



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:41 AM GMT

PDB ID : 3BRJ  
Title : Crystal structure of mannitol operon repressor (MtlR) from *Vibrio parahaemolyticus* RIMD 2210633  
Authors : Tan, K.; Zhou, M.; Moy, S.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2007-12-21  
Resolution : 2.75 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

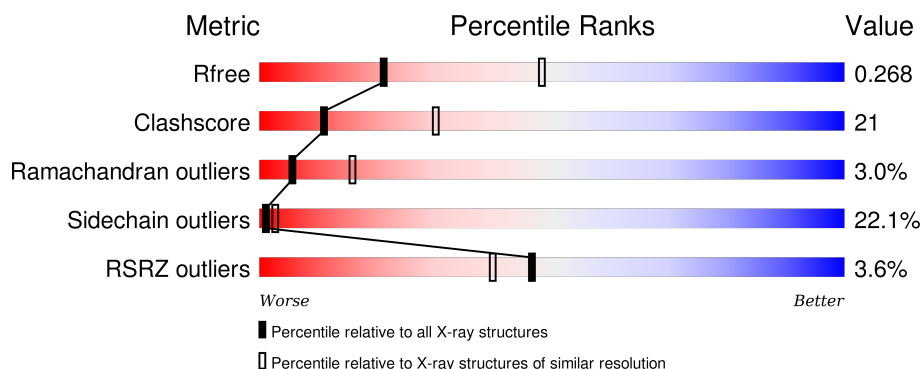
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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	175	
1	B	175	
1	C	175	
1	D	175	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5361 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 Mannitol operon repressor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	167	Total	C	N	O	S	Se	0	1	0
			1333	851	220	258	1	3			
1	B	169	Total	C	N	O	S	Se	0	0	0
			1344	857	223	261	1	2			
1	C	163	Total	C	N	O	S	Se	0	0	0
			1296	829	216	248	1	2			
1	D	168	Total	C	N	O	S	Se	0	0	0
			1336	853	221	259	1	2			

There are 12 discrepancies between the modelled and reference sequences:

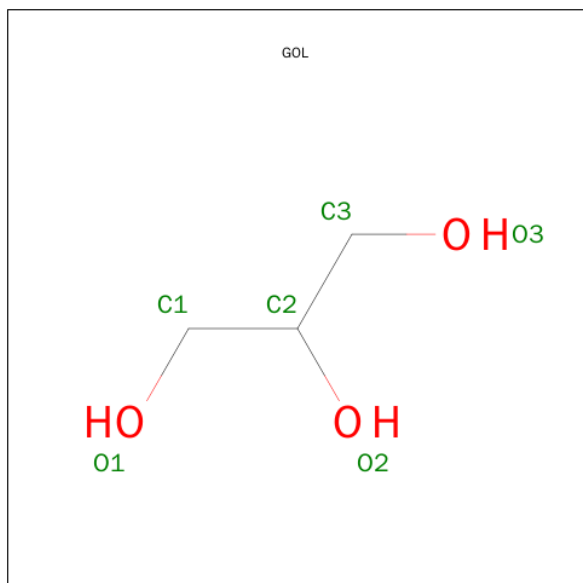
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP Q87SQ4
A	-1	ASN	-	EXPRESSION TAG	UNP Q87SQ4
A	0	ALA	-	EXPRESSION TAG	UNP Q87SQ4
B	-2	SER	-	EXPRESSION TAG	UNP Q87SQ4
B	-1	ASN	-	EXPRESSION TAG	UNP Q87SQ4
B	0	ALA	-	EXPRESSION TAG	UNP Q87SQ4
C	-2	SER	-	EXPRESSION TAG	UNP Q87SQ4
C	-1	ASN	-	EXPRESSION TAG	UNP Q87SQ4
C	0	ALA	-	EXPRESSION TAG	UNP Q87SQ4
D	-2	SER	-	EXPRESSION TAG	UNP Q87SQ4
D	-1	ASN	-	EXPRESSION TAG	UNP Q87SQ4
D	0	ALA	-	EXPRESSION TAG	UNP Q87SQ4

- 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	C	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		

