



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 25, 2024 – 10:11 AM EST

PDB ID : 8VRM
Title : Crystal structure of the Pcryo_0619 N-acetyltransferase from *Psychrobacter cryohalolentis* K5
Authors : Dunsirn, M.M.; Bockhaus, N.J.; Thoden, J.B.; Holden, H.M.
Deposited on : 2024-01-22
Resolution : 1.75 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

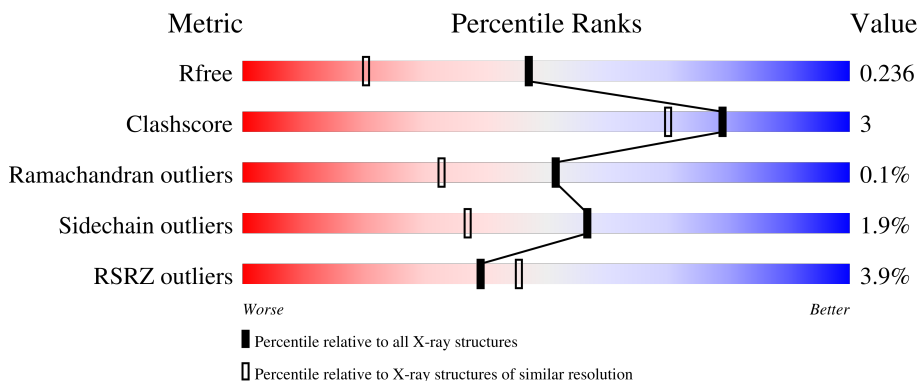
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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.



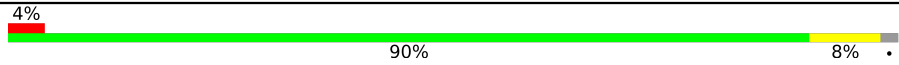
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	182	3% 91% 6% ..
1	B	182	5% 92% ..
1	C	182	% 89% 8% ..
1	D	182	5% 92% 5% .
1	E	182	3% 95% ..

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Mol	Chain	Length	Quality of chain
1	F	182	 A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a small red segment on the left labeled '4%', a large green segment in the middle labeled '90%', and a small yellow segment on the right labeled '8%'. There is a small grey dot at the end of the bar.

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	MPD	B	212	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8760 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 Acetyltransferase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	177	1333	851	223	254	5	0	0	0
1	B	176	1333	852	223	253	5	0	0	0
1	C	178	1341	856	225	255	5	0	0	0
1	D	177	1348	861	227	255	5	0	1	0
1	E	181	1373	874	233	261	5	0	0	0
1	F	178	1348	860	228	255	5	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

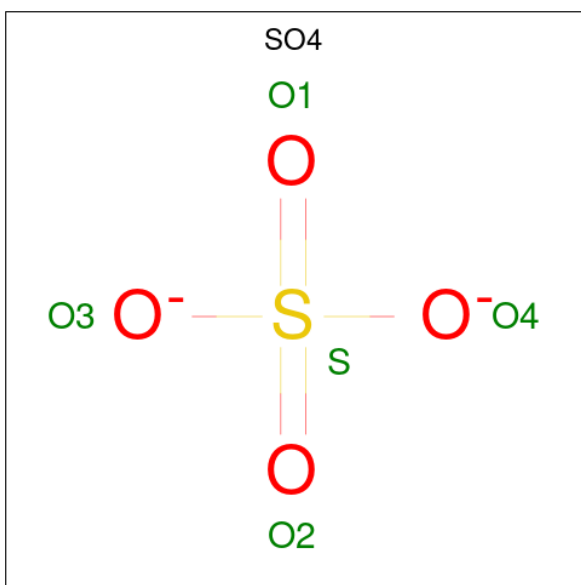
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q1QD51
A	-2	GLY	-	expression tag	UNP Q1QD51
A	-1	GLY	-	expression tag	UNP Q1QD51
A	0	HIS	-	expression tag	UNP Q1QD51
B	-3	GLY	-	expression tag	UNP Q1QD51
B	-2	GLY	-	expression tag	UNP Q1QD51
B	-1	GLY	-	expression tag	UNP Q1QD51
B	0	HIS	-	expression tag	UNP Q1QD51
C	-3	GLY	-	expression tag	UNP Q1QD51
C	-2	GLY	-	expression tag	UNP Q1QD51
C	-1	GLY	-	expression tag	UNP Q1QD51
C	0	HIS	-	expression tag	UNP Q1QD51
D	-3	GLY	-	expression tag	UNP Q1QD51
D	-2	GLY	-	expression tag	UNP Q1QD51
D	-1	GLY	-	expression tag	UNP Q1QD51
D	0	HIS	-	expression tag	UNP Q1QD51
E	-3	GLY	-	expression tag	UNP Q1QD51

