



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 03:25 am BST

PDB ID : 4FXT  
Title : Crystal structure of a DUF3823 family protein (BACOVA\_02663) from *Bacteroides ovatus* ATCC 8483 at 2.77 Å resolution  
Authors : Joint Center for Structural Genomics (JCSG)  
Deposited on : 2012-07-03  
Resolution : 2.77 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.

---

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

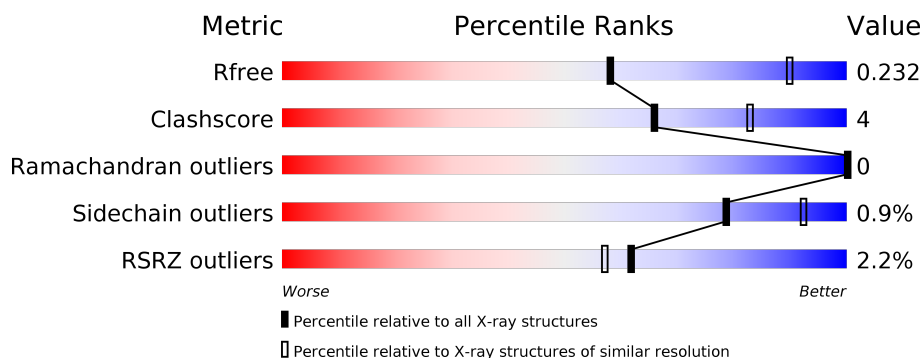
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.77 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	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	202	
1	B	202	
1	C	202	
1	D	202	
1	E	202	
1	F	202	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	202	
1	H	202	
1	I	202	
1	J	202	
1	K	202	
1	L	202	
1	M	202	
1	N	202	

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	EDO	B	302	-	-	-	X

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 21144 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	193	Total	C	N	O	S	Se	0	0	0
			1475	932	244	296	1	2			
1	B	193	Total	C	N	O	S	Se	0	1	0
			1489	941	248	297	1	2			
1	C	191	Total	C	N	O	S	Se	0	0	0
			1460	923	242	292	1	2			
1	D	192	Total	C	N	O	S	Se	0	0	0
			1470	927	246	294	1	2			
1	E	202	Total	C	N	O	S	Se	0	0	0
			1545	979	257	306	1	2			
1	F	197	Total	C	N	O	S	Se	0	0	0
			1515	958	252	302	1	2			
1	G	196	Total	C	N	O	S	Se	0	0	0
			1505	952	251	300	1	1			
1	H	196	Total	C	N	O	S	Se	0	0	0
			1502	951	248	300	1	2			
1	I	191	Total	C	N	O	S	Se	0	0	0
			1468	928	243	294	1	2			
1	J	197	Total	C	N	O	S	Se	0	0	0
			1509	953	252	301	1	2			
1	K	193	Total	C	N	O	S	Se	0	0	0
			1485	939	248	295	1	2			
1	L	191	Total	C	N	O	S	Se	0	1	0
			1473	929	247	294	1	2			
1	M	195	Total	C	N	O	S	Se	0	0	0
			1506	953	250	300	1	2			
1	N	188	Total	C	N	O	S	Se	0	1	0
			1447	915	240	289	1	2			

There are 14 discrepancies between the modelled and reference sequences:

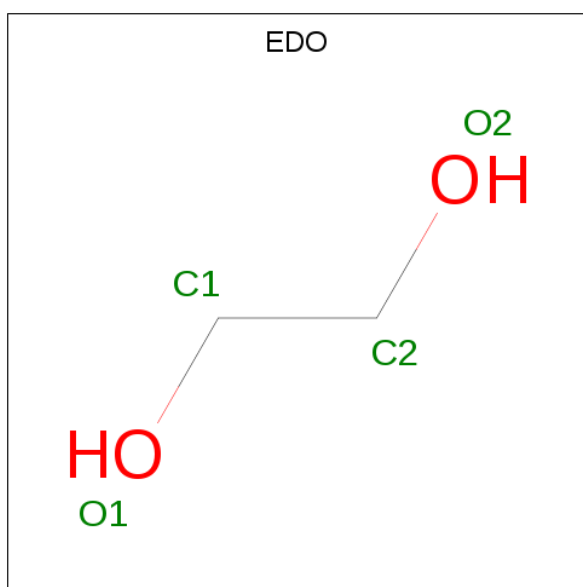
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	leader sequence	UNP A7LXU7

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	leader sequence	UNP A7LXU7
C	0	GLY	-	leader sequence	UNP A7LXU7
D	0	GLY	-	leader sequence	UNP A7LXU7
E	0	GLY	-	leader sequence	UNP A7LXU7
F	0	GLY	-	leader sequence	UNP A7LXU7
G	0	GLY	-	leader sequence	UNP A7LXU7
H	0	GLY	-	leader sequence	UNP A7LXU7
I	0	GLY	-	leader sequence	UNP A7LXU7
J	0	GLY	-	leader sequence	UNP A7LXU7
K	0	GLY	-	leader sequence	UNP A7LXU7
L	0	GLY	-	leader sequence	UNP A7LXU7
M	0	GLY	-	leader sequence	UNP A7LXU7
N	0	GLY	-	leader sequence	UNP A7LXU7

