



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 4, 2017 – 05:42 PM EDT

PDB ID : 2ASV  
Title : X-Ray studies on protein complexes: Enzymatic catalysis in Crystals of E. coli  
Maltodextrin Phosphorylase (MalP)  
Authors : Geremia, S.; Campagnolo, M.  
Deposited on : unknown  
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

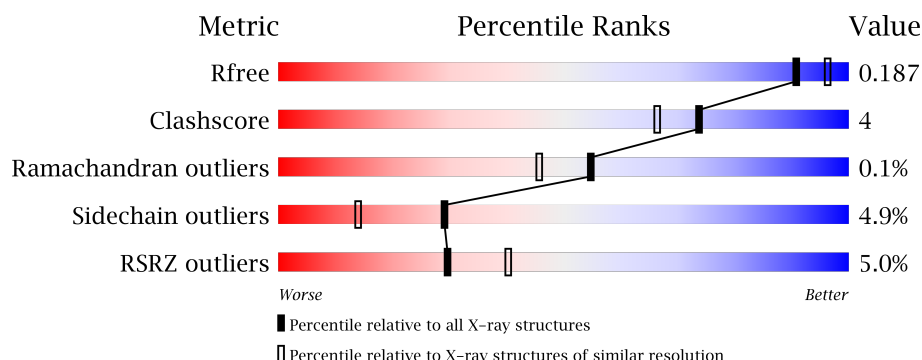
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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))
$R_{free}$	100719	2004 (1.96-1.96)
Clashscore	112137	2136 (1.96-1.96)
Ramachandran outliers	110173	2117 (1.96-1.96)
Sidechain outliers	110143	2117 (1.96-1.96)
RSRZ outliers	101464	2018 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	796	<div> <div>4%</div> <div>86%</div> <div>13%</div> <div>.</div> </div>
1	B	796	<div> <div>6%</div> <div>86%</div> <div>13%</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
3	GLC	B	996	-	-	-	X
4	ASO	A	1998	-	-	-	X
4	ASO	B	2998	-	-	X	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 14136 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.

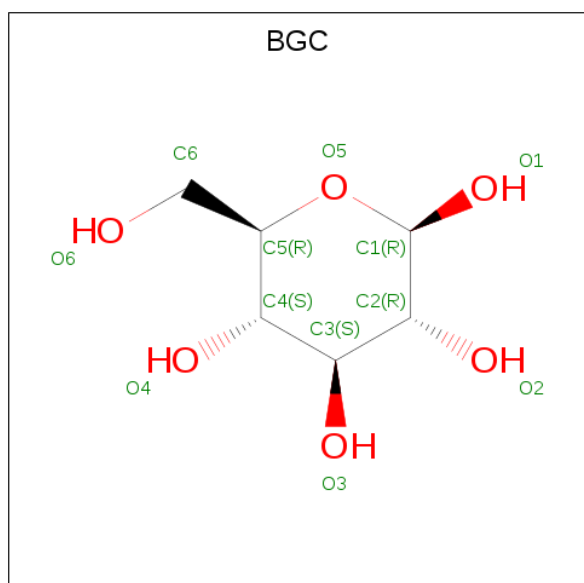
- Molecule 1 is a protein called Maltodextrin phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	796	Total	C	N	O	S	0	0	0
			6389	4079	1128	1162	20			
1	B	796	Total	C	N	O	S	0	0	0
			6389	4079	1128	1162	20			

There are 6 discrepancies between the modelled and reference sequences:

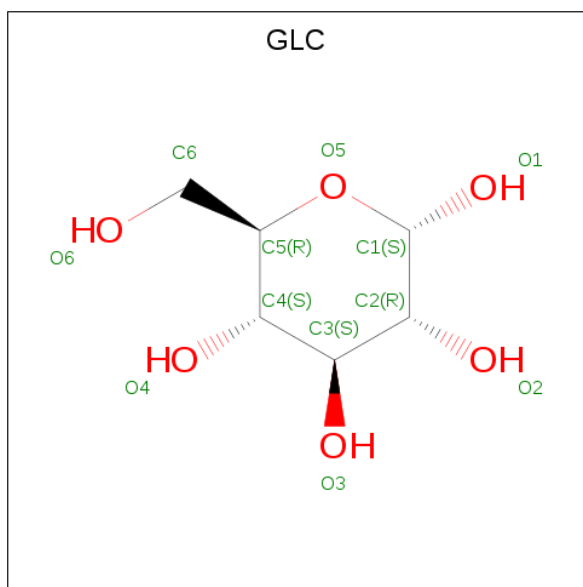
Chain	Residue	Modelled	Actual	Comment	Reference
A	261	ALA	HIS	ENGINEERED	UNP P00490
A	262	PHE	THR	ENGINEERED	UNP P00490
A	263	GLU	ALA	ENGINEERED	UNP P00490
B	261	ALA	HIS	ENGINEERED	UNP P00490
B	262	PHE	THR	ENGINEERED	UNP P00490
B	263	GLU	ALA	ENGINEERED	UNP P00490

- Molecule 2 is BETA-D-GLUCOSE (three-letter code: BGC) (formula:  $C_6H_{12}O_6$ ).