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP Q1QD51
E	-1	GLY	-	expression tag	UNP Q1QD51
E	0	HIS	-	expression tag	UNP Q1QD51
F	-3	GLY	-	expression tag	UNP Q1QD51
F	-2	GLY	-	expression tag	UNP Q1QD51
F	-1	GLY	-	expression tag	UNP Q1QD51
F	0	HIS	-	expression tag	UNP Q1QD51

- Molecule 2 is SULFATE ION (three-letter code: 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	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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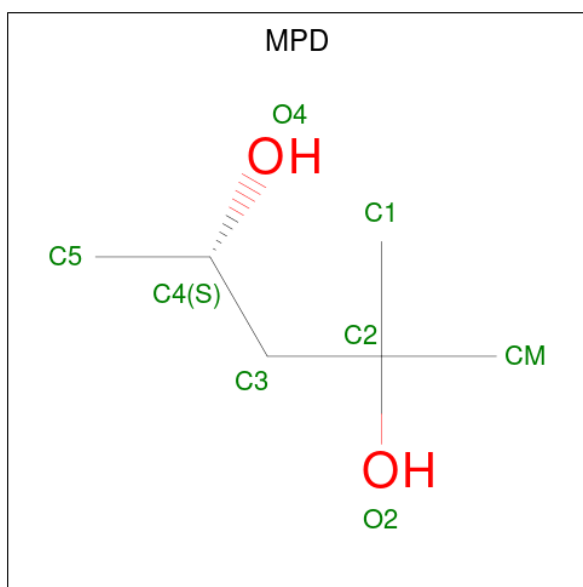
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0
2	B	1	5	4	1	0	0
2	B	1	5	4	1	0	0
2	B	1	5	4	1	0	0
2	B	1	5	4	1	0	0
2	B	1	5	4	1	0	0
2	B	1	5	4	1	0	0
2	B	1	5	4	1	0	0
2	B	1	5	4	1	0	0
2	B	1	5	4	1	0	0
2	B	1	5	4	1	0	0
2	B	1	5	4	1	0	0
2	B	1	5	4	1	0	0
2	B	1	5	4	1	0	0
2	C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

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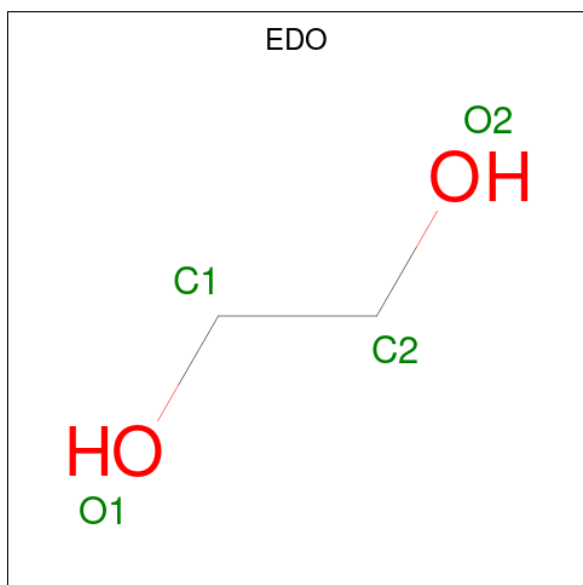
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			8	6	2		
3	D	1	Total	C	O	0	0
			8	6	2		
3	E	1	Total	C	O	0	0
			8	6	2		
3	F	1	Total	C	O	0	0
			8	6	2		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		

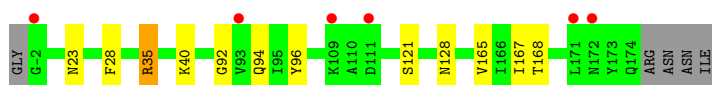
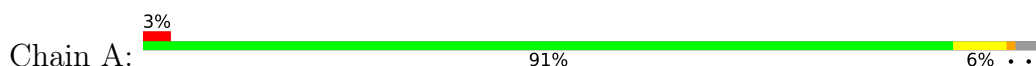
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	62	Total	O	0	0
			62	62		
5	B	74	Total	O	0	0
			74	74		
5	C	86	Total	O	0	0
			86	86		
5	D	50	Total	O	0	0
			50	50		
5	E	77	Total	O	0	0
			77	77		
5	F	65	Total	O	0	0
			65	65		

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.

