



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:48 PM GMT

PDB ID : 4MT4  
Title : Crystal structure of the Campylobacter jejuni CmeC outer membrane channel  
Authors : Su, C.-C.; Yu, E.W.  
Deposited on : 2013-09-19  
Resolution : 2.37 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

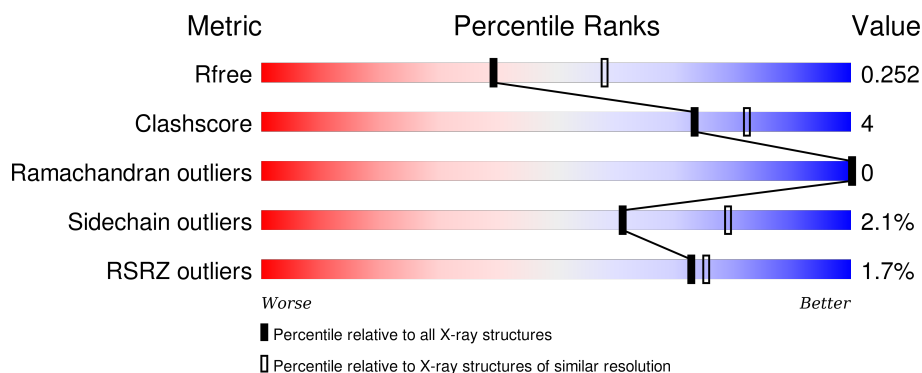
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*




The reported resolution of this entry is 2.37 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))
$R_{free}$	91344	4019 (2.40-2.36)
Clashscore	102246	4595 (2.40-2.36)
Ramachandran outliers	100387	4520 (2.40-2.36)
Sidechain outliers	100360	4522 (2.40-2.36)
RSRZ outliers	91569	4034 (2.40-2.36)

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. 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	479	
1	B	479	
1	C	479	

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	C8E	A	1005	-	-	-	X
2	C8E	B	502	-	-	-	X
2	C8E	C	501	-	-	-	X
2	C8E	C	502	-	-	-	X
2	C8E	C	504	-	-	-	X
3	SO4	B	501	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12304 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.

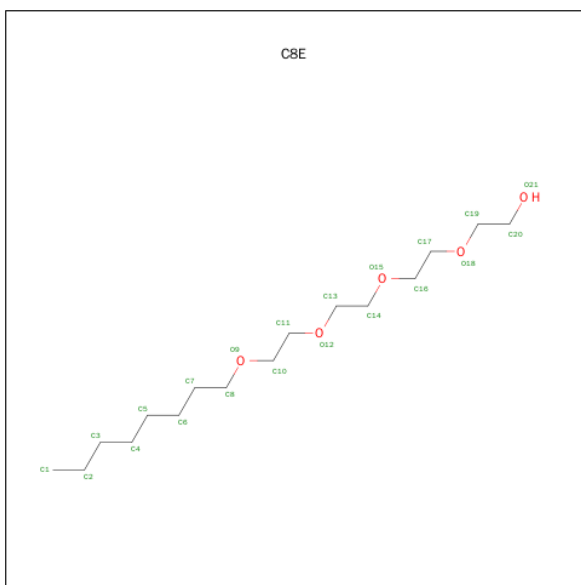
- Molecule 1 is a protein called CmeC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	472	Total	C	N	O	S	0	0	0
			3765	2384	630	745	6			
1	B	473	Total	C	N	O	S	0	0	0
			3774	2389	631	748	6			
1	C	472	Total	C	N	O	S	0	1	0
			3772	2389	632	745	6			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	474	HIS	-	EXPRESSION TAG	UNP Q8RTE3
A	475	HIS	-	EXPRESSION TAG	UNP Q8RTE3
A	476	HIS	-	EXPRESSION TAG	UNP Q8RTE3
A	477	HIS	-	EXPRESSION TAG	UNP Q8RTE3
A	478	HIS	-	EXPRESSION TAG	UNP Q8RTE3
A	479	HIS	-	EXPRESSION TAG	UNP Q8RTE3
B	474	HIS	-	EXPRESSION TAG	UNP Q8RTE3
B	475	HIS	-	EXPRESSION TAG	UNP Q8RTE3
B	476	HIS	-	EXPRESSION TAG	UNP Q8RTE3
B	477	HIS	-	EXPRESSION TAG	UNP Q8RTE3
B	478	HIS	-	EXPRESSION TAG	UNP Q8RTE3
B	479	HIS	-	EXPRESSION TAG	UNP Q8RTE3
C	474	HIS	-	EXPRESSION TAG	UNP Q8RTE3
C	475	HIS	-	EXPRESSION TAG	UNP Q8RTE3
C	476	HIS	-	EXPRESSION TAG	UNP Q8RTE3
C	477	HIS	-	EXPRESSION TAG	UNP Q8RTE3
C	478	HIS	-	EXPRESSION TAG	UNP Q8RTE3
C	479	HIS	-	EXPRESSION TAG	UNP Q8RTE3

