



# Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 10:46 pm BST

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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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 : 2.11  
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) : 2.11

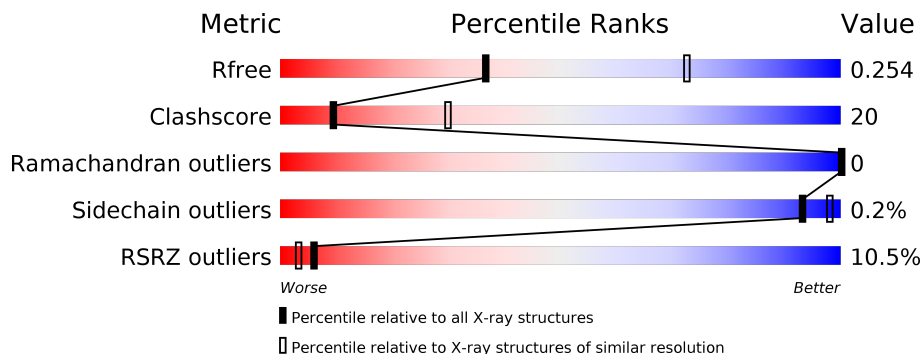
# 1 Overall quality at a glance

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	 6% 66% 16% 18%
1	B	173	 8% 72% 19% 9%
1	C	173	 12% 65% 27% 9%
1	D	173	 10% 73% 18% 9%
1	E	173	 6% 66% 16% 17%
1	F	173	 10% 73% 18% 9%

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Mol	Chain	Length	Quality of chain
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
			Total	C	N	O	S	Se			
1	A	142	1069	679	186	198	2	4	0	0	0
1	B	158	1195	755	213	221	2	4	0	0	0
1	C	158	1195	755	213	221	2	4	0	0	0
1	D	158	1195	755	213	221	2	4	0	0	0
1	E	143	1079	685	189	199	2	4	0	0	0
1	F	158	1195	755	213	221	2	4	0	0	0
1	G	158	1195	755	213	221	2	4	0	0	0
1	H	158	1195	755	213	221	2	4	0	0	0

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

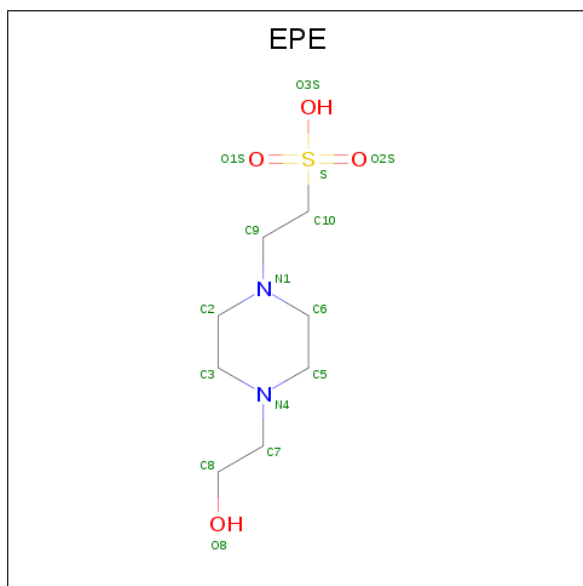
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Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	GLY	-	expression tag	UNP Q63XZ4
E	-3	GLY	-	expression tag	UNP Q63XZ4
E	-2	GLY	-	expression tag	UNP Q63XZ4
E	-1	GLY	-	expression tag	UNP Q63XZ4
E	0	GLY	-	expression tag	UNP Q63XZ4
F	-11	MSE	-	expression 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: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



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

- Molecule 3 is water.

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

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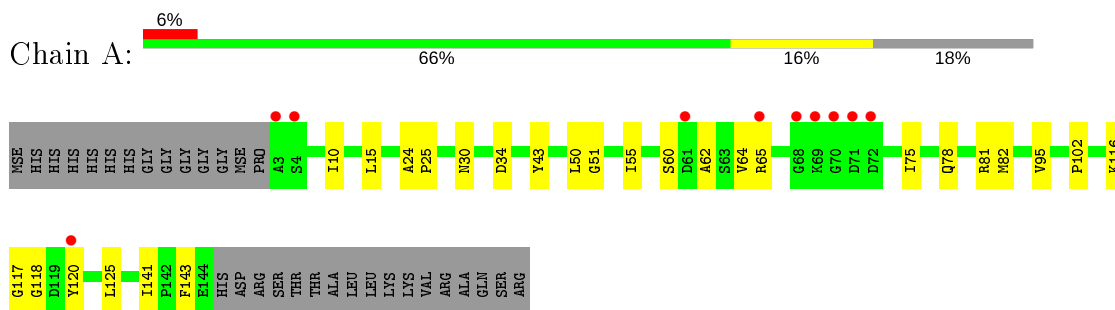
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	H	4	Total	O	0	0
			4	4		



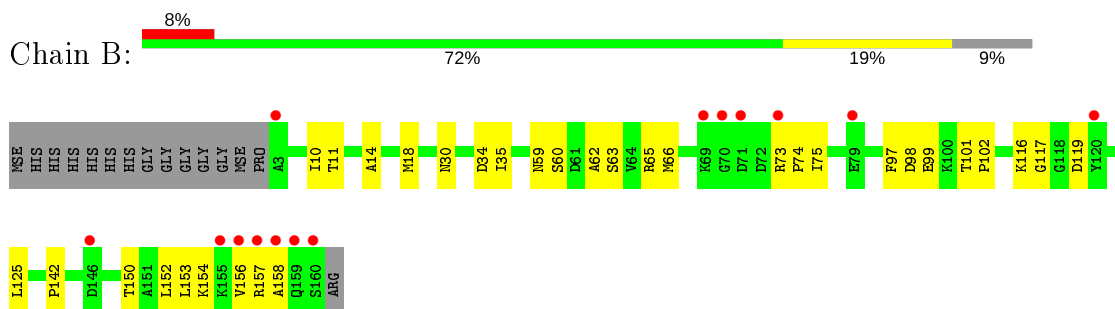
### 3 Residue-property plots [i](#)

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 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.