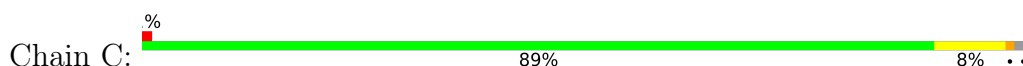
- Molecule 1: Acetyltransferase, putative



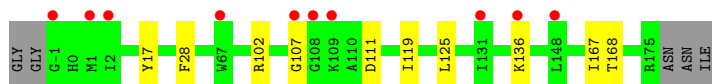
- Molecule 1: Acetyltransferase, putative



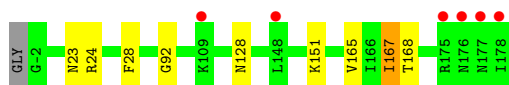
- Molecule 1: Acetyltransferase, putative



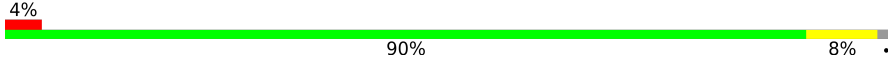
- Molecule 1: Acetyltransferase, putative



- Molecule 1: Acetyltransferase, putative



- Molecule 1: Acetyltransferase, putative

Chain F: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	106.67Å 106.67Å 180.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.19 – 1.75 46.19 – 1.75	Depositor EDS
% Data completeness (in resolution range)	98.4 (46.19-1.75) 98.4 (46.19-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 1.75Å)	Xtrriage
Refinement program	REFMAC 5.8.0405	Depositor
R, R_{free}	0.187 , 0.230 0.196 , 0.236	Depositor DCC
R_{free} test set	5779 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	24.0	Xtrriage
Anisotropy	0.213	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 48.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.035 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8760	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.40% 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: EDO, MPD, 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	0.41	0/1355	0.72	1/1830 (0.1%)
1	B	0.41	0/1355	0.71	0/1829
1	C	0.41	0/1363	0.68	0/1839
1	D	0.40	0/1371	0.68	0/1851
1	E	0.42	0/1395	0.70	0/1881
1	F	0.42	0/1370	0.67	0/1848
All	All	0.41	0/8209	0.69	1/11078 (0.0%)