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total C O 4 2 2	0	0
2	E	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	G	1	Total C O 4 2 2	0	0
2	H	1	Total C O 4 2 2	0	0
2	I	1	Total C O 4 2 2	0	0
2	J	1	Total C O 4 2 2	0	0
2	K	1	Total C O 4 2 2	0	0
2	L	1	Total C O 4 2 2	0	0
2	M	1	Total C O 4 2 2	0	0
2	N	1	Total C O 4 2 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	24	Total O 24 24	0	0
3	B	31	Total O 31 31	0	0
3	C	13	Total O 13 13	0	0
3	D	21	Total O 21 21	0	0
3	E	15	Total O 15 15	0	0
3	F	19	Total O 19 19	0	0
3	G	21	Total O 21 21	0	0
3	H	16	Total O 16 16	0	0

*Continued on next page...*

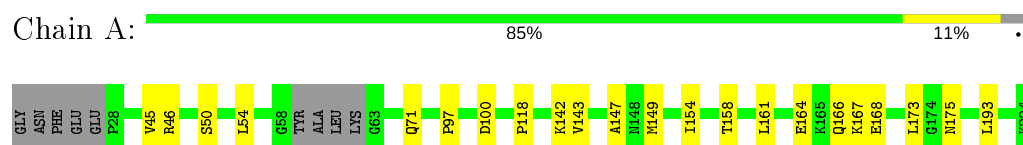
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	I	17	Total 17	O 17	0	0
3	J	12	Total 12	O 12	0	0
3	K	14	Total 14	O 14	0	0
3	L	8	Total 8	O 8	0	0
3	M	10	Total 10	O 10	0	0
3	N	10	Total 10	O 10	0	0

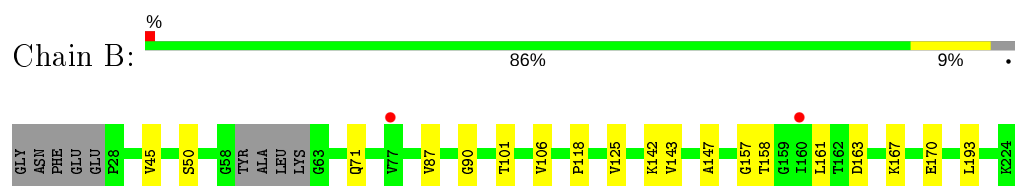
### 3 Residue-property plots [i](#)

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.

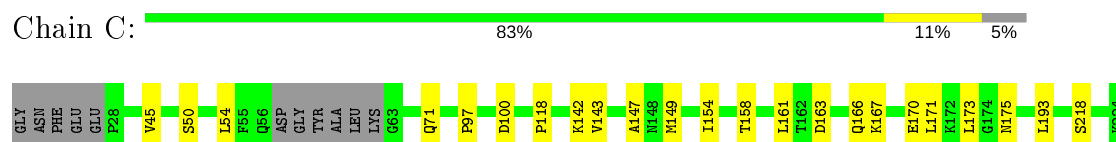
- Molecule 1: Uncharacterized protein



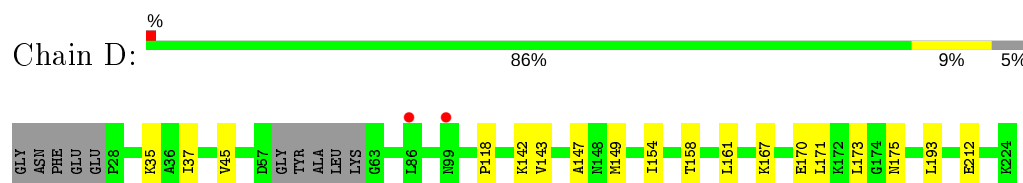
- Molecule 1: Uncharacterized protein



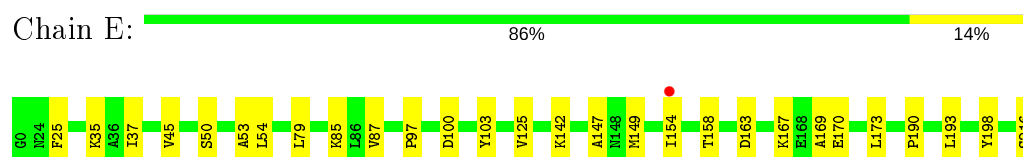
- Molecule 1: Uncharacterized protein



- Molecule 1: Uncharacterized protein

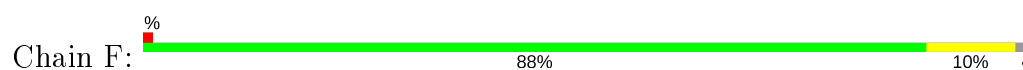


- Molecule 1: Uncharacterized protein



- Molecule 1: Uncharacterized protein

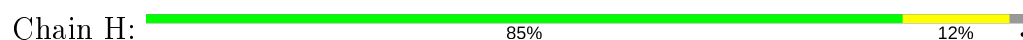




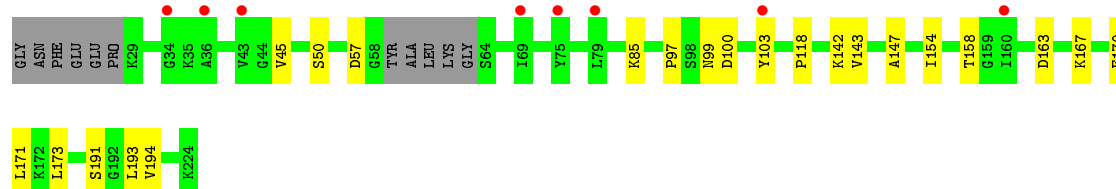
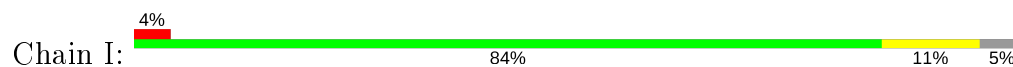
- Molecule 1: Uncharacterized protein



