



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:16 AM GMT

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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

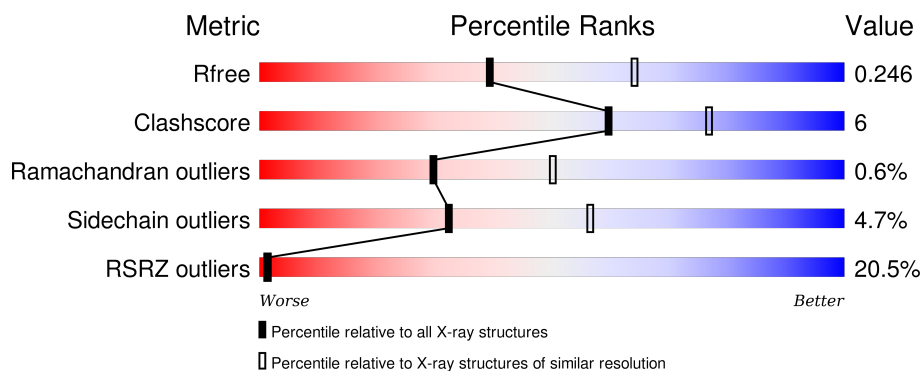
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

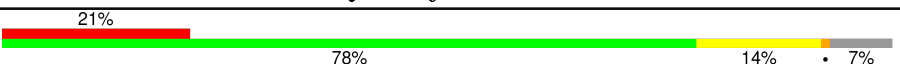
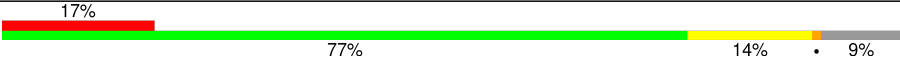
The reported resolution of this entry is 2.51 Å.

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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. 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	522	 21% 78% 14% • 7%
1	B	522	 17% 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	C	N	O	S	0	0	0
			3961	2543	677	722	19			
1	B	477	Total	C	N	O	S	0	1	0
			3902	2504	665	714	19			

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

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

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

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

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

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

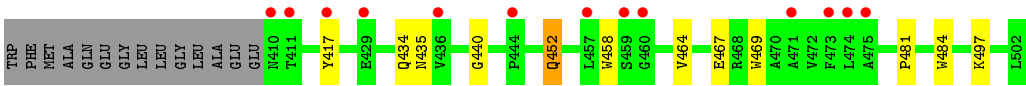
- Molecule 5 is water.

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

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



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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	2491 reflections (5.37%)	DCC
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 , 51.9	EDS
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 48972 reflections	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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

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: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:1:MET:HB2	1:A:127:GLY:HA3	1.91	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:259:TYR:HB3	1:A:301:MET:HE1	1.94	0.48
1:A:225:LEU:HD21	1:A:372:LEU:CD2	2.43	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:B:306:CYS:N	1:B:307:PRO:CD	2.80	0.45
1:A:421:LEU:HD11	1:A:431:LEU:HG	1.98	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:B:336:ARG:NE	1:B:338:GLU:OE2	2.51	0.43
1:A:234:MET:SD	1:A:327:VAL:HG21	2.59	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:B:69:ARG:NH1	1:B:146:ASP:OD1	2.49	0.42
1:A:268:ASP:HA	1:A:269:PRO:HD2	1.82	0.42
1:A:285:VAL:HG21	1:B:242:TRP:CG	2.54	0.42
1:A:262:CYS:HB2	1:A:294:ILE:HD12	2.01	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 [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	483/522 (92%)	449 (93%)	31 (6%)	3 (1%)	30	50
1	B	468/522 (90%)	452 (97%)	13 (3%)	3 (1%)	30	50
All	All	951/1044 (91%)	901 (95%)	44 (5%)	6 (1%)	30	50

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 ⓘ

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%)	28	50
1	B	412/444 (93%)	395 (96%)	17 (4%)	37	63
All	All	828/888 (93%)	789 (95%)	39 (5%)	32	56

