



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:45 PM GMT

PDB ID : 1YI7  
Title : Beta-d-xylosidase (selenomethionine) XYND from Clostridium Acetobutylicum  
Authors : Teplyakov, A.; Fedorov, E.; Gilliland, G.L.; Almo, S.C.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2005-01-11  
Resolution : 1.90 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.

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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 : 1.7 (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

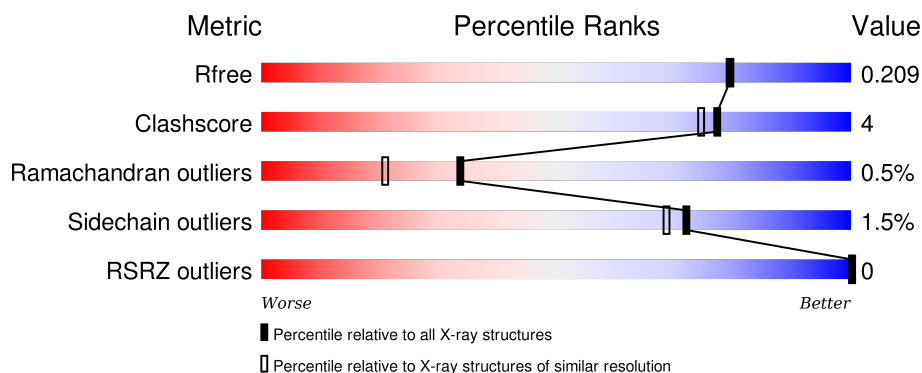
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	542	<div> <div>86%</div> <div>13%</div> <div>.</div> </div>
1	B	542	<div> <div>86%</div> <div>12%</div> <div>..</div> </div>
1	C	542	<div> <div>89%</div> <div>9%</div> <div>.</div> </div>
1	D	542	<div> <div>88%</div> <div>9%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CA	A	3001	-	-	-	X
2	CA	B	3002	-	-	-	X
3	SO4	B	3006	-	-	-	X
3	SO4	C	3007	-	-	-	X
5	GOL	A	3020	-	-	-	X
5	GOL	A	3024	-	-	-	X
5	GOL	A	3032	-	-	-	X
5	GOL	B	3021	-	-	-	X
5	GOL	B	3025	-	-	-	X
5	GOL	B	3033	-	-	-	X
5	GOL	C	3022	-	-	-	X
5	GOL	C	3026	-	-	-	X
5	GOL	C	3030	-	-	-	X
5	GOL	C	3034	-	-	-	X
5	GOL	D	3023	-	-	-	X
5	GOL	D	3027	-	-	-	X
5	GOL	D	3035	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 20181 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 Beta-xylosidase, family 43 glycosyl hydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	534	Total	C	N	O	S	Se	0	0	0
			4341	2783	723	821	10	4			
1	B	534	Total	C	N	O	S	Se	0	1	0
			4345	2785	723	823	10	4			
1	C	534	Total	C	N	O	S	Se	0	1	0
			4343	2784	723	821	11	4			
1	D	534	Total	C	N	O	S	Se	0	2	0
			4347	2786	723	823	11	4			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	CLONING ARTIFACT	UNP Q97DM1
A	2	SER	-	CLONING ARTIFACT	UNP Q97DM1
A	3	LEU	-	CLONING ARTIFACT	UNP Q97DM1
A	64	MSE	MET	MODIFIED RESIDUE	UNP Q97DM1
A	98	MSE	MET	MODIFIED RESIDUE	UNP Q97DM1
A	144	MSE	MET	MODIFIED RESIDUE	UNP Q97DM1
A	445	MSE	MET	MODIFIED RESIDUE	UNP Q97DM1
A	535	GLU	-	EXPRESSION TAG	UNP Q97DM1
A	536	GLY	-	EXPRESSION TAG	UNP Q97DM1
A	537	HIS	-	EXPRESSION TAG	UNP Q97DM1
A	538	HIS	-	EXPRESSION TAG	UNP Q97DM1
A	539	HIS	-	EXPRESSION TAG	UNP Q97DM1
A	540	HIS	-	EXPRESSION TAG	UNP Q97DM1
A	541	HIS	-	EXPRESSION TAG	UNP Q97DM1
A	542	HIS	-	EXPRESSION TAG	UNP Q97DM1
B	1	MSE	-	CLONING ARTIFACT	UNP Q97DM1
B	2	SER	-	CLONING ARTIFACT	UNP Q97DM1
B	3	LEU	-	CLONING ARTIFACT	UNP Q97DM1
B	64	MSE	MET	MODIFIED RESIDUE	UNP Q97DM1
B	98	MSE	MET	MODIFIED RESIDUE	UNP Q97DM1
B	144	MSE	MET	MODIFIED RESIDUE	UNP Q97DM1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	445	MSE	MET	MODIFIED RESIDUE	UNP Q97DM1
B	535	GLU	-	EXPRESSION TAG	UNP Q97DM1
B	536	GLY	-	EXPRESSION TAG	UNP Q97DM1
B	537	HIS	-	EXPRESSION TAG	UNP Q97DM1
B	538	HIS	-	EXPRESSION TAG	UNP Q97DM1
B	539	HIS	-	EXPRESSION TAG	UNP Q97DM1
B	540	HIS	-	EXPRESSION TAG	UNP Q97DM1
B	541	HIS	-	EXPRESSION TAG	UNP Q97DM1
B	542	HIS	-	EXPRESSION TAG	UNP Q97DM1
C	1	MSE	-	CLONING ARTIFACT	UNP Q97DM1
C	2	SER	-	CLONING ARTIFACT	UNP Q97DM1
C	3	LEU	-	CLONING ARTIFACT	UNP Q97DM1
C	64	MSE	MET	MODIFIED RESIDUE	UNP Q97DM1
C	98	MSE	MET	MODIFIED RESIDUE	UNP Q97DM1
C	144	MSE	MET	MODIFIED RESIDUE	UNP Q97DM1
C	445	MSE	MET	MODIFIED RESIDUE	UNP Q97DM1
C	535	GLU	-	EXPRESSION TAG	UNP Q97DM1
C	536	GLY	-	EXPRESSION TAG	UNP Q97DM1
C	537	HIS	-	EXPRESSION TAG	UNP Q97DM1
C	538	HIS	-	EXPRESSION TAG	UNP Q97DM1
C	539	HIS	-	EXPRESSION TAG	UNP Q97DM1
C	540	HIS	-	EXPRESSION TAG	UNP Q97DM1
C	541	HIS	-	EXPRESSION TAG	UNP Q97DM1
C	542	HIS	-	EXPRESSION TAG	UNP Q97DM1
D	1	MSE	-	CLONING ARTIFACT	UNP Q97DM1
D	2	SER	-	CLONING ARTIFACT	UNP Q97DM1
D	3	LEU	-	CLONING ARTIFACT	UNP Q97DM1
D	64	MSE	MET	MODIFIED RESIDUE	UNP Q97DM1
D	98	MSE	MET	MODIFIED RESIDUE	UNP Q97DM1
D	144	MSE	MET	MODIFIED RESIDUE	UNP Q97DM1
D	445	MSE	MET	MODIFIED RESIDUE	UNP Q97DM1
D	535	GLU	-	EXPRESSION TAG	UNP Q97DM1
D	536	GLY	-	EXPRESSION TAG	UNP Q97DM1
D	537	HIS	-	EXPRESSION TAG	UNP Q97DM1
D	538	HIS	-	EXPRESSION TAG	UNP Q97DM1
D	539	HIS	-	EXPRESSION TAG	UNP Q97DM1
D	540	HIS	-	EXPRESSION TAG	UNP Q97DM1
D	541	HIS	-	EXPRESSION TAG	UNP Q97DM1
D	542	HIS	-	EXPRESSION TAG	UNP Q97DM1