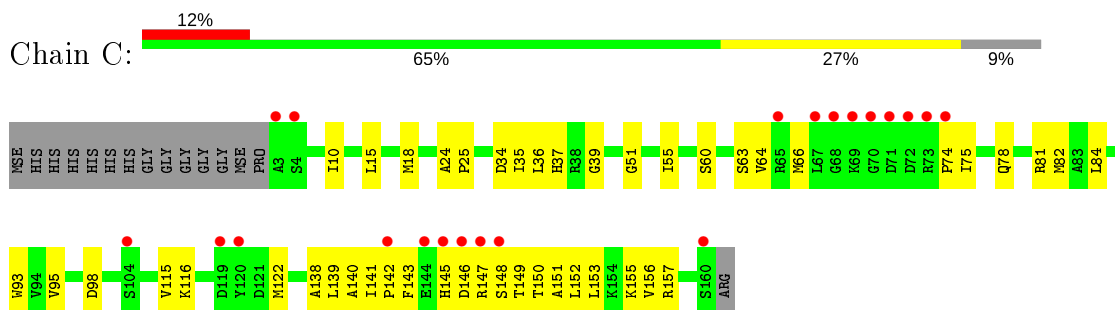
- Molecule 1: Putative cytidyltransferase



- Molecule 1: Putative cytidyltransferase

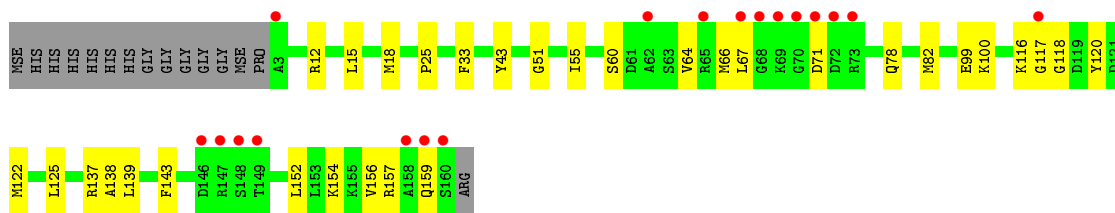


- Molecule 1: Putative cytidyltransferase

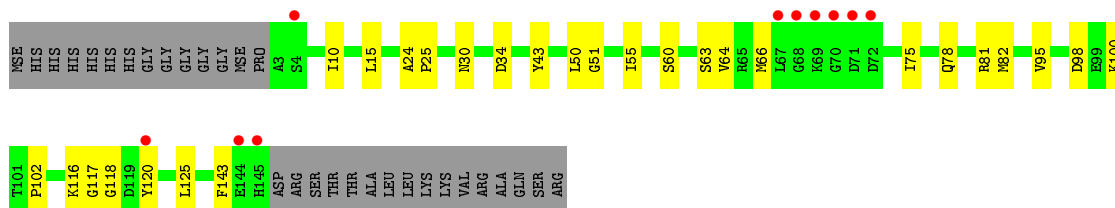


- Molecule 1: Putative cytidyltransferase

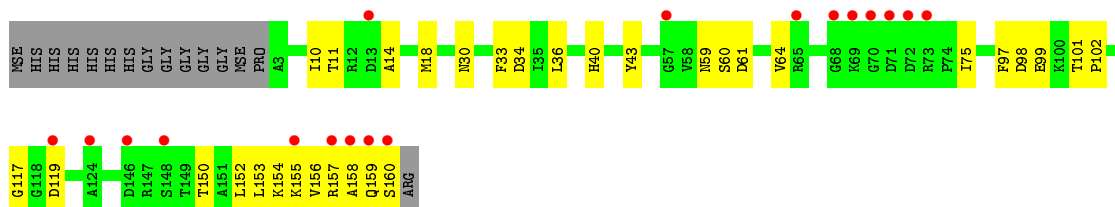
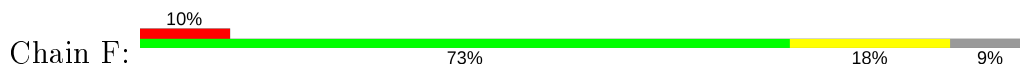




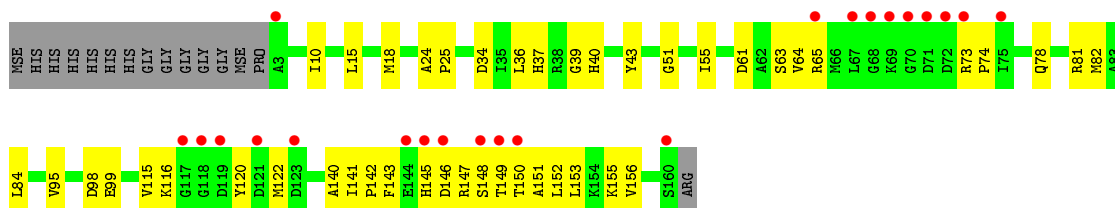
- Molecule 1: Putative cytidyltransferase



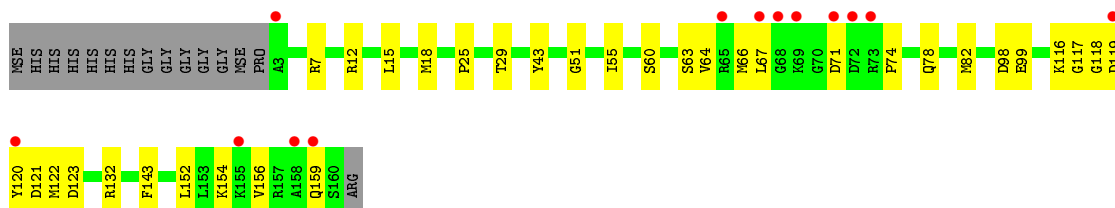
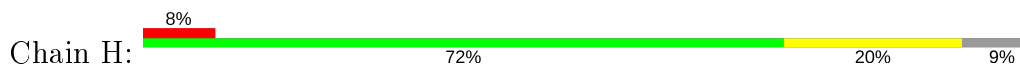
- Molecule 1: Putative cytidyltransferase



- Molecule 1: Putative cytidyltransferase



- Molecule 1: Putative cytidyltransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	30.6	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 0.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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.