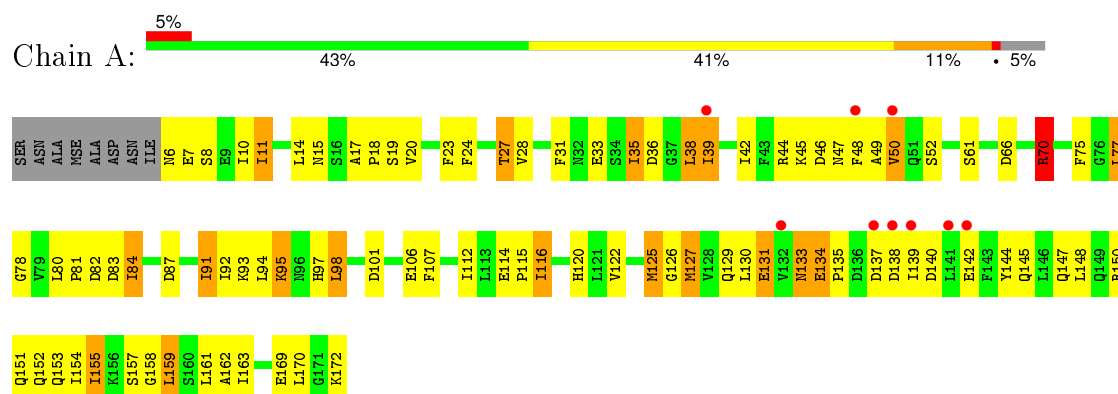
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	8	Total	O	0	0
			8	8		
4	B	9	Total	O	0	0
			9	9		
4	C	4	Total	O	0	0
			4	4		
4	D	9	Total	O	0	0
			9	9		

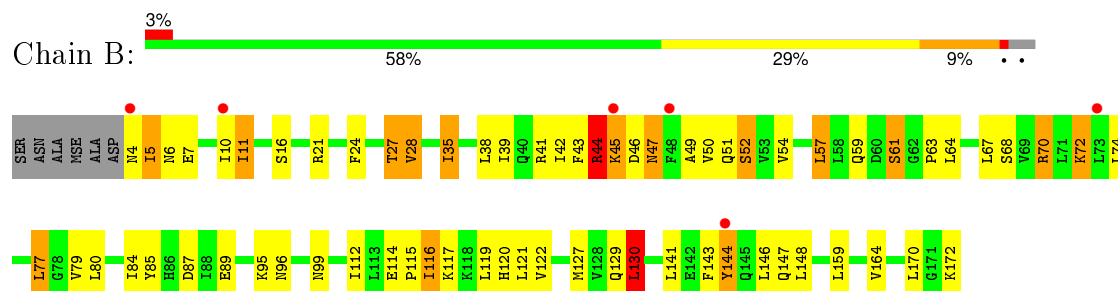
### 3 Residue-property plots [i](#)

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 ( $RSRZ > 2$ ). 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.

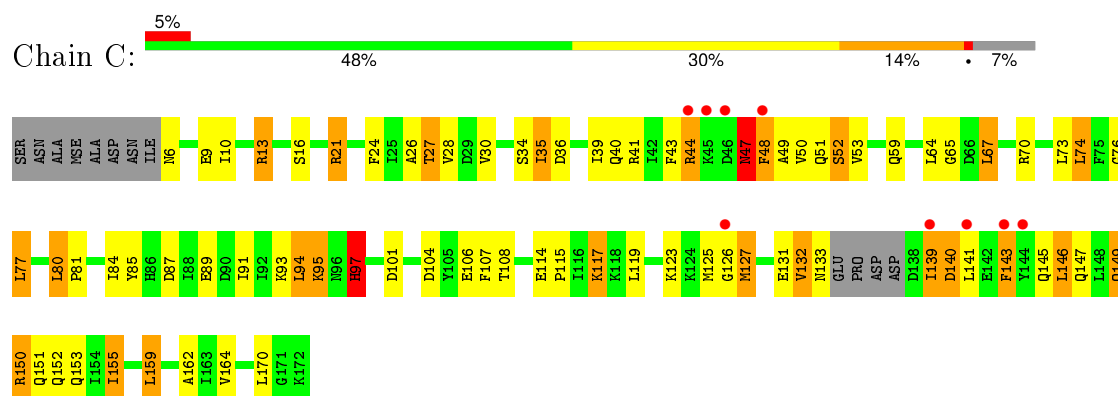
- Molecule 1: Mannitol operon repressor



- Molecule 1: Mannitol operon repressor



- Molecule 1: Mannitol operon repressor



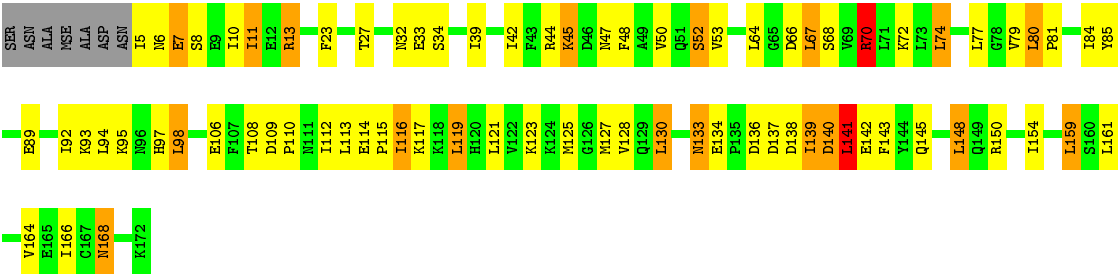
- Molecule 1: Mannitol operon repressor

Chain D: 

