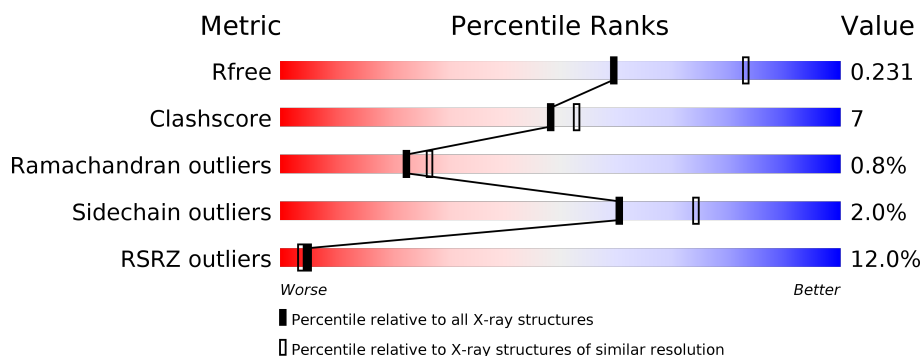
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	100719	1119 (2.48-2.44)
Clashscore	112137	1193 (2.48-2.44)
Ramachandran outliers	110173	1185 (2.48-2.44)
Sidechain outliers	110143	1185 (2.48-2.44)
RSRZ outliers	101464	1126 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	<div> <div>5%</div> <div>86%</div> <div>12%</div> <div>.</div> </div>
1	B	741	<div> <div>7%</div> <div>82%</div> <div>14%</div> <div>..</div> </div>
1	C	741	<div> <div>18%</div> <div>82%</div> <div>15%</div> <div>..</div> </div>
1	D	741	<div> <div>18%</div> <div>78%</div> <div>19%</div> <div>..</div> </div>

## 2 Entry composition

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
1	A	726	Total	C	N	O	S	0	0	0
			5428	3348	949	1123	8			
1	B	726	Total	C	N	O	S	0	0	0
			5428	3348	949	1123	8			
1	C	726	Total	C	N	O	S	0	0	0
			5428	3348	949	1123	8			
1	D	726	Total	C	N	O	S	0	0	0
			5428	3348	949	1123	8			

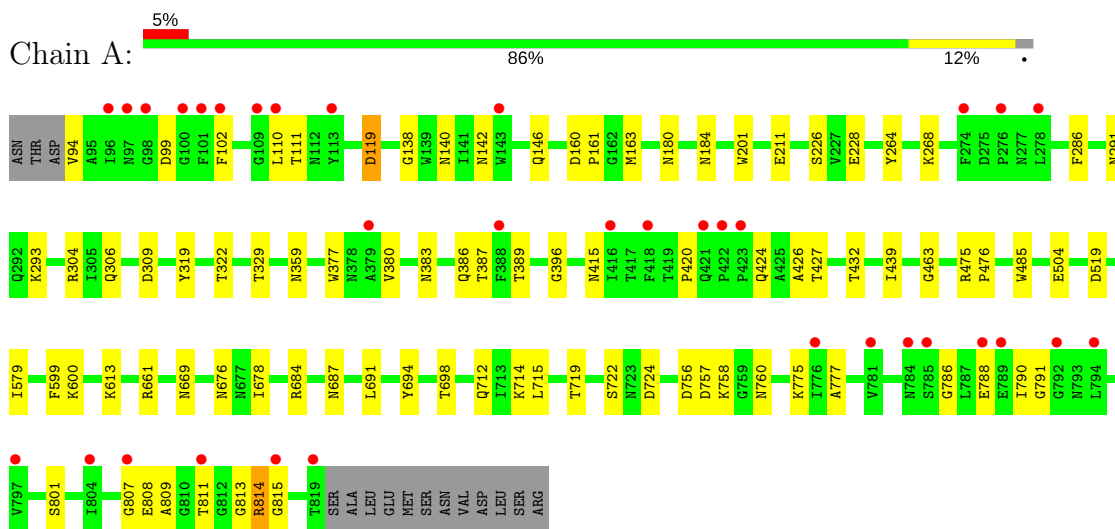
- Molecule 2 is water.