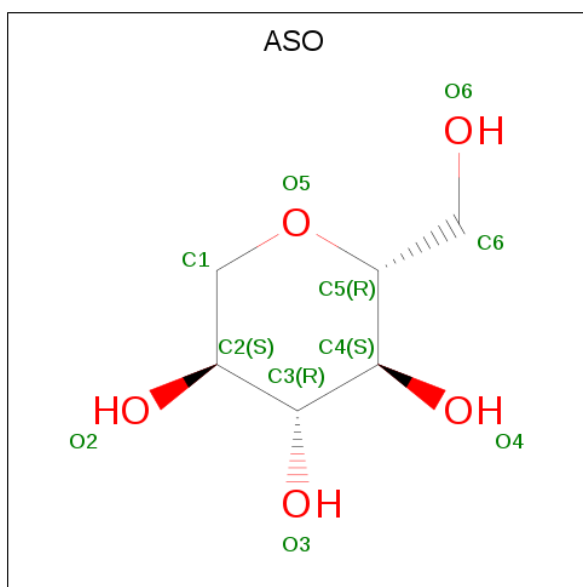
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is ALPHA-D-GLUCOSE (three-letter code: GLC) (formula:  $C_6H_{12}O_6$ ).



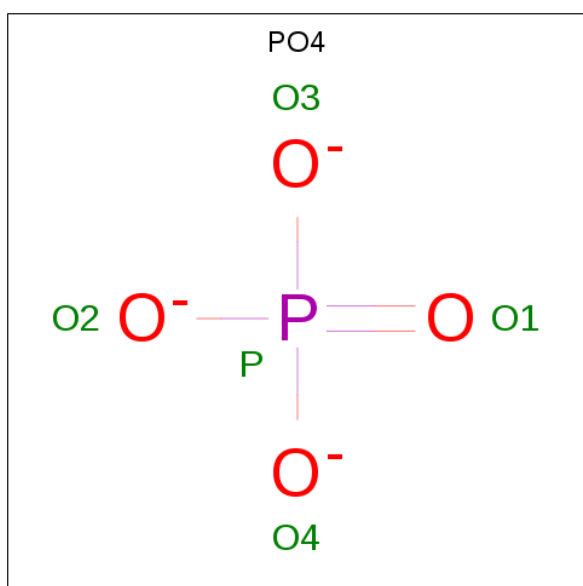
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 4 is 1,5-ANHYDROSORBITOL (three-letter code: ASO) (formula:  $C_6H_{12}O_5$ ).



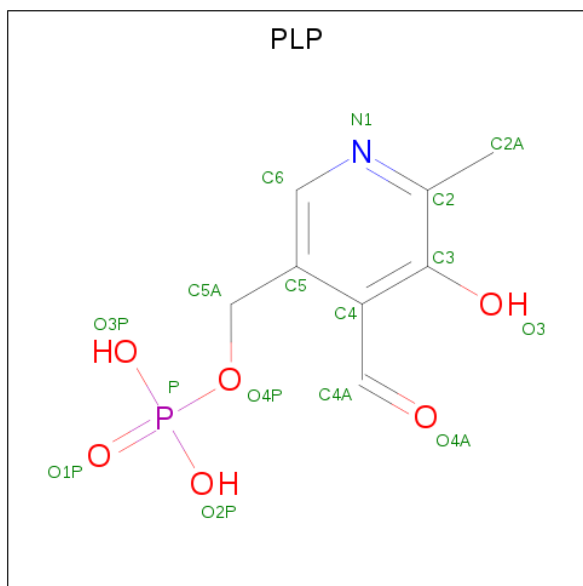
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula:  $C_8H_{10}NO_6P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
6	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

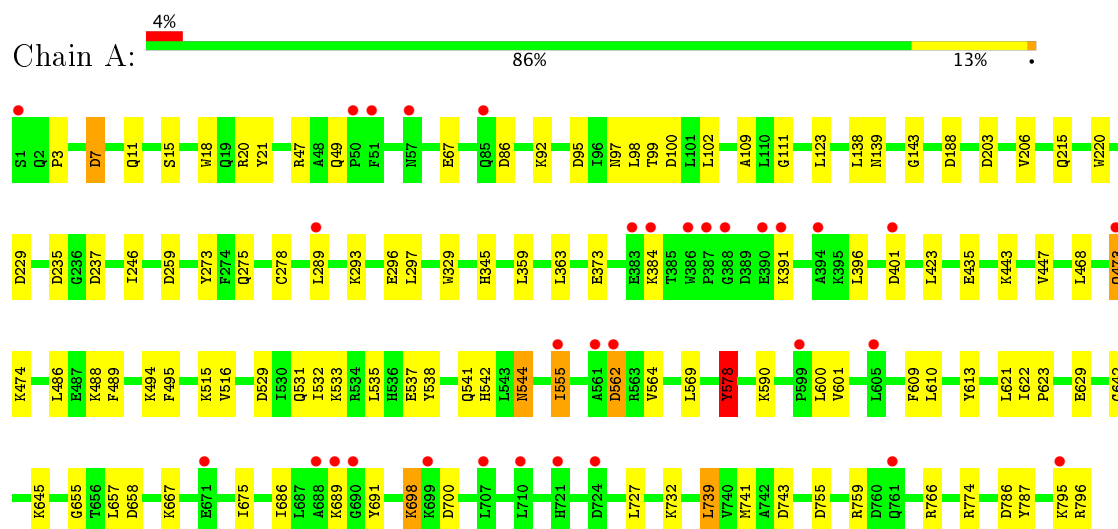
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	613	Total	O	0	0
			613	613		
7	B	571	Total	O	0	0
			571	571		