52%

33%

10%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.28 Å 63.28 Å 227.10 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.56 – 2.75 48.55 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.1 (48.56-2.75) 99.1 (48.55-2.75)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.71 (at 2.73 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.207 , 0.273 0.205 , 0.268	Depositor DCC
$R_{free}$ test set	1175 reflections (5.40%)	DCC
Wilson B-factor (Å <sup>2</sup> )	53.4	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 56.4	EDS
Estimated twinning fraction	0.054 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 22956 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5361	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 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	0.78	0/1354	0.95	3/1826 (0.2%)
1	B	0.77	0/1362	0.90	1/1838 (0.1%)
1	C	0.77	0/1312	0.90	3/1767 (0.2%)
1	D	0.88	0/1354	0.97	1/1827 (0.1%)
All	All	0.80	0/5382	0.93	8/7258 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	70	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	A	70	ARG	CB-CA-C	6.32	123.04	110.40
1	A	70	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	C	97	HIS	N-CA-CB	5.70	120.87	110.60
1	A	101	ASP	CB-CG-OD1	5.63	123.37	118.30
1	C	67	LEU	CB-CG-CD1	-5.34	101.92	111.00
1	C	80	LEU	CA-CB-CG	5.20	127.25	115.30
1	B	130	LEU	CA-CB-CG	5.07	126.95	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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	1333	0	1350	83	0
1	B	1344	0	1358	38	0
1	C	1296	0	1319	52	0
1	D	1336	0	1352	56	0
2	A	4	0	6	0	0
2	B	4	0	6	1	0
2	C	4	0	6	0	0
2	D	4	0	6	0	0
3	B	6	0	8	0	0
4	A	8	0	0	0	0
4	B	9	0	0	1	0
4	C	4	0	0	0	0
4	D	9	0	0	0	0
All	All	5361	0	5411	224	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 21.

All (224) 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:A:125:MSE:HE1	1:A:162:ALA:HA	1.22	1.17
1:A:47:ASN:HD21	1:A:49:ALA:HB3	1.22	1.03
1:D:32:ASN:HD22	1:D:67:LEU:HG	1.23	0.99
1:C:35:ILE:HD13	1:C:36:ASP:N	1.82	0.94
1:A:134:GLU:HB3	1:A:135:PRO:CA	1.98	0.92
1:A:125:MSE:CE	1:A:162:ALA:HA	2.05	0.86
1:A:134:GLU:HB3	1:A:135:PRO:HA	1.59	0.84
1:B:117:LYS:HG2	1:B:127:MSE:HE1	1.61	0.83
1:A:35:ILE:HD11	1:A:70:ARG:HG2	1.61	0.83
1:D:32:ASN:ND2	1:D:67:LEU:HG	1.96	0.81
1:C:106:GLU:HB3	1:C:152:GLN:NE2	1.97	0.79
1:D:45:LYS:HE3	1:D:45:LYS:H	1.48	0.79
1:A:150:ARG:O	1:A:150:ARG:HD2	1.83	0.78
1:A:78:GLY:HA2	1:B:44:ARG:NH2	2.00	0.77
1:B:7:GLU:O	1:B:11:ILE:HG22	1.86	0.75
1:A:44:ARG:HE	1:A:50:VAL:HG11	1.51	0.75
1:A:31:PHE:O	1:A:35:ILE:HG23	1.87	0.74
1:D:125:MSE:HB3	1:D:127:MSE:HE2	1.70	0.74
1:D:140:ASP:HB2	1:D:143:PHE:HB2	1.71	0.73
1:C:106:GLU:OE1	1:C:106:GLU:HA	1.88	0.72
1:D:112:ILE:O	1:D:116:ILE:HG23	1.90	0.72