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Ca 1 1	0	0
2	A	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0

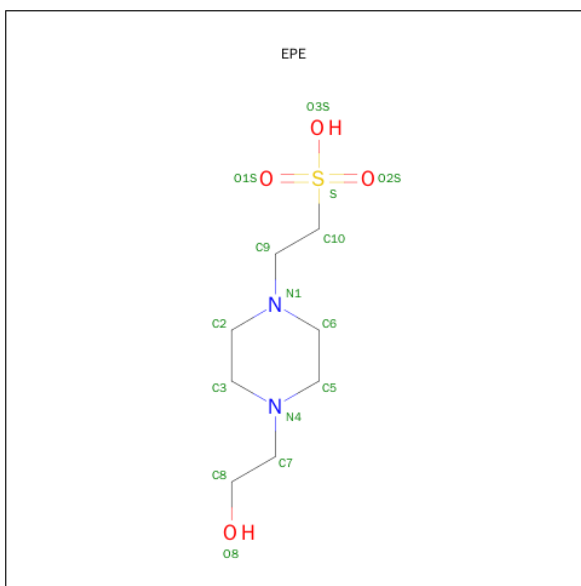
- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

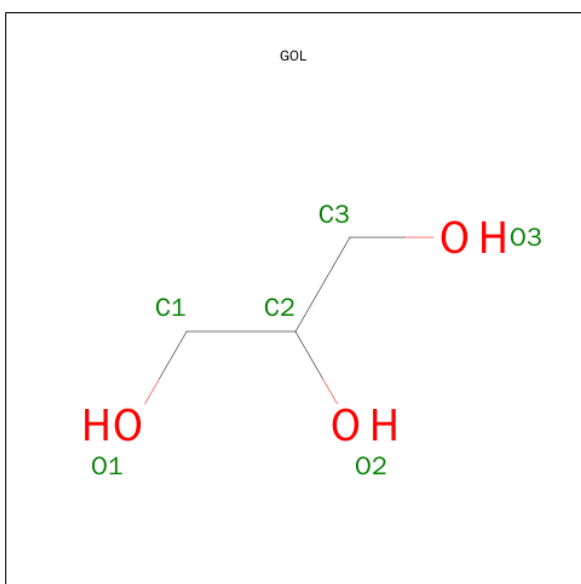
- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID

(three-letter code: EPE) (formula:  $C_8H_{18}N_2O_4S$ ).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 6 is water.

