



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 4, 2014 – 05:37 PM EST

PDB ID : 4RM1  
Title : The crystal structure of Y333Q mutant pyridoxal-dependent decarboxylase from *Sphaerobacter thermophilus* DSM 20745  
Authors : Wu, R.; Clancy, S.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2014-10-18  
Resolution : 1.99 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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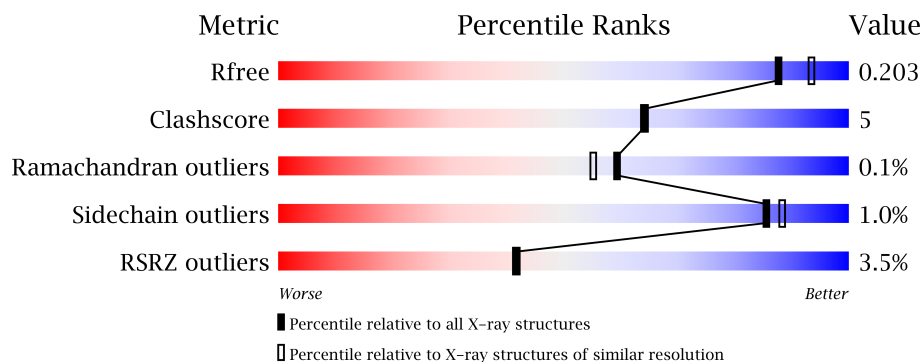
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable24103  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.1.3  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable24103

# 1 Overall quality at a glance

The reported resolution of this entry is 1.99 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))
$R_{free}$	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	486	
1	B	486	
1	C	486	
1	D	486	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	PMP	C	2000[B]	-	X
3	GOL	A	501	-	X
3	GOL	A	502	-	X
3	GOL	A	503	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	GOL	B	502	-	X
3	GOL	B	503	-	X
3	GOL	B	504	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15734 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

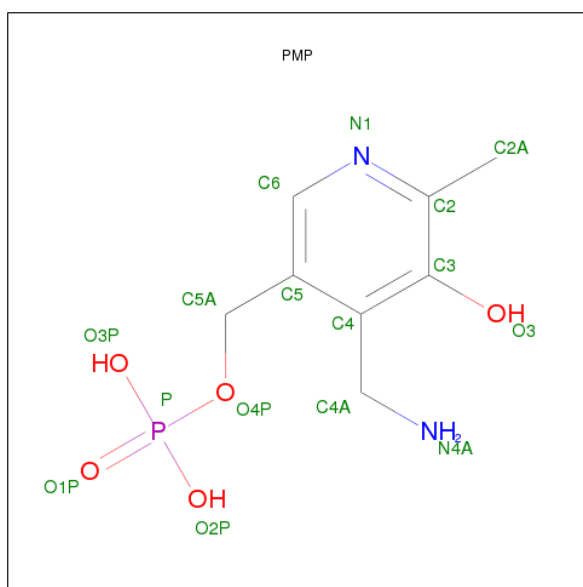
- Molecule 1 is a protein called Pyridoxal-dependent decarboxylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	473	Total	C	N	O	P	S	0	2	0
			3632	2295	652	667	1	17			
1	A	474	Total	C	N	O	P	S	0	3	0
			3653	2307	658	670	1	17			
1	C	476	Total	C	N	O	P	S	0	2	0
			3656	2312	658	668	1	17			
1	D	470	Total	C	N	O	P	S	0	3	0
			3607	2281	647	661	1	17			

There are 16 discrepancies between the modelled and reference sequences:

