



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2023 – 03:49 PM EDT

PDB ID : 4RIZ  
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 : 2014-10-07  
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.35.1  
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) : 2.35.1

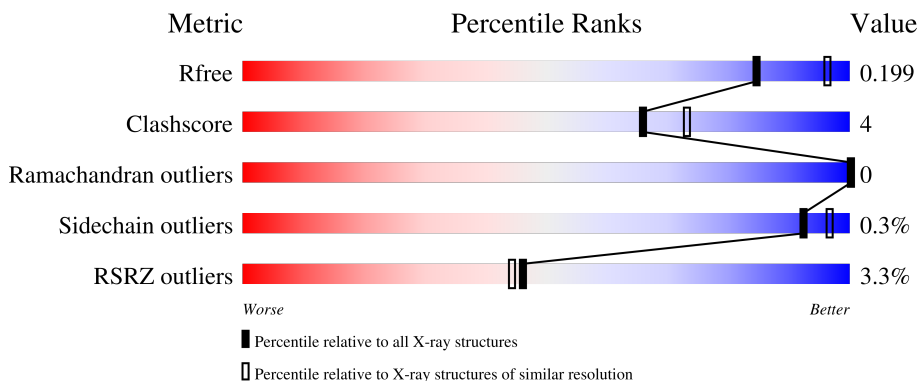
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 of 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	486	88% 8% .
1	B	486	87% 10% .
1	C	486	87% 10% .
1	D	486	88% 9% .

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
3	NA	B	504	-	-	-	X
4	GOL	B	503	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 15438 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.

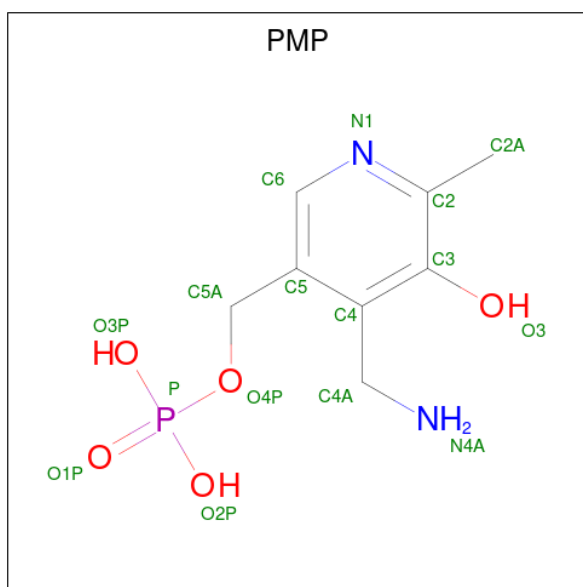
- Molecule 1 is a protein called Pyridoxal-dependent decarboxylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	470	3607	2282	648	660	1	16	0	2	0
1	B	475	3695	2330	668	678	1	18	0	6	0
1	C	476	3655	2312	657	668	1	17	0	2	0
1	D	472	3614	2286	647	663	1	17	0	2	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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
			Total	C	N	O	P		
2	A	1	16	8	2	5	1	0	1
2	C	1	16	8	2	5	1	0	1
2	D	1	16	8	2	5	1	0	1

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
3	A	1	1	1	0	0
3	B	1	1	1	0	0
3	D	1	1	1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

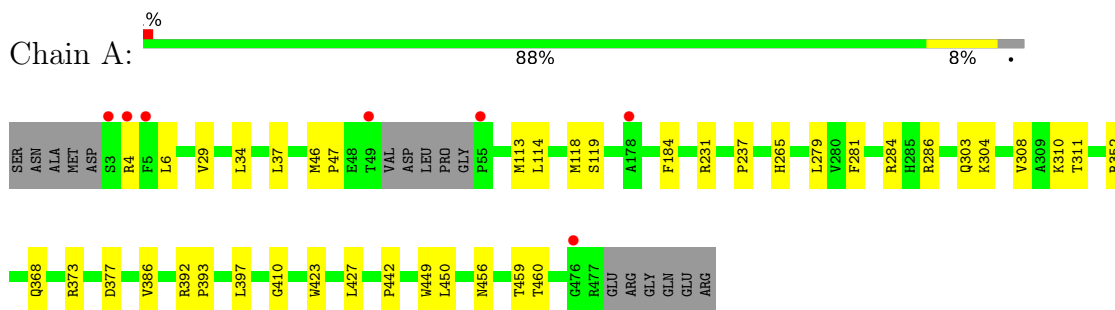
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	243	Total O 243 243	0	0
5	B	227	Total O 227 227	0	0
5	C	168	Total O 168 168	0	0
5	D	154	Total O 154 154	0	0