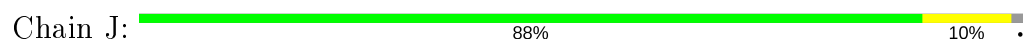
- Molecule 1: Uncharacterized protein



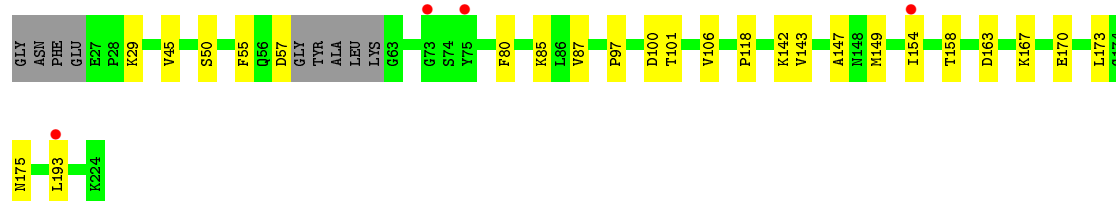
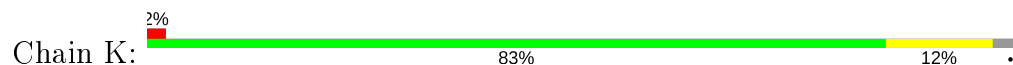
- Molecule 1: Uncharacterized protein