- Molecule 2 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: C<sub>16</sub>H<sub>34</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 21	C 16	O 5	0	0
2	A	1	Total 21	C 16	O 5	0	0
2	A	1	Total 21	C 16	O 5	0	0
2	A	1	Total 21	C 16	O 5	0	0
2	A	1	Total 21	C 16	O 5	0	0
2	A	1	Total 21	C 16	O 5	0	0
2	A	1	Total 21	C 16	O 5	0	0
2	A	1	Total 21	C 16	O 5	0	0
2	B	1	Total 21	C 16	O 5	0	0
2	B	1	Total 21	C 16	O 5	0	0
2	B	1	Total 21	C 16	O 5	0	0
2	B	1	Total 21	C 16	O 5	0	0
2	B	1	Total 21	C 16	O 5	0	0
2	C	1	Total 21	C 16	O 5	0	0
2	C	1	Total 21	C 16	O 5	0	0

*Continued on next page...*

Continued from previous page...

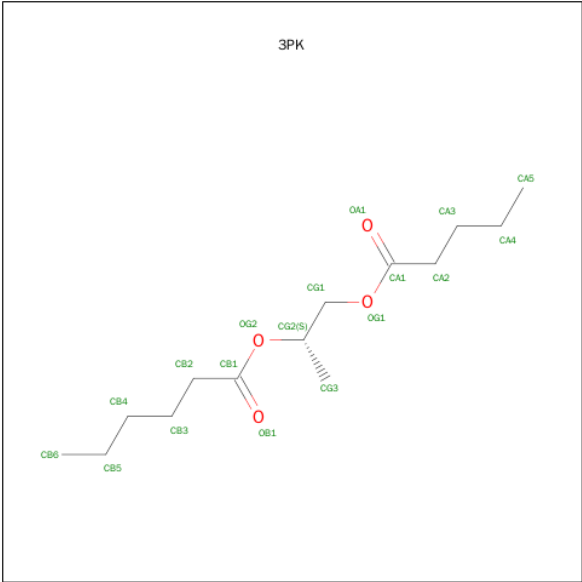
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			21	16	5		
2	C	1	Total	C	O	0	0
			21	16	5		
2	C	1	Total	C	O	0	0
			21	16	5		
2	C	1	Total	C	O	0	0
			21	16	5		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 4 is (2S)-1-(PENTANOYLOXY)PROPAN-2-YL HEXANOATE (three-letter code: 3PK) (formula: C<sub>14</sub>H<sub>26</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			17	13	4		
4	B	1	Total	C	O	0	0
			14	10	4		
4	C	1	Total	C	O	0	0
			15	11	4		

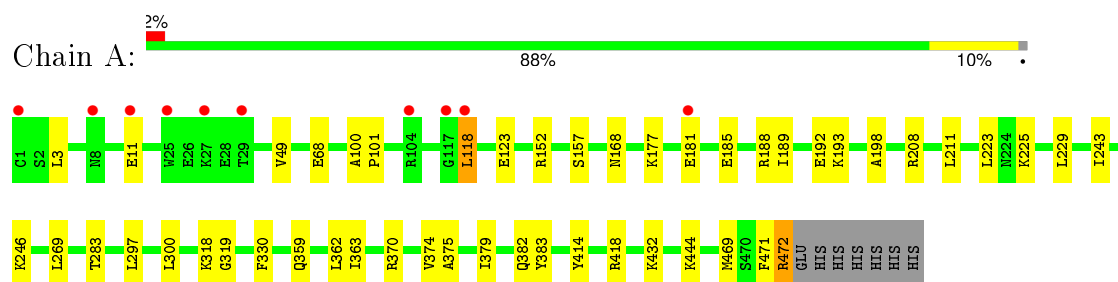
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	194	Total	O	0	0
			194	194		
5	B	185	Total	O	0	0
			185	185		
5	C	180	Total	O	0	0
			180	180		

