



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:03 AM UTC

PDB ID : 9CO2 / pdb_00009co2
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

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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

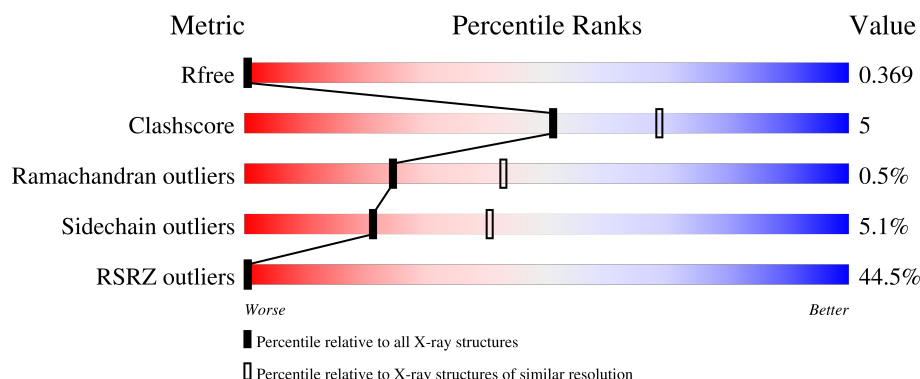
1 Overall quality at a glance

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}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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 $\leq 5\%$. 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	40% 86% 12% ..
1	B	382	34% 86% 12% .
1	C	382	54% 87% 11% .
1	D	382	48% 86% 12% .
2	E	17	35% 76% 18% 6%

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

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
1	A	382	Total	C	N	O	S	0	0	0
			3018	1918	484	606	10			
1	B	382	Total	C	N	O	S	0	0	0
			3018	1918	484	606	10			
1	C	382	Total	C	N	O	S	0	0	0
			3018	1918	484	606	10			
1	D	382	Total	C	N	O	S	0	0	0
			3018	1918	484	606	10			

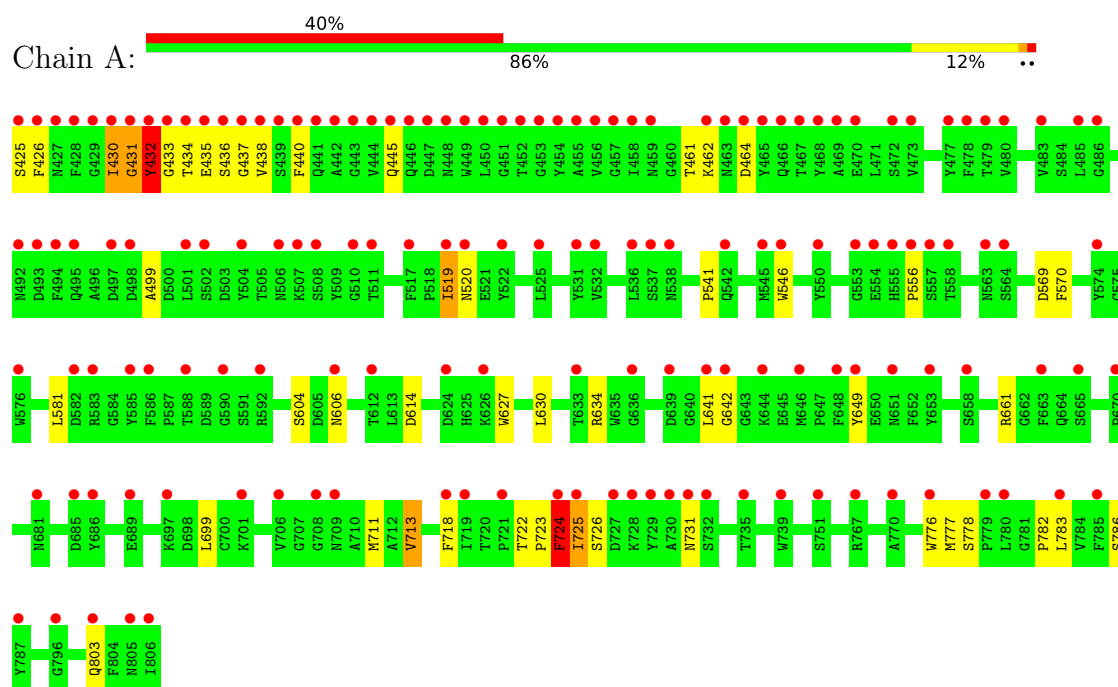
- Molecule 2 is a protein called PTB2 circular peptide.

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

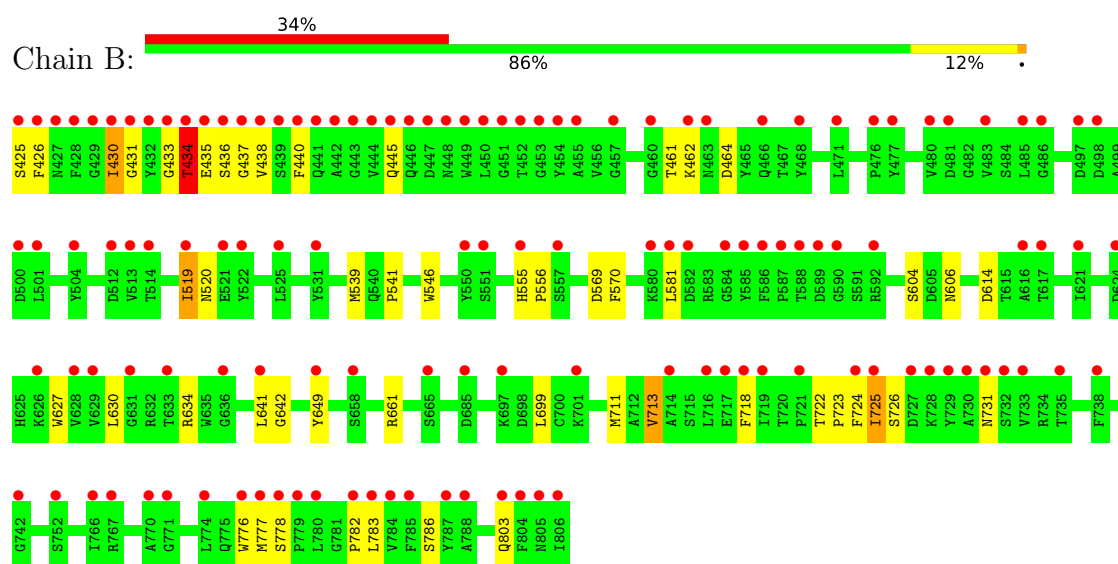
3 Residue-property plots [i](#)

