



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 14, 2024 – 10:15 PM EST

PDB ID : 4RLG  
Title : The clear crystal structure of pyridoxal-dependent decarboxylase from sphaerobacter thermophilus dsm 20745  
Authors : Wu, R.; Clancy, S.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2014-10-16  
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

<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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

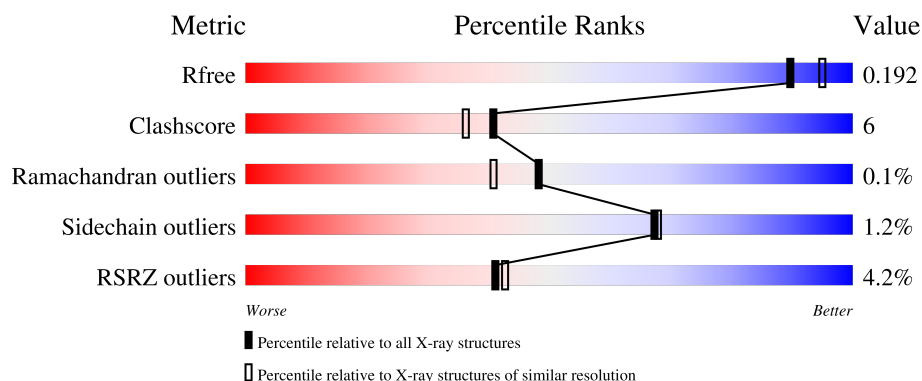
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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> <div>4%</div> <div> <div></div> <div>86%</div> <div>10%</div> <div>..</div> </div> </div>
1	B	486	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>9%</div> <div>.</div> </div> </div>
1	C	486	<div> <div>4%</div> <div> <div></div> <div>84%</div> <div>12%</div> <div>.</div> </div> </div>
1	D	486	<div> <div>5%</div> <div> <div></div> <div>84%</div> <div>13%</div> <div>.</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	ABU	D	502[A]	-	-	X	-
5	ABU	D	503[B]	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15766 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.

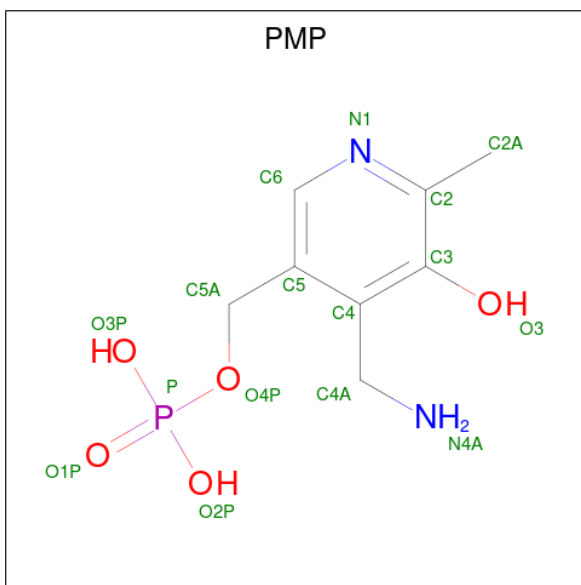
- Molecule 1 is a protein called Pyridoxal-dependent decarboxylase.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	472	Total	C	N	O	P	S	Se	0	3	0
			3640	2304	653	665	1	3	14			
1	B	470	Total	C	N	O	P	S	Se	0	5	0
			3625	2294	651	663	1	3	13			
1	D	470	Total	C	N	O	P	S	Se	0	3	0
			3628	2294	655	661	1	3	14			
1	C	469	Total	C	N	O	P	S	Se	0	2	0
			3612	2284	648	662	1	3	14			

There are 12 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
B	-2	SER	-	expression tag	UNP D1C7D8
B	-1	ASN	-	expression tag	UNP D1C7D8
B	0	ALA	-	expression tag	UNP D1C7D8
D	-2	SER	-	expression tag	UNP D1C7D8
D	-1	ASN	-	expression tag	UNP D1C7D8
D	0	ALA	-	expression tag	UNP D1C7D8
C	-2	SER	-	expression tag	UNP D1C7D8
C	-1	ASN	-	expression tag	UNP D1C7D8
C	0	ALA	-	expression tag	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	A	1	Total	C	N	O	P	0	1
			16	8	2	5	1		
2	B	1	Total	C	N	O	P	0	1
			16	8	2	5	1		
2	D	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<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).

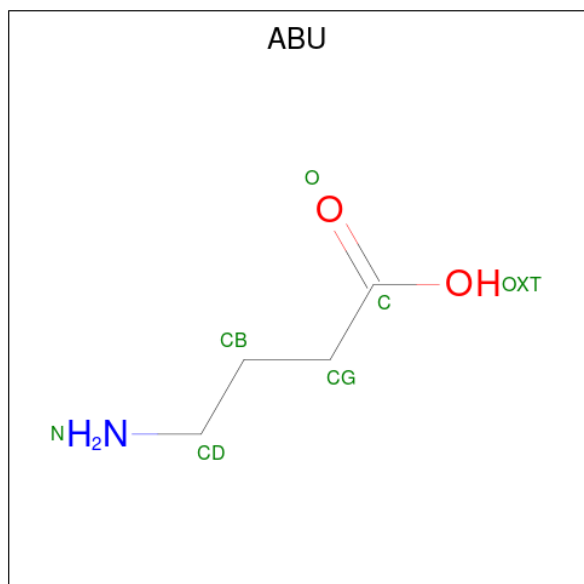


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total K 1 1	0	0
4	B	1	Total K 1 1	0	0
4	D	1	Total K 1 1	0	0
4	C	1	Total K 1 1	0	0