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:LYS:CG	1:B:127:MSE:HE1	2.20	0.71
1:A:127[B]:MSE:SE	1:A:127[B]:MSE:H	2.24	0.71
1:D:133:ASN:H	1:D:133:ASN:HD22	1.39	0.70
1:D:139:ILE:O	1:D:141:LEU:HG	1.92	0.70
1:A:134:GLU:HB3	1:A:135:PRO:C	2.10	0.70
1:A:112:ILE:O	1:A:116:ILE:HG23	1.94	0.68
1:D:64:LEU:O	1:D:70:ARG:HD3	1.95	0.67
1:C:35:ILE:HD13	1:C:35:ILE:C	2.16	0.67
1:D:74:LEU:HB3	1:D:80:LEU:HD22	1.76	0.67
1:B:50:VAL:O	1:B:54:VAL:HG23	1.95	0.66
1:C:81:PRO:HG2	1:C:84:ILE:HG13	1.77	0.66
1:C:24:PHE:HA	1:C:27:THR:HG23	1.77	0.66
1:C:117:LYS:NZ	1:C:127:MSE:HE1	2.11	0.66
1:D:128:VAL:O	1:D:128:VAL:HG12	1.94	0.65
1:A:125:MSE:HE3	1:A:127[B]:MSE:HE1	1.80	0.64
1:A:36:ASP:O	1:A:39:ILE:HG22	1.97	0.64
1:A:24:PHE:HA	1:A:27:THR:HG23	1.79	0.64
1:C:47:ASN:HB3	1:C:50:VAL:H	1.63	0.64
1:C:106:GLU:HB3	1:C:152:GLN:HE21	1.63	0.63
1:C:73:LEU:HG	1:C:77:LEU:HD22	1.80	0.63
1:A:116:ILE:O	1:A:116:ILE:HD12	1.97	0.62
1:C:21:ARG:NH1	1:C:104:ASP:OD2	2.32	0.62
1:D:98:LEU:HD11	1:D:112:ILE:HD11	1.81	0.62
1:C:10:ILE:HD11	1:C:164:VAL:HB	1.82	0.62
1:C:21:ARG:NH2	1:C:101:ASP:O	2.33	0.61
1:C:36:ASP:O	1:C:40:GLN:HG2	1.99	0.61
1:B:64:LEU:O	1:B:70:ARG:HD3	2.01	0.61
1:D:94:LEU:HA	1:D:97:HIS:HD2	1.65	0.61
1:A:8:SER:HA	1:A:11:ILE:HG13	1.83	0.61
1:A:23:PHE:O	1:A:27:THR:HG23	2.01	0.60
1:A:23:PHE:O	1:A:27:THR:CG2	2.49	0.60
1:C:6:ASN:HA	1:C:9:GLU:HG2	1.84	0.59
1:C:152:GLN:HA	1:C:155:ILE:HG22	1.85	0.59
1:A:8:SER:O	1:A:11:ILE:HG13	2.02	0.58
1:D:130:LEU:HD11	1:D:154:ILE:HG21	1.84	0.58
1:A:23:PHE:HE2	1:A:159:LEU:HD13	1.69	0.58
1:D:23:PHE:HE2	1:D:159:LEU:HD13	1.67	0.58
1:B:46:ASP:O	1:B:47:ASN:C	2.42	0.57
1:A:47:ASN:HD22	1:A:50:VAL:CG2	2.16	0.57
1:A:106:GLU:HG2	1:A:152:GLN:OE1	2.03	0.57
1:A:46:ASP:CG	1:A:47:ASN:H	2.05	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:GLN:O	1:C:65:GLY:HA3	2.05	0.57
1:A:81:PRO:HD2	1:A:84:ILE:HD13	1.87	0.57
1:D:139:ILE:HG22	1:D:139:ILE:O	2.05	0.56
1:D:45:LYS:HE3	1:D:45:LYS:N	2.19	0.56
1:A:131:GLU:OE1	1:A:131:GLU:N	2.38	0.56
1:D:6:ASN:C	1:D:8:SER:H	2.09	0.56
1:D:23:PHE:CE2	1:D:159:LEU:HD13	2.39	0.56
1:C:146:LEU:HD22	1:C:146:LEU:O	2.05	0.56
1:D:133:ASN:N	1:D:133:ASN:HD22	2.04	0.55
1:B:57:LEU:HD22	1:B:63:PRO:HG2	1.89	0.55
1:D:150:ARG:O	1:D:154:ILE:HG12	2.06	0.55
1:A:138:ASP:O	1:A:139:ILE:HG22	2.05	0.55
1:C:132:VAL:HG13	1:C:133:ASN:N	2.21	0.55
1:C:117:LYS:HZ2	1:C:127:MSE:HE1	1.70	0.55
1:C:132:VAL:HG13	1:C:133:ASN:H	1.72	0.55
1:B:87:ASP:OD1	1:B:120:HIS:HB2	2.06	0.55
1:C:74:LEU:HB3	1:C:80:LEU:HD22	1.89	0.55
1:A:47:ASN:HD22	1:A:50:VAL:HG22	1.70	0.55
1:C:94:LEU:HA	1:C:97:HIS:CE1	2.42	0.54
1:D:13:ARG:NH2	1:D:33:GLU:OE1	2.40	0.54
1:D:125:MSE:HE2	1:D:127:MSE:HE3	1.90	0.54
1:B:5:ILE:HG22	1:B:6:ASN:N	2.23	0.54
1:C:87:ASP:O	1:C:91:ILE:HG13	2.07	0.54
1:A:35:ILE:HD11	1:A:70:ARG:CG	2.36	0.54
1:A:159:LEU:HD22	1:A:163:ILE:CD1	2.38	0.53
1:A:159:LEU:HD22	1:A:163:ILE:HD11	1.91	0.53
1:D:94:LEU:HA	1:D:97:HIS:CD2	2.42	0.53
1:A:47:ASN:ND2	1:A:49:ALA:HB3	2.07	0.53