All (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:149:THR:O	1:G:153:LEU:HD13	1.46	1.12
1:G:73:ARG:HB2	1:G:74:PRO:HD2	1.30	1.12
1:G:61:ASP:O	1:G:64:VAL:HG12	1.47	1.11
1:A:60:SER:O	1:A:64:VAL:HG23	1.47	1.11
1:F:18:MSE:HE1	1:G:25:PRO:HB3	1.32	1.11
1:H:117:GLY:H	2:H:201:EPE:H72	1.08	1.11
1:G:149:THR:O	1:G:153:LEU:CD1	2.00	1.09
1:H:116:LYS:HD2	2:H:201:EPE:H71	1.29	1.08
1:B:116:LYS:CG	2:B:201:EPE:C8	2.24	1.08
1:B:18:MSE:HE1	1:C:25:PRO:HB3	1.09	1.07
1:H:43:TYR:OH	2:H:201:EPE:H82	1.56	1.06
1:G:141:ILE:HG23	1:G:142:PRO:HD2	1.32	1.05
1:G:63:SER:HB2	1:G:98:ASP:O	1.57	1.04
1:G:141:ILE:CG2	1:G:142:PRO:HD2	1.89	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:122:MSE:HE3	1:G:140:ALA:HB2	1.38	1.02
1:F:18:MSE:CE	1:G:25:PRO:HB3	1.93	0.99
1:B:116:LYS:HG3	2:B:201:EPE:O8	1.61	0.99
1:B:18:MSE:CE	1:C:25:PRO:HB3	1.93	0.98
1:C:156:VAL:HG22	1:D:156:VAL:HG21	1.47	0.95
1:G:64:VAL:HG11	1:G:74:PRO:HD3	1.51	0.92
1:F:150:THR:CG2	1:F:154:LYS:HE3	1.99	0.92
1:G:156:VAL:HG22	1:H:156:VAL:HG21	1.52	0.91
1:B:73:ARG:HG3	1:B:74:PRO:HD2	1.58	0.85
1:F:60:SER:HB3	1:F:98:ASP:OD1	1.76	0.85
2:D:201:EPE:C7	2:D:201:EPE:H91	2.07	0.84
1:F:117:GLY:H	2:F:201:EPE:C8	1.91	0.84
1:G:73:ARG:HB2	1:G:74:PRO:CD	2.09	0.83
1:H:117:GLY:N	2:H:201:EPE:H72	1.92	0.83
1:C:63:SER:HA	1:C:66:MSE:HG3	1.62	0.82
1:G:64:VAL:HG11	1:G:74:PRO:CD	2.10	0.80
1:B:73:ARG:CG	1:B:74:PRO:HD2	2.12	0.80
1:B:116:LYS:HG3	2:B:201:EPE:C8	2.02	0.80
1:E:116:LYS:HD3	1:E:125:LEU:HD11	1.63	0.80
1:E:66:MSE:SE	1:E:100:LYS:CB	2.79	0.80
1:C:153:LEU:O	1:C:157:ARG:HD3	1.81	0.79
1:F:60:SER:CB	1:F:98:ASP:OD1	2.30	0.79
1:C:141:ILE:HG23	1:C:142:PRO:HD2	1.64	0.79
1:A:116:LYS:CD	1:A:125:LEU:HD11	2.13	0.79
1:B:18:MSE:HE1	1:C:25:PRO:CB	2.04	0.79
1:B:117:GLY:H	2:B:201:EPE:H71	1.47	0.79
1:C:147:ARG:HA	1:C:150:THR:HG22	1.63	0.79
2:D:201:EPE:H71	2:D:201:EPE:H91	1.64	0.79
1:B:116:LYS:NZ	1:B:125:LEU:HD11	1.98	0.78
1:G:147:ARG:HA	1:G:150:THR:HG22	1.64	0.78
1:G:61:ASP:O	1:G:64:VAL:CG1	2.30	0.78
1:G:149:THR:O	1:G:153:LEU:HD12	1.85	0.77
1:B:75:ILE:HG21	1:B:158:ALA:HB1	1.67	0.77
1:D:71:ASP:HB3	1:D:154:LYS:HD3	1.67	0.77
1:B:116:LYS:HG2	2:B:201:EPE:H82	0.77	0.76
1:G:120:TYR:HB2	1:G:122:MSE:CE	2.16	0.76
1:A:116:LYS:HD3	1:A:125:LEU:HD11	1.68	0.75
1:D:71:ASP:CB	1:D:154:LYS:HD3	2.17	0.75
1:F:117:GLY:N	2:F:201:EPE:H81	2.01	0.75
1:H:119:ASP:O	1:H:120:TYR:CD1	2.39	0.75
1:G:64:VAL:HG13	1:G:65:ARG:N	2.03	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:153:LEU:O	1:F:157:ARG:HG2	1.88	0.74
1:H:116:LYS:HD2	2:H:201:EPE:C7	2.14	0.74
1:E:63:SER:O	1:E:66:MSE:HB2	1.88	0.73
1:H:117:GLY:H	2:H:201:EPE:C7	1.96	0.73
1:C:149:THR:O	1:C:153:LEU:HG	1.88	0.73
1:B:153:LEU:O	1:B:157:ARG:HG2	1.88	0.72
1:F:117:GLY:H	2:F:201:EPE:H81	1.53	0.72
1:B:62:ALA:HA	1:B:65:ARG:HD2	1.69	0.72
1:D:33:PHE:N	2:D:201:EPE:O3S	2.19	0.72
1:H:60:SER:O	1:H:64:VAL:HG23	1.88	0.72
1:B:60:SER:CB	1:B:98:ASP:OD1	2.37	0.71
1:F:150:THR:O	1:F:154:LYS:HG3	1.90	0.71
1:B:60:SER:OG	1:B:98:ASP:OD1	2.09	0.70
1:A:62:ALA:O	1:A:65:ARG:N	2.23	0.69
1:C:115:VAL:HG21	1:C:141:ILE:HD12	1.73	0.69
1:G:145:HIS:HE1	1:G:147:ARG:HG3	1.57	0.69
1:H:71:ASP:HB3	1:H:154:LYS:HD3	1.74	0.69
1:B:75:ILE:HG21	1:B:158:ALA:CB	2.23	0.69
1:C:152:LEU:O	1:C:156:VAL:HG23	1.93	0.69
1:C:141:ILE:CG2	1:C:142:PRO:HD2	2.21	0.69
1:D:66:MSE:SE	1:D:100:LYS:HD2	2.43	0.69
1:H:71:ASP:CB	1:H:154:LYS:HD3	2.23	0.68
1:G:36:LEU:HD12	1:G:84:LEU:HD12	1.76	0.68
1:D:117:GLY:O	1:D:120:TYR:CE2	2.47	0.68
1:G:152:LEU:O	1:G:156:VAL:HG23	1.93	0.67
1:C:35:ILE:HD13	1:C:153:LEU:HD21	1.76	0.67
1:B:73:ARG:HG2	1:B:74:PRO:N	2.10	0.67
1:C:36:LEU:HD12	1:C:84:LEU:HD12	1.76	0.67
1:D:116:LYS:HE3	2:D:201:EPE:C8	2.25	0.67
1:C:155:LYS:HD3	1:D:159:GLN:NE2	2.11	0.66
1:E:116:LYS:CD	1:E:125:LEU:HD11	2.25	0.66
1:E:25:PRO:HB3	1:H:18:MSE:HE1	1.77	0.66
1:E:63:SER:HB2	1:E:98:ASP:O	1.96	0.66
1:E:66:MSE:HB3	1:E:100:LYS:HG3	1.78	0.65
1:G:149:THR:C	1:G:153:LEU:HD13	2.15	0.65
1:A:25:PRO:HB3	1:D:18:MSE:HE1	1.79	0.65
1:F:155:LYS:O	1:F:159:GLN:HG3	1.96	0.65