- Molecule 5 is GAMMA-AMINO-BUTANOIC ACID (three-letter code: ABU) (formula: C<sub>4</sub>H<sub>9</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	N	O	0	1
			7	4	1	2		
5	D	1	Total	C	N	O	0	1
			7	4	1	2		

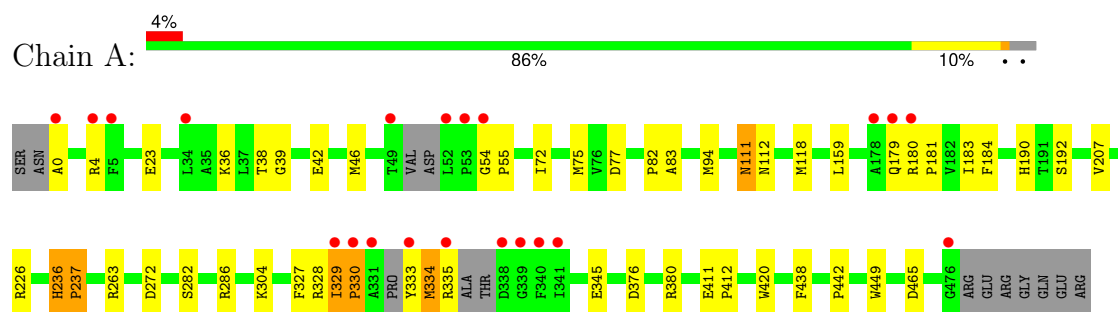
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	264	Total	O	0	0
			264	264		
6	B	305	Total	O	0	0
			305	305		
6	D	278	Total	O	0	0
			278	278		
6	C	302	Total	O	0	0
			302	302		

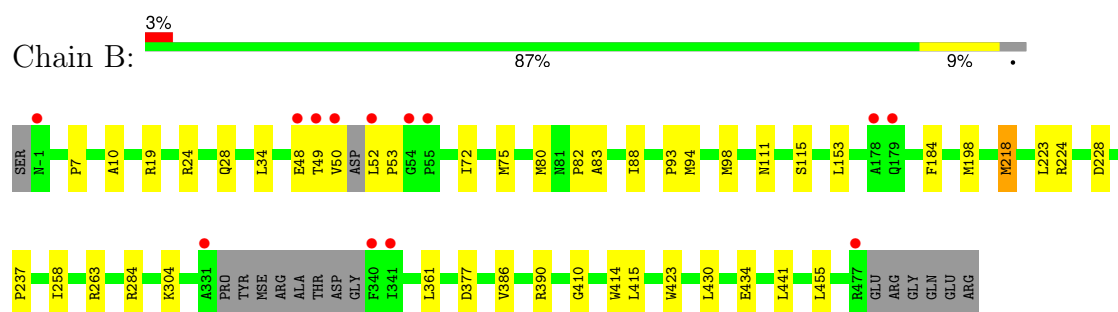
### 3 Residue-property plots

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.

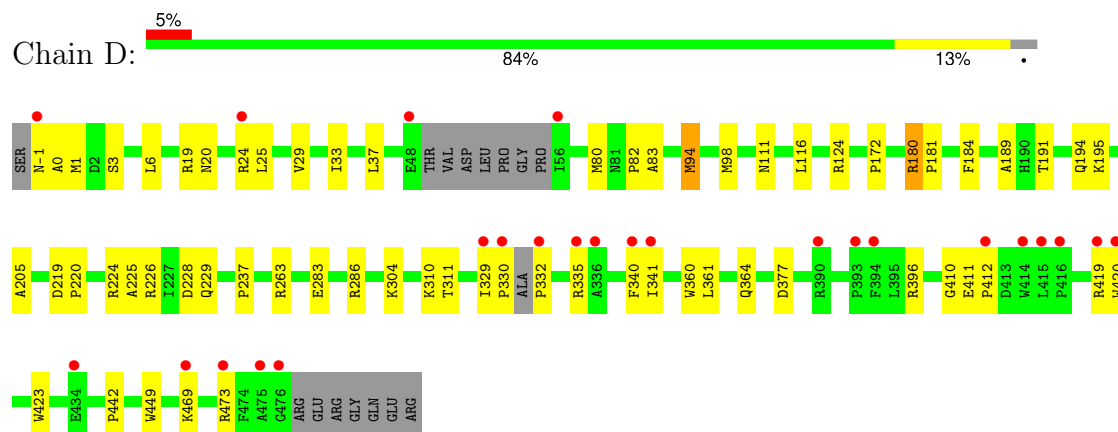
- Molecule 1: Pyridoxal-dependent decarboxylase



