



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 8, 2025 – 08:04 PM EST

PDB ID : 9CO2  
Title : Crystal structure of BamA in complex with the PTB2 open-state inhibitor  
(anisotropic data set)  
Authors : Sun, D.; Payandeh, J.  
Deposited on : 2024-07-16  
Resolution : 2.75 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.21  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.004 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

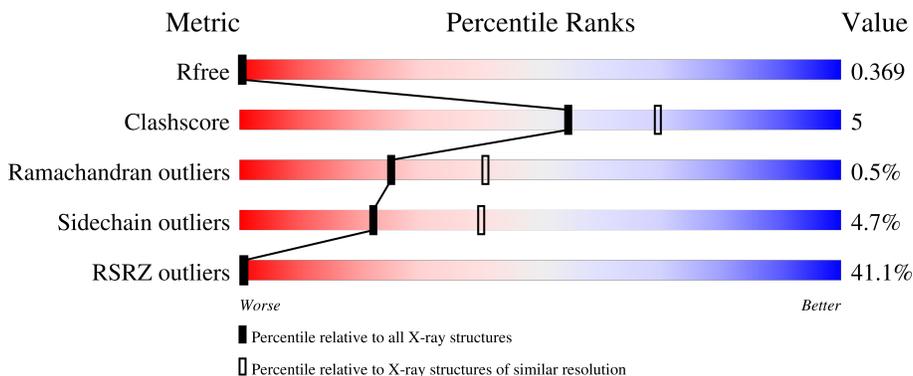
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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))
$R_{free}$	164625	1606 (2.78-2.74)
Clashscore	180529	1689 (2.78-2.74)
Ramachandran outliers	177936	1665 (2.78-2.74)
Sidechain outliers	177891	1665 (2.78-2.74)
RSRZ outliers	164620	1606 (2.78-2.74)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	382	
1	B	382	
1	C	382	
1	D	382	
2	E	17	

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Mol	Chain	Length	Quality of chain
2	F	17	<p>65% 82% 18%</p>
2	G	17	<p>47% 71% 24% 6%</p>
2	I	17	<p>65% 76% 18% 6%</p>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12648 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
			Total	C	N	O	S			
1	A	382	3018	1918	484	606	10	0	0	0
1	B	382	3018	1918	484	606	10	0	0	0
1	C	382	3018	1918	484	606	10	0	0	0
1	D	382	3018	1918	484	606	10	0	0	0

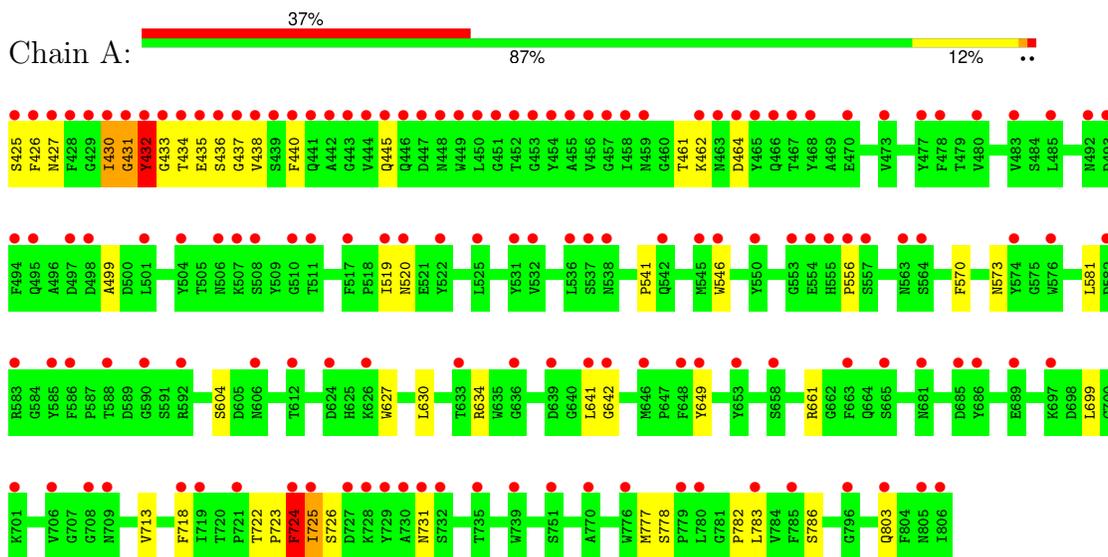
- Molecule 2 is a protein called PTB2 circular peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	E	17	144	96	29	18	1	0	0	1
2	F	17	144	96	29	18	1	0	0	1
2	G	17	144	96	29	18	1	0	0	1
2	I	17	144	96	29	18	1	0	0	1

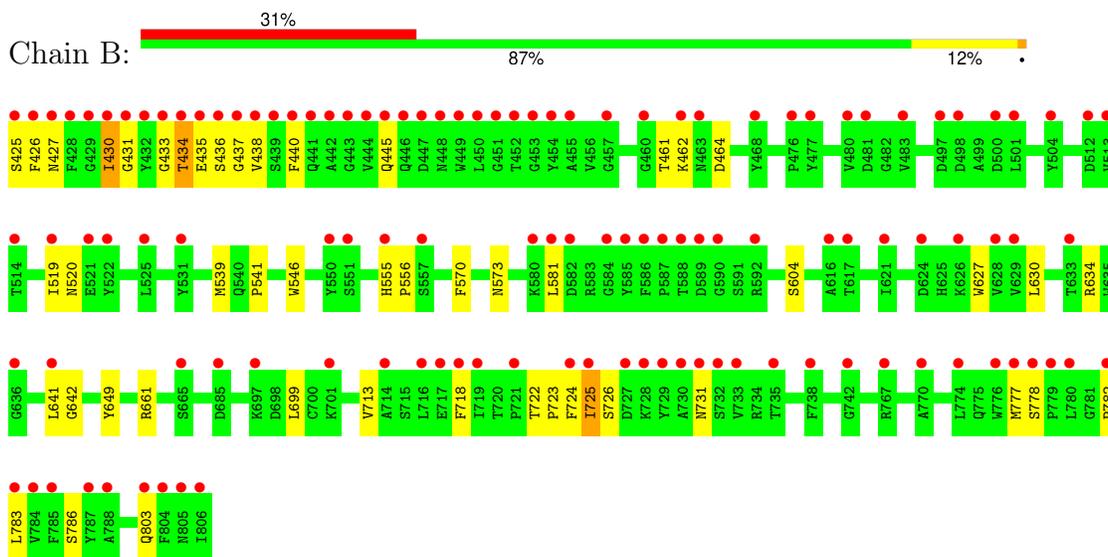
### 3 Residue-property plots [i](#)