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

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

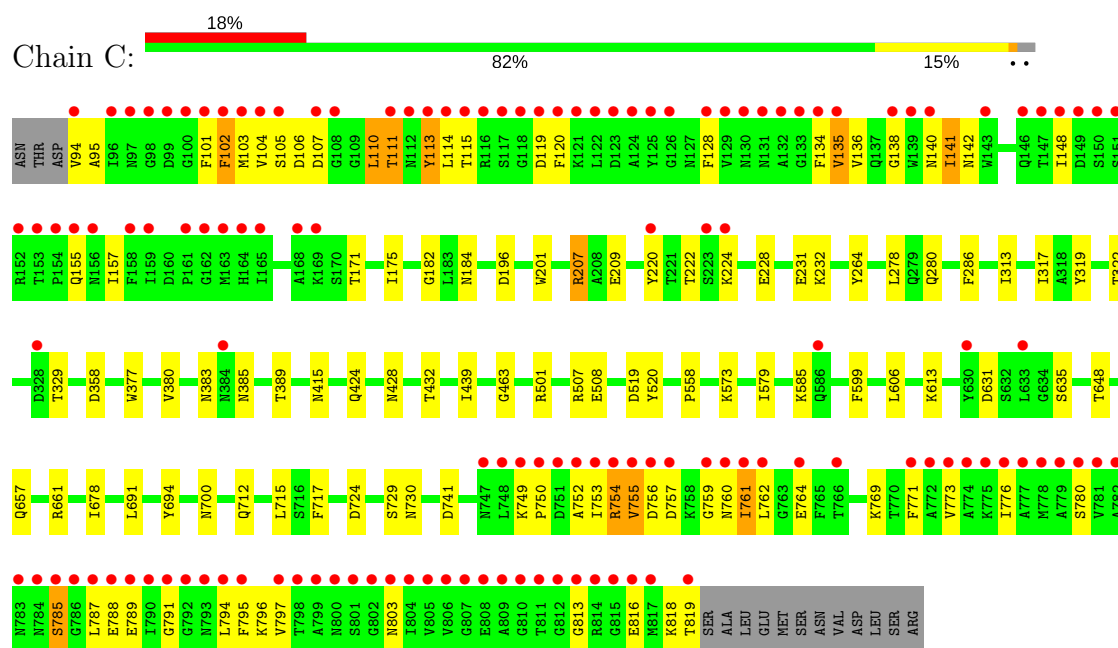
- Molecule 1: Flagellar hook subunit protein



