



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 04:02 am BST

PDB ID : 3LSA  
Title : Padron0.9-OFF (non-fluorescent state)  
Authors : Brakemann, T.; Weber, G.; Trowitzsch, S.; Wahl, M.C.; Jakobs, S.  
Deposited on : 2010-02-12  
Resolution : 1.79 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

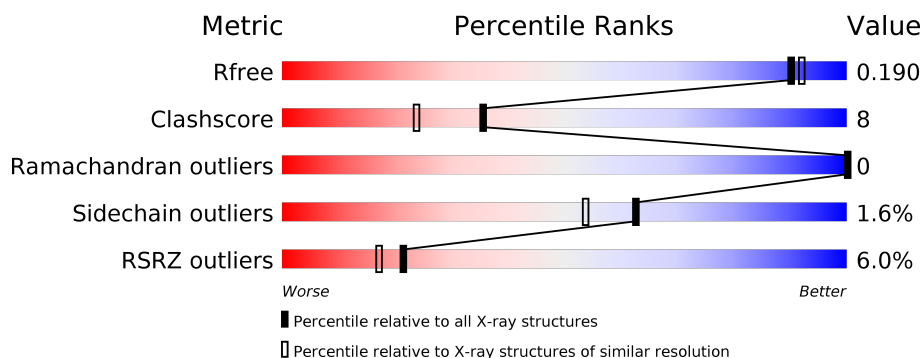
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.79 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	235	<div> <div>9%</div> <div> <div></div> <div>86%</div> <div>6%</div> <div>9%</div> </div> </div>
1	B	235	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>8%</div> <div>9%</div> </div> </div>
1	C	235	<div> <div>6%</div> <div> <div></div> <div>80%</div> <div>10%</div> <div>9%</div> </div> </div>
1	D	235	<div> <div>6%</div> <div> <div></div> <div>86%</div> <div>9%</div> <div>.</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	EPE	D	226[A]	-	-	X	X
5	EPE	D	226[B]	-	-	X	X

## 2 Entry composition [i](#)

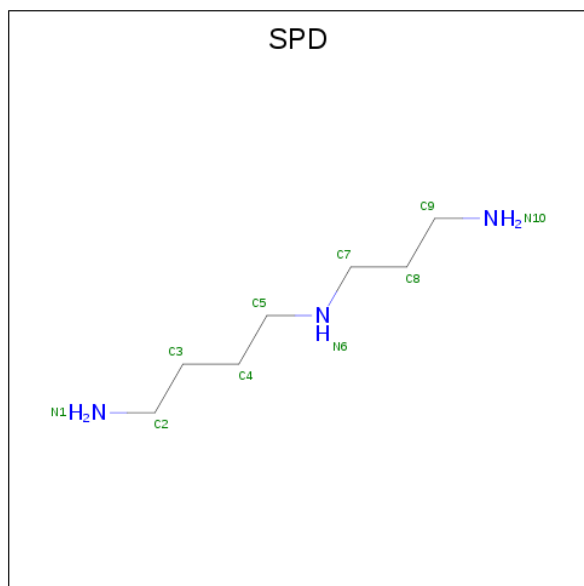
There are 6 unique types of molecules in this entry. The entry contains 8526 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Padron0.9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	13	0
			1819	1153	308	345	13			
1	B	214	Total	C	N	O	S	0	22	0
			1899	1201	323	362	13			
1	C	214	Total	C	N	O	S	0	23	0
			1887	1197	319	357	14			
1	D	225	Total	C	N	O	S	0	27	0
			2037	1286	356	381	14			

- Molecule 2 is SPERMIDINE (three-letter code: SPD) (formula: C<sub>7</sub>H<sub>19</sub>N<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			10	7	3		
2	B	1	Total	C	N	0	0
			10	7	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	N	0	0
			10	7	3		

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



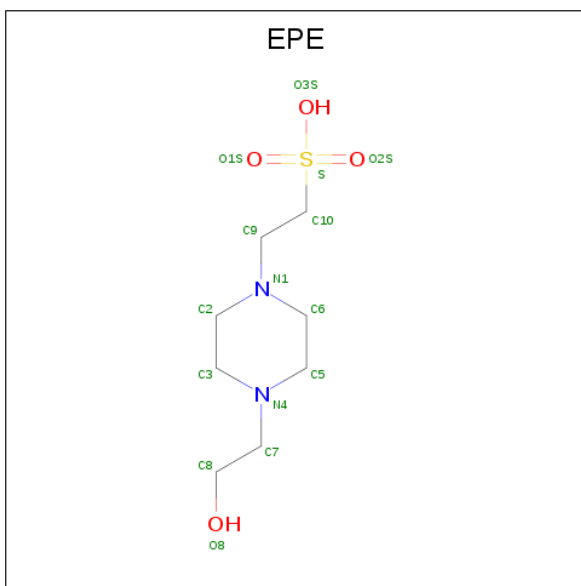
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



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

- Molecule 5 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
5	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	D	1	Total	C	N	O	S	0	1
			30	16	4	8	2		