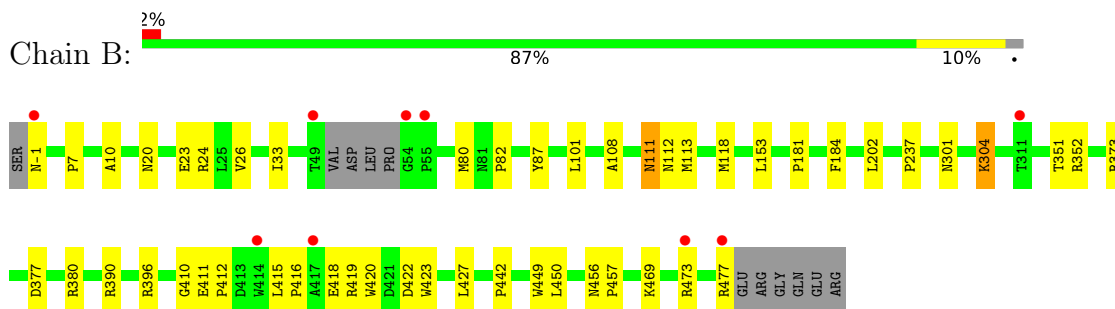
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

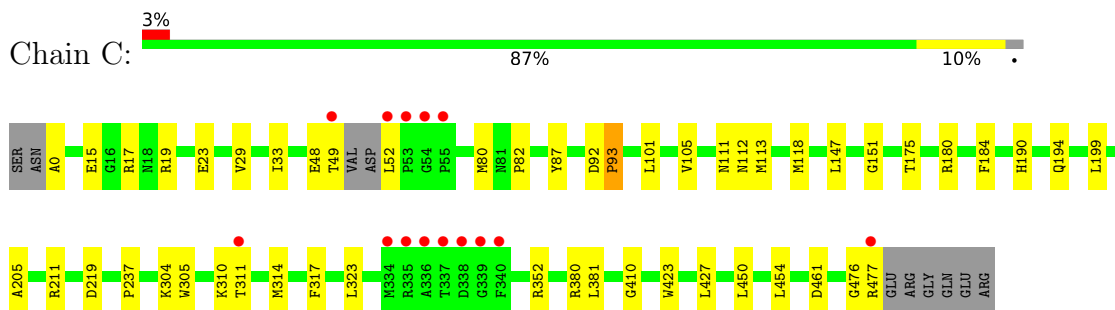
- Molecule 1: Pyridoxal-dependent decarboxylase



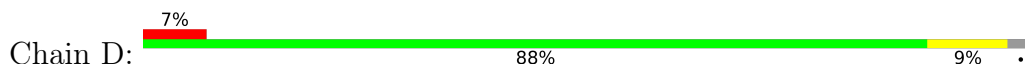
- Molecule 1: Pyridoxal-dependent decarboxylase