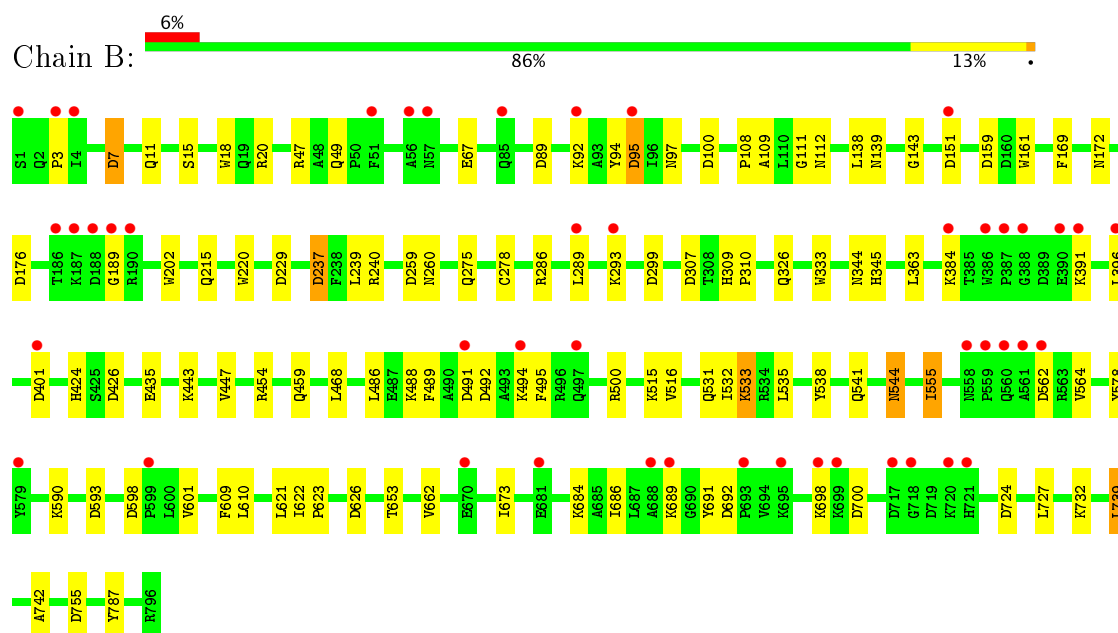
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ( $\text{RSRZ} > 2$ ). 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: Maltodextrin phosphorylase



#### • Molecule 1: Maltodextrin phosphorylase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.33Å 104.72Å 214.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 1.95 15.00 – 1.95	Depositor EDS
% Data completeness (in resolution range)	97.5 (15.00-1.95) 97.6 (15.00-1.95)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.42 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.179 , 0.226 0.191 , 0.187	Depositor DCC
$R_{free}$ test set	6000 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.8	Xtriage
Anisotropy	0.346	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 55.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	14136	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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: GLC, PO4, BGC, ASO, PLP

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	0.90	2/6539 (0.0%)	0.91	16/8865 (0.2%)
1	B	0.90	1/6539 (0.0%)	0.92	25/8865 (0.3%)
All	All	0.90	3/13078 (0.0%)	0.92	41/17730 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	273	TYR	CE2-CZ	-5.94	1.30	1.38
1	A	578	TYR	CD2-CE2	-5.72	1.30	1.39
1	B	333	TRP	CB-CG	-5.14	1.41	1.50