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



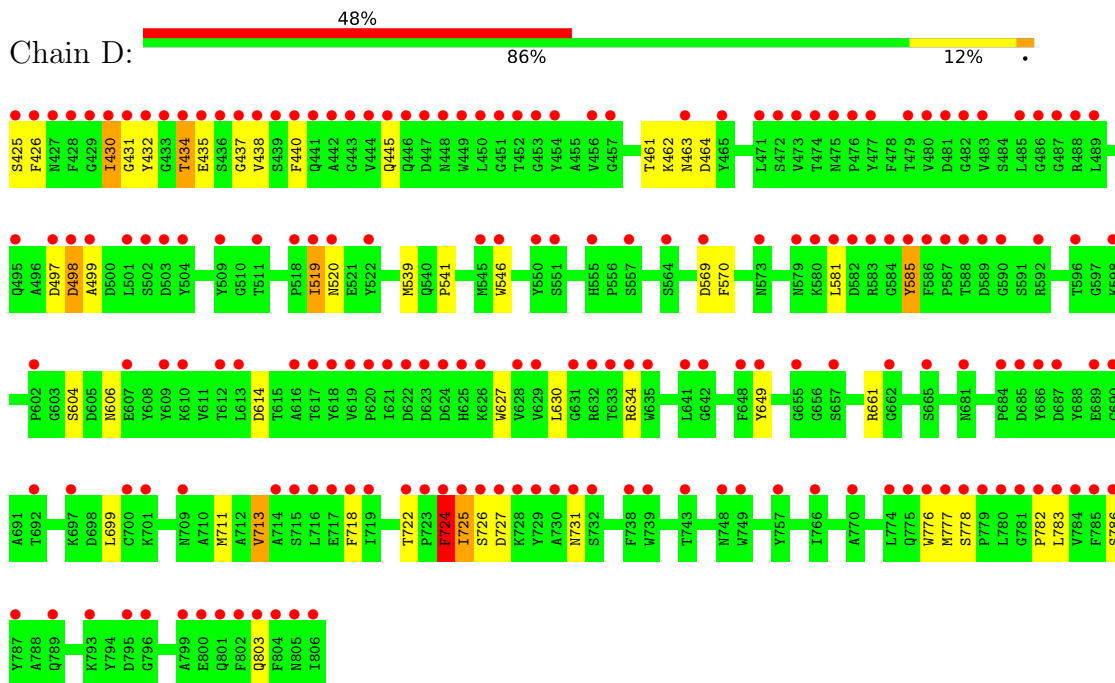
- Molecule 1: Outer membrane protein assembly factor BamA



Chain C:

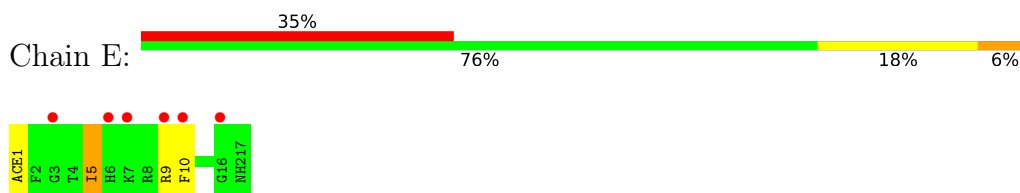


Chain D:

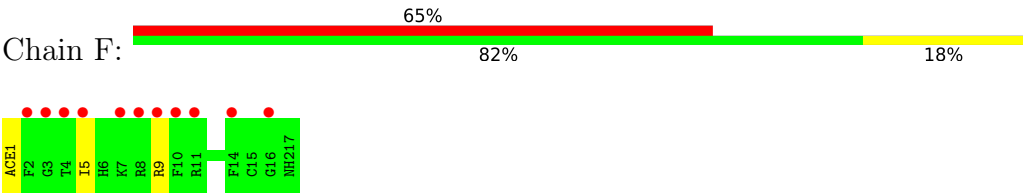


- Molecule 2: PTB2 circular peptide

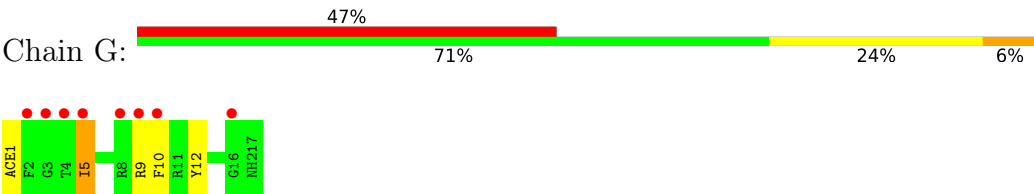
Chain E:



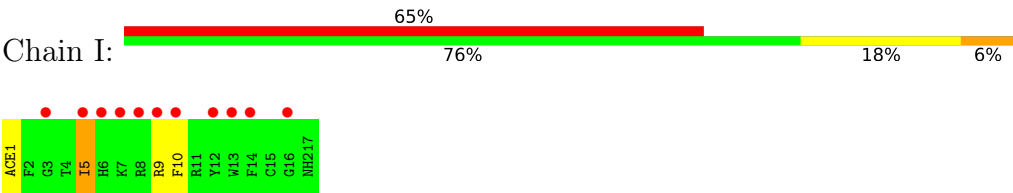
• Molecule 2: PTB2 circular peptide



• 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 2.76Å)	Xtriage
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	2430 reflections (2.94%)	wwPDB-VP
Wilson B-factor (Å ²)	52.9	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.58$, $\langle L^2 \rangle = 0.43$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	12648	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

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	0.22	0/3111	0.55	2/4238 (0.0%)
1	B	0.24	0/3111	0.54	1/4238 (0.0%)
1	C	0.30	2/3111 (0.1%)	0.60	9/4238 (0.2%)
1	D	0.30	1/3111 (0.0%)	0.56	7/4238 (0.2%)
2	E	0.43	1/147 (0.7%)	0.49	0/195
2	F	0.43	1/147 (0.7%)	0.49	0/195
2	G	0.43	1/147 (0.7%)	0.49	0/195
2	I	0.43	1/147 (0.7%)	0.49	0/195
All	All	0.28	7/13032 (0.1%)	0.56	19/17732 (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 (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	724	PHE	CD2-CE2	-6.18	1.20	1.38
1	C	431	GLY	C-N	5.44	1.43	1.33
1	C	432	TYR	CB-CG	5.23	1.63	1.51
2	G	1	ACE	C-N	5.10	1.43	1.33
2	E	1	ACE	C-N	5.10	1.43	1.33
2	F	1	ACE	C-N	5.10	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	1	ACE	C-N	5.07	1.43	1.33

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	432	TYR	CA-C-N	8.26	137.61	121.41
1	A	432	TYR	C-N-CA	8.26	137.61	121.41
1	B	434	THR	N-CA-C	-7.83	99.20	110.24
1	C	433	GLY	CA-C-N	-7.73	110.19	123.25
1	C	433	GLY	C-N-CA	-7.73	110.19	123.25
1	C	434	THR	CA-C-N	6.38	133.72	121.54
1	C	434	THR	C-N-CA	6.38	133.72	121.54
1	D	727	ASP	CA-C-N	-6.16	110.20	120.68
1	D	727	ASP	C-N-CA	-6.16	110.20	120.68
1	C	498	ASP	CA-C-N	-6.14	110.47	120.72
1	C	498	ASP	C-N-CA	-6.14	110.47	120.72
1	C	432	TYR	CA-CB-CG	5.88	124.48	113.90
1	D	434	THR	CA-C-N	5.62	132.28	121.54
1	D	434	THR	C-N-CA	5.62	132.28	121.54
1	D	724	PHE	CA-CB-CG	-5.15	108.65	113.80
1	D	585	TYR	CA-C-N	5.09	127.50	122.00
1	D	585	TYR	C-N-CA	5.09	127.50	122.00
1	C	584	GLY	CA-C-N	-5.08	111.89	120.58
1	C	584	GLY	C-N-CA	-5.08	111.89	120.58

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	37	0
1	B	3018	0	2740	31	0
1	C	3018	0	2740	29	0
1	D	3018	0	2740	30	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	126	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 (126) 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:D:776:TRP:CD1	1:D:777:MET:H	2.19	0.60
1:C:776:TRP:CD1	1:C:777:MET:H	2.20	0.60
1:B:776:TRP:CD1	1:B:777:MET:H	2.20	0.60
1:A:776:TRP:CD1	1:A:777:MET:H	2.19	0.59
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:A:627:TRP:HE3	1:A:718:PHE:CZ	2.26	0.54
1:C:497:ASP:O	1:C:498:ASP:HB3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:724:PHE:C	1:D:725:ILE:HG12	2.32	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:A:434:THR:C	1:A:436:SER:N	2.69	0.50
1:D:498:ASP:CG	1:D:499:ALA:N	2.69	0.49
1:D:634:ARG:HB2	1:D:713:VAL:HG22	1.94	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
1:C:545:MET:HE2	1:C:545:MET:HB3	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:569:ASP:CG	1:A:606:ASN:HD22	2.28	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:D:776:TRP:CG	1:D:777:MET:H	2.39	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:776:TRP:CG	1:A:777:MET:H	2.39	0.40
1:B:569:ASP:CG	1:B:606:ASN:HD22	2.29	0.40
1:D:569:ASP:CG	1:D:606:ASN:HD22	2.28	0.40
1:C:776:TRP:CG	1:C:777:MET:H	2.39	0.40
1:A:627:TRP:CE3	1:A:718:PHE:CZ	3.09	0.40
1:C:569:ASP:CG	1:C:606:ASN:HD22	2.28	0.40

There are no symmetry-related clashes.

