Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 09:24 pm BST

PDB ID	:	2CIM
Title	:	Crystal structure of Methanosarcina barkeri seryl-tRNA synthetase
Authors	:	Bilokapic, S.; Maier, T.; Ahel, D.; Gruic-Sovulj, I.; Soll, D.; Weygand-Durasevic, I.; Ban, N.
Deposited on	:	2006-03-24
Resolution	:	2.51 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 following versions of software and data (see references ⓘ) were used in the production of this report:

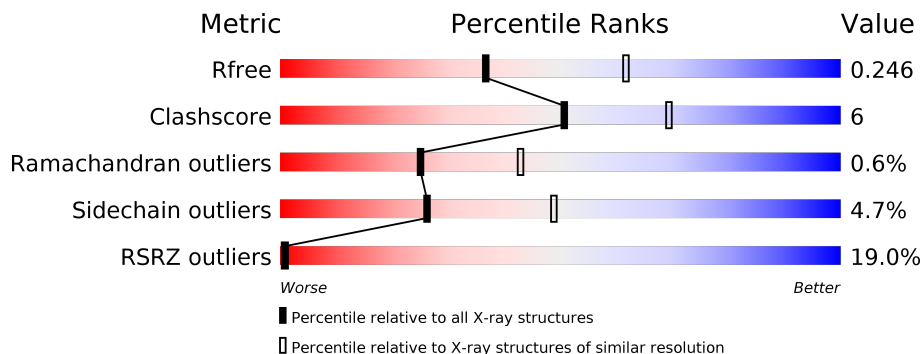|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.51 Å.

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

Metric	Percentile Ranks	Value
Rfree		0.246
Clashscore		6
Ramachandran outliers		0.6%
Sidechain outliers		4.7%
RSRZ outliers		19.0%

Worse　　　　　　　　　　　　　　　　　*Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	522	19%　78%　14%　•　7%
1	B	522	16%　77%　14%　•　9%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8131 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 SERYL-TRNA SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total 3961	C 2543	N 677	O 722	S 19	0	0	0
1	B	477	Total 3902	C 2504	N 665	O 714	S 19	0	1	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total 1	Zn 1	0	0
2	A	1	Total 1	Zn 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Cl 1	0	0
3	A	1	Total 1	Cl 1	0	0

- Molecule 4 is PLATINUM (II) ION (three-letter code: PT) (formula: Pt).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Pt 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	127	Total 127	O 127	0	0

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| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	136	Total 136	O 136	0	0