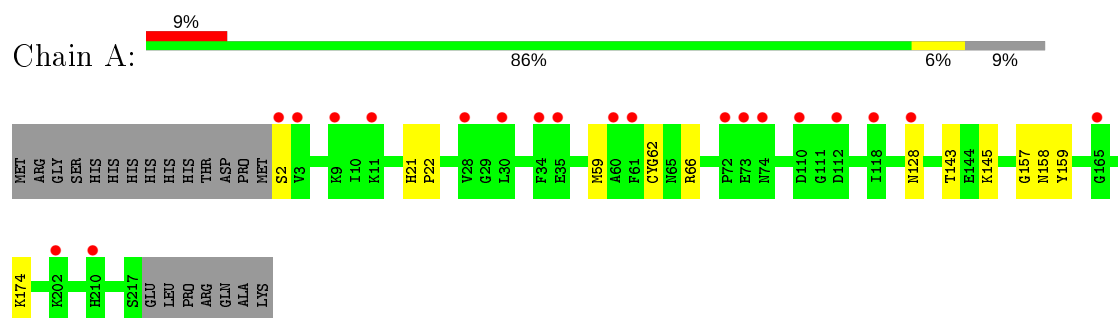
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	157	Total 169	O 169	0	12
6	B	185	Total 193	O 193	0	8
6	C	181	Total 189	O 189	0	8
6	D	220	Total 229	O 229	0	9

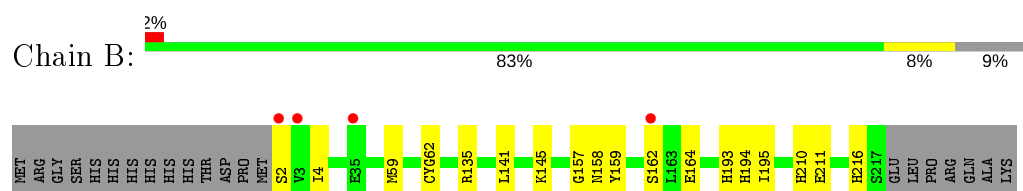
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

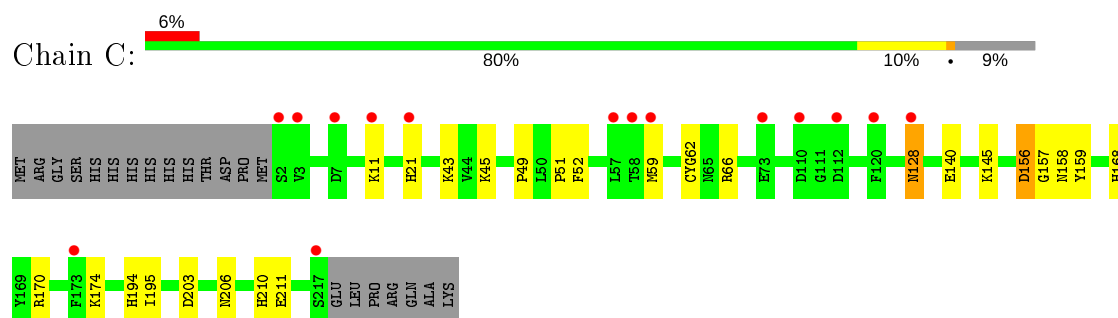
#### • Molecule 1: Padron0.9



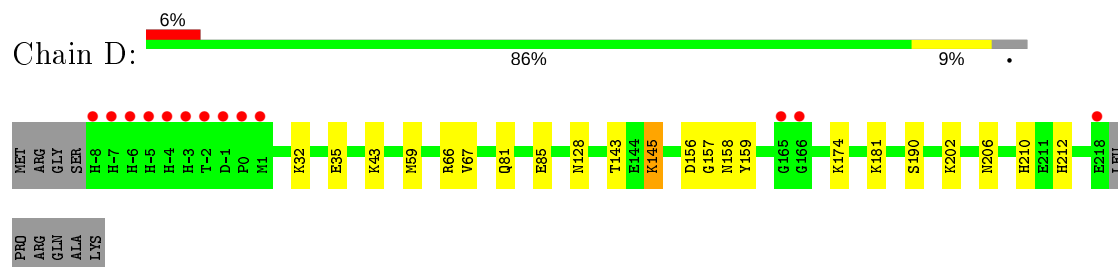
#### • Molecule 1: Padron0.9



#### • Molecule 1: Padron0.9



#### • Molecule 1: Padron0.9





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.33Å 104.26Å 123.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.79 29.99 – 1.79	Depositor EDS
% Data completeness (in resolution range)	99.2 (30.00-1.79) 99.2 (29.99-1.79)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.74 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.5.0063	Depositor
R, $R_{free}$	0.159 , 0.190 0.159 , 0.190	Depositor DCC
$R_{free}$ test set	4433 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.9	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 62.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	8526	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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: GOL, EPE, GYC, SO4, SPD