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	380/382 (100%)	358 (94%)	18 (5%)	4 (1%)	11	22
1	B	380/382 (100%)	358 (94%)	21 (6%)	1 (0%)	36	56
1	C	380/382 (100%)	362 (95%)	16 (4%)	2 (0%)	24	43
1	D	380/382 (100%)	361 (95%)	18 (5%)	1 (0%)	36	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	24	43

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 ⓘ

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%)	306 (96%)	14 (4%)	25	47
1	B	320/320 (100%)	307 (96%)	13 (4%)	27	49
1	C	320/320 (100%)	304 (95%)	16 (5%)	22	42
1	D	320/320 (100%)	303 (95%)	17 (5%)	20	39
2	E	13/13 (100%)	11 (85%)	2 (15%)	2	4
2	F	13/13 (100%)	11 (85%)	2 (15%)	2	4
2	G	13/13 (100%)	11 (85%)	2 (15%)	2	4
2	I	13/13 (100%)	11 (85%)	2 (15%)	2	4
All	All	1332/1332 (100%)	1264 (95%)	68 (5%)	21	40

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	430	ILE
1	A	519	ILE
1	A	581	LEU
1	A	614	ASP
1	A	630	LEU
1	A	649	TYR
1	A	661	ARG
1	A	699	LEU
1	A	711	MET
1	A	713	VAL
1	A	724	PHE
1	A	725	ILE
1	A	726	SER
1	A	731	ASN
1	B	430	ILE
1	B	519	ILE
1	B	581	LEU
1	B	614	ASP
1	B	630	LEU
1	B	649	TYR
1	B	661	ARG
1	B	699	LEU
1	B	711	MET
1	B	713	VAL
1	B	725	ILE
1	B	726	SER
1	B	731	ASN
1	C	430	ILE
1	C	432	TYR
1	C	519	ILE
1	C	581	LEU
1	C	585	TYR
1	C	614	ASP
1	C	630	LEU
1	C	649	TYR
1	C	661	ARG
1	C	699	LEU
1	C	711	MET
1	C	713	VAL
1	C	724	PHE
1	C	725	ILE
1	C	726	SER

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Mol	Chain	Res	Type
1	C	731	ASN
1	D	430	ILE
1	D	432	TYR
1	D	498	ASP
1	D	519	ILE
1	D	581	LEU
1	D	585	TYR
1	D	614	ASP
1	D	630	LEU
1	D	649	TYR
1	D	661	ARG
1	D	699	LEU
1	D	711	MET
1	D	713	VAL
1	D	724	PHE
1	D	725	ILE
1	D	726	SER
1	D	731	ASN
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. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	534	ASN
1	A	540	GLN
1	A	606	ASN
1	B	534	ASN
1	B	540	GLN
1	C	534	ASN
1	C	540	GLN
1	C	606	ASN
1	C	681	ASN
1	D	534	ASN
1	D	540	GLN
1	D	573	ASN

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, 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	382/382 (100%)	2.00	152 (39%) 1 0	17, 51, 109, 172	0
1	B	382/382 (100%)	1.82	129 (33%) 1 0	16, 51, 107, 160	0
1	C	382/382 (100%)	2.56	206 (53%) 0 0	25, 53, 124, 185	0
1	D	382/382 (100%)	2.41	184 (48%) 0 0	27, 56, 118, 184	0
2	E	15/17 (88%)	2.17	6 (40%) 1 0	29, 50, 79, 79	7 (46%)
2	F	15/17 (88%)	3.21	11 (73%) 0 0	38, 66, 97, 97	0
2	G	15/17 (88%)	2.49	8 (53%) 0 0	39, 70, 106, 111	0
2	I	15/17 (88%)	3.35	11 (73%) 0 0	22, 35, 74, 79	7 (46%)
All	All	1588/1596 (99%)	2.22	707 (44%) 0 0	16, 53, 116, 185	14 (0%)

All (707) 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	12.8
1	A	434	THR	11.5
1	C	432	TYR	11.3
1	D	432	TYR	11.2
1	A	432	TYR	10.2
1	A	437	GLY	9.9
1	C	426	PHE	9.6
1	B	432	TYR	9.5
1	C	429	GLY	9.4
1	B	434	THR	9.4
1	B	436	SER	9.1
1	D	586	PHE	9.1
1	D	587	PRO	9.1
1	C	430	ILE	9.1

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Mol	Chain	Res	Type	RSRZ
1	C	438	VAL	8.9
1	A	433	GLY	8.8
1	C	436	SER	8.7
1	D	430	ILE	8.7
1	D	426	PHE	8.6
1	D	437	GLY	8.5
1	C	437	GLY	8.5
1	C	435	GLU	8.2
1	D	438	VAL	8.2
2	I	16	GLY	8.0
1	A	436	SER	7.9
1	C	486	GLY	7.9
1	D	436	SER	7.6
1	D	582	ASP	7.6
1	D	588	THR	7.5
1	B	426	PHE	7.4
1	D	434	THR	7.4
1	C	428	PHE	7.4
1	A	430	ILE	7.3
1	C	449	TRP	7.3
2	I	3	GLY	6.9
1	D	642	GLY	6.9
1	D	442	ALA	6.9
1	A	435	GLU	6.9
1	D	501	LEU	6.8
1	C	487	GLY	6.6
1	B	780	LEU	6.6
2	F	3	GLY	6.5
1	D	435	GLU	6.5
1	C	434	THR	6.5
1	A	429	GLY	6.5
1	B	443	GLY	6.5
1	D	476	PRO	6.4
1	B	429	GLY	6.3
1	C	477	TYR	6.3
1	A	457	GLY	6.3
1	A	428	PHE	6.3
1	C	724	PHE	6.3
1	D	730	ALA	6.2
1	D	519	ILE	6.2
2	F	2	PHE	6.2
1	C	474	THR	6.1