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: SERYL-TRNA SYNTHETASE
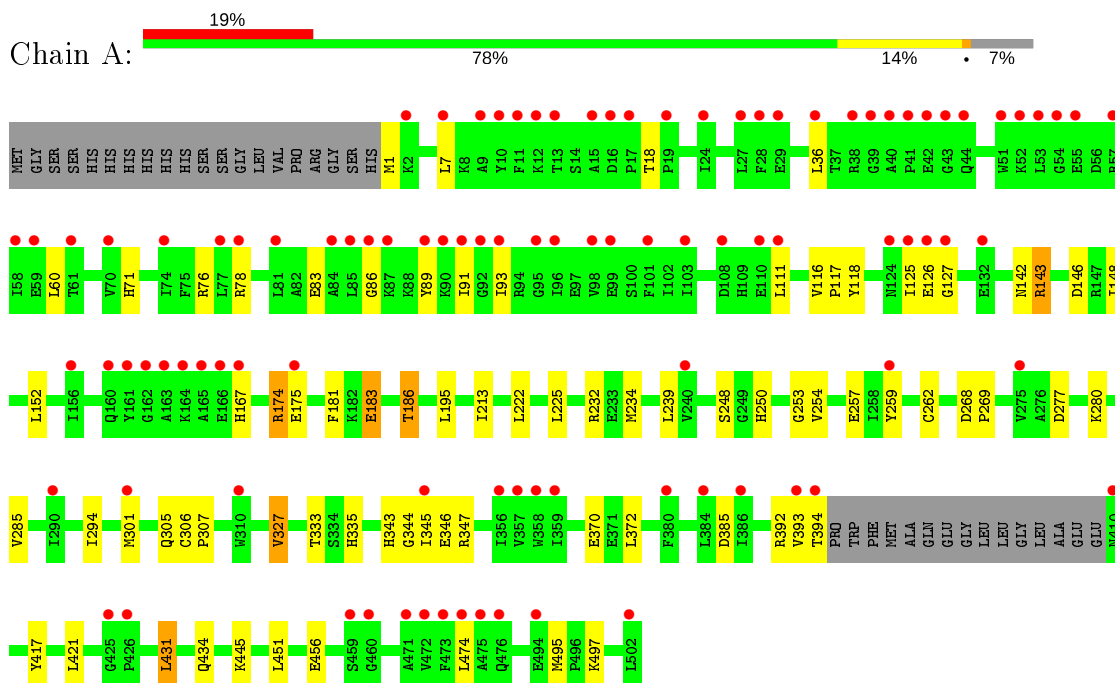
- Molecule 1: SERYL-TRNA SYNTHETASE
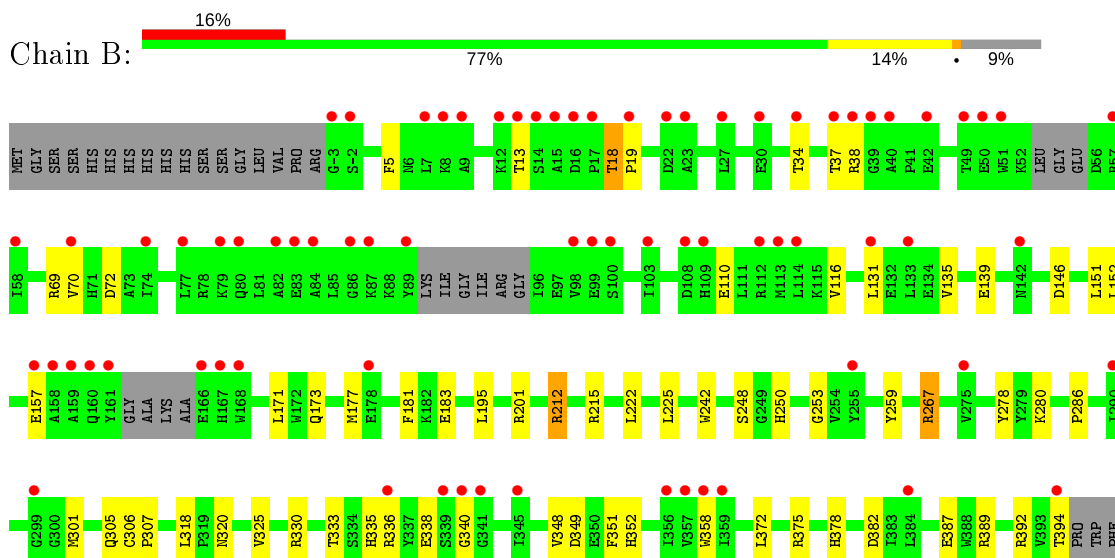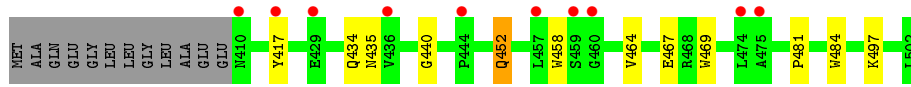
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	97.15Å 97.15Å 268.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.94 – 2.51 19.94 – 2.51	Depositor EDS
% Data completeness (in resolution range)	95.6 (19.94-2.51) 95.6 (19.94-2.51)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	3.29 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.199 , 0.252 0.199 , 0.246	Depositor DCC
R_{free} test set	2496 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	49.0	Xtriage
Anisotropy	0.362	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 51.8	EDS
L-test for twinning [2]	$<|L|> = 0.48$, $<L^2> = 0.31$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8131	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, PT, CL

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	0.43	1/4066 (0.0%)	0.57	0/5498
1	B	0.42	0/4005	0.54	0/5414
All	All	0.42	1/8071 (0.0%)	0.56	0/10912

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	183	GLU	CD-OE1	5.35	1.31	1.25

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	3961	0	3907	51	0
1	B	3902	0	3824	43	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
5	A	127	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	136	0	0	2	0
All	All	8131	0	7731	89	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 6.