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	0.48	0/1845	0.58	0/2488
1	B	0.53	0/1927	0.61	0/2596
1	C	0.58	0/1922	0.64	0/2588
1	D	0.62	2/2073 (0.1%)	0.66	0/2791
All	All	0.56	2/7767 (0.0%)	0.62	0/10463

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	202[A]	LYS	CG-CD	-5.07	1.35	1.52
1	D	202[B]	LYS	CG-CD	-5.07	1.35	1.52

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	1819	0	1730	15	0
1	B	1899	0	1795	17	0
1	C	1887	0	1804	34	0
1	D	2037	0	1919	58	0
2	A	10	0	19	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	20	0	38	2	0
3	B	6	0	8	0	0
3	C	12	0	16	0	0
3	D	6	0	8	1	0
4	B	5	0	0	0	0
5	D	45	0	51	40	0
6	A	169	0	0	3	0
6	B	193	0	0	8	0
6	C	189	0	0	9	0
6	D	229	0	0	9	0
All	All	8526	0	7388	123	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 8.

All (123) 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:D:174[B]:LYS:CE	5:D:226[B]:EPE:C5	1.87	1.53
1:D:174[B]:LYS:CE	5:D:226[B]:EPE:H52	1.09	1.52
1:D:174[B]:LYS:NZ	5:D:226[B]:EPE:C5	1.81	1.37
1:D:156[A]:ASP:OD1	5:D:226[A]:EPE:H51	1.24	1.29
1:D:174[B]:LYS:HZ1	5:D:226[B]:EPE:C5	1.36	1.29
1:D:156[A]:ASP:CG	5:D:226[A]:EPE:H51	1.56	1.24
1:D:212[B]:HIS:HD2	6:D:731[B]:HOH:O	1.18	1.23
1:D:156[A]:ASP:OD1	5:D:226[A]:EPE:C5	1.87	1.21
1:D:174[A]:LYS:HE2	5:D:226[A]:EPE:H62	1.26	1.17
1:D:174[B]:LYS:HE3	5:D:226[B]:EPE:C5	1.57	1.16
1:D:174[B]:LYS:NZ	5:D:226[B]:EPE:H51	1.47	1.16
1:D:174[B]:LYS:HE2	5:D:226[B]:EPE:H82	1.20	1.12
1:D:174[B]:LYS:HE2	5:D:226[B]:EPE:H52	1.15	1.09
1:D:174[B]:LYS:HE3	5:D:226[B]:EPE:H52	1.11	1.02
1:D:156[A]:ASP:OD1	5:D:226[A]:EPE:C6	2.08	1.01
1:D:156[A]:ASP:CG	5:D:226[A]:EPE:C5	2.26	0.99
1:D:156[A]:ASP:OD2	5:D:226[A]:EPE:C5	2.11	0.98
1:D:174[A]:LYS:NZ	5:D:226[A]:EPE:H92	1.79	0.97
1:D:174[B]:LYS:HZ1	5:D:226[B]:EPE:H51	0.81	0.95
1:D:158[A]:ASN:OD1	6:D:230:HOH:O	1.84	0.94
1:D:156[A]:ASP:OD2	5:D:226[A]:EPE:H52	1.67	0.93
1:D:174[A]:LYS:HE2	5:D:226[A]:EPE:C6	2.00	0.90
1:D:174[B]:LYS:HE2	5:D:226[B]:EPE:C8	2.02	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174[A]:LYS:CE	5:D:226[A]:EPE:H62	2.04	0.88
1:D:174[B]:LYS:CE	5:D:226[B]:EPE:H82	2.04	0.84
1:D:174[B]:LYS:HE3	5:D:226[B]:EPE:C6	2.08	0.84
1:D:174[B]:LYS:NZ	5:D:226[B]:EPE:H52	1.65	0.83
1:D:156[A]:ASP:OD2	5:D:226[A]:EPE:H51	1.79	0.81
1:C:156[B]:ASP:OD1	1:C:174:LYS:HD2	1.84	0.78
1:A:158[A]:ASN:OD1	6:A:363[A]:HOH:O	2.02	0.78
1:C:174:LYS:HE3	6:D:730:HOH:O	1.83	0.77