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Mol	Chain	Res	Type	RSRZ
1	D	806	ILE	6.1
1	C	582	ASP	6.1
1	B	477	TYR	6.0
1	D	780	LEU	5.9
1	D	445	GLN	5.9
1	C	796	GLY	5.9
2	F	8	ARG	5.9
1	B	449	TRP	5.9
1	B	438	VAL	5.9
1	A	450	LEU	5.8
1	C	450	LEU	5.8
1	C	799	ALA	5.8
1	B	770	ALA	5.8
1	B	776	TRP	5.7
1	B	433	GLY	5.7
1	A	779	PRO	5.7
1	D	449	TRP	5.7
1	D	450	LEU	5.6
1	C	662	GLY	5.6
1	D	729	TYR	5.6
1	A	449	TRP	5.6
1	A	446	GLN	5.6
1	C	642	GLY	5.6
1	D	550	TYR	5.5
1	A	438	VAL	5.5
1	D	725	ILE	5.5
1	B	592	ARG	5.5
1	A	462	LYS	5.5
1	D	728	LYS	5.5
1	C	431	GLY	5.5
1	B	729	TYR	5.5
1	C	445	GLN	5.4
1	D	626	LYS	5.4
1	C	727	ASP	5.4
1	B	428	PHE	5.4
1	B	435	GLU	5.4
1	D	665	SER	5.4
1	B	442	ALA	5.3
1	D	551	SER	5.3
1	A	440	PHE	5.3
1	C	501	LEU	5.3
1	B	587	PRO	5.3

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Mol	Chain	Res	Type	RSRZ
1	D	724	PHE	5.3
1	B	779	PRO	5.3
1	B	450	LEU	5.3
1	C	472	SER	5.3
1	C	551	SER	5.3
1	A	685	ASP	5.3
1	C	649	TYR	5.2
2	G	3	GLY	5.2
1	A	493	ASP	5.2
1	C	446	GLN	5.2
1	C	586	PHE	5.2
1	D	447	ASP	5.2
1	D	477	TYR	5.1
1	D	583	ARG	5.1
1	D	427	ASN	5.1
1	D	770	ALA	5.1
2	E	10	PHE	5.1
1	B	628	VAL	5.1
1	B	445	GLN	5.0
1	D	431	GLY	5.0
1	D	425	SER	5.0
1	B	724	PHE	5.0
1	C	585	TYR	5.0
1	D	429	GLY	5.0
1	C	550	TYR	5.0
1	C	588	THR	5.0
1	C	546	TRP	4.9
1	B	431	GLY	4.9
1	C	480	VAL	4.9
1	D	782	PRO	4.9
1	A	427	ASN	4.9
1	B	439	SER	4.9
1	D	727	ASP	4.9
1	C	718	PHE	4.8
1	B	785	PHE	4.8
1	A	780	LEU	4.8
1	A	426	PHE	4.7
1	A	805	ASN	4.7
1	D	585	TYR	4.7
1	D	522	TYR	4.7
1	C	511	THR	4.7
1	C	425	SER	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	440	PHE	4.7
2	I	10	PHE	4.6
1	A	550	TYR	4.6
1	B	730	ALA	4.6
1	D	474	THR	4.6
1	C	665	SER	4.6
1	B	550	TYR	4.6
1	C	739	TRP	4.6
1	C	730	ALA	4.6
1	A	553	GLY	4.6
1	A	641	LEU	4.6
1	C	447	ASP	4.6
1	C	565	PHE	4.6
2	G	10	PHE	4.6
1	A	466	GLN	4.6
1	C	519	ILE	4.6
1	B	581	LEU	4.6
1	D	428	PHE	4.6
1	A	477	TYR	4.5
1	A	504	TYR	4.5
1	A	686	TYR	4.5
1	A	725	ILE	4.5
1	C	729	TYR	4.5
1	A	642	GLY	4.5
1	C	448	ASN	4.5
1	B	425	SER	4.5
1	A	452	THR	4.5
1	B	588	THR	4.5
1	D	775	GLN	4.4
1	D	785	PHE	4.4
2	G	2	PHE	4.4
1	C	427	ASN	4.4
1	D	723	PRO	4.4
1	A	592	ARG	4.4
1	B	582	ASP	4.4
1	A	531	TYR	4.4
2	F	9	ARG	4.4
1	A	463	ASN	4.4
2	E	3	GLY	4.4
1	A	511	THR	4.4
1	D	633	THR	4.4
1	D	446	GLN	4.3

