



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 17, 2023 – 12:34 AM EDT

PDB ID : 4RJ0  
Title : The crystal structure of Y333N 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 : 1.95 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)  
Xtrriage (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

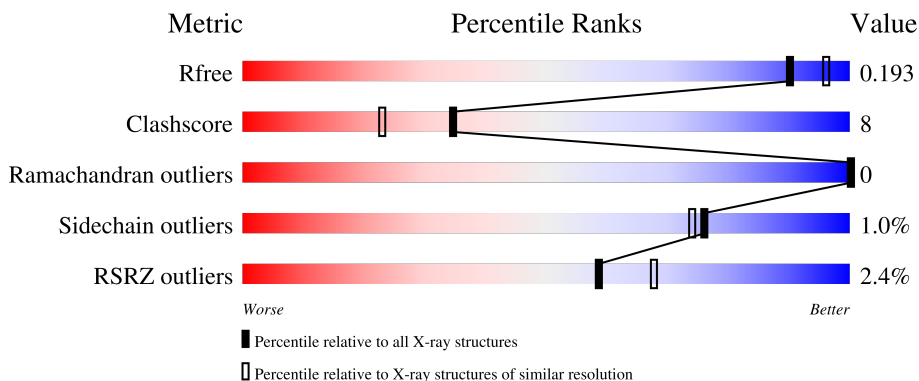
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 78%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">78%      17%      ..</p>
1	B	486	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 81%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">81%      15%      ..</p>
1	C	486	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 77%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 18%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">5%      77%      18%      5%</p>
1	D	486	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 77%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 19%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">2%      77%      19%      ..</p>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 15125 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	B	471	3617	2286	650	663	1	17	0	1	0
1	A	467	3601	2278	647	659	1	16	0	2	0
1	C	463	3543	2247	633	647	1	15	0	0	0
1	D	468	3584	2269	642	656	1	16	0	1	0

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	ASN	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	ASN	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	ASN	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	ASN	TYR	ENGINEERED MUTATION	UNP D1C7D8

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



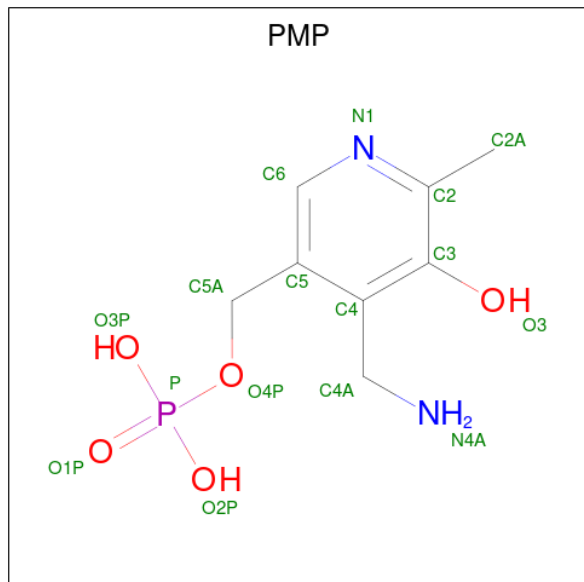
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (three-letter code: PMP) (formula:  $C_8H_{13}N_2O_5P$ ).



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

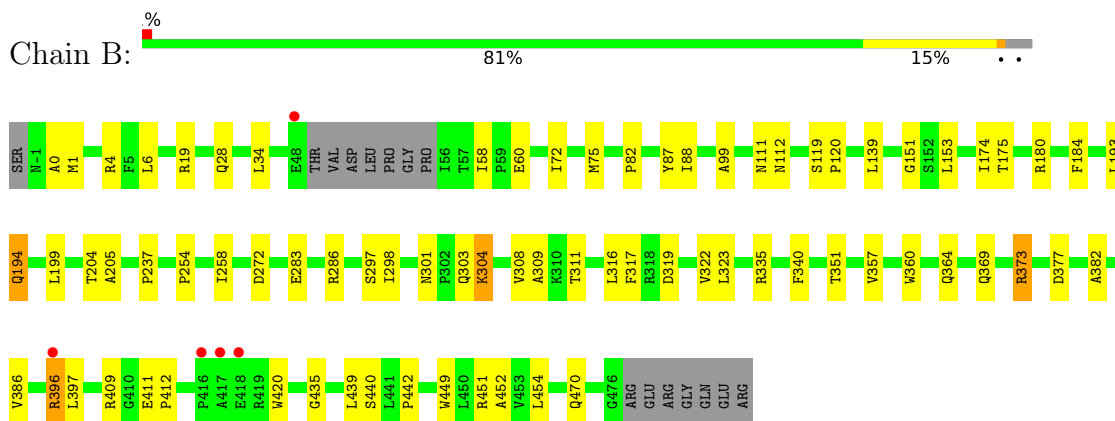
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	232	Total	O	0	0
			232	232		
5	A	238	Total	O	0	0
			238	238		
5	C	128	Total	O	0	0
			128	128		
5	D	143	Total	O	0	0
			143	143		

