



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 17, 2024 – 05:27 PM EDT

PDB ID : 3V0A
Title : 2.7 angstrom crystal structure of BoNT/Ai in complex with NTNHA
Authors : Gu, S.; Rumpel, S.; Zhou, J.; Strotmeier, J.; Bigalke, H.; Perry, K.; Shoemaker, C.B.; Rummel, A.; Jin, R.
Deposited on : 2011-12-07
Resolution : 2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 2.37.1
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) : 2.37.1

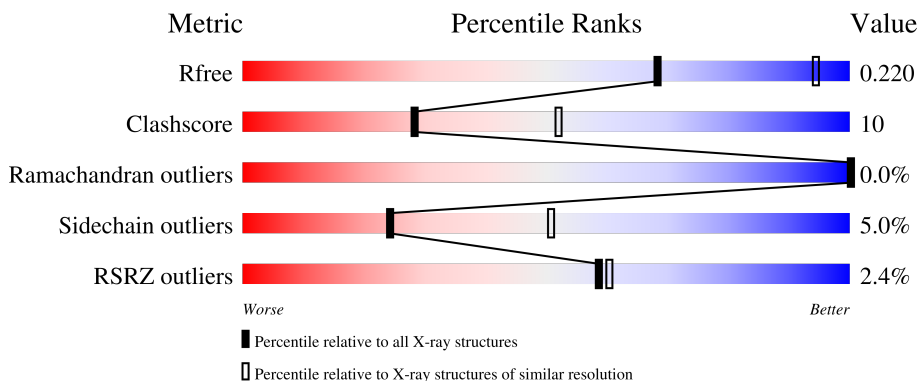
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	1296	 80% 17% ..
2	B	1196	 73% 21% . .
3	C	152	 43% 32% . 22%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 21163 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 BoNT/A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1280	10418	6681	1721	1983	33	36	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	224	GLN	GLU	ENGINEERED MUTATION	UNP Q7B8V4
A	363	ALA	ARG	ENGINEERED MUTATION	UNP Q7B8V4
A	366	PHE	TYR	ENGINEERED MUTATION	UNP Q7B8V4
A	1158	ALA	THR	CONFLICT	UNP Q7B8V4

- Molecule 2 is a protein called NTNH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	1150	9409	6022	1515	1840	32	46	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	EXPRESSION TAG	UNP Q45914
B	0	SER	-	EXPRESSION TAG	UNP Q45914
B	1194	PRO	-	EXPRESSION TAG	UNP Q45914

- Molecule 3 is a protein called Llama antibody F12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	119	892	551	156	181	4	4	0	0

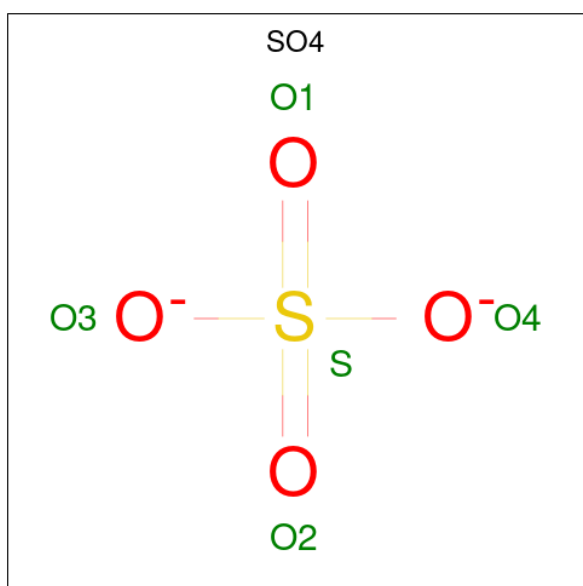
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



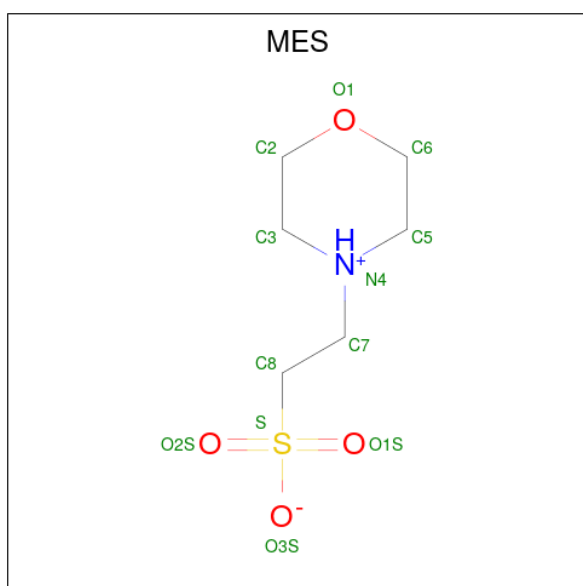
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
7	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
7	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
7	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