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Mol	Chain	Res	Type	RSRZ
2	F	10	PHE	4.3
1	C	732	SER	4.3
1	A	447	ASP	4.3
1	D	557	SER	4.3
1	C	775	GLN	4.3
1	C	522	TYR	4.3
1	D	480	VAL	4.3
1	D	628	VAL	4.3
1	A	448	ASN	4.3
2	E	9	ARG	4.2
1	C	442	ALA	4.2
1	D	803	GLN	4.2
1	D	453	GLY	4.2
1	A	425	SER	4.2
1	C	689	GLU	4.2
1	C	648	PHE	4.2
1	C	725	ILE	4.2
1	A	697	LYS	4.2
1	C	780	LEU	4.2
1	C	798	LYS	4.2
1	C	802	PHE	4.2
1	C	568	ASP	4.1
1	A	431	GLY	4.1
1	B	586	PHE	4.1
1	C	785	PHE	4.1
1	D	718	PHE	4.1
1	D	802	PHE	4.1
1	C	587	PRO	4.1
1	C	504	TYR	4.1
1	D	504	TYR	4.1
1	D	618	TYR	4.1
1	C	701	LYS	4.1
1	B	621	ILE	4.1
1	C	633	THR	4.1
1	C	495	GLN	4.1
1	C	753	GLN	4.1
1	C	803	GLN	4.1
1	C	583	ARG	4.1
1	D	766	ILE	4.1
1	A	439	SER	4.1
1	B	732	SER	4.1
1	A	468	TYR	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	501	LEU	4.0
1	C	440	PHE	4.0
1	D	440	PHE	4.0
1	B	522	TYR	4.0
1	C	609	TYR	4.0
1	D	454	TYR	4.0
1	D	497	ASP	4.0
1	D	487	GLY	4.0
1	A	729	TYR	4.0
1	B	427	ASN	4.0
1	B	557	SER	3.9
1	B	725	ILE	3.9
1	C	536	LEU	3.9
1	B	697	LYS	3.9
1	C	498	ASP	3.9
1	A	453	GLY	3.9
1	A	444	VAL	3.9
1	D	456	VAL	3.9
1	D	701	LYS	3.9
1	C	770	ALA	3.9
1	A	785	PHE	3.9
1	C	570	PHE	3.9
1	D	732	SER	3.8
1	C	707	GLY	3.8
1	D	739	TRP	3.8
1	A	522	TYR	3.8
1	C	463	ASN	3.8
1	C	755	SER	3.8
1	C	454	TYR	3.8
1	A	776	TRP	3.8
2	I	5	ILE	3.8
1	D	616	ALA	3.8
2	I	8	ARG	3.8
1	D	784	VAL	3.8
1	D	779	PRO	3.8
1	B	447	ASP	3.7
1	C	455	ALA	3.7
2	I	9	ARG	3.7
1	B	589	ASP	3.7
1	C	747	THR	3.7
1	D	471	LEU	3.7
1	D	439	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	590	GLY	3.7
1	B	728	LYS	3.7
1	A	582	ASP	3.7
1	B	616	ALA	3.7
1	B	444	VAL	3.7
1	C	493	ASP	3.7
1	D	448	ASN	3.7
1	A	455	ALA	3.7
1	D	502	SER	3.7
1	D	489	LEU	3.6
1	C	723	PRO	3.6
1	C	497	ASP	3.6
1	D	624	ASP	3.6
1	D	649	TYR	3.6
1	B	783	LEU	3.6
1	C	666	ASN	3.6
1	D	629	VAL	3.6
1	C	754	TYR	3.6
1	D	619	VAL	3.6
1	C	502	SER	3.6
1	D	613	LEU	3.6
1	A	519	ILE	3.5
1	B	727	ASP	3.5
2	F	16	GLY	3.5
1	D	609	TYR	3.5
1	B	685	ASP	3.5
1	D	589	ASP	3.5
2	E	16	GLY	3.5
1	B	738	PHE	3.5
1	A	458	ILE	3.5
1	A	497	ASP	3.5
1	B	437	GLY	3.5
1	C	483	VAL	3.5
1	B	468	TYR	3.5
1	D	793	LYS	3.5
1	C	530	GLY	3.5
1	C	643	GLY	3.5
1	B	782	PRO	3.5
1	D	774	LEU	3.5
1	B	774	LEU	3.4
1	B	480	VAL	3.4
2	G	5	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	674	TYR	3.4
1	C	475	ASN	3.4
1	C	569	ASP	3.4
1	D	444	VAL	3.4
1	A	443	GLY	3.4
1	C	485	LEU	3.4
1	D	716	LEU	3.4
1	B	718	PHE	3.4
1	C	462	LYS	3.4
1	A	525	LEU	3.4
1	C	532	VAL	3.4
1	C	539	MET	3.4
1	B	719	ILE	3.3
1	A	665	SER	3.3
1	C	439	SER	3.3
1	D	486	GLY	3.3
1	A	649	TYR	3.3
1	D	596	THR	3.3
1	C	782	PRO	3.3
1	D	783	LEU	3.3
1	A	719	ILE	3.3
1	D	498	ASP	3.3
1	D	546	TRP	3.3
1	B	452	THR	3.3
1	B	551	SER	3.3
1	C	790	PRO	3.3
1	A	636	GLY	3.3
1	A	770	ALA	3.3
1	A	624	ASP	3.3
1	C	481	ASP	3.3
1	A	576	TRP	3.2
1	B	446	GLN	3.2
1	D	584	GLY	3.2
1	A	520	ASN	3.2
1	C	592	ARG	3.2
1	C	632	ARG	3.2
1	A	545	MET	3.2
1	D	631	GLY	3.2
1	A	718	PHE	3.2
1	C	668	ILE	3.2
1	C	706	VAL	3.2
1	D	475	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	592	ARG	3.2
1	C	507	LYS	3.2
1	D	697	LYS	3.2
1	C	533	HIS	3.2
1	D	472	SER	3.2