1:B:44:ARG:O	1:B:46:ASP:N	2.42	0.52
1:A:48:PHE:O	1:A:52:SER:N	2.40	0.52
1:C:143:PHE:O	1:C:147:GLN:HG3	2.09	0.52
1:D:128:VAL:CG1	1:D:128:VAL:O	2.57	0.52
1:B:130:LEU:HD13	1:B:147:GLN:NE2	2.25	0.52
1:D:44:ARG:HH12	1:D:47:ASN:ND2	2.08	0.52
1:D:164:VAL:O	1:D:168:ASN:HB2	2.11	0.51
1:A:133:ASN:O	1:A:134:GLU:HG3	2.10	0.51
1:C:139:ILE:HD13	1:C:140:ASP:N	2.26	0.51
1:D:108:THR:HG21	1:D:148:LEU:HD22	1.92	0.51
1:B:49:ALA:O	1:B:52:SER:HB3	2.10	0.51
1:A:131:GLU:O	1:A:131:GLU:OE1	2.29	0.50
1:A:39:ILE:HD13	1:A:70:ARG:HG3	1.94	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ASN:HB3	1:A:50:VAL:HG23	1.94	0.50
1:C:44:ARG:CB	1:C:50:VAL:HG11	2.41	0.50
1:D:85:TYR:CZ	1:D:89:GLU:HG3	2.46	0.50
1:B:35:ILE:HD11	1:B:70:ARG:HB2	1.94	0.49
1:C:47:ASN:HB3	1:C:50:VAL:HG23	1.94	0.49
1:B:68:SER:O	1:B:72:LYS:HD2	2.13	0.49
1:D:6:ASN:C	1:D:8:SER:N	2.65	0.49
1:D:5:ILE:N	1:D:7:GLU:HB3	2.28	0.49
1:D:112:ILE:C	1:D:115:PRO:HD2	2.34	0.49
1:A:23:PHE:CE2	1:A:159:LEU:HD13	2.48	0.49
1:D:114:GLU:N	1:D:115:PRO:CD	2.76	0.48
1:A:134:GLU:CB	1:A:135:PRO:HA	2.39	0.48
1:D:116:ILE:HA	1:D:119:LEU:HD22	1.95	0.48
1:C:44:ARG:HB2	1:C:50:VAL:HG11	1.95	0.48
1:B:28:VAL:HG11	1:B:95:LYS:HD3	1.96	0.47
1:A:127[B]:MSE:HG2	1:A:158:GLY:HA3	1.95	0.47
1:A:66:ASP:O	1:A:70:ARG:HD2	2.14	0.47
1:C:139:ILE:HD13	1:C:140:ASP:H	1.79	0.47
1:B:38:LEU:O	1:B:41:ARG:N	2.44	0.47
1:D:98:LEU:HD11	1:D:112:ILE:CD1	2.45	0.47
1:A:80:LEU:HD22	1:A:84:ILE:HD11	1.97	0.47
1:C:76:GLY:O	1:D:44:ARG:HG2	2.15	0.47
1:C:64:LEU:O	1:C:70:ARG:HD2	2.14	0.47
1:C:43:PHE:O	1:C:44:ARG:C	2.53	0.47
1:C:26:ALA:O	1:C:30:VAL:HG23	2.15	0.47
1:D:141:LEU:HD12	1:D:142:GLU:H	1.79	0.47
1:A:14:LEU:HB3	1:A:23:PHE:HE1	1.80	0.47
1:A:8:SER:HA	1:A:11:ILE:CG1	2.44	0.47
1:A:77:LEU:HD21	1:B:77:LEU:HD11	1.97	0.47
1:D:44:ARG:HG3	1:D:50:VAL:HG21	1.98	0.46
1:B:43:PHE:O	1:B:44:ARG:C	2.53	0.46
1:D:140:ASP:O	1:D:141:LEU:C	2.54	0.46
1:B:41:ARG:NH2	1:B:172:LYS:O	2.49	0.46
1:A:92:ILE:O	1:A:93:LYS:C	2.54	0.46
1:C:73:LEU:HG	1:C:77:LEU:CD2	2.44	0.46
1:C:94:LEU:O	1:C:95:LYS:C	2.52	0.46
1:B:10:ILE:HD11	1:B:164:VAL:HG22	1.96	0.46
1:D:39:ILE:HD12	1:D:70:ARG:HB3	1.98	0.45
2:B:173:EDO:H11	4:B:183:HOH:O	2.15	0.45
1:D:139:ILE:C	1:D:141:LEU:H	2.19	0.45
1:C:44:ARG:HD3	1:C:50:VAL:HG21	1.99	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:ARG:NE	1:A:50:VAL:HG11	2.23	0.45
1:B:57:LEU:HD13	1:B:64:LEU:HD12	1.98	0.45
1:B:85:TYR:CZ	1:B:89:GLU:HG3	2.52	0.45
1:C:114:GLU:O	1:C:115:PRO:C	2.53	0.45
1:C:117:LYS:HZ1	1:C:127:MSE:HE1	1.82	0.45
1:C:107:PHE:HB3	1:C:155:ILE:CG2	2.47	0.45
1:A:75:PHE:HE2	1:A:82:ASP:OD2	1.99	0.45
1:A:126:GLY:H	1:A:127[B]:MSE:SE	2.49	0.44
1:B:47:ASN:HB2	1:B:50:VAL:HB	2.00	0.44
1:B:44:ARG:C	1:B:46:ASP:H	2.21	0.44
1:A:127[B]:MSE:HE2	1:A:158:GLY:O	2.17	0.44
1:D:66:ASP:O	1:D:70:ARG:HG2	2.16	0.44
1:A:75:PHE:CZ	1:B:50:VAL:HG22	2.53	0.44
1:D:133:ASN:N	1:D:133:ASN:ND2	2.66	0.44
1:B:95:LYS:HE3	1:B:96:ASN:OD1	2.18	0.44
1:B:35:ILE:HD11	1:B:70:ARG:CB	2.47	0.44