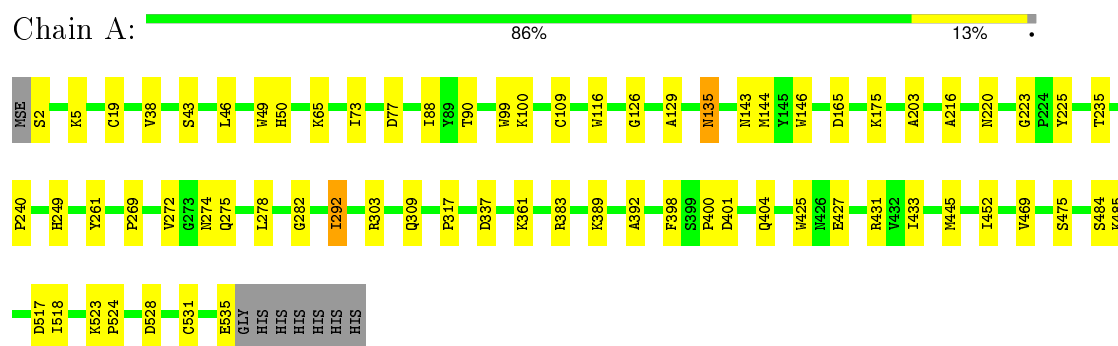


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	683	Total 683	O 683	0	0
6	B	614	Total 614	O 614	0	0
6	C	656	Total 656	O 656	0	0
6	D	633	Total 633	O 633	0	0

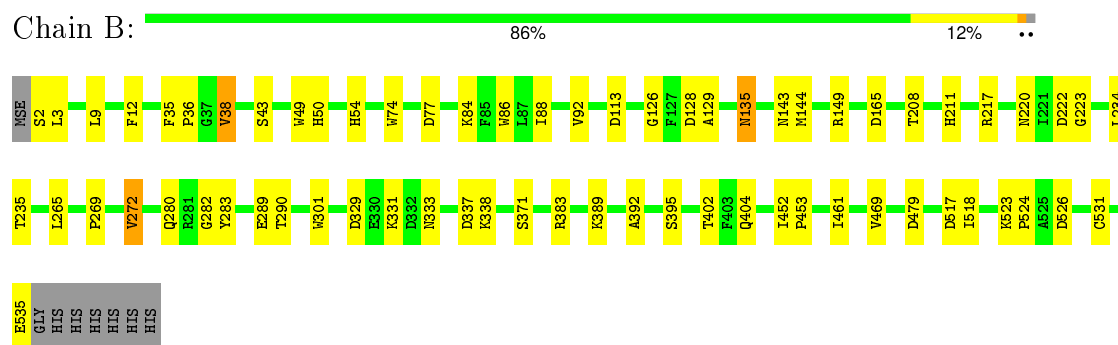
### 3 Residue-property plots

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.

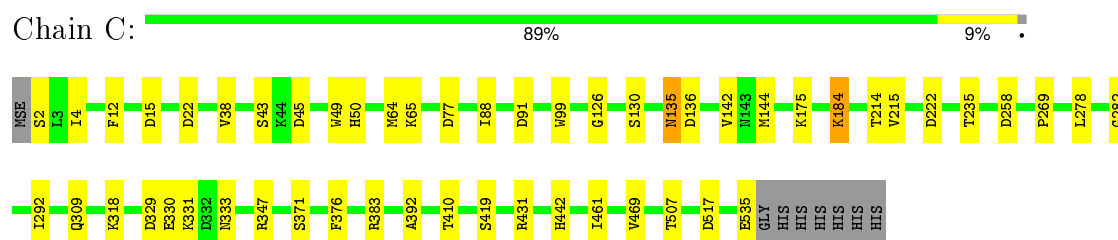
- Molecule 1: Beta-xylosidase, family 43 glycosyl hydrolase



- Molecule 1: Beta-xylosidase, family 43 glycosyl hydrolase

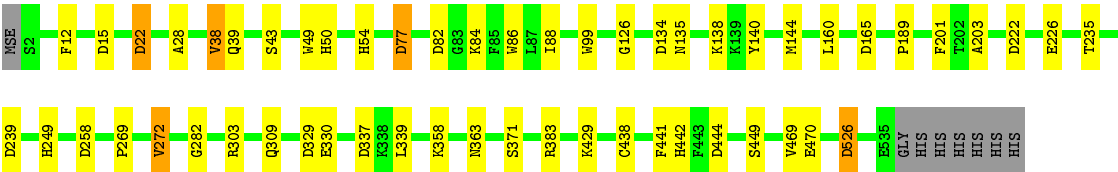


- Molecule 1: Beta-xylosidase, family 43 glycosyl hydrolase



- Molecule 1: Beta-xylosidase, family 43 glycosyl hydrolase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.13Å 143.73Å 188.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 38.52 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-1.90) 100.0 (38.52-1.90)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.85 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.142 , 0.202 0.148 , 0.209	Depositor DCC
$R_{free}$ test set	5740 reflections (3.11%)	DCC
Wilson B-factor (Å <sup>2</sup> )	17.6	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 51.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 190582 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	20181	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CA, EPE, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.64	1/4470 (0.0%)	0.80	4/6077 (0.1%)
1	B	0.61	0/4478	0.81	7/6088 (0.1%)
1	C	0.65	0/4476	0.82	9/6085 (0.1%)
1	D	0.64	0/4484	0.83	12/6096 (0.2%)
All	All	0.64	1/17908 (0.0%)	0.82	32/24346 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	19	CYS	CB-SG	-5.69	1.72	1.81