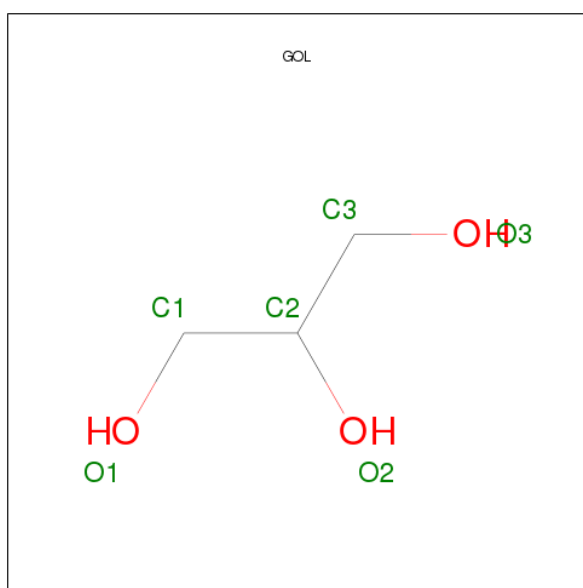
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	SER	-	EXPRESSION TAG	UNP D1C7D8
B	-1	ASN	-	EXPRESSION TAG	UNP D1C7D8
B	0	ALA	-	EXPRESSION TAG	UNP D1C7D8
B	333	GLN	TYR	ENGINEERED MUTATION	UNP D1C7D8
A	-2	SER	-	EXPRESSION TAG	UNP D1C7D8
A	-1	ASN	-	EXPRESSION TAG	UNP D1C7D8
A	0	ALA	-	EXPRESSION TAG	UNP D1C7D8
A	333	GLN	TYR	ENGINEERED MUTATION	UNP D1C7D8
C	-2	SER	-	EXPRESSION TAG	UNP D1C7D8
C	-1	ASN	-	EXPRESSION TAG	UNP D1C7D8
C	0	ALA	-	EXPRESSION TAG	UNP D1C7D8
C	333	GLN	TYR	ENGINEERED MUTATION	UNP D1C7D8
D	-2	SER	-	EXPRESSION TAG	UNP D1C7D8
D	-1	ASN	-	EXPRESSION TAG	UNP D1C7D8
D	0	ALA	-	EXPRESSION TAG	UNP D1C7D8
D	333	GLN	TYR	ENGINEERED MUTATION	UNP D1C7D8

- Molecule 2 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (three-letter code: PMP) (formula: C<sub>8</sub>H<sub>13</sub>N<sub>2</sub>O<sub>5</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	1
			16	8	2	5	1		
2	C	1	Total	C	N	O	P	0	1
			16	8	2	5	1		

- 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	B	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		
4	D	1	Total	Cl	0	0
			1	1		

- Molecule 5 is water.

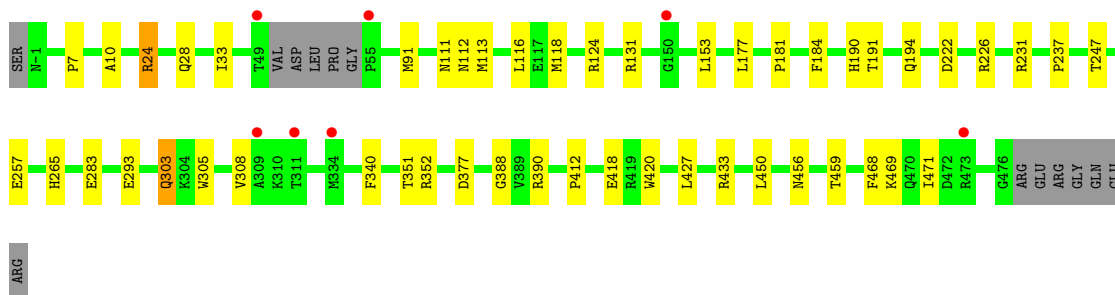
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	330	Total	O	0	0
			330	330		
5	A	351	Total	O	0	0
			351	351		
5	C	233	Total	O	0	0
			233	233		
5	D	202	Total	O	0	0
			202	202		

### 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.

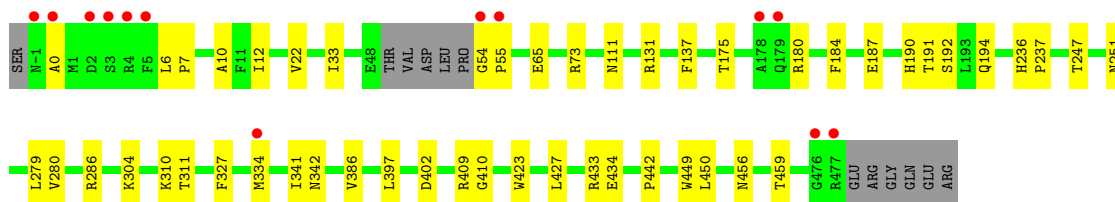
- Molecule 1: Pyridoxal-dependent decarboxylase

Chain B: 



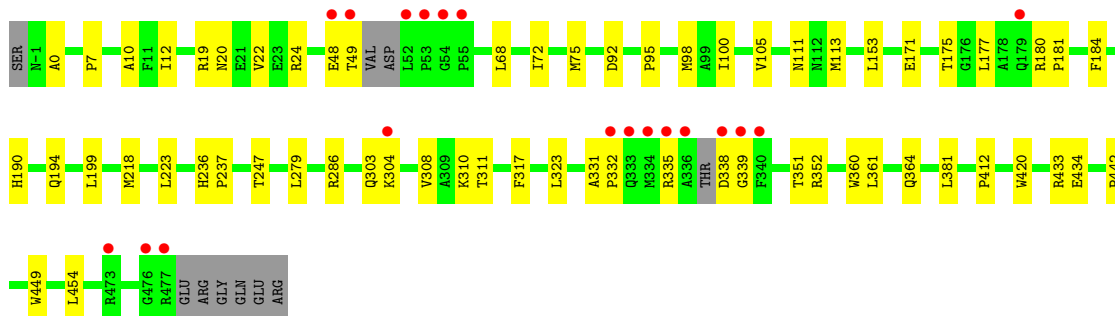
- Molecule 1: Pyridoxal-dependent decarboxylase