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: Outer membrane protein assembly factor BamA



- Molecule 1: Outer membrane protein assembly factor BamA

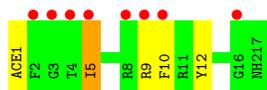


- Molecule 1: Outer membrane protein assembly factor BamA

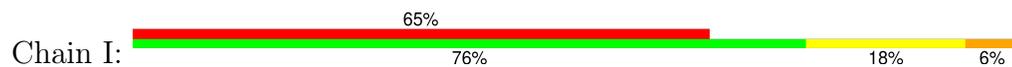




- Molecule 2: PTB2 circular peptide



- Molecule 2: PTB2 circular peptide



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.79Å 167.27Å 104.82Å 90.00° 110.99° 90.00°	Depositor
Resolution (Å)	29.59 – 2.75 29.59 – 2.75	Depositor EDS
% Data completeness (in resolution range)	57.3 (29.59-2.75) 57.4 (29.59-2.75)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.18 (at 2.76Å)	Xtrriage
Refinement program	PHENIX (1.20rc3-4406_final: ???)	Depositor
R, $R_{free}$	0.336 , 0.368 0.336 , 0.369	Depositor DCC
$R_{free}$ test set	4112 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.9	Xtrriage
Anisotropy	0.055	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 41.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.58$ , $\langle L^2 \rangle = 0.43$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	12648	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 60.43 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5235e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

Bond lengths and bond angles in the following residue types are not validated in this section: NH2, ACE

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	0.31	0/3111	0.60	1/4238 (0.0%)
1	B	0.33	0/3111	0.59	0/4238
1	C	0.38	1/3111 (0.0%)	0.63	3/4238 (0.1%)
1	D	0.40	3/3111 (0.1%)	0.61	1/4238 (0.0%)
2	E	0.43	0/147	0.80	1/195 (0.5%)
2	F	0.43	0/147	0.80	1/195 (0.5%)
2	G	0.43	0/147	0.80	1/195 (0.5%)
2	I	0.43	0/147	0.80	1/195 (0.5%)
All	All	0.36	4/13032 (0.0%)	0.62	9/17732 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	C	0	1
1	D	0	2
All	All	0	6

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	724	PHE	CD2-CE2	-9.57	1.20	1.39
1	C	432	TYR	CB-CG	7.67	1.63	1.51
1	D	498	ASP	CB-CG	5.68	1.63	1.51
1	D	724	PHE	CB-CG	-5.67	1.41	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	ACE	O-C-N	7.60	134.86	122.70
2	I	1	ACE	O-C-N	7.58	134.82	122.70
2	G	1	ACE	O-C-N	7.57	134.81	122.70
2	F	1	ACE	O-C-N	7.54	134.76	122.70
1	A	432	TYR	C-N-CA	7.29	137.61	122.30
1	D	724	PHE	CB-CG-CD2	-5.95	116.63	120.80
1	C	432	TYR	CA-CB-CG	5.83	124.48	113.40
1	C	432	TYR	CB-CG-CD2	5.79	124.48	121.00
1	C	585	TYR	CB-CG-CD1	5.09	124.05	121.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	431	GLY	Mainchain
1	B	433	GLY	Peptide
1	B	434	THR	Peptide
1	C	497	ASP	Peptide
1	D	434	THR	Peptide
1	D	497	ASP	Peptide

