



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:34 AM GMT

PDB ID : 2AZD
Title : X-Ray studies on Maltodextrin Phosphorylase (MalP) Complexes: recognition of substrates and CATALYTIC mechanism of phosphorylase family
Authors : Geremia, S.; Campagnolo, M.
Deposited on : 2005-09-10
Resolution : 2.16 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

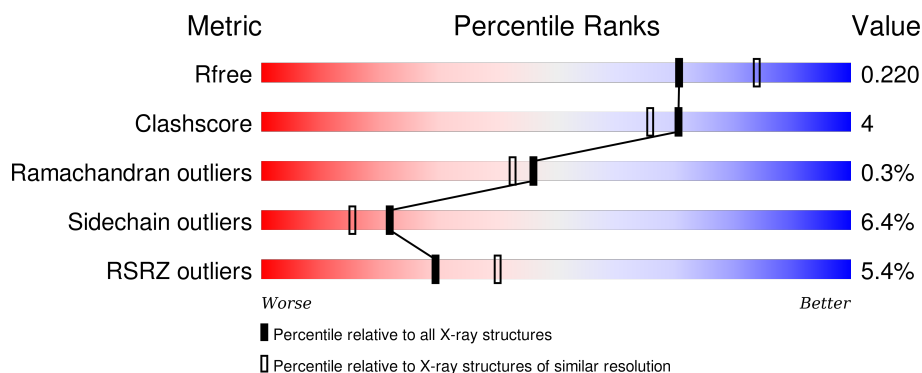
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.16 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}	91344	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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 ≥ 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>11%</div> <div>•</div> </div>
1	B	796	<div> <div>6%</div> <div>82%</div> <div>16%</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
2	GLC	A	997	-	-	-	X
2	GLC	B	995	-	-	-	X
2	GLC	B	996	-	-	-	X
2	GLC	B	997	-	-	-	X
3	VO4	A	999	-	-	X	X
3	VO4	B	1999	-	-	X	X
5	TRS	A	990	-	-	-	X
5	TRS	B	1990	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13556 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			

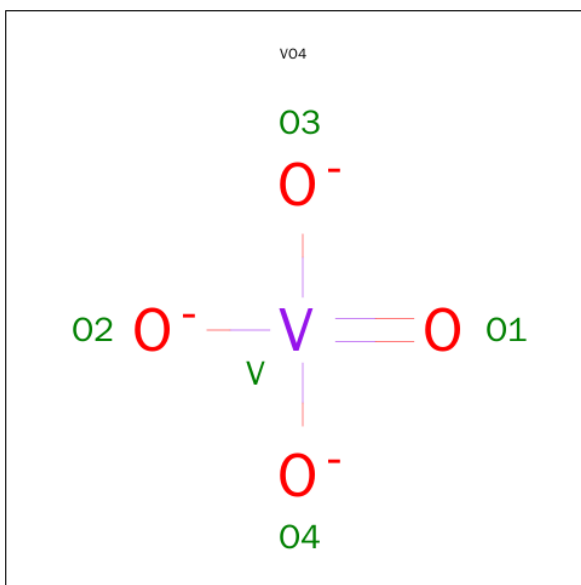
There are 6 discrepancies between the modelled and reference sequences:

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 a polymer of unknown type called SUGAR (4-MER).

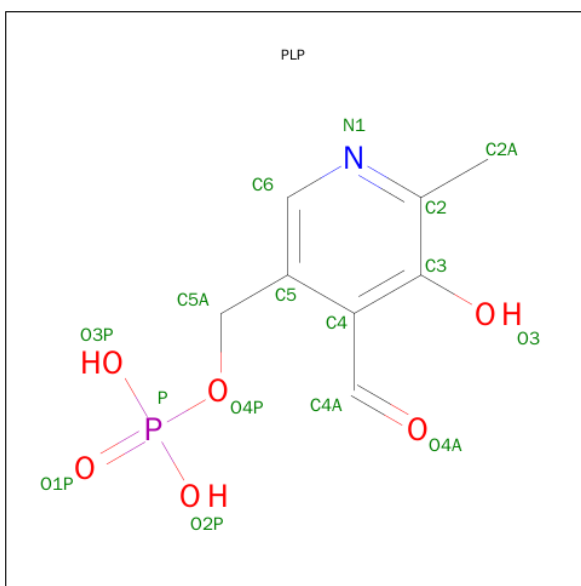
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	4	Total	C	O	0	0
			45	24	21		
2	B	4	Total	C	O	0	0
			45	24	21		

- Molecule 3 is VANADATE ION (three-letter code: VO4) (formula: O₄V).