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
1	C	0	1
1	E	0	1
1	F	0	1
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	ARG	NE-CZ-NH1	5.47	123.03	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	35	ARG	Sidechain
1	C	102	ARG	Sidechain
1	E	24	ARG	Sidechain
1	F	175	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	1333	0	1366	6	0
1	B	1333	0	1374	7	0
1	C	1341	0	1380	14	0
1	D	1348	0	1382	6	0
1	E	1373	0	1413	5	0
1	F	1348	0	1390	6	0
2	A	50	0	0	0	0
2	B	55	0	0	1	0
2	C	35	0	0	0	0
2	D	35	0	0	1	0
2	E	30	0	0	1	0
2	F	25	0	0	0	0
3	B	8	0	14	6	0
3	D	8	0	14	5	0
3	E	8	0	14	0	0
3	F	8	0	14	0	0
4	C	4	0	6	0	0
4	F	4	0	6	1	0
5	A	62	0	0	1	0
5	B	74	0	0	1	0
5	C	86	0	0	4	0
5	D	50	0	0	1	0
5	E	77	0	0	2	0
5	F	65	0	0	0	0
All	All	8760	0	8373	47	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 (47) 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)
3:B:212:MPD:H53	3:B:212:MPD:HM1	1.54	0.89
2:B:204:SO4:O3	5:B:301:HOH:O	1.93	0.83
1:C:20:LYS:HE2	3:D:208:MPD:HM2	1.67	0.75
2:E:203:SO4:O1	5:E:301:HOH:O	2.03	0.74
1:B:0:HIS:NE2	1:C:9:GLU:OE1	2.26	0.67
1:E:151:LYS:HE2	5:E:362:HOH:O	1.96	0.65
1:B:145:ALA:H	3:B:212:MPD:H32	1.62	0.65
1:E:165:VAL:O	1:E:167:ILE:HD13	1.99	0.62
1:C:103:LYS:HE2	5:C:302:HOH:O	1.99	0.61
3:B:212:MPD:HM1	3:B:212:MPD:C5	2.27	0.61
1:C:118:ARG:HD3	1:C:136:LYS:HE2	1.84	0.59
1:D:102:ARG:HD2	5:D:341:HOH:O	2.04	0.56
1:A:121:SER:OG	5:A:301:HOH:O	2.18	0.55
1:A:167:ILE:HG22	1:A:168:THR:HG22	1.87	0.55
1:C:20:LYS:NZ	3:D:208:MPD:H11	2.21	0.55
1:E:167:ILE:HG22	1:E:168:THR:HG22	1.89	0.53
1:B:127:PRO:HD2	3:B:212:MPD:H4	1.91	0.52
1:C:94:GLN:NE2	1:C:96:TYR:OH	2.42	0.52
1:C:139:ASP:OD1	5:C:301:HOH:O	2.19	0.52
1:A:92:GLY:HA3	1:A:128:ASN:ND2	2.26	0.52
1:D:111:ASP:HB3	2:D:202:SO4:O2	2.10	0.51
1:B:5:LYS:HE3	1:B:5:LYS:HA	1.92	0.51
1:E:165:VAL:HG23	1:E:167:ILE:CD1	2.42	0.50
1:D:17:TYR:OH	3:D:208:MPD:H53	2.13	0.49
1:C:151:LYS:HE3	5:C:375:HOH:O	2.13	0.49
1:F:-2:GLY:C	1:F:0:HIS:H	2.16	0.49
1:B:124:TYR:HH	3:B:212:MPD:HO4	1.57	0.48
1:A:92:GLY:HA3	1:A:128:ASN:HD22	1.81	0.46
1:D:167:ILE:HG22	1:D:168:THR:HG22	1.96	0.46
1:D:107:GLY:HA2	1:F:122:ASP:OD1	2.15	0.46
1:A:165:VAL:HG23	1:A:167:ILE:CD1	2.45	0.46
3:B:212:MPD:C5	3:B:212:MPD:CM	2.94	0.45
1:D:119:ILE:HD13	1:D:125:LEU:HD11	1.98	0.45
1:C:20:LYS:HZ1	3:D:208:MPD:H11	1.81	0.45
1:C:92:GLY:HA3	1:C:128:ASN:ND2	2.32	0.45
1:F:145:ALA:H	4:F:207:EDO:H21	1.82	0.45
1:B:0:HIS:CE1	1:C:9:GLU:OE1	2.71	0.44
1:E:92:GLY:HA3	1:E:128:ASN:ND2	2.32	0.44
1:B:5:LYS:O	1:B:9:GLU:HG3	2.19	0.43
1:F:67:TRP:HZ3	1:F:90:SER:HA	1.83	0.43
1:C:-3:GLY:CA	5:C:340:HOH:O	2.67	0.42
1:C:118:ARG:HD3	1:C:136:LYS:CE	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:GLN:NE2	1:A:96:TYR:OH	2.52	0.42
1:F:94:GLN:NE2	1:F:96:TYR:OH	2.53	0.42
3:D:208:MPD:H12	3:D:208:MPD:H4	1.66	0.42
1:F:35:ARG:HB3	1:F:49:SER:HB2	2.02	0.41
1:C:168:THR:OG1	1:C:169:ASP:N	2.53	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	175/182 (96%)	171 (98%)	4 (2%)	0	100	100
1	B	174/182 (96%)	171 (98%)	3 (2%)	0	100	100
1	C	176/182 (97%)	173 (98%)	3 (2%)	0	100	100
1	D	176/182 (97%)	170 (97%)	6 (3%)	0	100	100
1	E	179/182 (98%)	176 (98%)	3 (2%)	0	100	100
1	F	176/182 (97%)	171 (97%)	4 (2%)	1 (1%)	25	10
All	All	1056/1092 (97%)	1032 (98%)	23 (2%)	1 (0%)	51	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	-1	GLY