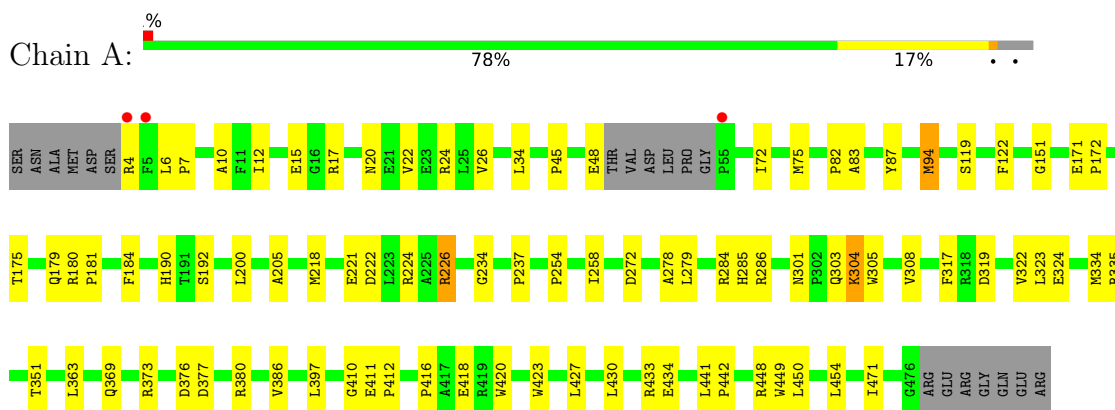
### 3 Residue-property plots

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.

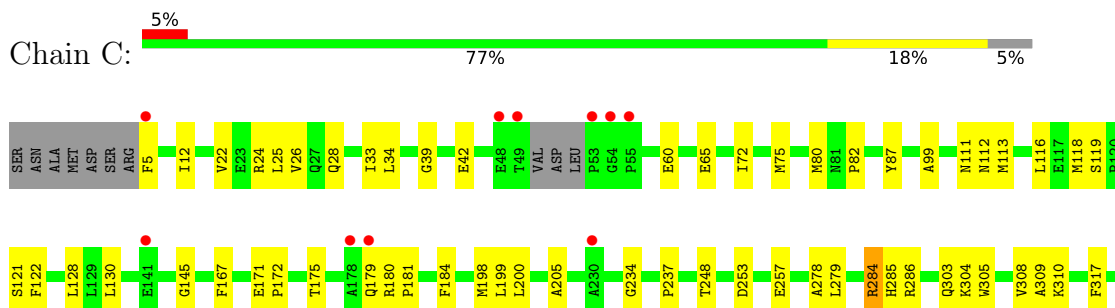
- Molecule 1: Pyridoxal-dependent decarboxylase

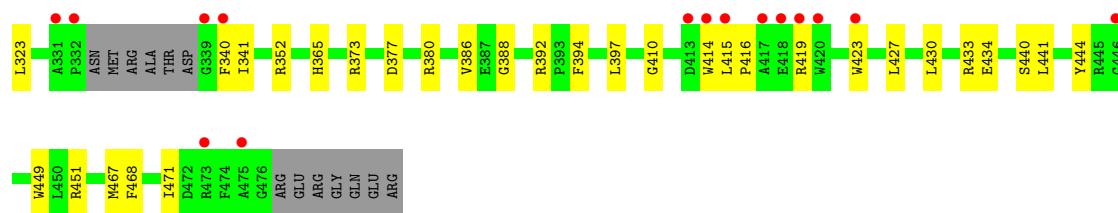


- Molecule 1: Pyridoxal-dependent decarboxylase

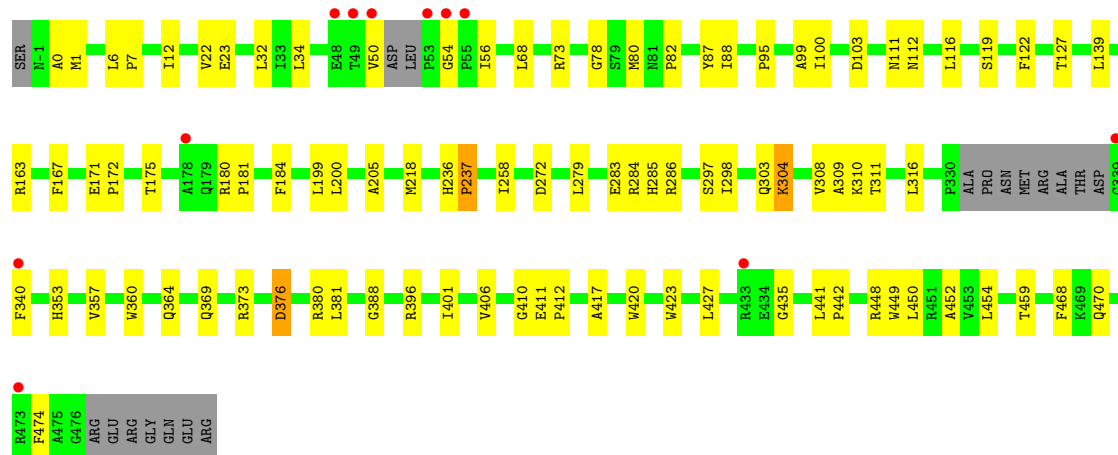
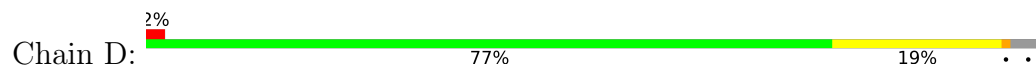


- Molecule 1: Pyridoxal-dependent decarboxylase





• 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, $\alpha$ , $\beta$ , $\gamma$	68.98Å 124.20Å 129.94Å 90.00° 99.56° 90.00°	Depositor
Resolution (Å)	32.56 – 1.95 32.56 – 1.92	Depositor EDS
% Data completeness (in resolution range)	91.0 (32.56-1.95) 89.0 (32.56-1.92)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.07 (at 1.92Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.168 , 0.193 0.170 , 0.193	Depositor DCC
$R_{free}$ test set	7349 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.2	Xtrriage
Anisotropy	0.118	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 49.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	15125	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% 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: PO4, GOL, PMP, LLP