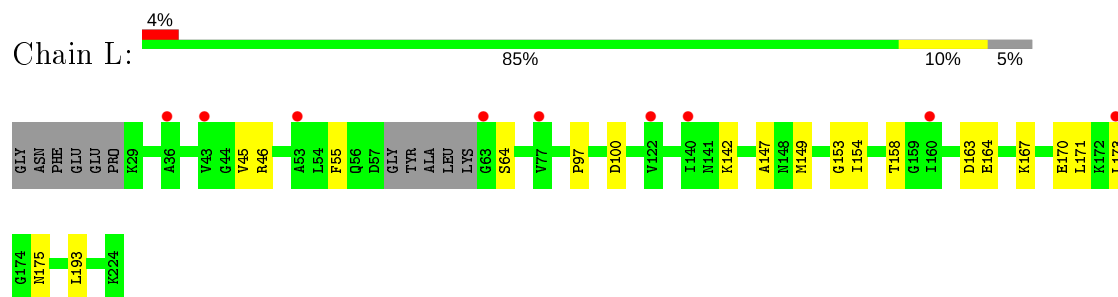
- Molecule 1: Uncharacterized protein



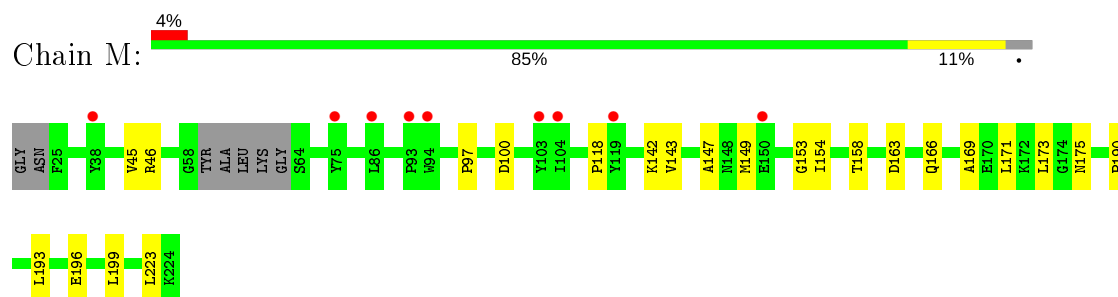
- Molecule 1: Uncharacterized protein



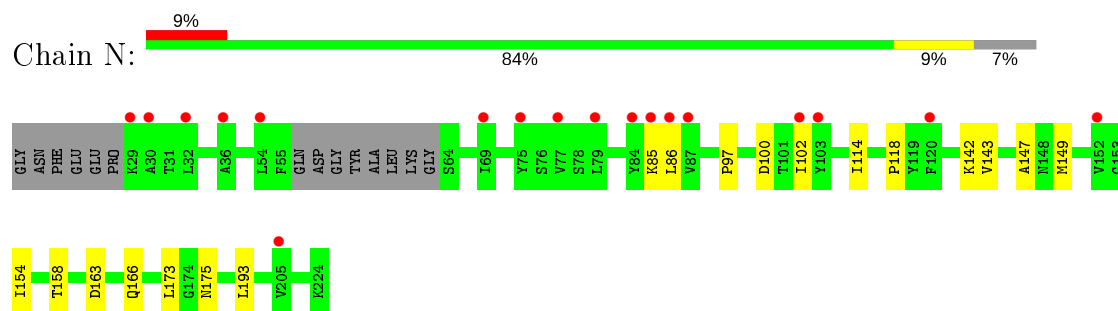
- Molecule 1: Uncharacterized protein



- Molecule 1: Uncharacterized protein



- Molecule 1: Uncharacterized protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.81Å 351.00Å 90.34Å 90.00° 93.42° 90.00°	Depositor
Resolution (Å)	49.08 – 2.77 48.06 – 2.77	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.08-2.77) 99.8 (48.06-2.77)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.97 (at 2.77Å)	Xtriage
Refinement program	BUSTER-TNT 2.10.0, BUSTER 2.10.0	Depositor
R, $R_{free}$	0.183 , 0.217 0.200 , 0.232	Depositor DCC
$R_{free}$ test set	4158 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.9	Xtriage
Anisotropy	0.607	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 58.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	21144	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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: 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	0.57	0/1498	0.75	0/2025
1	B	0.56	0/1515	0.78	0/2046
1	C	0.51	0/1483	0.73	0/2005
1	D	0.50	0/1492	0.73	0/2016
1	E	0.51	0/1571	0.74	0/2125
1	F	0.51	0/1539	0.74	0/2079
1	G	0.50	0/1529	0.75	0/2068
1	H	0.57	0/1526	0.76	0/2064
1	I	0.50	0/1490	0.72	0/2013
1	J	0.52	0/1534	0.76	0/2074
1	K	0.51	0/1508	0.74	0/2038
1	L	0.49	0/1497	0.73	0/2021
1	M	0.51	0/1530	0.74	0/2067
1	N	0.51	0/1471	0.74	0/1988
All	All	0.52	0/21183	0.74	0/28629

