Full wwPDB X-ray Structure Validation Report (i)

Mar 27, 2018 – 10:27 AM BST

PDB ID	:	6G26
Title	:	The crystal structure of the Burkholderia pseudomallei HicAB complex
Deposited on	:	2018-03-22
Resolution	:	2.49 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

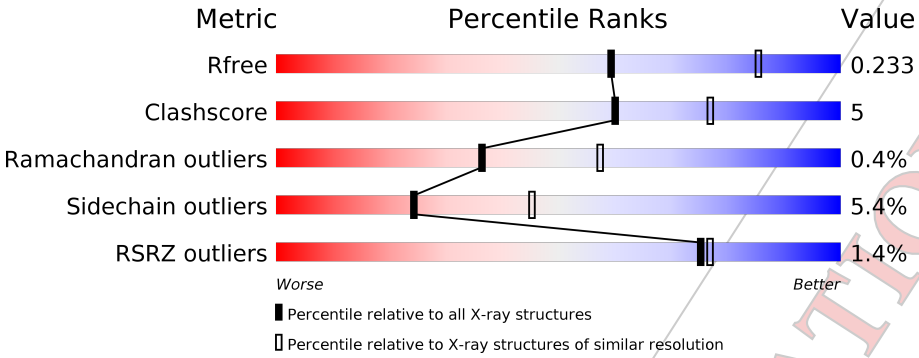
MolProbity	:	4.02b-467
Mogul	:	1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix)	:	1.13
EDS	:	rb-20031021
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20031021

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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}	111664	4155 (2.50-2.50)
Clashscore	122126	4827 (2.50-2.50)
Ramachandran outliers	120053	4735 (2.50-2.50)
Sidechain outliers	120020	4737 (2.50-2.50)
RSRZ outliers	108989	4058 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	142	82% 11%
1	B	142	87% 8%
1	C	142	3% 85% 11%
1	D	142	82% 11%
2	E	64	78% 16% 5%
2	F	64	88% 5% 6%

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Mol	Chain	Length	Quality of chain
2	G	64	2% 89% 6%
2	H	64	3% 73% 14% 5% 6%

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
4	EDO	C	202	-	-	-	X
5	PGE	D	206	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6648 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	137	Total	C	N	O	S	0	5	0
			1087	688	183	213	3			
1	B	136	Total	C	N	O	S	0	5	0
			1076	682	179	212	3			
1	C	136	Total	C	N	O	S	0	5	0
			1080	685	181	211	3			
1	D	136	Total	C	N	O	S	0	6	0
			1084	687	182	212	3			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q63NA5
A	136	LYS	VAL	conflict	UNP Q63NA5
A	137	HIS	ARG	conflict	UNP Q63NA5
A	139	HIS	-	expression tag	UNP Q63NA5
A	140	HIS	-	expression tag	UNP Q63NA5
A	141	HIS	-	expression tag	UNP Q63NA5
A	142	HIS	-	expression tag	UNP Q63NA5
B	1	MET	-	initiating methionine	UNP Q63NA5
B	136	LYS	VAL	conflict	UNP Q63NA5
B	137	HIS	ARG	conflict	UNP Q63NA5
B	139	HIS	-	expression tag	UNP Q63NA5
B	140	HIS	-	expression tag	UNP Q63NA5
B	141	HIS	-	expression tag	UNP Q63NA5
B	142	HIS	-	expression tag	UNP Q63NA5
C	1	MET	-	initiating methionine	UNP Q63NA5
C	136	LYS	VAL	conflict	UNP Q63NA5
C	137	HIS	ARG	conflict	UNP Q63NA5
C	139	HIS	-	expression tag	UNP Q63NA5
C	140	HIS	-	expression tag	UNP Q63NA5
C	141	HIS	-	expression tag	UNP Q63NA5
C	142	HIS	-	expression tag	UNP Q63NA5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MET	-	initiating methionine	UNP Q63NA5
D	136	LYS	VAL	conflict	UNP Q63NA5
D	137	HIS	ARG	conflict	UNP Q63NA5
D	139	HIS	-	expression tag	UNP Q63NA5
D	140	HIS	-	expression tag	UNP Q63NA5
D	141	HIS	-	expression tag	UNP Q63NA5
D	142	HIS	-	expression tag	UNP Q63NA5