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	299	ASP	CB-CG-OD2	7.45	125.00	118.30
1	B	307	ASP	CB-CG-OD2	7.20	124.78	118.30
1	B	626	ASP	CB-CG-OD2	6.74	124.37	118.30
1	A	259	ASP	CB-CG-OD2	6.49	124.14	118.30
1	B	500	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	B	259	ASP	CB-CG-OD2	6.43	124.08	118.30
1	B	176	ASP	CB-CG-OD1	6.39	124.05	118.30
1	A	235	ASP	CB-CG-OD2	6.37	124.03	118.30
1	A	229	ASP	CB-CG-OD2	6.31	123.98	118.30
1	A	786	ASP	CB-CG-OD2	6.09	123.78	118.30
1	B	229	ASP	CB-CG-OD2	6.01	123.71	118.30
1	B	237	ASP	CB-CG-OD1	5.96	123.66	118.30
1	A	562	ASP	CB-CG-OD2	5.95	123.65	118.30
1	B	401	ASP	CB-CG-OD2	5.88	123.59	118.30
1	B	151	ASP	CB-CG-OD2	5.87	123.58	118.30
1	A	86	ASP	CB-CG-OD2	5.81	123.53	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	95	ASP	CB-CG-OD2	5.78	123.50	118.30
1	A	237	ASP	CB-CG-OD2	5.72	123.44	118.30
1	B	598	ASP	CB-CG-OD2	5.68	123.41	118.30
1	A	95	ASP	CB-CG-OD2	5.62	123.36	118.30
1	B	700	ASP	CB-CG-OD2	5.57	123.31	118.30
1	B	159	ASP	CB-CG-OD2	5.54	123.28	118.30
1	B	7	ASP	CB-CG-OD2	5.53	123.28	118.30
1	A	188	ASP	CB-CG-OD2	5.48	123.23	118.30
1	A	7	ASP	CB-CG-OD2	5.40	123.16	118.30
1	B	426	ASP	CB-CG-OD2	5.35	123.11	118.30
1	A	658	ASP	CB-CG-OD2	5.34	123.11	118.30
1	B	89	ASP	CB-CG-OD2	5.33	123.09	118.30
1	B	562	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	203	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	286	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	A	796	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	A	743	ASP	CB-CG-OD2	5.19	122.97	118.30
1	B	492	ASP	CB-CG-OD2	5.18	122.96	118.30
1	B	692	ASP	CB-CG-OD2	5.14	122.93	118.30
1	B	286	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	A	401	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	700	ASP	CB-CG-OD2	5.07	122.86	118.30
1	B	491	ASP	CB-CG-OD2	5.05	122.85	118.30
1	B	724	ASP	CB-CG-OD2	5.05	122.85	118.30
1	B	593	ASP	CB-CG-OD2	5.02	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6389	0	6333	52	0
1	B	6389	0	6333	43	0
2	A	12	0	11	0	0
2	B	12	0	11	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	44	0	37	2	0
3	B	44	0	37	3	0
4	A	11	0	11	3	0
4	B	11	0	12	6	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
6	A	15	0	6	0	0
6	B	15	0	6	0	0
7	A	613	0	0	8	0
7	B	571	0	0	6	0
All	All	14136	0	12797	97	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 (97) 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)
3:A:997:GLC:O4	4:A:1998:ASO:H11	1.47	1.15
3:B:997:GLC:O4	4:B:2998:ASO:H11	1.65	0.95
1:B:345:HIS:O	4:B:2998:ASO:H12	1.74	0.86
1:A:97:ASN:HD22	1:A:100:ASP:H	1.33	0.76
3:A:997:GLC:HO4	4:A:1998:ASO:H11	1.49	0.74
1:A:3:PRO:HD2	7:A:2469:HOH:O	1.94	0.67
1:B:7:ASP:O	1:B:11:GLN:HG2	1.95	0.66
1:A:468:LEU:CD2	1:A:486:LEU:HD11	2.26	0.65
1:B:97:ASN:HD22	1:B:100:ASP:H	1.45	0.62
1:A:345:HIS:O	4:A:1998:ASO:H12	2.00	0.62
1:A:47:ARG:HD3	7:A:2181:HOH:O	1.99	0.62
1:B:468:LEU:CD2	1:B:486:LEU:HD11	2.30	0.61
1:A:21:TYR:O	1:B:172:ASN:HB2	2.01	0.61
1:B:3:PRO:HB3	1:B:49:GLN:OE1	2.00	0.61
3:B:997:GLC:C4	4:B:2998:ASO:H11	2.31	0.60
1:A:3:PRO:HB3	1:A:49:GLN:OE1	2.02	0.59
1:A:11:GLN:HG3	7:A:2565:HOH:O	2.03	0.58
1:A:531:GLN:HE22	1:A:541:GLN:HA	1.67	0.58
3:B:997:GLC:HO4	4:B:2998:ASO:H11	1.66	0.58
1:A:691:TYR:CE2	1:A:739:LEU:HD22	2.39	0.58
1:B:691:TYR:CE2	1:B:739:LEU:HD22	2.39	0.58
1:A:97:ASN:ND2	1:A:100:ASP:H	2.00	0.57
1:B:237:ASP:OD2	1:B:240:ARG:NH1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:VAL:HG11	1:A:787:TYR:CD2	2.41	0.56