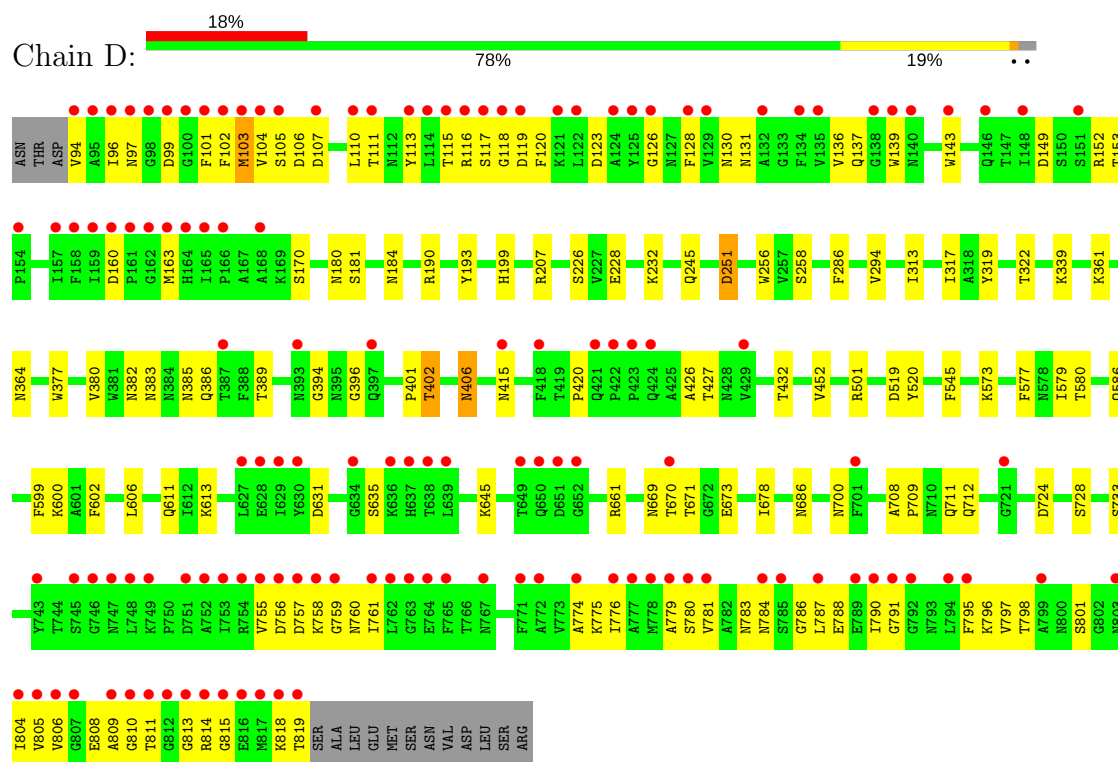
- Molecule 1: Flagellar hook subunit protein



- Molecule 1: Flagellar hook subunit protein



• Molecule 1: Flagellar hook subunit protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.72 (at 2.45Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.202 , 0.229 0.201 , 0.231	Depositor DCC
$R_{free}$ test set	7984 reflections (5.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.5	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 55.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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:N	1:B:803:ASN:OD1	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:OE1	1:D:586:GLN:N	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:N	1:A:99:ASP:OD1	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:758:LYS:HD2	1:D:810:GLY:HA3	1.99	0.45
1:D:97:ASN:ND2	1:D:99:ASP:O	2.50	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:787:LEU:HD12	1:D:788:GLU:N	2.28	0.45
1:D:775:LYS:HE3	1:D:808:GLU:OE1	2.17	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:724:ASP:N	1:C:724:ASP:OD1	2.50	0.45
1:C:94:VAL:O	1:C:818:LYS:NZ	2.36	0.45
1:D:102:PHE:CZ	1:D:116:ARG:HG3	2.52	0.45
1:D:94:VAL:HA	1:D:120:PHE:N	2.31	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:627:LEU:HB2	1:B:639:LEU:HB2	2.01	0.43
1:B:176:LYS:HD2	1:B:725:GLY:O	2.18	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:N	1:C:757:ASP:OD1	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:364:ASN:OD1	2:D:906:HOH:O	2.21	0.42
1:D:294:VAL:HG12	1:D:377:TRP:CZ2	2.54	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:N	1:A:724:ASP:OD1	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: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:D:96:ILE:HG22	1:D:97:ASN:N	2.36	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:ND2	1:D:406:ASN:O	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:687:ASN:O	1:B:586:GLN:HG3	2.20	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:811:THR:O	1:D:814:ARG:NE	2.54	0.41
1:A:396:GLY:HA2	1:A:427:THR:O	2.20	0.41
1:A:722:SER:OG	1:A:724:ASP:OD1	2.26	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: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%)	28	34
1	B	724/741 (98%)	681 (94%)	34 (5%)	9 (1%)	15	15
1	C	724/741 (98%)	699 (96%)	21 (3%)	4 (1%)	28	34
1	D	724/741 (98%)	699 (96%)	20 (3%)	5 (1%)	25	30
All	All	2896/2964 (98%)	2780 (96%)	94 (3%)	22 (1%)	22	26