- Molecule 2 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	61	Total	C	N	O	S	0	2	0
			492	317	93	81	1			
2	F	60	Total	C	N	O	S	0	2	0
			479	306	90	81	2			
2	G	60	Total	C	N	O	S	0	2	0
			485	312	92	80	1			
2	H	60	Total	C	N	O	S	0	4	0
			489	312	94	81	2			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	GLY	-	expression tag	UNP Q63NA6
E	-3	ILE	-	expression tag	UNP Q63NA6
E	-2	ASP	-	expression tag	UNP Q63NA6
E	-1	PRO	-	expression tag	UNP Q63NA6
E	0	PHE	-	expression tag	UNP Q63NA6
E	1	THR	-	expression tag	UNP Q63NA6
E	24	ALA	HIS	conflict	UNP Q63NA6
F	-4	GLY	-	expression tag	UNP Q63NA6
F	-3	ILE	-	expression tag	UNP Q63NA6
F	-2	ASP	-	expression tag	UNP Q63NA6
F	-1	PRO	-	expression tag	UNP Q63NA6
F	0	PHE	-	expression tag	UNP Q63NA6
F	1	THR	-	expression tag	UNP Q63NA6
F	24	ALA	HIS	conflict	UNP Q63NA6
G	-4	GLY	-	expression tag	UNP Q63NA6
G	-3	ILE	-	expression tag	UNP Q63NA6
G	-2	ASP	-	expression tag	UNP Q63NA6
G	-1	PRO	-	expression tag	UNP Q63NA6
G	0	PHE	-	expression tag	UNP Q63NA6

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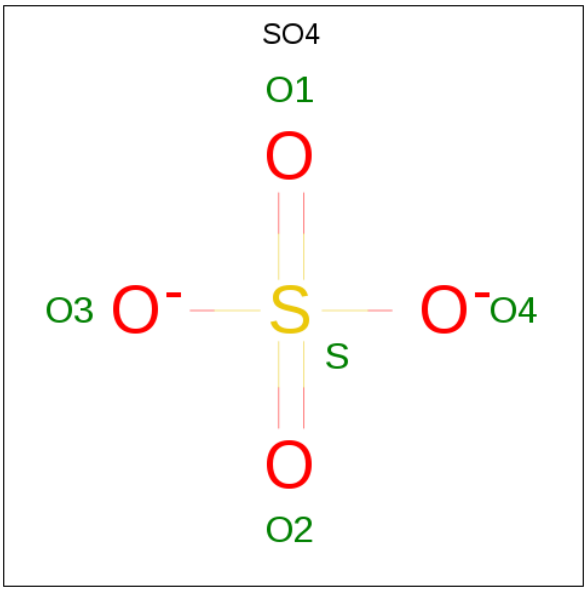
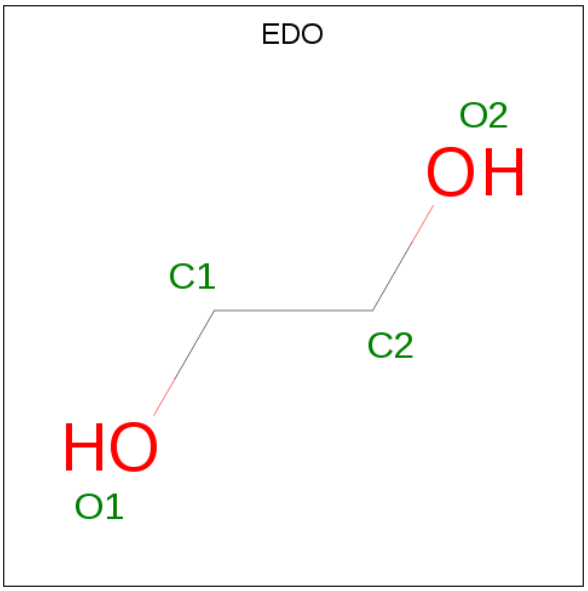
Chain	Residue	Modelled	Actual	Comment	Reference
G	1	THR	-	expression tag	UNP Q63NA6
G	24	ALA	HIS	conflict	UNP Q63NA6
H	-4	GLY	-	expression tag	UNP Q63NA6
H	-3	ILE	-	expression tag	UNP Q63NA6
H	-2	ASP	-	expression tag	UNP Q63NA6
H	-1	PRO	-	expression tag	UNP Q63NA6
H	0	PHE	-	expression tag	UNP Q63NA6
H	1	THR	-	expression tag	UNP Q63NA6
H	24	ALA	HIS	conflict	UNP Q63NA6