All (89) 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:143:ARG:HG2	1:A:143:ARG:HH11	0.97	1.13
1:A:125:ILE:HG22	1:A:126:GLU:H	1.23	1.04
1:B:352:HIS:HD2	1:B:467:GLU:OE2	1.45	0.98
1:A:143:ARG:HG2	1:A:143:ARG:NH1	1.77	0.86
1:A:259:TYR:CB	1:A:301:MET:HE2	2.06	0.85
5:A:2045:HOH:O	1:B:352:HIS:HE1	1.66	0.79
1:A:143:ARG:CG	1:A:143:ARG:HH11	1.88	0.79
1:A:186:THR:HG21	1:A:344:GLY:HA3	1.67	0.76
1:B:352:HIS:CD2	1:B:467:GLU:OE2	2.36	0.75
1:A:259:TYR:HB2	1:A:301:MET:HE2	1.70	0.74
1:A:259:TYR:HB3	1:A:301:MET:CE	2.21	0.71
1:A:259:TYR:CB	1:A:301:MET:CE	2.68	0.71
1:A:259:TYR:HB3	1:A:301:MET:HE2	1.73	0.69
1:B:259:TYR:HB3	1:B:301:MET:HE2	1.76	0.68
1:B:259:TYR:CB	1:B:301:MET:HE2	2.26	0.66
1:B:173:GLN:HG3	1:B:389:ARG:HB3	1.79	0.64
1:A:248:SER:OG	1:A:250:HIS:HD2	1.83	0.62
1:A:125:ILE:CG2	1:A:126:GLU:H	2.05	0.62
1:A:125:ILE:HG22	1:A:126:GLU:N	2.05	0.59
1:B:18:THR:H	1:B:19:PRO:HD2	1.68	0.58
1:A:280:LYS:HD2	1:B:151:LEU:HD13	1.87	0.57
1:A:250:HIS:HE1	5:A:2052:HOH:O	1.86	0.57
1:A:186:THR:HG21	1:A:345:ILE:H	1.69	0.56
1:B:417:TYR:HB2	1:B:434:GLN:HB3	1.87	0.56
1:B:278:TYR:HB3	1:B:286:PRO:HG3	1.89	0.55
1:B:375:ARG:HD3	5:B:2102:HOH:O	2.04	0.55
1:A:417:TYR:HB2	1:A:434:GLN:HB3	1.90	0.54
1:B:259:TYR:CB	1:B:301:MET:CE	2.85	0.54
1:A:186:THR:HG22	5:A:2082:HOH:O	2.07	0.54
1:A:343:HIS:CD2	1:A:347:ARG:HD2	2.43	0.53
1:B:212:ARG:HD3	5:B:2047:HOH:O	2.08	0.53
1:A:71:HIS:HE1	1:A:146:ASP:OD1	1.92	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:THR:HG22	1:B:38:ARG:HH12	1.73	0.53
1:A:257:GLU:HG2	1:B:267:ARG:HE	1.73	0.52
1:B:320:ASN:OD1	1:B:452:GLN:HG3	2.10	0.52
1:A:1:MET:HB2	1:A:127:GLY:HA3	1.91	0.52
1:B:135:VAL:HG13	1:B:139:GLU:HB2	1.92	0.52
1:B:248:SER:OG	1:B:250:HIS:HD2	1.93	0.52
1:A:306:CYS:SG	1:A:307:PRO:HD3	2.51	0.51
1:A:142:ASN:O	1:A:143:ARG:HB2	2.10	0.51
1:A:71:HIS:H	1:A:71:HIS:CD2	2.27	0.51
1:B:177:MET:HE3	1:B:387:GLU:HB2	1.92	0.51
1:A:445:LYS:NZ	1:A:456:GLU:OE1	2.40	0.51
1:B:306:CYS:SG	1:B:307:PRO:HD3	2.51	0.50
1:A:232:ARG:CD	5:A:2040:HOH:O	2.60	0.50
1:A:118:TYR:HB2	1:A:148:ILE:HD11	1.92	0.50