## 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	3018	0	2740	33	0
1	B	3018	0	2740	29	0
1	C	3018	0	2740	25	0
1	D	3018	0	2740	27	0
2	E	144	0	136	1	0
2	F	144	0	136	0	0
2	G	144	0	136	2	0
2	I	144	0	136	1	0
All	All	12648	0	11504	113	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (113) 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:434:THR:O	1:A:436:SER:N	1.95	0.99
1:A:430:ILE:HG12	1:A:431:GLY:H	1.41	0.86
1:B:430:ILE:HG12	1:B:431:GLY:H	1.41	0.86
1:C:430:ILE:HG12	1:C:431:GLY:H	1.41	0.85
1:D:430:ILE:HG12	1:D:431:GLY:H	1.41	0.84
1:C:425:SER:N	1:C:445:GLN:O	2.24	0.71
1:A:425:SER:N	1:A:445:GLN:O	2.24	0.70
1:D:425:SER:N	1:D:445:GLN:O	2.24	0.70
1:B:425:SER:N	1:B:445:GLN:O	2.24	0.70
1:D:722:THR:HB	1:D:725:ILE:HG13	1.81	0.63
1:A:722:THR:HB	1:A:725:ILE:HG13	1.81	0.63
1:B:722:THR:HB	1:B:725:ILE:HG13	1.81	0.62
1:B:723:PRO:O	1:B:724:PHE:CG	2.52	0.62
1:C:430:ILE:HG12	1:C:431:GLY:N	2.13	0.61
1:A:430:ILE:HG12	1:A:431:GLY:N	2.13	0.61
1:C:722:THR:HB	1:C:725:ILE:HG13	1.81	0.60
1:B:430:ILE:HG12	1:B:431:GLY:N	2.13	0.59
1:D:430:ILE:HG12	1:D:431:GLY:N	2.13	0.58
1:C:497:ASP:O	1:C:498:ASP:HB3	2.07	0.55
1:A:627:TRP:HE3	1:A:718:PHE:CZ	2.26	0.54
1:C:627:TRP:HE3	1:C:718:PHE:CZ	2.26	0.54
1:D:627:TRP:HE3	1:D:718:PHE:CZ	2.26	0.53
1:B:627:TRP:HE3	1:B:718:PHE:CZ	2.26	0.53
1:D:463:ASN:ND2	2:G:12:TYR:OH	2.39	0.52
1:D:430:ILE:HG13	1:D:440:PHE:HE1	1.75	0.52
1:C:430:ILE:HG13	1:C:440:PHE:HE1	1.75	0.51
1:A:430:ILE:HG13	1:A:440:PHE:HE1	1.75	0.51
1:A:440:PHE:O	1:A:461:THR:HA	2.11	0.50
1:D:440:PHE:O	1:D:461:THR:HA	2.11	0.50
1:B:430:ILE:HG13	1:B:440:PHE:HE1	1.75	0.50
1:B:440:PHE:O	1:B:461:THR:HA	2.11	0.50
1:C:440:PHE:O	1:C:461:THR:HA	2.11	0.50
1:D:634:ARG:HB2	1:D:713:VAL:HG22	1.94	0.49
1:D:724:PHE:C	1:D:725:ILE:HG12	2.32	0.49
1:B:634:ARG:HB2	1:B:713:VAL:HG22	1.94	0.49
1:C:634:ARG:HB2	1:C:713:VAL:HG22	1.94	0.49
1:A:634:ARG:HB2	1:A:713:VAL:HG22	1.94	0.48
1:D:437:GLY:HA3	1:D:464:ASP:H	1.78	0.48
1:A:519:ILE:HG13	1:A:520:ASN:H	1.78	0.48
1:C:437:GLY:HA3	1:C:464:ASP:H	1.78	0.48
1:D:778:SER:HB3	1:D:783:LEU:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:519:ILE:HG13	1:D:520:ASN:H	1.78	0.48
1:B:555:HIS:CD2	1:C:697:LYS:HG2	2.49	0.48
1:B:778:SER:HB3	1:B:783:LEU:HD11	1.96	0.48
1:C:519:ILE:HG13	1:C:520:ASN:H	1.78	0.48
1:B:519:ILE:HG13	1:B:520:ASN:H	1.78	0.47
1:A:778:SER:HB3	1:A:783:LEU:HD11	1.96	0.47
1:D:570:PHE:H	1:D:604:SER:HB3	1.79	0.47
1:B:570:PHE:H	1:B:604:SER:HB3	1.79	0.47
1:A:437:GLY:HA3	1:A:464:ASP:H	1.78	0.47
1:C:570:PHE:H	1:C:604:SER:HB3	1.79	0.47
1:C:778:SER:HB3	1:C:783:LEU:HD11	1.96	0.47
1:B:437:GLY:HA3	1:B:464:ASP:H	1.78	0.46
1:D:440:PHE:HB2	1:D:462:LYS:HB3	1.97	0.46
1:A:570:PHE:H	1:A:604:SER:HB3	1.79	0.46
1:B:440:PHE:HB2	1:B:462:LYS:HB3	1.97	0.46
1:C:440:PHE:HB2	1:C:462:LYS:HB3	1.97	0.46
1:A:641:LEU:O	1:B:642:GLY:HA3	2.15	0.46
1:A:430:ILE:CG1	1:A:431:GLY:H	2.22	0.45
1:A:786:SER:OG	1:A:803:GLN:HB2	2.16	0.45
1:C:786:SER:OG	1:C:803:GLN:HB2	2.16	0.45
1:A:642:GLY:HA3	1:B:641:LEU:O	2.16	0.45
1:B:786:SER:OG	1:B:803:GLN:HB2	2.16	0.45
1:D:498:ASP:CG	1:D:499:ALA:N	2.69	0.45
1:D:786:SER:OG	1:D:803:GLN:HB2	2.17	0.45
1:A:432:TYR:CG	1:A:433:GLY:N	2.85	0.45
1:A:541:PRO:HA	1:A:546:TRP:CE2	2.52	0.45
1:C:541:PRO:HA	1:C:546:TRP:NE1	2.32	0.45
1:C:430:ILE:CG1	1:C:431:GLY:N	2.80	0.44
1:A:777:MET:HA	1:A:782:PRO:HA	2.00	0.44
1:D:430:ILE:CG1	1:D:431:GLY:N	2.80	0.44
1:D:541:PRO:HA	1:D:546:TRP:NE1	2.32	0.44
1:B:777:MET:HA	1:B:782:PRO:HA	2.00	0.44
1:D:541:PRO:HA	1:D:546:TRP:CE2	2.52	0.44
1:D:777:MET:HA	1:D:782:PRO:HA	2.00	0.44
1:A:440:PHE:HB2	1:A:462:LYS:HB3	1.97	0.44
1:C:541:PRO:HA	1:C:546:TRP:CE2	2.52	0.44
1:B:541:PRO:HA	1:B:546:TRP:NE1	2.32	0.44
1:A:434:THR:O	1:A:434:THR:HG22	2.17	0.44
1:C:722:THR:CB	1:C:725:ILE:HG13	2.47	0.44
1:C:777:MET:HA	1:C:782:PRO:HA	2.00	0.44
1:A:541:PRO:HA	1:A:546:TRP:NE1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:434:THR:O	1:B:436:SER:O	2.36	0.44
1:B:541:PRO:HA	1:B:546:TRP:CE2	2.52	0.43
1:D:722:THR:CB	1:D:725:ILE:HG13	2.47	0.43
1:B:430:ILE:HG13	1:B:440:PHE:CE1	2.53	0.43
1:D:430:ILE:HG13	1:D:440:PHE:CE1	2.53	0.43
1:A:722:THR:CB	1:A:725:ILE:HG13	2.47	0.43
1:A:430:ILE:CG1	1:A:431:GLY:N	2.80	0.42
1:D:430:ILE:CG1	1:D:431:GLY:H	2.22	0.42
1:A:723:PRO:O	1:A:724:PHE:CD1	2.73	0.42
1:C:430:ILE:HG13	1:C:440:PHE:CE1	2.53	0.42
2:I:5:ILE:HD13	2:I:10:PHE:O	2.20	0.41
1:A:723:PRO:O	1:A:724:PHE:CB	2.68	0.41
1:B:539:MET:H	1:B:539:MET:HG2	1.64	0.41
1:B:722:THR:CB	1:B:725:ILE:HG13	2.47	0.41
2:E:5:ILE:HD13	2:E:10:PHE:O	2.20	0.41
1:B:555:HIS:CE1	1:C:697:LYS:HE3	2.55	0.41
1:A:430:ILE:HG13	1:A:440:PHE:CE1	2.53	0.41
1:D:425:SER:HA	1:D:426:PHE:CD2	2.56	0.41
1:C:425:SER:HA	1:C:426:PHE:CD2	2.56	0.41
1:A:425:SER:HA	1:A:426:PHE:CD2	2.56	0.41
1:B:425:SER:HA	1:B:426:PHE:CD2	2.56	0.41
1:C:546:TRP:CE3	1:C:556:PRO:HG2	2.56	0.41
2:G:5:ILE:HD13	2:G:10:PHE:O	2.20	0.41
1:A:546:TRP:CE3	1:A:556:PRO:HG2	2.56	0.41
1:B:546:TRP:CE3	1:B:556:PRO:HG2	2.56	0.40
1:D:438:VAL:HG23	1:D:464:ASP:OD1	2.21	0.40
1:D:539:MET:H	1:D:539:MET:HG2	1.64	0.40
1:A:438:VAL:HG23	1:A:464:ASP:OD1	2.22	0.40
1:A:723:PRO:O	1:A:724:PHE:CG	2.75	0.40
1:B:438:VAL:HG23	1:B:464:ASP:OD1	2.22	0.40
1:A:627:TRP:CE3	1:A:718:PHE:CZ	3.09	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	380/382 (100%)	358 (94%)	18 (5%)	4 (1%)	12	21
1	B	380/382 (100%)	358 (94%)	21 (6%)	1 (0%)	37	55
1	C	380/382 (100%)	362 (95%)	16 (4%)	2 (0%)	25	41
1	D	380/382 (100%)	361 (95%)	18 (5%)	1 (0%)	37	55
2	E	15/17 (88%)	15 (100%)	0	0	100	100
2	F	15/17 (88%)	15 (100%)	0	0	100	100
2	G	15/17 (88%)	15 (100%)	0	0	100	100
2	I	15/17 (88%)	15 (100%)	0	0	100	100
All	All	1580/1596 (99%)	1499 (95%)	73 (5%)	8 (0%)	25	41