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 ⓘ

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%)	75	85
1	B	581/595 (98%)	562 (97%)	19 (3%)	43	57
1	C	581/595 (98%)	567 (98%)	14 (2%)	54	69
1	D	581/595 (98%)	575 (99%)	6 (1%)	80	87
All	All	2324/2380 (98%)	2278 (98%)	46 (2%)	60	74

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

Some 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 carbohydrates 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

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	726/741 (97%)	0.22	34 (4%) 32 30	29, 51, 98, 126	0
1	B	726/741 (97%)	0.40	49 (6%) 19 16	23, 47, 118, 150	0
1	C	726/741 (97%)	1.51	133 (18%) 1 1	25, 48, 249, 302	0
1	D	726/741 (97%)	1.06	133 (18%) 1 1	27, 63, 190, 248	0
All	All	2904/2964 (97%)	0.80	349 (12%) 5 4	23, 53, 192, 302	0

All (349) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	777	ALA	66.6
1	C	776	ILE	53.1
1	C	781	VAL	43.9
1	D	812	GLY	20.3
1	C	133	GLY	19.6
1	C	790	ILE	18.6
1	C	807	GLY	18.0
1	C	100	GLY	17.2
1	C	803	ASN	16.8
1	D	98	GLY	16.3
1	C	102	PHE	15.8
1	D	810	GLY	15.5
1	C	802	GLY	15.5
1	C	778	MET	15.4
1	D	811	THR	14.9
1	C	132	ALA	14.7
1	C	113	TYR	14.7
1	D	813	GLY	14.5
1	C	124	ALA	13.9
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	12.7
1	C	750	PRO	12.5
1	C	138	GLY	12.4
1	C	129	VAL	12.3
1	C	814	ARG	12.3
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	11.0
1	C	139	TRP	10.7
1	C	130	ASN	10.6
1	C	101	PHE	10.6
1	C	810	GLY	10.6
1	C	804	ILE	10.5
1	B	819	THR	10.5
1	B	157	ILE	10.5
1	C	805	VAL	10.4
1	C	780	SER	10.1
1	B	803	ASN	10.0
1	C	122	LEU	10.0
1	D	159	ILE	9.5
1	C	787	LEU	9.4
1	D	815	GLY	9.4
1	C	751	ASP	9.3
1	C	135	VAL	9.2
1	D	746	GLY	9.1
1	C	819	THR	9.0
1	C	134	PHE	9.0
1	D	100	GLY	8.7
1	D	115	THR	8.7
1	C	116	ARG	8.7
1	C	159	ILE	8.5
1	D	158	PHE	8.4
1	C	773	VAL	8.2
1	D	819	THR	8.2
1	C	125	TYR	8.2
1	C	99	ASP	8.1