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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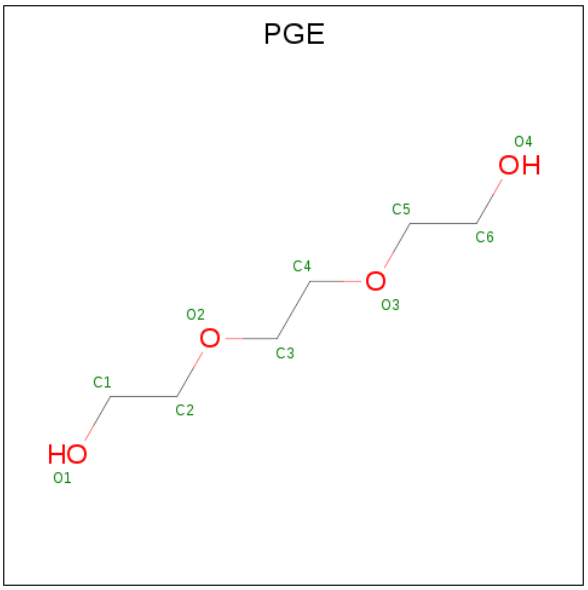
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	H	1	Total C O 4 2 2	0	0

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C O 10 6 4	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	66	Total O 66 66	0	0
6	B	44	Total O 44 44	0	0
6	C	34	Total O 34 34	0	0
6	D	53	Total O 53 53	0	0

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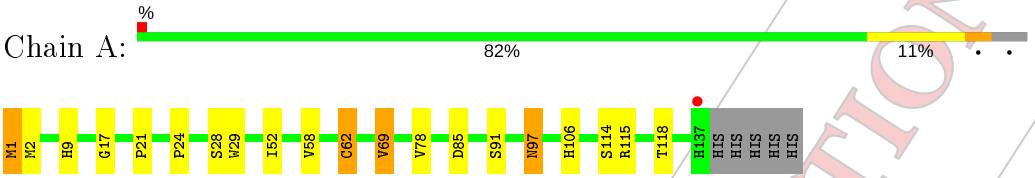
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	28	Total O 28 28	0	0
6	F	26	Total O 26 26	0	0
6	G	7	Total O 7 7	0	0
6	H	11	Total O 11 11	0	0

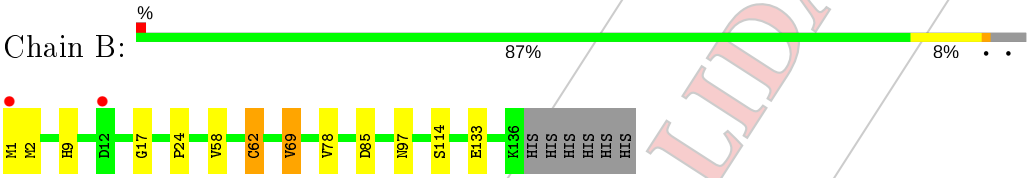
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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 geometryand 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.

