



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 02:39 PM UTC

PDB ID : 9FI1 / pdb_00009fi1
Title : Bacteroides ovatus polysaccharide lyase family 38 (BoPL38) mutant H297N at pH 3.5
Authors : Tandrup, T.; Wilkens, C.
Deposited on : 2024-05-28
Resolution : 2.36 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	:	4-5-2 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

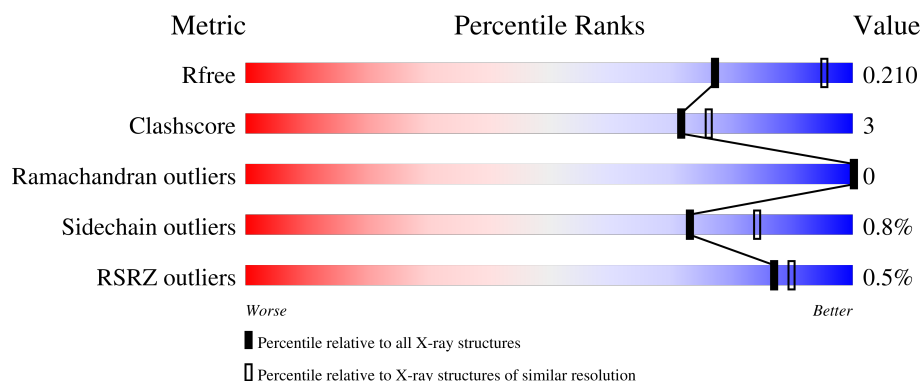
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.36 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	404	
1	B	404	
1	C	404	
1	D	404	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12939 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 Alginate lyase family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	381	Total	C	N	O	S	0	3	0
			3075	1969	518	575	13			
1	B	381	Total	C	N	O	S	0	4	0
			3079	1970	519	577	13			
1	C	381	Total	C	N	O	S	0	7	0
			3099	1985	524	577	13			
1	D	380	Total	C	N	O	S	0	2	0
			3064	1960	517	574	13			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A5M5BWR5
A	2	GLY	-	expression tag	UNP A0A5M5BWR5
A	3	SER	-	expression tag	UNP A0A5M5BWR5
A	4	SER	-	expression tag	UNP A0A5M5BWR5
A	5	HIS	-	expression tag	UNP A0A5M5BWR5
A	6	HIS	-	expression tag	UNP A0A5M5BWR5
A	7	HIS	-	expression tag	UNP A0A5M5BWR5
A	8	HIS	-	expression tag	UNP A0A5M5BWR5
A	9	HIS	-	expression tag	UNP A0A5M5BWR5
A	10	HIS	-	expression tag	UNP A0A5M5BWR5
A	11	SER	-	expression tag	UNP A0A5M5BWR5
A	12	SER	-	expression tag	UNP A0A5M5BWR5
A	13	GLY	-	expression tag	UNP A0A5M5BWR5
A	14	LEU	-	expression tag	UNP A0A5M5BWR5
A	15	VAL	-	expression tag	UNP A0A5M5BWR5
A	16	PRO	-	expression tag	UNP A0A5M5BWR5
A	17	ARG	-	expression tag	UNP A0A5M5BWR5
A	18	GLY	-	expression tag	UNP A0A5M5BWR5
A	19	SER	-	expression tag	UNP A0A5M5BWR5
A	20	HIS	-	expression tag	UNP A0A5M5BWR5
A	21	MET	-	expression tag	UNP A0A5M5BWR5