1:D:212[B]:HIS:CD2	6:D:731[B]:HOH:O	2.03	0.76
1:D:206:ASN:HB3	3:D:227:GOL:H11	1.68	0.75
1:A:158[A]:ASN:CG	6:A:363[A]:HOH:O	2.26	0.74
1:C:156[B]:ASP:OD1	1:C:174:LYS:CD	2.36	0.74
1:D:156[A]:ASP:OD1	5:D:226[A]:EPE:H61	1.88	0.73
1:A:158[A]:ASN:ND2	6:A:363[A]:HOH:O	2.23	0.71
1:D:174[B]:LYS:NZ	5:D:226[B]:EPE:N4	2.38	0.71
1:A:143:THR:H	1:B:145[A]:LYS:HZ1	1.36	0.71
1:C:158[B]:ASN:OD1	6:C:524:HOH:O	2.10	0.69
1:D:174[A]:LYS:HZ3	5:D:226[A]:EPE:H92	1.57	0.69
1:C:194:HIS:HD2	6:C:727:HOH:O	1.76	0.68
1:B:195[A]:ILE:HD13	1:B:211:GLU:HG3	1.75	0.67
1:C:21[B]:HIS:CD2	1:C:21[B]:HIS:O	2.48	0.67
1:C:158[A]:ASN:ND2	6:C:715[A]:HOH:O	2.29	0.65
1:C:140:GLU:OE2	1:C:168:HIS:HE1	1.80	0.65
1:D:174[A]:LYS:HZ1	5:D:226[A]:EPE:H92	1.63	0.64
1:B:216[B]:HIS:HD2	6:B:725:HOH:O	1.81	0.64
1:B:194:HIS:HD2	6:B:625:HOH:O	1.80	0.64
1:D:174[A]:LYS:CE	5:D:226[A]:EPE:H92	2.28	0.63
1:C:21[B]:HIS:CE1	1:C:51:PRO:HG2	2.35	0.62
1:A:174[A]:LYS:HE2	2:B:226:SPD:H31	1.82	0.61
1:D:128[B]:ASN:OD1	6:D:229:HOH:O	2.16	0.60
1:D:210[A]:HIS:HD2	6:D:626:HOH:O	1.85	0.59
1:C:145:LYS:HE3	6:D:255:HOH:O	2.03	0.58
6:C:250:HOH:O	1:D:145[B]:LYS:HE3	2.04	0.58
1:B:210:HIS:HD2	6:B:625:HOH:O	1.87	0.58
1:A:143:THR:H	1:B:145[A]:LYS:NZ	2.01	0.58
1:C:128[A]:ASN:H	1:C:128[A]:ASN:ND2	2.03	0.57
1:C:156[A]:ASP:HB3	1:C:174:LYS:HD3	1.86	0.56
1:C:170:ARG:HH21	5:D:226[A]:EPE:H61	1.71	0.56
1:C:43[A]:LYS:NZ	1:C:206:ASN:HD21	2.04	0.56
1:D:174[B]:LYS:CE	5:D:226[B]:EPE:H51	1.96	0.56
1:D:156[A]:ASP:OD1	1:D:174[A]:LYS:HG2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:145[A]:LYS:HB2	1:D:145[A]:LYS:NZ	2.24	0.53
1:B:210:HIS:CD2	6:B:625:HOH:O	2.61	0.53
1:C:21[B]:HIS:C	1:C:21[B]:HIS:CD2	2.83	0.53
1:D:210[A]:HIS:CD2	6:D:626:HOH:O	2.61	0.52
1:A:158[B]:ASN:N	1:B:158[B]:ASN:HD21	2.08	0.52
1:C:21[B]:HIS:CD2	6:C:293:HOH:O	2.62	0.52
1:C:168:HIS:HD2	6:D:305:HOH:O	1.92	0.52
1:D:145[A]:LYS:N	1:D:145[A]:LYS:HD3	2.25	0.52
1:A:174[A]:LYS:NZ	2:B:226:SPD:H51	2.25	0.51
1:C:43[A]:LYS:HZ2	1:C:206:ASN:HD21	1.57	0.51
1:C:62:GYC:O2	1:C:62:GYC:HD2	2.10	0.51
1:D:32:LYS:HD3	1:D:35[B]:GLU:OE2	2.11	0.50
1:D:157:GLY:HA3	1:D:159:TYR:CZ	2.47	0.50
1:C:45:LYS:HA	1:C:45:LYS:HE2	1.94	0.50
1:C:21[B]:HIS:O	1:C:21[B]:HIS:CG	2.64	0.49
1:D:143:THR:HG22	1:D:145[B]:LYS:HE2	1.93	0.49
1:C:156[B]:ASP:OD1	1:C:174:LYS:HD3	2.11	0.49
1:B:194:HIS:CD2	6:B:625:HOH:O	2.59	0.49
1:D:174[A]:LYS:HE2	5:D:226[A]:EPE:H92	1.94	0.48