1:B:189:GLY:HA2	7:B:3544:HOH:O	2.06	0.55
1:A:7:ASP:O	1:A:11:GLN:HG2	2.07	0.54
1:A:610:LEU:HD12	1:A:621:LEU:HD21	1.89	0.54
1:B:220:TRP:CD2	1:B:278:CYS:HB3	2.42	0.54
1:B:684:LYS:NZ	7:B:3242:HOH:O	2.42	0.53
1:B:345:HIS:O	4:B:2998:ASO:C1	2.53	0.53
1:A:532:ILE:HG21	1:A:621:LEU:HD13	1.91	0.53
1:A:246:ILE:HD13	1:B:239:LEU:HD12	1.91	0.53
1:A:138:LEU:HD21	1:A:275:GLN:HB2	1.93	0.51
1:B:97:ASN:ND2	1:B:100:ASP:H	2.08	0.51
1:A:655:GLY:O	1:A:675:ILE:HA	2.11	0.50
1:B:555:ILE:HD11	1:B:601:VAL:HG22	1.93	0.50
1:A:562:ASP:O	1:A:759:ARG:NH2	2.42	0.50
1:A:473:GLN:OE1	1:A:474:LYS:HE2	2.12	0.50
1:A:396:LEU:HD21	1:A:435:GLU:HB2	1.94	0.49
1:B:544:ASN:HD22	1:B:544:ASN:C	2.15	0.49
1:B:344:ASN:O	1:B:424:HIS:HE1	1.96	0.49
1:A:555:ILE:HD11	1:A:601:VAL:HG22	1.95	0.48
1:B:67:GLU:HB2	1:B:111:GLY:HA2	1.95	0.48
1:A:447:VAL:HG11	1:A:787:TYR:CE2	2.49	0.48
1:A:293:LYS:O	1:A:296:GLU:HG2	2.14	0.47
1:A:359:LEU:HD12	7:A:2451:HOH:O	2.15	0.47
1:A:67:GLU:HB2	1:A:111:GLY:HA2	1.96	0.47
1:A:423:LEU:HD23	1:A:423:LEU:O	2.15	0.47
1:B:610:LEU:HD12	1:B:621:LEU:HD21	1.97	0.47
1:B:653:THR:HB	1:B:673:ILE:HG13	1.96	0.47
1:B:220:TRP:CE2	1:B:278:CYS:HB3	2.50	0.46
1:A:766:ARG:HD2	7:A:2218:HOH:O	2.16	0.46
1:B:447:VAL:HG11	1:B:787:TYR:CD2	2.50	0.46
1:B:109:ALA:HB1	1:B:143:GLY:HA3	1.97	0.45
1:A:489:PHE:HB3	1:A:495:PHE:CG	2.52	0.45
1:B:138:LEU:HD21	1:B:275:GLN:HB2	1.99	0.45
1:B:15:SER:HA	1:B:18:TRP:NE1	2.32	0.44
1:B:237:ASP:OD2	1:B:240:ARG:HD2	2.18	0.44
1:B:531:GLN:HE22	1:B:541:GLN:HA	1.82	0.44
1:A:3:PRO:HB3	1:A:49:GLN:CD	2.38	0.43
1:A:473:GLN:HB2	1:A:473:GLN:HE21	1.59	0.43
1:B:169:PHE:CE1	1:B:202:TRP:HB3	2.53	0.43
1:A:220:TRP:CD2	1:A:278:CYS:HB3	2.54	0.43
1:B:489:PHE:HB3	1:B:495:PHE:CG	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:HIS:O	4:B:2998:ASO:H2	2.18	0.43
1:A:691:TYR:OH	1:A:741:MET:HB2	2.19	0.43
1:A:3:PRO:CD	7:A:2469:HOH:O	2.62	0.43
1:B:47:ARG:HD3	7:B:3205:HOH:O	2.19	0.43
1:A:11:GLN:CG	7:A:2565:HOH:O	2.66	0.43
1:B:108:PRO:HA	1:B:161:TRP:CE3	2.54	0.42
1:A:544:ASN:ND2	7:A:2050:HOH:O	2.52	0.42
1:A:97:ASN:HD21	1:A:99:THR:HB	1.83	0.42
1:A:246:ILE:CD1	1:B:239:LEU:HD12	2.49	0.42
1:A:544:ASN:HD22	1:A:544:ASN:C	2.22	0.42
1:A:622:ILE:N	1:A:623:PRO:CD	2.83	0.42
1:B:532:ILE:HG21	1:B:621:LEU:HD13	2.00	0.42
1:B:396:LEU:HD21	1:B:435:GLU:HB2	2.01	0.42
1:A:98:LEU:O	1:A:102:LEU:HG	2.20	0.42
1:B:459:GLN:NE2	7:B:3263:HOH:O	2.46	0.41
1:B:94:TYR:O	1:B:95:ASP:HB2	2.20	0.41
1:A:109:ALA:HB1	1:A:143:GLY:HA3	2.03	0.41
1:A:529:ASP:OD1	1:A:629:GLU:OE2	2.38	0.41
1:A:123:LEU:HB3	1:A:206:VAL:HG11	2.01	0.41
1:A:532:ILE:HB	1:A:613:TYR:CZ	2.55	0.41
1:A:698:LYS:HD2	1:A:698:LYS:HA	1.93	0.41
1:A:657:LEU:HA	1:A:657:LEU:HD23	1.97	0.41
1:B:590:LYS:HD2	1:B:590:LYS:HA	1.83	0.41
1:B:260:ASN:ND2	7:B:3437:HOH:O	2.54	0.41
1:A:15:SER:HA	1:A:18:TRP:NE1	2.36	0.41
1:B:309:HIS:N	1:B:310:PRO:CD	2.84	0.41
1:A:329:TRP:CZ3	1:A:373:GLU:HG2	2.57	0.41
1:B:739:LEU:HB3	1:B:742:ALA:HB3	2.03	0.41
1:A:642:GLY:HA2	1:A:645:LYS:HD2	2.04	0.40
1:A:537:GLU:HB2	1:A:578:TYR:OH	2.22	0.40
1:B:112:ASN:OD1	7:B:3563:HOH:O	2.22	0.40
1:B:622:ILE:N	1:B:623:PRO:CD	2.84	0.40
1:A:667:LYS:O	1:A:774:ARG:HD3	2.22	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	794/796 (100%)	770 (97%)	23 (3%)	1 (0%)	55	46
1	B	794/796 (100%)	770 (97%)	23 (3%)	1 (0%)	55	46
All	All	1588/1592 (100%)	1540 (97%)	46 (3%)	2 (0%)	55	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	533	LYS
1	B	533	LYS