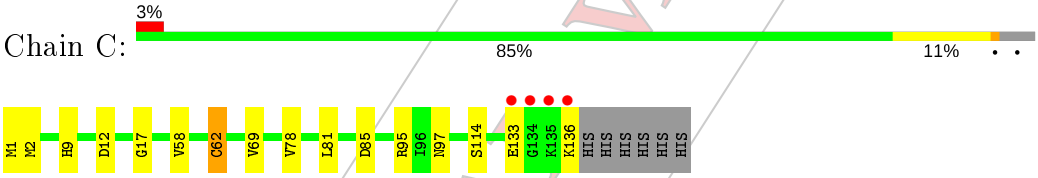
- Molecule 1: Uncharacterized protein



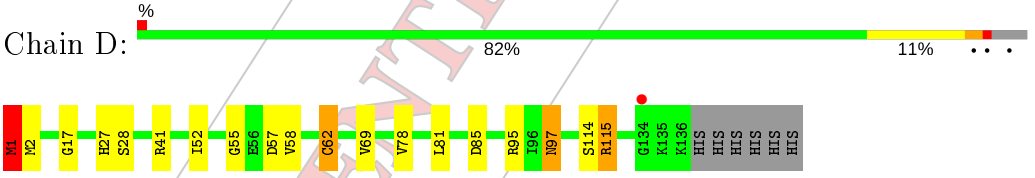
- Molecule 1: Uncharacterized protein



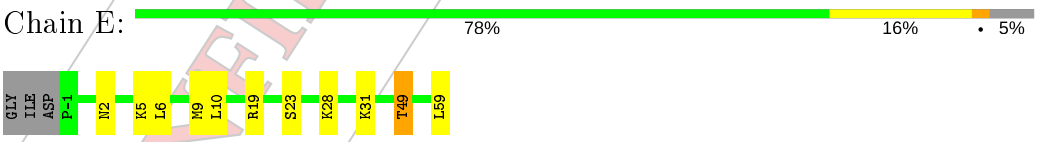
- Molecule 1: Uncharacterized protein



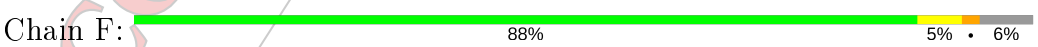
- Molecule 1: Uncharacterized protein

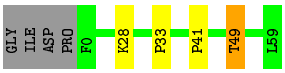


- Molecule 2: Uncharacterized protein



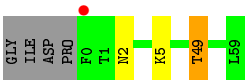
- Molecule 2: Uncharacterized protein





• Molecule 2: Uncharacterized protein

Chain G:



• Molecule 2: Uncharacterized protein

Chain H:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	85.14Å 74.19Å 85.31Å 90.00° 90.05° 90.00°	Depositor
Resolution (Å)	34.02 – 2.49 38.15 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.8 (34.02-2.49) 99.9 (38.15-2.49)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.67 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.187 , 0.233 0.188 , 0.233	Depositor DCC
R_{free} test set	1722 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å^2)	51.8	Xtriage
Anisotropy	0.320	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 41.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.005 for l,k,-h 0.034 for h,-k,-l 0.024 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6648	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.72% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PGE, SO4, EDO

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	0.66	0/1124	0.85	2/1527 (0.1%)
1	B	0.62	0/1113	0.78	0/1513
1	C	0.62	0/1118	0.79	2/1520 (0.1%)
1	D	0.67	0/1124	0.83	3/1527 (0.2%)
2	E	0.69	0/511	0.90	1/685 (0.1%)
2	F	0.67	0/493	0.89	0/661
2	G	0.63	0/503	0.84	0/674
2	H	0.70	0/512	0.99	2/686 (0.3%)
All	All	0.65	0/6498	0.84	10/8793 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	10	LEU	CB-CG-CD2	6.62	122.26	111.00
1	D	41	ARG	NE-CZ-NH2	5.73	123.16	120.30
2	H	10	LEU	CB-CG-CD1	-5.44	101.76	111.00
1	A	115[A]	ARG	CG-CD-NE	-5.41	100.45	111.80
1	A	115[B]	ARG	CG-CD-NE	-5.41	100.45	111.80
1	D	115	ARG	NE-CZ-NH1	5.34	122.97	120.30
2	E	10	LEU	CB-CG-CD2	-5.29	102.00	111.00
1	D	1	MET	CA-CB-CG	5.15	122.06	113.30
1	C	12[A]	ASP	CB-CG-OD1	5.07	122.86	118.30
1	C	12[B]	ASP	CB-CG-OD1	5.07	122.86	118.30