1:D:145[B]:LYS:HD3	1:D:190:SER:HB3	1.96	0.48
1:A:158[B]:ASN:N	1:A:158[B]:ASN:OD1	2.43	0.48
1:A:157:GLY:HA3	1:A:159:TYR:CZ	2.49	0.48
1:D:174[B]:LYS:HE3	5:D:226[B]:EPE:H62	1.93	0.47
1:C:128[A]:ASN:OD1	6:C:642:HOH:O	2.21	0.46
1:B:135:ARG:HD3	6:B:530[B]:HOH:O	2.15	0.46
1:C:157:GLY:HA3	1:C:159:TYR:CZ	2.51	0.46
1:C:43[B]:LYS:HG2	1:C:206:ASN:ND2	2.31	0.46
1:B:62:GYC:HD2	1:B:62:GYC:O2	2.15	0.45
1:A:62:GYC:HD2	1:A:62:GYC:O2	2.15	0.45
1:A:145:LYS:HE3	6:B:285:HOH:O	2.16	0.45
1:A:21[A]:HIS:HA	1:A:22:PRO:HD3	1.79	0.45
1:B:162[A]:SER:OG	6:B:235[A]:HOH:O	2.21	0.45
1:D:81:GLN:O	1:D:181:LYS:HE2	2.17	0.45
1:C:49:PRO:HB3	1:C:203:ASP:HB2	2.00	0.44
1:C:174:LYS:HE2	6:C:729:HOH:O	2.18	0.44
1:C:21[B]:HIS:HE1	1:C:52:PHE:HD2	1.66	0.44
1:D:43[B]:LYS:HD3	1:D:206:ASN:ND2	2.33	0.43
5:D:226[B]:EPE:H82	5:D:226[B]:EPE:H52	1.50	0.43
1:A:128[B]:ASN:C	1:A:128[B]:ASN:OD1	2.56	0.43
1:B:2:SER:HB3	1:B:4:ILE:HG22	2.00	0.42
1:C:195[B]:ILE:HD13	1:C:211:GLU:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174[B]:LYS:HZ3	5:D:226[B]:EPE:C7	2.31	0.42
1:D:85:GLU:OE1	1:D:181:LYS:HD3	2.18	0.42
1:C:21[B]:HIS:CE1	1:C:52:PHE:CD2	3.07	0.42
1:B:4:ILE:O	1:B:4:ILE:HG23	2.20	0.42
1:B:157:GLY:HA3	1:B:159:TYR:CZ	2.54	0.42
1:C:157:GLY:HA3	1:C:159:TYR:CE1	2.55	0.42
1:C:21[B]:HIS:CE1	1:C:52:PHE:HD2	2.38	0.42
1:B:141[A]:LEU:HD22	1:B:193:HIS:O	2.20	0.42
1:D:174[A]:LYS:CD	5:D:226[A]:EPE:H62	2.50	0.41
1:A:157:GLY:HA3	1:A:159:TYR:CE1	2.56	0.41
1:D:143:THR:CG2	1:D:145[B]:LYS:HE2	2.51	0.41
1:C:210[A]:HIS:ND1	6:C:727:HOH:O	2.37	0.41
6:C:524:HOH:O	1:D:145[A]:LYS:HE2	2.21	0.40
1:C:11[A]:LYS:HE2	1:C:11[A]:LYS:HB3	1.86	0.40
1:D:174[B]:LYS:NZ	5:D:226[B]:EPE:C7	2.84	0.40
1:D:32:LYS:HD3	1:D:35[B]:GLU:CD	2.41	0.40
1:B:164[A]:GLU:CD	1:B:164[A]:GLU:O	2.60	0.40
5:D:226[A]:EPE:H81	5:D:226[A]:EPE:H32	1.73	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	224/235 (95%)	223 (100%)	1 (0%)	0	100	100
1	B	234/235 (100%)	232 (99%)	2 (1%)	0	100	100
1	C	233/235 (99%)	232 (100%)	1 (0%)	0	100	100
1	D	249/235 (106%)	249 (100%)	0	0	100	100
All	All	940/940 (100%)	936 (100%)	4 (0%)	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	196/202 (97%)	192 (98%)	4 (2%)	55	44
1	B	206/202 (102%)	204 (99%)	2 (1%)	76	71
1	C	206/202 (102%)	199 (97%)	7 (3%)	37	22
1	D	220/202 (109%)	214 (97%)	6 (3%)	44	31
All	All	828/808 (102%)	809 (98%)	19 (2%)	62	37