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	147/152 (97%)	144 (98%)	3 (2%)	55	34
1	B	148/152 (97%)	144 (97%)	4 (3%)	44	22
1	C	148/152 (97%)	145 (98%)	3 (2%)	55	34
1	D	149/152 (98%)	147 (99%)	2 (1%)	69	54
1	E	152/152 (100%)	149 (98%)	3 (2%)	55	34
1	F	149/152 (98%)	147 (99%)	2 (1%)	69	54
All	All	893/912 (98%)	876 (98%)	17 (2%)	57	37

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	28	PHE
1	A	40	LYS
1	B	5	LYS
1	B	28	PHE
1	B	46	GLU
1	B	136	LYS
1	C	20	LYS
1	C	28	PHE
1	C	136	LYS
1	D	28	PHE
1	D	136	LYS
1	E	23	ASN
1	E	28	PHE
1	E	167	ILE
1	F	23	ASN
1	F	28	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	GLN
1	A	128	ASN
1	B	94	GLN
1	B	128	ASN
1	C	94	GLN

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Mol	Chain	Res	Type
1	C	128	ASN
1	D	94	GLN
1	E	23	ASN
1	E	128	ASN
1	F	94	GLN
1	F	128	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](#)

52 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	E	203	-	4,4,4	0.37	0	6,6,6	0.10	0
2	SO4	B	211	-	4,4,4	0.34	0	6,6,6	0.07	0
2	SO4	F	202	-	4,4,4	0.42	0	6,6,6	0.07	0
2	SO4	A	209	-	4,4,4	0.34	0	6,6,6	0.08	0
2	SO4	B	208	-	4,4,4	0.30	0	6,6,6	0.08	0
4	EDO	F	207	-	3,3,3	0.31	0	2,2,2	0.14	0
2	SO4	C	203	-	4,4,4	0.37	0	6,6,6	0.12	0
2	SO4	D	202	-	4,4,4	0.35	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	B	207	-	4,4,4	0.31	0	6,6,6	0.04	0
2	SO4	A	203	-	4,4,4	0.32	0	6,6,6	0.11	0
2	SO4	B	203	-	4,4,4	0.37	0	6,6,6	0.07	0
3	MPD	B	212	-	7,7,7	0.41	0	9,10,10	0.99	1 (11%)
2	SO4	D	204	-	4,4,4	0.36	0	6,6,6	0.11	0
2	SO4	A	204	-	4,4,4	0.33	0	6,6,6	0.09	0
2	SO4	B	204	-	4,4,4	0.35	0	6,6,6	0.08	0
2	SO4	C	205	-	4,4,4	0.44	0	6,6,6	0.17	0
2	SO4	C	201	-	4,4,4	0.46	0	6,6,6	0.14	0
2	SO4	D	201	-	4,4,4	0.43	0	6,6,6	0.14	0
3	MPD	E	207	-	7,7,7	0.28	0	9,10,10	0.49	0
2	SO4	B	209	-	4,4,4	0.30	0	6,6,6	0.11	0
2	SO4	A	210	-	4,4,4	0.30	0	6,6,6	0.13	0
2	SO4	B	206	-	4,4,4	0.25	0	6,6,6	0.16	0
3	MPD	D	208	-	7,7,7	0.32	0	9,10,10	0.95	0
2	SO4	F	203	-	4,4,4	0.35	0	6,6,6	0.04	0
4	EDO	C	208	-	3,3,3	0.18	0	2,2,2	0.38	0
2	SO4	D	207	-	4,4,4	0.31	0	6,6,6	0.12	0
2	SO4	D	206	-	4,4,4	0.33	0	6,6,6	0.05	0
2	SO4	D	203	-	4,4,4	0.38	0	6,6,6	0.12	0
2	SO4	A	207	-	4,4,4	0.29	0	6,6,6	0.08	0
2	SO4	A	206	-	4,4,4	0.32	0	6,6,6	0.09	0
2	SO4	C	207	-	4,4,4	0.34	0	6,6,6	0.07	0
2	SO4	E	206	-	4,4,4	0.33	0	6,6,6	0.08	0
2	SO4	F	204	-	4,4,4	0.32	0	6,6,6	0.11	0
2	SO4	E	204	-	4,4,4	0.29	0	6,6,6	0.11	0
2	SO4	F	201	-	4,4,4	0.27	0	6,6,6	0.13	0
2	SO4	E	201	-	4,4,4	0.46	0	6,6,6	0.10	0
2	SO4	D	205	-	4,4,4	0.35	0	6,6,6	0.04	0
2	SO4	B	202	-	4,4,4	0.37	0	6,6,6	0.11	0
2	SO4	B	205	-	4,4,4	0.34	0	6,6,6	0.16	0
2	SO4	A	205	-	4,4,4	0.33	0	6,6,6	0.10	0
2	SO4	C	206	-	4,4,4	0.34	0	6,6,6	0.06	0
2	SO4	B	210	-	4,4,4	0.32	0	6,6,6	0.10	0
2	SO4	A	202	-	4,4,4	0.37	0	6,6,6	0.21	0
2	SO4	C	202	-	4,4,4	0.33	0	6,6,6	0.08	0
2	SO4	A	201	-	4,4,4	0.39	0	6,6,6	0.11	0
2	SO4	F	205	-	4,4,4	0.31	0	6,6,6	0.15	0
2	SO4	C	204	-	4,4,4	0.29	0	6,6,6	0.08	0
2	SO4	E	205	-	4,4,4	0.36	0	6,6,6	0.05	0
2	SO4	E	202	-	4,4,4	0.34	0	6,6,6	0.11	0
2	SO4	B	201	-	4,4,4	0.40	0	6,6,6	0.11	0
2	SO4	A	208	-	4,4,4	0.36	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MPD	F	206	-	7,7,7	0.21	0	9,10,10	0.62	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
4	EDO	C	208	-	-	1/1/1/1	-
3	MPD	B	212	-	-	1/5/5/5	-
4	EDO	F	207	-	-	1/1/1/1	-
3	MPD	E	207	-	-	2/5/5/5	-
3	MPD	F	206	-	-	2/5/5/5	-
3	MPD	D	208	-	-	2/5/5/5	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	212	MPD	C5-C4-C3	2.47	123.34	111.69