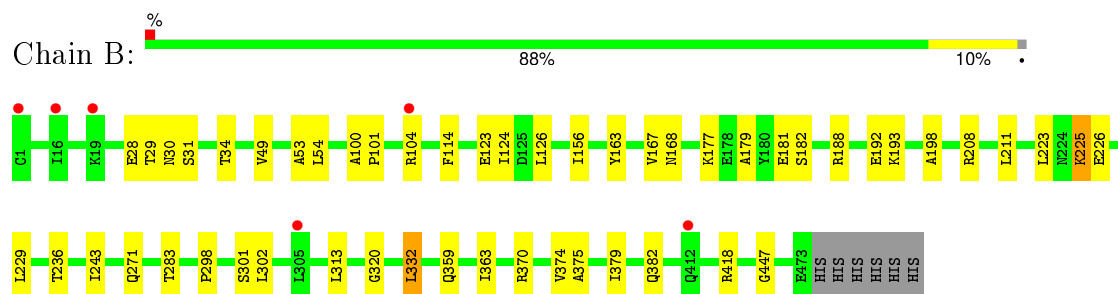
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). 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.

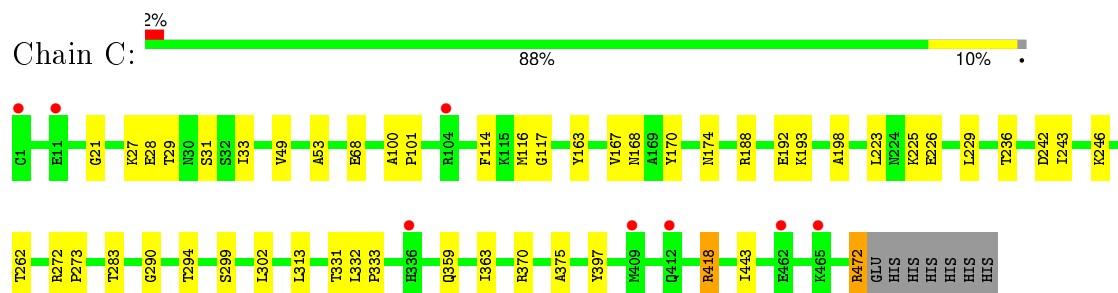
#### • Molecule 1: CmeC



#### • Molecule 1: CmeC



#### • Molecule 1: CmeC





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.83Å 146.32Å 418.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.37 104.72 – 2.37	Depositor EDS
% Data completeness (in resolution range)	98.2 (100.00-2.37) 98.4 (104.72-2.37)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 2.37Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1439)	Depositor
R, $R_{free}$	0.210 , 0.243 0.222 , 0.252	Depositor DCC
$R_{free}$ test set	5631 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.1	Xtriage
Anisotropy	0.732	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 51.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 112440 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12304	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.51% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 3PK, C8E, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.23	0/3835	0.35	0/5184
1	B	0.21	0/3844	0.35	0/5196
1	C	0.22	0/3846	0.35	0/5199
All	All	0.22	0/11525	0.35	0/15579

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	3765	0	3675	31	0
1	B	3774	0	3681	31	0
1	C	3772	0	3682	31	0
2	A	147	0	238	9	0
2	B	105	0	170	6	0
2	C	126	0	204	5	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	17	0	18	0	0
4	B	14	0	12	6	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	15	0	14	0	0
5	A	194	0	0	2	0
5	B	185	0	0	1	0
5	C	180	0	0	0	0
All	All	12304	0	11694	97	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 4.

