



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 15, 2025 – 11:15 am BST

PDB ID : 9GRW / pdb_00009grw
Title : Structure of Heparinase I from Bacteroides eggerthii in complex with calcium cofactor
Authors : Mycroft-West, C.; Wu, L.
Deposited on : 2024-09-12
Resolution : 1.85 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 Phenix2.0rc1
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

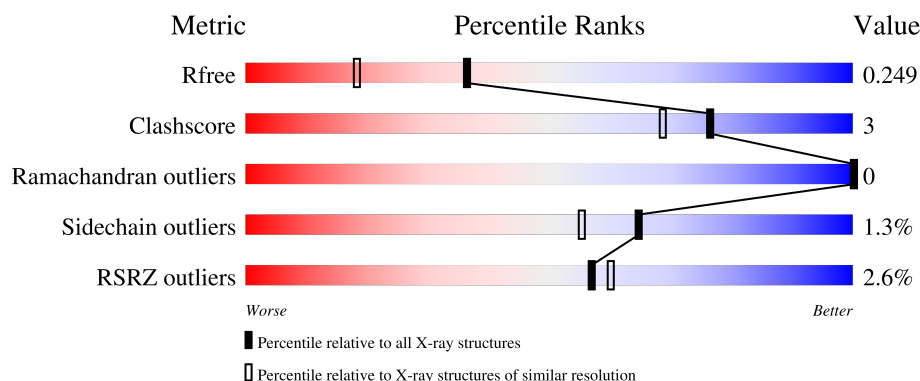
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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}	164625	3097 (1.86-1.86)
Clashscore	180529	3359 (1.86-1.86)
Ramachandran outliers	177936	3335 (1.86-1.86)
Sidechain outliers	177891	3335 (1.86-1.86)
RSRZ outliers	164620	3097 (1.86-1.86)

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	382	
1	B	382	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ACT	A	402	-	-	X	-
3	ACT	A	405	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12657 atoms, of which 5889 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 Heparin lyase I.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	370	Total	C	H	N	O	S	85	2	0
			5921	1900	2945	511	555	10			
1	B	367	Total	C	H	N	O	S	83	0	0
			5858	1880	2914	505	549	10			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP E5WZ15
A	375	LEU	-	expression tag	UNP E5WZ15
A	376	GLU	-	expression tag	UNP E5WZ15
A	377	HIS	-	expression tag	UNP E5WZ15
A	378	HIS	-	expression tag	UNP E5WZ15
A	379	HIS	-	expression tag	UNP E5WZ15
A	380	HIS	-	expression tag	UNP E5WZ15
A	381	HIS	-	expression tag	UNP E5WZ15
A	382	HIS	-	expression tag	UNP E5WZ15
B	1	MET	-	initiating methionine	UNP E5WZ15
B	375	LEU	-	expression tag	UNP E5WZ15
B	376	GLU	-	expression tag	UNP E5WZ15
B	377	HIS	-	expression tag	UNP E5WZ15
B	378	HIS	-	expression tag	UNP E5WZ15
B	379	HIS	-	expression tag	UNP E5WZ15
B	380	HIS	-	expression tag	UNP E5WZ15
B	381	HIS	-	expression tag	UNP E5WZ15
B	382	HIS	-	expression tag	UNP E5WZ15

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

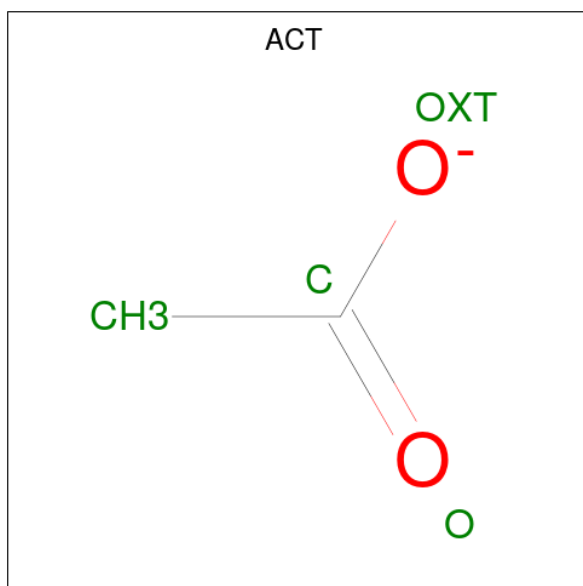
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

Continued on next page...

