



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 25, 2024 – 12:09 PM EDT

PDB ID : 5XF2
Title : Crystal structure of SeMet-HldC from Burkholderia pseudomallei
Authors : Park, J.; Kim, H.; Kim, S.; Lee, D.; Shin, D.H.
Deposited on : 2017-04-07
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.37.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

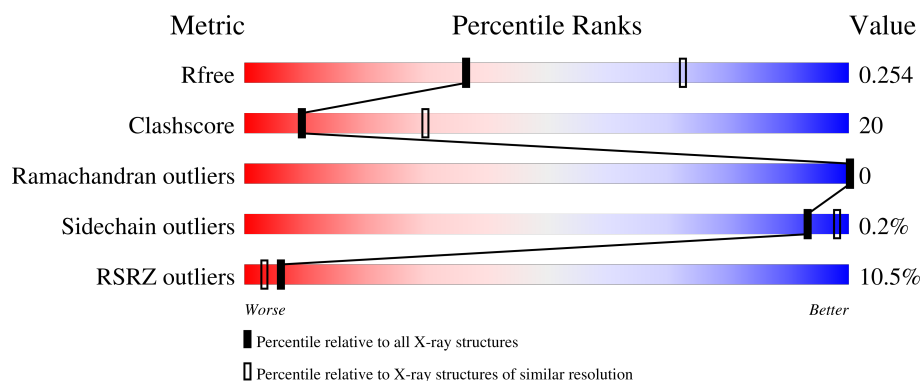
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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.



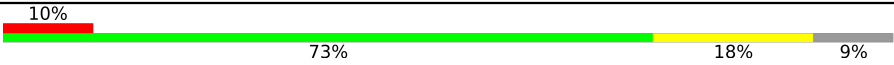


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	173	<div> <div>6%</div> <div> <div></div> <div>66%</div> <div>16%</div> <div>18%</div> </div> </div>
1	B	173	<div> <div>8%</div> <div> <div></div> <div>72%</div> <div>19%</div> <div>9%</div> </div> </div>
1	C	173	<div> <div>12%</div> <div> <div></div> <div>65%</div> <div>27%</div> <div>9%</div> </div> </div>
1	D	173	<div> <div>10%</div> <div> <div></div> <div>73%</div> <div>18%</div> <div>9%</div> </div> </div>
1	E	173	<div> <div>6%</div> <div> <div></div> <div>66%</div> <div>16%</div> <div>17%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	173	
1	G	173	
1	H	173	