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	1087	0	1078	19	0
1	B	1076	0	1065	11	0
1	C	1080	0	1067	11	0
1	D	1084	0	1078	16	0
2	E	492	0	534	9	0
2	F	479	0	515	5	0
2	G	485	0	527	4	0
2	H	489	0	534	10	0
3	A	10	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	A	28	0	42	5	0
4	B	16	0	24	2	0
4	C	8	0	12	0	0
4	D	16	0	24	1	0
4	H	4	0	6	0	0
5	D	10	0	14	8	0
6	A	66	0	0	1	0
6	B	44	0	0	0	0
6	C	34	0	0	1	0
6	D	53	0	0	0	0
6	E	28	0	0	0	0
6	F	26	0	0	1	0
6	G	7	0	0	0	0
6	H	11	0	0	0	0
All	All	6648	0	6520	65	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 5.

All (65) 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)
2:H:23:SER:HB2	2:H:41:PRO:HD2	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1:MET:HA	1:D:62:CYS:SG	2.12	0.89
1:B:17:GLY:HA3	2:E:49:THR:HG21	1.68	0.75
1:C:17:GLY:HA3	2:G:49:THR:HG21	1.72	0.71
2:H:23:SER:HB2	2:H:41:PRO:CD	2.19	0.71
1:A:17:GLY:HA3	2:F:49:THR:HG21	1.71	0.70
1:A:1:MET:HA	1:A:62:CYS:SG	2.34	0.67
1:B:1:MET:HA	1:B:62:CYS:SG	2.34	0.67
1:C:1:MET:HA	1:C:62:CYS:SG	2.34	0.67
1:D:17:GLY:HA3	2:H:49:THR:HG21	1.79	0.65
2:H:40:HIS:O	2:H:41:PRO:C	2.36	0.62
1:D:27:HIS:HE1	2:H:52:SER:OG	1.85	0.59
1:A:69:VAL:HG11	1:C:81:LEU:HD12	1.86	0.58
1:D:55:GLY:HA2	5:D:206:PGE:H12	1.88	0.56
1:C:136:LYS:HG2	6:C:334:HOH:O	2.06	0.56
2:E:9:MET:CE	2:E:59:LEU:HD13	2.36	0.55
1:D:52:ILE:HA	5:D:206:PGE:H1	1.89	0.55
1:B:24:PRO:HA	4:B:204:EDO:H22	1.90	0.54
1:A:52:ILE:HG22	4:A:204:EDO:H11	1.90	0.53
1:A:17:GLY:CA	2:F:49:THR:HG21	2.39	0.53
1:B:17:GLY:CA	2:E:49:THR:HG21	2.37	0.52
1:A:28:SER:OG	4:A:203:EDO:H12	2.10	0.52
1:A:1:MET:CA	1:A:62:CYS:SG	2.98	0.52
2:H:1:THR:HG21	2:H:42:LYS:C	2.30	0.52
1:A:91:SER:H	4:A:204:EDO:H12	1.74	0.51
1:A:106:HIS:HD2	5:D:206:PGE:H32	1.76	0.51
1:C:9:HIS:HB2	2:G:49:THR:HG22	1.92	0.51
2:E:2:ASN:HB3	2:E:5:LYS:HG3	1.93	0.50
1:B:1:MET:CA	1:B:62:CYS:SG	3.00	0.49
1:B:9:HIS:HB2	2:E:49:THR:HG22	1.94	0.49
1:C:1:MET:CA	1:C:62:CYS:SG	2.99	0.49
1:A:118:THR:HA	6:A:322:HOH:O	2.13	0.49
1:D:57:ASP:HB3	5:D:206:PGE:H6	1.95	0.49
1:A:24:PRO:HA	4:A:206:EDO:H22	1.95	0.48
2:E:9:MET:HE3	2:E:59:LEU:HD13	1.94	0.48
1:C:17:GLY:CA	2:G:49:THR:HG21	2.42	0.48
1:A:97:ASN:ND2	1:D:97:ASN:OD1	2.47	0.48
2:H:11:GLU:O	2:H:16[B]:ARG:NH2	2.47	0.47
1:B:1:MET:N	1:B:62:CYS:SG	2.86	0.47
1:B:97:ASN:HD21	1:C:97:ASN:HD21	1.62	0.47
1:C:1:MET:N	1:C:62:CYS:SG	2.87	0.47
1:D:52:ILE:HG22	4:D:202:EDO:H22	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2:ASN:HB3	2:G:5[B]:LYS:HD2	1.98	0.46
1:A:1:MET:N	1:A:62:CYS:SG	2.85	0.45
1:D:57:ASP:CB	5:D:206:PGE:H6	2.46	0.45
1:D:52:ILE:HA	5:D:206:PGE:C1	2.46	0.45
2:F:33:PRO:HD2	6:F:107:HOH:O	2.17	0.45
1:D:2:MET:HG2	1:D:85:ASP:HA	1.99	0.44
2:H:1:THR:HG21	2:H:42:LYS:O	2.18	0.44
1:D:57:ASP:CA	5:D:206:PGE:H6	2.49	0.43
1:D:17:GLY:CA	2:H:49:THR:HG21	2.46	0.43
1:B:69:VAL:HG11	1:D:81:LEU:HD12	2.01	0.43
1:D:28:SER:HA	2:H:39:PRO:HB3	2.01	0.43
1:A:9:HIS:HB2	2:F:49:THR:HG22	2.02	0.42
4:B:203:EDO:H12	2:E:23:SER:H	1.84	0.42
1:A:106:HIS:HB2	5:D:206:PGE:H42	2.01	0.42
1:C:2:MET:HG2	1:C:85:ASP:HA	2.02	0.41
2:E:9:MET:HE2	2:E:59:LEU:HD13	2.02	0.41
1:A:21:PRO:HA	4:A:206:EDO:H21	2.03	0.41
1:A:2:MET:HG2	1:A:85:ASP:HA	2.03	0.40
2:E:6:LEU:HD12	2:E:9:MET:HE1	2.03	0.40
1:A:29:TRP:CD2	2:F:41:PRO:HB3	2.56	0.40
1:B:2:MET:HG2	1:B:85:ASP:HA	2.03	0.40
1:B:78:VAL:HG21	1:D:78:VAL:HG21	2.04	0.40
1:A:78:VAL:HG21	1:C:78:VAL:HG21	2.04	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	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
1	B	139/142 (98%)	137 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	139/142 (98%)	136 (98%)	3 (2%)	0	100	100
1	D	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
2	E	61/64 (95%)	60 (98%)	1 (2%)	0	100	100
2	F	60/64 (94%)	60 (100%)	0	0	100	100
2	G	60/64 (94%)	60 (100%)	0	0	100	100
2	H	62/64 (97%)	59 (95%)	0	3 (5%)	2	3
All	All	801/824 (97%)	786 (98%)	12 (2%)	3 (0%)	36	57