Continued from previous page...

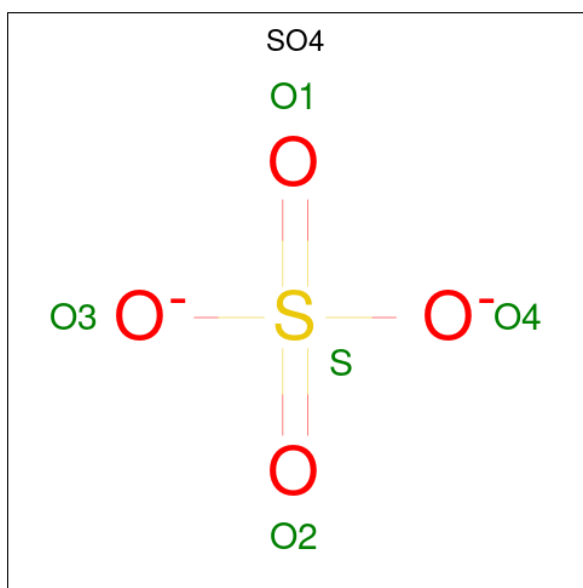
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	3	0
			7	2	3	2		
3	A	1	Total	C	H	O	3	0
			7	2	3	2		
3	A	1	Total	C	H	O	3	0
			7	2	3	2		
3	A	1	Total	C	H	O	3	0
			7	2	3	2		
3	A	1	Total	C	H	O	3	0
			7	2	3	2		
3	B	1	Total	C	H	O	3	0
			7	2	3	2		
3	B	1	Total	C	H	O	3	0
			7	2	3	2		
3	B	1	Total	C	H	O	3	0
			7	2	3	2		
3	B	1	Total	C	H	O	3	0
			7	2	3	2		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

Continued on next page...

Continued from previous page...

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

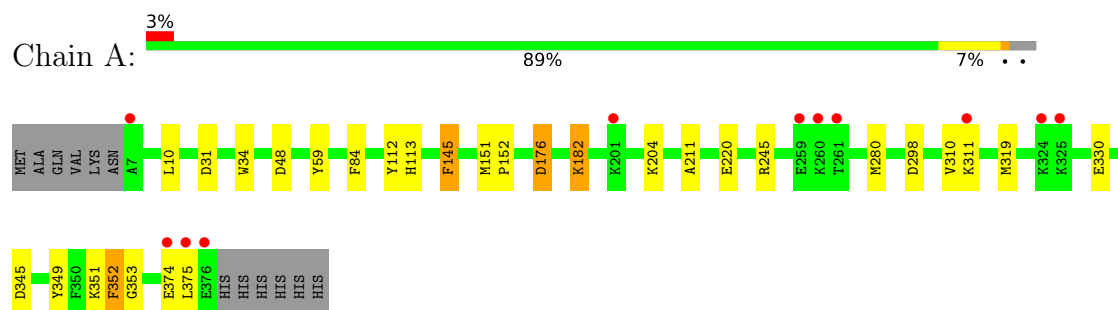
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	357	Total O 357 357	0	0
5	B	314	Total O 314 314	0	0

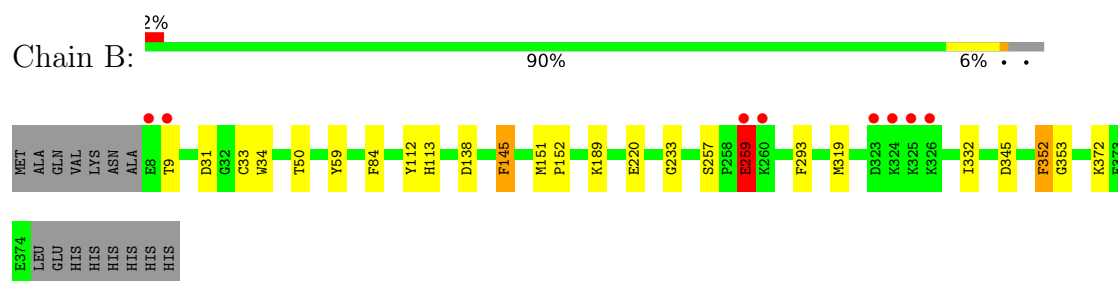
3 Residue-property plots [i](#)