1:G:64:VAL:CG1	1:G:74:PRO:HD3	2.25	0.65
1:A:118:GLY:CA	1:A:143:PHE:CE2	2.81	0.64
1:C:25:PRO:HG2	1:C:51:GLY:HA2	1.79	0.64
1:A:24:ALA:HB1	1:D:18:MSE:CE	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:116:LYS:CD	2:H:201:EPE:H71	2.18	0.63
1:G:25:PRO:HG2	1:G:51:GLY:HA2	1.79	0.63
1:A:75:ILE:CD1	1:B:154:LYS:HG2	2.28	0.63
1:E:75:ILE:CD1	1:F:154:LYS:HG2	2.28	0.63
1:E:118:GLY:CA	1:E:143:PHE:CE2	2.82	0.63
1:B:152:LEU:O	1:B:156:VAL:HG23	1.99	0.62
1:F:152:LEU:O	1:F:156:VAL:HG23	1.99	0.62
1:B:116:LYS:HZ2	1:B:125:LEU:HD11	1.62	0.62
1:E:24:ALA:HB1	1:H:18:MSE:CE	2.29	0.62
1:H:117:GLY:O	1:H:120:TYR:CE2	2.53	0.62
1:G:156:VAL:HG11	1:H:152:LEU:HD11	1.82	0.62
1:F:59:ASN:OD1	1:F:97:PHE:HZ	1.82	0.61
1:D:156:VAL:O	1:D:159:GLN:HG2	2.00	0.61
1:B:59:ASN:OD1	1:B:97:PHE:HZ	1.82	0.61
1:F:75:ILE:HG21	1:F:158:ALA:CB	2.30	0.61
1:B:10:ILE:HD11	1:B:14:ALA:CB	2.30	0.61
1:H:43:TYR:CZ	2:H:201:EPE:H82	2.36	0.61
1:A:116:LYS:HD2	1:A:125:LEU:HD11	1.82	0.61
1:B:150:THR:HG22	1:B:154:LYS:HE3	1.83	0.61
1:B:73:ARG:CG	1:B:74:PRO:CD	2.79	0.61
1:A:60:SER:O	1:A:64:VAL:CG2	2.37	0.60
2:D:201:EPE:C9	2:D:201:EPE:H71	2.30	0.60
1:D:116:LYS:HE3	2:D:201:EPE:H81	1.82	0.60
1:G:145:HIS:CE1	1:G:150:THR:HG21	2.36	0.60
1:B:59:ASN:OD1	1:B:97:PHE:CZ	2.54	0.60
1:D:15:LEU:HD21	1:D:55:ILE:HD13	1.83	0.60
1:F:43:TYR:CE2	2:F:201:EPE:H82	2.36	0.60
1:G:150:THR:HG23	1:G:151:ALA:N	2.16	0.60
1:H:156:VAL:O	1:H:159:GLN:HG2	2.00	0.60
1:C:156:VAL:HG11	1:D:152:LEU:HD11	1.84	0.60
1:F:59:ASN:OD1	1:F:97:PHE:CZ	2.54	0.60
1:F:10:ILE:HD11	1:F:14:ALA:CB	2.30	0.60
1:H:15:LEU:HD21	1:H:55:ILE:HD13	1.82	0.60
2:H:201:EPE:H91	2:H:201:EPE:N4	2.16	0.60
1:B:59:ASN:CG	1:B:97:PHE:CZ	2.76	0.60
1:C:150:THR:HG23	1:C:151:ALA:N	2.16	0.59
1:H:123:ASP:OD1	1:H:132:ARG:NH1	2.33	0.59
1:B:116:LYS:HA	2:B:201:EPE:H71	1.85	0.59
1:F:59:ASN:CG	1:F:97:PHE:CZ	2.76	0.59
1:C:18:MSE:O	1:C:18:MSE:HG2	2.03	0.59
2:F:201:EPE:H72	2:F:201:EPE:N1	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:64:VAL:CG1	1:G:65:ARG:N	2.65	0.59
1:H:43:TYR:OH	2:H:201:EPE:C8	2.44	0.59
1:G:141:ILE:CG2	1:G:142:PRO:CD	2.73	0.59
1:H:118:GLY:N	1:H:143:PHE:HB3	2.18	0.58
1:C:115:VAL:HG21	1:C:141:ILE:CD1	2.33	0.58
1:G:143:PHE:CE2	1:G:145:HIS:HB3	2.38	0.58
1:D:118:GLY:N	1:D:143:PHE:HB3	2.18	0.58
1:F:34:ASP:OD2	1:F:75:ILE:HD12	2.03	0.58
1:G:155:LYS:HD3	1:H:159:GLN:NE2	2.18	0.58
1:B:116:LYS:HA	2:B:201:EPE:C7	2.33	0.58
1:D:25:PRO:HG2	1:D:51:GLY:HA2	1.85	0.58
1:F:18:MSE:HE2	1:G:25:PRO:HB3	1.85	0.58
1:G:64:VAL:HG13	1:G:65:ARG:H	1.69	0.58
1:C:122:MSE:CE	1:C:138:ALA:HB1	2.34	0.57
1:H:25:PRO:HG2	1:H:51:GLY:HA2	1.85	0.57
1:H:12:ARG:NH2	1:H:99:GLU:OE1	2.37	0.57
1:B:34:ASP:OD2	1:B:75:ILE:HD12	2.03	0.57
1:E:118:GLY:HA2	1:E:143:PHE:CE2	2.40	0.57
1:H:120:TYR:O	1:H:121:ASP:C	2.43	0.57
1:B:35:ILE:HD11	1:B:75:ILE:HD13	1.86	0.57
1:A:75:ILE:HD11	1:B:154:LYS:HG2	1.85	0.57
1:C:75:ILE:HD12	1:C:153:LEU:HD22	1.86	0.56
1:G:148:SER:O	1:G:152:LEU:HD12	2.06	0.56
1:E:75:ILE:HD12	1:F:154:LYS:HG2	1.87	0.56
1:F:117:GLY:CA	2:F:201:EPE:H81	2.35	0.56
1:C:141:ILE:CG2	1:C:142:PRO:CD	2.83	0.56
1:A:15:LEU:HD21	1:A:55:ILE:HD13	1.87	0.55
1:C:148:SER:O	1:C:152:LEU:HD12	2.05	0.55
1:F:40:HIS:HE2	2:F:201:EPE:H92	1.70	0.55
1:D:60:SER:O	1:D:64:VAL:HG23	2.06	0.55
1:G:115:VAL:HG21	1:G:141:ILE:CD1	2.37	0.55
1:C:37:HIS:HB2	1:C:146:ASP:CB	2.36	0.55
1:F:75:ILE:HG21	1:F:158:ALA:HB1	1.89	0.55
1:E:24:ALA:HB1	1:H:18:MSE:HE2	1.89	0.55
1:H:116:LYS:HB2	1:H:122:MSE:SE	2.56	0.55
1:H:63:SER:HB2	1:H:98:ASP:O	2.07	0.55
2:D:201:EPE:H72	2:D:201:EPE:H91	1.87	0.54
1:E:15:LEU:HD21	1:E:55:ILE:HD13	1.87	0.54
1:A:24:ALA:HB1	1:D:18:MSE:HE2	1.89	0.54
1:E:66:MSE:SE	1:E:100:LYS:CA	3.06	0.54
1:F:117:GLY:HA3	2:F:201:EPE:H81	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:117:GLY:O	1:H:120:TYR:HE2	1.91	0.54
1:D:71:ASP:HB3	1:D:154:LYS:CD	2.36	0.53
1:D:71:ASP:HB3	1:D:154:LYS:NZ	2.23	0.53
1:F:43:TYR:CZ	2:F:201:EPE:H82	2.42	0.53
1:F:117:GLY:N	2:F:201:EPE:C8	2.64	0.53
1:D:116:LYS:HE3	2:D:201:EPE:H82	1.91	0.53
1:G:18:MSE:HG2	1:G:18:MSE:O	2.09	0.53