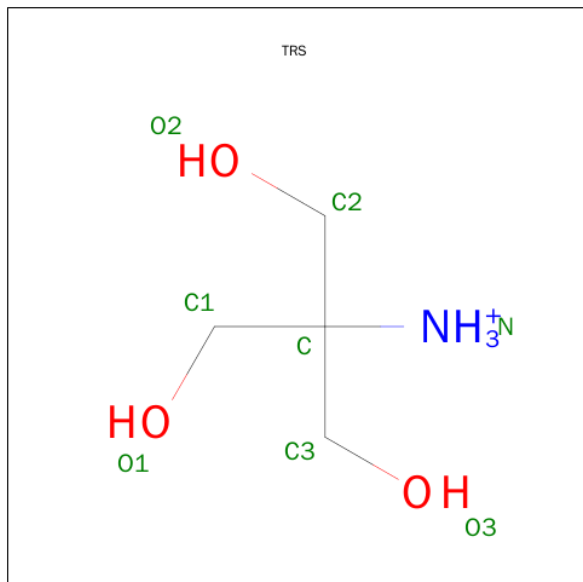
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	V	0	0
			5	4	1		
3	B	1	Total	O	V	0	0
			5	4	1		

- Molecule 4 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



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

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			8	4	1	3		
5	B	1	Total	C	N	O	0	0
			8	4	1	3		

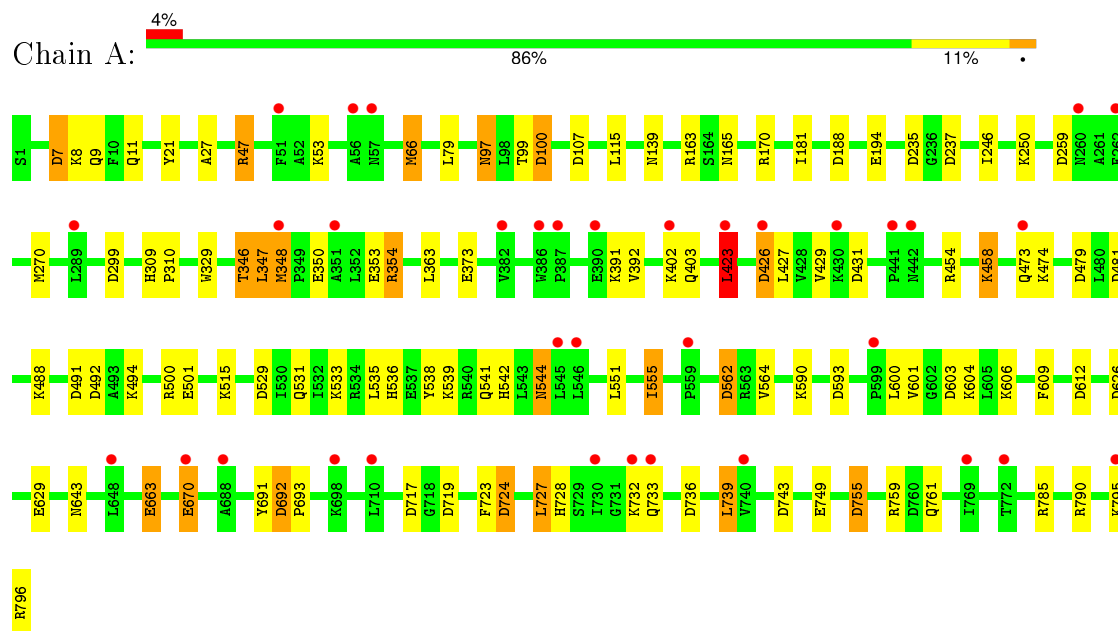
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	339	Total	O	0	0
			339	339		
6	B	293	Total	O	0	0
			293	293		