### 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	667/667 (100%)	633 (95%)	34 (5%)	28	13
1	B	667/667 (100%)	635 (95%)	32 (5%)	30	14
All	All	1334/1334 (100%)	1268 (95%)	66 (5%)	29	14

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ARG
1	A	92	LYS
1	A	139	ASN
1	A	215	GLN

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Mol	Chain	Res	Type
1	A	289	LEU
1	A	297	LEU
1	A	363	LEU
1	A	384	LYS
1	A	391	LYS
1	A	443	LYS
1	A	473	GLN
1	A	488	LYS
1	A	494	LYS
1	A	515	LYS
1	A	516	VAL
1	A	535	LEU
1	A	538	TYR
1	A	542	HIS
1	A	544	ASN
1	A	555	ILE
1	A	564	VAL
1	A	569	LEU
1	A	578	TYR
1	A	590	LYS
1	A	600	LEU
1	A	609	PHE
1	A	686	ILE
1	A	689	LYS
1	A	698	LYS
1	A	727	LEU
1	A	732	LYS
1	A	739	LEU
1	A	755	ASP
1	A	795	LYS
1	B	20	ARG
1	B	92	LYS
1	B	139	ASN
1	B	215	GLN
1	B	289	LEU
1	B	293	LYS
1	B	326	GLN
1	B	363	LEU
1	B	384	LYS
1	B	391	LYS
1	B	443	LYS
1	B	454	ARG

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Mol	Chain	Res	Type
1	B	488	LYS
1	B	494	LYS
1	B	515	LYS
1	B	516	VAL
1	B	533	LYS
1	B	535	LEU
1	B	538	TYR
1	B	544	ASN
1	B	555	ILE
1	B	564	VAL
1	B	578	TYR
1	B	609	PHE
1	B	662	VAL
1	B	686	ILE
1	B	689	LYS
1	B	698	LYS
1	B	727	LEU
1	B	732	LYS
1	B	739	LEU
1	B	755	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	97	ASN
1	A	112	ASN
1	A	139	ASN
1	A	178	GLN
1	A	221	GLN
1	A	260	ASN
1	A	446	ASN
1	A	459	GLN
1	A	531	GLN
1	A	544	ASN
1	A	678	HIS
1	B	9	GLN
1	B	57	ASN
1	B	97	ASN
1	B	112	ASN
1	B	139	ASN
1	B	178	GLN

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Mol	Chain	Res	Type
1	B	221	GLN
1	B	260	ASN
1	B	446	ASN
1	B	459	GLN
1	B	531	GLN
1	B	544	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

16 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	$\# Z  > 2$
4	ASO	A	1998	-	11,11,11	3.48	4 (36%)	13,15,15	4.25	7 (53%)
6	PLP	A	900	1	15,15,16	2.02	3 (20%)	20,22,23	1.77	6 (30%)
2	BGC	A	993	3	12,12,12	0.56	0	17,17,17	1.02	1 (5%)
3	GLC	A	994	3,2	11,11,12	0.96	0	13,15,17	1.51	3 (23%)
3	GLC	A	995	3	11,11,12	0.91	0	13,15,17	1.21	2 (15%)
3	GLC	A	996	3	11,11,12	0.94	0	13,15,17	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GLC	A	997	3	11,11,12	0.97	0	13,15,17	1.59	2 (15%)
5	PO4	A	999	-	4,4,4	0.71	0	6,6,6	0.98	0
5	PO4	B	1999	-	4,4,4	1.24	1 (25%)	6,6,6	0.79	0
4	ASO	B	2998	-	11,11,11	3.36	4 (36%)	13,15,15	3.88	5 (38%)
6	PLP	B	900	1	15,15,16	2.13	3 (20%)	20,22,23	1.91	6 (30%)
2	BGC	B	993	3	12,12,12	0.65	0	17,17,17	1.03	1 (5%)
3	GLC	B	994	3,2	11,11,12	0.52	0	13,15,17	1.32	3 (23%)
3	GLC	B	995	3	11,11,12	0.84	1 (9%)	13,15,17	1.54	1 (7%)
3	GLC	B	996	3	11,11,12	0.76	0	13,15,17	1.45	3 (23%)
3	GLC	B	997	3	11,11,12	0.85	0	13,15,17	1.89	4 (30%)