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	208	MPD	C2-C3-C4-C5
3	F	206	MPD	C2-C3-C4-O4
4	C	208	EDO	O1-C1-C2-O2
4	F	207	EDO	O1-C1-C2-O2
3	B	212	MPD	C2-C3-C4-C5
3	F	206	MPD	C2-C3-C4-C5
3	E	207	MPD	C1-C2-C3-C4
3	E	207	MPD	O2-C2-C3-C4
3	D	208	MPD	C2-C3-C4-O4

There are no ring outliers.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	203	SO4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	207	EDO	1	0
2	D	202	SO4	1	0
3	B	212	MPD	6	0
2	B	204	SO4	1	0
3	D	208	MPD	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

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	177/182 (97%)	0.17	6 (3%) 45 51	18, 30, 49, 79	0
1	B	176/182 (96%)	0.19	10 (5%) 23 29	18, 29, 47, 68	0
1	C	178/182 (97%)	-0.00	2 (1%) 80 86	18, 28, 47, 73	0
1	D	177/182 (97%)	0.33	10 (5%) 24 30	19, 33, 52, 65	0
1	E	181/182 (99%)	0.19	6 (3%) 46 53	17, 28, 48, 68	0
1	F	178/182 (97%)	0.20	8 (4%) 33 39	18, 29, 47, 68	0
All	All	1067/1092 (97%)	0.18	42 (3%) 39 45	17, 30, 49, 79	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	175	ARG	5.7
1	E	178	ILE	5.4
1	C	-3	GLY	4.9
1	E	109	LYS	4.9
1	F	1	MET	4.1
1	D	109	LYS	4.1
1	F	-2	GLY	4.0
1	E	177	ASN	3.9
1	E	176	ASN	3.9
1	A	-2	GLY	3.5
1	A	109	LYS	3.4
1	F	-1	GLY	3.1
1	E	175	ARG	2.8
1	B	-1	GLY	2.8
1	B	109	LYS	2.7
1	A	172	ASN	2.7
1	D	136	LYS	2.7
1	B	111	ASP	2.6
1	B	107	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	171	LEU	2.6
1	B	148	LEU	2.5
1	D	-1	GLY	2.5
1	B	1	MET	2.4
1	D	148	LEU	2.4
1	D	2	ILE	2.3
1	F	0	HIS	2.3
1	F	2	ILE	2.3
1	B	162	SER	2.2
1	B	165	VAL	2.2
1	D	1	MET	2.2
1	F	146	ASN	2.2
1	D	107	GLY	2.2
1	D	108	GLY	2.2
1	D	131	ILE	2.2
1	A	93	VAL	2.1
1	A	111	ASP	2.1
1	D	67	TRP	2.1
1	C	160	PHE	2.1
1	B	127	PRO	2.0
1	B	163	PRO	2.0
1	E	148	LEU	2.0
1	F	171	LEU	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 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	EDO	C	208	4/4	0.64	0.15	55,58,60,62	0
2	SO4	B	208	5/5	0.75	0.36	72,90,101,103	0
2	SO4	C	205	5/5	0.79	0.17	50,62,69,82	0
2	SO4	D	205	5/5	0.80	0.26	97,107,114,117	0
2	SO4	F	205	5/5	0.80	0.25	71,80,88,92	0