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	0.91	1/3649 (0.0%)	0.71	0/4961
1	B	0.93	0/3664	0.72	3/4981 (0.1%)
1	C	0.86	1/3591 (0.0%)	0.66	2/4884 (0.0%)
1	D	0.85	2/3631 (0.1%)	0.68	2/4936 (0.0%)
All	All	0.89	4/14535 (0.0%)	0.69	7/19762 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	376	ASP	CB-CG	-5.90	1.39	1.51
1	A	45	PRO	N-CD	5.33	1.55	1.47
1	C	257	GLU	CD-OE1	-5.18	1.20	1.25
1	D	237	PRO	N-CD	5.04	1.54	1.47

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	193	LEU	O-C-N	-6.02	113.06	122.70
1	B	193	LEU	CA-C-N	5.68	129.69	117.20
1	D	236	HIS	C-N-CD	5.58	140.11	128.40
1	B	19	ARG	NE-CZ-NH1	-5.53	117.54	120.30
1	C	253	ASP	CB-CG-OD1	5.43	123.19	118.30
1	D	376	ASP	CB-CG-OD1	-5.07	113.73	118.30
1	C	253	ASP	C-N-CD	5.02	138.94	128.40

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3601	0	3596	76	0
1	B	3617	0	3611	59	0
1	C	3543	0	3543	70	0
1	D	3584	0	3585	72	0
2	A	12	0	16	2	0
2	D	6	0	8	0	0
3	C	5	0	0	0	0
4	D	16	0	11	2	0
5	A	238	0	0	4	0
5	B	232	0	0	3	0
5	C	128	0	0	0	0
5	D	143	0	0	1	0
All	All	15125	0	14370	238	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (238) 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:B:396:ARG:HD2	1:B:411:GLU:OE1	1.47	1.12
1:A:430:LEU:CD1	1:A:434:GLU:HG3	1.97	0.95
1:C:179:GLN:HB3	1:C:234:GLY:O	1.71	0.90
1:A:430:LEU:HD12	1:A:434:GLU:HG3	1.54	0.89
1:C:25:LEU:HD13	1:C:65:GLU:HG2	1.55	0.89
1:C:284:ARG:HH11	1:C:284:ARG:HB2	1.39	0.88
1:B:396:ARG:HD2	1:B:411:GLU:CD	1.98	0.83
1:A:12:ILE:HG12	1:A:22:VAL:HG11	1.61	0.81
1:A:386:VAL:HG13	1:A:397:LEU:HD11	1.64	0.80
1:B:396:ARG:CD	1:B:411:GLU:OE1	2.31	0.79
1:B:184:PHE:HE2	1:B:237:PRO:HB3	1.49	0.78
1:C:373:ARG:NH1	1:C:377:ASP:OD1	2.17	0.76
1:B:194[A]:GLN:H	1:B:194[A]:GLN:HE21	1.33	0.75
1:A:7:PRO:HG2	1:A:10:ALA:HB2	1.71	0.73
1:C:12:ILE:HG12	1:C:22:VAL:HG11	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:LEU:HD11	1:A:434:GLU:HG3	1.71	0.72
1:A:454:LEU:N	1:A:454:LEU:HD22	2.04	0.71
1:C:5:PHE:HD2	1:D:373:ARG:NH1	1.89	0.70
1:C:440:SER:OG	1:C:451:ARG:HB3	1.89	0.70
1:C:72:ILE:HA	1:C:75:MET:HE2	1.73	0.69
1:A:184:PHE:HE2	1:A:237:PRO:HB3	1.58	0.69
1:C:5:PHE:CD2	1:D:373:ARG:NH1	2.61	0.69
1:C:380:ARG:HH11	1:C:380:ARG:HG2	1.58	0.68
1:D:139:LEU:HD11	1:D:298:ILE:HD12	1.77	0.67
1:B:194[A]:GLN:H	1:B:194[A]:GLN:NE2	1.93	0.66
1:C:380:ARG:HG2	1:C:380:ARG:NH1	2.11	0.65
1:A:20:ASN:HB3	1:A:24:ARG:HH22	1.62	0.65
1:A:430:LEU:HD12	1:A:434:GLU:CG	2.24	0.65
1:B:72:ILE:HA	1:B:75:MET:HE2	1.79	0.65
1:A:376:ASP:O	1:A:380:ARG:HG3	1.96	0.65
1:D:116:LEU:HD13	1:D:116:LEU:O	1.96	0.64
1:C:171:GLU:H	1:C:172:PRO:HD2	1.63	0.64
1:B:412:PRO:HD2	1:B:420:TRP:CD1	2.32	0.63
1:C:184:PHE:HE2	1:C:237:PRO:HB3	1.63	0.63
1:C:427:LEU:HD12	1:C:427:LEU:O	1.98	0.63
1:A:218:MET:SD	1:A:258:ILE:HD12	2.38	0.63
1:A:15:GLU:OE1	1:A:17:ARG:NH1	2.31	0.62
1:A:442:PRO:HD2	1:A:449:TRP:O	1.98	0.62
1:B:440:SER:OG	1:B:451:ARG:HB3	1.99	0.62
1:D:410:GLY:HA3	1:D:423:TRP:CZ3	2.34	0.62
1:A:317:PHE:CE2	1:A:323:LEU:HD21	2.35	0.62
1:C:128:LEU:HD13	1:D:54:GLY:O	1.99	0.62