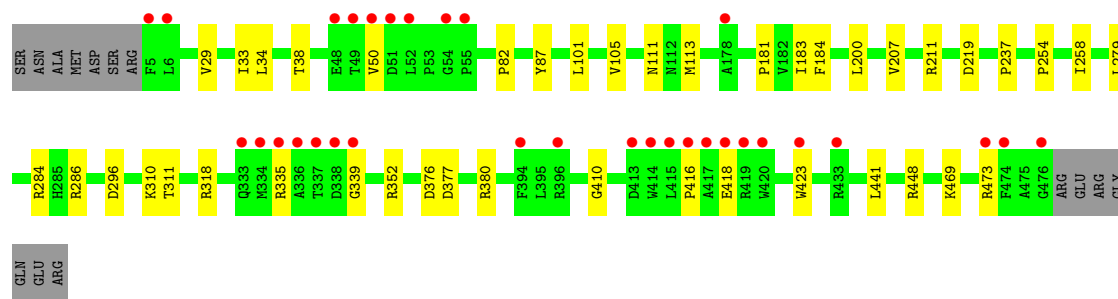


- Molecule 1: Pyridoxal-dependent decarboxylase



- Molecule 1: Pyridoxal-dependent decarboxylase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.41Å 124.66Å 131.85Å 90.00° 99.42° 90.00°	Depositor
Resolution (Å)	39.58 – 2.20 41.25 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.58-2.20) 99.3 (41.25-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.51 (at 2.20Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.157 , 0.199 0.160 , 0.199	Depositor DCC
$R_{free}$ test set	5611 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.9	Xtrriage
Anisotropy	0.657	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 48.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	15438	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% 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: PMP, LLP, NA, GOL

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	0.30	1/3655 (0.0%)	0.44	2/4970 (0.0%)
1	B	0.25	0/3743	0.41	0/5087
1	C	0.31	1/3704 (0.0%)	0.43	1/5037 (0.0%)
1	D	0.25	0/3663	0.41	0/4986
All	All	0.28	2/14765 (0.0%)	0.42	3/20080 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	47	PRO	N-CD	5.27	1.55	1.47
1	C	93	PRO	N-CD	5.25	1.55	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	C	92	ASP	C-N-CD	5.68	140.32	128.40
1	A	119	SER	C-N-CD	5.45	139.85	128.40
1	A	46	MET	C-N-CD	5.36	139.65	128.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	304[A]	LLP	Mainchain