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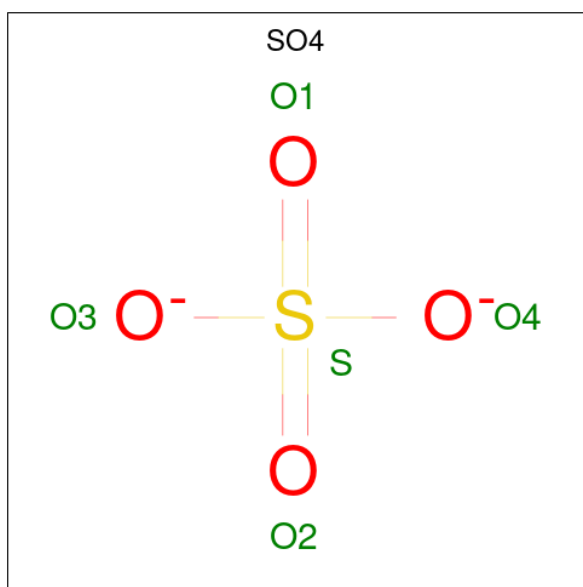
Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ALA	-	expression tag	UNP A0A5M5BWR5
A	23	SER	-	expression tag	UNP A0A5M5BWR5
A	297	ASN	HIS	engineered mutation	UNP A0A5M5BWR5
B	1	MET	-	initiating methionine	UNP A0A5M5BWR5
B	2	GLY	-	expression tag	UNP A0A5M5BWR5
B	3	SER	-	expression tag	UNP A0A5M5BWR5
B	4	SER	-	expression tag	UNP A0A5M5BWR5
B	5	HIS	-	expression tag	UNP A0A5M5BWR5
B	6	HIS	-	expression tag	UNP A0A5M5BWR5
B	7	HIS	-	expression tag	UNP A0A5M5BWR5
B	8	HIS	-	expression tag	UNP A0A5M5BWR5
B	9	HIS	-	expression tag	UNP A0A5M5BWR5
B	10	HIS	-	expression tag	UNP A0A5M5BWR5
B	11	SER	-	expression tag	UNP A0A5M5BWR5
B	12	SER	-	expression tag	UNP A0A5M5BWR5
B	13	GLY	-	expression tag	UNP A0A5M5BWR5
B	14	LEU	-	expression tag	UNP A0A5M5BWR5
B	15	VAL	-	expression tag	UNP A0A5M5BWR5
B	16	PRO	-	expression tag	UNP A0A5M5BWR5
B	17	ARG	-	expression tag	UNP A0A5M5BWR5
B	18	GLY	-	expression tag	UNP A0A5M5BWR5
B	19	SER	-	expression tag	UNP A0A5M5BWR5
B	20	HIS	-	expression tag	UNP A0A5M5BWR5
B	21	MET	-	expression tag	UNP A0A5M5BWR5
B	22	ALA	-	expression tag	UNP A0A5M5BWR5
B	23	SER	-	expression tag	UNP A0A5M5BWR5
B	297	ASN	HIS	engineered mutation	UNP A0A5M5BWR5
C	1	MET	-	initiating methionine	UNP A0A5M5BWR5
C	2	GLY	-	expression tag	UNP A0A5M5BWR5
C	3	SER	-	expression tag	UNP A0A5M5BWR5
C	4	SER	-	expression tag	UNP A0A5M5BWR5
C	5	HIS	-	expression tag	UNP A0A5M5BWR5
C	6	HIS	-	expression tag	UNP A0A5M5BWR5
C	7	HIS	-	expression tag	UNP A0A5M5BWR5
C	8	HIS	-	expression tag	UNP A0A5M5BWR5
C	9	HIS	-	expression tag	UNP A0A5M5BWR5
C	10	HIS	-	expression tag	UNP A0A5M5BWR5
C	11	SER	-	expression tag	UNP A0A5M5BWR5
C	12	SER	-	expression tag	UNP A0A5M5BWR5
C	13	GLY	-	expression tag	UNP A0A5M5BWR5
C	14	LEU	-	expression tag	UNP A0A5M5BWR5
C	15	VAL	-	expression tag	UNP A0A5M5BWR5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	16	PRO	-	expression tag	UNP A0A5M5BWR5
C	17	ARG	-	expression tag	UNP A0A5M5BWR5
C	18	GLY	-	expression tag	UNP A0A5M5BWR5
C	19	SER	-	expression tag	UNP A0A5M5BWR5
C	20	HIS	-	expression tag	UNP A0A5M5BWR5
C	21	MET	-	expression tag	UNP A0A5M5BWR5
C	22	ALA	-	expression tag	UNP A0A5M5BWR5
C	23	SER	-	expression tag	UNP A0A5M5BWR5
C	297	ASN	HIS	engineered mutation	UNP A0A5M5BWR5
D	1	MET	-	initiating methionine	UNP A0A5M5BWR5
D	2	GLY	-	expression tag	UNP A0A5M5BWR5
D	3	SER	-	expression tag	UNP A0A5M5BWR5
D	4	SER	-	expression tag	UNP A0A5M5BWR5
D	5	HIS	-	expression tag	UNP A0A5M5BWR5
D	6	HIS	-	expression tag	UNP A0A5M5BWR5
D	7	HIS	-	expression tag	UNP A0A5M5BWR5
D	8	HIS	-	expression tag	UNP A0A5M5BWR5
D	9	HIS	-	expression tag	UNP A0A5M5BWR5
D	10	HIS	-	expression tag	UNP A0A5M5BWR5
D	11	SER	-	expression tag	UNP A0A5M5BWR5
D	12	SER	-	expression tag	UNP A0A5M5BWR5
D	13	GLY	-	expression tag	UNP A0A5M5BWR5
D	14	LEU	-	expression tag	UNP A0A5M5BWR5
D	15	VAL	-	expression tag	UNP A0A5M5BWR5
D	16	PRO	-	expression tag	UNP A0A5M5BWR5
D	17	ARG	-	expression tag	UNP A0A5M5BWR5
D	18	GLY	-	expression tag	UNP A0A5M5BWR5
D	19	SER	-	expression tag	UNP A0A5M5BWR5
D	20	HIS	-	expression tag	UNP A0A5M5BWR5
D	21	MET	-	expression tag	UNP A0A5M5BWR5
D	22	ALA	-	expression tag	UNP A0A5M5BWR5
D	23	SER	-	expression tag	UNP A0A5M5BWR5
D	297	ASN	HIS	engineered mutation	UNP A0A5M5BWR5