Chain A: 



- Molecule 1: Pyridoxal-dependent decarboxylase

Chain C: 



- Molecule 1: Pyridoxal-dependent decarboxylase

Chain D: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.55Å 125.00Å 132.24Å 90.00° 99.62° 90.00°	Depositor
Resolution (Å)	45.12 – 1.99 45.12 – 1.98	Depositor EDS
% Data completeness (in resolution range)	95.5 (45.12-1.99) 95.5 (45.12-1.98)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.16 (at 1.98Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.169 , 0.203 0.169 , 0.203	Depositor DCC
$R_{free}$ test set	7222 reflections (4.94%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.7	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 36.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 146612 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	15734	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, LLP, PMP, CL

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	0.54	0/3701	0.60	0/5031
1	B	0.53	0/3680	0.60	0/5003
1	C	0.51	0/3704	0.55	0/5035
1	D	0.49	0/3655	0.57	0/4972
All	All	0.52	0/14740	0.58	0/20041

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3653	0	3652	41	0
1	B	3632	0	3625	43	0
1	C	3656	0	3653	43	0
1	D	3607	0	3596	35	0
2	B	16	0	10	4	0
2	C	16	0	10	3	0
3	A	18	0	24	3	0
3	B	18	0	24	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	A	351	0	0	15	1
5	B	330	0	0	16	1
5	C	233	0	0	7	0
5	D	202	0	0	4	0
All	All	15734	0	14594	159	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (159) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:194:GLN:HG3	5:A:941:HOH:O	1.50	1.10
1:C:335:ARG:HD3	1:C:339:GLY:O	1.56	1.06
1:C:153:LEU:HG	5:C:2240:HOH:O	1.61	1.00
1:A:131:ARG:HD2	5:A:849:HOH:O	1.65	0.97
1:A:190:HIS:HE1	5:A:949:HOH:O	1.53	0.90
3:B:504:GOL:O3	5:B:906:HOH:O	1.91	0.85
1:D:179:GLN:HG2	1:D:234:GLY:C	1.97	0.85
1:D:153:LEU:HG	5:D:748:HOH:O	1.76	0.84
1:A:334:MET:O	5:A:943:HOH:O	1.97	0.83
1:D:179:GLN:HG2	1:D:234:GLY:O	1.79	0.83
3:B:502:GOL:H32	5:B:924:HOH:O	1.80	0.81
1:B:194:GLN:HG2	5:B:822:HOH:O	1.84	0.78
1:D:113:MET:HB2	1:D:352:ARG:HB3	1.68	0.76
1:D:179:GLN:CG	1:D:234:GLY:O	2.35	0.75
1:A:236:HIS:HE1	5:A:946:HOH:O	1.71	0.73
1:A:190:HIS:CE1	5:A:949:HOH:O	2.34	0.73
1:C:0:ALA:HB2	1:D:377:ASP:OD2	1.89	0.73
1:C:236:HIS:HE1	5:C:2249:HOH:O	1.70	0.73
3:B:504:GOL:H31	5:B:835:HOH:O	1.89	0.73
1:C:335:ARG:HD3	1:C:339:GLY:C	2.10	0.72
1:B:257:GLU:HG3	5:B:798:HOH:O	1.89	0.72
1:B:153:LEU:HG	5:B:925:HOH:O	1.88	0.71
1:A:73:ARG:HG2	5:A:844:HOH:O	1.88	0.71
1:B:247:THR:HB	3:B:504:GOL:H32	1.76	0.66
1:A:192:SER:HB3	5:A:949:HOH:O	1.94	0.66
1:B:412:PRO:HD2	1:B:420:TRP:CD1	2.31	0.66
1:B:191:THR:HG22	5:B:927:HOH:O	1.96	0.65
1:B:283:GLU:HG3	5:B:861:HOH:O	1.97	0.64