1:E:118:GLY:HA2	1:E:143:PHE:CD2	2.44	0.53
1:F:43:TYR:CZ	2:F:201:EPE:C8	2.91	0.53
1:G:37:HIS:HB2	1:G:146:ASP:CB	2.39	0.53
1:G:64:VAL:CG1	1:G:65:ARG:H	2.20	0.53
1:F:33:PHE:H	2:F:201:EPE:H102	1.74	0.53
1:G:141:ILE:HG22	1:G:142:PRO:HD2	1.83	0.52
1:C:141:ILE:HG23	1:C:142:PRO:CD	2.37	0.52
1:C:60:SER:O	1:C:64:VAL:HG23	2.09	0.52
2:D:201:EPE:C7	2:D:201:EPE:C9	2.85	0.52
1:E:25:PRO:HB3	1:H:18:MSE:CE	2.37	0.52
1:B:116:LYS:NZ	1:B:125:LEU:CD1	2.71	0.52
1:C:155:LYS:HB2	1:D:156:VAL:CG1	2.38	0.52
1:D:12:ARG:NH2	1:D:99:GLU:OE1	2.37	0.52
1:F:40:HIS:NE2	2:F:201:EPE:H92	2.25	0.52
1:D:43:TYR:CE2	2:D:201:EPE:H21	2.45	0.52
1:B:73:ARG:HG2	1:B:74:PRO:CD	2.40	0.52
1:G:143:PHE:HE2	1:G:145:HIS:HB3	1.74	0.52
1:B:116:LYS:HD2	1:B:125:LEU:HD11	1.92	0.52
1:G:73:ARG:CB	1:G:74:PRO:HD2	2.20	0.51
1:G:155:LYS:HB2	1:H:156:VAL:CG1	2.40	0.51
1:C:15:LEU:HD21	1:C:55:ILE:HD13	1.93	0.51
1:H:29:THR:OG1	2:H:201:EPE:H81	2.10	0.51
1:B:150:THR:CG2	1:B:154:LYS:HE3	2.41	0.51
1:B:18:MSE:CE	1:C:25:PRO:CB	2.78	0.51
1:G:15:LEU:HD21	1:G:55:ILE:HD13	1.93	0.51
1:C:37:HIS:HE1	1:C:143:PHE:CZ	2.28	0.51
1:A:118:GLY:HA2	1:A:143:PHE:CE2	2.46	0.51
1:G:61:ASP:C	1:G:64:VAL:HG12	2.28	0.50
1:C:75:ILE:CD1	1:C:153:LEU:HD22	2.41	0.50
1:H:71:ASP:HB3	1:H:154:LYS:NZ	2.26	0.50
1:B:18:MSE:SE	1:C:24:ALA:HB1	2.62	0.50
1:A:25:PRO:HB3	1:D:18:MSE:CE	2.40	0.50
1:G:145:HIS:ND1	1:G:150:THR:HG21	2.26	0.50
1:E:25:PRO:CB	1:H:18:MSE:HE1	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:ILE:HD11	1:B:14:ALA:HB1	1.94	0.49
1:A:116:LYS:HD2	1:A:125:LEU:CD1	2.41	0.49
1:C:122:MSE:HE2	1:C:139:LEU:N	2.27	0.49
1:G:115:VAL:HG23	1:G:141:ILE:HG13	1.93	0.49
1:G:122:MSE:CE	1:G:140:ALA:HB2	2.26	0.49
1:B:101:THR:HB	1:B:102:PRO:CD	2.43	0.49
1:F:101:THR:HB	1:F:102:PRO:CD	2.43	0.49
1:G:150:THR:CG2	1:G:151:ALA:N	2.75	0.49
1:B:117:GLY:N	2:B:201:EPE:H71	2.22	0.49
1:F:10:ILE:HD11	1:F:14:ALA:HB1	1.94	0.49
1:G:156:VAL:CG2	1:H:156:VAL:HG21	2.36	0.49
1:A:25:PRO:CB	1:D:18:MSE:HE1	2.43	0.48
1:E:50:LEU:O	1:H:7:ARG:HG3	2.13	0.48
1:F:10:ILE:HD11	1:F:14:ALA:HB3	1.96	0.48
1:C:18:MSE:HE1	1:C:93:TRP:CH2	2.48	0.48
1:D:66:MSE:O	1:D:67:LEU:HB2	2.13	0.48
1:F:159:GLN:O	1:F:160:SER:C	2.51	0.48
1:C:156:VAL:CG2	1:D:156:VAL:HG21	2.30	0.48
1:C:150:THR:CG2	1:C:151:ALA:N	2.75	0.48
1:A:117:GLY:O	1:A:120:TYR:HE2	1.96	0.48
1:A:50:LEU:HD11	1:A:141:ILE:HD11	1.96	0.48
1:H:64:VAL:HG11	1:H:74:PRO:HD3	1.96	0.48
1:F:119:ASP:OD1	1:F:119:ASP:O	2.32	0.48
1:C:34:ASP:HA	1:C:81:ARG:HD3	1.96	0.47
1:E:117:GLY:O	1:E:120:TYR:HE2	1.96	0.47
1:E:25:PRO:HA	1:H:18:MSE:HE3	1.96	0.47
1:H:66:MSE:O	1:H:67:LEU:HB2	2.13	0.47
1:C:63:SER:HB2	1:C:98:ASP:O	2.14	0.47
1:B:119:ASP:OD1	1:B:119:ASP:O	2.32	0.47
1:C:35:ILE:HD13	1:C:153:LEU:CD2	2.44	0.47
1:D:122:MSE:HE3	1:D:138:ALA:HB1	1.96	0.47
1:A:25:PRO:HG2	1:A:51:GLY:HA2	1.97	0.47
1:B:10:ILE:HD11	1:B:14:ALA:HB3	1.95	0.47
1:C:37:HIS:HB2	1:C:146:ASP:HB2	1.96	0.47
1:G:145:HIS:CE1	1:G:147:ARG:HG3	2.45	0.47
1:F:60:SER:O	1:F:61:ASP:C	2.54	0.47
1:F:75:ILE:HG21	1:F:158:ALA:HB3	1.97	0.46
1:G:141:ILE:HG22	1:G:142:PRO:CD	2.44	0.46
1:G:40:HIS:HA	1:G:143:PHE:HE1	1.80	0.46
1:B:60:SER:O	1:B:63:SER:N	2.49	0.46
1:B:73:ARG:CG	1:B:74:PRO:N	2.76	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:GLY:HA2	1:A:143:PHE:CD2	2.51	0.46
1:D:122:MSE:CE	1:D:138:ALA:HB1	2.46	0.46
1:G:39:GLY:O	1:G:143:PHE:CE1	2.68	0.46
1:G:34:ASP:HA	1:G:81:ARG:HD3	1.96	0.46
1:E:25:PRO:HG2	1:E:51:GLY:HA2	1.97	0.46
1:E:60:SER:O	1:E:64:VAL:HG23	2.16	0.46
1:A:78:GLN:O	1:A:82:MSE:HG3	2.16	0.46
1:C:39:GLY:C	1:C:143:PHE:CE1	2.89	0.46
1:G:143:PHE:HE2	1:G:145:HIS:CB	2.29	0.46
1:G:63:SER:OG	1:G:99:GLU:O	2.11	0.46
2:H:201:EPE:C9	2:H:201:EPE:N4	2.76	0.46
1:A:116:LYS:CD	1:A:125:LEU:CD1	2.90	0.45
1:B:116:LYS:HG3	2:B:201:EPE:HO8	1.74	0.45
1:B:142:PRO:HB3	3:B:303:HOH:O	2.16	0.45
1:E:78:GLN:O	1:E:82:MSE:HG3	2.16	0.45
1:F:30:ASN:OD1	1:F:102:PRO:HG3	2.17	0.45
1:B:30:ASN:OD1	1:B:102:PRO:HG3	2.16	0.45
1:G:147:ARG:HA	1:G:150:THR:CG2	2.40	0.45
1:H:60:SER:HA	1:H:78:GLN:CD	2.37	0.45