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	1475	0	1448	14	0
1	B	1489	0	1471	11	0
1	C	1460	0	1432	14	0
1	D	1470	0	1449	12	0
1	E	1545	0	1518	17	0
1	F	1515	0	1488	13	0
1	G	1505	0	1483	13	0
1	H	1502	0	1479	14	0
1	I	1468	0	1448	11	0
1	J	1509	0	1480	10	0
1	K	1485	0	1465	11	0
1	L	1473	0	1460	12	0
1	M	1506	0	1483	12	0
1	N	1447	0	1434	9	0
2	A	4	0	6	0	0
2	B	12	0	18	2	0
2	C	4	0	6	1	0
2	D	4	0	6	0	0
2	E	4	0	6	0	0
2	F	4	0	6	2	0
2	G	4	0	6	0	0
2	H	4	0	6	0	0
2	I	4	0	6	0	0
2	J	4	0	6	0	0
2	K	4	0	6	0	0
2	L	4	0	6	0	0
2	M	4	0	6	1	0
2	N	4	0	6	1	0
3	A	24	0	0	0	0
3	B	31	0	0	2	0
3	C	13	0	0	0	0
3	D	21	0	0	1	0
3	E	15	0	0	2	0
3	F	19	0	0	0	0
3	G	21	0	0	0	0
3	H	16	0	0	0	0
3	I	17	0	0	1	0
3	J	12	0	0	0	0
3	K	14	0	0	0	0
3	L	8	0	0	0	0
3	M	10	0	0	0	0
3	N	10	0	0	0	0
All	All	21144	0	20634	164	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 (164) 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:E:169:ALA:HB2	1:E:190:PRO:HG3	1.64	0.79
1:H:164:GLU:O	1:H:167:LYS:HE3	1.83	0.78
1:A:168:GLU:HG2	1:A:193:LEU:HD13	1.72	0.70
1:F:158:THR:H	2:F:301:EDO:H21	1.57	0.70
1:D:161:LEU:HD11	1:G:171:LEU:HD11	1.73	0.69
1:C:161:LEU:HD11	1:D:171:LEU:HD11	1.79	0.65
1:B:161:LEU:HD11	1:C:171:LEU:HD11	1.80	0.63
1:K:167:LYS:HD2	1:K:170:GLU:HB3	1.80	0.63
1:B:157:GLY:HA3	2:B:301:EDO:H12	1.81	0.62
1:L:164:GLU:O	1:L:167:LYS:HE3	2.00	0.61
1:A:158:THR:HG22	1:A:193:LEU:HD11	1.84	0.59
1:G:158:THR:HG22	1:G:193:LEU:HD13	1.85	0.58
1:M:169:ALA:HB2	1:M:190:PRO:HG3	1.85	0.58
1:K:55:PHE:HB2	1:K:85:LYS:HG3	1.86	0.57
1:I:142:LYS:HE3	1:I:147:ALA:O	2.05	0.57
1:I:158:THR:HG22	1:I:193:LEU:HD13	1.87	0.57
1:M:142:LYS:HE3	1:M:147:ALA:O	2.05	0.56
1:L:158:THR:HG22	1:L:193:LEU:HD13	1.86	0.56
1:C:142:LYS:HE3	1:C:147:ALA:O	2.06	0.56
1:K:142:LYS:HE3	1:K:147:ALA:O	2.06	0.56
1:E:158:THR:HG22	1:E:193:LEU:HD13	1.89	0.55
1:G:97:PRO:HG2	1:G:100:ASP:HB3	1.87	0.55
1:K:87:VAL:CG1	1:K:101:THR:HG22	2.37	0.55
1:M:158:THR:HG22	1:M:193:LEU:HD13	1.88	0.55
1:B:142:LYS:HE3	1:B:147:ALA:O	2.07	0.54
1:H:142:LYS:HE3	1:H:147:ALA:O	2.07	0.54
1:L:142:LYS:HE3	1:L:147:ALA:O	2.08	0.54
1:J:142:LYS:HE3	1:J:147:ALA:O	2.07	0.54
1:A:142:LYS:HE3	1:A:147:ALA:O	2.08	0.54
1:J:158:THR:HG22	1:J:193:LEU:HD13	1.90	0.54
1:D:142:LYS:HE3	1:D:147:ALA:O	2.06	0.54
1:E:142:LYS:HE3	1:E:147:ALA:O	2.07	0.54
1:B:167:LYS:HD2	1:B:170:GLU:HB3	1.91	0.53
1:K:118:PRO:O	1:K:143:VAL:HB	2.08	0.53
1:A:164:GLU:O	1:A:167:LYS:HE3	2.08	0.53
1:F:142:LYS:HE3	1:F:147:ALA:O	2.09	0.53
1:L:154:ILE:HD11	1:L:173:LEU:HD11	1.91	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:GLY:HA3	3:B:430:HOH:O	2.10	0.52
1:I:154:ILE:HD11	1:I:173:LEU:HD11	1.91	0.52
1:D:161:LEU:CD1	1:G:171:LEU:HD11	2.39	0.52
1:L:167:LYS:HD2	1:L:170:GLU:HB3	1.90	0.52
1:N:142:LYS:HE3	1:N:147:ALA:O	2.09	0.52
1:G:142:LYS:HE3	1:G:147:ALA:O	2.10	0.51
1:K:154:ILE:HD11	1:K:173:LEU:HD11	1.92	0.51
1:B:71:GLN:NE2	3:B:407:HOH:O	2.43	0.51
1:F:154:ILE:HD11	1:F:173:LEU:HD11	1.93	0.51
1:I:191:SER:O	1:I:194:VAL:HG12	2.11	0.51
1:D:158:THR:HG22	1:D:193:LEU:HD13	1.92	0.51
1:B:158:THR:HG22	1:B:193:LEU:HD13	1.91	0.51
1:A:154:ILE:HD11	1:A:173:LEU:HD11	1.92	0.50
1:D:118:PRO:O	1:D:143:VAL:HB	2.12	0.50
1:E:149:MSE:CE	3:E:408:HOH:O	2.59	0.50
1:C:71:GLN:HE22	1:C:218:SER:HB3	1.77	0.50
1:K:158:THR:HG22	1:K:193:LEU:HD21	1.95	0.49
1:J:154:ILE:HD11	1:J:173:LEU:HD11	1.95	0.49
1:I:99:ASN:ND2	3:I:406:HOH:O	2.46	0.49
1:H:154:ILE:HD11	1:H:173:LEU:HD11	1.95	0.48
1:M:154:ILE:HD11	1:M:173:LEU:HD11	1.94	0.48
1:N:158:THR:HG22	1:N:193:LEU:HD13	1.95	0.48
1:D:154:ILE:HD11	1:D:173:LEU:HD11	1.94	0.48
1:F:158:THR:HG22	1:F:193:LEU:HD13	1.95	0.48
1:K:29:LYS:HE2	1:K:80:PHE:CE2	2.49	0.48
1:C:149:MSE:HE3	1:C:175:ASN:O	2.14	0.48
1:F:161:LEU:HD11	1:I:171:LEU:HD11	1.95	0.48
1:F:158:THR:H	2:F:301:EDO:C2	2.25	0.47
1:N:85:LYS:HA	1:N:102:ILE:O	2.14	0.47
1:N:154:ILE:HD11	1:N:173:LEU:HD11	1.97	0.47
1:F:97:PRO:HG2	1:F:100:ASP:HB3	1.96	0.47
1:F:35:LYS:HE3	1:F:37:ILE:HD11	1.96	0.47
1:I:167:LYS:HD2	1:I:170:GLU:HB3	1.96	0.47
1:E:154:ILE:HD11	1:E:173:LEU:HD11	1.97	0.47
1:C:154:ILE:HD11	1:C:173:LEU:HD11	1.97	0.47
1:N:118:PRO:O	1:N:143:VAL:HB	2.14	0.47
1:F:167:LYS:HD2	1:F:170:GLU:HB3	1.96	0.47
1:H:149:MSE:HE3	1:H:175:ASN:O	2.14	0.47
1:M:166:GLN:HB3	2:M:301:EDO:H11	1.96	0.47
1:J:97:PRO:HG2	1:J:100:ASP:HB3	1.95	0.47
1:I:45:VAL:HG21	1:I:50:SER:OG	2.15	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:149:MSE:HE3	1:K:175:ASN:O	2.14	0.47
1:F:149:MSE:HE3	1:F:175:ASN:O	2.14	0.46
1:I:85:LYS:HE2	1:I:103:TYR:HE2	1.79	0.46
1:H:31:THR:HG22	1:H:33:THR:HG23	1.97	0.46
1:J:118:PRO:O	1:J:143:VAL:HB	2.14	0.46
1:E:35:LYS:HE3	1:E:37:ILE:HD11	1.98	0.45
1:M:199:LEU:HD12	1:M:199:LEU:C	2.36	0.45
1:D:167:LYS:HD2	1:D:170:GLU:HB3	1.98	0.45
1:H:61:LEU:H	1:H:61:LEU:HD23	1.81	0.45