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Mol	Chain	Res	Type	RSRZ
1	C	793	ASN	8.1
1	C	791	GLY	8.1
1	C	782	ALA	8.0
1	C	146	GLN	8.0
1	C	762	LEU	8.0
1	C	161	PRO	8.0
1	C	772	ALA	7.9
1	C	115	THR	7.9
1	C	811	THR	7.8
1	C	150	SER	7.8
1	C	783	ASN	7.8
1	D	752	ALA	7.6
1	D	790	ILE	7.4
1	C	795	PHE	7.4
1	D	791	GLY	7.4
1	C	131	ASN	7.3
1	D	781	VAL	7.2
1	C	147	THR	7.0
1	D	99	ASP	7.0
1	D	113	TYR	6.9
1	C	809	ALA	6.9
1	C	112	ASN	6.9
1	D	424	GLN	6.8
1	D	784	ASN	6.8
1	C	114	LEU	6.8
1	D	163	MET	6.7
1	D	804	ILE	6.4
1	B	424	GLN	6.4
1	D	794	LEU	6.3
1	C	149	ASP	6.3
1	D	125	TYR	6.3
1	C	162	GLY	6.3
1	D	162	GLY	6.3
1	B	158	PHE	6.2
1	D	787	LEU	6.1
1	A	819	THR	6.1
1	C	817	MET	6.1
1	D	814	ARG	6.1
1	C	117	SER	6.0
1	D	764	GLU	6.0
1	C	111	THR	6.0
1	C	756	ASP	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	C	784	ASN	5.9
1	B	148	ILE	5.9
1	C	121	LYS	5.8
1	D	122	LEU	5.8
1	C	154	PRO	5.8
1	C	759	GLY	5.8
1	D	165	ILE	5.7
1	C	94	VAL	5.7
1	D	772	ALA	5.7
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	94	VAL	5.4
1	D	135	VAL	5.4
1	D	778	MET	5.3
1	B	797	VAL	5.3
1	D	164	HIS	5.3
1	C	151	SER	5.3
1	D	748	LEU	5.2
1	D	629	ILE	5.1
1	C	120	PHE	5.0
1	B	109	GLY	5.0
1	D	780	SER	5.0
1	D	785	SER	5.0
1	C	103	MET	5.0
1	D	128	PHE	5.0
1	C	96	ILE	4.9
1	C	771	PHE	4.9
1	C	812	GLY	4.7
1	C	786	GLY	4.7
1	B	792	GLY	4.7
1	A	102	PHE	4.7
1	B	776	ILE	4.7
1	D	747	ASN	4.6
1	C	128	PHE	4.6
1	D	792	GLY	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	108	GLY	4.6
1	D	107	ASP	4.6
1	D	806	VAL	4.6
1	C	97	ASN	4.6
1	B	423	PRO	4.5
1	C	785	SER	4.5
1	D	116	ARG	4.5
1	A	96	ILE	4.5
1	B	779	ALA	4.5
1	C	775	LYS	4.5
1	C	749	LYS	4.4
1	C	774	ALA	4.4
1	B	781	VAL	4.3
1	D	126	GLY	4.3
1	D	117	SER	4.2
1	D	818	LYS	4.2
1	C	155	GLN	4.2
1	C	126	GLY	4.2
1	D	121	LYS	4.1
1	B	159	ILE	4.1
1	D	102	PHE	4.0
1	D	110	LEU	4.0
1	D	803	ASN	4.0
1	C	223	SER	4.0
1	B	421	GLN	4.0
1	D	103	MET	4.0
1	D	757	ASP	4.0
1	A	792	GLY	4.0
1	B	125	TYR	3.9
1	B	794	LEU	3.9
1	D	161	PRO	3.9
1	B	804	ILE	3.9
1	D	96	ILE	3.9
1	D	95	ALA	3.9
1	C	143	TRP	3.9
1	D	776	ILE	3.9
1	A	110	LEU	3.9
1	D	140	ASN	3.8
1	B	802	GLY	3.8
1	B	799	ALA	3.7
1	C	105	SER	3.7
1	D	649	THR	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	797	VAL	3.6
1	D	771	PHE	3.6
1	A	109	GLY	3.5
1	D	111	THR	3.5
1	C	384	ASN	3.5
1	D	132	ALA	3.5
1	C	766	THR	3.5
1	C	754	ARG	3.4
1	C	156	ASN	3.4
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	3.4
1	C	764	GLU	3.3
1	A	423	PRO	3.3