1:D:116:LEU:HD13	1:D:116:LEU:C	2.21	0.61
1:B:357:VAL:HG13	1:A:75:MET:HE1	1.81	0.61
1:B:180:ARG:HH22	1:B:205:ALA:HB3	1.65	0.61
1:B:357:VAL:HG13	1:A:75:MET:CE	2.31	0.60
1:B:386:VAL:HG13	1:B:397:LEU:HD11	1.81	0.60
1:A:6:LEU:HD13	2:A:501:GOL:H2	1.83	0.59
1:A:433:ARG:HD3	5:A:814:HOH:O	2.01	0.59
1:A:179:GLN:HG2	1:A:234:GLY:O	2.01	0.59
1:A:410:GLY:HA3	1:A:423:TRP:CZ3	2.39	0.58
1:D:80:MET:HG2	1:D:82:PRO:HD3	1.86	0.58
1:D:381:LEU:HD21	1:D:459:THR:HG22	1.86	0.57
1:C:386:VAL:HG13	1:C:397:LEU:HD11	1.87	0.57
1:B:373:ARG:NH2	1:B:377:ASP:OD2	2.37	0.56
1:C:39:GLY:O	1:C:42:GLU:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:284:ARG:HB2	1:C:284:ARG:NH1	2.15	0.56
1:B:60:GLU:HG2	1:A:369:GLN:OE1	2.05	0.56
1:B:194[A]:GLN:NE2	1:B:194[A]:GLN:N	2.54	0.56
1:B:369:GLN:HB3	1:A:4:ARG:CG	2.36	0.56
1:A:373:ARG:NH2	1:A:377:ASP:OD1	2.39	0.55
1:C:171:GLU:N	1:C:172:PRO:HD2	2.22	0.55
1:B:369:GLN:HB3	1:A:4:ARG:HG3	1.89	0.55
1:D:423:TRP:CE2	1:D:474:PHE:HE2	2.25	0.55
1:A:190:HIS:ND1	1:A:192:SER:HB3	2.22	0.55
1:C:410:GLY:HA3	1:C:423:TRP:CZ3	2.42	0.55
1:D:0:ALA:C	1:D:6:LEU:HD12	2.27	0.55
1:D:171:GLU:HB2	1:D:172:PRO:HD3	1.88	0.54
1:D:184:PHE:HE2	1:D:237:PRO:HB3	1.71	0.54
1:A:324:GLU:OE1	1:A:335:ARG:NH2	2.39	0.54
1:C:181:PRO:CD	1:D:175:THR:HG21	2.38	0.54
1:B:283:GLU:HG2	1:B:286:ARG:NH2	2.23	0.54
1:A:180:ARG:HH12	1:A:205:ALA:HB3	1.72	0.54
1:D:272:ASP:OD2	4:D:2001[B]:PMP:N1	2.41	0.54
1:A:412:PRO:HD2	1:A:420:TRP:CD1	2.43	0.54
1:A:180:ARG:HH12	1:A:205:ALA:CB	2.20	0.54
1:B:351:THR:OG1	1:A:304:LLP:OP1	2.16	0.53
1:D:441:LEU:HD23	1:D:448:ARG:HH11	1.73	0.53
1:B:442:PRO:HD2	1:B:449:TRP:O	2.09	0.53
1:D:435:GLY:HA2	1:D:470:GLN:HE22	1.72	0.53
1:A:20:ASN:O	1:A:24:ARG:HG3	2.08	0.52
1:C:279:LEU:O	1:C:286:ARG:HB3	2.09	0.52
1:D:82:PRO:HA	1:D:87:TYR:CG	2.44	0.52
1:D:1:MET:SD	1:D:6:LEU:HD13	2.49	0.52
1:C:112:ASN:HB3	1:C:118:MET:HB3	1.91	0.52
1:A:279:LEU:O	1:A:286:ARG:HB3	2.10	0.51
1:C:414:TRP:O	1:C:415:LEU:HD23	2.10	0.51
1:C:82:PRO:HD2	5:D:2195:HOH:O	2.10	0.51
1:D:272:ASP:OD2	1:D:304[A]:LLP:N1	2.43	0.51
1:B:317:PHE:CE2	1:B:323:LEU:HD21	2.45	0.51
1:A:20:ASN:HB3	1:A:24:ARG:NH2	2.24	0.51
1:B:435:GLY:HA3	1:B:470:GLN:OE1	2.11	0.51
1:A:184:PHE:CE2	1:A:237:PRO:HB3	2.43	0.51
1:B:204:THR:OG1	1:A:171:GLU:HG2	2.11	0.50
1:D:435:GLY:HA3	1:D:470:GLN:OE1	2.11	0.50
1:A:151:GLY:HA3	1:A:301:ASN:HD21	1.76	0.50
1:D:279:LEU:O	1:D:286:ARG:HB3	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:THR:HG21	1:A:181:PRO:HD2	1.94	0.49
1:C:181:PRO:HD2	1:D:175:THR:HG21	1.94	0.49
1:D:103:ASP:OD1	1:D:353:HIS:HE1	1.96	0.49
1:D:396:ARG:HE	1:D:411:GLU:CD	2.16	0.49
1:B:194[B]:GLN:CD	5:B:723:HOH:O	2.50	0.49
1:C:467:MET:O	1:C:471:ILE:HG13	2.13	0.49
1:C:80:MET:HG2	1:C:82:PRO:HD3	1.95	0.49
1:D:360:TRP:O	1:D:364:GLN:HG3	2.13	0.49
1:B:435:GLY:CA	1:B:470:GLN:OE1	2.61	0.49
1:D:12:ILE:HG12	1:D:22:VAL:HG11	1.95	0.49
1:C:284:ARG:HH11	1:C:284:ARG:CB	2.20	0.48
1:C:430:LEU:HD12	1:C:433:ARG:HH11	1.78	0.48
1:D:50:VAL:HG13	1:D:50:VAL:O	2.12	0.48