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	432	TYR
1	A	435	GLU
1	B	435	GLU
1	C	498	ASP
1	A	499	ALA
1	A	724	PHE
1	D	435	GLU
1	C	433	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	320/320 (100%)	308 (96%)	12 (4%)	28	49
1	B	320/320 (100%)	309 (97%)	11 (3%)	32	54
1	C	320/320 (100%)	305 (95%)	15 (5%)	22	40
1	D	320/320 (100%)	304 (95%)	16 (5%)	20	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	13/13 (100%)	11 (85%)	2 (15%)	2	3
2	F	13/13 (100%)	11 (85%)	2 (15%)	2	3
2	G	13/13 (100%)	11 (85%)	2 (15%)	2	3
2	I	13/13 (100%)	11 (85%)	2 (15%)	2	3
All	All	1332/1332 (100%)	1270 (95%)	62 (5%)	22	40

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	427	ASN
1	A	430	ILE
1	A	573	ASN
1	A	581	LEU
1	A	630	LEU
1	A	649	TYR
1	A	661	ARG
1	A	699	LEU
1	A	724	PHE
1	A	725	ILE
1	A	726	SER
1	A	731	ASN
1	B	427	ASN
1	B	430	ILE
1	B	573	ASN
1	B	581	LEU
1	B	630	LEU
1	B	649	TYR
1	B	661	ARG
1	B	699	LEU
1	B	725	ILE
1	B	726	SER
1	B	731	ASN
1	C	427	ASN
1	C	430	ILE
1	C	432	TYR
1	C	498	ASP
1	C	573	ASN
1	C	581	LEU
1	C	585	TYR
1	C	630	LEU
1	C	649	TYR