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	528	ASP	CB-CG-OD2	7.31	124.88	118.30
1	B	526	ASP	CB-CG-OD2	7.13	124.72	118.30
1	D	526	ASP	CB-CG-OD2	6.57	124.21	118.30
1	C	15	ASP	CB-CG-OD2	6.40	124.06	118.30
1	D	77	ASP	CB-CG-OD2	6.22	123.90	118.30
1	C	329	ASP	CB-CG-OD2	6.20	123.88	118.30
1	A	517	ASP	CB-CG-OD2	6.08	123.77	118.30
1	C	136	ASP	CB-CG-OD2	6.06	123.75	118.30
1	D	258	ASP	CB-CG-OD2	5.97	123.68	118.30
1	B	517	ASP	CB-CG-OD2	5.93	123.64	118.30
1	A	165	ASP	CB-CG-OD2	5.87	123.58	118.30
1	D	239	ASP	CB-CG-OD2	5.82	123.53	118.30
1	B	128	ASP	CB-CG-OD2	5.73	123.46	118.30
1	D	82	ASP	CB-CG-OD2	5.67	123.41	118.30
1	C	517	ASP	CB-CG-OD2	5.67	123.41	118.30
1	C	45	ASP	CB-CG-OD2	5.60	123.34	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	444	ASP	CB-CG-OD2	5.52	123.27	118.30
1	D	22[A]	ASP	CB-CG-OD2	5.35	123.11	118.30
1	D	22[B]	ASP	CB-CG-OD2	5.35	123.11	118.30
1	B	165	ASP	CB-CG-OD2	5.34	123.11	118.30
1	B	329	ASP	CB-CG-OD2	5.33	123.10	118.30
1	C	91	ASP	CB-CG-OD2	5.32	123.08	118.30
1	D	134	ASP	CB-CG-OD2	5.25	123.03	118.30
1	D	329	ASP	CB-CG-OD2	5.24	123.01	118.30
1	C	258	ASP	CB-CG-OD2	5.23	123.00	118.30
1	B	113	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	401	ASP	CB-CG-OD2	5.21	122.99	118.30
1	B	479	ASP	CB-CG-OD2	5.21	122.99	118.30
1	C	222	ASP	CB-CG-OD2	5.18	122.96	118.30
1	D	165	ASP	CB-CG-OD2	5.17	122.95	118.30
1	D	15	ASP	CB-CG-OD2	5.13	122.92	118.30
1	C	22	ASP	CB-CG-OD2	5.03	122.83	118.30

