



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:55 AM UTC

PDB ID : 2CIM / pdb_00002cim
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 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
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

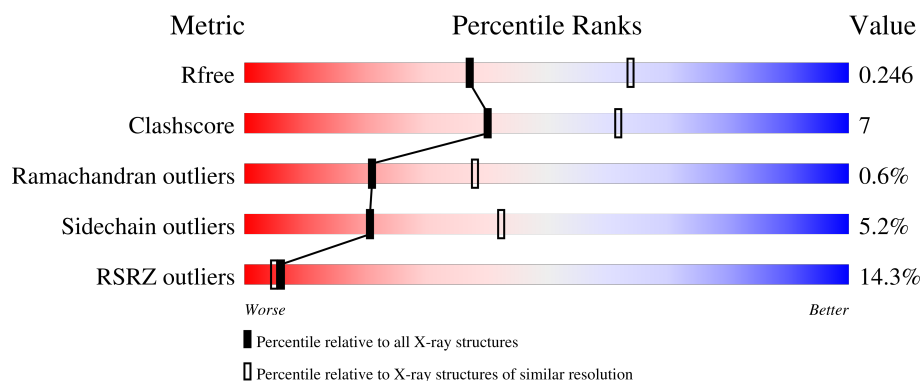
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 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	522	20% 77% 15% 7%
1	B	522	6% 75% 16% 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 (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 4 is PLATINUM (II) ION (CCD ID: PT) (formula: Pt).

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

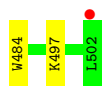
- Molecule 5 is water.

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) 95.4 (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	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)	0.28 , 56.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	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, 0.333 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: PT, ZN, 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	0.53	0/4066	0.80	3/5498 (0.1%)
1	B	0.50	0/4005	0.79	1/5414 (0.0%)
All	All	0.51	0/8071	0.80	4/10912 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	332	GLY	N-CA-C	5.99	118.65	110.69
1	A	116	VAL	CA-C-N	5.36	126.54	119.84
1	A	116	VAL	C-N-CA	5.36	126.54	119.84
1	A	332	GLY	N-CA-C	5.01	117.35	110.69

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	60	0
1	B	3902	0	3824	51	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
4	A	1	0	0	0	0
5	A	127	0	0	7	0
5	B	136	0	0	2	0
All	All	8131	0	7731	103	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 7.

All (103) 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:HH11	1:A:143:ARG:HG2	0.97	1.13
1:A:125:ILE:HG22	1:A:126:GLU:H	1.23	1.04
1:A:259:TYR:HB3	1:A:301:MET:HE2	1.43	0.98
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
5:A:2045:HOH:O	1:B:352:HIS:HE1	1.66	0.79
1:A:143:ARG:HH11	1:A:143:ARG:CG	1.88	0.79
1:A:259:TYR:CB	1:A:301:MET:HE2	2.16	0.76
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:CB	1:A:301:MET:CE	2.68	0.71
1:A:259:TYR:HB3	1:A:301:MET:CE	2.21	0.68
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:B:177:MET:HE3	1:B:387:GLU:HB2	1.82	0.61
1:B:259:TYR:HB3	1:B:301:MET:HE2	1.82	0.61
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:A:243:GLU:HA	1:A:246:MET:HE3	1.88	0.55
1:B:375:ARG:HD3	5:B:2102:HOH:O	2.04	0.55
1:B:259:TYR:CB	1:B:301:MET:HE2	2.36	0.55
1:A:492:VAL:CG1	1:A:495:MET:HE2	2.37	0.55
1:B:98:VAL:HG21	1:B:140:MET:HE3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:484:TRP:CH2	1:A:495:MET:HE3	2.45	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:A:445:LYS:NZ	1:A:456:GLU:OE1	2.40	0.51
1:B:259:TYR:HB2	1:B:301:MET:HE3	1.93	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:234:MET:HE3	1:B:207:GLY:HA2	1.93	0.50
1:A:118:TYR:HB2	1:A:148:ILE:HD11	1.92	0.50
1:B:101:PHE:CD1	1:B:140:MET:HE2	2.47	0.49
1:A:186:THR:HA	1:A:189:MET:HE3	1.95	0.49
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:B:101:PHE:HD1	1:B:140:MET:HE2	1.78	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:492:VAL:HG11	1:A:495:MET:HE2	1.97	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:A:239:LEU:HD12	1:B:301:MET:HE1	1.97	0.46
1:B:131:LEU:HD11	1:B:152:LEU:HD22	1.97	0.46
1:A:484:TRP:CZ3	1:A:495:MET:HE3	2.51	0.45
1:B:338:GLU:HB2	1:B:349:ASP:OD1	2.16	0.45
1:A:186:THR:HG21	1:A:344:GLY:CA	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:259:TYR:HB2	1:A:301:MET:HE3	1.99	0.45
1:A:421:LEU:HD11	1:A:431:LEU:HG	1.98	0.45
1:A:492:VAL:HG13	1:A:495:MET:HE2	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:B:174:ARG:CZ	1:B:177:MET:HE1	2.48	0.44
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:259:TYR:CB	1:A:301:MET:HE3	2.48	0.43
1:A:234:MET:SD	1:A:327:VAL:HG21	2.59	0.43
1:B:5:PHE:HB3	1:B:70:VAL:HG22	1.99	0.43
1:B:336:ARG:NE	1:B:338:GLU:OE2	2.51	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:A:301:MET:HE1	1:B:239:LEU:HD12	2.03	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%)	21	38
1	B	468/522 (90%)	452 (97%)	13 (3%)	3 (1%)	21	38
All	All	951/1044 (91%)	901 (95%)	44 (5%)	6 (1%)	21	38