1	D	479	THR	3.2
1	D	722	THR	3.2
1	D	719	ILE	3.2
1	D	607	GLU	3.1
1	A	441	GLN	3.1
2	G	9	ARG	3.1
1	B	457	GLY	3.1
1	A	483	VAL	3.1
1	C	628	VAL	3.1
1	C	610	LYS	3.1
1	B	481	ASP	3.1
1	C	476	PRO	3.1
1	A	588	THR	3.1
1	A	451	GLY	3.1
1	C	697	LYS	3.1
1	D	580	LYS	3.1
1	A	480	VAL	3.1
1	D	483	VAL	3.1
1	C	681	ASN	3.1
1	B	521	GLU	3.1
1	C	540	GLN	3.1
1	C	692	THR	3.1
1	D	778	SER	3.1
1	C	760	TYR	3.0
2	E	6	HIS	3.0
1	D	441	GLN	3.0
1	C	749	TRP	3.0
1	D	804	PHE	3.0
1	D	786	SER	3.0
2	I	12	TYR	3.0
1	D	518	PRO	3.0
1	A	806	ILE	3.0
1	C	655	GLY	3.0
1	A	456	VAL	3.0
1	A	464	ASP	3.0
1	A	728	LYS	3.0
1	B	636	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	452	THR	3.0
1	B	804	PHE	3.0
1	B	717	GLU	3.0
1	C	557	SER	3.0
1	A	454	TYR	3.0
1	B	454	TYR	3.0
1	A	467	THR	3.0
1	D	662	GLY	3.0
2	G	16	GLY	3.0
1	A	721	PRO	2.9
1	A	495	GLN	2.9
1	D	579	ASN	2.9
1	A	498	ASP	2.9
1	B	617	THR	2.9
1	A	724	PHE	2.9
1	C	673	VAL	2.9
1	D	555	HIS	2.9
1	C	671	LYS	2.9
1	A	612	THR	2.9
1	A	536	LEU	2.9
1	A	470	GLU	2.9
1	A	538	ASN	2.9
1	A	563	ASN	2.9
1	C	686	TYR	2.9
1	A	510	GLY	2.9
1	A	485	LEU	2.9
1	C	529	LEU	2.9
2	I	14	PHE	2.9
1	C	661	ARG	2.9
1	D	634	ARG	2.9
1	D	564	SER	2.9
1	D	621	ILE	2.9
1	C	728	LYS	2.9
1	D	581	LEU	2.9
1	D	681	ASN	2.8
1	B	453	GLY	2.8
1	D	481	ASP	2.8
1	C	806	ILE	2.8
1	A	442	ALA	2.8
1	B	531	TYR	2.8
1	B	714	ALA	2.8
1	A	478	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	456	VAL	2.8
2	I	7	LYS	2.8
1	D	641	LEU	2.8
1	D	617	THR	2.8
1	C	545	MET	2.8
1	D	717	GLU	2.8
1	B	519	ILE	2.8
1	A	658	SER	2.8
1	B	525	LEU	2.8
1	D	451	GLY	2.8
1	D	795	ASP	2.8
1	A	706	VAL	2.8
1	D	488	ARG	2.8
1	D	632	ARG	2.8
1	A	556	PRO	2.7
1	D	749	TRP	2.7
1	C	584	GLY	2.7
1	A	633	THR	2.7
1	C	478	PHE	2.7
1	A	732	SER	2.7
1	C	606	ASN	2.7
1	C	776	TRP	2.7
1	D	573	ASN	2.7
1	D	777	MET	2.7
1	D	743	THR	2.7
1	C	598	LYS	2.7
1	D	485	LEU	2.7
1	B	742	GLY	2.7
1	B	448	ASN	2.7
1	C	520	ASN	2.7
1	D	520	ASN	2.7
1	B	784	VAL	2.7
1	C	499	ALA	2.7
1	C	687	ASP	2.7
1	A	445	GLN	2.7
1	C	482	GLY	2.7
1	D	443	GLY	2.7
1	B	455	ALA	2.7
2	F	14	PHE	2.7
1	C	704	ASP	2.7
1	A	542	GLN	2.6
1	B	641	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	708	GLY	2.6
1	D	482	GLY	2.6
1	D	657	SER	2.6
1	D	799	ALA	2.6
1	B	476	PRO	2.6
1	B	633	THR	2.6
1	B	498	ASP	2.6
1	C	625	HIS	2.6
1	A	564	SER	2.6
1	A	751	SER	2.6
1	C	721	PRO	2.6
1	D	692	THR	2.6
1	D	738	PHE	2.6
1	C	624	ASP	2.6
1	A	653	TYR	2.6
1	C	669	GLY	2.6
1	D	796	GLY	2.6
1	A	473	VAL	2.6
1	A	681	ASN	2.6
1	B	629	VAL	2.6
1	C	705	ALA	2.6
1	B	514	THR	2.6
1	C	612	THR	2.6
2	G	4	THR	2.6
1	B	512	ASP	2.6
1	B	451	GLY	2.6
1	B	721	PRO	2.6
1	C	490	PHE	2.6
1	B	665	SER	2.5
1	B	624	ASP	2.5
1	B	626	LYS	2.5
1	A	689	GLU	2.5
1	C	684	PRO	2.5
1	C	514	THR	2.5
1	C	534	ASN	2.5
1	C	626	LYS	2.5
1	D	473	VAL	2.5
1	A	586	PHE	2.5
1	A	803	GLN	2.5
1	A	606	ASN	2.5
1	A	557	SER	2.5
1	B	580	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	776	TRP	2.5
1	C	685	ASP	2.5
1	C	762	ASP	2.5
1	D	687	ASP	2.5
1	D	620	PRO	2.5
1	D	684	PRO	2.5
1	A	459	ASN	2.5
1	A	731	ASN	2.5
1	C	793	LYS	2.5
1	D	709	ASN	2.5
2	F	7	LYS	2.5
1	C	489	LEU	2.5
1	C	726	SER	2.5
1	A	727	ASP	2.5
1	A	465	TYR	2.5
1	B	585	TYR	2.5