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	4341	0	4127	40	0
1	B	4345	0	4127	32	0
1	C	4343	0	4128	29	0
1	D	4347	0	4128	32	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	10	0	0	1	0
3	B	10	0	0	0	0
3	C	5	0	0	0	0
3	D	10	0	0	0	0
4	A	30	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	15	0	17	1	0
4	D	15	0	17	0	0
5	A	30	0	40	0	0
5	B	30	0	40	2	0
5	C	30	0	40	1	0
5	D	30	0	40	0	0
6	A	683	0	0	5	0
6	B	614	0	0	2	0
6	C	656	0	0	5	0
6	D	633	0	0	13	0
All	All	20181	0	16738	126	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 (126) 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:C:331:LYS:HE2	1:C:333:ASN:HD21	1.46	0.79
1:A:475:SER:HB3	1:A:485:LYS:HA	1.63	0.78
1:D:358:LYS:HE3	6:D:3636:HOH:O	1.84	0.77
1:A:65:LYS:HA	6:A:3696:HOH:O	1.87	0.74
1:A:269:PRO:HB3	1:A:282:GLY:HA3	1.71	0.72
1:D:84:LYS:HE3	1:D:86:TRP:CZ2	2.25	0.72
1:A:65:LYS:HG3	6:A:3707:HOH:O	1.90	0.69
1:D:337:ASP:HB3	6:D:3543:HOH:O	1.93	0.69
1:D:449:SER:HA	6:D:3426:HOH:O	1.92	0.68
1:D:272:VAL:HG12	6:D:3442:HOH:O	1.94	0.67
1:C:65:LYS:HD2	6:D:3621:HOH:O	1.94	0.66
1:B:269:PRO:HB3	1:B:282:GLY:HA3	1.79	0.64
1:C:175:LYS:HD3	6:C:3669:HOH:O	1.97	0.64
1:C:126:GLY:HA3	1:C:144:MSE:O	2.00	0.62
1:B:272:VAL:HG21	1:B:280:GLN:O	2.02	0.59
1:C:442:HIS:HB2	6:C:3679:HOH:O	2.03	0.58
1:D:269:PRO:HB3	1:D:282:GLY:HA3	1.86	0.57
1:C:331:LYS:CE	1:C:333:ASN:HD21	2.15	0.57
1:B:9:LEU:HB2	1:B:290:THR:HB	1.88	0.56
1:C:65:LYS:HA	6:C:3525:HOH:O	2.05	0.55
1:C:135:ASN:C	1:C:135:ASN:HD22	2.09	0.54
1:A:261:TYR:HB3	1:A:292:ILE:CD1	2.38	0.54
1:B:217:ARG:HG2	1:B:301:TRP:CH2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:SER:HB2	1:A:484:SER:O	2.08	0.53
1:D:337:ASP:HB2	6:D:3636:HOH:O	2.10	0.51
1:B:220:ASN:ND2	1:B:223:GLY:O	2.43	0.51
1:C:99:TRP:CD2	1:D:371:SER:HB2	2.45	0.51
1:A:126:GLY:HA3	1:A:144:MSE:O	2.11	0.51
1:A:274:ASN:OD1	1:C:184:LYS:HE2	2.10	0.51
1:A:129:ALA:HA	1:A:143:ASN:HB3	1.93	0.51
1:C:269:PRO:HB3	1:C:282:GLY:HA3	1.94	0.50
1:A:235:THR:O	1:A:309:GLN:HA	2.11	0.50
1:C:371:SER:HB2	1:D:99:TRP:CD2	2.46	0.50
1:B:392:ALA:HA	1:B:531:CYS:O	2.13	0.49
1:D:429:LYS:NZ	1:D:449:SER:O	2.45	0.49
1:D:203:ALA:HB2	1:D:249:HIS:HA	1.95	0.49
1:A:216:ALA:HB1	1:A:225:TYR:HB3	1.94	0.49
1:A:99:TRP:CD2	1:B:371:SER:HB2	2.47	0.48
1:B:404:GLN:HB3	1:B:518:ILE:HB	1.96	0.48
1:C:376:PHE:HA	6:C:3525:HOH:O	2.13	0.48
5:B:3029:GOL:H11	6:D:3307:HOH:O	2.12	0.48
1:A:425:TRP:CH2	1:A:427:GLU:HA	2.49	0.48
1:D:22[B]:ASP:HB3	6:D:3306:HOH:O	2.13	0.47
1:A:389:LYS:HE3	1:A:389:LYS:HB2	1.62	0.47
1:A:475:SER:CB	1:A:484:SER:O	2.62	0.47
1:A:220:ASN:ND2	1:A:223:GLY:O	2.48	0.47
1:D:470:GLU:HG2	6:D:3656:HOH:O	2.14	0.47
1:A:361:LYS:HG3	6:A:3617:HOH:O	2.15	0.47
1:A:445:MSE:HE1	1:B:149:ARG:HG2	1.97	0.47
1:A:272:VAL:HG22	1:A:275:GLN:HB2	1.96	0.47
1:C:4:ILE:HG21	1:C:292:ILE:CG2	2.45	0.46
1:B:129:ALA:HA	1:B:143:ASN:HB3	1.98	0.46
1:D:303:ARG:HB3	6:D:3632:HOH:O	2.15	0.46
1:B:523:LYS:HG3	1:B:524:PRO:HD2	1.97	0.46
1:C:461:ILE:N	1:C:461:ILE:HD12	2.30	0.46
1:B:337:ASP:HB2	6:B:3599:HOH:O	2.15	0.46
1:A:99:TRP:CE3	1:B:371:SER:HB2	2.50	0.46
1:B:265:LEU:HA	1:B:289:GLU:O	2.16	0.45
1:A:100:LYS:HE2	1:A:146:TRP:CH2	2.52	0.45
1:B:84:LYS:HE3	1:B:86:TRP:CZ2	2.52	0.45
1:D:126:GLY:HA3	1:D:144:MSE:O	2.16	0.45
1:D:358:LYS:HG3	6:D:3636:HOH:O	2.17	0.45
1:D:442:HIS:HB2	6:D:3611:HOH:O	2.15	0.45
1:C:99:TRP:CD2	1:D:371:SER:CB	2.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:TRP:CE3	1:D:371:SER:HB2	2.52	0.45
1:A:5:LYS:HD2	6:A:3341:HOH:O	2.15	0.45
1:B:77:ASP:HB3	1:B:88:ILE:HB	1.99	0.45
1:A:433:ILE:HB	1:A:452:ILE:HB	1.98	0.45
1:A:240:PRO:HG3	1:A:278:LEU:HD23	2.00	0.44
1:A:261:TYR:HB3	1:A:292:ILE:HD12	1.99	0.44
1:C:410:THR:HG23	1:C:419:SER:O	2.17	0.44
1:B:35:PHE:CG	1:B:36:PRO:HA	2.52	0.44
1:B:2:SER:C	1:B:3:LEU:HD12	2.38	0.44
1:C:130:SER:HB3	1:C:142:VAL:HG23	2.00	0.44
1:C:278:LEU:HD11	5:C:3030:GOL:H31	2.00	0.44
1:A:77:ASP:HB3	1:A:88:ILE:HB	1.99	0.44
1:D:77:ASP:HB3	1:D:88:ILE:HB	2.00	0.44
1:D:28:ALA:HA	1:D:39:GLN:O	2.18	0.44
1:A:392:ALA:HA	1:A:531:CYS:O	2.18	0.43
1:A:135:ASN:HD22	1:A:135:ASN:C	2.22	0.43
1:A:99:TRP:CD2	1:B:371:SER:CB	3.01	0.43
1:A:523:LYS:HG3	1:A:524:PRO:HD2	2.00	0.43
1:B:234:LEU:O	1:B:235:THR:HB	2.19	0.43
1:B:43:SER:HB2	1:B:49:TRP:CD2	2.54	0.43
1:B:126:GLY:HA3	1:B:144:MSE:O	2.18	0.43
1:A:5:LYS:HE3	3:A:3011:SO4:O1	2.19	0.42
1:C:318:LYS:CE	6:C:3487:HOH:O	2.67	0.42
1:D:226:GLU:O	1:D:226:GLU:HG3	2.18	0.42
1:A:404:GLN:HB3	1:A:518:ILE:HB	2.00	0.42
1:D:438:CYS:SG	1:D:441:PHE:HA	2.59	0.42
1:D:189:PRO:HA	1:D:201:PHE:O	2.19	0.42
1:A:398:PHE:CD2	1:A:400:PRO:HD3	2.54	0.42
1:A:46:LEU:HD12	1:A:317:PRO:HG3	2.01	0.42
1:D:363:ASN:OD1	1:D:526:ASP:HB3	2.20	0.42
1:A:43:SER:HB2	1:A:49:TRP:CD2	2.55	0.42
1:C:43:SER:HB2	1:C:49:TRP:CD2	2.55	0.42
1:D:38:VAL:O	1:D:54:HIS:HA	2.20	0.42
1:B:331:LYS:HE2	1:B:333:ASN:HD21	1.85	0.42
1:C:12:PHE:CE1	1:C:507:THR:HA	2.55	0.41
1:B:135:ASN:HD22	1:B:135:ASN:C	2.24	0.41
4:C:3015:EPE:H81	4:C:3015:EPE:H31	1.76	0.41
1:A:73:ILE:HA	1:A:90:THR:O	2.20	0.41
1:C:77:ASP:HB3	1:C:88:ILE:HB	2.03	0.41
1:A:303:ARG:HA	1:A:303:ARG:HD3	1.92	0.41
1:D:138:LYS:HE2	6:D:3668:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:CYS:HB2	1:A:116:TRP:CD2	2.56	0.41
1:B:208:THR:O	1:B:211:HIS:HB2	2.20	0.41
1:D:303:ARG:HD3	1:D:303:ARG:HA	1.93	0.41
1:B:74:TRP:CD2	1:B:92:VAL:HG21	2.55	0.41
1:D:43:SER:HB2	1:D:49:TRP:CD2	2.55	0.41
1:D:235:THR:O	1:D:309:GLN:HA	2.21	0.41
1:B:283:TYR:CE1	5:B:3033:GOL:H32	2.56	0.41
1:B:395:SER:HA	1:B:461:ILE:O	2.22	0.40
1:A:203:ALA:HB2	1:A:249:HIS:HA	2.03	0.40
1:B:38:VAL:O	1:B:54:HIS:HA	2.21	0.40
1:B:389:LYS:HB3	1:B:389:LYS:HE2	1.96	0.40
1:C:214:THR:HG22	1:C:215:VAL:N	2.37	0.40
1:D:140:TYR:HB3	1:D:160:LEU:HD11	2.03	0.40
1:B:452:ILE:HA	1:B:453:PRO:HD3	1.96	0.40
1:C:64:MSE:HE3	1:C:347:ARG:HA	2.03	0.40
1:A:337:ASP:HB2	6:A:3601:HOH:O	2.21	0.40
1:B:535:GLU:HG3	6:B:3646:HOH:O	2.21	0.40
1:C:235:THR:O	1:C:309:GLN:HA	2.22	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	532/542 (98%)	503 (94%)	27 (5%)	2 (0%)	39	27
1	B	533/542 (98%)	504 (95%)	26 (5%)	3 (1%)	30	17
1	C	533/542 (98%)	503 (94%)	28 (5%)	2 (0%)	39	27
1	D	534/542 (98%)	504 (94%)	27 (5%)	3 (1%)	30	17
All	All	2132/2168 (98%)	2014 (94%)	108 (5%)	10 (0%)	34	21