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	305	GLN
1	B	18	THR
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%)	391 (94%)	25 (6%)	17	36
1	B	412/444 (93%)	394 (96%)	18 (4%)	25	50
All	All	828/888 (93%)	785 (95%)	43 (5%)	21	42

All (43) 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	81	LEU
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	285	VAL
1	A	327	VAL
1	A	342	ILE
1	A	346	GLU
1	A	370	GLU
1	A	394	THR
1	A	414	THR
1	A	431	LEU
1	A	451	LEU
1	A	474	LEU
1	A	479	LEU
1	B	13	THR
1	B	37	THR
1	B	72	ASP
1	B	110	GLU
1	B	114	LEU
1	B	152	LEU
1	B	195	LEU
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	393	VAL
1	B	394	THR
1	B	435	ASN
1	B	452	GLN
1	B	497	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	6	ASN
1	A	71	HIS
1	A	250	HIS
1	A	283	HIS
1	A	335	HIS
1	A	343	HIS
1	A	378	HIS
1	A	448	ASN
1	A	452	GLN
1	B	4	GLN
1	B	142	ASN
1	B	250	HIS
1	B	265	GLN
1	B	335	HIS
1	B	343	HIS
1	B	352	HIS
1	B	378	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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%)	1.18	106 (21%) 2 2	55, 66, 120, 123	0
1	B	477/522 (91%)	0.81	32 (6%) 24 21	34, 66, 79, 96	1 (0%)
All	All	964/1044 (92%)	0.99	138 (14%) 6 5	34, 66, 114, 123	1 (0%)