1:C:10:ILE:O	1:C:13:ARG:HB2	2.18	0.44
1:A:8:SER:C	1:A:10:ILE:N	2.71	0.44
1:D:68:SER:O	1:D:72:LYS:HG3	2.18	0.44
1:A:112:ILE:O	1:A:116:ILE:CG2	2.63	0.44
1:A:47:ASN:ND2	1:A:50:VAL:H	2.15	0.44
1:A:122:VAL:HA	1:A:127[B]:MSE:SE	2.68	0.43
1:C:85:TYR:CZ	1:C:89:GLU:HG3	2.53	0.43
1:D:81:PRO:HD2	1:D:84:ILE:HG13	2.00	0.43
1:A:94:LEU:O	1:A:97:HIS:HB2	2.18	0.43
1:D:121:LEU:HD23	1:D:166:ILE:HG13	2.00	0.43
1:A:87:ASP:OD1	1:A:120:HIS:N	2.52	0.43
1:C:47:ASN:CB	1:C:50:VAL:HG23	2.49	0.43
1:A:78:GLY:HA2	1:B:44:ARG:HH22	1.79	0.43
1:A:87:ASP:O	1:A:91:ILE:HG23	2.19	0.43
1:A:31:PHE:HE1	1:A:91:ILE:CD1	2.32	0.42
1:A:23:PHE:O	1:A:27:THR:HG22	2.18	0.42
1:A:116:ILE:HD12	1:A:122:VAL:HG21	2.01	0.42
1:D:112:ILE:O	1:D:115:PRO:HD2	2.19	0.42
1:A:107:PHE:HB3	1:A:155:ILE:HG12	2.01	0.42
1:B:24:PHE:HA	1:B:27:THR:HG23	2.01	0.42
1:A:127[B]:MSE:HG2	1:A:158:GLY:CA	2.50	0.42
1:C:48:PHE:HA	1:C:51:GLN:HG2	2.01	0.42
1:A:114:GLU:HB2	1:A:115:PRO:HD3	2.01	0.42
1:B:112:ILE:O	1:B:116:ILE:HG23	2.19	0.42
1:D:127:MSE:HG2	1:D:161:LEU:HD12	2.00	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:PHE:O	1:B:45:LYS:N	2.52	0.42
1:C:48:PHE:HD1	1:C:48:PHE:HA	1.74	0.42
1:D:67:LEU:HD13	1:D:92:ILE:HD11	2.02	0.42
1:A:148:LEU:O	1:A:151:GLN:N	2.51	0.42
1:B:21:ARG:HD3	1:B:99:ASN:OD1	2.19	0.42
1:A:17:ALA:HA	1:A:18:PRO:HD3	1.77	0.42
1:C:35:ILE:C	1:C:35:ILE:CD1	2.83	0.42
1:D:113:LEU:HG	1:D:117:LYS:HD2	2.00	0.42
1:A:95:LYS:C	1:A:95:LYS:HD2	2.41	0.41
1:A:137:ASP:HB3	1:A:138:ASP:H	1.67	0.41
1:A:6:ASN:O	1:A:8:SER:N	2.54	0.41
1:D:11:ILE:HG12	1:D:164:VAL:HG21	2.03	0.41
1:B:59:GLN:HE21	1:B:61:SER:HB2	1.86	0.41
1:A:78:GLY:CA	1:B:44:ARG:NH2	2.79	0.41
1:B:87:ASP:OD2	1:B:119:LEU:HG	2.20	0.41
1:D:48:PHE:O	1:D:52:SER:HB3	2.20	0.41
1:C:49:ALA:HA	1:C:52:SER:HG	1.86	0.41
1:A:116:ILE:HD12	1:A:116:ILE:C	2.41	0.41
1:D:109:ASP:HA	1:D:110:PRO:HD3	1.94	0.41
1:A:116:ILE:CD1	1:A:122:VAL:HG11	2.51	0.41
1:A:46:ASP:CG	1:A:47:ASN:N	2.73	0.41
1:A:151:GLN:O	1:A:155:ILE:HG23	2.21	0.41
1:A:98:LEU:HD11	1:A:112:ILE:HD11	2.03	0.41
1:D:6:ASN:O	1:D:8:SER:N	2.54	0.41
1:C:149:GLN:OE1	1:C:149:GLN:HA	2.21	0.41
1:A:19:SER:O	1:A:20:VAL:C	2.57	0.41
1:D:42:ILE:HD13	1:D:79:VAL:HG21	2.03	0.41
1:D:80:LEU:HA	1:D:80:LEU:HD12	1.87	0.41
1:B:143:PHE:O	1:B:144:TYR:C	2.60	0.41
1:A:127[B]:MSE:HE3	1:A:161:LEU:HD23	2.03	0.40
1:C:150:ARG:O	1:C:152:GLN:N	2.54	0.40
1:A:14:LEU:HB3	1:A:23:PHE:CE1	2.55	0.40
1:B:114:GLU:O	1:B:115:PRO:C	2.58	0.40
1:A:38:LEU:HG	1:A:170:LEU:O	2.21	0.40
1:C:159:LEU:O	1:C:162:ALA:HB3	2.20	0.40
1:C:125:MSE:O	1:C:127:MSE:N	2.50	0.40
1:A:35:ILE:HG22	1:A:170:LEU:HD21	2.02	0.40
1:C:95:LYS:HE3	1:C:95:LYS:HB3	1.85	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	166/175 (95%)	144 (87%)	17 (10%)	5 (3%)	5	16
1	B	167/175 (95%)	153 (92%)	10 (6%)	4 (2%)	7	22
1	C	159/175 (91%)	138 (87%)	13 (8%)	8 (5%)	3	6
1	D	166/175 (95%)	150 (90%)	13 (8%)	3 (2%)	11	30
All	All	658/700 (94%)	585 (89%)	53 (8%)	20 (3%)	5	16