1:B:272:ASP:OD2	1:B:304:LLP:N1	2.46	0.48
1:D:442:PRO:HD2	1:D:449:TRP:O	2.14	0.48
1:B:254:PRO:O	1:B:258:ILE:HG12	2.14	0.48
1:D:180:ARG:HH22	1:D:205:ALA:HB3	1.78	0.48
1:C:26:VAL:HG21	1:D:34:LEU:HD21	1.95	0.48
1:A:418:GLU:CD	1:A:418:GLU:H	2.16	0.48
1:D:284:ARG:HG2	1:D:285:HIS:CD2	2.48	0.48
1:A:72:ILE:HA	1:A:75:MET:HE2	1.94	0.47
1:A:454:LEU:N	1:A:454:LEU:CD2	2.73	0.47
1:A:119:SER:HB2	1:A:122:PHE:HB2	1.96	0.47
1:B:82:PRO:HA	1:B:87:TYR:CG	2.49	0.47
1:A:319:ASP:O	1:A:322:VAL:HG12	2.14	0.47
1:B:99:ALA:HB1	1:B:309:ALA:H	1.78	0.47
1:C:24:ARG:O	1:C:28:GLN:HG3	2.15	0.47
1:B:369:GLN:CB	1:A:4:ARG:HG3	2.43	0.47
1:A:373:ARG:NH2	1:A:377:ASP:OD2	2.47	0.47
1:C:284:ARG:HD3	1:C:285:HIS:NE2	2.30	0.47
1:D:381:LEU:HB3	1:D:454:LEU:HG	1.96	0.47
1:D:417:ALA:HA	1:D:420:TRP:CD2	2.49	0.47
1:C:416:PRO:HD2	1:C:419:ARG:HD2	1.96	0.47
1:D:95:PRO:HG2	1:D:100:ILE:HD11	1.97	0.47
1:D:127:THR:HG1	1:D:340:PHE:HE1	1.63	0.47
1:A:222:ASP:O	1:A:226:ARG:HG2	2.15	0.47
1:C:317:PHE:CE2	1:C:323:LEU:HD21	2.50	0.47
1:A:303:GLN:HA	1:A:308:VAL:O	2.15	0.46
1:D:303:GLN:HA	1:D:308:VAL:O	2.15	0.46
1:A:34:LEU:HD23	1:A:34:LEU:HA	1.80	0.46
1:A:221:GLU:HG3	5:A:822:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:GLN:O	1:A:4:ARG:HD2	2.16	0.46
1:B:382:ALA:HA	1:B:454:LEU:HD13	1.98	0.46
1:C:116:LEU:HD12	1:C:340:PHE:CD2	2.51	0.46
1:D:99:ALA:HB1	1:D:309:ALA:H	1.80	0.46
1:C:200:LEU:HA	1:D:199:LEU:O	2.16	0.46
1:B:175:THR:HG21	1:A:181:PRO:CD	2.46	0.45
1:C:82:PRO:HA	1:C:87:TYR:CG	2.52	0.45
1:D:167:PHE:CZ	1:D:181:PRO:HB3	2.51	0.45
1:B:151:GLY:HA3	1:B:301:ASN:HD21	1.82	0.45
1:B:319:ASP:O	1:B:322:VAL:HG12	2.17	0.45
1:C:121:SER:HB3	1:D:78:GLY:C	2.37	0.45
1:B:153:LEU:HG	5:B:581:HOH:O	2.17	0.45
1:A:83:ALA:HA	1:A:94:MET:HE3	1.99	0.45
1:A:278:ALA:CB	1:A:305:TRP:HB3	2.46	0.45
1:C:310:LYS:HE3	1:D:112:ASN:HB2	1.99	0.45
1:C:441:LEU:HD12	1:C:449:TRP:O	2.17	0.45
1:A:254:PRO:O	1:A:258:ILE:HG12	2.17	0.45
1:A:272:ASP:OD2	1:A:304:LLP:N1	2.50	0.45
1:D:412:PRO:HD2	1:D:420:TRP:CD1	2.52	0.45
1:C:60:GLU:HG3	1:D:369:GLN:HG3	1.99	0.45
1:A:441:LEU:HG	1:A:448:ARG:HD2	1.99	0.45
1:B:335:ARG:HG3	1:B:340:PHE:O	2.17	0.44
1:C:180:ARG:HH22	1:C:205:ALA:HB3	1.82	0.44
1:C:5:PHE:HD2	1:D:373:ARG:HH12	1.58	0.44
1:C:392:ARG:HB3	1:C:394:PHE:CE2	2.52	0.44
1:C:278:ALA:CB	1:C:305:TRP:HB3	2.47	0.44
1:D:441:LEU:HD23	1:D:448:ARG:NH1	2.32	0.44
1:B:88:ILE:HG13	1:B:439:LEU:HD23	1.99	0.44
1:C:130:LEU:HD23	1:C:145:GLY:C	2.37	0.44
1:B:4:ARG:NH2	1:D:1:MET:O	2.49	0.44
1:A:82:PRO:HA	1:A:87:TYR:CG	2.53	0.44
1:C:34:LEU:HD13	1:D:23:GLU:HG2	2.00	0.44
1:B:0:ALA:HB2	1:A:377:ASP:OD2	2.18	0.43
1:A:286:ARG:O	2:A:502:GOL:H11	2.17	0.43
1:D:119:SER:HB2	1:D:122:PHE:HB2	2.00	0.43
1:B:409:ARG:HD3	1:B:449:TRP:CE2	2.53	0.43
1:A:427:LEU:HD23	1:A:450:LEU:HD11	2.00	0.43
1:C:121:SER:HB3	1:D:78:GLY:O	2.17	0.43
1:C:175:THR:HG21	1:D:181:PRO:CD	2.49	0.43
1:C:388:GLY:HA3	1:C:468:PHE:CZ	2.54	0.43
1:D:116:LEU:C	1:D:116:LEU:CD1	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:ILE:HD12	1:A:175:THR:CG2	2.49	0.43