All (97) 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)
4:B:507:3PK:H1A2	4:B:507:3PK:CB2	1.43	1.47
4:B:507:3PK:CB2	4:B:507:3PK:CA2	2.30	1.09
2:A:1005:C8E:H82	2:A:1006:C8E:H31	1.49	0.94
4:B:507:3PK:OG1	4:B:507:3PK:CB2	2.30	0.79
4:B:507:3PK:CG1	4:B:507:3PK:CB2	2.66	0.74
1:B:298:PRO:HG3	1:B:332:LEU:HG	1.73	0.70
4:B:507:3PK:CA1	4:B:507:3PK:CB2	2.71	0.68
1:A:375:ALA:HA	1:B:223:LEU:HD11	1.76	0.67
1:A:471:PHE:CD1	1:A:472:ARG:N	2.65	0.65
1:A:319:GLY:H	2:A:1007:C8E:H171	1.62	0.65
1:B:182:SER:HB2	1:B:418:ARG:HH22	1.63	0.64
2:A:1004:C8E:H171	2:B:503:C8E:H171	1.80	0.61
2:A:1009:C8E:H31	1:C:302:LEU:HD21	1.83	0.60
1:B:49:VAL:HG22	1:B:236:THR:HG21	1.84	0.60
1:C:27:LYS:NZ	1:C:28:GLU:O	2.30	0.60
1:C:313:LEU:H	2:C:504:C8E:H191	1.68	0.59
1:A:223:LEU:HD11	1:C:375:ALA:HA	1.85	0.58
1:B:320:GLY:H	2:B:506:C8E:H202	1.67	0.58
1:C:29:THR:HG22	1:C:31:SER:H	1.70	0.57
1:B:126:LEU:HD23	4:B:507:3PK:H2A2	1.88	0.55
1:B:375:ALA:HA	1:C:223:LEU:HD11	1.88	0.55
1:A:188:ARG:NH1	1:A:192:GLU:OE2	2.39	0.55
1:A:469:MET:O	1:A:472:ARG:HG3	2.07	0.54
1:C:116:MET:HG2	2:C:502:C8E:H141	1.90	0.54
1:B:379:ILE:HA	1:B:382:GLN:HE21	1.73	0.53
1:A:118:LEU:HD22	2:A:1006:C8E:H131	1.91	0.53
1:A:68:GLU:OE1	1:A:472:ARG:NH2	2.39	0.53
1:B:313:LEU:H	2:B:502:C8E:H192	1.74	0.53
1:C:188:ARG:NH1	1:C:192:GLU:OE2	2.42	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:ILE:HD11	1:B:302:LEU:HD22	1.91	0.52
1:A:300:LEU:HD13	1:A:330:PHE:HD1	1.74	0.52
1:A:370:ARG:HD2	1:B:243:ILE:O	2.10	0.51
1:A:193:LYS:HB3	1:A:198:ALA:HB3	1.91	0.51
1:B:123:GLU:OE2	1:B:301:SER:OG	2.28	0.51
1:B:29:THR:HG22	1:B:31:SER:H	1.75	0.50
1:A:374:VAL:HG11	1:B:226:GLU:HG3	1.94	0.50
1:C:193:LYS:HB3	1:C:198:ALA:HB3	1.93	0.50
1:C:299:SER:OG	1:C:331:THR:OG1	2.30	0.50
1:B:182:SER:HB2	1:B:418:ARG:NH2	2.27	0.50
1:A:243:ILE:O	1:C:370:ARG:HD2	2.12	0.49
1:A:3:LEU:HD11	1:A:297:LEU:HD12	1.94	0.49
1:B:114:PHE:HZ	2:B:502:C8E:H162	1.79	0.48
1:A:359:GLN:O	1:A:363:ILE:HG12	2.14	0.48
1:B:193:LYS:HB3	1:B:198:ALA:HB3	1.96	0.48
2:A:1002:C8E:H71	2:C:501:C8E:H82	1.97	0.47
1:A:208:ARG:NH2	5:A:1267:HOH:O	2.48	0.47
1:B:370:ARG:HD2	1:C:243:ILE:O	2.14	0.47
1:C:33:ILE:HG21	1:C:443:ILE:HG23	1.97	0.47
1:B:53:ALA:HB2	1:B:236:THR:HG22	1.97	0.46
1:C:114:PHE:HZ	2:C:504:C8E:H162	1.81	0.46
2:B:502:C8E:H12	2:B:503:C8E:H13	1.97	0.46
1:B:374:VAL:HG11	1:C:226:GLU:HG3	1.98	0.45
1:B:223:LEU:HD12	1:B:223:LEU:HA	1.82	0.45