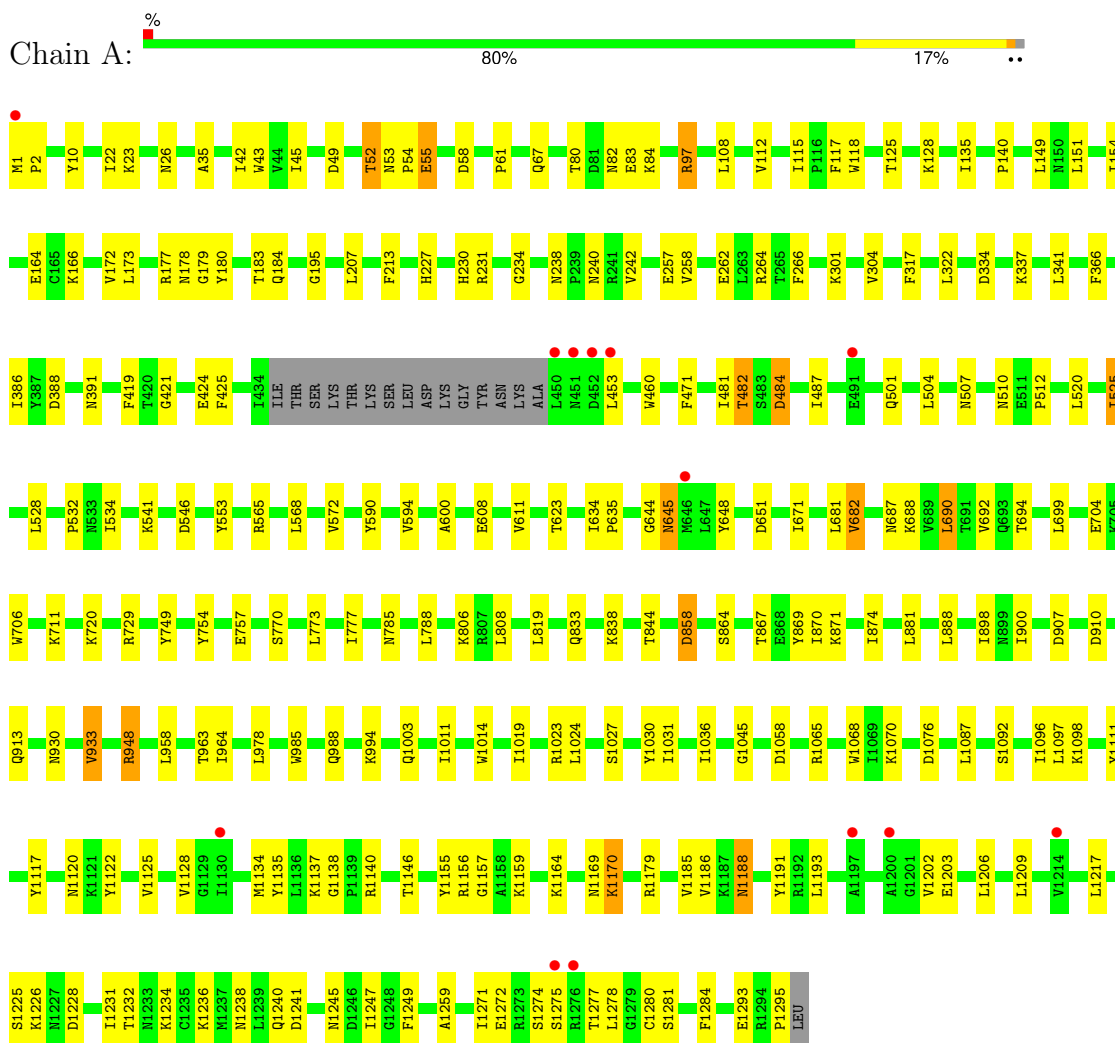
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	181	Total	O	0	0
			181	181		
8	B	112	Total	O	0	0
			112	112		
8	C	1	Total	O	0	0
			1	1		