1:C:18:MSE:CG	1:C:18:MSE:O	2.64	0.45
1:G:15:LEU:HD22	1:G:95:VAL:HG21	1.98	0.45
1:C:15:LEU:HD22	1:C:95:VAL:HG21	1.98	0.45
1:F:43:TYR:CZ	2:F:201:EPE:H81	2.52	0.45
1:G:115:VAL:HG21	1:G:141:ILE:HD12	1.98	0.45
1:H:71:ASP:HB3	1:H:154:LYS:CD	2.43	0.45
1:A:25:PRO:HA	1:D:18:MSE:HE3	1.98	0.44
1:H:29:THR:OG1	2:H:201:EPE:C8	2.65	0.44
1:C:37:HIS:CE1	1:C:143:PHE:CZ	3.05	0.44
1:G:120:TYR:HB2	1:G:122:MSE:HE1	1.97	0.44
1:G:78:GLN:O	1:G:82:MSE:HG3	2.18	0.44
1:E:51:GLY:CA	1:H:7:ARG:HD2	2.48	0.44
1:C:37:HIS:HB2	1:C:146:ASP:HB3	2.00	0.44
1:A:15:LEU:HD22	1:A:95:VAL:HG21	2.00	0.44
1:B:116:LYS:HZ1	1:B:125:LEU:CD1	2.29	0.44
1:D:60:SER:HA	1:D:78:GLN:CD	2.37	0.44
1:G:37:HIS:HB2	1:G:146:ASP:HB2	1.98	0.44
1:B:99:GLU:H	1:B:99:GLU:CD	2.21	0.44
1:G:155:LYS:HB2	1:H:156:VAL:HG11	1.98	0.44
1:C:78:GLN:O	1:C:82:MSE:HG3	2.18	0.44
1:A:117:GLY:O	1:A:120:TYR:CE2	2.71	0.43
1:C:18:MSE:HE1	1:C:93:TRP:CZ2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:201:EPE:H22	2:F:201:EPE:H101	1.75	0.43
1:G:156:VAL:CG1	1:H:152:LEU:HD11	2.46	0.43
1:F:60:SER:O	1:F:64:VAL:HG23	2.18	0.43
1:G:39:GLY:C	1:G:143:PHE:CE1	2.92	0.43
1:C:141:ILE:HG22	1:C:142:PRO:N	2.33	0.43
1:F:99:GLU:H	1:F:99:GLU:CD	2.21	0.43
1:C:34:ASP:OD2	1:C:74:PRO:HA	2.19	0.43
1:A:118:GLY:HA3	1:A:120:TYR:CE2	2.54	0.43
1:A:62:ALA:C	1:A:64:VAL:N	2.72	0.43
1:C:155:LYS:HB2	1:D:156:VAL:HG11	1.99	0.43
1:E:117:GLY:O	1:E:120:TYR:CE2	2.71	0.43
1:G:115:VAL:CG2	1:G:141:ILE:HG13	2.49	0.43
1:E:118:GLY:HA3	1:E:120:TYR:CE2	2.54	0.43
1:B:116:LYS:CD	1:B:125:LEU:HD11	2.49	0.42
1:E:15:LEU:HD22	1:E:95:VAL:HG21	2.00	0.42
1:C:122:MSE:HE2	1:C:138:ALA:HB1	2.01	0.42
1:C:122:MSE:HE3	1:C:138:ALA:HB1	2.02	0.42
1:E:10:ILE:HG23	1:E:95:VAL:HG22	2.00	0.42
1:F:101:THR:HB	1:F:102:PRO:HD2	2.02	0.42
2:B:201:EPE:H21	2:B:201:EPE:H101	1.90	0.42
1:G:155:LYS:CB	1:H:156:VAL:CG1	2.97	0.42
1:B:101:THR:HB	1:B:102:PRO:HD2	2.02	0.42
1:C:116:LYS:O	1:C:140:ALA:HA	2.20	0.42
1:A:75:ILE:HD12	1:B:154:LYS:CG	2.50	0.41
1:A:75:ILE:HG22	1:B:153:LEU:HD21	2.01	0.41
1:C:145:HIS:HD2	1:C:150:THR:HG21	1.85	0.41
1:D:116:LYS:CE	2:D:201:EPE:H81	2.50	0.41
1:A:30:ASN:OD1	1:A:102:PRO:HG3	2.20	0.41
1:A:10:ILE:HG23	1:A:95:VAL:HG22	2.00	0.41
1:C:18:MSE:HE1	1:C:93:TRP:CZ3	2.55	0.41
1:E:116:LYS:CD	1:E:125:LEU:CD1	2.97	0.41
1:C:116:LYS:O	1:C:141:ILE:N	2.50	0.41
1:C:155:LYS:CB	1:D:156:VAL:CG1	2.98	0.41
1:F:10:ILE:HG12	1:F:11:THR:N	2.35	0.41
1:B:10:ILE:HG12	1:B:11:THR:N	2.35	0.41
1:D:116:LYS:CE	2:D:201:EPE:C8	2.97	0.41
1:E:75:ILE:HG22	1:F:153:LEU:HD21	2.01	0.41
1:F:159:GLN:O	1:F:160:SER:O	2.38	0.41
1:G:37:HIS:HB2	1:G:146:ASP:HB3	2.03	0.41
1:C:63:SER:CA	1:C:66:MSE:HG3	2.44	0.41
1:G:43:TYR:HB2	1:G:143:PHE:HD1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:34:ASP:HA	1:E:81:ARG:HD3	2.03	0.41
1:A:34:ASP:HA	1:A:81:ARG:HD3	2.03	0.41
1:E:30:ASN:OD1	1:E:102:PRO:HG3	2.20	0.41
1:F:18:MSE:SE	1:G:24:ALA:HB1	2.71	0.41
1:G:116:LYS:O	1:G:140:ALA:HA	2.20	0.41
1:H:78:GLN:O	1:H:82:MSE:HG3	2.21	0.41
1:A:75:ILE:CD1	1:B:154:LYS:CG	2.98	0.41
1:B:60:SER:HB3	1:B:98:ASP:OD1	2.20	0.41
1:E:60:SER:HA	1:E:78:GLN:CD	2.42	0.41
2:F:201:EPE:C7	2:F:201:EPE:N1	2.76	0.41
1:G:10:ILE:O	1:G:95:VAL:HG13	2.21	0.41
1:D:116:LYS:HD2	1:D:125:LEU:HD11	2.04	0.40
1:D:137:ARG:CD	1:D:139:LEU:HD22	2.51	0.40
1:D:157:ARG:HE	1:D:157:ARG:HB3	1.60	0.40
2:B:201:EPE:H62	2:B:201:EPE:H102	1.78	0.40
1:F:36:LEU:HA	1:F:36:LEU:HD23	1.94	0.40
1:F:59:ASN:ND2	1:F:97:PHE:CE1	2.90	0.40
1:C:10:ILE:O	1:C:95:VAL:HG13	2.21	0.40
1:A:60:SER:HA	1:A:78:GLN:CD	2.42	0.40
1:C:25:PRO:HG2	1:C:51:GLY:CA	2.51	0.40
1:B:63:SER:O	1:B:66:MSE:HB2	2.22	0.40
1:B:59:ASN:ND2	1:B:97:PHE:CE1	2.90	0.40
1:C:147:ARG:HA	1:C:150:THR:CG2	2.42	0.40
1:D:78:GLN:O	1:D:82:MSE:HG3	2.21	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	140/173 (81%)	138 (99%)	2 (1%)	0	<a href="#">100</a> <a href="#">100</a>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 [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	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