- Molecule 1: Pyridoxal-dependent decarboxylase

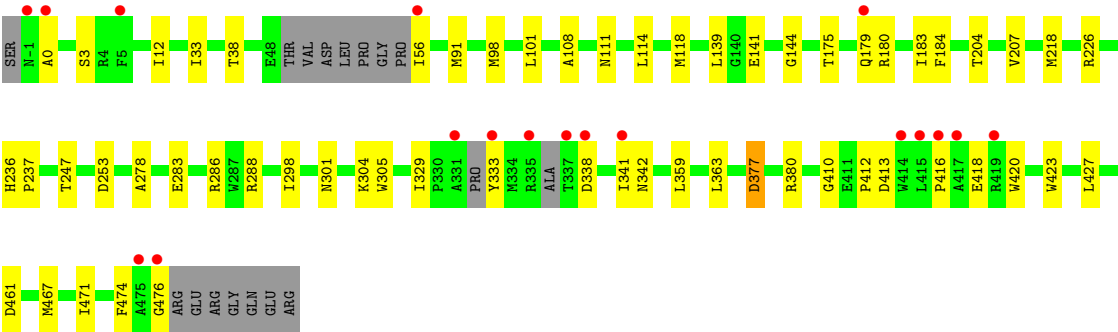
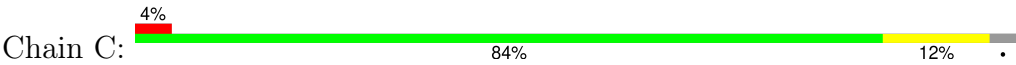


- Molecule 1: Pyridoxal-dependent decarboxylase



- 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, $\alpha$ , $\beta$ , $\gamma$	69.32Å 124.98Å 132.76Å 90.00° 99.49° 90.00°	Depositor
Resolution (Å)	39.70 – 1.90 39.70 – 1.90	Depositor EDS
% Data completeness (in resolution range)	88.1 (39.70-1.90) 88.0 (39.70-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.93 (at 1.89Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.162 , 0.191 0.165 , 0.192	Depositor DCC
$R_{free}$ test set	7746 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.4	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 44.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	15766	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, K, ABU, 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	0.78	3/3673 (0.1%)	0.76	3/4968 (0.1%)
1	B	0.77	0/3657	0.73	0/4951
1	C	0.80	0/3643	0.78	3/4925 (0.1%)
1	D	0.77	0/3661	0.75	1/4950 (0.0%)
All	All	0.78	3/14634 (0.0%)	0.76	7/19794 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	237	PRO	N-CD	5.24	1.55	1.47
1	A	55	PRO	N-CD	5.14	1.55	1.47
1	A	330	PRO	N-CD	5.02	1.54	1.47

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	195	LYS	CD-CE-NZ	5.59	124.55	111.70
1	A	329	ILE	C-N-CD	5.58	140.11	128.40
1	C	377	ASP	CB-CG-OD1	5.56	123.31	118.30
1	A	54	GLY	C-N-CD	5.52	140.00	128.40
1	C	288	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	A	236	HIS	C-N-CD	5.32	139.57	128.40
1	C	286	ARG	NE-CZ-NH2	-5.29	117.66	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3640	0	3622	38	0
1	B	3625	0	3620	43	0
1	C	3612	0	3595	49	0
1	D	3628	0	3618	64	0
2	A	16	0	9	0	0
2	B	16	0	10	4	0
2	C	16	0	10	4	0
2	D	16	0	11	5	0
3	A	6	0	8	1	0
3	B	12	0	16	1	0
3	C	6	0	8	1	0
3	D	6	0	8	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	D	14	0	0	10	0
6	A	264	0	0	3	0
6	B	305	0	0	8	0
6	C	302	0	0	7	0
6	D	278	0	0	9	0
All	All	15766	0	14535	187	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 6.