1:C:71:GLN:HE22	1:C:218:SER:CB	2.30	0.45
1:L:158:THR:HG22	1:L:193:LEU:CD1	2.47	0.45
1:L:149:MSE:HE3	1:L:175:ASN:O	2.17	0.45
1:C:166:GLN:HB3	2:C:301:EDO:H11	1.99	0.45
1:E:97:PRO:HG2	1:E:100:ASP:HB3	1.98	0.45
1:C:161:LEU:CD1	1:D:171:LEU:HD11	2.46	0.45
1:N:97:PRO:HG2	1:N:100:ASP:HB3	1.98	0.45
1:E:149:MSE:HE1	3:E:408:HOH:O	2.17	0.45
1:M:97:PRO:HG2	1:M:100:ASP:HB3	1.99	0.45
1:A:161:LEU:HD11	1:H:171:LEU:HD11	1.98	0.44
1:J:199:LEU:C	1:J:199:LEU:HD12	2.37	0.44
1:A:149:MSE:HE3	1:A:175:ASN:O	2.17	0.44
1:A:97:PRO:HG2	1:A:100:ASP:HB3	1.98	0.44
1:H:97:PRO:HG2	1:H:100:ASP:HB3	2.00	0.44
1:I:97:PRO:HG2	1:I:100:ASP:HB3	2.00	0.44
1:A:158:THR:HG22	1:A:193:LEU:CD1	2.46	0.44
1:G:154:ILE:HD11	1:G:173:LEU:HD11	2.00	0.44
1:M:149:MSE:HE3	1:M:175:ASN:O	2.17	0.44
1:J:45:VAL:HG21	1:J:50:SER:OG	2.18	0.44
1:L:97:PRO:HG2	1:L:100:ASP:HB3	1.99	0.44
1:M:118:PRO:O	1:M:143:VAL:HB	2.18	0.44
1:J:149:MSE:HE3	1:J:175:ASN:O	2.18	0.43
1:C:158:THR:HG22	1:C:193:LEU:HD13	2.00	0.43
1:A:45:VAL:HG21	1:A:50:SER:OG	2.19	0.43
1:H:71:GLN:OE1	1:H:161:LEU:HA	2.19	0.43
1:N:166[A]:GLN:HB3	2:N:301:EDO:H22	2.00	0.43
1:B:125:VAL:H	2:B:302:EDO:H11	1.84	0.43
1:C:97:PRO:HG2	1:C:100:ASP:HB3	2.00	0.43
1:E:53:ALA:HB3	1:E:87:VAL:HG23	1.99	0.43
1:H:153:GLY:HA2	1:H:171:LEU:O	2.18	0.43
1:I:118:PRO:O	1:I:143:VAL:HB	2.18	0.43
1:K:97:PRO:HG2	1:K:100:ASP:HB3	2.00	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:167:LYS:HD2	1:E:170:GLU:HB3	2.01	0.43
1:M:45:VAL:HG22	1:M:46:ARG:H	1.83	0.43
1:D:35:LYS:HE3	1:D:37:ILE:HD11	2.00	0.42
1:E:125:VAL:HG21	1:E:216:SER:CB	2.48	0.42
1:H:45:VAL:HG22	1:H:46:ARG:H	1.83	0.42
1:F:71:GLN:OE1	1:F:161:LEU:HA	2.19	0.42
1:G:45:VAL:HG21	1:G:50:SER:OG	2.20	0.42
1:E:85:LYS:NZ	1:E:103:TYR:HE2	2.17	0.42
1:J:153:GLY:HA2	1:J:171:LEU:O	2.19	0.42
1:H:158:THR:HG22	1:H:193:LEU:HD13	2.00	0.42
1:C:45:VAL:HG21	1:C:50:SER:OG	2.19	0.42
1:E:45:VAL:HG21	1:E:50:SER:OG	2.20	0.42
1:K:45:VAL:HG21	1:K:50:SER:OG	2.20	0.42
1:B:87:VAL:CG1	1:B:101:THR:HG22	2.49	0.42
1:B:118:PRO:O	1:B:143:VAL:HB	2.20	0.42
1:A:54:LEU:HD12	1:A:54:LEU:HA	1.92	0.42
1:E:54:LEU:HD21	1:E:79:LEU:HD11	2.02	0.42
1:L:55:PHE:HB3	1:L:64:SER:HA	2.02	0.42
1:N:149:MSE:HE3	1:N:175:ASN:O	2.20	0.42
1:D:212:GLU:HG3	3:D:401:HOH:O	2.19	0.41
1:E:25:PHE:HB2	1:L:64:SER:O	2.20	0.41
1:A:45:VAL:HG22	1:A:46:ARG:H	1.85	0.41
1:F:45:VAL:HG21	1:F:50:SER:OG	2.20	0.41
1:G:45:VAL:HG22	1:G:46:ARG:H	1.85	0.41
1:D:149:MSE:HE3	1:D:175:ASN:O	2.20	0.41
1:G:167:LYS:HD2	1:G:170:GLU:HB3	2.03	0.41
1:A:118:PRO:O	1:A:143:VAL:HB	2.20	0.41
1:B:45:VAL:HG21	1:B:50:SER:OG	2.21	0.41
1:C:118:PRO:O	1:C:143:VAL:HB	2.20	0.41
1:L:153:GLY:HA2	1:L:171:LEU:O	2.21	0.41
1:M:153:GLY:HA2	1:M:171:LEU:O	2.21	0.40
1:N:86:LEU:HD13	1:N:114:ILE:HG13	2.03	0.40
1:C:167:LYS:HD2	1:C:170:GLU:HB3	2.03	0.40
1:G:149:MSE:HE3	1:G:175:ASN:O	2.21	0.40
1:G:54:LEU:CD2	1:G:79:LEU:HD11	2.51	0.40
1:E:125:VAL:HG21	1:E:216:SER:HB2	2.03	0.40
1:G:61:LEU:N	1:G:61:LEU:HD12	2.36	0.40
1:H:198:TYR:CG	1:H:220:LYS:HE3	2.56	0.40
1:E:198:TYR:CG	1:E:220:LYS:HE3	2.56	0.40
1:G:153:GLY:HA2	1:G:171:LEU:O	2.21	0.40
1:L:45:VAL:HG22	1:L:46:ARG:H	1.86	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:GLN:HE21	1:H:133:LYS:NZ	2.20	0.40
1:F:45:VAL:HG22	1:F:46:ARG:H	1.86	0.40
1:J:158:THR:HG22	1:J:193:LEU:CD1	2.52	0.40
1:M:196:GLU:O	1:M:223:LEU:HB2	2.21	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	189/202 (94%)	186 (98%)	3 (2%)	0	100	100
1	B	190/202 (94%)	184 (97%)	6 (3%)	0	100	100
1	C	187/202 (93%)	183 (98%)	4 (2%)	0	100	100
1	D	188/202 (93%)	185 (98%)	3 (2%)	0	100	100
1	E	200/202 (99%)	193 (96%)	7 (4%)	0	100	100
1	F	193/202 (96%)	189 (98%)	4 (2%)	0	100	100
1	G	194/202 (96%)	189 (97%)	5 (3%)	0	100	100
1	H	194/202 (96%)	189 (97%)	5 (3%)	0	100	100
1	I	187/202 (93%)	184 (98%)	3 (2%)	0	100	100
1	J	195/202 (96%)	192 (98%)	3 (2%)	0	100	100
1	K	189/202 (94%)	185 (98%)	4 (2%)	0	100	100
1	L	188/202 (93%)	185 (98%)	3 (2%)	0	100	100
1	M	191/202 (95%)	185 (97%)	6 (3%)	0	100	100
1	N	185/202 (92%)	182 (98%)	3 (2%)	0	100	100
All	All	2670/2828 (94%)	2611 (98%)	59 (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	160/167 (96%)	159 (99%)	1 (1%)	86	95
1	B	162/167 (97%)	160 (99%)	2 (1%)	71	90
1	C	158/167 (95%)	156 (99%)	2 (1%)	69	89
1	D	160/167 (96%)	159 (99%)	1 (1%)	86	95
1	E	165/167 (99%)	164 (99%)	1 (1%)	86	95
1	F	164/167 (98%)	163 (99%)	1 (1%)	86	95
1	G	162/167 (97%)	162 (100%)	0	100	100
1	H	162/167 (97%)	161 (99%)	1 (1%)	86	95
1	I	160/167 (96%)	158 (99%)	2 (1%)	69	89
1	J	162/167 (97%)	159 (98%)	3 (2%)	57	83
1	K	161/167 (96%)	158 (98%)	3 (2%)	57	83
1	L	161/167 (96%)	160 (99%)	1 (1%)	86	95
1	M	164/167 (98%)	163 (99%)	1 (1%)	86	95
1	N	158/167 (95%)	157 (99%)	1 (1%)	86	95
All	All	2259/2338 (97%)	2239 (99%)	20 (1%)	78	92