2	SO4	C	204	5/5	0.80	0.27	71,84,96,101	0
3	MPD	D	208	8/8	0.82	0.23	47,58,63,69	0
3	MPD	B	212	8/8	0.82	0.21	45,48,53,53	0
2	SO4	F	204	5/5	0.83	0.33	88,89,90,91	0
4	EDO	F	207	4/4	0.83	0.20	40,42,45,48	0
2	SO4	D	202	5/5	0.84	0.25	62,87,88,89	0
2	SO4	E	204	5/5	0.85	0.20	75,77,84,86	0
3	MPD	F	206	8/8	0.85	0.17	61,65,73,73	0
2	SO4	A	204	5/5	0.86	0.24	65,72,83,85	0
2	SO4	B	209	5/5	0.87	0.12	70,77,87,88	0
2	SO4	B	207	5/5	0.87	0.24	79,93,95,105	0
3	MPD	E	207	8/8	0.87	0.15	34,45,49,50	0
2	SO4	B	202	5/5	0.88	0.13	81,82,89,93	0
2	SO4	D	204	5/5	0.89	0.13	90,99,108,108	0
2	SO4	B	205	5/5	0.89	0.26	59,60,77,78	0
2	SO4	D	206	5/5	0.89	0.21	82,84,85,94	0
2	SO4	E	206	5/5	0.90	0.30	77,78,85,96	0
2	SO4	A	203	5/5	0.90	0.33	72,88,95,110	0
2	SO4	E	205	5/5	0.90	0.39	71,84,98,99	0
2	SO4	E	203	5/5	0.91	0.22	60,73,74,76	0
2	SO4	C	207	5/5	0.91	0.14	75,78,85,91	0
2	SO4	A	206	5/5	0.91	0.29	72,72,77,91	0
2	SO4	B	210	5/5	0.91	0.12	72,76,77,87	0
2	SO4	A	207	5/5	0.91	0.35	70,72,83,85	0
2	SO4	A	205	5/5	0.91	0.34	83,89,93,94	0
2	SO4	B	203	5/5	0.92	0.22	71,79,81,87	0
2	SO4	B	206	5/5	0.92	0.15	44,70,83,87	0
2	SO4	C	206	5/5	0.92	0.11	85,86,92,95	0
2	SO4	B	204	5/5	0.92	0.21	67,73,77,85	0
2	SO4	C	202	5/5	0.92	0.27	69,70,85,92	0
2	SO4	F	203	5/5	0.93	0.28	76,81,85,87	0
2	SO4	A	210	5/5	0.93	0.16	66,69,76,78	0
2	SO4	E	202	5/5	0.93	0.20	51,62,67,70	0
2	SO4	C	203	5/5	0.94	0.25	66,67,69,72	0
2	SO4	B	211	5/5	0.94	0.23	76,82,88,91	0
2	SO4	D	201	5/5	0.94	0.14	64,68,71,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO4	F	201	5/5	0.94	0.22	45,55,62,67	0
2	SO4	F	202	5/5	0.94	0.12	59,60,64,70	0
2	SO4	A	209	5/5	0.94	0.10	71,71,81,81	0
2	SO4	D	203	5/5	0.94	0.25	65,70,74,78	0
2	SO4	D	207	5/5	0.95	0.20	54,64,71,73	0
2	SO4	A	202	5/5	0.96	0.10	60,63,66,67	0
2	SO4	A	208	5/5	0.96	0.21	74,79,88,88	0
2	SO4	B	201	5/5	0.96	0.12	63,63,70,70	0
2	SO4	C	201	5/5	0.97	0.05	62,62,66,72	0
2	SO4	E	201	5/5	0.97	0.08	47,52,59,65	0
2	SO4	A	201	5/5	0.98	0.05	41,44,47,48	0

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

There are no such residues in this entry.