1	C	531	TYR	2.5
1	B	441	GLN	2.5
1	B	701	LYS	2.4
1	A	735	THR	2.4
1	C	667	THR	2.4
1	A	506	ASN	2.4
1	D	805	ASN	2.4
1	A	783	LEU	2.4
1	C	524	SER	2.4
1	B	497	ASP	2.4
1	B	590	GLY	2.4
1	A	648	PHE	2.4
1	C	663	PHE	2.4
1	C	672	ALA	2.4
1	A	492	ASN	2.4
1	B	805	ASN	2.4
1	B	806	ILE	2.4
1	C	698	ASP	2.4
1	A	554	GLU	2.4
1	B	777	MET	2.4
1	A	507	LYS	2.4
1	C	757	TYR	2.4
1	D	648	PHE	2.4
1	C	719	ILE	2.4
1	C	748	ASN	2.4
1	A	639	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	739	TRP	2.4
1	C	473	VAL	2.4
1	A	574	TYR	2.4
1	C	579	ASN	2.4
1	C	805	ASN	2.4
1	D	731	ASN	2.4
1	A	537	SER	2.4
1	C	559	SER	2.4
1	C	703	ASP	2.4
1	A	546	TRP	2.4
1	B	460	GLY	2.4
1	D	457	GLY	2.4
1	D	789	GLN	2.4
2	F	4	THR	2.3
1	D	622	ASP	2.3
1	B	767	ARG	2.3
1	A	730	ALA	2.3
1	D	509	TYR	2.3
1	D	715	SER	2.3
1	C	789	GLN	2.3
1	D	714	ALA	2.3
1	D	726	SER	2.3
1	C	779	PRO	2.3
2	I	13	TRP	2.3
1	C	771	GLY	2.3
1	B	501	LEU	2.3
1	A	701	LYS	2.3
1	C	722	THR	2.3
1	C	743	THR	2.3
1	B	787	TYR	2.3
1	A	709	ASN	2.3
1	C	488	ARG	2.3
1	D	623	ASP	2.3
1	C	756	GLY	2.3
1	C	549	LEU	2.3
1	A	517	PHE	2.3
1	B	788	ALA	2.2
1	C	766	ILE	2.2
1	A	646	MET	2.2
1	C	800	GLU	2.2
1	C	618	TYR	2.2
1	C	506	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	614	ASP	2.2
1	A	796	GLY	2.2
1	B	584	GLY	2.2
1	C	745	TRP	2.2
1	C	580	LYS	2.2
1	D	625	HIS	2.2
1	B	735	THR	2.2
1	B	504	TYR	2.2
1	B	500	ASP	2.2
1	B	778	SER	2.2
1	C	774	LEU	2.2
1	A	532	VAL	2.2
1	A	626	LYS	2.2
1	C	494	PHE	2.2
1	D	689	GLU	2.2
1	D	690	CYS	2.2
1	D	800	GLU	2.2
1	C	734	ARG	2.2
2	F	11	ARG	2.2
1	B	463	ASN	2.2
1	B	731	ASN	2.2
1	C	653	TYR	2.2
1	D	602	PRO	2.2
1	A	590	GLY	2.2
1	C	783	LEU	2.2
1	D	655	GLY	2.2
1	C	777	MET	2.2
1	A	494	PHE	2.2
1	A	663	PHE	2.2
1	B	555	HIS	2.2
2	F	5	ILE	2.2
1	B	803	GLN	2.2
1	B	716	LEU	2.2
1	A	555	HIS	2.2
1	B	513	VAL	2.2
2	I	6	HIS	2.2
1	A	583	ARG	2.1
1	A	585	TYR	2.1
1	B	462	LYS	2.1
1	D	463	ASN	2.1
1	C	656	GLY	2.1
1	A	508	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	483	VAL	2.1
1	B	733	VAL	2.1
1	C	616	ALA	2.1
1	D	499	ALA	2.1
1	C	576	TRP	2.1
1	D	635	TRP	2.1
1	C	518	PRO	2.1
1	D	598	LYS	2.1
1	B	771	GLY	2.1
1	C	761	SER	2.1
1	A	469	ALA	2.1
1	D	610	LYS	2.1
1	B	466	GLN	2.1
1	D	545	MET	2.1
1	B	485	LEU	2.1
1	D	700	CYS	2.1
1	A	787	TYR	2.1
1	B	486	GLY	2.1
1	C	453	GLY	2.1
1	C	638	GLY	2.1
1	B	766	ILE	2.1
1	D	569	ASP	2.1
1	C	535	SER	2.1
1	A	644	LYS	2.1
1	A	558	THR	2.1
1	D	801	GLN	2.1
1	B	471	LEU	2.1
1	C	581	LEU	2.1
1	A	486	GLY	2.1
1	B	631	GLY	2.1
1	D	781	GLY	2.1
1	B	649	TYR	2.1
1	A	767	ARG	2.0
1	C	639	ASP	2.0
1	C	795	ASP	2.0
1	D	503	ASP	2.0
2	G	8	ARG	2.0
1	A	479	THR	2.0
1	D	511	THR	2.0
1	D	612	THR	2.0
1	A	670	PRO	2.0
1	C	664	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	651	ASN	2.0
1	C	573	ASN	2.0
1	C	574	TYR	2.0
1	D	465	TYR	2.0
1	D	757	TYR	2.0
1	D	787	TYR	2.0
1	C	607	GLU	2.0
1	C	746	ASP	2.0
1	D	685	ASP	2.0
2	E	7	LYS	2.0
1	A	472	SER	2.0
1	A	502	SER	2.0
1	B	658	SER	2.0
1	B	752	SER	2.0
1	C	741	MET	2.0
1	D	495	GLN	2.0
1	D	748	ASN	2.0
1	C	547	ARG	2.0
1	D	686	TYR	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 oligosaccharides 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.