1:B:225:LYS:HB3	1:B:225:LYS:HE3	1.88	0.45
1:B:179:ALA:O	1:B:418:ARG:NH2	2.47	0.44
1:B:54:LEU:HD21	1:B:156:ILE:HD11	1.98	0.44
1:A:157:SER:HB3	1:A:444:LYS:HE2	2.00	0.44
1:A:471:PHE:CE1	1:A:472:ARG:HG2	2.53	0.44
1:B:177:LYS:O	1:B:181:GLU:HG2	2.18	0.44
1:C:170:TYR:CZ	1:C:225:LYS:HD3	2.53	0.43
1:A:246:LYS:HE2	1:A:246:LYS:HB3	1.79	0.43
1:A:225:LYS:HB3	1:A:225:LYS:HE3	1.89	0.43
1:C:332:LEU:HD22	1:C:333:PRO:HD2	2.00	0.43
1:A:269:LEU:HD11	1:A:362:LEU:HD21	2.01	0.43
1:B:188:ARG:NH1	1:B:192:GLU:OE2	2.51	0.43
1:A:177:LYS:O	1:A:181:GLU:HG2	2.19	0.43
1:C:242:ASP:HA	1:C:246:LYS:HD3	2.01	0.43
1:A:471:PHE:CD1	1:A:471:PHE:C	2.92	0.43
1:C:68:GLU:OE1	1:C:472:ARG:NH2	2.47	0.43
2:A:1005:C8E:H102	2:A:1005:C8E:H132	1.78	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:502:C8E:H171	2:B:502:C8E:H201	1.70	0.42
1:C:359:GLN:O	1:C:363:ILE:HG12	2.19	0.42
1:C:100:ALA:HA	1:C:101:PRO:HD3	1.93	0.42
1:A:152:ARG:NH2	5:A:1215:HOH:O	2.53	0.42
1:C:21:GLY:N	1:C:262:THR:O	2.49	0.42
1:C:397:TYR:CE1	1:C:418:ARG:HG2	2.55	0.42
1:A:379:ILE:HA	1:A:382:GLN:HE21	1.84	0.41
1:C:163:TYR:O	1:C:167:VAL:HG23	2.20	0.41
1:C:272:ARG:HA	1:C:273:PRO:HD3	1.90	0.41
1:A:414:TYR:O	1:A:418:ARG:HG3	2.21	0.41
1:A:318:LYS:HD2	2:A:1007:C8E:H172	2.03	0.41
1:C:223:LEU:HA	1:C:223:LEU:HD12	1.86	0.41
1:C:225:LYS:HB3	1:C:225:LYS:HE2	1.87	0.41
1:B:163:TYR:O	1:B:167:VAL:HG23	2.21	0.41
1:A:100:ALA:HA	1:A:101:PRO:HD3	1.92	0.41
1:B:359:GLN:O	1:B:363:ILE:HG12	2.20	0.40
1:A:68:GLU:CD	1:A:472:ARG:HH22	2.24	0.40
1:B:30:ASN:ND2	5:B:711:HOH:O	2.46	0.40
1:C:53:ALA:HB2	1:C:236:THR:HG22	2.02	0.40
1:A:185:GLU:O	1:A:189:ILE:HG12	2.21	0.40
1:C:290:GLY:O	1:C:294:THR:HG23	2.21	0.40
2:A:1005:C8E:H161	2:A:1005:C8E:H191	1.78	0.40
1:C:117:GLY:HA2	2:C:502:C8E:H102	2.03	0.40
1:C:33:ILE:HD13	1:C:443:ILE:HG23	2.03	0.40
1:B:100:ALA:HA	1:B:101:PRO:HD3	1.91	0.40
1:B:271:GLN:O	1:B:447:GLY:HA3	2.22	0.40
1:A:383:TYR:HE2	1:A:432:LYS:HG3	1.87	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	470/479 (98%)	463 (98%)	7 (2%)	0	100	100
1	B	471/479 (98%)	465 (99%)	6 (1%)	0	100	100
1	C	471/479 (98%)	465 (99%)	6 (1%)	0	100	100
All	All	1412/1437 (98%)	1393 (99%)	19 (1%)	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	403/410 (98%)	394 (98%)	9 (2%)	60	78
1	B	404/410 (98%)	394 (98%)	10 (2%)	55	74
1	C	404/410 (98%)	397 (98%)	7 (2%)	68	84
All	All	1211/1230 (98%)	1185 (98%)	26 (2%)	61	79