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLN
1	B	106	VAL
1	B	163	ASP
1	C	54	LEU
1	C	163	ASP
1	D	45	VAL
1	E	163	ASP
1	F	99	ASN
1	H	106	VAL
1	I	57	ASP
1	I	163	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	J	37	ILE
1	J	54	LEU
1	J	167	LYS
1	K	57	ASP
1	K	106	VAL
1	K	163	ASP
1	L	163	ASP
1	M	163	ASP
1	N	163	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	GLN
1	C	71	GLN
1	D	71	GLN
1	F	99	ASN
1	J	112	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

16 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	EDO	F	301	-	3,3,3	0.65	0	2,2,2	0.35	0
2	EDO	L	301	-	3,3,3	0.78	0	2,2,2	0.28	0
2	EDO	B	301	-	3,3,3	0.66	0	2,2,2	0.09	0
2	EDO	H	301	-	3,3,3	0.87	0	2,2,2	0.31	0
2	EDO	N	301	-	3,3,3	0.74	0	2,2,2	0.04	0
2	EDO	B	302	-	3,3,3	1.11	0	2,2,2	0.10	0
2	EDO	J	301	-	3,3,3	0.71	0	2,2,2	0.10	0
2	EDO	G	301	-	3,3,3	0.84	0	2,2,2	0.22	0
2	EDO	B	303	-	3,3,3	0.70	0	2,2,2	0.22	0
2	EDO	E	301	-	3,3,3	0.70	0	2,2,2	0.11	0
2	EDO	C	301	-	3,3,3	0.68	0	2,2,2	0.08	0
2	EDO	A	301	-	3,3,3	0.77	0	2,2,2	0.27	0
2	EDO	M	301	-	3,3,3	0.65	0	2,2,2	0.33	0
2	EDO	K	301	-	3,3,3	0.69	0	2,2,2	0.13	0
2	EDO	D	301	-	3,3,3	0.66	0	2,2,2	0.10	0
2	EDO	I	301	-	3,3,3	0.68	0	2,2,2	0.22	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
2	EDO	F	301	-	-	1/1/1/1	-
2	EDO	L	301	-	-	0/1/1/1	-
2	EDO	B	301	-	-	0/1/1/1	-
2	EDO	H	301	-	-	0/1/1/1	-
2	EDO	N	301	-	-	0/1/1/1	-
2	EDO	B	302	-	-	0/1/1/1	-
2	EDO	J	301	-	-	0/1/1/1	-
2	EDO	G	301	-	-	0/1/1/1	-
2	EDO	B	303	-	-	0/1/1/1	-
2	EDO	E	301	-	-	0/1/1/1	-
2	EDO	C	301	-	-	0/1/1/1	-
2	EDO	A	301	-	-	0/1/1/1	-
2	EDO	M	301	-	-	0/1/1/1	-
2	EDO	K	301	-	-	0/1/1/1	-
2	EDO	D	301	-	-	0/1/1/1	-
2	EDO	I	301	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	301	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	301	EDO	2	0
2	B	301	EDO	1	0
2	N	301	EDO	1	0
2	B	302	EDO	1	0
2	C	301	EDO	1	0
2	M	301	EDO	1	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	191/202 (94%)	-0.02	0 <span>100</span> <span>100</span>	38, 57, 102, 142	0
1	B	191/202 (94%)	0.08	2 (1%) <span>82</span> <span>80</span>	44, 61, 87, 108	0
1	C	189/202 (93%)	0.07	0 <span>100</span> <span>100</span>	41, 67, 104, 124	0
1	D	190/202 (94%)	0.28	2 (1%) <span>80</span> <span>78</span>	46, 68, 108, 140	0
1	E	200/202 (99%)	0.13	1 (0%) <span>91</span> <span>90</span>	47, 68, 104, 132	0
1	F	195/202 (96%)	0.08	3 (1%) <span>73</span> <span>71</span>	43, 66, 108, 132	0
1	G	194/202 (96%)	0.09	0 <span>100</span> <span>100</span>	43, 68, 94, 117	0
1	H	194/202 (96%)	0.06	1 (0%) <span>91</span> <span>90</span>	34, 61, 102, 122	0
1	I	189/202 (93%)	0.32	8 (4%) <span>36</span> <span>30</span>	50, 70, 117, 164	0
1	J	195/202 (96%)	0.15	1 (0%) <span>91</span> <span>90</span>	43, 64, 102, 132	0
1	K	191/202 (94%)	0.22	4 (2%) <span>63</span> <span>59</span>	58, 75, 104, 123	0
1	L	189/202 (93%)	0.37	9 (4%) <span>30</span> <span>24</span>	61, 82, 108, 126	0
1	M	193/202 (95%)	0.43	9 (4%) <span>31</span> <span>25</span>	62, 88, 141, 157	0
1	N	186/202 (92%)	0.51	18 (9%) <span>7</span> <span>5</span>	56, 83, 152, 170	0
All	All	2687/2828 (95%)	0.20	58 (2%) <span>62</span> <span>57</span>	34, 70, 113, 170	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	77	VAL	6.7
1	N	86	LEU	6.0
1	N	79	LEU	5.9
1	N	87	VAL	4.5
1	N	103	TYR	4.0
1	M	75	TYR	3.6
1	L	36	ALA	3.1
1	N	84	TYR	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	M	94	TRP	3.0
1	K	75	TYR	2.9
1	N	85	LYS	2.9
1	L	77	VAL	2.8
1	N	102	ILE	2.8
1	M	103	TYR	2.8
1	J	103	TYR	2.7
1	I	160	ILE	2.7
1	I	103	TYR	2.7
1	N	29	LYS	2.6
1	N	120	PHE	2.6
1	D	99	ASN	2.6
1	I	34	GLY	2.6
1	L	122	VAL	2.6
1	N	54	LEU	2.5
1	N	75	TYR	2.5
1	L	63	GLY	2.5
1	M	86	LEU	2.5
1	N	32	LEU	2.5
1	K	154	ILE	2.5
1	L	140	ILE	2.5
1	M	104	ILE	2.5
1	N	36	ALA	2.5
1	N	205	VAL	2.5
1	H	31	THR	2.4
1	I	69	ILE	2.4
1	I	75	TYR	2.4
1	M	93	PRO	2.3
1	L	160	ILE	2.3
1	D	86	LEU	2.2
1	M	150	GLU	2.2
1	I	43	VAL	2.2
1	N	69	ILE	2.2
1	B	77	VAL	2.2
1	M	38	TYR	2.2
1	B	160	ILE	2.2
1	L	53	ALA	2.2
1	L	43	VAL	2.2
1	L	173	LEU	2.2
1	F	58	GLY	2.1
1	K	73	GLY	2.1
1	I	79	LEU	2.1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	N	30	ALA	2.1
1	N	152	VAL	2.1
1	E	154	ILE	2.0
1	I	36	ALA	2.0
1	F	26	GLU	2.0
1	F	160	ILE	2.0
1	M	119	TYR	2.0
1	K	193	LEU	2.0