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	42	LYS
2	H	41	PRO
2	H	40	HIS

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	120/120 (100%)	113 (94%)	7 (6%)	22	41
1	B	119/120 (99%)	113 (95%)	6 (5%)	27	49
1	C	119/120 (99%)	113 (95%)	6 (5%)	27	49
1	D	120/120 (100%)	110 (92%)	10 (8%)	12	23
2	E	56/56 (100%)	51 (91%)	5 (9%)	11	21
2	F	54/56 (96%)	52 (96%)	2 (4%)	37	64
2	G	55/56 (98%)	54 (98%)	1 (2%)	62	84
2	H	56/56 (100%)	50 (89%)	6 (11%)	7	14
All	All	699/704 (99%)	656 (94%)	43 (6%)	24	38

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	58	VAL
1	A	62	CYS
1	A	69	VAL
1	A	97	ASN
1	A	114[A]	SER
1	A	114[B]	SER
1	B	58	VAL
1	B	62	CYS
1	B	69	VAL
1	B	114[A]	SER
1	B	114[B]	SER
1	B	133	GLU
1	C	58	VAL
1	C	62	CYS
1	C	69	VAL
1	C	95	ARG
1	C	114	SER
1	C	133	GLU
1	D	1	MET
1	D	58	VAL
1	D	62	CYS
1	D	69	VAL
1	D	95[A]	ARG
1	D	95[B]	ARG
1	D	97	ASN
1	D	114[A]	SER
1	D	114[B]	SER
1	D	115	ARG
2	E	19	ARG
2	E	28	LYS
2	E	31[A]	LYS
2	E	31[B]	LYS
2	E	49	THR
2	F	28	LYS
2	F	49	THR
2	G	49	THR
2	H	9[A]	MET
2	H	9[B]	MET
2	H	19[A]	ARG
2	H	19[B]	ARG
2	H	41	PRO
2	H	49	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	HIS
1	C	97	ASN
1	D	27	HIS
2	H	40	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

24 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	$\#\|Z\| > 2$
3	SO4	A	201	-	4,4,4	0.31	0	6,6,6	0.78	0
3	SO4	A	202	-	4,4,4	0.43	0	6,6,6	1.26	1 (16%)
4	EDO	A	203	-	3,3,3	0.79	0	2,2,2	0.92	0
4	EDO	A	204	-	3,3,3	0.51	0	2,2,2	0.66	0
4	EDO	A	205	-	3,3,3	0.66	0	2,2,2	0.24	0
4	EDO	A	206	-	3,3,3	0.44	0	2,2,2	0.40	0
4	EDO	A	207	-	3,3,3	0.61	0	2,2,2	1.06	0
4	EDO	A	208	-	3,3,3	0.55	0	2,2,2	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	EDO	A	209	-	3,3,3	0.71	0	2,2,2	0.43	0
3	SO4	B	201	-	4,4,4	0.38	0	6,6,6	0.69	0
4	EDO	B	202	-	3,3,3	0.34	0	2,2,2	0.97	0
4	EDO	B	203	-	3,3,3	0.63	0	2,2,2	0.83	0
4	EDO	B	204	-	3,3,3	0.42	0	2,2,2	0.68	0
4	EDO	B	205	-	3,3,3	0.69	0	2,2,2	0.28	0
3	SO4	C	201	-	4,4,4	0.44	0	6,6,6	0.52	0
4	EDO	C	202	-	3,3,3	0.93	0	2,2,2	0.11	0
4	EDO	C	203	-	3,3,3	0.43	0	2,2,2	0.77	0
3	SO4	D	201	-	4,4,4	0.12	0	6,6,6	1.02	0