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	134	GLU
1	B	5	ILE
1	B	45	LYS
1	D	7	GLU
1	A	7	GLU
1	B	16	SER
1	B	44	ARG
1	C	47	ASN
1	C	132	VAL
1	C	140	ASP
1	C	151	GLN
1	C	44	ARG
1	C	126	GLY
1	C	150	ARG
1	D	141	LEU
1	A	129	GLN
1	A	140	ASP
1	C	170	LEU
1	A	142	GLU
1	D	139	ILE



### 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	153/155 (99%)	117 (76%)	36 (24%)	1	2
1	B	154/155 (99%)	122 (79%)	32 (21%)	1	3
1	C	148/155 (96%)	113 (76%)	35 (24%)	1	2
1	D	153/155 (99%)	121 (79%)	32 (21%)	1	3
All	All	608/620 (98%)	473 (78%)	135 (22%)	1	3

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ILE
1	A	15	ASN
1	A	27	THR
1	A	28	VAL
1	A	33	GLU
1	A	35	ILE
1	A	38	LEU
1	A	39	ILE
1	A	42	ILE
1	A	45	LYS
1	A	50	VAL
1	A	61	SER
1	A	70	ARG
1	A	77	LEU
1	A	83	ASP
1	A	84	ILE
1	A	91	ILE
1	A	95	LYS
1	A	98	LEU
1	A	116	ILE
1	A	125	MSE
1	A	127[A]	MSE
1	A	127[B]	MSE
1	A	130	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	131	GLU
1	A	133	ASN
1	A	144	TYR
1	A	145	GLN
1	A	147	GLN
1	A	153	GLN
1	A	154	ILE
1	A	155	ILE
1	A	157	SER
1	A	159	LEU
1	A	169	GLU
1	A	172	LYS
1	B	4	ASN
1	B	11	ILE
1	B	27	THR
1	B	28	VAL
1	B	35	ILE
1	B	39	ILE
1	B	42	ILE
1	B	44	ARG
1	B	47	ASN
1	B	51	GLN
1	B	52	SER
1	B	57	LEU
1	B	61	SER
1	B	67	LEU
1	B	70	ARG
1	B	72	LYS
1	B	74	LEU
1	B	77	LEU
1	B	79	VAL
1	B	80	LEU
1	B	84	ILE
1	B	116	ILE
1	B	121	LEU
1	B	122	VAL
1	B	129	GLN
1	B	130	LEU
1	B	141	LEU
1	B	144	TYR
1	B	146	LEU
1	B	148	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	159	LEU
1	B	170	LEU
1	C	13	ARG
1	C	16	SER
1	C	21	ARG
1	C	27	THR
1	C	28	VAL
1	C	34	SER
1	C	35	ILE
1	C	39	ILE
1	C	41	ARG
1	C	47	ASN
1	C	48	PHE
1	C	52	SER
1	C	53	VAL
1	C	67	LEU
1	C	74	LEU
1	C	77	LEU
1	C	93	LYS
1	C	94	LEU
1	C	95	LYS
1	C	97	HIS
1	C	108	THR
1	C	117	LYS
1	C	119	LEU
1	C	123	LYS
1	C	127	MSE
1	C	131	GLU
1	C	139	ILE
1	C	141	LEU
1	C	143	PHE
1	C	145	GLN
1	C	146	LEU
1	C	149	GLN
1	C	153	GLN
1	C	155	ILE
1	C	159	LEU
1	D	10	ILE
1	D	11	ILE
1	D	13	ARG
1	D	27	THR
1	D	34	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	45	LYS
1	D	52	SER
1	D	53	VAL
1	D	67	LEU
1	D	70	ARG
1	D	74	LEU
1	D	77	LEU
1	D	80	LEU
1	D	93	LYS
1	D	95	LYS
1	D	98	LEU
1	D	106	GLU
1	D	116	ILE
1	D	119	LEU
1	D	123	LYS
1	D	130	LEU
1	D	133	ASN
1	D	134	GLU
1	D	136	ASP
1	D	137	ASP
1	D	138	ASP
1	D	140	ASP
1	D	141	LEU
1	D	145	GLN
1	D	148	LEU
1	D	159	LEU
1	D	168	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	47	ASN
1	A	51	GLN
1	A	153	GLN
1	B	51	GLN
1	B	129	GLN
1	B	152	GLN
1	C	6	ASN
1	C	51	GLN
1	C	97	HIS
1	C	99	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	152	GLN
1	C	153	GLN
1	D	32	ASN
1	D	47	ASN
1	D	51	GLN
1	D	59	GLN
1	D	133	ASN
1	D	152	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](#)