## 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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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(Å <sup>2</sup> )	Q<0.9
2	EDO	B	302	4/4	0.75	0.47	63,64,67,68	0
2	EDO	L	301	4/4	0.89	0.16	54,58,61,62	0
2	EDO	B	303	4/4	0.89	0.21	77,79,80,81	0
2	EDO	G	301	4/4	0.90	0.30	61,63,63,64	0
2	EDO	H	301	4/4	0.90	0.40	56,59,64,66	0
2	EDO	J	301	4/4	0.91	0.27	64,66,69,71	0
2	EDO	I	301	4/4	0.91	0.19	56,58,64,70	0
2	EDO	N	301	4/4	0.92	0.31	57,58,60,60	0
2	EDO	F	301	4/4	0.92	0.21	66,68,69,71	0
2	EDO	K	301	4/4	0.93	0.19	57,58,58,59	0
2	EDO	D	301	4/4	0.93	0.23	53,54,54,54	0
2	EDO	M	301	4/4	0.93	0.31	55,55,57,57	0
2	EDO	A	301	4/4	0.94	0.28	67,67,68,68	0
2	EDO	E	301	4/4	0.96	0.17	68,70,72,73	0
2	EDO	B	301	4/4	0.96	0.19	52,54,57,61	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	EDO	C	301	4/4	0.98	0.20	66,66,68,69	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.