1:B:1:MET:SD	1:B:6:LEU:HD13	2.58	0.43
1:D:401:ILE:HG21	1:D:406:VAL:HG22	2.01	0.43
1:B:199:LEU:O	1:A:200:LEU:HA	2.19	0.43
1:D:283:GLU:HG2	1:D:286:ARG:NH2	2.34	0.43
1:A:171:GLU:N	1:A:172:PRO:HD2	2.34	0.43
1:C:365:HIS:CD2	1:D:68:LEU:HD11	2.54	0.43
1:C:303:GLN:HA	1:C:308:VAL:O	2.19	0.43
1:B:34:LEU:HD21	1:A:26:VAL:HG21	2.01	0.42
1:B:58:ILE:HG12	1:A:363:LEU:HD13	1.99	0.42
1:B:139:LEU:HD11	1:B:298:ILE:HD12	2.00	0.42
1:D:310:LYS:HA	1:D:311:THR:HA	1.79	0.42
1:C:175:THR:HG21	1:D:181:PRO:HD3	2.02	0.42
1:B:360:TRP:O	1:B:364:GLN:HG3	2.19	0.42
1:A:180:ARG:CZ	5:A:746:HOH:O	2.67	0.42
1:C:199:LEU:O	1:D:200:LEU:HA	2.20	0.42
4:D:2001[B]:PMP:O3P	4:D:2001[B]:PMP:H4A1	2.19	0.42
1:C:171:GLU:N	1:C:172:PRO:CD	2.82	0.42
1:D:297:SER:HA	1:D:316:LEU:O	2.19	0.42
1:D:388:GLY:HA3	1:D:468:PHE:CZ	2.55	0.42
1:C:119:SER:HB2	1:C:122:PHE:HB2	2.01	0.42
1:A:411:GLU:HG2	1:A:420:TRP:CE3	2.54	0.42
1:C:75:MET:CE	1:D:357:VAL:HG13	2.50	0.42
1:C:113:MET:HB2	1:C:352:ARG:HB3	2.02	0.42
1:D:0:ALA:O	1:D:6:LEU:HD12	2.20	0.42
1:B:369:GLN:HB3	1:A:4:ARG:HG2	2.00	0.42
1:A:284:ARG:O	1:A:284:ARG:HG2	2.18	0.42
1:A:284:ARG:HD2	1:A:285:HIS:NE2	2.34	0.42
1:C:99:ALA:HB1	1:C:309:ALA:H	1.85	0.42
1:C:171:GLU:HB2	1:C:172:PRO:HD3	2.01	0.42
1:B:88:ILE:O	1:B:452:ALA:HA	2.20	0.41
1:A:278:ALA:HB2	1:A:305:TRP:HB3	2.02	0.41
1:A:427:LEU:HD21	1:A:471:ILE:HG12	2.01	0.41
1:C:128:LEU:HB3	1:D:56:ILE:HG12	2.02	0.41
1:B:396:ARG:HD2	1:B:411:GLU:CG	2.50	0.41
1:C:198:MET:O	1:D:163:ARG:NH2	2.53	0.41
1:C:388:GLY:O	1:C:392:ARG:HG3	2.20	0.41
1:B:382:ALA:HA	1:B:454:LEU:CD1	2.51	0.41
1:B:303:GLN:HA	1:B:308:VAL:O	2.21	0.41
1:D:454:LEU:N	1:D:454:LEU:HD22	2.35	0.41
1:C:365:HIS:O	1:D:7:PRO:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:415:LEU:HD13	1:C:419:ARG:CB	2.51	0.41
1:D:88:ILE:O	1:D:452:ALA:HA	2.20	0.41
1:B:120:PRO:HB3	5:B:664:HOH:O	2.21	0.41
1:B:297:SER:HA	1:B:316:LEU:O	2.21	0.41
1:C:341:ILE:HG23	1:C:341:ILE:O	2.21	0.41
1:D:427:LEU:HD23	1:D:450:LEU:HD11	2.03	0.41
1:C:167:PHE:CZ	1:C:181:PRO:HB3	2.56	0.40
1:D:218:MET:CE	1:D:258:ILE:HD13	2.52	0.40
1:D:401:ILE:O	1:D:401:ILE:HG13	2.21	0.40
1:C:248:THR:HG21	1:C:444:TYR:CD1	2.56	0.40
1:B:112:ASN:O	1:B:119:SER:HB3	2.21	0.40
1:B:311:THR:HG22	1:A:351:THR:HG22	2.04	0.40
1:D:32:LEU:HD13	1:D:73:ARG:NH1	2.36	0.40
1:A:224:ARG:HD3	5:A:837:HOH:O	2.21	0.40
1:A:416:PRO:HB2	1:A:418:GLU:HG2	2.03	0.40
1:D:380:ARG:HD2	1:D:380:ARG:HA	1.96	0.40
1:A:411:GLU:HG2	1:A:420:TRP:CZ3	2.57	0.40
1:C:33:ILE:HD13	1:C:33:ILE:HA	1.74	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	464/486 (96%)	452 (97%)	12 (3%)	0	100	100
1	B	467/486 (96%)	457 (98%)	10 (2%)	0	100	100
1	C	456/486 (94%)	444 (97%)	12 (3%)	0	100	100
1	D	461/486 (95%)	454 (98%)	7 (2%)	0	100	100
All	All	1848/1944 (95%)	1807 (98%)	41 (2%)	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%)	358 (99%)	4 (1%)	73	71
1	B	363/376 (96%)	357 (98%)	6 (2%)	60	55
1	C	356/376 (95%)	353 (99%)	3 (1%)	81	80
1	D	361/376 (96%)	359 (99%)	2 (1%)	86	85
All	All	1442/1504 (96%)	1427 (99%)	15 (1%)	76	74