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	173	Total	O	0	0
			173	173		
3	B	164	Total	O	0	0
			164	164		
3	C	132	Total	O	0	0
			132	132		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	108	Total 108	O 108	0	1

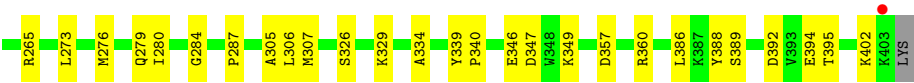
- Molecule 1: Alginate lyase family protein

H238	W246	Y247	E248	R260	L296	A305	N327	D336	Y342	W348	Q358	Q375	K376	Y377	V378	D379	K387	Y388	S389	E394	K403	LYS																					
Met	Gly	Ser	Ser	His	His	His	His	Ser	Ser	Gly	Leu	Val	Pro	Arg	Gly	Ser	His	His	Met	Ala	S23	E45	V48	L54	S59	D95	S96	T97	X98	I99	D100	G101	R121	Y132	L137	R155	Q173	K180	R194	V198	A199	K200	K215

Relative abundance of 32 amino acids. The chart shows the relative abundance of 32 amino acids. The y-axis represents relative abundance from 0 to 100. The x-axis lists the amino acids: MET, GLY, SER, HIS, HIS, HIS, HIS, HIS, HIS, SER, SER, SER, GLY, LEU, VAL, PRO, ARG, GLY, SER, HIS, MET, MET, MET, ALA, S23, L26, E45, R50, L54, E60, I63, D95, G101, K179, S184, Y247, A256, S271, K275, M276, E304, A305, L306, M307, E308, A309, and N310. The bars are color-coded: yellow for most, green for SER, HIS, and MET, and grey for MET, GLY, SER, and LYS. A red dot is placed above the K179 bar.

L286	P287	T293	L306	K351	K387	K403	LYS	NET	GLY	SER	HIS	HIS	HIS	HIS	HIS	HIS	SER	GLY	LEU	VAL	PRO	ARG	GLY	SER	HIS	NET	ALA	G23
E248	D262	E263	L264	K276	L280	C285		L34	E45	K46	K80	W93	P94	D95	G101	L102	K107	R101	T231	R235	E248	L252	D262	E263	L264	K276	L280	C285

MET	GLY	SER	SER	SER	HTS	HTS	HTS	HTS	HTS	HTS	SER	SER	GLY	VAL	PRO	ARG	GLY	SER	HTS	MET	ALA	SER	A24	P25	L26	Q42	E45	A46	L54	K61	Y62	D95	G101	L102	M112	P113	E114	L137	K179	V198	L201	L245	W246	E247	Y248	A256
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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	197.44Å 89.09Å 146.66Å 90.00° 120.55° 90.00°	Depositor
Resolution (Å)	48.48 – 2.36 48.48 – 2.36	Depositor EDS
% Data completeness (in resolution range)	97.4 (48.48-2.36) 97.4 (48.48-2.36)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.37Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.179 , 0.222 (Not available) , 0.210	Depositor DCC
R_{free} test set	4452 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	44.9	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 32.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12939	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% 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: SO4

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	0.37	0/3161	0.52	0/4282
1	B	0.36	0/3168	0.53	0/4291
1	C	0.35	0/3194	0.50	0/4324
1	D	0.34	0/3147	0.51	0/4264
All	All	0.36	0/12670	0.52	0/17161

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	3075	0	3062	22	1
1	B	3079	0	3064	16	0
1	C	3099	0	3101	18	0
1	D	3064	0	3041	26	1
2	A	10	0	0	1	0
2	B	15	0	0	0	0
2	C	5	0	0	0	0
2	D	15	0	0	0	0
3	A	173	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	164	0	0	1	0
3	C	132	0	0	3	1
3	D	108	0	0	0	1
All	All	12939	0	12268	80	2

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 3.