All (187) 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:191:THR:HG22	5:D:503[B]:ABU:CD	1.76	1.15
1:A:333:TYR:HB2	1:A:334:MSE:CE	1.80	1.10
1:D:191:THR:HG22	5:D:502[A]:ABU:N	1.72	1.01
1:A:333:TYR:HB2	1:A:334:MSE:HE3	1.02	0.99
3:C:502:GOL:H11	6:C:810:HOH:O	1.64	0.96
1:D:191:THR:HA	5:D:503[B]:ABU:CB	1.94	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:TYR:CB	1:A:334:MSE:HE3	1.94	0.95
1:D:98:MSE:CE	1:D:361:LEU:HD13	1.95	0.95
1:D:80:MSE:HG2	1:D:82:PRO:HD3	1.52	0.91
1:D:191:THR:HA	5:D:502[A]:ABU:CD	1.99	0.91
1:A:0:ALA:HB2	1:B:377:ASP:OD2	1.71	0.88
1:D:283:GLU:HG2	1:D:286:ARG:NH2	1.94	0.82
1:A:82:PRO:HD2	6:A:2362:HOH:O	1.81	0.80
1:B:98:MSE:HE3	1:B:361:LEU:HB3	1.65	0.79
1:D:283:GLU:HG2	1:D:286:ARG:HH22	1.48	0.76
1:D:0:ALA:HB2	1:C:377:ASP:OD2	1.86	0.76
1:D:98:MSE:HE1	1:D:361:LEU:HD13	1.67	0.75
1:D:194:GLN:HG3	5:D:503[B]:ABU:OXT	1.87	0.74
1:C:416:PRO:HB2	1:C:418:GLU:OE2	1.87	0.74
1:D:98:MSE:HE2	1:D:361:LEU:HB3	1.69	0.72
1:A:39:GLY:O	1:A:42:GLU:HG2	1.88	0.72
1:D:20:ASN:O	1:D:24:ARG:HG3	1.89	0.71
1:D:25:LEU:HD21	1:C:98:MSE:CE	2.21	0.70
1:B:390:ARG:HG2	6:B:902:HOH:O	1.92	0.70
1:B:98:MSE:CE	1:B:361:LEU:HD13	2.22	0.70
1:C:380:ARG:NH2	1:C:461:ASP:OD1	2.24	0.70
1:C:183:ILE:HD11	1:C:207:VAL:HG22	1.75	0.68
1:D:-1:ASN:ND2	6:D:878:HOH:O	2.26	0.67
1:A:179:GLN:N	1:A:179:GLN:OE1	2.28	0.65
1:D:25:LEU:HD21	1:C:98:MSE:HE3	1.80	0.63
1:B:98:MSE:CE	1:B:361:LEU:HB3	2.28	0.63
1:B:153:LEU:HG	6:B:896:HOH:O	1.98	0.63
1:C:474:PHE:C	1:C:476:GLY:N	2.52	0.62
1:B:390:ARG:CG	6:B:902:HOH:O	2.46	0.62
1:D:191:THR:CA	5:D:503[B]:ABU:CB	2.72	0.62
1:D:377:ASP:OD2	1:C:0:ALA:HB2	1.98	0.62
1:A:179:GLN:HG2	1:A:236:HIS:HB2	1.81	0.62
1:C:474:PHE:C	1:C:476:GLY:H	2.04	0.60
1:B:50:VAL:HG23	1:B:52:LEU:N	2.16	0.59
1:C:423:TRP:CE2	1:C:474:PHE:HE2	2.19	0.59
1:D:263:ARG:NH2	6:D:715:HOH:O	2.35	0.59
1:D:80:MSE:HE2	1:C:111:ASN:HA	1.84	0.59
1:D:184:PHE:HE2	1:D:237:PRO:HB3	1.67	0.59
1:A:83:ALA:HA	1:A:94:MSE:HE2	1.85	0.59
1:B:98:MSE:HE3	1:B:361:LEU:HD13	1.83	0.59
1:C:179:GLN:N	1:C:179:GLN:OE1	2.35	0.59
1:C:341:ILE:HG12	1:C:342:ASN:N	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:172:PRO:O	1:C:180:ARG:NH1	2.31	0.58
1:D:191:THR:HG22	5:D:503[B]:ABU:CB	2.32	0.58
1:B:93:PRO:HB3	1:B:455:LEU:HD13	1.85	0.57
1:C:410:GLY:HA3	1:C:423:TRP:CZ3	2.39	0.57
1:A:184:PHE:HE2	1:A:237:PRO:HB3	1.70	0.56
1:D:410:GLY:HA3	1:D:423:TRP:CZ3	2.41	0.56
1:A:46:MSE:HE2	1:A:438:PHE:CE1	2.40	0.56
1:B:80:MSE:HG2	1:B:82:PRO:HD3	1.89	0.55
1:B:98:MSE:HE1	1:B:361:LEU:HD13	1.87	0.55
1:D:124:ARG:HD2	6:D:842:HOH:O	2.05	0.55
1:D:304[A]:LLP:H5'1	6:D:660:HOH:O	2.05	0.55
1:D:191:THR:HG23	1:C:333:TYR:OH	2.05	0.55
1:D:329:ILE:HG23	1:C:204:THR:HG21	1.89	0.55
1:D:469:LYS:N	1:D:469:LYS:HD3	2.21	0.55
1:C:56:ILE:HA	6:C:855:HOH:O	2.06	0.55
1:D:224:ARG:NH1	1:D:228:ASP:OD1	2.27	0.54
1:A:190:HIS:CD2	1:A:192:SER:H	2.26	0.54
1:D:98:MSE:CE	1:D:361:LEU:HB3	2.35	0.54
1:C:184:PHE:HE2	1:C:237:PRO:HB3	1.73	0.53
1:B:410:GLY:HA3	1:B:423:TRP:CZ3	2.44	0.53
1:D:191:THR:CG2	5:D:502[A]:ABU:N	2.62	0.53
1:A:36:LYS:NZ	1:A:77:ASP:OD1	2.41	0.53
1:D:19[B]:ARG:HG3	1:C:38:THR:HG21	1.91	0.53
1:D:98:MSE:HE3	1:D:361:LEU:HD13	1.85	0.53
1:C:380:ARG:HH21	1:C:461:ASP:CG	2.11	0.52
1:D:83:ALA:HA	1:D:94:MSE:HE3	1.92	0.52
1:B:218:MSE:HE2	1:B:258[B]:ILE:HD12	1.92	0.52
1:C:412:PRO:HD2	1:C:420:TRP:CD1	2.45	0.52
1:A:183[B]:ILE:HD11	1:A:207:VAL:HG22	1.92	0.51
1:A:190:HIS:HD2	1:A:192:SER:OG	1.93	0.51
1:B:72:ILE:HA	1:B:75:MSE:HE2	1.93	0.51
1:D:329:ILE:HG23	1:D:330:PRO:HD2	1.92	0.51
1:C:329:ILE:HG12	6:C:870:HOH:O	2.11	0.50
1:A:335:ARG:HB2	1:B:441:LEU:HB3	1.94	0.50
1:D:473:ARG:HG3	1:D:473:ARG:HH11	1.74	0.50
2:D:501[B]:PMP:H5A1	6:D:660:HOH:O	2.11	0.50
1:B:224:ARG:HH12	1:B:228:ASP:CG	2.15	0.49
1:D:180:ARG:HH22	1:D:205:ALA:HB3	1.78	0.49
1:D:412:PRO:HD2	1:D:420:TRP:NE1	2.27	0.49
1:B:98:MSE:HE3	1:B:361:LEU:CB	2.41	0.48