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
2	EPE	B	201	-	-	X	-
2	EPE	D	201	-	-	X	-
2	EPE	F	201	-	-	X	-
2	EPE	H	201	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9419 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 Putative cytidylyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	142	Total	C	N	O	S	Se	0	0	0
			1069	679	186	198	2	4			
1	B	158	Total	C	N	O	S	Se	0	0	0
			1195	755	213	221	2	4			
1	C	158	Total	C	N	O	S	Se	0	0	0
			1195	755	213	221	2	4			
1	D	158	Total	C	N	O	S	Se	0	0	0
			1195	755	213	221	2	4			
1	E	143	Total	C	N	O	S	Se	0	0	0
			1079	685	189	199	2	4			
1	F	158	Total	C	N	O	S	Se	0	0	0
			1195	755	213	221	2	4			
1	G	158	Total	C	N	O	S	Se	0	0	0
			1195	755	213	221	2	4			
1	H	158	Total	C	N	O	S	Se	0	0	0
			1195	755	213	221	2	4			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MSE	-	expression tag	UNP Q63XZ4
A	-10	HIS	-	expression tag	UNP Q63XZ4
A	-9	HIS	-	expression tag	UNP Q63XZ4
A	-8	HIS	-	expression tag	UNP Q63XZ4
A	-7	HIS	-	expression tag	UNP Q63XZ4
A	-6	HIS	-	expression tag	UNP Q63XZ4
A	-5	HIS	-	expression tag	UNP Q63XZ4
A	-4	GLY	-	expression tag	UNP Q63XZ4
A	-3	GLY	-	expression tag	UNP Q63XZ4
A	-2	GLY	-	expression tag	UNP Q63XZ4
A	-1	GLY	-	expression tag	UNP Q63XZ4
A	0	GLY	-	expression tag	UNP Q63XZ4
B	-11	MSE	-	expression tag	UNP Q63XZ4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	HIS	-	expression tag	UNP Q63XZ4
B	-9	HIS	-	expression tag	UNP Q63XZ4
B	-8	HIS	-	expression tag	UNP Q63XZ4
B	-7	HIS	-	expression tag	UNP Q63XZ4
B	-6	HIS	-	expression tag	UNP Q63XZ4
B	-5	HIS	-	expression tag	UNP Q63XZ4
B	-4	GLY	-	expression tag	UNP Q63XZ4
B	-3	GLY	-	expression tag	UNP Q63XZ4
B	-2	GLY	-	expression tag	UNP Q63XZ4
B	-1	GLY	-	expression tag	UNP Q63XZ4
B	0	GLY	-	expression tag	UNP Q63XZ4
C	-11	MSE	-	expression tag	UNP Q63XZ4
C	-10	HIS	-	expression tag	UNP Q63XZ4
C	-9	HIS	-	expression tag	UNP Q63XZ4
C	-8	HIS	-	expression tag	UNP Q63XZ4
C	-7	HIS	-	expression tag	UNP Q63XZ4
C	-6	HIS	-	expression tag	UNP Q63XZ4
C	-5	HIS	-	expression tag	UNP Q63XZ4
C	-4	GLY	-	expression tag	UNP Q63XZ4
C	-3	GLY	-	expression tag	UNP Q63XZ4
C	-2	GLY	-	expression tag	UNP Q63XZ4
C	-1	GLY	-	expression tag	UNP Q63XZ4
C	0	GLY	-	expression tag	UNP Q63XZ4
D	-11	MSE	-	expression tag	UNP Q63XZ4
D	-10	HIS	-	expression tag	UNP Q63XZ4
D	-9	HIS	-	expression tag	UNP Q63XZ4
D	-8	HIS	-	expression tag	UNP Q63XZ4
D	-7	HIS	-	expression tag	UNP Q63XZ4
D	-6	HIS	-	expression tag	UNP Q63XZ4
D	-5	HIS	-	expression tag	UNP Q63XZ4
D	-4	GLY	-	expression tag	UNP Q63XZ4
D	-3	GLY	-	expression tag	UNP Q63XZ4
D	-2	GLY	-	expression tag	UNP Q63XZ4
D	-1	GLY	-	expression tag	UNP Q63XZ4
D	0	GLY	-	expression tag	UNP Q63XZ4
E	-11	MSE	-	expression tag	UNP Q63XZ4
E	-10	HIS	-	expression tag	UNP Q63XZ4
E	-9	HIS	-	expression tag	UNP Q63XZ4
E	-8	HIS	-	expression tag	UNP Q63XZ4
E	-7	HIS	-	expression tag	UNP Q63XZ4
E	-6	HIS	-	expression tag	UNP Q63XZ4
E	-5	HIS	-	expression tag	UNP Q63XZ4

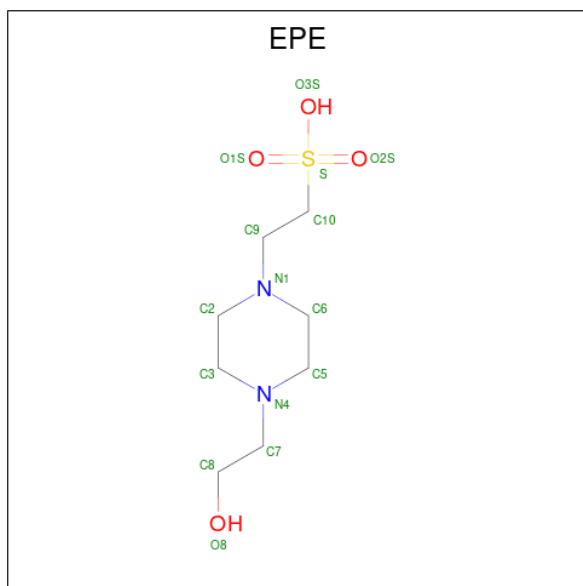
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Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	GLY	-	expression tag	UNP Q63XZ4
E	-3	GLY	-	expression tag	UNP Q63XZ4
E	-2	GLY	-	expression tag	UNP Q63XZ4
E	-1	GLY	-	expression tag	UNP Q63XZ4
E	0	GLY	-	expression tag	UNP Q63XZ4
F	-11	MSE	-	expression tag	UNP Q63XZ4
F	-10	HIS	-	expression tag	UNP Q63XZ4
F	-9	HIS	-	expression tag	UNP Q63XZ4
F	-8	HIS	-	expression tag	UNP Q63XZ4
F	-7	HIS	-	expression tag	UNP Q63XZ4
F	-6	HIS	-	expression tag	UNP Q63XZ4
F	-5	HIS	-	expression tag	UNP Q63XZ4
F	-4	GLY	-	expression tag	UNP Q63XZ4
F	-3	GLY	-	expression tag	UNP Q63XZ4
F	-2	GLY	-	expression tag	UNP Q63XZ4
F	-1	GLY	-	expression tag	UNP Q63XZ4
F	0	GLY	-	expression tag	UNP Q63XZ4
G	-11	MSE	-	expression tag	UNP Q63XZ4
G	-10	HIS	-	expression tag	UNP Q63XZ4
G	-9	HIS	-	expression tag	UNP Q63XZ4
G	-8	HIS	-	expression tag	UNP Q63XZ4
G	-7	HIS	-	expression tag	UNP Q63XZ4
G	-6	HIS	-	expression tag	UNP Q63XZ4
G	-5	HIS	-	expression tag	UNP Q63XZ4
G	-4	GLY	-	expression tag	UNP Q63XZ4
G	-3	GLY	-	expression tag	UNP Q63XZ4
G	-2	GLY	-	expression tag	UNP Q63XZ4
G	-1	GLY	-	expression tag	UNP Q63XZ4
G	0	GLY	-	expression tag	UNP Q63XZ4
H	-11	MSE	-	expression tag	UNP Q63XZ4
H	-10	HIS	-	expression tag	UNP Q63XZ4
H	-9	HIS	-	expression tag	UNP Q63XZ4
H	-8	HIS	-	expression tag	UNP Q63XZ4
H	-7	HIS	-	expression tag	UNP Q63XZ4
H	-6	HIS	-	expression tag	UNP Q63XZ4
H	-5	HIS	-	expression tag	UNP Q63XZ4
H	-4	GLY	-	expression tag	UNP Q63XZ4
H	-3	GLY	-	expression tag	UNP Q63XZ4
H	-2	GLY	-	expression tag	UNP Q63XZ4
H	-1	GLY	-	expression tag	UNP Q63XZ4
H	0	GLY	-	expression tag	UNP Q63XZ4

- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID

(three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	F	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	H	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	O	0	0
			3	3		
3	B	3	Total	O	0	0
			3	3		
3	C	6	Total	O	0	0
			6	6		
3	D	6	Total	O	0	0
			6	6		
3	E	8	Total	O	0	0
			8	8		
3	F	5	Total	O	0	0
			5	5		
3	G	6	Total	O	0	0
			6	6		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	4	Total	O	0	0
			4	4		

- Molecule 1: Putative cytidyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	73.95Å 73.95Å 74.88Å 108.38° 108.38° 108.02°	Depositor
Resolution (Å)	31.27 – 2.80 34.64 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.8 (31.27-2.80) 96.8 (34.64-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.70 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.243 , 0.252 0.245 , 0.254	Depositor DCC
R_{free} test set	1382 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å ²)	30.6	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 0.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.005 for k,l,h 0.005 for l,h,k 0.427 for -k,-h,-l 0.009 for -l,-k,-h 0.008 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	9419	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.13% 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: EPE

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	0.52	0/1085	0.67	0/1467
1	B	0.45	0/1212	0.64	0/1637
1	C	0.46	0/1212	0.65	0/1637
1	D	0.40	0/1212	0.60	0/1637
1	E	0.51	0/1096	0.67	0/1482
1	F	0.45	0/1212	0.69	0/1637
1	G	0.44	0/1212	0.60	0/1637
1	H	0.40	0/1212	0.61	0/1637
All	All	0.45	0/9453	0.64	0/12771

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	1069	0	1075	35	0
1	B	1195	0	1211	61	0
1	C	1195	0	1211	62	0
1	D	1195	0	1211	40	0
1	E	1079	0	1082	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1195	0	1211	50	0
1	G	1195	0	1211	73	0
1	H	1195	0	1211	48	0
2	B	15	0	18	13	0
2	D	15	0	18	12	0
2	F	15	0	18	16	0
2	H	15	0	18	13	0
3	A	3	0	0	0	0
3	B	3	0	0	1	0
3	C	6	0	0	0	0
3	D	6	0	0	0	0
3	E	8	0	0	0	0
3	F	5	0	0	0	0
3	G	6	0	0	0	0
3	H	4	0	0	0	0
All	All	9419	0	9495	370	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 20.