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: Heparin lyase I



• Molecule 1: Heparin lyase I



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	140.19Å 91.48Å 73.45Å 90.00° 95.46° 90.00°	Depositor
Resolution (Å)	54.29 – 1.85 54.29 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (54.29-1.85) 99.9 (54.29-1.85)	Depositor EDS
R_{merge}	0.39	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.210 , 0.247 0.211 , 0.249	Depositor DCC
R_{free} test set	3925 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	19.1	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 36.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12657	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, CA, ACT

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	0.51	0/3060	0.87	5/4135 (0.1%)
1	B	0.50	0/3019	0.89	5/4079 (0.1%)
All	All	0.51	0/6079	0.88	10/8214 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	352	PHE	CA-CB-CG	8.24	122.04	113.80
1	B	352	PHE	CA-CB-CG	7.55	121.35	113.80
1	A	145	PHE	CA-CB-CG	6.20	120.00	113.80
1	B	145	PHE	CA-CB-CG	6.11	119.91	113.80
1	B	138	ASP	CA-CB-CG	5.86	118.46	112.60
1	A	345	ASP	CA-CB-CG	5.50	118.09	112.60
1	A	176	ASP	CA-CB-CG	5.34	117.94	112.60
1	B	345	ASP	CA-CB-CG	5.15	117.75	112.60
1	A	298	ASP	CA-CB-CG	5.09	117.69	112.60
1	B	259	GLU	CB-CA-C	5.08	118.79	110.96

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	245	ARG	Sidechain

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	2976	2945	2924	18	0
1	B	2944	2914	2906	14	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	24	18	18	7	0
3	B	16	12	12	0	0
4	A	80	0	0	0	0
4	B	55	0	0	0	0
5	A	357	0	0	3	0
5	B	314	0	0	1	0
All	All	6768	5889	5860	33	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 3.

All (33) 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:10:LEU:HD12	3:A:405:ACT:H3	1.21	1.13
1:B:31:ASP:OD2	1:B:59:TYR:OH	1.75	1.02
1:B:319:MET:HE3	1:B:332:ILE:HD13	1.57	0.85
1:A:31:ASP:OD2	1:A:59:TYR:OH	1.96	0.83
1:A:330:GLU:OE2	5:A:501:HOH:O	2.04	0.74
1:A:349:TYR:OH	3:A:402:ACT:CH3	2.48	0.61
1:A:10:LEU:HD12	3:A:405:ACT:CH3	2.14	0.59
1:A:349:TYR:OH	3:A:402:ACT:H2	2.05	0.56
1:B:293:PHE:CE1	1:B:319:MET:HE2	2.43	0.54
1:A:204:LYS:HE2	5:A:816:HOH:O	2.08	0.53
1:B:9:THR:HB	1:B:50:THR:CG2	2.39	0.52
1:A:349:TYR:OH	3:A:402:ACT:H3	2.10	0.50
1:A:351:LYS:NZ	3:A:402:ACT:H1	2.26	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:GLY:HA3	1:B:259:GLU:OE2	2.12	0.49
1:A:182:LYS:HD3	1:A:211:ALA:HB2	1.96	0.48
1:A:310:VAL:HG12	1:A:311:LYS:HG3	1.96	0.47
1:A:280:MET:HE1	1:A:319:MET:HE1	1.97	0.47
1:B:257:SER:OG	1:B:259:GLU:HG2	2.14	0.47
1:B:189:LYS:NZ	5:B:514:HOH:O	2.49	0.46
1:B:293:PHE:HE1	1:B:319:MET:HE2	1.81	0.43
1:A:113:HIS:CD2	1:A:151:MET:HE2	2.53	0.43
1:B:33:CYS:HG	1:B:34:TRP:CD1	2.38	0.42
1:B:113:HIS:CD2	1:B:151:MET:HE2	2.55	0.42
1:B:152:PRO:HB3	1:B:220:GLU:HG2	2.02	0.42
1:B:145:PHE:HA	1:B:353:GLY:O	2.20	0.41
1:A:145:PHE:HA	1:A:353:GLY:O	2.20	0.41
1:A:10:LEU:HD23	1:A:48:ASP:HA	2.03	0.41
1:A:374:GLU:O	1:A:375:LEU:C	2.64	0.41
1:A:152:PRO:HB3	1:A:220:GLU:HG2	2.02	0.41
1:B:34:TRP:CE3	1:B:84:PHE:HB3	2.55	0.41
1:A:34:TRP:CE3	1:A:84:PHE:HB3	2.55	0.41
1:B:293:PHE:HE1	1:B:319:MET:CE	2.34	0.41
3:A:402:ACT:CH3	5:A:763:HOH:O	2.70	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	370/382 (97%)	357 (96%)	13 (4%)	0	100	100
1	B	365/382 (96%)	355 (97%)	10 (3%)	0	100	100
All	All	735/764 (96%)	712 (97%)	23 (3%)	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	319/328 (97%)	315 (99%)	4 (1%)	65	55
1	B	315/328 (96%)	311 (99%)	4 (1%)	65	55
All	All	634/656 (97%)	626 (99%)	8 (1%)	65	55