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLU
1	A	49	VAL
1	A	118	LEU
1	A	123	GLU
1	A	168	ASN
1	A	211	LEU
1	A	229	LEU
1	A	283	THR
1	A	472	ARG
1	B	28	GLU
1	B	34	THR
1	B	104	ARG
1	B	168	ASN
1	B	208	ARG
1	B	211	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	225	LYS
1	B	229	LEU
1	B	283	THR
1	B	332	LEU
1	C	49	VAL
1	C	168	ASN
1	C	174	ASN
1	C	229	LEU
1	C	283	THR
1	C	418	ARG
1	C	472	ARG

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

Mol	Chain	Res	Type
1	A	382	GLN
1	B	382	GLN

### 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](#)

23 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	C8E	A	1001	-	20,20,20	0.62	0	19,19,19	1.39	1 (5%)
2	C8E	A	1002	-	20,20,20	0.63	0	19,19,19	1.30	0
3	SO4	A	1003	-	4,4,4	0.24	0	6,6,6	0.11	0
2	C8E	A	1004	-	20,20,20	0.63	0	19,19,19	1.34	0
2	C8E	A	1005	-	20,20,20	0.62	0	19,19,19	1.34	0
2	C8E	A	1006	-	20,20,20	1.15	1 (5%)	19,19,19	1.58	6 (31%)
2	C8E	A	1007	-	20,20,20	0.61	0	19,19,19	1.35	0
4	3PK	A	1008	1	16,16,17	1.93	3 (18%)	18,18,19	2.03	7 (38%)
2	C8E	A	1009	-	20,20,20	0.61	0	19,19,19	1.34	0
3	SO4	B	501	-	4,4,4	0.25	0	6,6,6	0.10	0
2	C8E	B	502	-	20,20,20	0.63	0	19,19,19	1.29	0
2	C8E	B	503	-	20,20,20	0.61	0	19,19,19	1.34	1 (5%)
2	C8E	B	504	-	20,20,20	0.60	0	19,19,19	1.36	1 (5%)
2	C8E	B	505	-	20,20,20	0.61	0	19,19,19	1.37	1 (5%)
2	C8E	B	506	-	20,20,20	0.62	0	19,19,19	1.33	0
4	3PK	B	507	1	13,13,17	2.30	2 (15%)	14,15,19	2.15	4 (28%)
2	C8E	C	501	-	20,20,20	0.60	0	19,19,19	1.37	1 (5%)
2	C8E	C	502	-	20,20,20	0.62	0	19,19,19	1.32	1 (5%)
2	C8E	C	503	-	20,20,20	0.61	0	19,19,19	1.34	1 (5%)
2	C8E	C	504	-	20,20,20	0.62	0	19,19,19	1.29	0
2	C8E	C	505	-	20,20,20	0.61	0	19,19,19	1.33	0
2	C8E	C	506	-	20,20,20	0.62	0	19,19,19	1.38	0
4	3PK	C	507	1	14,14,17	1.95	2 (14%)	16,16,19	1.88	6 (37%)