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	469	VAL
1	B	469	VAL
1	C	469	VAL
1	D	469	VAL
1	B	12	PHE
1	D	12	PHE
1	A	38	VAL
1	B	38	VAL
1	C	38	VAL
1	D	38	VAL

### 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	475/477 (100%)	467 (98%)	8 (2%)	68	64
1	B	476/477 (100%)	469 (98%)	7 (2%)	72	69
1	C	476/477 (100%)	469 (98%)	7 (2%)	72	69
1	D	477/477 (100%)	471 (99%)	6 (1%)	76	73
All	All	1904/1908 (100%)	1876 (98%)	28 (2%)	72	69

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	50	HIS
1	A	135	ASN
1	A	175	LYS
1	A	292	ILE
1	A	383	ARG
1	A	431	ARG
1	A	535	GLU
1	B	50	HIS
1	B	135	ASN
1	B	222	ASP
1	B	272	VAL

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Mol	Chain	Res	Type
1	B	338	LYS
1	B	383	ARG
1	B	402	THR
1	C	2	SER
1	C	50	HIS
1	C	135	ASN
1	C	184	LYS
1	C	383	ARG
1	C	431	ARG
1	C	535	GLU
1	D	50	HIS
1	D	135	ASN
1	D	222	ASP
1	D	272	VAL
1	D	339	LEU
1	D	383	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	ASN
1	A	333	ASN
1	B	135	ASN
1	B	333	ASN
1	C	135	ASN
1	C	333	ASN
1	D	135	ASN
1	D	333	ASN

### 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

Of 35 ligands modelled in this entry, 4 are monoatomic - leaving 31 for Mogul analysis.