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Mol	Chain	Res	Type
1	C	661	ARG
1	C	699	LEU
1	C	724	PHE
1	C	725	ILE
1	C	726	SER
1	C	731	ASN
1	D	427	ASN
1	D	430	ILE
1	D	432	TYR
1	D	498	ASP
1	D	573	ASN
1	D	581	LEU
1	D	585	TYR
1	D	630	LEU
1	D	649	TYR
1	D	661	ARG
1	D	699	LEU
1	D	724	PHE
1	D	725	ILE
1	D	726	SER
1	D	731	ASN
1	D	739	TRP
2	E	5	ILE
2	E	9	ARG
2	F	5	ILE
2	F	9	ARG
2	G	5	ILE
2	G	9	ARG
2	I	5	ILE
2	I	9	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 oligosaccharides 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	382/382 (100%)	1.88	141 (36%)	1   1	17, 51, 109, 172	0
1	B	382/382 (100%)	1.71	119 (31%)	1   1	16, 51, 107, 160	0
1	C	382/382 (100%)	2.45	190 (49%)	0   0	25, 53, 124, 185	0
1	D	382/382 (100%)	2.30	167 (43%)	1   0	27, 56, 118, 184	0
2	E	15/17 (88%)	2.07	5 (33%)	1   1	29, 50, 79, 79	7 (46%)
2	F	15/17 (88%)	3.11	11 (73%)	0   0	38, 66, 97, 97	0
2	G	15/17 (88%)	2.39	8 (53%)	0   0	39, 70, 106, 111	0
2	I	15/17 (88%)	3.25	11 (73%)	0   0	22, 35, 74, 79	7 (46%)
All	All	1588/1596 (99%)	2.11	652 (41%)	1   0	16, 53, 116, 185	14 (0%)