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 ⓘ

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 ⓘ

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	487/522 (93%)	1.17	108 (22%) ⓘ ⓘ	55, 66, 120, 123	0
1	B	477/522 (91%)	0.95	90 (18%) ⓘ ⓘ	55, 66, 79, 96	0
All	All	964/1044 (92%)	1.06	198 (20%) ⓘ ⓘ	55, 66, 114, 123	0

All (198) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	58	ILE	10.5
1	A	11	PHE	10.5
1	A	165	ALA	8.5
1	B	113	MET	8.4
1	A	91	ILE	8.4
1	A	161	TYR	8.3
1	B	167	HIS	8.0
1	A	39	GLY	7.9
1	A	163	ALA	7.8
1	B	161	TYR	7.6
1	A	53	LEU	6.5
1	A	15	ALA	6.3
1	A	160	GLN	6.1
1	B	166	GLU	5.6
1	A	17	PRO	5.4
1	A	162	GLY	5.4
1	A	167	HIS	5.3
1	B	114	LEU	5.1
1	A	93	ILE	5.1
1	B	51	TRP	5.0
1	A	42	GLU	4.9
1	A	108	ASP	4.8
1	B	168	TRP	4.7
1	A	81	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	40	ALA	4.6
1	A	166	GLU	4.5
1	A	28	PHE	4.5
1	B	394	THR	4.5
1	A	57	ARG	4.5
1	A	164	LYS	4.5
1	A	51	TRP	4.4
1	A	74	ILE	4.3
1	A	24	ILE	4.3
1	A	474	LEU	4.2
1	B	357	VAL	4.1
1	A	126	GLU	4.1
1	B	160	GLN	4.1
1	B	359	ILE	4.1
1	A	44	GLN	4.0
1	A	393	VAL	4.0
1	B	22	ASP	4.0
1	B	98	VAL	3.9
1	A	394	THR	3.9
1	A	357	VAL	3.8
1	A	426	PRO	3.8
1	B	12	LYS	3.8
1	B	133	LEU	3.8
1	B	27	LEU	3.7
1	A	52	LYS	3.7
1	B	83	GLU	3.7
1	B	40	ALA	3.7
1	B	459	SER	3.7
1	A	12	LYS	3.6
1	B	410	ASN	3.6
1	A	55	GLU	3.6
1	B	89	TYR	3.6
1	A	89	TYR	3.6
1	B	86	GLY	3.6
1	B	13	THR	3.5
1	B	8	LYS	3.5
1	A	7	LEU	3.5
1	A	10	TYR	3.5
1	B	356	ILE	3.5
1	B	474	LEU	3.5
1	B	340	GLY	3.5
1	B	9	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	159	ALA	3.4
1	A	85	LEU	3.4
1	B	339	SER	3.4
1	A	358	TRP	3.3
1	B	108	ASP	3.3
1	A	475	ALA	3.3
1	B	49	THR	3.3
1	A	2	LYS	3.3
1	A	27	LEU	3.3
1	B	290	ILE	3.3
1	B	275	VAL	3.3
1	B	19	PRO	3.3
1	A	472	VAL	3.2
1	B	15	ALA	3.2
1	B	84	ALA	3.2
1	B	112	ARG	3.2
1	A	473	PHE	3.2
1	A	103	ILE	3.2
1	B	14	SER	3.2
1	A	471	ALA	3.1
1	A	96	ILE	3.1
1	A	92	GLY	3.1
1	A	175	GLU	3.1
1	A	259	TYR	3.1
1	A	61	THR	3.1
1	B	457	LEU	3.1
1	A	90	LYS	3.0
1	A	459	SER	3.0
1	A	87	LYS	3.0
1	A	356	ILE	3.0
1	A	43	GLY	3.0
1	A	16	ASP	3.0
1	B	34	THR	3.0