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	C8E	A	1001	-	-	0/18/18/18	0/0/0/0
2	C8E	A	1002	-	-	0/18/18/18	0/0/0/0
3	SO4	A	1003	-	-	0/0/0/0	0/0/0/0
2	C8E	A	1004	-	-	0/18/18/18	0/0/0/0
2	C8E	A	1005	-	-	0/18/18/18	0/0/0/0
2	C8E	A	1006	-	-	0/18/18/18	0/0/0/0
2	C8E	A	1007	-	-	0/18/18/18	0/0/0/0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	3PK	A	1008	1	-	0/17/17/18	0/0/0/0
2	C8E	A	1009	-	-	0/18/18/18	0/0/0/0
3	SO4	B	501	-	-	0/0/0/0	0/0/0/0
2	C8E	B	502	-	-	0/18/18/18	0/0/0/0
2	C8E	B	503	-	-	0/18/18/18	0/0/0/0
2	C8E	B	504	-	-	0/18/18/18	0/0/0/0
2	C8E	B	505	-	-	0/18/18/18	0/0/0/0
2	C8E	B	506	-	-	0/18/18/18	0/0/0/0
4	3PK	B	507	1	-	0/13/13/18	0/0/0/0
2	C8E	C	501	-	-	0/18/18/18	0/0/0/0
2	C8E	C	502	-	-	0/18/18/18	0/0/0/0
2	C8E	C	503	-	-	0/18/18/18	0/0/0/0
2	C8E	C	504	-	-	0/18/18/18	0/0/0/0
2	C8E	C	505	-	-	0/18/18/18	0/0/0/0
2	C8E	C	506	-	-	0/18/18/18	0/0/0/0
4	3PK	C	507	1	-	0/15/15/18	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	507	3PK	OG2-CG2	-6.94	1.34	1.47
4	A	1008	3PK	OG2-CG2	-6.01	1.36	1.47
4	C	507	3PK	OG2-CG2	-5.66	1.36	1.47
4	C	507	3PK	OG1-CG1	-3.87	1.36	1.45
4	B	507	3PK	OG1-CG1	-3.79	1.36	1.45
4	A	1008	3PK	OG1-CG1	-3.56	1.37	1.45
2	A	1006	C8E	O18-C19	-2.57	1.31	1.42
4	A	1008	3PK	CB5-CB4	-2.07	1.36	1.51

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	507	3PK	OG2-CB1-OB1	-5.34	112.25	122.92
4	C	507	3PK	OG1-CA1-OA1	-4.24	112.54	123.49
2	A	1006	C8E	C6-C7-C8	-2.75	101.17	113.47
4	A	1008	3PK	OG1-CA1-OA1	-2.40	117.31	123.49
4	C	507	3PK	OG2-CB1-OB1	-2.35	117.36	123.67
4	B	507	3PK	OG1-CA1-OA1	-2.25	117.69	123.49
4	B	507	3PK	OB1-CB1-CB2	-2.05	117.28	124.85
2	A	1006	C8E	O15-C16-C17	2.01	119.29	110.36
2	A	1001	C8E	O18-C17-C16	2.01	119.30	110.36
2	C	503	C8E	O9-C8-C7	2.01	117.93	109.87