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	59[A]	MET
1	A	59[B]	MET
1	A	66	ARG
1	B	59[A]	MET
1	B	59[B]	MET
1	C	59[A]	MET
1	C	59[B]	MET
1	C	66	ARG
1	C	128[A]	ASN
1	C	128[B]	ASN
1	C	156[A]	ASP
1	C	156[B]	ASP
1	D	59[A]	MET
1	D	59[B]	MET
1	D	66	ARG
1	D	67	VAL
1	D	145[A]	LYS
1	D	145[B]	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	184	GLN
1	B	184	GLN
1	B	194	HIS
1	B	210	HIS
1	C	168	HIS
1	C	184	GLN
1	C	206	ASN
1	D	-4	HIS
1	D	38	GLN
1	D	194	HIS
1	D	206	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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$
1	GYC	B	62	1	22,22,23	2.76	6 (27%)	26,30,32	3.07	10 (38%)
1	GYC	A	62	1	22,22,23	2.79	7 (31%)	26,30,32	3.13	10 (38%)
1	GYC	D	62	1	22,22,23	2.59	5 (22%)	26,30,32	2.83	9 (34%)
1	GYC	C	62	1	22,22,23	2.69	6 (27%)	26,30,32	2.70	7 (26%)

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
1	GYC	B	62	1	-	3/9/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	GYC	A	62	1	-	3/9/29/30	0/2/2/2
1	GYC	D	62	1	-	3/9/29/30	0/2/2/2
1	GYC	C	62	1	-	3/9/29/30	0/2/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	62	GYC	CB2-CA2	7.87	1.41	1.35
1	D	62	GYC	CB2-CA2	7.64	1.41	1.35
1	B	62	GYC	CB2-CA2	7.55	1.41	1.35
1	C	62	GYC	CB2-CA2	7.37	1.41	1.35
1	B	62	GYC	CA2-C2	-7.04	1.41	1.48
1	A	62	GYC	CA2-C2	-6.95	1.41	1.48
1	C	62	GYC	CA2-C2	-6.58	1.42	1.48
1	D	62	GYC	CA2-C2	-6.25	1.42	1.48
1	A	62	GYC	OH-CZ	-5.41	1.24	1.37
1	B	62	GYC	OH-CZ	-5.36	1.24	1.37
1	C	62	GYC	OH-CZ	-5.19	1.24	1.37
1	D	62	GYC	OH-CZ	-4.61	1.26	1.37
1	B	62	GYC	CG2-CB2	-2.77	1.41	1.46
1	C	62	GYC	CG2-CB2	-2.76	1.41	1.46
1	D	62	GYC	CG2-CB2	-2.74	1.41	1.46
1	A	62	GYC	CG2-CB2	-2.65	1.41	1.46
1	B	62	GYC	C2-N3	-2.62	1.33	1.39
1	C	62	GYC	C2-N3	-2.54	1.33	1.39
1	A	62	GYC	C2-N3	-2.47	1.34	1.39
1	A	62	GYC	C1-N3	-2.36	1.33	1.37
1	B	62	GYC	CA2-N2	-2.36	1.33	1.38
1	A	62	GYC	CA2-N2	-2.28	1.33	1.38
1	D	62	GYC	C2-N3	-2.26	1.34	1.39
1	C	62	GYC	CB1-CA1	2.01	1.55	1.53

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	GYC	CA2-C2-N3	10.26	108.22	103.37
1	C	62	GYC	CA2-C2-N3	9.33	107.78	103.37
1	B	62	GYC	CA2-C2-N3	9.19	107.72	103.37
1	B	62	GYC	CB2-CA2-C2	7.29	130.97	122.28
1	D	62	GYC	CA2-C2-N3	7.14	106.75	103.37
1	D	62	GYC	CB2-CA2-C2	6.75	130.33	122.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	62	GYC	CB2-CA2-C2	6.25	129.73	122.28
1	A	62	GYC	CB2-CA2-C2	6.21	129.69	122.28
1	A	62	GYC	C2-CA2-N2	-5.14	105.33	108.93
1	B	62	GYC	C2-CA2-N2	-4.88	105.52	108.93
1	B	62	GYC	CA2-N2-C1	4.87	109.36	105.77
1	D	62	GYC	CA2-N2-C1	4.59	109.15	105.77
1	A	62	GYC	CA2-N2-C1	4.30	108.94	105.77
1	D	62	GYC	C2-CA2-N2	-4.17	106.01	108.93
1	B	62	GYC	CB2-CA2-N2	-3.86	123.48	128.83
1	C	62	GYC	C2-CA2-N2	-3.81	106.27	108.93
1	A	62	GYC	O2-C2-CA2	-3.80	128.82	130.96
1	D	62	GYC	CB2-CA2-N2	-3.78	123.58	128.83
1	D	62	GYC	O-C-CA3	-3.75	115.07	126.39
1	C	62	GYC	CB2-CA2-N2	-3.50	123.97	128.83
1	C	62	GYC	O-C-CA3	-3.22	116.67	126.39
1	A	62	GYC	O-C-CA3	-3.05	117.17	126.39
1	B	62	GYC	O-C-CA3	-2.96	117.47	126.39
1	D	62	GYC	N3-C1-N2	-2.87	109.47	111.45
1	A	62	GYC	CB2-CA2-N2	-2.78	124.97	128.83
1	A	62	GYC	CG2-CB2-CA2	2.69	133.24	129.94
1	C	62	GYC	CA2-N2-C1	2.56	107.66	105.77
1	C	62	GYC	CG2-CB2-CA2	2.51	133.02	129.94
1	D	62	GYC	CA1-CB1-SG1	-2.48	109.10	114.44
1	B	62	GYC	CA3-N3-C1	-2.38	124.30	127.16
1	B	62	GYC	N3-C1-N2	-2.35	109.83	111.45
1	A	62	GYC	CA3-N3-C1	-2.35	124.34	127.16
1	D	62	GYC	CA3-N3-C1	-2.28	124.43	127.16
1	B	62	GYC	O2-C2-CA2	-2.12	129.77	130.96
1	B	62	GYC	CG2-CB2-CA2	2.03	132.43	129.94
1	A	62	GYC	CA3-N3-C2	2.01	128.42	123.80