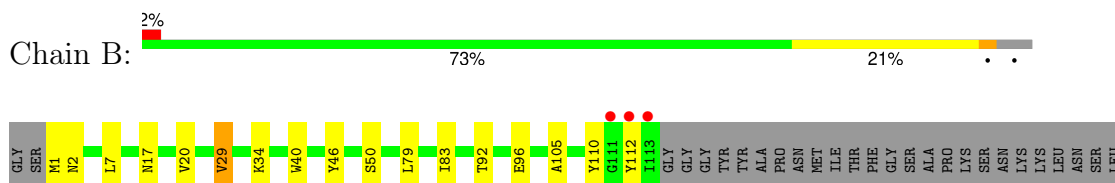
3 Residue-property plots

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: BoNT/A



• Molecule 2: NTNH



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	156.08Å 156.08Å 324.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.36 – 2.70 49.54 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.36-2.70) 99.7 (49.54-2.70)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.89 (at 2.69Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.176 , 0.224 0.173 , 0.220	Depositor DCC
R_{free} test set	5477 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	50.5	Xtrriage
Anisotropy	0.556	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 49.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	21163	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.96% 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: ZN, SO4, CA, MES

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.31	0/10639	0.49	0/14405
2	B	0.32	0/9604	0.51	0/13015
3	C	0.24	0/912	0.45	0/1238
All	All	0.31	0/21155	0.50	0/28658

There are no bond length outliers.

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	10418	0	10297	180	0
2	B	9409	0	9202	194	0
3	C	892	0	840	41	0
4	A	1	0	0	0	0
5	A	1	0	0	0	0
6	A	60	0	0	2	0
6	B	35	0	0	1	0
6	C	5	0	0	0	0
7	B	48	0	52	1	0
8	A	181	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	112	0	0	2	0
8	C	1	0	0	1	0
All	All	21163	0	20391	404	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 10.

The worst 5 of 404 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:1275:SER:HA	2:B:827:LEU:HD21	1.22	1.21
2:B:528:ASP:HB2	2:B:530:SER:H	1.07	1.13
2:B:528:ASP:HB2	2:B:530:SER:N	1.76	1.00
2:B:426:THR:HB	2:B:427:VAL:CA	1.91	0.99
2:B:426:THR:HB	2:B:427:VAL:HA	1.02	0.98

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	1276/1296 (98%)	1242 (97%)	34 (3%)	0	100	100
2	B	1144/1196 (96%)	1105 (97%)	38 (3%)	1 (0%)	51	78
3	C	117/152 (77%)	112 (96%)	5 (4%)	0	100	100
All	All	2537/2644 (96%)	2459 (97%)	77 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	429	ASP

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	1162/1176 (99%)	1125 (97%)	37 (3%)	39 68
2	B	1076/1114 (97%)	1008 (94%)	68 (6%)	18 40
3	C	94/123 (76%)	83 (88%)	11 (12%)	5 12
All	All	2332/2413 (97%)	2216 (95%)	116 (5%)	24 51

5 of 116 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	493	ILE
3	C	29	LEU
2	B	674	THR
3	C	28	THR
2	B	1128	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	913	GLN
2	B	961	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 2 are monoatomic - leaving 24 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SO4	A	1304	-	4,4,4	0.23	0	6,6,6	0.08	0
6	SO4	B	1196	-	4,4,4	0.24	0	6,6,6	0.07	0
6	SO4	C	144	-	4,4,4	0.26	0	6,6,6	0.06	0
6	SO4	A	1300	-	4,4,4	0.24	0	6,6,6	0.09	0
7	MES	B	1204	-	12,12,12	1.32	2 (16%)	15,16,16	1.93	4 (26%)
6	SO4	A	1301	-	4,4,4	0.23	0	6,6,6	0.12	0
7	MES	B	1205	-	12,12,12	1.32	2 (16%)	15,16,16	1.87	4 (26%)
6	SO4	B	1201	-	4,4,4	0.24	0	6,6,6	0.12	0
6	SO4	B	1199	-	4,4,4	0.25	0	6,6,6	0.16	0
6	SO4	A	1299	-	4,4,4	0.25	0	6,6,6	0.10	0
6	SO4	A	1308	-	4,4,4	0.23	0	6,6,6	0.14	0
6	SO4	A	1309	-	4,4,4	0.24	0	6,6,6	0.06	0
6	SO4	B	1198	-	4,4,4	0.25	0	6,6,6	0.11	0
6	SO4	A	1305	-	4,4,4	0.24	0	6,6,6	0.08	0
6	SO4	A	1307	-	4,4,4	0.24	0	6,6,6	0.11	0
6	SO4	A	1303	-	4,4,4	0.22	0	6,6,6	0.16	0
6	SO4	A	1306	-	4,4,4	0.23	0	6,6,6	0.10	0
6	SO4	B	1195	-	4,4,4	0.25	0	6,6,6	0.06	0
6	SO4	B	1197	-	4,4,4	0.25	0	6,6,6	0.13	0
7	MES	B	1202	-	12,12,12	1.25	1 (8%)	15,16,16	1.88	5 (33%)
6	SO4	A	1310	-	4,4,4	0.26	0	6,6,6	0.11	0
7	MES	B	1203	-	12,12,12	1.31	1 (8%)	15,16,16	1.85	4 (26%)
6	SO4	A	1302	-	4,4,4	0.24	0	6,6,6	0.11	0
6	SO4	B	1200	-	4,4,4	0.22	0	6,6,6	0.17	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MES	B	1202	-	-	3/6/14/14	0/1/1/1
7	MES	B	1205	-	-	1/6/14/14	0/1/1/1
7	MES	B	1204	-	-	1/6/14/14	0/1/1/1
7	MES	B	1203	-	-	0/6/14/14	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1205	MES	C5-N4	-3.12	1.38	1.46
7	B	1203	MES	C5-N4	-3.10	1.38	1.46
7	B	1204	MES	C5-N4	-3.07	1.38	1.46
7	B	1202	MES	C5-N4	-2.90	1.39	1.46
7	B	1205	MES	C8-S	2.09	1.80	1.77