The worst 5 of 370 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:B:116:LYS:CG	2:B:201:EPE:H82	1.53	1.37
1:B:116:LYS:HG2	2:B:201:EPE:C8	1.67	1.23
1:F:150:THR:HG22	1:F:154:LYS:HE3	1.27	1.16
1:E:66:MSE:SE	1:E:100:LYS:HB2	1.98	1.14
1:G:73:ARG:HB2	1:G:74:PRO:HD2	1.30	1.12

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	140/173 (81%)	138 (99%)	2 (1%)	0	100	100
1	B	156/173 (90%)	153 (98%)	3 (2%)	0	100	100
1	C	156/173 (90%)	155 (99%)	1 (1%)	0	100	100
1	D	156/173 (90%)	153 (98%)	3 (2%)	0	100	100
1	E	141/173 (82%)	139 (99%)	2 (1%)	0	100	100
1	F	156/173 (90%)	153 (98%)	3 (2%)	0	100	100
1	G	156/173 (90%)	155 (99%)	1 (1%)	0	100	100
1	H	156/173 (90%)	153 (98%)	3 (2%)	0	100	100
All	All	1217/1384 (88%)	1199 (98%)	18 (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	111/129 (86%)	110 (99%)	1 (1%)	78	94
1	B	125/129 (97%)	125 (100%)	0	100	100
1	C	125/129 (97%)	125 (100%)	0	100	100
1	D	125/129 (97%)	125 (100%)	0	100	100
1	E	112/129 (87%)	111 (99%)	1 (1%)	78	94
1	F	125/129 (97%)	125 (100%)	0	100	100
1	G	125/129 (97%)	125 (100%)	0	100	100
1	H	125/129 (97%)	125 (100%)	0	100	100
All	All	973/1032 (94%)	971 (100%)	2 (0%)	93	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	TYR
1	E	43	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	159	GLN
1	D	159	GLN
1	G	145	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	EPE	F	201	-	15,15,15	1.66	3 (20%)	18,20,20	1.82	4 (22%)
2	EPE	D	201	-	15,15,15	1.66	3 (20%)	18,20,20	2.08	8 (44%)
2	EPE	H	201	-	15,15,15	1.64	4 (26%)	18,20,20	1.88	4 (22%)
2	EPE	B	201	-	15,15,15	1.64	4 (26%)	18,20,20	1.85	4 (22%)

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
2	EPE	F	201	-	-	5/9/19/19	0/1/1/1
2	EPE	D	201	-	-	2/9/19/19	0/1/1/1
2	EPE	H	201	-	-	6/9/19/19	0/1/1/1
2	EPE	B	201	-	-	4/9/19/19	0/1/1/1

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	201	EPE	O1S-S	3.48	1.55	1.45
2	F	201	EPE	O1S-S	3.48	1.55	1.45
2	B	201	EPE	O1S-S	3.46	1.55	1.45
2	H	201	EPE	O2S-S	3.37	1.55	1.45
2	F	201	EPE	O2S-S	3.36	1.54	1.45

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	201	EPE	O3S-S-O2S	-4.20	101.01	111.27
2	B	201	EPE	O3S-S-O1S	-4.17	101.08	111.27
2	H	201	EPE	O2S-S-C10	3.80	111.49	106.92
2	D	201	EPE	O2S-S-C10	3.79	111.48	106.92
2	F	201	EPE	O2S-S-C10	3.76	111.44	106.92

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	201	EPE	C9-C10-S-O1S
2	B	201	EPE	C9-C10-S-O3S
2	F	201	EPE	S-C10-C9-N1
2	F	201	EPE	C9-C10-S-O1S
2	F	201	EPE	C9-C10-S-O2S

There are no ring outliers.

4 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	201	EPE	16	0
2	D	201	EPE	12	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	201	EPE	13	0
2	B	201	EPE	13	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	138/173 (79%)	0.39	10 (7%) 15 8	4, 15, 63, 100	0
1	B	154/173 (89%)	0.43	14 (9%) 9 5	3, 15, 66, 112	0
1	C	154/173 (89%)	0.80	21 (13%) 3 1	5, 20, 84, 116	0
1	D	154/173 (89%)	0.58	18 (11%) 4 2	7, 21, 67, 103	0
1	E	139/173 (80%)	0.44	10 (7%) 15 8	4, 16, 71, 99	0
1	F	154/173 (89%)	0.66	18 (11%) 4 2	3, 14, 70, 115	0
1	G	154/173 (89%)	0.93	22 (14%) 2 1	5, 20, 77, 102	0
1	H	154/173 (89%)	0.55	13 (8%) 11 5	7, 23, 68, 101	0
All	All	1201/1384 (86%)	0.60	126 (10%) 6 3	3, 18, 72, 116	0

The worst 5 of 126 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	70	GLY	17.9
1	G	68	GLY	15.7
1	C	146	ASP	10.4
1	C	71	ASP	10.3
1	D	69	LYS	9.2

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	EPE	B	201	15/15	0.82	0.29	17,23,33,35	0
2	EPE	F	201	15/15	0.84	0.34	16,30,56,60	0
2	EPE	D	201	15/15	0.90	0.23	19,30,38,42	0
2	EPE	H	201	15/15	0.93	0.22	23,28,35,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.