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

Mol	Chain	Res	Type
1	B	28	GLN
1	B	111	ASN
1	B	194[A]	GLN
1	B	194[B]	GLN
1	B	373	ARG
1	B	396	ARG
1	A	48	GLU
1	A	94	MET
1	A	226	ARG
1	A	334	MET
1	C	111	ASN
1	C	284	ARG
1	C	434	GLU
1	D	111	ASN
1	D	376	ASP

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

Mol	Chain	Res	Type
1	A	28	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	23,24,25	2.65	9 (39%)	25,32,34	2.05	6 (24%)
1	LLP	C	304	1	23,24,25	2.56	9 (39%)	25,32,34	2.27	6 (24%)
1	LLP	B	304	1	23,24,25	2.87	8 (34%)	25,32,34	2.62	6 (24%)
1	LLP	D	304[A]	1	23,24,25	1.97	5 (21%)	25,32,34	1.49	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	A	304	1	-	7/16/17/19	0/1/1/1
1	LLP	C	304	1	-	6/16/17/19	0/1/1/1
1	LLP	B	304	1	-	4/16/17/19	0/1/1/1
1	LLP	D	304[A]	1	-	4/16/17/19	0/1/1/1

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	304	LLP	C3-C2	8.39	1.49	1.40
1	A	304	LLP	C3-C2	6.38	1.47	1.40
1	D	304[A]	LLP	C4'-NZ	6.34	1.48	1.27
1	A	304	LLP	C4'-NZ	6.01	1.47	1.27
1	B	304	LLP	C4'-NZ	5.88	1.47	1.27
1	C	304	LLP	C3-C2	5.79	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	304	LLP	C4-C3	5.08	1.48	1.40
1	C	304	LLP	C4'-NZ	4.98	1.44	1.27
1	B	304	LLP	C4-C5	4.95	1.48	1.42
1	C	304	LLP	C4-C5	4.29	1.47	1.42
1	C	304	LLP	C4-C3	4.12	1.47	1.40
1	B	304	LLP	C4-C3	4.09	1.47	1.40
1	B	304	LLP	P-OP3	-3.58	1.41	1.54
1	A	304	LLP	P-OP2	-3.44	1.41	1.54
1	D	304[A]	LLP	C4-C4'	3.39	1.53	1.46
1	C	304	LLP	P-OP2	-3.23	1.42	1.54
1	C	304	LLP	CB-CA	-3.18	1.49	1.53
1	D	304[A]	LLP	CB-CA	-3.06	1.49	1.53
1	C	304	LLP	P-OP1	-2.92	1.41	1.50
1	B	304	LLP	P-OP2	-2.89	1.43	1.54
1	A	304	LLP	P-OP3	-2.80	1.44	1.54
1	C	304	LLP	CE-NZ	-2.72	1.40	1.46
1	A	304	LLP	C4-C5	2.65	1.45	1.42
1	A	304	LLP	C4-C4'	2.53	1.51	1.46
1	A	304	LLP	CE-NZ	-2.48	1.41	1.46
1	D	304[A]	LLP	C2'-C2	2.35	1.54	1.50
1	A	304	LLP	P-OP1	-2.31	1.43	1.50
1	B	304	LLP	CA-N	-2.13	1.41	1.48
1	C	304	LLP	CA-N	-2.09	1.41	1.48
1	D	304[A]	LLP	CE-NZ	-2.08	1.42	1.46
1	B	304	LLP	P-OP1	-2.06	1.43	1.50

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	304	LLP	C4-C3-C2	-9.74	114.16	120.19
1	C	304	LLP	OP4-C5'-C5	7.55	123.73	109.35
1	C	304	LLP	C4-C3-C2	-5.38	116.86	120.19
1	A	304	LLP	C4-C3-C2	-5.01	117.09	120.19
1	A	304	LLP	OP4-C5'-C5	4.66	118.23	109.35
1	D	304[A]	LLP	OP4-C5'-C5	4.30	117.54	109.35
1	B	304	LLP	OP4-C5'-C5	4.03	117.03	109.35
1	A	304	LLP	OP2-P-OP4	-3.98	96.16	106.73
1	B	304	LLP	C4-C4'-NZ	-3.75	107.09	124.31
1	B	304	LLP	O3-C3-C2	3.22	124.50	117.49
1	A	304	LLP	C4-C4'-NZ	-3.20	109.64	124.31
1	C	304	LLP	C4-C4'-NZ	-3.17	109.75	124.31
1	C	304	LLP	C6-N1-C2	3.14	124.98	119.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	304	LLP	C6-N1-C2	3.12	124.94	119.17
1	B	304	LLP	C6-N1-C2	3.03	124.78	119.17
1	D	304[A]	LLP	CD-CE-NZ	2.91	118.06	110.93
1	A	304	LLP	O3-C3-C2	2.63	123.23	117.49
1	C	304	LLP	OP2-P-OP1	2.45	120.26	110.68
1	B	304	LLP	OP3-P-OP2	2.13	115.78	107.64
1	C	304	LLP	O3-C3-C2	2.11	122.10	117.49
1	D	304[A]	LLP	C6-N1-C2	2.01	122.89	119.17