1:C:381:LEU:HB3	1:C:454:LEU:HD22	1.80	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:24:ARG:HD2	5:B:858:HOH:O	1.97	0.63
1:C:335:ARG:HD3	1:C:339:GLY:CA	2.29	0.63
1:D:324:GLU:OE1	1:D:335:ARG:NH2	2.32	0.63
1:C:335:ARG:HB3	1:C:339:GLY:HA2	1.81	0.63
1:D:337:THR:HG23	1:D:337:THR:O	1.99	0.62
1:A:73:ARG:CG	5:A:844:HOH:O	2.48	0.60
1:C:335:ARG:CD	1:C:339:GLY:O	2.43	0.59
1:B:184:PHE:HE2	1:B:237:PRO:HB3	1.67	0.59
1:A:386:VAL:HG13	1:A:397:LEU:HD11	1.85	0.58
1:B:433:ARG:NH2	5:B:841:HOH:O	2.35	0.58
1:D:410:GLY:HA3	1:D:423:TRP:CZ3	2.38	0.58
1:B:190:HIS:HA	3:B:504:GOL:O1	2.03	0.57
1:D:179:GLN:CB	1:D:234:GLY:O	2.53	0.56
1:A:184:PHE:HE2	1:A:237:PRO:HB3	1.71	0.56
1:D:179:GLN:HG3	1:D:235:GLN:HA	1.89	0.55
1:D:139:LEU:HD11	1:D:298:ILE:HD12	1.89	0.54
1:A:187:GLU:HA	3:A:503:GOL:H31	1.89	0.54
1:B:131:ARG:NH1	5:B:766:HOH:O	2.31	0.54
1:A:409:ARG:HH12	3:A:501:GOL:H12	1.72	0.54
1:B:222:ASP:O	1:B:226:ARG:HG2	2.08	0.54
1:D:389:VAL:HG11	1:D:397:LEU:HG	1.91	0.53
1:B:351:THR:HB	1:A:304:LLP:OP1	2.08	0.53
1:C:279:LEU:O	1:C:286:ARG:HB3	2.09	0.53
1:B:231:ARG:HH12	1:B:265:HIS:HD2	1.56	0.53
1:C:72:ILE:HA	1:C:75:MET:HE2	1.90	0.53
1:B:191:THR:HG23	3:B:504:GOL:O2	2.08	0.53
1:C:351:THR:HB	1:D:304[A]:LLP:OP1	2.09	0.52
1:A:304:LLP:H2'2	5:A:840:HOH:O	2.10	0.52
1:C:412:PRO:HD2	1:C:420:TRP:CD1	2.44	0.52
1:C:98:MET:HE3	1:C:361:LEU:HD13	1.91	0.51
1:C:181:PRO:CD	1:D:175:THR:HG21	2.40	0.51
1:B:184:PHE:CE2	1:B:237:PRO:HB3	2.44	0.51
1:A:442:PRO:HD2	1:A:449:TRP:O	2.12	0.50
1:C:236:HIS:CE1	5:C:2249:HOH:O	2.52	0.50
1:C:105:VAL:HG22	1:D:33:ILE:HD11	1.94	0.50
1:A:304:LLP:C2'	5:A:840:HOH:O	2.60	0.49
1:A:12:ILE:HG12	1:A:22[B]:VAL:HG11	1.94	0.49
1:A:279:LEU:O	1:A:286:ARG:HB3	2.12	0.49
1:C:304[A]:LLP:H5'1	5:C:2302:HOH:O	2.12	0.49
1:D:179:GLN:CG	1:D:234:GLY:C	2.75	0.49
1:D:469:LYS:HE2	1:D:473:ARG:NH2	2.28	0.49
1:A:7:PRO:HG2	1:A:10:ALA:HB2	1.95	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:410:GLY:HA3	1:A:423:TRP:CZ3	2.48	0.48
5:C:2210:HOH:O	1:D:82:PRO:HD2	2.13	0.48
1:A:180:ARG:NH2	5:A:785:HOH:O	2.34	0.48
1:C:175:THR:HG21	1:D:181:PRO:HD2	1.94	0.48
1:C:19:ARG:HG3	1:C:20:ASN:N	2.29	0.47
1:B:377:ASP:OD2	1:A:0:ALA:HB2	2.15	0.47
1:B:124:ARG:HG2	1:B:340:PHE:CD1	2.50	0.47
1:B:116:LEU:HB3	3:B:503:GOL:C1	2.45	0.47
1:A:191:THR:HG22	5:A:942:HOH:O	2.15	0.47
1:B:24:ARG:O	1:B:28:GLN:HG3	2.15	0.46
1:D:179:GLN:HB3	1:D:234:GLY:O	2.14	0.46
1:D:279:LEU:O	1:D:286:ARG:HB3	2.14	0.46
1:C:7:PRO:HG2	1:C:10:ALA:HB2	1.98	0.46
1:C:113:MET:HB2	1:C:352:ARG:HB3	1.97	0.46
1:D:278:ALA:CB	1:D:305:TRP:HB3	2.46	0.46
1:B:390:ARG:NH1	5:B:776:HOH:O	2.42	0.46
1:D:352:ARG:HG2	5:D:720:HOH:O	2.16	0.46
1:B:427:LEU:HD23	1:B:450:LEU:HD11	1.97	0.45
1:C:181:PRO:HD2	1:D:175:THR:HG21	1.97	0.45
1:C:95:PRO:HG2	1:C:100:ILE:HD11	1.98	0.45
1:C:92:ASP:HB3	5:C:2219:HOH:O	2.16	0.45