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	TYR
1	A	176	ASP
1	A	182	LYS
1	A	352	PHE
1	B	112	TYR
1	B	259	GLU
1	B	352	PHE
1	B	372	LYS

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

Mol	Chain	Res	Type
1	B	114	HIS
1	B	187	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 39 ligands modelled in this entry, 2 are monoatomic - leaving 37 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	$\# Z > 2$
3	ACT	B	405	-	3,3,3	1.00	0	3,3,3	0.71	0
3	ACT	A	405	-	3,3,3	1.04	0	3,3,3	0.72	0
4	SO4	A	423	-	4,4,4	0.36	0	6,6,6	0.07	0
4	SO4	A	417	-	4,4,4	0.30	0	6,6,6	0.07	0
3	ACT	A	407	-	3,3,3	1.07	0	3,3,3	0.65	0
4	SO4	B	410	-	4,4,4	0.43	0	6,6,6	0.11	0
4	SO4	A	409	-	4,4,4	0.33	0	6,6,6	0.11	0
3	ACT	B	404	-	3,3,3	0.89	0	3,3,3	1.00	0
4	SO4	B	412	-	4,4,4	0.35	0	6,6,6	0.07	0
4	SO4	B	413	-	4,4,4	0.35	0	6,6,6	0.07	0
3	ACT	A	404	-	3,3,3	0.99	0	3,3,3	0.80	0
4	SO4	B	408	-	4,4,4	0.36	0	6,6,6	0.16	0
3	ACT	A	403	-	3,3,3	1.10	0	3,3,3	0.73	0
4	SO4	B	406	-	4,4,4	0.44	0	6,6,6	0.15	0
4	SO4	B	409	-	4,4,4	0.37	0	6,6,6	0.08	0
4	SO4	A	419	-	4,4,4	0.32	0	6,6,6	0.08	0
4	SO4	A	413	-	4,4,4	0.35	0	6,6,6	0.12	0
4	SO4	A	408	-	4,4,4	0.38	0	6,6,6	0.12	0
4	SO4	A	421	-	4,4,4	0.35	0	6,6,6	0.07	0
3	ACT	B	403	-	3,3,3	1.05	0	3,3,3	0.81	0
4	SO4	A	418	-	4,4,4	0.31	0	6,6,6	0.15	0
4	SO4	A	422	-	4,4,4	0.38	0	6,6,6	0.06	0
3	ACT	A	406	-	3,3,3	0.98	0	3,3,3	0.90	0
4	SO4	B	414	-	4,4,4	0.33	0	6,6,6	0.12	0
4	SO4	A	410	-	4,4,4	0.50	0	6,6,6	0.14	0
4	SO4	B	416	-	4,4,4	0.35	0	6,6,6	0.20	0
4	SO4	B	411	-	4,4,4	0.29	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SO4	A	412	-	4,4,4	0.39	0	6,6,6	0.15	0
3	ACT	A	402	-	3,3,3	0.87	0	3,3,3	0.87	0
4	SO4	B	415	-	4,4,4	0.37	0	6,6,6	0.08	0
3	ACT	B	402	-	3,3,3	1.15	0	3,3,3	0.84	0
4	SO4	B	407	-	4,4,4	0.31	0	6,6,6	0.08	0
4	SO4	A	411	-	4,4,4	0.32	0	6,6,6	0.10	0
4	SO4	A	414	-	4,4,4	0.37	0	6,6,6	0.08	0
4	SO4	A	416	-	4,4,4	0.39	0	6,6,6	0.06	0
4	SO4	A	415	-	4,4,4	0.28	0	6,6,6	0.11	0
4	SO4	A	420	-	4,4,4	0.33	0	6,6,6	0.15	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.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	405	ACT	2	0
3	A	402	ACT	5	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	370/382 (96%)	-0.09	11 (2%) 52 56	9, 20, 42, 84	1 (0%)