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	39	GLY	5.2
1	A	28	PHE	5.1
1	A	163	ALA	5.0
1	A	90	LYS	4.5
1	B	58	ILE	4.4
1	B	167	HIS	4.4
1	A	161	TYR	4.3
1	A	11	PHE	4.1
1	A	46	ALA	4.1
1	B	161	TYR	4.1
1	A	88	LYS	3.8
1	A	19	PRO	3.8
1	A	45	GLY	3.7
1	A	77	LEU	3.7
1	B	156	ILE	3.7
1	A	275	VAL	3.6
1	A	58	ILE	3.4
1	B	27	LEU	3.4
1	A	272	TRP	3.4
1	A	36	LEU	3.3
1	B	336	ARG	3.3
1	A	165	ALA	3.3
1	A	129	ILE	3.3
1	A	285	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	166	GLU	3.2
1	A	5	PHE	3.2
1	A	35	LEU	3.2
1	A	101	PHE	3.2
1	B	80	GLN	3.1
1	A	27	LEU	3.1
1	A	167	HIS	3.1
1	B	-1	HIS	3.1
1	B	11	PHE	3.1
1	A	94	ARG	3.1
1	A	51	TRP	3.1
1	B	166	GLU	3.1
1	A	133	LEU	3.1
1	A	68	VAL	3.0
1	A	159	ALA	3.0
1	A	413	GLY	3.0
1	A	158	ALA	3.0
1	B	-3	GLY	3.0
1	A	105	VAL	2.9
1	B	456[A]	GLU	2.9
1	A	84	ALA	2.9
1	B	15	ALA	2.9
1	A	149	LEU	2.9
1	A	111	LEU	2.9
1	A	54	GLY	2.9
1	A	281	VAL	2.9
1	B	394	THR	2.9
1	A	160	GLN	2.9
1	A	156	ILE	2.8
1	A	162	GLY	2.8
1	A	96	ILE	2.8
1	A	70	VAL	2.8
1	B	17	PRO	2.8
1	A	87	LYS	2.8
1	B	73	ALA	2.8
1	B	107	ALA	2.8
1	B	51	TRP	2.7
1	B	105	VAL	2.7
1	A	103	ILE	2.7
1	A	393	VAL	2.7
1	A	93	ILE	2.7
1	A	38	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	48	VAL	2.6
1	A	7	LEU	2.6
1	B	9	ALA	2.6
1	A	152	LEU	2.6
1	A	107	ALA	2.6
1	A	21	LYS	2.6
1	A	10	TYR	2.6
1	A	24	ILE	2.5
1	A	114	LEU	2.5
1	A	276	ALA	2.5
1	B	10	TYR	2.5
1	A	82	ALA	2.5
1	A	239	LEU	2.4
1	B	60	LEU	2.4
1	A	266	THR	2.4
1	A	86	GLY	2.4
1	B	114	LEU	2.4
1	A	116	VAL	2.4
1	A	47	LYS	2.4
1	A	14	SER	2.4
1	A	55	GLU	2.4
1	A	175	GLU	2.4
1	A	374	ASP	2.3
1	B	111	LEU	2.3
1	A	89	TYR	2.3
1	A	41	PRO	2.3
1	A	44	GLN	2.3
1	A	289	LEU	2.3
1	A	155	LYS	2.3
1	A	62	LEU	2.3
1	A	117	PRO	2.3
1	A	267	ARG	2.3
1	A	135	VAL	2.3
1	A	43	GLY	2.2
1	A	95	GLY	2.2
1	B	502	LEU	2.2
1	A	124	ASN	2.2
1	A	53	LEU	2.2
1	A	108	ASP	2.2
1	A	99	GLU	2.2
1	A	178	GLU	2.2
1	A	17	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	152	LEU	2.2
1	A	261	VAL	2.2
1	A	65	GLY	2.2
1	A	92	GLY	2.2
1	A	262	CYS	2.2
1	A	299	GLY	2.2
1	B	160	GLN	2.1
1	B	393	VAL	2.1
1	A	57	ARG	2.1
1	A	168	TRP	2.1
1	A	300	GLY	2.1
1	B	57	ARG	2.1
1	B	99	GLU	2.1
1	A	164	LYS	2.1
1	A	240	VAL	2.1
1	B	98	VAL	2.1
1	A	15	ALA	2.1
1	A	40	ALA	2.1
1	A	118	TYR	2.1
1	B	113	MET	2.1
1	A	60	LEU	2.0
1	A	83	GLU	2.0
1	A	61	THR	2.0
1	A	74	ILE	2.0
1	A	254	VAL	2.0
1	A	12	LYS	2.0
1	A	18	THR	2.0
1	A	245	TRP	2.0
1	A	71	HIS	2.0
1	A	100	SER	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
4	PT	A	1505	1/1	0.94	0.07	67,67,67,67	1
3	CL	A	1504	1/1	0.95	0.22	38,38,38,38	0
3	CL	B	1504	1/1	0.97	0.21	43,43,43,43	0
2	ZN	B	1503	1/1	0.98	0.18	73,73,73,73	0
2	ZN	A	1503	1/1	0.98	0.21	70,70,70,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.