1:A:65:GLU:HG3	5:A:917:HOH:O	2.17	0.45
1:C:338:ASP:N	5:C:2252:HOH:O	2.48	0.45
1:D:92:ASP:HB3	5:D:722:HOH:O	2.15	0.45
1:A:180:ARG:HD3	5:A:874:HOH:O	2.16	0.45
1:A:433:ARG:NH2	1:A:434:GLU:OE2	2.49	0.45
1:A:251:ASN:HA	1:A:402:ASP:HB2	1.99	0.45
1:C:303:GLN:HA	1:C:308:VAL:O	2.17	0.45
1:B:112:ASN:HB3	1:B:118:MET:HB3	1.98	0.45
1:D:442:PRO:HD2	1:D:449:TRP:O	2.17	0.45
1:B:190:HIS:HD2	1:B:247:THR:OG1	2.01	0.44
1:B:124:ARG:HH12	3:B:503:GOL:C2	2.30	0.44
1:B:469:LYS:HD2	5:B:727:HOH:O	2.17	0.44
1:B:293:GLU:HB3	3:B:502:GOL:H11	2.00	0.44
1:C:442:PRO:HD2	1:C:449:TRP:O	2.18	0.44
1:D:223:LEU:O	1:D:227:ILE:HG13	2.18	0.44
1:B:33:ILE:HA	1:B:33:ILE:HD13	1.87	0.43
1:B:231:ARG:HH12	1:B:265:HIS:CD2	2.35	0.43
1:C:48:GLU:O	1:C:49:THR:OG1	2.28	0.43
2:B:501[B]:PMP:H5A1	5:B:787:HOH:O	2.18	0.43
1:C:317:PHE:CE2	1:C:323:LEU:HD21	2.53	0.43
1:A:190:HIS:HD2	1:A:247:THR:OG1	2.01	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:373:ARG:NH1	1:D:377:ASP:OD1	2.51	0.43
1:B:7:PRO:HG2	1:B:10:ALA:HB2	2.01	0.43
1:C:433:ARG:NH2	1:C:434:GLU:OE1	2.52	0.43
1:A:310:LYS:HA	1:A:311:THR:HA	1.82	0.42
1:B:190:HIS:CE1	5:B:787:HOH:O	2.72	0.42
1:C:184:PHE:HE2	1:C:237:PRO:HB3	1.84	0.42
1:C:190:HIS:HD2	1:C:247:THR:OG1	2.01	0.42
1:B:388:GLY:HA3	1:B:468:PHE:CZ	2.55	0.42
1:C:338:ASP:N	1:C:338:ASP:OD1	2.52	0.42
1:B:113:MET:HB2	1:B:352:ARG:HB3	2.02	0.42
1:B:91:MET:HE1	1:B:247:THR:HA	2.01	0.42
1:C:12:ILE:HG12	1:C:22[B]:VAL:HG11	2.02	0.42
1:A:137:PHE:CD1	1:A:280:VAL:HG11	2.55	0.42
1:B:456:ASN:HB3	1:B:459:THR:OG1	2.19	0.42
1:C:199:LEU:O	1:D:200:LEU:HA	2.19	0.42
1:D:177:LEU:HD23	1:D:181:PRO:CG	2.50	0.42
1:A:33:ILE:HA	1:A:33:ILE:HD13	1.96	0.41
1:B:418:GLU:CD	1:B:418:GLU:H	2.24	0.41
1:C:180:ARG:HE	1:C:180:ARG:HB2	1.69	0.41
1:A:54:GLY:HA2	1:A:55:PRO:HA	1.87	0.41
1:C:310:LYS:HA	1:C:311:THR:HA	1.70	0.41
1:B:469:LYS:HG3	5:B:920:HOH:O	2.20	0.41
1:B:427:LEU:HD21	1:B:471:ILE:HG12	2.02	0.41
1:C:360:TRP:O	1:C:364:GLN:HG3	2.19	0.41
1:C:68:LEU:HD11	1:D:365:HIS:CD2	2.56	0.41
1:D:401:ILE:HG21	1:D:406:VAL:HG22	2.02	0.41
1:B:190:HIS:CG	2:B:501[B]:PMP:C6	3.04	0.41
1:C:218:MET:CE	1:C:223:LEU:HD22	2.50	0.41
1:C:335:ARG:CB	1:C:339:GLY:HA2	2.50	0.41
1:A:341:ILE:HG12	1:A:342:ASN:N	2.36	0.41
1:A:427:LEU:HD23	1:A:450:LEU:HD11	2.03	0.41
1:B:303:GLN:HA	1:B:308:VAL:O	2.21	0.41
1:C:331:ALA:HB1	1:C:332:PRO:HD2	2.03	0.41
1:B:181:PRO:CD	1:A:175:THR:HG21	2.51	0.40
1:A:409:ARG:HH12	3:A:501:GOL:C1	2.34	0.40
1:A:6:LEU:HA	1:A:6:LEU:HD23	1.95	0.40
1:D:254:PRO:O	1:D:258:ILE:HG12	2.21	0.40
1:A:6:LEU:HA	1:A:7:PRO:HD2	1.91	0.40
1:D:329:ILE:HG12	5:D:726:HOH:O	2.22	0.40
1:A:456:ASN:HB3	1:A:459:THR:OG1	2.20	0.40
1:B:181:PRO:HD2	1:A:175:THR:HG21	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:B:896:HOH:O	5:A:945:HOH:O[1_655]	2.18	0.02