All (652) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	433	GLY	22.1
1	D	433	GLY	15.0
1	B	430	ILE	12.7
1	A	434	THR	11.5
1	C	432	TYR	11.1
1	D	432	TYR	11.1
1	A	432	TYR	10.0
1	A	437	GLY	9.8
1	B	432	TYR	9.4
1	C	426	PHE	9.4
1	B	434	THR	9.4
1	C	429	GLY	9.3
1	B	436	SER	9.2
1	C	430	ILE	9.0
1	D	587	PRO	9.0
1	D	586	PHE	8.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	438	VAL	8.8
1	C	436	SER	8.8
1	A	433	GLY	8.8
1	D	430	ILE	8.6
1	D	437	GLY	8.5
1	C	437	GLY	8.4
1	D	426	PHE	8.4
1	C	435	GLU	8.3
1	D	438	VAL	8.1
1	A	436	SER	7.9
1	C	486	GLY	7.8
2	I	16	GLY	7.8
1	D	436	SER	7.7
1	D	582	ASP	7.7
1	D	588	THR	7.5
1	D	434	THR	7.4
1	B	426	PHE	7.3
1	C	428	PHE	7.2
1	A	430	ILE	7.2
1	C	449	TRP	7.1
1	A	435	GLU	7.0
2	I	3	GLY	6.8
1	D	442	ALA	6.8
1	D	642	GLY	6.8
1	D	501	LEU	6.6
1	D	435	GLU	6.6
1	C	487	GLY	6.4
2	F	3	GLY	6.4
1	C	434	THR	6.4
1	B	780	LEU	6.4
1	B	443	GLY	6.3
1	A	429	GLY	6.3
1	D	476	PRO	6.3
1	C	477	TYR	6.2
1	B	429	GLY	6.2
1	A	457	GLY	6.2
1	A	428	PHE	6.1
1	C	724	PHE	6.1
1	D	730	ALA	6.1
1	C	582	ASP	6.1
1	D	519	ILE	6.1
1	C	474	THR	6.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	806	ILE	6.0
2	F	2	PHE	6.0
2	F	8	ARG	5.9
1	B	477	TYR	5.9
1	D	445	GLN	5.9
1	C	796	GLY	5.8
1	D	780	LEU	5.8
1	B	438	VAL	5.7
1	B	449	TRP	5.7
1	B	770	ALA	5.7
1	A	450	LEU	5.7
1	C	450	LEU	5.7
1	C	799	ALA	5.7
1	A	446	GLN	5.6
1	B	776	TRP	5.6
1	A	779	PRO	5.6
1	B	433	GLY	5.5
1	D	450	LEU	5.5
1	B	592	ARG	5.5
1	A	449	TRP	5.5
1	D	449	TRP	5.5
1	C	642	GLY	5.5
1	D	729	TYR	5.5
1	C	662	GLY	5.5
1	A	462	LYS	5.5
1	D	728	LYS	5.5
1	D	725	ILE	5.5
1	A	438	VAL	5.4
1	D	550	TYR	5.4
1	C	445	GLN	5.4
1	D	626	LYS	5.4
1	B	435	GLU	5.4
1	D	665	SER	5.4
1	C	727	ASP	5.4
1	C	431	GLY	5.3
1	B	729	TYR	5.3
1	D	551	SER	5.3
1	C	472	SER	5.3
2	G	3	GLY	5.3
1	B	442	ALA	5.3
1	C	551	SER	5.2
1	A	685	ASP	5.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	587	PRO	5.2
1	B	428	PHE	5.2
1	A	493	ASP	5.2
1	B	779	PRO	5.2
1	C	501	LEU	5.2
1	A	440	PHE	5.2
1	D	724	PHE	5.2
1	D	583	ARG	5.1
1	B	450	LEU	5.1
1	C	446	GLN	5.1
1	D	447	ASP	5.1
1	C	649	TYR	5.1
1	D	427	ASN	5.1
1	B	445	GLN	5.0
1	D	477	TYR	5.0
1	C	586	PHE	5.0
1	D	425	SER	5.0
1	D	770	ALA	5.0
1	D	429	GLY	5.0
2	E	10	PHE	5.0
1	B	628	VAL	4.9
1	C	585	TYR	4.9
1	C	588	THR	4.9
1	D	431	GLY	4.9
1	D	727	ASP	4.9
1	B	724	PHE	4.9
1	C	550	TYR	4.9
1	A	427	ASN	4.8
1	B	439	SER	4.8
1	C	546	TRP	4.8
1	C	480	VAL	4.8
1	D	782	PRO	4.8
1	B	431	GLY	4.8
1	C	718	PHE	4.7
1	A	805	ASN	4.6
1	A	780	LEU	4.6
1	B	785	PHE	4.6
1	C	425	SER	4.6
1	A	426	PHE	4.6
1	C	665	SER	4.6
1	D	585	TYR	4.6
1	C	511	THR	4.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	466	GLN	4.6
1	D	522	TYR	4.6
1	D	474	THR	4.5
1	C	447	ASP	4.5
1	B	440	PHE	4.5
1	A	550	TYR	4.5
1	B	730	ALA	4.5
1	C	730	ALA	4.5
2	I	10	PHE	4.5
1	B	550	TYR	4.5
1	A	725	ILE	4.5
1	A	553	GLY	4.5
1	C	739	TRP	4.5
1	A	641	LEU	4.5
1	A	686	TYR	4.4
1	C	448	ASN	4.4
1	C	519	ILE	4.4
1	B	425	SER	4.4
1	C	565	PHE	4.4
2	G	10	PHE	4.4
1	A	477	TYR	4.4
1	A	504	TYR	4.4
1	C	729	TYR	4.4
1	B	581	LEU	4.4
1	A	592	ARG	4.4
1	D	428	PHE	4.4
1	A	642	GLY	4.4
1	A	452	THR	4.4
1	B	588	THR	4.4
1	D	775	GLN	4.4
2	F	9	ARG	4.4
1	C	427	ASN	4.4
1	B	582	ASP	4.4
1	A	463	ASN	4.3
1	D	446	GLN	4.3
1	D	723	PRO	4.3
1	D	785	PHE	4.3
2	G	2	PHE	4.3
1	C	732	SER	4.3
1	D	557	SER	4.3
1	A	511	THR	4.3
1	D	633	THR	4.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	447	ASP	4.2
2	E	9	ARG	4.2
1	C	775	GLN	4.2
1	A	531	TYR	4.2
2	E	3	GLY	4.2
1	A	448	ASN	4.2
1	C	689	GLU	4.2
1	D	803	GLN	4.2
2	F	10	PHE	4.2
1	A	425	SER	4.2
1	D	480	VAL	4.2
1	C	522	TYR	4.2
1	C	798	LYS	4.2
1	D	628	VAL	4.1
1	A	697	LYS	4.1
1	C	442	ALA	4.1
1	D	453	GLY	4.1
1	C	568	ASP	4.1
1	C	725	ILE	4.1
1	C	780	LEU	4.1
1	C	701	LYS	4.1
1	C	648	PHE	4.1
1	A	431	GLY	4.0
1	C	803	GLN	4.0
1	C	583	ARG	4.0
1	D	504	TYR	4.0
1	C	495	GLN	4.0
1	C	753	GLN	4.0
1	C	587	PRO	4.0
1	C	802	PHE	4.0
1	D	718	PHE	4.0
1	A	439	SER	4.0