1:B:201:ARG:NH2	1:B:338:GLU:O	2.43	0.49
1:A:186:THR:CG2	1:A:344:GLY:HA3	2.39	0.48
1:A:225:LEU:HD21	1:A:372:LEU:CD2	2.43	0.48
1:A:259:TYR:HB3	1:A:301:MET:HE1	1.94	0.48
1:A:89:TYR:HB3	1:A:91:ILE:HD12	1.96	0.47
1:A:174:ARG:NH2	1:A:385:ASP:OD1	2.47	0.47
1:B:181:PHE:CZ	1:B:183:GLU:HB2	2.49	0.47
1:A:232:ARG:HD3	5:A:2040:HOH:O	2.14	0.47
1:A:186:THR:CG2	5:A:2082:HOH:O	2.61	0.47
1:A:167:HIS:O	1:A:393:VAL:HA	2.15	0.46
1:B:378:HIS:HD2	1:B:382:ASP:OD2	1.99	0.46
1:B:131:LEU:HD11	1:B:152:LEU:HD22	1.97	0.46
1:B:338:GLU:HB2	1:B:349:ASP:OD1	2.16	0.45
1:A:213:ILE:HD11	1:A:495:MET:HE3	1.98	0.45
1:A:186:THR:HG21	1:A:344:GLY:CA	2.43	0.45
1:B:171:LEU:HD11	1:B:392:ARG:HE	1.82	0.45
1:B:201:ARG:HH12	1:B:340:GLY:HA2	1.82	0.45
1:B:481:PRO:HA	1:B:484:TRP:CD2	2.52	0.45
1:A:116:VAL:HG13	1:A:117:PRO:HD2	1.99	0.45
1:A:421:LEU:HD11	1:A:431:LEU:HG	1.98	0.45
1:B:306:CYS:N	1:B:307:PRO:CD	2.80	0.45
1:B:440:GLY:HA2	1:B:458:TRP:CD2	2.52	0.45
1:A:250:HIS:O	1:A:254:VAL:HG22	2.17	0.44
1:B:259:TYR:HB2	1:B:301:MET:CE	2.47	0.44
1:A:239:LEU:CD1	1:B:301:MET:HE1	2.48	0.43
1:A:234:MET:SD	1:A:327:VAL:HG21	2.59	0.43
1:B:336:ARG:NE	1:B:338:GLU:OE2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:PHE:HB3	1:B:70:VAL:HG22	1.99	0.43
1:B:325:VAL:O	1:B:358:TRP:HA	2.18	0.42
1:B:378:HIS:CD2	1:B:382:ASP:OD2	2.72	0.42
1:A:268:ASP:HA	1:A:269:PRO:HD2	1.82	0.42
1:B:69:ARG:NH1	1:B:146:ASP:OD1	2.49	0.42
1:A:262:CYS:HB2	1:A:294:ILE:HD12	2.01	0.42
1:A:285:VAL:HG21	1:B:242:TRP:CG	2.54	0.42
1:A:333:THR:OG1	1:A:335:HIS:CE1	2.73	0.42
1:B:225:LEU:HD21	1:B:372:LEU:CD2	2.50	0.41
1:A:277:ASP:HB3	1:B:116:VAL:HG22	2.02	0.41
1:A:36:LEU:HD23	1:A:76:ARG:HD2	2.02	0.41
1:B:333:THR:OG1	1:B:335:HIS:HE1	2.04	0.41
1:B:348:VAL:CG2	1:B:351:PHE:HB3	2.51	0.40
1:B:464:VAL:HG13	1:B:469:TRP:CE2	2.57	0.40
1:A:181:PHE:CZ	1:A:183:GLU:HB3	2.56	0.40
1:A:392:ARG:NH1	5:A:2091:HOH:O	2.55	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	483/522 (92%)	449 (93%)	31 (6%)	3 (1%)	25	43
1	B	468/522 (90%)	452 (97%)	13 (3%)	3 (1%)	25	43
All	All	951/1044 (91%)	901 (95%)	44 (5%)	6 (1%)	25	43