## 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	472/486 (97%)	463 (98%)	8 (2%)	1 (0%)	56	51
1	B	469/486 (96%)	457 (97%)	12 (3%)	0	100	100
1	C	470/486 (97%)	454 (97%)	16 (3%)	0	100	100
1	D	467/486 (96%)	452 (97%)	14 (3%)	1 (0%)	56	51
All	All	1878/1944 (97%)	1826 (97%)	50 (3%)	2 (0%)	59	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	338	ASP
1	A	327	PHE

### 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	368/376 (98%)	367 (100%)	1 (0%)	96	97
1	B	366/376 (97%)	361 (99%)	5 (1%)	78	81
1	C	368/376 (98%)	363 (99%)	5 (1%)	78	81
1	D	363/376 (96%)	359 (99%)	4 (1%)	84	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1465/1504 (97%)	1450 (99%)	15 (1%)	85	88

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	24	ARG
1	B	111	ASN
1	B	177	LEU
1	B	303	GLN
1	B	305	TRP
1	A	111	ASN
1	C	24	ARG
1	C	111	ASN
1	C	171	GLU
1	C	177	LEU
1	C	194	GLN
1	D	111	ASN
1	D	305	TRP
1	D	334	MET
1	D	376	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	190	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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	LLP	A	304	1	24,24,25	4.18	5 (20%)	30,32,34	1.64	3 (10%)
1	LLP	B	304[A]	-	24,24,25	3.78	3 (12%)	30,32,34	1.84	4 (13%)
1	LLP	C	304[A]	-	24,24,25	3.88	6 (25%)	30,32,34	2.30	8 (26%)
1	LLP	D	304[A]	-	24,24,25	3.85	3 (12%)	30,32,34	2.85	6 (20%)

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	LLP	A	304	1	-	0/15/17/19	0/1/1/1
1	LLP	B	304[A]	-	-	0/15/17/19	0/1/1/1
1	LLP	C	304[A]	-	-	0/15/17/19	0/1/1/1
1	LLP	D	304[A]	-	-	0/15/17/19	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	304	LLP	O-C	19.45	1.24	1.11
1	B	304[A]	LLP	O-C	17.49	1.23	1.11
1	D	304[A]	LLP	O-C	15.70	1.22	1.11
1	C	304[A]	LLP	O-C	14.54	1.21	1.11
1	D	304[A]	LLP	CE-NZ	-9.06	1.17	1.46
1	C	304[A]	LLP	C3-C2	8.39	1.46	1.40
1	C	304[A]	LLP	C5-C4	5.37	1.48	1.40
1	C	304[A]	LLP	C3-C4	4.86	1.48	1.40
1	B	304[A]	LLP	CB-CA	-3.83	1.49	1.53
1	A	304	LLP	CB-CA	-3.55	1.49	1.53
1	C	304[A]	LLP	P-OP3	-2.83	1.44	1.54
1	C	304[A]	LLP	P-OP2	-2.60	1.45	1.54
1	A	304	LLP	C3-C2	-2.53	1.39	1.40
1	B	304[A]	LLP	O3-C3	2.35	1.42	1.37
1	D	304[A]	LLP	C3-C2	-2.29	1.39	1.40
1	A	304	LLP	O3-C3	2.13	1.42	1.37
1	A	304	LLP	CE-NZ	-2.05	1.40	1.46