The worst 5 of 80 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:215:LYS:NZ	3:A:601:HOH:O	2.18	0.76
1:A:336:ASP:OD1	1:A:377:TYR:OH	2.08	0.71
1:D:276:MET:HE3	1:D:306:LEU:HD13	1.77	0.65
1:A:180:LYS:HD3	1:A:180:LYS:H	1.66	0.61
1:D:347:ASP:O	1:D:349:LYS:HD2	2.03	0.58

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:718:HOH:O	3:D:699:HOH:O[4_456]	2.07	0.13
1:A:327:ASN:O	1:D:265:ARG:NH1[2_556]	2.15	0.05

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	382/404 (95%)	373 (98%)	9 (2%)	0	100	100
1	B	383/404 (95%)	375 (98%)	8 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	386/404 (96%)	379 (98%)	7 (2%)	0	100	100
1	D	380/404 (94%)	372 (98%)	8 (2%)	0	100	100
All	All	1531/1616 (95%)	1499 (98%)	32 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	328/344 (95%)	325 (99%)	3 (1%)	70	82
1	B	329/344 (96%)	328 (100%)	1 (0%)	86	92
1	C	332/344 (96%)	328 (99%)	4 (1%)	63	77
1	D	326/344 (95%)	322 (99%)	4 (1%)	63	77
All	All	1315/1376 (96%)	1303 (99%)	12 (1%)	73	82

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	275[B]	LYS
1	D	42	GLN
1	D	326	SER
1	D	45	GLU
1	B	184	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	42	GLN
1	D	288	GLN
1	D	375	GLN
1	C	125	ASN
1	A	39	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](#)

9 ligands are modelled in this entry.

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	$\# Z > 2$
2	SO4	A	502	-	4,4,4	0.60	0	6,6,6	0.39	0
2	SO4	B	502	-	4,4,4	0.67	0	6,6,6	0.20	0
2	SO4	D	503	-	4,4,4	0.61	0	6,6,6	0.26	0
2	SO4	C	501	-	4,4,4	0.61	0	6,6,6	0.31	0
2	SO4	D	502	-	4,4,4	0.66	0	6,6,6	0.10	0
2	SO4	D	501	-	4,4,4	0.67	0	6,6,6	0.07	0
2	SO4	B	501	-	4,4,4	0.69	0	6,6,6	0.18	0
2	SO4	B	503	-	4,4,4	0.68	0	6,6,6	0.29	0
2	SO4	A	501	-	4,4,4	0.70	0	6,6,6	0.25	0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	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	381/404 (94%)	-0.35	1 (0%) 90 92	25, 45, 64, 88	3 (0%)
1	B	381/404 (94%)	-0.32	2 (0%) 87 90	27, 45, 64, 83	4 (1%)
1	C	381/404 (94%)	-0.25	1 (0%) 90 92	24, 47, 68, 92	7 (1%)
1	D	380/404 (94%)	-0.09	3 (0%) 82 86	27, 51, 75, 93	2 (0%)
All	All	1523/1616 (94%)	-0.25	7 (0%) 87 90	24, 47, 70, 93	16 (1%)

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	403	LYS	2.8
1	D	46	LYS	2.4
1	C	45	GLU	2.2
1	B	179	LYS	2.2
1	B	403	LYS	2.1

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 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
2	SO4	D	501	5/5	0.42	0.20	76,76,90,98	5
2	SO4	B	502	5/5	0.70	0.15	75,101,109,123	5
2	SO4	B	501	5/5	0.72	0.15	110,110,137,144	0
2	SO4	D	502	5/5	0.82	0.14	59,65,72,77	5
2	SO4	A	501	5/5	0.84	0.13	88,100,131,136	0
2	SO4	A	502	5/5	0.96	0.12	41,50,59,65	0
2	SO4	B	503	5/5	0.96	0.10	46,55,58,71	0
2	SO4	D	503	5/5	0.96	0.09	57,58,73,74	0
2	SO4	C	501	5/5	0.97	0.08	52,55,66,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.