1:A:329:ILE:HG23	1:A:330:PRO:HD2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:335:ARG:HD2	6:D:871:HOH:O	2.14	0.48
1:B:24:ARG:O	1:B:28:GLN:HG3	2.14	0.47
1:B:414:TRP:CD1	1:B:415:LEU:HD13	2.49	0.47
1:C:278:ALA:CB	1:C:305:TRP:HB3	2.44	0.47
1:A:190:HIS:HD2	1:A:192:SER:CB	2.27	0.47
1:A:236:HIS:HE1	6:A:2337:HOH:O	1.97	0.47
1:C:141:GLU:HA	1:C:141:GLU:OE1	2.15	0.47
1:A:23:GLU:HG2	1:B:34:LEU:HD13	1.96	0.47
1:B:430:LEU:HD12	1:B:434:GLU:HG2	1.95	0.47
1:C:236:HIS:CE1	6:C:801:HOH:O	2.68	0.47
1:A:376:ASP:O	1:A:380:ARG:HG3	2.15	0.46
1:D:191:THR:CA	5:D:502[A]:ABU:CD	2.82	0.46
1:A:282:SER:O	1:A:286:ARG:HB2	2.15	0.46
1:B:52:LEU:C	1:B:52:LEU:HD23	2.36	0.46
1:C:218:MSE:HE3	1:C:253:ASP:OD2	2.15	0.46
1:D:116:LEU:HD21	1:D:124:ARG:NH2	2.30	0.46
1:B:7:PRO:HG2	1:B:10:ALA:HB2	1.97	0.46
1:B:284:ARG:NH2	6:B:721:HOH:O	2.36	0.46
1:D:473:ARG:HG3	1:D:473:ARG:NH1	2.31	0.46
1:B:263:ARG:NH2	6:B:762:HOH:O	2.49	0.46
1:B:83:ALA:HA	1:B:94:MSE:HE2	1.98	0.46
1:C:380:ARG:NH2	1:C:461:ASP:CG	2.68	0.45
1:C:91:MSE:HE1	1:C:247:THR:HA	1.97	0.45
1:A:411:GLU:HG2	1:A:420:TRP:CE3	2.52	0.45
1:D:33:ILE:HG23	1:D:33:ILE:HD12	1.77	0.45
1:A:442:PRO:HD2	1:A:449:TRP:O	2.16	0.45
1:D:225:ALA:O	1:D:229:GLN:HG3	2.17	0.45
1:A:46:MSE:HE2	1:A:438:PHE:CZ	2.53	0.44
1:B:115:SER:HB3	3:B:502:GOL:H2	1.98	0.44
1:B:184:PHE:HE2	1:B:237:PRO:HB3	1.81	0.44
1:D:37:LEU:HD13	1:C:12:ILE:HD12	1.99	0.44
1:A:465:ASP:OD1	3:A:2002:GOL:C1	2.65	0.44
1:D:1:MSE:SE	1:D:6:LEU:HD13	2.67	0.44
1:A:327:PHE:O	1:B:198:MSE:HE2	2.17	0.44
1:D:29:VAL:HG21	1:C:101:LEU:HD13	1.99	0.44
1:D:33:ILE:HD13	1:D:33:ILE:HA	1.85	0.44
1:A:111:ASN:HA	1:B:80:MSE:HE2	2.00	0.43
1:C:179:GLN:H	1:C:179:GLN:CD	2.20	0.43
1:D:360:TRP:O	1:D:364:GLN:HG3	2.19	0.43
1:A:72:ILE:HA	1:A:75:MSE:HE2	2.00	0.43
1:D:412:PRO:HA	6:D:716:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:ILE:HG23	1:C:33:ILE:HD12	1.78	0.42
1:B:48:GLU:CD	1:B:49:THR:N	2.73	0.42
1:B:284:ARG:NE	6:B:721:HOH:O	2.40	0.42
1:A:412:PRO:HD2	1:A:420:TRP:CD1	2.54	0.42
1:D:189:ALA:O	5:D:502[A]:ABU:O	2.37	0.42
1:C:412:PRO:HD2	1:C:420:TRP:NE1	2.35	0.42
1:A:263:ARG:NH2	6:A:2203:HOH:O	2.47	0.42
1:C:139:LEU:HD11	1:C:298:ILE:HD12	2.02	0.42
1:B:390:ARG:HG3	6:B:902:HOH:O	2.17	0.42
1:B:386:VAL:O	1:B:390:ARG:HG3	2.20	0.42
1:D:419:ARG:HA	6:D:767:HOH:O	2.20	0.42
1:C:33:ILE:HD13	1:C:33:ILE:HA	1.83	0.41
1:C:236:HIS:HE1	6:C:801:HOH:O	2.01	0.41
1:D:219:ASP:HA	1:D:220:PRO:HD3	1.80	0.41
1:C:283:GLU:HG2	6:C:899:HOH:O	2.19	0.41
1:A:112:ASN:HB3	1:A:118:MSE:HB3	2.01	0.41
1:A:159:LEU:HD22	1:A:183[A]:ILE:HD13	2.02	0.41
1:A:272:ASP:OD2	1:A:304[A]:LLP:N1	2.53	0.41
1:D:396:ARG:HD3	1:D:411:GLU:OE1	2.19	0.41
1:C:359:LEU:O	1:C:363:LEU:HG	2.20	0.41
1:C:144:GLY:HA3	6:C:876:HOH:O	2.20	0.41
1:D:310:LYS:HA	1:D:311:THR:HA	1.83	0.41
1:A:180:ARG:HA	1:A:181:PRO:HD3	1.89	0.41
1:D:37:LEU:HD11	1:C:108:ALA:HB1	2.02	0.41
1:A:38:THR:OG1	1:B:19:ARG:NH2	2.54	0.41
1:A:328:ARG:NH2	1:A:345:GLU:OE1	2.54	0.41
1:D:442:PRO:HD2	1:D:449:TRP:O	2.21	0.41
1:D:181:PRO:CD	1:C:175:THR:HG21	2.50	0.41
1:D:332:PRO:N	6:D:843:HOH:O	2.54	0.41
1:B:50:VAL:O	1:B:52:LEU:N	2.54	0.40
1:B:52:LEU:HG	1:B:53:PRO:HD2	2.04	0.40
1:B:218:MSE:CE	1:B:223:LEU:HD22	2.51	0.40
1:D:412:PRO:HD2	1:D:420:TRP:CD1	2.56	0.40
1:B:88:ILE:HG22	6:B:666:HOH:O	2.20	0.40
1:D:19[A]:ARG:NH1	1:C:38:THR:OG1	2.55	0.40
1:C:114:LEU:HD23	1:C:118:MSE:SE	2.71	0.40
1:C:329:ILE:HD13	1:C:329:ILE:HG21	1.67	0.40
1:C:427:LEU:HD21	1:C:471:ILE:HG12	2.03	0.40
1:A:335:ARG:HD2	1:B:441:LEU:CD2	2.52	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	466/486 (96%)	458 (98%)	8 (2%)	0	100	100
1	B	467/486 (96%)	456 (98%)	11 (2%)	0	100	100
1	C	461/486 (95%)	451 (98%)	9 (2%)	1 (0%)	44	36
1	D	465/486 (96%)	455 (98%)	10 (2%)	0	100	100
All	All	1859/1944 (96%)	1820 (98%)	38 (2%)	1 (0%)	48	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	413	ASP