1	B	367/382 (96%)	-0.06	8 (2%) 62 65	13, 22, 40, 78	0
All	All	737/764 (96%)	-0.08	19 (2%) 57 60	9, 21, 41, 84	1 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	375	LEU	6.6
1	B	325	LYS	4.5
1	A	376	GLU	4.2
1	B	324	LYS	3.8
1	B	326	LYS	3.1
1	A	324	LYS	2.6
1	B	323	ASP	2.6
1	B	8	GLU	2.5
1	A	374	GLU	2.5
1	A	7	ALA	2.4
1	A	259	GLU	2.4
1	B	9	THR	2.4
1	A	311	LYS	2.3
1	A	325	LYS	2.3
1	A	261	THR	2.3
1	A	201	LYS	2.3
1	A	260	LYS	2.2
1	B	260	LYS	2.2
1	B	259	GLU	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(\AA^2)	Q<0.9
3	ACT	A	406	4/4	0.56	0.24	39,39,51,55	3
4	SO4	B	413	5/5	0.67	0.16	77,77,82,84	0
4	SO4	A	420	5/5	0.73	0.14	55,55,64,66	0
4	SO4	B	415	5/5	0.73	0.17	65,65,67,74	0
4	SO4	A	415	5/5	0.74	0.14	52,54,59,62	0
4	SO4	B	414	5/5	0.77	0.14	52,53,63,64	0
4	SO4	A	418	5/5	0.77	0.14	49,54,56,57	0
4	SO4	A	419	5/5	0.80	0.15	48,61,64,64	0
4	SO4	B	411	5/5	0.81	0.14	53,53,57,59	0
4	SO4	A	421	5/5	0.82	0.13	60,61,62,63	0
3	ACT	A	405	4/4	0.83	0.30	39,39,43,44	3
3	ACT	A	404	4/4	0.83	0.23	39,39,51,52	3
4	SO4	B	412	5/5	0.83	0.13	55,61,64,66	0
4	SO4	B	409	5/5	0.84	0.14	51,53,58,59	0
3	ACT	B	402	4/4	0.84	0.16	30,32,39,39	3
3	ACT	A	407	4/4	0.84	0.15	39,39,41,42	3
4	SO4	A	422	5/5	0.85	0.11	61,63,68,68	0
4	SO4	A	416	5/5	0.87	0.11	48,49,54,55	0
4	SO4	A	414	5/5	0.87	0.12	55,56,58,59	0
4	SO4	B	407	5/5	0.87	0.12	43,47,50,52	0
3	ACT	B	403	4/4	0.88	0.15	30,30,39,39	3
3	ACT	A	403	4/4	0.89	0.15	32,37,39,39	3
4	SO4	A	417	5/5	0.89	0.10	36,40,46,48	0
4	SO4	A	423	5/5	0.90	0.10	45,48,51,54	0
4	SO4	A	413	5/5	0.90	0.12	51,53,53,57	0
4	SO4	B	416	5/5	0.90	0.12	38,40,49,49	0
4	SO4	B	410	5/5	0.92	0.11	43,45,48,50	0
3	ACT	A	402	4/4	0.93	0.10	17,23,39,39	3
3	ACT	B	404	4/4	0.93	0.14	25,29,39,39	3
4	SO4	A	412	5/5	0.96	0.14	34,34,36,38	0
3	ACT	B	405	4/4	0.96	0.06	17,18,39,39	3
4	SO4	A	410	5/5	0.96	0.09	34,34,35,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SO4	B	406	5/5	0.97	0.07	32,32,35,35	0
4	SO4	B	408	5/5	0.97	0.07	26,26,28,30	0
4	SO4	A	411	5/5	0.98	0.07	27,27,31,31	0
4	SO4	A	409	5/5	0.98	0.07	25,25,26,28	0
4	SO4	A	408	5/5	0.98	0.05	22,24,25,25	0
2	CA	B	401	1/1	0.99	0.04	17,17,17,17	0
2	CA	A	401	1/1	0.99	0.02	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.