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	305	GLN
1	B	18	THR

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Mol	Chain	Res	Type
1	B	253	GLY
1	B	305	GLN
1	A	253	GLY
1	A	86	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	416/444 (94%)	394 (95%)	22 (5%)	22	43
1	B	412/444 (93%)	395 (96%)	17 (4%)	30	55
All	All	828/888 (93%)	789 (95%)	39 (5%)	26	49

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	18	THR
1	A	60	LEU
1	A	78	ARG
1	A	83	GLU
1	A	93	ILE
1	A	111	LEU
1	A	143	ARG
1	A	152	LEU
1	A	174	ARG
1	A	175	GLU
1	A	186	THR
1	A	195	LEU
1	A	222	LEU
1	A	327	VAL
1	A	346	GLU
1	A	370	GLU
1	A	394	THR
1	A	431	LEU

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Mol	Chain	Res	Type
1	A	451	LEU
1	A	474	LEU
1	A	497	LYS
1	B	13	THR
1	B	37	THR
1	B	72	ASP
1	B	110	GLU
1	B	157	GLU
1	B	195	LEU
1	B	212	ARG
1	B	215	ARG
1	B	222	LEU
1	B	267	ARG
1	B	280	LYS
1	B	318	LEU
1	B	330	ARG
1	B	394	THR
1	B	435	ASN
1	B	452	GLN
1	B	497	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	HIS
1	A	250	HIS
1	A	283	HIS
1	A	335	HIS
1	A	378	HIS
1	A	448	ASN
1	B	187	GLN
1	B	250	HIS
1	B	335	HIS
1	B	352	HIS
1	B	378	HIS
1	B	448	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	487/522 (93%)	1.08	99 (20%)	1	0	55, 66, 120, 123	0
1	B	477/522 (91%)	0.86	84 (17%)	1	1	55, 66, 79, 96	0
All	All	964/1044 (92%)	0.97	183 (18%)	1	1	55, 66, 114, 123	0