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1204	MES	O3S-S-O2S	-4.26	100.73	111.40
7	B	1202	MES	O3S-S-O2S	-4.14	101.04	111.40
7	B	1205	MES	O3S-S-O2S	-4.12	101.09	111.40
7	B	1203	MES	O3S-S-O2S	-3.85	101.78	111.40
7	B	1204	MES	O2S-S-C8	3.33	111.76	106.73

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	1202	MES	C8-C7-N4-C5
7	B	1204	MES	N4-C7-C8-S
7	B	1202	MES	C8-C7-N4-C3
7	B	1205	MES	C8-C7-N4-C5
7	B	1202	MES	C7-C8-S-O3S

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1196	SO4	1	0
7	B	1204	MES	1	0
6	A	1303	SO4	1	0
6	A	1306	SO4	1	0

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(Å ²)	Q<0.9
1	A	1280/1296 (98%)	-0.27	13 (1%) 82 83	32, 56, 101, 170	10 (0%)
2	B	1150/1196 (96%)	-0.15	23 (2%) 65 67	29, 54, 111, 166	14 (1%)
3	C	119/152 (78%)	1.04	26 (21%) 0 0	79, 115, 158, 187	1 (0%)
All	All	2549/2644 (96%)	-0.16	62 (2%) 59 60	29, 56, 117, 187	25 (0%)

The worst 5 of 62 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	9	GLY	5.7
3	C	14	PRO	5.7
1	A	450	LEU	4.6
3	C	93	TYR	4.2
3	C	118	VAL	4.1

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
6	SO4	A	1306	5/5	0.78	0.26	157,160,162,162	0
6	SO4	C	144	5/5	0.78	0.22	161,162,165,165	0
6	SO4	A	1305	5/5	0.81	0.30	155,157,160,161	0
6	SO4	A	1307	5/5	0.83	0.36	172,173,174,176	0
7	MES	B	1204	12/12	0.83	0.22	82,100,176,178	0
7	MES	B	1202	12/12	0.84	0.21	88,96,189,190	0
6	SO4	A	1309	5/5	0.85	0.23	159,159,160,160	0
6	SO4	A	1303	5/5	0.85	0.23	132,136,137,140	0
7	MES	B	1205	12/12	0.85	0.28	105,116,150,150	0
6	SO4	B	1201	5/5	0.86	0.20	151,152,155,160	0
6	SO4	B	1199	5/5	0.87	0.35	122,125,128,130	0
6	SO4	A	1310	5/5	0.88	0.30	133,139,139,142	0
6	SO4	B	1196	5/5	0.88	0.27	157,159,161,162	0
6	SO4	A	1302	5/5	0.89	0.26	137,137,138,139	0
6	SO4	B	1200	5/5	0.90	0.15	112,117,119,121	0
6	SO4	A	1304	5/5	0.90	0.16	136,137,138,139	0
6	SO4	A	1301	5/5	0.90	0.24	120,121,125,125	0
6	SO4	B	1197	5/5	0.93	0.22	129,131,132,135	0
6	SO4	B	1195	5/5	0.93	0.14	96,102,104,104	0
6	SO4	B	1198	5/5	0.95	0.15	86,94,105,105	0
6	SO4	A	1308	5/5	0.95	0.21	139,142,142,143	0
6	SO4	A	1300	5/5	0.96	0.14	98,103,108,110	0
7	MES	B	1203	12/12	0.96	0.17	74,79,111,112	0
5	CA	A	1298	1/1	0.97	0.05	67,67,67,67	1
6	SO4	A	1299	5/5	0.98	0.16	97,99,101,103	0
4	ZN	A	1297	1/1	0.99	0.17	62,62,62,62	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.