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	62	GYC	N2-CA2-CB2-CG2
1	B	62	GYC	C2-CA2-CB2-CG2
1	A	62	GYC	N2-CA2-CB2-CG2
1	A	62	GYC	C2-CA2-CB2-CG2
1	D	62	GYC	N2-CA2-CB2-CG2
1	D	62	GYC	C2-CA2-CB2-CG2
1	C	62	GYC	N2-CA2-CB2-CG2

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Mol	Chain	Res	Type	Atoms
1	C	62	GYC	C2-CA2-CB2-CG2
1	B	62	GYC	C-CA3-N3-C2
1	A	62	GYC	C-CA3-N3-C2
1	D	62	GYC	C-CA3-N3-C2
1	C	62	GYC	C-CA3-N3-C2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	62	GYC	1	0
1	A	62	GYC	1	0
1	C	62	GYC	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

11 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	SPD	B	227	-	9,9,9	0.28	0	8,8,8	0.61	0
5	EPE	D	226[A]	-	15,15,15	0.88	1 (6%)	18,20,20	1.69	5 (27%)
2	SPD	A	225	-	9,9,9	0.30	0	8,8,8	0.77	0
3	GOL	B	225	-	5,5,5	0.42	0	5,5,5	0.24	0
2	SPD	B	226	-	9,9,9	0.28	0	8,8,8	0.68	0
5	EPE	D	226[B]	-	15,15,15	0.96	1 (6%)	18,20,20	1.92	5 (27%)
5	EPE	D	225	-	15,15,15	0.88	1 (6%)	18,20,20	1.72	5 (27%)
3	GOL	C	226	-	5,5,5	0.44	0	5,5,5	0.24	0
3	GOL	D	227	-	5,5,5	0.41	0	5,5,5	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	C	225	-	5,5,5	0.38	0	5,5,5	0.20	0
4	SO4	B	228	-	4,4,4	0.13	0	6,6,6	0.10	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	SPD	B	227	-	-	4/7/7/7	-
5	EPE	D	226[A]	-	-	5/9/19/19	0/1/1/1
2	SPD	A	225	-	-	3/7/7/7	-
3	GOL	B	225	-	-	4/4/4/4	-
2	SPD	B	226	-	-	6/7/7/7	-
5	EPE	D	226[B]	-	-	8/9/19/19	0/1/1/1
5	EPE	D	225	-	-	3/9/19/19	0/1/1/1
3	GOL	C	226	-	-	4/4/4/4	-
3	GOL	D	227	-	-	4/4/4/4	-
3	GOL	C	225	-	-	2/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	226[B]	EPE	C10-S	3.30	1.82	1.77
5	D	225	EPE	C10-S	2.94	1.81	1.77
5	D	226[A]	EPE	C10-S	2.90	1.81	1.77

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	225	EPE	C5-N4-C3	4.37	118.66	108.83
5	D	226[B]	EPE	C5-N4-C3	4.32	118.54	108.83
5	D	226[B]	EPE	C7-N4-C3	3.36	119.82	111.23
5	D	226[A]	EPE	C7-N4-C5	3.28	119.63	111.23
5	D	226[B]	EPE	O2S-S-C10	3.18	110.75	106.92
5	D	226[B]	EPE	O1S-S-C10	3.13	110.68	106.92
5	D	226[B]	EPE	C7-N4-C5	3.08	119.11	111.23
5	D	226[A]	EPE	C5-N4-C3	3.03	115.65	108.83
5	D	226[A]	EPE	C7-N4-C3	2.91	118.69	111.23
5	D	225	EPE	C7-N4-C5	2.65	118.01	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	226[A]	EPE	O3S-S-C10	2.57	109.93	105.77
5	D	225	EPE	O2S-S-C10	2.37	109.76	106.92
5	D	226[A]	EPE	O1S-S-C10	2.27	109.64	106.92
5	D	225	EPE	C6-C5-N4	2.18	115.12	110.64
5	D	225	EPE	C7-N4-C3	2.06	116.50	111.23

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	226[A]	EPE	C8-C7-N4-C3
3	B	225	GOL	O1-C1-C2-C3
3	B	225	GOL	C1-C2-C3-O3
5	D	226[B]	EPE	C8-C7-N4-C5
5	D	225	EPE	C9-C10-S-O1S
5	D	225	EPE	C9-C10-S-O3S
3	C	226	GOL	O1-C1-C2-C3
3	C	226	GOL	C1-C2-C3-O3
3	C	226	GOL	O2-C2-C3-O3
3	D	227	GOL	O1-C1-C2-C3
5	D	226[B]	EPE	N4-C7-C8-O8
2	B	226	SPD	C3-C4-C5-N6
2	B	227	SPD	N6-C7-C8-C9
2	B	227	SPD	C3-C4-C5-N6
3	D	227	GOL	C1-C2-C3-O3
3	C	225	GOL	C1-C2-C3-O3
2	A	225	SPD	C3-C4-C5-N6
3	B	225	GOL	O1-C1-C2-O2
3	B	225	GOL	O2-C2-C3-O3
2	B	226	SPD	C4-C5-N6-C7
2	A	225	SPD	N6-C7-C8-C9
3	D	227	GOL	O2-C2-C3-O3
5	D	226[A]	EPE	N4-C7-C8-O8
2	A	225	SPD	C2-C3-C4-C5
2	B	226	SPD	C2-C3-C4-C5
5	D	226[A]	EPE	C10-C9-N1-C2
5	D	226[B]	EPE	C10-C9-N1-C2
5	D	226[B]	EPE	C10-C9-N1-C6
5	D	226[B]	EPE	C9-C10-S-O3S
2	B	226	SPD	C7-C8-C9-N10
3	C	226	GOL	O1-C1-C2-O2
3	D	227	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	B	226	SPD	C8-C7-N6-C5
5	D	226[B]	EPE	C9-C10-S-O1S
5	D	226[B]	EPE	C9-C10-S-O2S
5	D	225	EPE	C9-C10-S-O2S
3	C	225	GOL	O2-C2-C3-O3
2	B	227	SPD	C4-C5-N6-C7
2	B	226	SPD	N6-C7-C8-C9
5	D	226[A]	EPE	C10-C9-N1-C6
2	B	227	SPD	C8-C7-N6-C5
5	D	226[A]	EPE	C9-C10-S-O2S
5	D	226[B]	EPE	C8-C7-N4-C3