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	$\# Z  > 2$
3	SO4	A	3005	-	4,4,4	0.11	0	6,6,6	0.12	0
3	SO4	A	3011	-	4,4,4	0.22	0	6,6,6	0.29	0
4	EPE	A	3012	-	14,15,15	0.39	0	18,20,20	1.34	2 (11%)
4	EPE	A	3013	-	14,15,15	0.46	0	18,20,20	1.98	4 (22%)
5	GOL	A	3016	-	5,5,5	0.44	0	5,5,5	0.40	0
5	GOL	A	3020	-	5,5,5	0.48	0	5,5,5	1.24	1 (20%)
5	GOL	A	3024	-	5,5,5	0.37	0	5,5,5	0.36	0
5	GOL	A	3028	-	5,5,5	0.40	0	5,5,5	0.40	0
5	GOL	A	3032	-	5,5,5	0.51	0	5,5,5	0.41	0
3	SO4	B	3006	-	4,4,4	0.10	0	6,6,6	0.23	0
3	SO4	B	3009	-	4,4,4	0.20	0	6,6,6	0.20	0
5	GOL	B	3017	-	5,5,5	0.23	0	5,5,5	0.38	0
5	GOL	B	3021	-	5,5,5	0.36	0	5,5,5	1.34	1 (20%)
5	GOL	B	3025	-	5,5,5	0.37	0	5,5,5	0.46	0
5	GOL	B	3029	-	5,5,5	0.37	0	5,5,5	0.84	0
5	GOL	B	3033	-	5,5,5	0.44	0	5,5,5	0.38	0
3	SO4	C	3007	-	4,4,4	0.31	0	6,6,6	0.18	0
4	EPE	C	3015	-	14,15,15	0.51	0	18,20,20	1.84	3 (16%)
5	GOL	C	3018	-	5,5,5	0.41	0	5,5,5	0.54	0
5	GOL	C	3022	-	5,5,5	0.33	0	5,5,5	0.83	0
5	GOL	C	3026	-	5,5,5	0.43	0	5,5,5	0.55	0
5	GOL	C	3030	-	5,5,5	0.44	0	5,5,5	0.26	0
5	GOL	C	3034	-	5,5,5	0.37	0	5,5,5	0.44	0
3	SO4	D	3008	-	4,4,4	0.10	0	6,6,6	0.27	0
3	SO4	D	3010	-	4,4,4	0.31	0	6,6,6	0.59	0
4	EPE	D	3014	-	14,15,15	0.39	0	18,20,20	1.66	3 (16%)
5	GOL	D	3019	-	5,5,5	0.19	0	5,5,5	0.37	0
5	GOL	D	3023	-	5,5,5	0.41	0	5,5,5	1.09	0
5	GOL	D	3027	-	5,5,5	0.39	0	5,5,5	0.42	0
5	GOL	D	3031	-	5,5,5	0.21	0	5,5,5	0.57	0
5	GOL	D	3035	-	5,5,5	0.42	0	5,5,5	0.35	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
3	SO4	A	3005	-	-	0/0/0/0	0/0/0/0
3	SO4	A	3011	-	-	0/0/0/0	0/0/0/0
4	EPE	A	3012	-	-	0/9/19/19	0/1/1/1
4	EPE	A	3013	-	-	0/9/19/19	0/1/1/1
5	GOL	A	3016	-	-	0/4/4/4	0/0/0/0
5	GOL	A	3020	-	-	0/4/4/4	0/0/0/0
5	GOL	A	3024	-	-	0/4/4/4	0/0/0/0
5	GOL	A	3028	-	-	0/4/4/4	0/0/0/0
5	GOL	A	3032	-	-	0/4/4/4	0/0/0/0
3	SO4	B	3006	-	-	0/0/0/0	0/0/0/0
3	SO4	B	3009	-	-	0/0/0/0	0/0/0/0
5	GOL	B	3017	-	-	0/4/4/4	0/0/0/0
5	GOL	B	3021	-	-	0/4/4/4	0/0/0/0
5	GOL	B	3025	-	-	0/4/4/4	0/0/0/0
5	GOL	B	3029	-	-	0/4/4/4	0/0/0/0
5	GOL	B	3033	-	-	0/4/4/4	0/0/0/0
3	SO4	C	3007	-	-	0/0/0/0	0/0/0/0
4	EPE	C	3015	-	-	0/9/19/19	0/1/1/1
5	GOL	C	3018	-	-	0/4/4/4	0/0/0/0
5	GOL	C	3022	-	-	0/4/4/4	0/0/0/0
5	GOL	C	3026	-	-	0/4/4/4	0/0/0/0
5	GOL	C	3030	-	-	0/4/4/4	0/0/0/0
5	GOL	C	3034	-	-	0/4/4/4	0/0/0/0
3	SO4	D	3008	-	-	0/0/0/0	0/0/0/0
3	SO4	D	3010	-	-	0/0/0/0	0/0/0/0
4	EPE	D	3014	-	-	0/9/19/19	0/1/1/1
5	GOL	D	3019	-	-	0/4/4/4	0/0/0/0
5	GOL	D	3023	-	-	0/4/4/4	0/0/0/0
5	GOL	D	3027	-	-	0/4/4/4	0/0/0/0
5	GOL	D	3031	-	-	0/4/4/4	0/0/0/0
5	GOL	D	3035	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	3013	EPE	C9-N1-C2	-2.66	104.45	111.27
5	B	3021	GOL	C3-C2-C1	-2.43	101.58	111.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	3020	GOL	C3-C2-C1	-2.08	102.98	111.12
4	C	3015	EPE	C7-N4-C5	2.11	116.69	111.27
4	A	3012	EPE	C7-N4-C5	2.14	116.76	111.27
4	D	3014	EPE	C7-N4-C5	2.18	116.86	111.27
4	A	3013	EPE	C6-C5-N4	2.28	114.72	110.63
4	D	3014	EPE	O1S-S-C10	2.79	109.28	106.91
4	C	3015	EPE	O1S-S-C10	3.20	109.64	106.91
4	A	3012	EPE	C5-N4-C3	3.26	115.96	108.90
4	A	3013	EPE	C5-N4-C3	4.15	117.88	108.90
4	D	3014	EPE	C5-N4-C3	4.78	119.25	108.90
4	A	3013	EPE	O1S-S-C10	4.84	111.03	106.91
4	C	3015	EPE	C5-N4-C3	4.85	119.40	108.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3011	SO4	1	0
5	B	3029	GOL	1	0
5	B	3033	GOL	1	0
4	C	3015	EPE	1	0
5	C	3030	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	530/542 (97%)	-0.37	0 100 100	13, 20, 40, 67	0
1	B	530/542 (97%)	-0.30	0 100 100	16, 22, 40, 75	0
1	C	530/542 (97%)	-0.40	0 100 100	14, 21, 41, 91	0
1	D	530/542 (97%)	-0.48	0 100 100	14, 20, 39, 77	0
All	All	2120/2168 (97%)	-0.39	0 100 100	13, 21, 40, 91	0