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	304	LLP	C4-C4'-NZ-CE
1	B	304	LLP	O-C-CA-CB
1	A	304	LLP	C4-C4'-NZ-CE
1	A	304	LLP	C4-C5-C5'-OP4
1	A	304	LLP	C6-C5-C5'-OP4
1	A	304	LLP	C5'-OP4-P-OP1
1	A	304	LLP	C5'-OP4-P-OP2
1	C	304	LLP	C4-C4'-NZ-CE
1	C	304	LLP	C4-C5-C5'-OP4
1	C	304	LLP	C6-C5-C5'-OP4
1	C	304	LLP	O-C-CA-CB
1	D	304[A]	LLP	C4-C4'-NZ-CE
1	D	304[A]	LLP	CG-CD-CE-NZ
1	C	304	LLP	CD-CE-NZ-C4'
1	C	304	LLP	C3-C4-C4'-NZ
1	B	304	LLP	C3-C4-C4'-NZ
1	A	304	LLP	C3-C4-C4'-NZ
1	D	304[A]	LLP	CD-CE-NZ-C4'
1	B	304	LLP	CD-CE-NZ-C4'
1	D	304[A]	LLP	C3-C4-C4'-NZ
1	A	304	LLP	CG-CD-CE-NZ

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	304	LLP	2	0
1	B	304	LLP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	304[A]	LLP	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GOL	A	501	-	5,5,5	0.45	0	5,5,5	0.23	0
2	GOL	A	502	-	5,5,5	0.36	0	5,5,5	0.27	0
2	GOL	D	2002	-	5,5,5	0.24	0	5,5,5	0.43	0
4	PMP	D	2001[B]	-	16,16,16	1.37	3 (18%)	21,23,23	0.85	0
3	PO4	C	501	-	4,4,4	0.83	0	6,6,6	0.60	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	GOL	A	502	-	-	4/4/4/4	-
4	PMP	D	2001[B]	-	-	1/8/8/8	0/1/1/1
2	GOL	D	2002	-	-	2/4/4/4	-
2	GOL	A	501	-	-	2/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	2001[B]	PMP	C3-C2	-2.79	1.38	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	2001[B]	PMP	P-O1P	2.09	1.57	1.50
4	D	2001[B]	PMP	O3-C3	2.04	1.41	1.37

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	502	GOL	O1-C1-C2-C3
2	A	502	GOL	C1-C2-C3-O3
2	D	2002	GOL	O2-C2-C3-O3
2	A	501	GOL	O1-C1-C2-C3
2	D	2002	GOL	C1-C2-C3-O3
2	A	502	GOL	O1-C1-C2-O2
2	A	502	GOL	O2-C2-C3-O3
2	A	501	GOL	O1-C1-C2-O2
4	D	2001[B]	PMP	C5-C4-C4A-N4A

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	GOL	1	0
2	A	502	GOL	1	0
4	D	2001[B]	PMP	2	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	466/486 (95%)	-0.29	3 (0%) 89 93	8, 16, 37, 57	0
1	B	470/486 (96%)	-0.26	5 (1%) 80 85	8, 17, 40, 53	0
1	C	462/486 (95%)	0.10	25 (5%) 25 34	12, 25, 47, 62	1 (0%)
1	D	467/486 (96%)	-0.08	11 (2%) 59 68	14, 24, 44, 63	0
All	All	1865/1944 (95%)	-0.13	44 (2%) 59 68	8, 21, 43, 63	1 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	50	VAL	6.7
1	D	339	GLY	6.6
1	C	49	THR	6.6
1	A	5	PHE	6.0
1	C	54	GLY	6.0
1	D	54	GLY	6.0
1	D	49	THR	5.5
1	C	414	TRP	5.2
1	A	55	PRO	4.6
1	C	53	PRO	4.3
1	D	48	GLU	4.3
1	C	331	ALA	4.0
1	C	178	ALA	4.0
1	C	55	PRO	4.0
1	C	419	ARG	4.0
1	C	415	LEU	4.0
1	B	48	GLU	3.9
1	A	4	ARG	3.7
1	B	418	GLU	3.6
1	C	340	PHE	3.5
1	D	340	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	423	TRP	3.3
1	C	413	ASP	3.3
1	C	5	PHE	3.2
1	C	339	GLY	3.2
1	B	416	PRO	3.0
1	C	417	ALA	2.9
1	C	418	GLU	2.8
1	C	420	TRP	2.8
1	D	53	PRO	2.8
1	C	179	GLN	2.8
1	C	48	GLU	2.7
1	D	433	ARG	2.7
1	C	332	PRO	2.7
1	C	141	GLU	2.5
1	C	475	ALA	2.5
1	C	230	ALA	2.4
1	D	473	ARG	2.4
1	D	178	ALA	2.4
1	C	473	ARG	2.3
1	D	55	PRO	2.2
1	B	396	ARG	2.2
1	B	417	ALA	2.1
1	C	446	GLY	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	D	304[A]	24/25	0.92	0.16	12,28,33,38	15
1	LLP	A	304	24/25	0.94	0.12	6,23,30,34	0
1	LLP	C	304	24/25	0.94	0.13	13,27,38,41	0
1	LLP	B	304	24/25	0.94	0.16	9,23,32,37	4

## 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
2	GOL	A	501	6/6	0.79	0.20	30,37,46,48	0
2	GOL	A	502	6/6	0.84	0.14	43,46,48,52	0
2	GOL	D	2002	6/6	0.85	0.17	43,52,54,58	0
3	PO4	C	501	5/5	0.87	0.15	63,66,68,70	0
4	PMP	D	2001[B]	16/16	0.92	0.14	27,31,36,40	16

## 6.5 Other polymers [i](#)

There are no such residues in this entry.