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
4	ASO	A	1998	-	-	0/2/19/19	0/1/1/1
6	PLP	A	900	1	-	0/6/6/8	0/1/1/1
2	BGC	A	993	3	-	0/2/22/22	0/1/1/1
3	GLC	A	994	3,2	-	0/2/19/22	0/1/1/1
3	GLC	A	995	3	-	0/2/19/22	0/1/1/1
3	GLC	A	996	3	-	0/2/19/22	0/1/1/1
3	GLC	A	997	3	-	0/2/19/22	0/1/1/1
5	PO4	A	999	-	-	0/0/0/0	0/0/0/0
5	PO4	B	1999	-	-	0/0/0/0	0/0/0/0
4	ASO	B	2998	-	-	0/2/19/19	0/1/1/1
6	PLP	B	900	1	-	0/6/6/8	0/1/1/1
2	BGC	B	993	3	-	0/2/22/22	0/1/1/1
3	GLC	B	994	3,2	-	0/2/19/22	0/1/1/1
3	GLC	B	995	3	-	0/2/19/22	0/1/1/1
3	GLC	B	996	3	-	0/2/19/22	0/1/1/1
3	GLC	B	997	3	-	0/2/19/22	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1998	ASO	O5-C1	-10.16	1.27	1.43
4	B	2998	ASO	O5-C1	-9.69	1.27	1.43
6	B	900	PLP	C3-C2	-6.85	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	900	PLP	C3-C2	-5.65	1.36	1.40
4	A	1998	ASO	O2-C2	-3.40	1.35	1.43
4	A	1998	ASO	C1-C2	-2.99	1.45	1.52
6	A	900	PLP	C5-C4	-2.97	1.37	1.40
6	A	900	PLP	C4A-C4	-2.89	1.45	1.51
4	B	2998	ASO	C1-C2	-2.85	1.45	1.52
4	B	2998	ASO	O2-C2	-2.84	1.37	1.43
6	B	900	PLP	C4A-C4	-2.63	1.46	1.51
4	A	1998	ASO	O5-C5	2.01	1.47	1.43
3	B	995	GLC	C2-C3	2.05	1.55	1.52
6	B	900	PLP	C6-N1	2.21	1.39	1.34
5	B	1999	PO4	P-O1	2.36	1.55	1.50
4	B	2998	ASO	O5-C5	3.28	1.50	1.43