4	EDO	D	202	-	3,3,3	0.44	0	2,2,2	0.68	0
4	EDO	D	203	-	3,3,3	0.60	0	2,2,2	0.35	0
4	EDO	D	204	-	3,3,3	0.48	0	2,2,2	0.62	0
4	EDO	D	205	-	3,3,3	0.60	0	2,2,2	0.25	0
5	PGE	D	206	-	9,9,9	0.52	0	8,8,8	0.38	0
4	EDO	H	101	-	3,3,3	0.55	0	2,2,2	0.50	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
3	SO4	A	201	-	-	0/0/0/0	0/0/0/0
3	SO4	A	202	-	-	0/0/0/0	0/0/0/0
4	EDO	A	203	-	-	0/1/1/1	0/0/0/0
4	EDO	A	204	-	-	0/1/1/1	0/0/0/0
4	EDO	A	205	-	-	0/1/1/1	0/0/0/0
4	EDO	A	206	-	-	0/1/1/1	0/0/0/0
4	EDO	A	207	-	-	0/1/1/1	0/0/0/0
4	EDO	A	208	-	-	0/1/1/1	0/0/0/0
4	EDO	A	209	-	-	0/1/1/1	0/0/0/0
3	SO4	B	201	-	-	0/0/0/0	0/0/0/0
4	EDO	B	202	-	-	0/1/1/1	0/0/0/0
4	EDO	B	203	-	-	0/1/1/1	0/0/0/0
4	EDO	B	204	-	-	0/1/1/1	0/0/0/0
4	EDO	B	205	-	-	0/1/1/1	0/0/0/0
3	SO4	C	201	-	-	0/0/0/0	0/0/0/0
4	EDO	C	202	-	-	0/1/1/1	0/0/0/0
4	EDO	C	203	-	-	0/1/1/1	0/0/0/0
3	SO4	D	201	-	-	0/0/0/0	0/0/0/0
4	EDO	D	202	-	-	0/1/1/1	0/0/0/0
4	EDO	D	203	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	D	204	-	-	0/1/1/1	0/0/0/0
4	EDO	D	205	-	-	0/1/1/1	0/0/0/0
5	PGE	D	206	-	-	0/7/7/7	0/0/0/0
4	EDO	H	101	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	202	SO4	O3-S-O1	-2.12	97.78	109.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	203	EDO	1	0
4	A	204	EDO	2	0
4	A	206	EDO	2	0
4	B	203	EDO	1	0
4	B	204	EDO	1	0
4	D	202	EDO	1	0
5	D	206	PGE	8	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	137/142 (96%)	-0.17	1 (0%)	87	88	30, 43, 78, 157	0
1	B	136/142 (95%)	-0.12	2 (1%)	73	75	33, 55, 96, 129	0
1	C	136/142 (95%)	-0.05	4 (2%)	51	55	39, 57, 95, 142	0
1	D	136/142 (95%)	-0.13	1 (0%)	87	88	34, 46, 78, 124	0
2	E	61/64 (95%)	-0.18	0	100	100	34, 46, 66, 116	0
2	F	60/64 (93%)	-0.01	0	100	100	27, 41, 65, 105	0
2	G	60/64 (93%)	0.07	1 (1%)	70	72	47, 68, 102, 133	0
2	H	60/64 (93%)	-0.07	2 (3%)	46	50	38, 59, 95, 122	0
All	All	786/824 (95%)	-0.10	11 (1%)	75	77	27, 51, 93, 157	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	134	GLY	4.9
1	C	133	GLU	3.9
2	G	0	PHE	3.6
1	D	134	GLY	3.5
1	A	137	HIS	3.1
1	C	136	LYS	3.0
1	C	135	LYS	3.0
2	H	0	PHE	2.7
1	B	1	MET	2.6
2	H	41	PRO	2.5
1	B	12[A]	ASP	2.2