1	D	651	ASP	3.3
1	D	129	VAL	3.3
1	B	100	GLY	3.3
1	A	98	GLY	3.3
1	D	779	ALA	3.2
1	D	755	VAL	3.2
1	A	815	GLY	3.2
1	C	760	ASN	3.2
1	D	639	LEU	3.2
1	D	114	LEU	3.2
1	C	168	ALA	3.1
1	B	790	ILE	3.1
1	C	815	GLY	3.1
1	B	111	THR	3.1
1	C	761	ILE	3.1
1	D	638	THR	3.1
1	D	157	ILE	3.1
1	B	379	ALA	3.1
1	C	123	ASP	3.1
1	A	788	GLU	3.1
1	C	152	ARG	3.1
1	D	763	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	774	ALA	3.1
1	B	114	LEU	3.1
1	B	138	GLY	3.0
1	D	762	LEU	3.0
1	B	274	PHE	3.0
1	B	795	PHE	3.0
1	D	143	TRP	3.0
1	A	379	ALA	3.0
1	D	160	ASP	3.0
1	B	150	SER	3.0
1	A	785	SER	3.0
1	D	630	TYR	3.0
1	C	586	GLN	3.0
1	C	816	GLU	2.9
1	D	134	PHE	2.9
1	B	796	LYS	2.9
1	C	757	ASP	2.9
1	B	143	TRP	2.9
1	D	636	LYS	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	D	816	GLU	2.8
1	B	147	THR	2.8
1	B	129	VAL	2.8
1	A	274	PHE	2.8
1	C	753	ILE	2.7
1	D	104	VAL	2.7
1	C	779	ALA	2.7
1	D	817	MET	2.7
1	D	397	GLN	2.7
1	B	791	GLY	2.6
1	D	627	LEU	2.6
1	D	119	ASP	2.6
1	C	158	PHE	2.6
1	D	154	PRO	2.6
1	C	163	MET	2.6
1	B	773	VAL	2.6
1	D	751	ASP	2.6
1	A	789	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	808	GLU	2.6
1	A	794	LEU	2.5
1	D	652	GLY	2.5
1	C	224	LYS	2.5
1	D	805	VAL	2.5
1	C	165	ILE	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	D	418	PHE	2.5
1	C	169	LYS	2.5
1	B	140	ASN	2.5
1	D	759	GLY	2.5
1	C	630	TYR	2.5
1	B	156	ASN	2.5
1	A	278	LEU	2.4
1	A	418	PHE	2.4
1	A	422	PRO	2.4
1	D	745	SER	2.4
1	A	416	ILE	2.4
1	C	140	ASN	2.4
1	C	798	THR	2.4
1	D	151	SER	2.4
1	C	747	ASN	2.4
1	D	789	GLU	2.4
1	A	97	ASN	2.4
1	D	767	ASN	2.4
1	D	761	ILE	2.4
1	C	748	LEU	2.4
1	A	101	PHE	2.3
1	A	811	THR	2.3
1	D	753	ILE	2.3
1	C	107	ASP	2.3
1	A	388	PHE	2.2
1	D	758	LYS	2.2
1	A	113	TYR	2.2
1	B	771	PHE	2.2
1	D	124	ALA	2.2
1	D	701	PHE	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	118	GLY	2.2
1	D	799	ALA	2.2
1	B	757	ASP	2.2
1	C	800	ASN	2.2
1	D	138	GLY	2.2
1	A	143	TRP	2.2
1	B	774	ALA	2.2
1	A	804	ILE	2.2
1	B	149	ASP	2.2
1	A	781	VAL	2.2
1	A	807	GLY	2.2
1	C	220	TYR	2.1
1	D	634	GLY	2.1
1	D	429	VAL	2.1
1	D	749	LYS	2.1
1	C	633	LEU	2.1
1	D	146	GLN	2.1
1	D	721	GLY	2.1
1	C	799	ALA	2.1
1	B	153	THR	2.1
1	A	421	GLN	2.1
1	C	164	HIS	2.1
1	D	387	THR	2.1
1	D	422	PRO	2.1
1	B	787	LEU	2.1
1	D	743	TYR	2.1
1	D	166	PRO	2.1
1	B	756	ASP	2.1
1	C	801	SER	2.1
1	D	105	SER	2.1
1	D	756	ASP	2.0
1	D	670	THR	2.0

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

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.