There are no RSRZ outliers to report.

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	SO4	C	3007	5/5	0.97	0.18	9.51	38,44,58,125	0
5	GOL	C	3030	6/6	0.97	0.14	7.20	27,37,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	GOL	D	3023	6/6	0.95	0.17	5.46	16,23,26,30	0
5	GOL	D	3035	6/6	0.98	0.13	4.33	20,28,38,56	0
5	GOL	A	3020	6/6	0.97	0.23	4.30	11,17,25,28	0
5	GOL	C	3022	6/6	0.97	0.20	3.40	19,24,25,43	0
3	SO4	B	3006	5/5	0.97	0.15	3.39	40,46,56,68	0
5	GOL	D	3027	6/6	0.92	0.15	3.31	37,45,47,49	0
2	CA	B	3002	1/1	0.98	0.19	3.11	42,42,42,42	0
5	GOL	C	3026	6/6	0.87	0.19	3.02	30,37,41,54	0
5	GOL	B	3025	6/6	0.91	0.17	3.00	33,50,59,78	0
2	CA	A	3001	1/1	1.00	0.18	2.96	43,43,43,43	0
5	GOL	C	3034	6/6	0.94	0.14	2.80	21,28,46,56	0
5	GOL	A	3024	6/6	0.91	0.18	2.79	31,42,49,51	0
5	GOL	A	3032	6/6	0.95	0.14	2.74	20,25,33,42	0
5	GOL	B	3021	6/6	0.97	0.21	2.49	15,19,25,28	0
5	GOL	B	3033	6/6	0.96	0.14	2.28	20,32,43,44	0
3	SO4	D	3008	5/5	0.97	0.17	1.73	44,47,50,75	0
2	CA	C	3003	1/1	0.99	0.17	1.67	38,38,38,38	0
4	EPE	A	3012	15/15	0.95	0.11	1.46	18,27,50,56	0
3	SO4	A	3005	5/5	0.95	0.18	1.36	37,54,59,63	0
5	GOL	D	3031	6/6	0.96	0.08	0.72	27,34,40,44	0
5	GOL	B	3029	6/6	0.98	0.08	0.69	28,32,35,38	0
2	CA	D	3004	1/1	0.99	0.08	0.03	41,41,41,41	0
4	EPE	A	3013	15/15	0.97	0.08	0.00	17,24,38,52	0
5	GOL	A	3028	6/6	0.98	0.07	-0.22	24,39,43,44	0
5	GOL	C	3018	6/6	0.97	0.08	-0.41	17,20,23,25	0
5	GOL	B	3017	6/6	0.97	0.07	-0.55	20,24,25,27	0
5	GOL	A	3016	6/6	0.98	0.07	-0.71	16,19,22,22	0
5	GOL	D	3019	6/6	0.98	0.07	-0.71	14,16,22,22	0
4	EPE	C	3015	15/15	0.96	0.07	-0.72	17,25,42,46	0
4	EPE	D	3014	15/15	0.97	0.07	-1.34	18,24,45,49	0
3	SO4	B	3009	5/5	0.96	0.19	-	30,40,53,67	0
3	SO4	A	3011	5/5	0.95	0.28	-	64,65,75,78	0
3	SO4	D	3010	5/5	0.97	0.10	-	31,37,52,54	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.