## 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	3607	0	3595	26	0
1	B	3695	0	3688	41	0
1	C	3655	0	3654	33	0
1	D	3614	0	3605	25	0
2	A	16	0	11	3	0
2	C	16	0	11	4	0
2	D	16	0	11	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	B	18	0	24	4	0
4	D	6	0	8	0	0
5	A	243	0	0	1	0
5	B	227	0	0	4	0
5	C	168	0	0	1	0
5	D	154	0	0	0	0
All	All	15438	0	14607	114	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 (114) 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:469:LYS:HE2	1:D:473:ARG:HH22	1.42	0.84
1:A:114:LEU:HB3	1:A:118:MET:HE3	1.67	0.76
1:C:15:GLU:OE1	1:C:17:ARG:NH2	2.24	0.70
1:D:335:ARG:NH1	1:D:339:GLY:O	2.24	0.70
1:A:114:LEU:HB3	1:A:118:MET:CE	2.24	0.68
1:B:456:ASN:O	4:B:503:GOL:C3	2.45	0.65
1:A:184:PHE:HE2	1:A:237:PRO:HB3	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:211:ARG:NH2	1:C:219:ASP:OD2	2.30	0.64
1:D:377:ASP:OD1	1:D:380:ARG:NH1	2.32	0.62
1:B:456:ASN:O	4:B:503:GOL:H31	1.98	0.62
1:B:456:ASN:C	4:B:503:GOL:H31	2.22	0.59
1:B:184:PHE:HE2	1:B:237:PRO:HB3	1.67	0.59
1:B:113:MET:HB2	1:B:352:ARG:HB3	1.84	0.59
1:C:381:LEU:HB3	1:C:454:LEU:HD22	1.85	0.58
1:C:80:MET:H	1:D:111:ASN:HD21	1.50	0.58
1:B:153:LEU:HG	5:B:814:HOH:O	2.03	0.58
1:C:52:LEU:C	1:C:52:LEU:HD13	2.24	0.58
1:C:23:GLU:HG2	1:D:34:LEU:HD13	1.86	0.58
1:B:419:ARG:NH2	1:B:422:ASP:OD2	2.37	0.56
1:C:48:GLU:CD	1:C:48:GLU:H	2.09	0.56
1:D:184:PHE:HE2	1:D:237:PRO:HB3	1.69	0.56
1:B:416:PRO:HG2	1:B:419:ARG:HG2	1.86	0.56
1:A:460:THR:HG22	1:B:-1:ASN:HD21	1.72	0.55
2:A:501[B]:PMP:O2P	1:B:351:THR:HB	2.08	0.54
1:B:469:LYS:HE2	1:B:473:ARG:NH2	2.23	0.54
1:C:380:ARG:NH2	1:C:461:ASP:OD1	2.40	0.54
1:A:113:MET:HB2	1:A:352:ARG:HB3	1.89	0.53
1:A:373:ARG:NH2	1:A:377:ASP:OD1	2.42	0.53
1:D:113:MET:HB2	1:D:352:ARG:HB3	1.89	0.53
1:B:416:PRO:HB2	1:B:418:GLU:OE2	2.09	0.53
1:C:180:ARG:HH22	1:C:205:ALA:HB3	1.74	0.52
1:B:111:ASN:HD22	1:B:111:ASN:N	2.08	0.52
1:C:49:THR:HG22	1:C:49:THR:O	2.08	0.52
1:B:377:ASP:OD1	1:B:380:ARG:NH1	2.37	0.50
1:D:279:LEU:O	1:D:286:ARG:HB3	2.11	0.50
1:A:279:LEU:O	1:A:286:ARG:HB3	2.11	0.50
1:B:390:ARG:NH1	5:B:749:HOH:O	2.42	0.50
1:A:37:LEU:HD11	1:B:108:ALA:HB1	1.93	0.49
1:C:33:ILE:HD11	1:D:105:VAL:HG22	1.94	0.49
1:C:113:MET:HB2	1:C:352:ARG:HB3	1.94	0.49
1:C:175:THR:HG21	1:D:181:PRO:HD2	1.95	0.49
1:D:416:PRO:HB2	1:D:418:GLU:OE1	2.13	0.49
1:A:410:GLY:HA3	1:A:423:TRP:CZ3	2.47	0.49
1:A:34:LEU:HD21	1:B:26:VAL:HG21	1.96	0.48
1:B:80:MET:HG3	1:B:82:PRO:HD3	1.95	0.48
1:B:7:PRO:HG2	1:B:10:ALA:HB2	1.96	0.48
1:A:4:ARG:HB2	1:B:373:ARG:HE	1.78	0.48
1:C:19:ARG:NH2	1:D:38:THR:OG1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:ARG:HH12	1:A:265:HIS:HD2	1.62	0.47
1:B:469:LYS:HE2	1:B:473:ARG:HH21	1.78	0.47
1:A:386:VAL:HG13	1:A:397:LEU:HD11	1.97	0.47
1:C:476:GLY:O	1:C:477:ARG:HG3	2.14	0.47
1:C:184:PHE:HE2	1:C:237:PRO:HB3	1.79	0.47
1:C:190:HIS:HB2	2:C:2001[B]:PMP:H2A3	1.96	0.47
1:B:457:PRO:HA	4:B:503:GOL:H31	1.96	0.47