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	900	PLP	C3-C2-N1	-3.80	115.76	120.75
3	B	997	GLC	O3-C3-C2	-3.44	103.77	110.02
6	B	900	PLP	C4A-C4-C3	-3.35	114.76	120.54
6	B	900	PLP	C6-C5-C4	-3.11	115.58	118.18
6	B	900	PLP	C3-C2-N1	-3.10	116.68	120.75
6	A	900	PLP	C4A-C4-C3	-3.07	115.25	120.54
3	A	994	GLC	O5-C1-C2	-2.91	106.24	110.79
3	B	996	GLC	O2-C2-C3	-2.61	105.05	110.17
3	B	996	GLC	O3-C3-C2	-2.43	105.60	110.02
6	B	900	PLP	C5-C6-N1	-2.42	119.78	123.87
3	B	997	GLC	O4-C4-C5	-2.41	103.21	109.28
6	A	900	PLP	C6-C5-C4	-2.33	116.23	118.18
4	B	2998	ASO	O3-C3-C2	-2.27	105.90	110.02
2	B	993	BGC	O3-C3-C2	-2.21	105.55	110.36
4	A	1998	ASO	O3-C3-C2	-2.19	106.05	110.02
3	B	994	GLC	O4-C4-C3	-2.11	105.76	110.36
3	B	994	GLC	O2-C2-C3	-2.09	106.06	110.17
3	A	995	GLC	O5-C1-C2	-2.00	107.65	110.79
2	A	993	BGC	O5-C5-C6	2.02	111.25	106.41
3	A	994	GLC	C1-O5-C5	2.09	115.04	112.17
3	B	994	GLC	C1-C2-C3	2.10	112.31	109.65
3	B	997	GLC	O2-C2-C3	2.11	114.31	110.17
3	B	996	GLC	O2-C2-C1	2.24	113.73	109.18
4	A	1998	ASO	C2-C3-C4	2.28	114.84	110.88
3	A	994	GLC	C1-C2-C3	2.28	112.54	109.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	900	PLP	C2A-C2-N1	2.31	122.50	117.89
3	A	995	GLC	C1-C2-C3	2.46	112.77	109.65
3	B	997	GLC	O4-C4-C3	2.49	115.78	110.36
3	A	997	GLC	O5-C1-C2	2.61	114.89	110.79
6	A	900	PLP	C6-N1-C2	2.64	124.34	119.26
6	B	900	PLP	C6-N1-C2	2.79	124.63	119.26
4	A	1998	ASO	C6-C5-C4	3.02	120.08	113.00
6	A	900	PLP	C3-C4-C5	3.24	122.30	118.63
3	A	997	GLC	O2-C2-C3	3.59	117.22	110.17
3	B	995	GLC	C1-O5-C5	4.15	117.89	112.17
4	B	2998	ASO	C1-C2-C3	4.40	115.23	109.65
4	B	2998	ASO	O2-C2-C3	4.44	118.90	110.17
6	B	900	PLP	C3-C4-C5	4.47	123.70	118.63
4	A	1998	ASO	O2-C2-C3	4.53	119.07	110.17
4	A	1998	ASO	C1-C2-C3	4.70	115.61	109.65
4	A	1998	ASO	O5-C1-C2	6.71	121.30	110.79
4	B	2998	ASO	O5-C1-C2	7.92	123.20	110.79
4	B	2998	ASO	C1-O5-C5	8.81	124.30	112.17
4	A	1998	ASO	C1-O5-C5	11.15	127.54	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1998	ASO	3	0
3	A	997	GLC	2	0
4	B	2998	ASO	6	0
3	B	997	GLC	3	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	796/796 (100%)	0.31	32 (4%)	39 49	20, 31, 50, 67	0
1	B	796/796 (100%)	0.32	47 (5%)	23 32	20, 31, 49, 67	0
All	All	1592/1592 (100%)	0.32	79 (4%)	30 40	20, 31, 49, 67	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	187	LYS	8.7
1	B	57	ASN	7.6
1	B	559	PRO	6.7
1	A	51	PHE	6.7
1	B	562	ASP	5.6
1	B	560	GLN	5.3
1	B	189	GLY	4.3
1	B	387	PRO	4.1
1	A	473	GLN	4.0
1	B	689	LYS	4.0
1	B	56	ALA	3.9
1	B	186	THR	3.9
1	B	188	ASP	3.8
1	A	1	SER	3.6
1	B	51	PHE	3.6
1	A	688	ALA	3.5
1	A	391	LYS	3.5
1	B	695	LYS	3.4
1	B	92	LYS	3.4
1	A	390	GLU	3.3
1	A	57	ASN	3.2
1	B	579	TYR	3.2
1	B	151	ASP	3.2
1	A	386	TRP	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	721	HIS	3.1
1	B	386	TRP	3.1
1	B	388	GLY	3.1
1	B	561	ALA	3.0
1	A	689	LYS	3.0
1	A	289	LEU	2.9
1	A	555	ILE	2.9
1	B	289	LEU	2.9
1	A	561	ALA	2.9
1	B	85	GLN	2.8
1	B	390	GLU	2.8
1	A	690	GLY	2.7
1	B	396	LEU	2.7
1	B	391	LYS	2.7
1	A	599	PRO	2.7
1	B	681	GLU	2.7
1	B	401	ASP	2.6
1	A	795	LYS	2.5
1	A	383	GLU	2.5
1	B	494	LYS	2.5
1	B	95	ASP	2.5
1	A	710	LEU	2.4
1	B	721	HIS	2.4
1	B	688	ALA	2.4
1	A	388	GLY	2.4
1	B	718	GLY	2.4
1	B	599	PRO	2.4
1	B	4	ILE	2.4
1	B	693	PRO	2.3
1	B	190	ARG	2.3
1	A	605	LEU	2.3
1	B	1	SER	2.3
1	A	761	GLN	2.3
1	B	699	LYS	2.3
1	A	401	ASP	2.3
1	A	707	LEU	2.3
1	B	720	LYS	2.2
1	A	85	GLN	2.2
1	B	491	ASP	2.2
1	B	670	GLU	2.2
1	B	717	ASP	2.2
1	B	698	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	293	LYS	2.1
1	B	384	LYS	2.1
1	A	387	PRO	2.1
1	A	562	ASP	2.1
1	A	699	LYS	2.1
1	A	724	ASP	2.1
1	B	558	ASN	2.1
1	A	394	ALA	2.1
1	B	3	PRO	2.1
1	B	497	GLN	2.1
1	A	671	GLU	2.1
1	A	50	PRO	2.0
1	A	384	LYS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	ASO	B	2998	11/11	0.86	0.20	4.16	34,41,45,47	0
3	GLC	B	996	11/12	0.91	0.14	4.00	31,32,36,36	0
4	ASO	A	1998	11/11	0.89	0.17	2.44	29,39,42,43	0
3	GLC	A	997	11/12	0.93	0.13	0.93	27,28,31,35	0
3	GLC	B	995	11/12	0.92	0.14	0.70	30,34,37,39	0
3	GLC	A	995	11/12	0.91	0.11	0.27	30,32,34,35	0
3	GLC	B	997	11/12	0.95	0.10	0.01	26,30,31,34	0
6	PLP	A	900	15/16	0.96	0.10	-0.12	21,24,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	PLP	B	900	15/16	0.96	0.09	-0.40	21,24,31,31	0
3	GLC	B	994	11/12	0.93	0.12	-0.46	38,40,43,44	0
3	GLC	A	996	11/12	0.96	0.09	-0.66	28,30,32,35	0
3	GLC	A	994	11/12	0.96	0.09	-0.81	34,37,41,42	0
5	PO4	A	999	5/5	0.98	0.07	-1.24	31,33,38,38	0
5	PO4	B	1999	5/5	0.97	0.08	-1.80	30,33,36,38	0
2	BGC	A	993	12/12	0.61	0.41	-	49,53,54,54	10
2	BGC	B	993	12/12	0.60	0.42	-	49,53,54,55	10

## 6.5 Other polymers [i](#)

There are no such residues in this entry.