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 (i)

There are no carbohydrates 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, 95^{th} 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(Å^2)	Q<0.9
4	EDO	D	205	4/4	0.71	0.30	83,88,105,118	0
4	EDO	B	203	4/4	0.74	0.30	65,68,76,111	0
4	EDO	C	202	4/4	0.78	0.41	64,66,78,92	0
4	EDO	D	204	4/4	0.80	0.45	74,82,84,90	0
4	EDO	B	205	4/4	0.80	0.26	72,73,99,130	0
4	EDO	C	203	4/4	0.81	0.23	74,86,87,93	0
4	EDO	A	209	4/4	0.83	0.25	47,56,67,77	0
5	PGE	D	206	10/10	0.84	0.33	41,55,64,76	10
4	EDO	A	208	4/4	0.86	0.21	59,74,77,85	0
4	EDO	A	207	4/4	0.86	0.23	54,64,71,81	0
4	EDO	A	205	4/4	0.86	0.21	62,69,79,101	0
4	EDO	D	202	4/4	0.87	0.26	69,70,86,89	0
4	EDO	B	202	4/4	0.88	0.17	63,81,82,89	0
4	EDO	D	203	4/4	0.88	0.16	88,92,94,98	0
4	EDO	H	101	4/4	0.90	0.28	69,78,80,88	0
4	EDO	A	204	4/4	0.92	0.19	67,68,78,97	0
4	EDO	A	203	4/4	0.92	0.34	43,65,79,107	0
4	EDO	A	206	4/4	0.95	0.22	37,44,69,84	0
3	SO4	B	201	5/5	0.97	0.12	70,72,83,85	0
4	EDO	B	204	4/4	0.97	0.46	46,49,75,92	0
3	SO4	A	201	5/5	0.97	0.16	39,44,47,58	0
3	SO4	C	201	5/5	0.98	0.12	65,67,76,79	0
3	SO4	D	201	5/5	0.99	0.10	43,45,54,58	0
3	SO4	A	202	5/5	1.00	0.12	28,36,41,42	0

6.5 Other polymers (i)

There are no such residues in this entry.