1:C:82:PRO:HA	1:C:87:TYR:CG	2.49	0.47
1:C:410:GLY:HA3	1:C:423:TRP:CZ3	2.50	0.46
1:B:20:ASN:ND2	5:B:755:HOH:O	2.33	0.46
1:B:82:PRO:HA	1:B:87:TYR:CG	2.51	0.45
1:D:296:ASP:HA	1:D:318:ARG:HG2	1.98	0.45
1:A:34:LEU:HD13	1:B:23:GLU:HG2	1.99	0.45
1:D:254:PRO:O	1:D:258:ILE:HG12	2.17	0.45
1:B:442:PRO:HD2	1:B:449:TRP:O	2.17	0.45
1:A:303:GLN:HA	1:A:308:VAL:O	2.17	0.44
1:C:52:LEU:C	1:C:52:LEU:CD1	2.85	0.44
1:D:211:ARG:NH1	1:D:219:ASP:OD2	2.50	0.44
1:A:118:MET:HB2	1:A:118:MET:HE2	1.70	0.44
1:A:427:LEU:HD23	1:A:450:LEU:HD11	2.00	0.44
1:B:112:ASN:HB3	1:B:118:MET:HB3	1.98	0.44
1:D:310:LYS:HA	1:D:311:THR:HA	1.69	0.44
1:C:112:ASN:HB3	1:C:118:MET:HB3	2.00	0.44
1:B:410:GLY:HA3	1:B:423:TRP:CZ3	2.53	0.44
1:D:284:ARG:HD2	1:D:376:ASP:OD1	2.17	0.44
1:B:412:PRO:HD2	1:B:420:TRP:CD1	2.53	0.44
1:C:310:LYS:HA	1:C:311:THR:HA	1.68	0.43
1:B:418:GLU:H	1:B:418:GLU:CD	2.20	0.43
1:B:24:ARG:NH2	5:B:680:HOH:O	2.44	0.43
1:C:101:LEU:HD13	1:D:29:VAL:HG21	2.00	0.43
1:D:410:GLY:HA3	1:D:423:TRP:CZ3	2.54	0.43
1:B:427:LEU:HD23	1:B:450:LEU:HD11	2.00	0.43
1:D:441:LEU:O	1:D:448:ARG:NH1	2.51	0.43
1:B:396:ARG:HD2	1:B:411:GLU:OE1	2.18	0.42
1:A:442:PRO:HD2	1:A:449:TRP:O	2.19	0.42
1:B:184:PHE:CE2	1:B:237:PRO:HB3	2.51	0.42
1:A:456:ASN:HB3	1:A:459:THR:OG1	2.19	0.42
1:B:181:PRO:HB2	1:B:202:LEU:HD22	2.01	0.42
1:D:82:PRO:HA	1:D:87:TYR:CG	2.54	0.42
1:A:6:LEU:HD23	1:A:6:LEU:HA	1.89	0.42
1:B:301:ASN:HD22	1:B:304:LLP:HE2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:477:ARG:HB3	1:B:477:ARG:NH1	2.34	0.42
1:C:199:LEU:O	1:D:200:LEU:HA	2.19	0.42
1:A:310:LYS:HA	1:A:311:THR:HA	1.72	0.41
1:C:151:GLY:HA3	2:C:2001[B]:PMP:H5A1	2.02	0.41
1:C:194:GLN:OE1	1:C:194:GLN:N	2.53	0.41
1:A:284:ARG:NH1	5:A:793:HOH:O	2.53	0.41
1:C:105:VAL:HG22	1:D:33:ILE:HD11	2.01	0.41
1:A:392:ARG:HA	1:A:393:PRO:HD2	1.87	0.41
1:C:147:LEU:HD23	1:C:314:MET:HB3	2.03	0.41
1:C:29:VAL:HG21	1:D:101:LEU:HD13	2.02	0.41
1:B:33:ILE:HD13	1:B:33:ILE:HA	1.93	0.41
1:B:415:LEU:HG	1:B:419:ARG:HB2	2.02	0.41
1:A:29:VAL:HG21	1:B:101:LEU:HD13	2.03	0.41
1:A:304[A]:LLP:OP1	1:B:351:THR:HB	2.20	0.41
1:C:427:LEU:HD23	1:C:450:LEU:HD11	2.03	0.41
1:C:317:PHE:CE2	1:C:323:LEU:HD21	2.56	0.40
1:C:476:GLY:O	1:C:477:ARG:CG	2.69	0.40
1:D:183:ILE:HD11	1:D:207:VAL:HG22	2.04	0.40
1:C:0:ALA:N	5:C:2159:HOH:O	2.53	0.40
1:A:281:PHE:HD1	1:A:368:GLN:HG2	1.87	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	466/486 (96%)	453 (97%)	13 (3%)	0	100	100
1	B	477/486 (98%)	463 (97%)	14 (3%)	0	100	100
1	C	472/486 (97%)	457 (97%)	15 (3%)	0	100	100
1	D	470/486 (97%)	458 (97%)	12 (3%)	0	100	100
All	All	1885/1944 (97%)	1831 (97%)	54 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	362/376 (96%)	362 (100%)	0	100	100
1	B	373/376 (99%)	372 (100%)	1 (0%)	92	97
1	C	368/376 (98%)	365 (99%)	3 (1%)	81	90
1	D	364/376 (97%)	363 (100%)	1 (0%)	92	97
All	All	1467/1504 (98%)	1462 (100%)	5 (0%)	92	97