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	C8E	O9-C8-C7	2.02	117.97	109.87
2	B	504	C8E	O9-C8-C7	2.03	118.02	109.87
4	C	507	3PK	OG1-CG1-CG2	2.06	114.14	108.61
2	C	502	C8E	O9-C8-C7	2.12	118.36	109.87
4	C	507	3PK	OG2-CB1-CB2	2.14	118.73	110.96
2	B	503	C8E	O9-C8-C7	2.16	118.51	109.87
2	B	505	C8E	O9-C8-C7	2.16	118.51	109.87
4	C	507	3PK	OG2-CG2-CG1	2.35	111.22	105.90
4	A	1008	3PK	OG1-CA1-CA2	2.37	119.13	111.90
2	A	1006	C8E	O21-C20-C19	2.37	126.68	112.03
4	A	1008	3PK	CG2-OG2-CB1	2.45	121.08	117.92
4	A	1008	3PK	OG2-CG2-CG3	2.54	113.61	107.88
2	A	1006	C8E	O9-C8-C7	2.54	120.05	109.87
2	A	1006	C8E	C16-O15-C14	2.54	124.23	113.31
4	C	507	3PK	OG1-CA1-CA2	2.70	120.13	111.90
4	A	1008	3PK	CG1-OG1-CA1	2.79	124.64	116.85
4	A	1008	3PK	OG1-CG1-CG2	2.92	116.42	108.61
2	A	1006	C8E	O18-C17-C16	3.07	124.01	110.36
4	B	507	3PK	OG2-CG2-CG1	3.26	113.29	105.90
4	A	1008	3PK	OG2-CB1-CB2	4.27	120.80	111.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1002	C8E	1	0
2	A	1004	C8E	1	0
2	A	1005	C8E	3	0
2	A	1006	C8E	2	0
2	A	1007	C8E	2	0
2	A	1009	C8E	1	0
2	B	502	C8E	4	0
2	B	503	C8E	2	0
2	B	506	C8E	1	0
4	B	507	3PK	6	0
2	C	501	C8E	1	0
2	C	502	C8E	2	0
2	C	504	C8E	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	472/479 (98%)	0.60	10 (2%) 67 70	36, 52, 77, 101	0
1	B	473/479 (98%)	0.57	6 (1%) 79 81	37, 52, 76, 107	0
1	C	472/479 (98%)	0.61	8 (1%) 73 75	38, 52, 76, 105	0
All	All	1417/1437 (98%)	0.60	24 (1%) 73 75	36, 52, 77, 107	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	104	ARG	6.2
1	A	104	ARG	4.2
1	A	27	LYS	3.9
1	C	409	MET	3.5
1	A	29	THR	3.3
1	C	336[A]	HIS	3.3
1	B	104	ARG	3.2
1	A	11	GLU	3.1
1	C	462	GLU	3.1
1	A	25	TRP	2.7
1	B	16	ILE	2.7
1	B	1	CYS	2.5
1	B	412	GLN	2.4
1	C	1	CYS	2.4
1	A	118	LEU	2.3
1	C	412	GLN	2.3
1	B	19	LYS	2.2
1	A	1	CYS	2.1
1	A	8	ASN	2.1
1	A	117	GLY	2.1
1	C	11	GLU	2.1
1	C	465	LYS	2.1
1	B	305	LEU	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	181	GLU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	C8E	A	1005	21/21	0.81	0.29	6.07	48,68,91,92	0
2	C8E	C	502	21/21	0.78	0.28	5.82	51,66,94,108	0
2	C8E	B	502	21/21	0.85	0.34	5.39	50,66,94,100	0
2	C8E	C	504	21/21	0.78	0.31	5.08	46,69,98,102	0
3	SO4	B	501	5/5	0.93	0.24	4.39	58,61,73,73	0
2	C8E	C	501	21/21	0.90	0.23	2.47	44,60,69,71	0
2	C8E	B	504	21/21	0.89	0.24	1.94	40,61,77,78	0
2	C8E	A	1004	21/21	0.84	0.24	1.72	44,56,71,76	0
2	C8E	B	505	21/21	0.79	0.24	1.66	57,72,93,109	0
2	C8E	A	1009	21/21	0.85	0.23	1.50	59,66,95,105	0
2	C8E	B	506	21/21	0.71	0.23	1.41	57,78,95,111	0
4	3PK	C	507	15/18	0.83	0.21	0.85	68,77,96,96	0
2	C8E	A	1006	21/21	0.74	0.22	0.39	57,71,87,95	0
4	3PK	A	1008	17/18	0.89	0.18	0.09	63,76,89,91	0
2	C8E	C	503	21/21	0.84	0.18	-0.10	58,72,84,96	0
2	C8E	A	1007	21/21	0.80	0.15	-1.16	55,75,91,94	0
3	SO4	A	1003	5/5	0.96	0.16	-1.18	55,63,73,74	0
2	C8E	C	505	21/21	0.85	0.37	-	42,80,95,110	0
2	C8E	C	506	21/21	0.81	0.27	-	55,74,89,96	0
2	C8E	A	1001	21/21	0.81	0.30	-	33,76,91,95	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	C8E	B	503	21/21	0.86	0.34	-	28,64,97,111	0
2	C8E	A	1002	21/21	0.83	0.24	-	44,68,84,87	0
4	3PK	B	507	14/18	0.88	0.27	-	77,85,92,101	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.