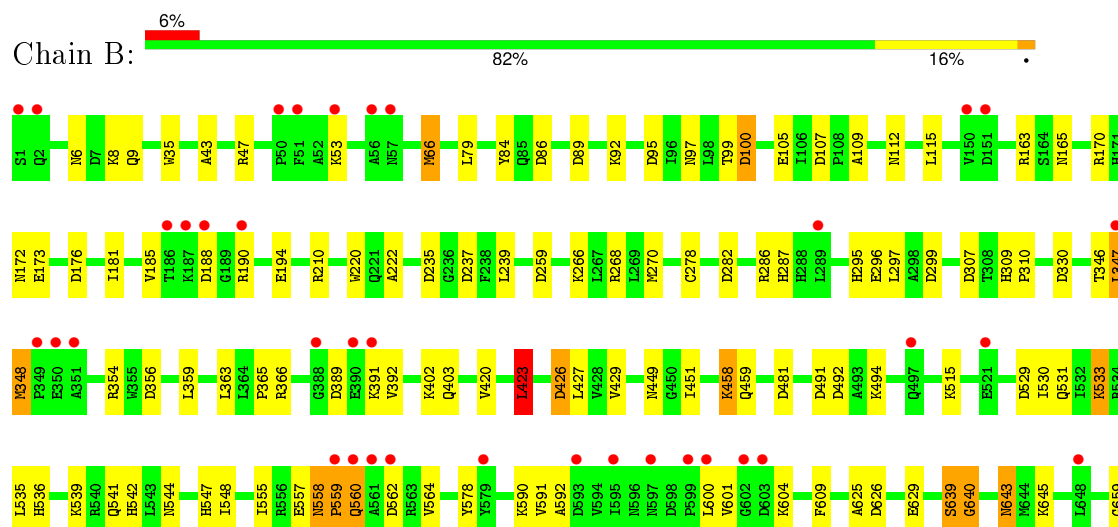
3 Residue-property plots

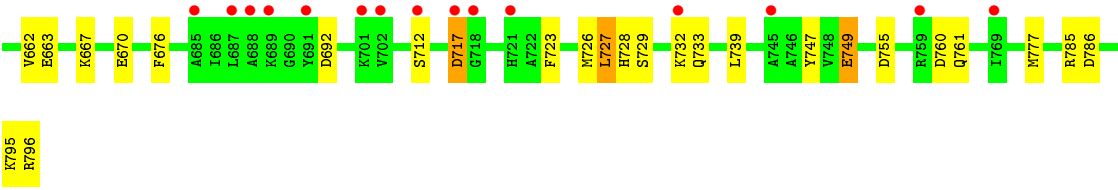
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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, α , β , γ	76.78Å 105.89Å 220.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.83 – 2.16 21.71 – 2.16	Depositor EDS
% Data completeness (in resolution range)	91.5 (6.83-2.16) 91.7 (21.71-2.16)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.15Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.205 , 0.250 0.217 , 0.220	Depositor DCC
R_{free} test set	4325 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	31.8	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 88853 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13556	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, VO4, TRS, BGC, 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	1.15	9/6539 (0.1%)	1.01	33/8865 (0.4%)
1	B	1.17	10/6539 (0.2%)	1.04	31/8865 (0.3%)
All	All	1.16	19/13078 (0.1%)	1.03	64/17730 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	761	GLN	CG-CD	7.97	1.69	1.51
1	B	173	GLU	CD-OE2	6.89	1.33	1.25
1	A	474	LYS	CD-CE	6.59	1.67	1.51
1	B	662	VAL	CA-CB	6.37	1.68	1.54
1	B	420	VAL	CB-CG2	6.36	1.66	1.52
1	B	222	ALA	CA-CB	-5.93	1.40	1.52
1	A	27	ALA	CA-CB	5.84	1.64	1.52
1	B	761	GLN	CG-CD	5.75	1.64	1.51
1	A	474	LYS	CE-NZ	5.70	1.63	1.49
1	A	663	GLU	CD-OE2	5.46	1.31	1.25
1	B	726	MET	CG-SD	5.39	1.95	1.81
1	B	643	ASN	CG-OD1	5.30	1.35	1.24
1	A	353	GLU	CD-OE1	5.27	1.31	1.25
1	B	717	ASP	CB-CG	5.26	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	473	GLN	CG-CD	5.24	1.63	1.51
1	B	109	ALA	CA-CB	-5.22	1.41	1.52
1	B	749	GLU	CD-OE2	5.20	1.31	1.25
1	A	501	GLU	CG-CD	5.07	1.59	1.51
1	A	423	LEU	CG-CD1	5.04	1.70	1.51