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	111	ASN
1	C	93	PRO
1	C	111	ASN
1	C	305	TRP
1	D	50	VAL

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

Mol	Chain	Res	Type
1	B	-1	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	B	304	1	23,24,25	1.96	5 (21%)	25,32,34	1.57	3 (12%)

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	B	304	1	-	2/16/17/19	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	304	LLP	C4'-NZ	6.31	1.48	1.27
1	B	304	LLP	C4-C4'	3.39	1.53	1.46
1	B	304	LLP	CB-CA	-3.01	1.49	1.53
1	B	304	LLP	C2'-C2	2.35	1.54	1.50
1	B	304	LLP	O3-C3	2.02	1.41	1.37

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	304	LLP	OP4-C5'-C5	4.98	118.84	109.35
1	B	304	LLP	CD-CE-NZ	2.94	118.13	110.93
1	B	304	LLP	CE-NZ-C4'	-2.04	112.65	118.90

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	304	LLP	C4-C4'-NZ-CE
1	B	304	LLP	CG-CD-CE-NZ

There are no ring outliers.



1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	304	LLP	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 3 are monoatomic - leaving 7 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$
2	PMP	A	501[B]	-	16,16,16	1.89	6 (37%)	21,23,23	1.69	3 (14%)
4	GOL	D	502	-	5,5,5	0.34	0	5,5,5	0.37	0
4	GOL	B	502	-	5,5,5	0.36	0	5,5,5	0.72	0
2	PMP	C	2001[B]	-	16,16,16	1.85	4 (25%)	21,23,23	1.84	2 (9%)
2	PMP	D	501[B]	-	16,16,16	1.92	6 (37%)	21,23,23	1.31	2 (9%)
4	GOL	B	503	-	5,5,5	0.70	0	5,5,5	0.83	0
4	GOL	B	501	-	5,5,5	0.36	0	5,5,5	0.34	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	PMP	A	501[B]	-	-	0/8/8/8	0/1/1/1
4	GOL	D	502	-	-	2/4/4/4	-
4	GOL	B	502	-	-	4/4/4/4	-
2	PMP	C	2001[B]	-	-	3/8/8/8	0/1/1/1
2	PMP	D	501[B]	-	-	0/8/8/8	0/1/1/1
4	GOL	B	503	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	B	501	-	-	2/4/4/4	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2001[B]	PMP	C3-C2	-4.09	1.36	1.40
2	D	501[B]	PMP	C3-C2	-3.83	1.37	1.40
2	A	501[B]	PMP	C6-N1	-3.53	1.27	1.34
2	D	501[B]	PMP	P-O3P	-3.27	1.42	1.54
2	A	501[B]	PMP	C3-C2	-3.14	1.37	1.40
2	C	2001[B]	PMP	P-O3P	-3.07	1.43	1.54
2	D	501[B]	PMP	C6-N1	-3.02	1.28	1.34
2	A	501[B]	PMP	P-O3P	-3.00	1.43	1.54
2	D	501[B]	PMP	C2A-C2	-2.97	1.45	1.50
2	C	2001[B]	PMP	C6-N1	-2.94	1.28	1.34
2	A	501[B]	PMP	C2A-C2	-2.87	1.45	1.50
2	C	2001[B]	PMP	C2A-C2	-2.85	1.45	1.50
2	A	501[B]	PMP	P-O4P	-2.38	1.52	1.60
2	A	501[B]	PMP	P-O2P	-2.36	1.45	1.54
2	D	501[B]	PMP	P-O4P	-2.15	1.53	1.60
2	D	501[B]	PMP	P-O2P	-2.10	1.46	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2001[B]	PMP	O4P-C5A-C5	5.60	120.02	109.35
2	C	2001[B]	PMP	O3P-P-O4P	4.68	119.18	106.73
2	A	501[B]	PMP	O4P-C5A-C5	4.63	118.17	109.35
2	D	501[B]	PMP	O4P-C5A-C5	3.82	116.64	109.35
2	A	501[B]	PMP	C6-C5-C4	-3.40	115.71	118.12
2	A	501[B]	PMP	O3P-P-O4P	2.31	112.87	106.73
2	D	501[B]	PMP	C5A-C5-C6	-2.21	115.74	119.37