1	B	732	SER	4.0
1	C	633	THR	4.0
1	B	586	PHE	4.0
1	C	785	PHE	4.0
1	B	621	ILE	4.0
1	C	504	TYR	4.0
1	D	618	TYR	4.0
1	D	802	PHE	4.0
1	D	766	ILE	4.0
1	D	497	ASP	3.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	468	TYR	3.9
1	B	427	ASN	3.9
1	A	501	LEU	3.9
1	B	557	SER	3.9
1	B	522	TYR	3.9
1	C	609	TYR	3.9
1	D	454	TYR	3.9
1	B	697	LYS	3.9
1	B	725	ILE	3.9
1	C	440	PHE	3.9
1	D	440	PHE	3.9
1	C	498	ASP	3.8
1	D	487	GLY	3.8
1	D	701	LYS	3.8
1	A	729	TYR	3.8
1	C	536	LEU	3.8
1	D	732	SER	3.8
1	A	444	VAL	3.8
1	D	456	VAL	3.8
1	C	755	SER	3.8
1	A	453	GLY	3.8
1	C	463	ASN	3.8
1	C	707	GLY	3.7
2	I	8	ARG	3.7
2	I	9	ARG	3.7
1	C	770	ALA	3.7
1	A	785	PHE	3.7
1	A	522	TYR	3.7
1	D	739	TRP	3.7
1	B	447	ASP	3.7
1	C	570	PHE	3.7
1	C	454	TYR	3.7
1	D	616	ALA	3.7
1	C	747	THR	3.7
1	B	589	ASP	3.7
2	I	5	ILE	3.7
1	D	439	SER	3.7
1	B	728	LYS	3.6
1	D	779	PRO	3.6
1	A	776	TRP	3.6
1	D	502	SER	3.6
1	D	448	ASN	3.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	455	ALA	3.6
1	D	784	VAL	3.6
1	D	590	GLY	3.6
1	A	582	ASP	3.6
1	C	493	ASP	3.6
1	D	471	LEU	3.6
1	B	444	VAL	3.6
1	D	624	ASP	3.6
1	A	455	ALA	3.6
1	B	616	ALA	3.6
1	C	497	ASP	3.6
1	D	489	LEU	3.5
1	C	723	PRO	3.5
1	D	649	TYR	3.5
1	B	727	ASP	3.5
1	C	502	SER	3.5
1	C	666	ASN	3.5
1	D	629	VAL	3.5
1	B	783	LEU	3.5
1	B	685	ASP	3.4
1	D	589	ASP	3.4
1	D	619	VAL	3.4
1	A	519	ILE	3.4
1	C	754	TYR	3.4
1	D	609	TYR	3.4
1	A	497	ASP	3.4
1	D	793	LYS	3.4
2	F	16	GLY	3.4
1	D	613	LEU	3.4
2	E	16	GLY	3.4
1	A	458	ILE	3.4
1	C	483	VAL	3.4
1	B	738	PHE	3.4
1	B	468	TYR	3.3
1	B	782	PRO	3.3
1	C	569	ASP	3.3
1	D	444	VAL	3.3
1	B	437	GLY	3.3
1	C	475	ASN	3.3
1	C	530	GLY	3.3
1	D	774	LEU	3.3
2	G	5	ILE	3.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	480	VAL	3.3
1	B	774	LEU	3.3
1	C	643	GLY	3.3
1	C	462	LYS	3.3
1	C	674	TYR	3.3
1	A	443	GLY	3.3
1	A	665	SER	3.3
1	C	439	SER	3.3
1	C	485	LEU	3.3
1	C	539	MET	3.2
1	B	719	ILE	3.2
1	C	532	VAL	3.2
1	D	716	LEU	3.2
1	B	718	PHE	3.2
1	C	782	PRO	3.2
1	A	649	TYR	3.2
1	D	486	GLY	3.2
1	D	592	ARG	3.2
1	D	596	THR	3.2
1	B	551	SER	3.2
1	A	719	ILE	3.2
1	A	525	LEU	3.2
1	D	783	LEU	3.2
1	C	592	ARG	3.2
1	C	632	ARG	3.2
1	D	498	ASP	3.2
1	B	452	THR	3.2
1	A	770	ALA	3.2
1	B	446	GLN	3.2
1	A	624	ASP	3.2
1	C	481	ASP	3.2
1	C	790	PRO	3.1
1	A	520	ASN	3.1
1	D	472	SER	3.1
1	D	546	TRP	3.1
1	A	636	GLY	3.1
1	C	507	LYS	3.1
1	D	697	LYS	3.1
1	A	576	TRP	3.1
1	D	584	GLY	3.1
1	A	545	MET	3.1
1	D	607	GLU	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	533	HIS	3.1
1	C	668	ILE	3.1
1	D	475	ASN	3.1
1	C	706	VAL	3.1
1	D	719	ILE	3.1
2	G	9	ARG	3.1
1	A	441	GLN	3.1
1	D	631	GLY	3.1
1	B	481	ASP	3.0
1	D	722	THR	3.0
1	A	718	PHE	3.0
1	C	610	LYS	3.0
1	D	580	LYS	3.0
1	C	697	LYS	3.0
1	B	457	GLY	3.0
1	C	476	PRO	3.0
1	B	521	GLU	3.0
1	A	588	THR	3.0
1	D	479	THR	3.0
1	A	483	VAL	3.0
1	C	628	VAL	3.0
1	C	681	ASN	3.0
1	C	540	GLN	3.0
1	D	441	GLN	3.0
1	A	451	GLY	3.0
1	D	778	SER	3.0
1	C	692	THR	3.0
1	A	480	VAL	3.0
1	D	483	VAL	3.0
2	E	6	HIS	2.9
1	C	760	TYR	2.9
1	C	557	SER	2.9
1	D	786	SER	2.9
1	B	717	GLU	2.9
2	I	12	TYR	2.9
1	A	728	LYS	2.9
1	D	804	PHE	2.9
1	C	655	GLY	2.9
1	D	518	PRO	2.9
1	D	452	THR	2.9
1	A	456	VAL	2.9
1	A	464	ASP	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	806	ILE	2.9
1	C	749	TRP	2.9
1	A	454	TYR	2.9
1	A	467	THR	2.9
1	A	495	GLN	2.9
1	B	636	GLY	2.9
1	D	579	ASN	2.9
1	D	662	GLY	2.9
1	A	470	GLU	2.8
1	C	671	LYS	2.8
1	B	617	THR	2.8
1	B	454	TYR	2.8
1	A	498	ASP	2.8
1	A	721	PRO	2.8
2	G	16	GLY	2.8
1	D	555	HIS	2.8
1	C	661	ARG	2.8
1	D	634	ARG	2.8
1	D	564	SER	2.8
1	C	673	VAL	2.8
1	A	724	PHE	2.8
1	B	804	PHE	2.8
1	A	538	ASN	2.8
1	A	536	LEU	2.8
1	A	563	ASN	2.8
2	I	14	PHE	2.8
1	A	485	LEU	2.8
1	C	686	TYR	2.8
1	A	510	GLY	2.8
1	C	728	LYS	2.8
1	D	621	ILE	2.7
1	D	681	ASN	2.7
1	A	612	THR	2.7
1	C	529	LEU	2.7
1	D	581	LEU	2.7
1	D	488	ARG	2.7
1	C	806	ILE	2.7
1	D	481	ASP	2.7
1	D	717	GLU	2.7
1	C	456	VAL	2.7
1	A	442	ALA	2.7