Some 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 carbohydrates 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	D	201	-	15,15,15	1.66	3 (20%)	18,20,20	2.08	8 (44%)
2	EPE	F	201	-	15,15,15	1.66	3 (20%)	18,20,20	1.82	4 (22%)
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	D	201	-	-	2/9/19/19	0/1/1/1
2	EPE	F	201	-	-	5/9/19/19	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

All (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
2	D	201	EPE	O2S-S	3.33	1.54	1.45
2	H	201	EPE	O1S-S	3.14	1.54	1.45
2	B	201	EPE	O2S-S	3.12	1.54	1.45
2	B	201	EPE	C7-N4	-2.18	1.42	1.47
2	F	201	EPE	C7-N4	-2.17	1.42	1.47
2	D	201	EPE	C7-N4	-2.17	1.42	1.47
2	H	201	EPE	C7-N4	-2.15	1.42	1.47
2	H	201	EPE	O3S-S	2.14	1.55	1.47
2	B	201	EPE	O3S-S	2.07	1.55	1.47

All (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
2	F	201	EPE	O2S-S-O1S	-3.73	101.05	113.95
2	D	201	EPE	O2S-S-O1S	-3.73	101.05	113.95
2	B	201	EPE	O3S-S-C10	3.52	111.47	105.77
2	D	201	EPE	O1S-S-C10	3.49	111.11	106.92
2	F	201	EPE	O1S-S-C10	3.48	111.10	106.92
2	B	201	EPE	O1S-S-C10	3.47	111.09	106.92
2	H	201	EPE	O3S-S-C10	3.33	111.16	105.77
2	H	201	EPE	O1S-S-C10	2.78	110.26	106.92
2	D	201	EPE	O3S-S-C10	2.76	110.22	105.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	201	EPE	O3S-S-C10	2.75	110.22	105.77
2	B	201	EPE	O2S-S-C10	2.74	110.21	106.92
2	D	201	EPE	C6-N1-C2	2.70	114.91	108.83
2	D	201	EPE	C5-N4-C3	2.66	114.83	108.83
2	D	201	EPE	C6-C5-N4	2.12	114.99	110.64
2	D	201	EPE	C3-C2-N1	2.11	114.98	110.64