1	A	38	ARG	2.9
1	A	99	GLU	2.9
1	B	17	PRO	2.9
1	A	84	ALA	2.9
1	B	417	TYR	2.9
1	A	77	LEU	2.9
1	B	178	GLU	2.9
1	A	386	ILE	2.9
1	B	16	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	95	GLY	2.9
1	B	255	TYR	2.8
1	A	425	GLY	2.8
1	B	77	LEU	2.8
1	B	131	LEU	2.7
1	B	109	HIS	2.7
1	B	157	GLU	2.7
1	B	80	GLN	2.7
1	B	-2	SER	2.7
1	A	29	GLU	2.7
1	B	-3	GLY	2.6
1	B	87	LYS	2.6
1	B	475	ALA	2.6
1	A	125	ILE	2.6
1	B	70	VAL	2.6
1	A	19	PRO	2.6
1	A	70	VAL	2.6
1	B	345	ILE	2.6
1	A	54	GLY	2.5
1	A	59	GLU	2.5
1	A	132	GLU	2.5
1	B	336	ARG	2.5
1	A	476	GLN	2.5
1	A	359	ILE	2.5
1	A	301	MET	2.5
1	A	410	ASN	2.5
1	A	86	GLY	2.5
1	A	460	GLY	2.5
1	A	110	GLU	2.5
1	B	74	ILE	2.4
1	A	78	ARG	2.4
1	A	111	LEU	2.4
1	B	42	GLU	2.4
1	B	142	ASN	2.4
1	B	37	THR	2.4
1	B	58	ILE	2.4
1	A	380	PHE	2.4
1	B	436	VAL	2.4
1	B	100	SER	2.4
1	A	290	ILE	2.4
1	A	41	PRO	2.4
1	B	444	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	345	ILE	2.3
1	A	384	LEU	2.3
1	A	502	LEU	2.3
1	B	82	ALA	2.3
1	A	240	VAL	2.3
1	B	299	GLY	2.3
1	A	156	ILE	2.3
1	B	50	GLU	2.3
1	A	124	ASN	2.3
1	B	460	GLY	2.3
1	B	23	ALA	2.3
1	B	103	ILE	2.3
1	B	341	GLY	2.3
1	A	275	VAL	2.3
1	A	494	GLU	2.2
1	A	98	VAL	2.2
1	B	38	ARG	2.2
1	B	158	ALA	2.2
1	A	101	PHE	2.2
1	B	57	ARG	2.2
1	B	79	LYS	2.2
1	A	36	LEU	2.2
1	B	39	GLY	2.2
1	B	358	TRP	2.2
1	B	411	THR	2.2
1	B	7	LEU	2.2
1	A	9	ALA	2.1
1	A	127	GLY	2.1
1	A	13	THR	2.1
1	A	157	GLU	2.1
1	A	1	MET	2.1
1	A	5	PHE	2.1
1	B	384	LEU	2.1
1	A	31	ALA	2.1
1	A	73	ALA	2.1
1	B	30	GLU	2.1
1	A	310	TRP	2.1
1	B	473	PHE	2.1
1	B	429	GLU	2.1
1	A	372	LEU	2.1
1	B	99	GLU	2.1
1	A	470	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	109	HIS	2.0
1	A	469	TRP	2.0
1	B	35	LEU	2.0
1	B	471	ALA	2.0
1	B	110	GLU	2.0
1	B	21	LYS	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	CL	A	1504	1/1	0.97	0.15	-0.83	38,38,38,38	0
3	CL	B	1504	1/1	0.98	0.09	-2.60	43,43,43,43	0
4	PT	A	1505	1/1	0.97	0.08	-	67,67,67,67	1
2	ZN	A	1503	1/1	0.97	0.22	-	70,70,70,70	0
2	ZN	B	1503	1/1	0.95	0.16	-	73,73,73,73	0

6.5 Other polymers [i](#)

There are no such residues in this entry.