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	299	ASP	CB-CG-OD2	8.70	126.13	118.30
1	B	692	ASP	CB-CG-OD2	8.70	126.13	118.30
1	B	626	ASP	CB-CG-OD2	8.15	125.64	118.30
1	B	86	ASP	CB-CG-OD2	7.46	125.01	118.30
1	B	176	ASP	CB-CG-OD1	7.22	124.80	118.30
1	B	286	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	B	760	ASP	CB-CG-OD2	7.21	124.79	118.30
1	A	299	ASP	CB-CG-OD2	7.21	124.79	118.30
1	A	593	ASP	CB-CG-OD1	6.79	124.41	118.30
1	B	95	ASP	CB-CG-OD2	6.75	124.38	118.30
1	A	717	ASP	CB-CG-OD2	6.75	124.37	118.30
1	A	100	ASP	CB-CG-OD1	6.73	124.36	118.30
1	A	755	ASP	CB-CG-OD2	6.70	124.33	118.30
1	B	786	ASP	CB-CG-OD2	6.55	124.19	118.30
1	B	426	ASP	CB-CG-OD2	6.54	124.18	118.30
1	A	47	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	A	426	ASP	CB-CG-OD2	6.38	124.04	118.30
1	A	719	ASP	CB-CG-OD2	6.29	123.96	118.30
1	B	268	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	B	307	ASP	CB-CG-OD2	6.26	123.94	118.30
1	B	717	ASP	CB-CG-OD1	6.19	123.87	118.30
1	A	724	ASP	CB-CG-OD2	6.12	123.81	118.30
1	A	790	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	A	500	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	A	736	ASP	CB-CG-OD2	6.03	123.72	118.30
1	A	743	ASP	CB-CG-OD2	6.03	123.72	118.30
1	A	479	ASP	CB-CG-OD1	5.99	123.69	118.30
1	B	481	ASP	CB-CG-OD2	5.95	123.65	118.30
1	A	431	ASP	CB-CG-OD2	5.91	123.62	118.30
1	A	107	ASP	CB-CG-OD2	5.91	123.62	118.30
1	B	259	ASP	CB-CG-OD2	5.88	123.59	118.30
1	A	7	ASP	CB-CG-OD2	5.81	123.53	118.30
1	A	354	ARG	NE-CZ-NH2	-5.79	117.40	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	491	ASP	CB-CG-OD2	5.76	123.48	118.30
1	A	692	ASP	CB-CG-OD2	5.70	123.43	118.30
1	B	163	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	492	ASP	CB-CG-OD2	5.65	123.39	118.30
1	B	389	ASP	CB-CG-OD2	5.63	123.37	118.30
1	B	210	ARG	NE-CZ-NH2	5.62	123.11	120.30
1	A	474	LYS	CD-CE-NZ	5.57	124.51	111.70
1	A	562	ASP	CB-CG-OD2	5.56	123.31	118.30
1	A	259	ASP	CB-CG-OD2	5.54	123.29	118.30
1	A	423	LEU	CA-CB-CG	5.50	127.95	115.30
1	A	612	ASP	CB-CG-OD2	5.43	123.19	118.30
1	B	423	LEU	CA-CB-CG	5.40	127.71	115.30
1	B	330	ASP	CB-CG-OD2	5.38	123.14	118.30
1	B	356	ASP	CB-CG-OD2	5.38	123.14	118.30
1	B	562	ASP	CB-CG-OD2	5.36	123.13	118.30
1	B	235	ASP	CB-CG-OD2	5.34	123.10	118.30
1	B	66	MET	CG-SD-CE	-5.33	91.67	100.20
1	A	626	ASP	CB-CG-OD2	5.28	123.05	118.30
1	B	640	GLY	N-CA-C	-5.25	99.96	113.10
1	A	163	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	A	235	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	759	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	A	491	ASP	CB-CG-OD2	5.15	122.93	118.30
1	A	603	ASP	CB-CG-OD2	5.14	122.93	118.30
1	A	188	ASP	CB-CG-OD2	5.11	122.90	118.30
1	B	366	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	B	89	ASP	CB-CG-OD1	5.04	122.84	118.30
1	B	282	ASP	CB-CG-OD2	5.04	122.83	118.30
1	B	100	ASP	CB-CG-OD1	5.03	122.83	118.30
1	B	423	LEU	CB-CG-CD2	5.03	119.55	111.00
1	A	481	ASP	CB-CG-OD2	5.03	122.82	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	562	ASP	Peptide
1	B	559	PRO	Peptide