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2001[B]	PMP	C5A-O4P-P-O2P
2	C	2001[B]	PMP	C5A-O4P-P-O3P
4	B	501	GOL	C1-C2-C3-O3
4	B	501	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	B	503	GOL	C1-C2-C3-O3
4	B	502	GOL	O1-C1-C2-C3
4	D	502	GOL	O1-C1-C2-C3
2	C	2001[B]	PMP	C5A-O4P-P-O1P
4	B	502	GOL	O1-C1-C2-O2
4	B	503	GOL	O2-C2-C3-O3
4	B	502	GOL	C1-C2-C3-O3
4	B	502	GOL	O2-C2-C3-O3
4	D	502	GOL	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501[B]	PMP	3	0
2	C	2001[B]	PMP	4	0
2	D	501[B]	PMP	1	0
4	B	503	GOL	4	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	469/486 (96%)	-0.34	7 (1%) 73 72	16, 27, 52, 78	0
1	B	474/486 (97%)	-0.29	9 (1%) 66 65	16, 29, 56, 78	0
1	C	475/486 (97%)	-0.21	14 (2%) 51 49	21, 36, 60, 81	0
1	D	471/486 (96%)	0.04	32 (6%) 17 16	22, 37, 72, 90	0
All	All	1889/1944 (97%)	-0.20	62 (3%) 46 44	16, 33, 61, 90	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	54	GLY	6.1
1	C	52	LEU	5.9
1	D	52	LEU	5.6
1	D	337	THR	5.6
1	D	49	THR	5.3
1	D	51	ASP	5.3
1	D	50	VAL	5.0
1	D	339	GLY	4.9
1	D	55	PRO	4.9
1	D	414	TRP	4.8
1	C	337	THR	4.8
1	C	54	GLY	4.6
1	B	54	GLY	4.5
1	A	55	PRO	4.4
1	A	5	PHE	4.4
1	A	3	SER	4.4
1	C	339	GLY	4.2
1	A	49	THR	4.0
1	B	-1	ASN	3.8
1	D	334	MET	3.7
1	D	413	ASP	3.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	416	PRO	3.4
1	D	415	LEU	3.2
1	C	338	ASP	3.2
1	D	5	PHE	3.1
1	D	48	GLU	3.1
1	C	336	ALA	3.1
1	D	335	ARG	3.1
1	D	419	ARG	3.1
1	D	417	ALA	3.0
1	C	477	ARG	3.0
1	D	473	ARG	3.0
1	D	476	GLY	3.0
1	C	49	THR	3.0
1	D	418	GLU	2.9
1	C	334	MET	2.9
1	B	311	THR	2.8
1	D	474	PHE	2.8
1	D	338	ASP	2.8
1	B	49	THR	2.8
1	C	55	PRO	2.7
1	A	4	ARG	2.6
1	D	396	ARG	2.6
1	B	417	ALA	2.5
1	C	311	THR	2.5
1	D	420	TRP	2.3
1	C	335	ARG	2.3
1	B	55	PRO	2.3
1	B	477	ARG	2.3
1	B	473	ARG	2.3
1	C	340	PHE	2.3
1	D	333	GLN	2.3
1	D	6	LEU	2.2
1	D	336	ALA	2.2
1	D	433	ARG	2.2
1	B	414	TRP	2.2
1	D	178	ALA	2.2
1	D	423	TRP	2.1
1	A	178	ALA	2.1
1	D	394	PHE	2.1
1	A	476	GLY	2.0
1	C	53	PRO	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(Å <sup>2</sup> )	Q<0.9
1	LLP	C	304[A]	24/25	0.91	0.23	27,57,63,65	16
1	LLP	B	304	24/25	0.96	0.20	16,34,49,51	0
1	LLP	A	304[A]	24/25	0.96	0.15	17,41,51,55	15
1	LLP	D	304[A]	24/25	0.96	0.18	23,43,55,66	16

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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(Å <sup>2</sup> )	Q<0.9
3	NA	B	504	1/1	0.74	0.44	59,59,59,59	0
3	NA	D	503	1/1	0.77	0.33	75,75,75,75	0
4	GOL	B	501	6/6	0.83	0.16	48,56,62,67	0
4	GOL	B	502	6/6	0.84	0.34	91,94,96,98	0
4	GOL	D	502	6/6	0.89	0.17	55,66,66,69	0
4	GOL	B	503	6/6	0.91	0.31	67,78,81,89	0
2	PMP	C	2001[B]	16/16	0.93	0.18	27,36,42,46	16
2	PMP	A	501[B]	16/16	0.96	0.15	14,27,36,38	16
2	PMP	D	501[B]	16/16	0.97	0.14	20,39,42,43	16
3	NA	A	502	1/1	0.99	0.28	18,18,18,18	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.