2	I	7	LYS	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	453	GLY	2.7
1	D	632	ARG	2.7
1	A	658	SER	2.7
1	B	531	TYR	2.7
1	D	795	ASP	2.7
1	C	545	MET	2.7
1	A	706	VAL	2.7
1	B	784	VAL	2.7
1	A	478	PHE	2.7
1	B	525	LEU	2.7
1	D	641	LEU	2.7
1	D	617	THR	2.7
1	B	519	ILE	2.7
1	C	687	ASP	2.6
1	B	714	ALA	2.6
1	A	633	THR	2.6
1	A	732	SER	2.6
1	D	451	GLY	2.6
1	C	598	LYS	2.6
1	C	606	ASN	2.6
1	D	573	ASN	2.6
1	A	556	PRO	2.6
1	D	743	THR	2.6
1	C	704	ASP	2.6
1	B	448	ASN	2.6
1	C	520	ASN	2.6
1	D	520	ASN	2.6
1	A	445	GLN	2.6
1	C	478	PHE	2.6
1	B	742	GLY	2.6
1	C	584	GLY	2.6
1	C	776	TRP	2.6
1	D	749	TRP	2.6
1	D	777	MET	2.6
1	D	485	LEU	2.6
1	A	542	GLN	2.6
1	B	498	ASP	2.5
1	B	455	ALA	2.5
1	C	499	ALA	2.5
2	F	14	PHE	2.5
1	B	633	THR	2.5
1	C	482	GLY	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	443	GLY	2.5
1	A	751	SER	2.5
1	D	657	SER	2.5
1	B	641	LEU	2.5
1	B	476	PRO	2.5
1	C	624	ASP	2.5
1	C	625	HIS	2.5
1	A	708	GLY	2.5
1	D	482	GLY	2.5
1	A	564	SER	2.5
1	C	721	PRO	2.5
1	A	473	VAL	2.5
1	B	512	ASP	2.5
1	A	459	ASN	2.5
1	A	681	ASN	2.5
1	C	705	ALA	2.5
1	D	799	ALA	2.5
1	B	626	LYS	2.5
1	B	514	THR	2.5
1	C	612	THR	2.5
1	D	692	THR	2.5
2	G	4	THR	2.5
1	A	689	GLU	2.5
1	B	665	SER	2.5
1	B	629	VAL	2.5
1	A	653	TYR	2.5
1	D	738	PHE	2.5
1	D	796	GLY	2.5
1	B	721	PRO	2.4
1	C	684	PRO	2.4
1	C	626	LYS	2.4
1	B	624	ASP	2.4
1	C	534	ASN	2.4
1	C	685	ASP	2.4
1	C	762	ASP	2.4
1	B	451	GLY	2.4
1	C	669	GLY	2.4
1	A	557	SER	2.4
1	A	803	GLN	2.4
1	B	580	LYS	2.4
1	C	490	PHE	2.4
1	A	606	ASN	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	727	ASP	2.4
1	D	709	ASN	2.4
1	C	514	THR	2.4
1	D	684	PRO	2.4
1	C	793	LYS	2.4
2	F	7	LYS	2.4
1	B	441	GLN	2.4
1	C	524	SER	2.4
1	D	473	VAL	2.4
1	A	731	ASN	2.4
1	D	687	ASP	2.4
1	A	554	GLU	2.4
1	C	489	LEU	2.4
1	B	701	LYS	2.4
1	D	620	PRO	2.4
1	D	776	TRP	2.4
1	A	586	PHE	2.4
1	C	726	SER	2.4
1	C	531	TYR	2.4
1	A	492	ASN	2.4
1	A	506	ASN	2.4
1	B	497	ASP	2.4
1	B	805	ASN	2.4
1	C	698	ASP	2.4
1	D	805	ASN	2.4
1	A	735	THR	2.3
1	C	672	ALA	2.3
1	B	585	TYR	2.3
1	C	748	ASN	2.3
1	A	783	LEU	2.3
1	C	667	THR	2.3
1	B	806	ILE	2.3
1	B	590	GLY	2.3
1	A	465	TYR	2.3
1	A	507	LYS	2.3
1	A	639	ASP	2.3
1	C	579	ASN	2.3
1	B	767	ARG	2.3
1	A	648	PHE	2.3
1	C	663	PHE	2.3
1	C	719	ILE	2.3
1	A	537	SER	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	559	SER	2.3
1	B	777	MET	2.3
1	C	757	TYR	2.3
1	C	703	ASP	2.3
1	C	805	ASN	2.3
1	D	731	ASN	2.3
2	F	4	THR	2.3
1	C	473	VAL	2.3
1	D	648	PHE	2.3
1	D	789	GLN	2.3
1	A	739	TRP	2.3
1	A	574	TYR	2.2
1	D	622	ASP	2.2
1	B	460	GLY	2.2
1	D	457	GLY	2.2
1	D	715	SER	2.2
1	C	789	GLN	2.2
1	A	730	ALA	2.2
1	A	546	TRP	2.2
1	C	488	ARG	2.2
1	D	726	SER	2.2
1	C	800	GLU	2.2
1	C	722	THR	2.2
1	A	701	LYS	2.2
1	D	714	ALA	2.2
1	C	771	GLY	2.2
1	C	743	THR	2.2
1	A	709	ASN	2.2
1	D	509	TYR	2.2
1	D	623	ASP	2.2
1	C	580	LYS	2.2
1	B	501	LEU	2.2
1	C	756	GLY	2.2
2	I	13	TRP	2.1
1	C	779	PRO	2.1
1	C	506	ASN	2.1
1	B	500	ASP	2.1
1	C	614	ASP	2.1
1	B	803	GLN	2.1
1	A	646	MET	2.1
1	C	549	LEU	2.1
1	C	734	ARG	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	F	11	ARG	2.1
1	D	689	GLU	2.1
1	D	800	GLU	2.1
1	D	625	HIS	2.1
1	B	787	TYR	2.1
1	C	618	TYR	2.1
1	C	766	ILE	2.1
1	B	788	ALA	2.1
1	B	584	GLY	2.1
1	C	745	TRP	2.1
1	A	626	LYS	2.1
1	B	735	THR	2.1
1	B	778	SER	2.1
1	A	517	PHE	2.1
1	B	463	ASN	2.1
1	B	504	TYR	2.1
1	C	774	LEU	2.1
1	A	796	GLY	2.1
1	D	690	CYS	2.1
1	D	602	PRO	2.1
1	A	555	HIS	2.1
1	B	555	HIS	2.1
1	B	462	LYS	2.1
1	C	777	MET	2.1
2	F	5	ILE	2.1
1	A	532	VAL	2.1
1	C	494	PHE	2.1
1	B	731	ASN	2.1
1	C	783	LEU	2.1
1	C	653	TYR	2.1
1	A	583	ARG	2.1
1	A	590	GLY	2.1
1	D	655	GLY	2.1
1	D	598	LYS	2.0
2	I	6	HIS	2.0
1	A	494	PHE	2.0
1	A	508	SER	2.0
1	A	663	PHE	2.0
1	B	513	VAL	2.0
1	C	761	SER	2.0
1	B	716	LEU	2.0
1	D	463	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	483	VAL	2.0
1	B	733	VAL	2.0
2	G	8	ARG	2.0
1	A	585	TYR	2.0
1	C	616	ALA	2.0
1	D	499	ALA	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.