5 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	A	173	-	3,3,3	0.76	0	2,2,2	0.11	0
2	EDO	B	173	-	3,3,3	0.64	0	2,2,2	0.13	0
3	GOL	B	174	-	5,5,5	0.67	0	5,5,5	1.14	0
2	EDO	C	173	-	3,3,3	0.89	0	2,2,2	0.14	0
2	EDO	D	173	-	3,3,3	0.83	0	2,2,2	0.18	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	A	173	-	-	0/1/1/1	0/0/0/0
2	EDO	B	173	-	-	0/1/1/1	0/0/0/0
3	GOL	B	174	-	-	0/4/4/4	0/0/0/0
2	EDO	C	173	-	-	0/1/1/1	0/0/0/0
2	EDO	D	173	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	173	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	165/175 (94%)	0.33	9 (5%)	29	22	35, 49, 74, 78	0
1	B	167/175 (95%)	0.24	6 (3%)	46	40	39, 49, 66, 74	0
1	C	161/175 (92%)	0.34	9 (5%)	28	21	40, 50, 69, 78	0
1	D	166/175 (94%)	0.12	0	100	100	36, 49, 67, 87	0
All	All	659/700 (94%)	0.26	24 (3%)	46	40	35, 49, 69, 87	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	139	ILE	6.2
1	C	139	ILE	5.0
1	C	141	LEU	4.4
1	C	143	PHE	4.3
1	C	126	GLY	4.1
1	A	138	ASP	4.0
1	B	4	ASN	3.4
1	A	137	ASP	3.3
1	B	144	TYR	2.8
1	B	10	ILE	2.7
1	C	46	ASP	2.6
1	A	48	PHE	2.6
1	C	144	TYR	2.5
1	A	39	ILE	2.5
1	C	48	PHE	2.5
1	B	45	LYS	2.3
1	C	45	LYS	2.3
1	C	44	ARG	2.3
1	B	48	PHE	2.2
1	B	73	LEU	2.2
1	A	132	VAL	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	50	VAL	2.1
1	A	141	LEU	2.1
1	A	142	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( $\text{\AA}^2$ )	Q<0.9
2	EDO	B	173	4/4	0.78	0.19	0.45	55,55,56,56	0
2	EDO	A	173	4/4	0.86	0.11	-2.18	52,52,53,53	0
3	GOL	B	174	6/6	0.89	0.14	-2.33	39,42,42,43	0
2	EDO	C	173	4/4	0.84	0.17	-	45,48,49,49	0
2	EDO	D	173	4/4	0.77	0.21	-	50,52,53,54	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.