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	201	EPE	S-C10-C9-N1
2	F	201	EPE	C9-C10-S-O1S
2	F	201	EPE	C9-C10-S-O2S
2	F	201	EPE	C9-C10-S-O3S
2	H	201	EPE	C9-C10-S-O2S
2	B	201	EPE	C9-C10-S-O1S
2	B	201	EPE	C9-C10-S-O3S
2	H	201	EPE	N4-C7-C8-O8
2	B	201	EPE	N4-C7-C8-O8
2	F	201	EPE	N4-C7-C8-O8
2	H	201	EPE	C8-C7-N4-C3
2	H	201	EPE	C9-C10-S-O3S
2	H	201	EPE	C8-C7-N4-C5
2	H	201	EPE	C9-C10-S-O1S
2	B	201	EPE	C9-C10-S-O2S
2	D	201	EPE	C8-C7-N4-C5
2	D	201	EPE	C8-C7-N4-C3

There are no ring outliers.

4 monomers are involved in 54 short contacts:

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

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, 95<sup>th</sup> 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 <sup>2</sup> )	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

All (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
1	F	69	LYS	8.8
1	H	69	LYS	8.8
1	G	146	ASP	8.6
1	D	70	GLY	8.2
1	A	70	GLY	8.1
1	B	158	ALA	8.1
1	C	67	LEU	7.9
1	F	68	GLY	7.6
1	E	68	GLY	7.5
1	C	119	ASP	7.4
1	B	160	SER	7.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	69	LYS	7.2
1	E	71	ASP	6.8
1	C	145	HIS	6.6
1	E	145	HIS	6.2
1	G	70	GLY	5.9
1	H	67	LEU	5.8
1	D	3	ALA	5.5
1	G	69	LYS	5.4
1	D	68	GLY	5.4
1	B	71	ASP	5.3
1	E	70	GLY	5.1
1	C	68	GLY	5.0
1	C	70	GLY	5.0
1	G	123	ASP	4.7
1	H	65	ARG	4.7
1	C	72	ASP	4.7
1	D	71	ASP	4.7
1	C	65	ARG	4.7
1	H	68	GLY	4.6
1	D	67	LEU	4.6
1	G	117	GLY	4.6
1	B	69	LYS	4.5
1	B	156	VAL	4.5
1	F	71	ASP	4.4
1	G	65	ARG	4.4
1	D	160	SER	4.3
1	F	159	GLN	4.3
1	G	75	ILE	4.2
1	A	61	ASP	4.2
1	G	144	GLU	4.2
1	A	71	ASP	4.1
1	H	119	ASP	4.1
1	A	68	GLY	4.0
1	C	69	LYS	4.0
1	C	144	GLU	3.9
1	B	70	GLY	3.9
1	D	159	GLN	3.7
1	A	69	LYS	3.6
1	C	147	ARG	3.6
1	B	3	ALA	3.6
1	D	149	THR	3.5
1	A	3	ALA	3.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	148	SER	3.5
1	G	148	SER	3.5
1	F	146	ASP	3.4
1	H	158	ALA	3.4
1	G	160	SER	3.4
1	G	118	GLY	3.4
1	F	72	ASP	3.4
1	E	72	ASP	3.3
1	G	149	THR	3.3
1	C	104	SER	3.3
1	B	146	ASP	3.3
1	F	119	ASP	3.2
1	F	157	ARG	3.2
1	H	3	ALA	3.2
1	E	144	GLU	3.2
1	F	65	ARG	3.1
1	F	13	ASP	3.1
1	D	158	ALA	3.0
1	D	65	ARG	3.0
1	D	147	ARG	3.0
1	B	159	GLN	3.0
1	G	119	ASP	3.0
1	D	73	ARG	2.9
1	G	71	ASP	2.9
1	D	148	SER	2.9
1	A	65	ARG	2.9
1	B	157	ARG	2.8
1	F	148	SER	2.8
1	C	120	TYR	2.8
1	C	3	ALA	2.8
1	F	158	ALA	2.8
1	G	121	ASP	2.7
1	H	159	GLN	2.7
1	G	3	ALA	2.7
1	G	72	ASP	2.6
1	D	117	GLY	2.6
1	C	160	SER	2.6
1	C	74	PRO	2.6
1	B	73	ARG	2.6
1	B	120	TYR	2.6
1	B	155	LYS	2.6
1	F	160	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	120	TYR	2.6
1	G	150	THR	2.5
1	A	4	SER	2.4
1	H	73	ARG	2.4
1	C	4	SER	2.4
1	H	72	ASP	2.4
1	G	145	HIS	2.4
1	C	73	ARG	2.4
1	F	124	ALA	2.4
1	F	155	LYS	2.4
1	E	120	TYR	2.3
1	F	73	ARG	2.3
1	E	67	LEU	2.3
1	C	142	PRO	2.2
1	G	73	ARG	2.2
1	D	72	ASP	2.2
1	H	71	ASP	2.1
1	D	146	ASP	2.1
1	A	120	TYR	2.1
1	G	67	LEU	2.1
1	B	79	GLU	2.1
1	H	155	LYS	2.1
1	A	72	ASP	2.1
1	D	62	ALA	2.1
1	E	4	SER	2.1
1	F	57	GLY	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 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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	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.