There are no ring outliers.

4 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	226[A]	EPE	20	0
2	B	226	SPD	2	0
5	D	226[B]	EPE	20	0
3	D	227	GOL	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	213/235 (90%)	0.43	20 (9%) 8 6	12, 17, 22, 32	2 (0%)
1	B	213/235 (90%)	0.20	4 (1%) 66 63	12, 17, 23, 33	4 (1%)
1	C	213/235 (90%)	0.29	15 (7%) 16 13	11, 15, 22, 33	1 (0%)
1	D	224/235 (95%)	0.19	13 (5%) 23 18	11, 15, 25, 42	4 (1%)
All	All	863/940 (91%)	0.28	52 (6%) 21 17	11, 16, 23, 42	11 (1%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	-2	THR	8.5
1	D	-8	HIS	7.5
1	B	2	SER	7.1
1	D	0	PRO	6.7
1	D	1	MET	5.8
1	C	2	SER	5.3
1	A	2	SER	5.0
1	D	-3	HIS	4.9
1	D	-1	ASP	4.3
1	D	-5	HIS	3.9
1	A	165	GLY	3.8
1	B	3	VAL	3.7
1	A	3	VAL	3.7
1	D	165[A]	GLY	3.5
1	D	-7	HIS	3.5
1	C	3	VAL	3.4
1	A	128[A]	ASN	3.4
1	A	74	ASN	3.3
1	D	218	GLU	3.2
1	C	59[A]	MET	3.1
1	A	30	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	202	LYS	3.1
1	A	73	GLU	3.0
1	A	34	PHE	2.9
1	D	-4	HIS	2.9
1	A	60	ALA	2.8
1	B	162[A]	SER	2.8
1	D	-6	HIS	2.7
1	A	112	ASP	2.7
1	C	110	ASP	2.6
1	C	120	PHE	2.6
1	C	112	ASP	2.6
1	C	57	LEU	2.5
1	C	21[A]	HIS	2.4
1	C	7	ASP	2.4
1	D	166	GLY	2.3
1	C	128[A]	ASN	2.3
1	C	11[A]	LYS	2.3
1	C	73	GLU	2.2
1	A	28[A]	VAL	2.2
1	A	210	HIS	2.2
1	C	173	PHE	2.1
1	A	9	LYS	2.1
1	A	61	PHE	2.1
1	C	58	THR	2.1
1	A	118	ILE	2.1
1	A	35	GLU	2.1
1	A	11	LYS	2.0
1	A	72	PRO	2.0
1	B	35	GLU	2.0
1	A	110	ASP	2.0
1	C	217[A]	SER	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	GYC	A	62	21/22	0.96	0.16	15,17,18,20	0
1	GYC	C	62	21/22	0.96	0.15	13,14,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	GYC	B	62	21/22	0.97	0.09	16,18,20,22	0
1	GYC	D	62	21/22	0.98	0.10	12,14,19,19	0

### 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
3	GOL	C	225	6/6	0.60	0.19	60,61,61,62	0
5	EPE	D	226[B]	15/15	0.62	0.44	42,50,55,55	15
5	EPE	D	226[A]	15/15	0.62	0.44	65,68,72,72	15
2	SPD	B	227	10/10	0.69	0.18	50,54,56,57	0
3	GOL	C	226	6/6	0.72	0.23	71,71,71,71	0
2	SPD	B	226	10/10	0.73	0.18	52,52,53,53	0
2	SPD	A	225	10/10	0.74	0.25	50,51,54,54	0
3	GOL	D	227	6/6	0.78	0.25	56,58,58,59	0
4	SO4	B	228	5/5	0.81	0.19	87,87,87,87	0
3	GOL	B	225	6/6	0.84	0.15	56,58,58,58	0
5	EPE	D	225	15/15	0.84	0.33	47,58,62,63	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.