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	304[A]	LLP	CD-CE-NZ	10.74	139.63	111.96
1	C	304[A]	LLP	CD-CE-NZ	7.07	130.18	111.96
1	D	304[A]	LLP	OP4-C5'-C5	6.24	121.94	109.26
1	B	304[A]	LLP	OP4-C5'-C5	5.43	120.31	109.26
1	A	304	LLP	OP4-C5'-C5	5.10	119.62	109.26
1	D	304[A]	LLP	C4-C4'-NZ	4.91	121.44	111.37
1	C	304[A]	LLP	C4-C4'-NZ	-4.72	101.68	111.37
1	B	304[A]	LLP	C-CA-N	-4.45	109.39	113.83
1	A	304	LLP	C-CA-N	-4.24	109.60	113.83
1	C	304[A]	LLP	C4'-NZ-CE	4.01	128.10	113.43
1	B	304[A]	LLP	C4'-C4-C5	3.84	123.19	119.70
1	D	304[A]	LLP	C-CA-N	-3.81	110.03	113.83
1	D	304[A]	LLP	C4'-C4-C5	3.66	123.03	119.70
1	C	304[A]	LLP	C4'-C4-C5	3.66	123.03	119.70
1	D	304[A]	LLP	P-OP4-C5'	-3.65	112.73	120.67
1	C	304[A]	LLP	C-CA-N	-3.38	110.45	113.83
1	C	304[A]	LLP	P-OP4-C5'	-3.32	113.44	120.67
1	B	304[A]	LLP	P-OP4-C5'	-2.77	114.65	120.67
1	C	304[A]	LLP	OP2-P-OP1	2.66	119.06	110.36
1	A	304	LLP	P-OP4-C5'	-2.61	114.99	120.67
1	C	304[A]	LLP	C6-N1-C2	2.34	124.30	119.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	GOL	A	501	-	5,5,5	0.28	0	5,5,5	0.24	0
3	GOL	A	502	-	5,5,5	0.43	0	5,5,5	1.78	2 (40%)
3	GOL	A	503	-	5,5,5	0.21	0	5,5,5	0.25	0
2	PMP	B	501[B]	-	16,16,16	3.72	7 (43%)	23,23,23	1.53	6 (26%)
3	GOL	B	502	-	5,5,5	0.67	0	5,5,5	1.06	0
3	GOL	B	503	-	5,5,5	0.53	0	5,5,5	1.24	0
3	GOL	B	504	-	5,5,5	0.21	0	5,5,5	0.26	0
2	PMP	C	2000[B]	-	16,16,16	3.31	6 (37%)	23,23,23	1.48	4 (17%)

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	GOL	A	501	-	-	0/4/4/4	0/0/0/0
3	GOL	A	502	-	-	0/4/4/4	0/0/0/0
3	GOL	A	503	-	-	0/4/4/4	0/0/0/0
2	PMP	B	501[B]	-	-	0/8/8/8	0/1/1/1
3	GOL	B	502	-	-	0/4/4/4	0/0/0/0
3	GOL	B	503	-	-	0/4/4/4	0/0/0/0
3	GOL	B	504	-	-	0/4/4/4	0/0/0/0
2	PMP	C	2000[B]	-	-	0/8/8/8	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501[B]	PMP	C3-C2	12.15	1.49	1.40
2	C	2000[B]	PMP	C3-C2	9.80	1.47	1.40
2	C	2000[B]	PMP	C5-C4	5.64	1.48	1.40
2	B	501[B]	PMP	C5-C4	5.34	1.48	1.40
2	C	2000[B]	PMP	C3-C4	4.43	1.47	1.40
2	B	501[B]	PMP	C3-C4	3.64	1.46	1.40
2	B	501[B]	PMP	P-O2P	-3.14	1.43	1.54
2	C	2000[B]	PMP	P-O3P	-2.97	1.44	1.54
2	C	2000[B]	PMP	P-O2P	-2.86	1.44	1.54
2	B	501[B]	PMP	P-O1P	-2.73	1.42	1.51
2	B	501[B]	PMP	P-O3P	-2.32	1.46	1.54
2	C	2000[B]	PMP	P-O1P	-2.31	1.43	1.51
2	B	501[B]	PMP	P-O4P	-2.18	1.52	1.60