### 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	365/362 (101%)	361 (99%)	4 (1%)	70	71
1	B	365/362 (101%)	363 (100%)	2 (0%)	86	88
1	C	363/362 (100%)	359 (99%)	4 (1%)	70	71
1	D	364/362 (101%)	357 (98%)	7 (2%)	52	49
All	All	1457/1448 (101%)	1440 (99%)	17 (1%)	67	68

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	111	ASN
1	A	226	ARG
1	A	334	MSE
1	B	111	ASN
1	B	218	MSE
1	D	3	SER
1	D	94	MSE
1	D	111	ASN
1	D	180	ARG
1	D	226	ARG
1	D	340	PHE
1	D	341	ILE
1	C	3	SER
1	C	226	ARG
1	C	338	ASP
1	C	467	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	190	HIS
1	A	236	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 4 are monoatomic - leaving 11 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
5	ABU	D	502[A]	-	6,6,6	1.00	0	6,6,6	2.50	3 (50%)
3	GOL	C	502	-	5,5,5	0.56	0	5,5,5	0.85	0
3	GOL	B	502	-	5,5,5	0.41	0	5,5,5	0.51	0
3	GOL	A	2002	-	5,5,5	0.37	0	5,5,5	0.46	0
5	ABU	D	503[B]	-	6,6,6	0.79	0	6,6,6	2.43	3 (50%)
3	GOL	B	503	-	5,5,5	0.39	0	5,5,5	0.63	0
3	GOL	D	504	-	5,5,5	0.29	0	5,5,5	0.73	0
2	PMP	B	501[B]	-	16,16,16	3.18	6 (37%)	22,23,23	1.52	5 (22%)
2	PMP	D	501[B]	-	16,16,16	3.05	6 (37%)	22,23,23	1.44	5 (22%)
2	PMP	A	2001[B]	-	16,16,16	2.99	6 (37%)	22,23,23	1.63	7 (31%)
2	PMP	C	501[B]	-	16,16,16	2.83	5 (31%)	22,23,23	1.65	5 (22%)