All (183) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	11	PHE	10.1
1	A	58	ILE	10.1
1	A	91	ILE	8.2
1	A	165	ALA	8.1
1	A	161	TYR	8.1
1	B	113	MET	8.0
1	B	167	HIS	7.7
1	A	39	GLY	7.6
1	A	163	ALA	7.4
1	B	161	TYR	7.4
1	A	53	LEU	6.3
1	A	160	GLN	5.9
1	A	15	ALA	5.8
1	B	166	GLU	5.4
1	A	17	PRO	5.2
1	A	162	GLY	5.1
1	A	167	HIS	5.1
1	A	93	ILE	4.9
1	B	114	LEU	4.9
1	B	51	TRP	4.8
1	A	42	GLU	4.7
1	B	168	TRP	4.6
1	A	108	ASP	4.5
1	A	81	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	40	ALA	4.4
1	A	166	GLU	4.4
1	A	164	LYS	4.3
1	A	28	PHE	4.3
1	B	394	THR	4.3
1	A	57	ARG	4.3
1	A	51	TRP	4.2
1	A	24	ILE	4.1
1	A	74	ILE	4.1
1	A	474	LEU	4.0
1	A	126	GLU	4.0
1	A	44	GLN	3.9
1	B	160	GLN	3.9
1	B	357	VAL	3.9
1	B	359	ILE	3.9
1	A	393	VAL	3.8
1	B	22	ASP	3.8
1	B	98	VAL	3.8
1	B	12	LYS	3.7
1	A	357	VAL	3.6
1	A	394	THR	3.6
1	B	133	LEU	3.6
1	A	52	LYS	3.6
1	A	426	PRO	3.6
1	B	27	LEU	3.5
1	A	12	LYS	3.5
1	B	83	GLU	3.5
1	B	459	SER	3.5
1	B	410	ASN	3.5
1	B	40	ALA	3.4
1	A	89	TYR	3.4
1	B	8	LYS	3.4
1	B	89	TYR	3.4
1	A	10	TYR	3.4
1	A	55	GLU	3.4
1	B	474	LEU	3.3
1	B	9	ALA	3.3
1	B	13	THR	3.3
1	B	356	ILE	3.3
1	A	7	LEU	3.3
1	A	85	LEU	3.3
1	B	86	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	340	GLY	3.3
1	B	159	ALA	3.2
1	A	358	TRP	3.2
1	A	2	LYS	3.2
1	A	27	LEU	3.2
1	B	108	ASP	3.2
1	B	339	SER	3.2
1	B	49	THR	3.2
1	B	290	ILE	3.2
1	B	84	ALA	3.1
1	A	475	ALA	3.1
1	B	275	VAL	3.1
1	B	19	PRO	3.1
1	B	112	ARG	3.1
1	B	14	SER	3.1
1	A	473	PHE	3.1
1	A	92	GLY	3.1
1	A	472	VAL	3.1
1	B	15	ALA	3.0
1	A	96	ILE	3.0
1	A	103	ILE	3.0
1	A	471	ALA	3.0
1	A	175	GLU	3.0
1	A	259	TYR	3.0
1	A	87	LYS	2.9
1	B	457	LEU	2.9
1	A	90	LYS	2.9
1	A	459	SER	2.9
1	A	61	THR	2.9
1	A	16	ASP	2.8
1	A	356	ILE	2.8
1	A	38	ARG	2.8
1	B	34	THR	2.8
1	A	77	LEU	2.8
1	A	43	GLY	2.8
1	B	17	PRO	2.8
1	B	417	TYR	2.8
1	A	99	GLU	2.8
1	B	178	GLU	2.8
1	B	16	ASP	2.8
1	A	386	ILE	2.7
1	A	84	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	255	TYR	2.7
1	A	95	GLY	2.7
1	B	80	GLN	2.6
1	B	109	HIS	2.6
1	A	425	GLY	2.6
1	B	77	LEU	2.6
1	B	157	GLU	2.6
1	B	87	LYS	2.6
1	B	131	LEU	2.6
1	A	29	GLU	2.5
1	A	125	ILE	2.5
1	B	-2	SER	2.5
1	B	-3	GLY	2.5
1	A	59	GLU	2.5
1	B	475	ALA	2.5
1	B	70	VAL	2.4
1	A	70	VAL	2.4
1	B	336	ARG	2.4
1	A	132	GLU	2.4
1	B	345	ILE	2.4
1	A	54	GLY	2.4
1	A	19	PRO	2.4
1	A	476	GLN	2.4
1	A	359	ILE	2.4
1	A	111	LEU	2.4
1	A	110	GLU	2.4
1	A	460	GLY	2.3
1	A	78	ARG	2.3
1	A	301	MET	2.3
1	A	410	ASN	2.3
1	B	74	ILE	2.3
1	B	100	SER	2.3
1	B	142	ASN	2.3
1	B	42	GLU	2.3
1	A	380	PHE	2.3
1	A	290	ILE	2.2
1	B	37	THR	2.2
1	B	436	VAL	2.2
1	B	58	ILE	2.2
1	A	156	ILE	2.2
1	A	345	ILE	2.2
1	A	41	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	444	PRO	2.2
1	A	86	GLY	2.2
1	B	82	ALA	2.2
1	A	384	LEU	2.2
1	B	299	GLY	2.2
1	A	124	ASN	2.2
1	B	57	ARG	2.2
1	A	240	VAL	2.1
1	B	23	ALA	2.1
1	A	494	GLU	2.1
1	B	50	GLU	2.1
1	A	502	LEU	2.1
1	B	79	LYS	2.1
1	B	460	GLY	2.1
1	A	275	VAL	2.1
1	B	158	ALA	2.1
1	A	101	PHE	2.1
1	B	341	GLY	2.1
1	B	103	ILE	2.1
1	B	38	ARG	2.1
1	A	98	VAL	2.1
1	A	36	LEU	2.1
1	B	358	TRP	2.1
1	A	127	GLY	2.0
1	B	39	GLY	2.0
1	A	13	THR	2.0
1	B	7	LEU	2.0
1	B	30	GLU	2.0
1	A	9	ALA	2.0
1	A	310	TRP	2.0
1	B	384	LEU	2.0
1	B	99	GLU	2.0
1	B	429	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	B	1503	1/1	0.95	0.17	73,73,73,73	0
4	PT	A	1505	1/1	0.97	0.08	67,67,67,67	1
3	CL	A	1504	1/1	0.97	0.15	38,38,38,38	0
2	ZN	A	1503	1/1	0.97	0.22	70,70,70,70	0
3	CL	B	1504	1/1	0.98	0.09	43,43,43,43	0

6.5 Other polymers (i)

There are no such residues in this entry.