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501[B]	PMP	O4P-C5A-C5	4.18	117.76	109.26
2	B	501[B]	PMP	O3-C3-C2	3.46	123.78	117.69
2	C	2000[B]	PMP	O3-C3-C2	2.91	122.82	117.69
2	C	2000[B]	PMP	O4P-C5A-C5	2.87	115.09	109.26
2	C	2000[B]	PMP	P-O4P-C5A	-2.84	114.49	120.67
3	A	502	GOL	O1-C1-C2	-2.49	99.30	110.37
2	B	501[B]	PMP	C6-N1-C2	2.37	124.36	119.29
3	A	502	GOL	O2-C2-C1	-2.35	97.56	108.44
2	B	501[B]	PMP	P-O4P-C5A	-2.26	115.75	120.67
2	C	2000[B]	PMP	C6-N1-C2	2.24	124.08	119.29
2	B	501[B]	PMP	C4-C3-C2	-2.17	116.06	119.82
2	B	501[B]	PMP	O2P-P-O1P	2.08	117.17	110.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	474/486 (97%)	-0.16	13 (2%) 52 52	12, 22, 46, 81	0
1	B	473/486 (97%)	-0.22	7 (1%) 70 70	12, 22, 45, 64	1 (0%)
1	C	476/486 (97%)	-0.02	19 (3%) 36 36	17, 30, 54, 75	1 (0%)
1	D	470/486 (96%)	0.17	28 (5%) 21 20	17, 31, 61, 89	1 (0%)
All	All	1893/1944 (97%)	-0.06	67 (3%) 42 41	12, 26, 52, 89	3 (0%)

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	339	GLY	8.0
1	C	52	LEU	8.0
1	D	335	ARG	6.9
1	D	334	MET	6.8
1	A	477	ARG	6.3
1	A	4	ARG	6.3
1	C	334	MET	5.9
1	C	336	ALA	5.9
1	D	337	THR	5.7
1	D	54	GLY	5.6
1	C	338	ASP	5.4
1	C	339	GLY	5.4
1	D	49	THR	5.3
1	A	54	GLY	5.1
1	D	414	TRP	4.9
1	A	5	PHE	4.8
1	C	335	ARG	4.7
1	C	49	THR	4.7
1	D	333	GLN	4.6
1	D	336	ALA	4.5
1	D	50	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	55	PRO	4.3
1	C	54	GLY	4.0
1	C	333	GLN	3.9
1	D	340	PHE	3.8
1	A	3	SER	3.7
1	D	415	LEU	3.7
1	A	0	ALA	3.5
1	B	49	THR	3.4
1	A	476	GLY	3.3
1	C	53	PRO	3.3
1	B	55	PRO	3.2
1	A	334	MET	3.1
1	D	338	ASP	3.1
1	C	55	PRO	3.0
1	C	332	PRO	3.0
1	A	178	ALA	3.0
1	D	55	PRO	3.0
1	D	423	TRP	3.0
1	C	477	ARG	2.9
1	C	340	PHE	2.8
1	D	474	PHE	2.7
1	D	48	GLU	2.7
1	D	412	PRO	2.7
1	D	476	GLY	2.7
1	B	473	ARG	2.6
1	C	179	GLN	2.5
1	D	178	ALA	2.5
1	D	473	ARG	2.5
1	A	2	ASP	2.5
1	B	334	MET	2.5
1	D	420	TRP	2.4
1	D	418	GLU	2.4
1	C	304[A]	LLP	2.4
1	B	150	GLY	2.4
1	C	473	ARG	2.4
1	D	394	PHE	2.4
1	D	413	ASP	2.4
1	D	332	PRO	2.3
1	D	53	PRO	2.3
1	B	309	ALA	2.3
1	C	48	GLU	2.2
1	A	179	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	179	GLN	2.2
1	C	476	GLY	2.1
1	A	-1	ASN	2.1
1	B	311	THR	2.1

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

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	LLP	C	304[A]	24/25	0.30	6.40	17,84,106,111	15
1	LLP	D	304[A]	24/25	0.23	3.62	18,29,39,44	16
1	LLP	B	304[A]	24/25	0.20	1.22	13,42,53,54	16
1	LLP	A	304	24/25	0.16	0.91	10,22,38,39	7

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	GOL	B	503	6/6	0.26	19.87	28,32,41,41	0
2	PMP	C	2000[B]	16/16	0.40	9.76	52,65,86,95	16
3	GOL	B	504	6/6	0.27	8.02	63,73,76,78	0
3	GOL	B	502	6/6	0.20	7.63	54,57,59,60	0
3	GOL	A	501	6/6	0.16	4.36	38,51,56,60	0
3	GOL	A	503	6/6	0.18	3.47	33,49,55,68	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	A	502	6/6	0.14	2.54	54,55,58,58	0
2	PMP	B	501[B]	16/16	0.20	1.14	18,31,37,43	15
4	CL	D	501	1/1	0.08	-4.07	26,26,26,26	0
4	CL	B	505	1/1	0.13	-4.42	22,22,22,22	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.