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
5	ABU	D	502[A]	-	-	2/4/4/4	-
3	GOL	C	502	-	-	0/4/4/4	-
3	GOL	B	502	-	-	2/4/4/4	-
3	GOL	A	2002	-	-	4/4/4/4	-
5	ABU	D	503[B]	-	-	3/4/4/4	-
3	GOL	B	503	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	D	504	-	-	4/4/4/4	-
2	PMP	B	501[B]	-	-	0/8/8/8	0/1/1/1
2	PMP	D	501[B]	-	-	0/8/8/8	0/1/1/1
2	PMP	A	2001[B]	-	-	0/8/8/8	0/1/1/1
2	PMP	C	501[B]	-	-	2/8/8/8	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501[B]	PMP	C3-C2	7.71	1.49	1.41
2	B	501[B]	PMP	C3-C2	7.50	1.48	1.41
2	A	2001[B]	PMP	C3-C2	6.73	1.48	1.41
2	C	501[B]	PMP	C3-C2	6.27	1.47	1.41
2	B	501[B]	PMP	C3-C4	6.14	1.49	1.40
2	A	2001[B]	PMP	C3-C4	5.95	1.48	1.40
2	B	501[B]	PMP	C5-C4	5.67	1.48	1.40
2	D	501[B]	PMP	C3-C4	5.46	1.48	1.40
2	A	2001[B]	PMP	C5-C4	5.28	1.47	1.40
2	C	501[B]	PMP	C5-C4	5.15	1.47	1.40
2	C	501[B]	PMP	C3-C4	4.92	1.47	1.40
2	D	501[B]	PMP	C5-C4	4.48	1.46	1.40
2	C	501[B]	PMP	P-O3P	-3.99	1.40	1.54
2	D	501[B]	PMP	P-O2P	-3.64	1.41	1.54
2	D	501[B]	PMP	P-O3P	-3.50	1.41	1.54
2	B	501[B]	PMP	P-O2P	-3.40	1.42	1.54
2	A	2001[B]	PMP	P-O2P	-3.37	1.42	1.54
2	B	501[B]	PMP	P-O3P	-3.10	1.43	1.54
2	A	2001[B]	PMP	P-O1P	-3.04	1.41	1.50
2	C	501[B]	PMP	P-O2P	-3.02	1.43	1.54
2	B	501[B]	PMP	P-O1P	-2.46	1.42	1.50
2	D	501[B]	PMP	P-O1P	-2.14	1.43	1.50
2	A	2001[B]	PMP	P-O3P	-2.07	1.47	1.54

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	502[A]	ABU	CB-CG-C	-4.40	103.03	114.51
5	D	503[B]	ABU	CB-CG-C	-4.27	103.36	114.51
2	B	501[B]	PMP	O4P-C5A-C5	3.82	116.52	109.36
2	A	2001[B]	PMP	O4P-C5A-C5	3.54	115.98	109.36
2	C	501[B]	PMP	C2A-C2-C3	-3.39	116.82	120.80
2	D	501[B]	PMP	O3-C3-C2	3.09	124.00	117.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	503[B]	ABU	OXT-C-CG	3.04	123.59	114.00
2	D	501[B]	PMP	C4-C3-C2	-3.02	115.35	119.91
5	D	502[A]	ABU	OXT-C-CG	2.82	122.90	114.00
2	B	501[B]	PMP	C6-N1-C2	2.77	124.21	119.20
2	D	501[B]	PMP	O3P-P-O2P	2.76	118.14	107.80
2	C	501[B]	PMP	O4P-C5A-C5	2.74	114.50	109.36
2	A	2001[B]	PMP	C2A-C2-C3	-2.74	117.59	120.80
2	D	501[B]	PMP	C6-N1-C2	2.74	124.17	119.20
2	A	2001[B]	PMP	C6-N1-C2	2.72	124.13	119.20
2	C	501[B]	PMP	O3P-P-O4P	-2.67	99.70	106.67
5	D	503[B]	ABU	O-C-CG	-2.67	114.61	123.09
5	D	502[A]	ABU	O-C-CG	-2.64	114.72	123.09
2	C	501[B]	PMP	C4-C3-C2	-2.59	115.99	119.91
2	B	501[B]	PMP	O3-C3-C2	2.53	122.82	117.58
2	A	2001[B]	PMP	O3P-P-O2P	2.51	117.21	107.80
2	A	2001[B]	PMP	C4-C3-C2	-2.38	116.32	119.91
2	B	501[B]	PMP	O3P-P-O2P	2.31	116.46	107.80
2	B	501[B]	PMP	C4-C3-C2	-2.18	116.62	119.91
2	A	2001[B]	PMP	C2A-C2-N1	2.08	121.56	117.64
2	D	501[B]	PMP	O4P-C5A-C5	2.04	113.19	109.36
2	C	501[B]	PMP	C2A-C2-N1	2.04	121.48	117.64
2	A	2001[B]	PMP	O3-C3-C4	2.02	124.05	118.18

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	501[B]	PMP	C3-C4-C4A-N4A
2	C	501[B]	PMP	C5-C4-C4A-N4A
3	A	2002	GOL	C1-C2-C3-O3
3	D	504	GOL	O1-C1-C2-C3
5	D	503[B]	ABU	CD-CB-CG-C
3	A	2002	GOL	O1-C1-C2-C3
3	B	502	GOL	O1-C1-C2-C3
3	D	504	GOL	C1-C2-C3-O3
3	A	2002	GOL	O2-C2-C3-O3
3	B	502	GOL	O1-C1-C2-O2
3	D	504	GOL	O2-C2-C3-O3
3	A	2002	GOL	O1-C1-C2-O2
3	D	504	GOL	O1-C1-C2-O2
5	D	503[B]	ABU	O-C-CG-CB
5	D	502[A]	ABU	OXT-C-CG-CB

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Mol	Chain	Res	Type	Atoms
5	D	502[A]	ABU	O-C-CG-CB
5	D	503[B]	ABU	OXT-C-CG-CB

There are no ring outliers.

8 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	502[A]	ABU	5	0
3	C	502	GOL	1	0
3	B	502	GOL	1	0
3	A	2002	GOL	1	0
5	D	503[B]	ABU	5	0
2	B	501[B]	PMP	4	0
2	D	501[B]	PMP	5	0
2	C	501[B]	PMP	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	457/486 (94%)	-0.04	21 (4%) 38 39	8, 25, 52, 70	9 (1%)
1	B	456/486 (93%)	-0.21	13 (2%) 54 56	10, 24, 48, 65	5 (1%)
1	C	454/486 (93%)	-0.26	18 (3%) 43 44	9, 21, 48, 73	6 (1%)
1	D	455/486 (93%)	-0.11	25 (5%) 32 33	12, 23, 54, 68	10 (2%)
All	All	1822/1944 (93%)	-0.15	77 (4%) 41 43	8, 23, 51, 73	30 (1%)

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	476	GLY	5.2
1	D	340	PHE	5.0
1	D	476	GLY	4.9
1	B	340	PHE	4.8
1	A	0	ALA	4.8
1	A	49	THR	4.7
1	A	52	LEU	4.4
1	A	54	GLY	4.4
1	D	416	PRO	4.2
1	B	54	GLY	4.2
1	A	4	ARG	4.1
1	D	335	ARG	4.1
1	A	340	PHE	3.9
1	D	336	ALA	3.9
1	A	335	ARG	3.8
1	D	415	LEU	3.8
1	B	331	ALA	3.7
1	B	50	VAL	3.6
1	A	5	PHE	3.6
1	D	419	ARG	3.6
1	B	52	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	337	THR	3.4
1	C	338	ASP	3.4
1	C	331	ALA	3.3
1	B	341	ILE	3.2
1	C	475	ALA	3.2
1	A	339	GLY	3.1
1	D	332	PRO	3.0
1	D	420	TRP	3.0
1	C	0	ALA	2.9
1	C	179	GLN	2.9
1	D	56	ILE	2.8
1	A	331	ALA	2.8
1	B	477	ARG	2.8
1	A	178	ALA	2.8
1	A	333	TYR	2.7
1	A	53	PRO	2.7
1	C	5	PHE	2.6
1	D	473	ARG	2.6
1	A	476	GLY	2.6
1	A	338	ASP	2.6
1	C	335	ARG	2.6
1	B	49	THR	2.6
1	D	390	ARG	2.6
1	D	330	PRO	2.6
1	C	416	PRO	2.5
1	A	179	GLN	2.5
1	C	341	ILE	2.5
1	B	55	PRO	2.5
1	A	329	ILE	2.5
1	A	341	ILE	2.5
1	D	412	PRO	2.4
1	D	24	ARG	2.4
1	C	333	TYR	2.4
1	A	34	LEU	2.4
1	D	329	ILE	2.4
1	D	469	LYS	2.4
1	B	-1	ASN	2.4
1	D	394	PHE	2.4
1	D	341	ILE	2.3
1	C	419	ARG	2.3
1	B	178	ALA	2.3
1	A	180	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	414	TRP	2.2
1	C	-1	ASN	2.2
1	C	417	ALA	2.2
1	D	414	TRP	2.2
1	D	434	GLU	2.2
1	D	393	PRO	2.2
1	B	48	GLU	2.1
1	D	48	GLU	2.1
1	C	415	LEU	2.1
1	B	179	GLN	2.1
1	D	475	ALA	2.1
1	A	330	PRO	2.1
1	C	56	ILE	2.0
1	D	-1	ASN	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	A	304[A]	24/25	0.95	0.09	14,25,31,33	15
1	LLP	B	304[A]	24/25	0.97	0.07	13,24,29,31	15
1	LLP	D	304[A]	24/25	0.97	0.08	12,23,30,30	15
1	LLP	C	304[A]	24/25	0.97	0.07	11,21,25,27	15

## 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( $\text{\AA}^2$ )	Q<0.9
3	GOL	C	502	6/6	0.70	0.15	56,58,60,63	0
5	ABU	D	503[B]	7/7	0.71	0.20	27,30,33,35	7
3	GOL	D	504	6/6	0.75	0.17	62,63,65,67	0
3	GOL	B	502	6/6	0.82	0.13	41,47,55,57	0
3	GOL	A	2002	6/6	0.82	0.17	50,59,62,67	0
3	GOL	B	503	6/6	0.90	0.10	59,62,65,65	0
5	ABU	D	502[A]	7/7	0.93	0.11	24,25,33,33	6
2	PMP	A	2001[B]	16/16	0.93	0.10	21,27,31,33	16
2	PMP	D	501[B]	16/16	0.94	0.10	16,27,30,30	16
2	PMP	B	501[B]	16/16	0.94	0.09	19,25,30,31	16
2	PMP	C	501[B]	16/16	0.95	0.09	10,22,26,27	16
4	K	D	505	1/1	0.95	0.08	49,49,49,49	0
4	K	C	503	1/1	0.97	0.06	40,40,40,40	0
4	K	A	2003	1/1	0.98	0.04	44,44,44,44	0
4	K	B	504	1/1	0.98	0.04	38,38,38,38	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.