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	6332	41	0
1	B	6389	0	6333	58	0
2	A	45	0	39	3	0
2	B	45	0	39	4	0
3	A	5	0	0	7	0
3	B	5	0	0	8	0
4	A	15	0	6	0	0
4	B	15	0	7	1	0
5	A	8	0	12	1	0
5	B	8	0	12	1	0
6	A	339	0	0	9	0
6	B	293	0	0	6	0
All	All	13556	0	12780	112	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 (112) 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:348:MET:SD	1:B:348:MET:CE	2.02	1.47
1:B:557:GLU:O	1:B:558:ASN:HB2	1.76	0.86
1:B:347:LEU:O	1:B:348:MET:HB2	1.74	0.85
1:A:347:LEU:O	1:A:348:MET:HB2	1.82	0.77
1:B:295:HIS:CD2	1:B:296:GLU:HG3	2.22	0.74
2:A:997:GLC:H62	3:A:999:VO4:O3	1.87	0.73
1:B:97:ASN:HD21	1:B:99:THR:HB	1.54	0.72
1:B:729:SER:HB2	6:B:2164:HOH:O	1.89	0.71
3:B:1999:VO4:O1	3:B:1999:VO4:V	1.49	0.69
1:B:547:HIS:O	1:B:548:ILE:C	2.31	0.67
3:B:1999:VO4:O2	3:B:1999:VO4:V	1.51	0.67
3:A:999:VO4:V	3:A:999:VO4:O4	1.51	0.67
3:A:999:VO4:O1	3:A:999:VO4:V	1.50	0.67
3:B:1999:VO4:O3	3:B:1999:VO4:V	1.50	0.67
3:A:999:VO4:O3	3:A:999:VO4:V	1.50	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:997:GLC:H62	3:B:1999:VO4:O3	1.95	0.67
3:A:999:VO4:O2	3:A:999:VO4:V	1.53	0.64
1:A:97:ASN:HD21	1:A:99:THR:HB	1.61	0.64
3:B:1999:VO4:O4	3:B:1999:VO4:V	1.54	0.64
1:B:97:ASN:HD22	1:B:100:ASP:H	1.46	0.63
1:A:531:GLN:HE22	1:A:541:GLN:HA	1.64	0.63
1:A:97:ASN:HD22	1:A:100:ASP:H	1.47	0.62
1:B:79:LEU:HD11	1:B:458:LYS:HG2	1.82	0.61
1:A:79:LEU:HD11	1:A:458:LYS:HG2	1.85	0.59
1:B:459:GLN:NE2	6:B:2274:HOH:O	2.36	0.58
1:A:606:LYS:HG3	6:A:1122:HOH:O	2.04	0.58
1:A:270:MET:HG2	1:A:363:LEU:HD21	1.86	0.57
3:B:1999:VO4:O1	5:B:1990:TRS:H31	2.05	0.57
1:A:66:MET:HG3	1:A:309:HIS:CB	2.35	0.56
1:B:533:LYS:HB2	6:B:2223:HOH:O	2.05	0.56
1:A:423:LEU:HD13	6:A:1264:HOH:O	2.05	0.56
1:B:530:ILE:HD12	1:B:625:ALA:HB2	1.87	0.56
1:B:97:ASN:ND2	1:B:99:THR:HB	2.20	0.55
1:B:423:LEU:HD13	6:B:2257:HOH:O	2.05	0.55
1:B:66:MET:HG3	1:B:309:HIS:HB3	1.89	0.55
1:A:97:ASN:ND2	1:A:99:THR:HB	2.21	0.54
1:B:66:MET:HG3	1:B:309:HIS:CB	2.38	0.54
1:A:728:HIS:HB3	1:A:733:GLN:HB2	1.89	0.54
1:A:246:ILE:HD13	1:B:239:LEU:HD12	1.89	0.53
1:B:270:MET:HG2	1:B:363:LEU:HD21	1.90	0.53
1:B:531:GLN:HE22	1:B:541:GLN:HA	1.74	0.53
1:B:115:LEU:H	2:B:997:GLC:H61	1.74	0.53
1:A:723:PHE:HB2	1:A:727:LEU:HD22	1.91	0.53
1:B:112:ASN:HD22	2:B:996:GLC:H61	1.74	0.52
1:B:558:ASN:H	1:B:559:PRO:HD3	1.75	0.52
1:B:639:SER:OG	1:B:640:GLY:N	2.40	0.52
1:A:9:GLN:HG3	6:A:1239:HOH:O	2.10	0.51
1:A:670:GLU:HB3	6:A:1321:HOH:O	2.10	0.51
1:A:115:LEU:H	2:A:997:GLC:H61	1.75	0.50
1:A:309:HIS:N	1:A:310:PRO:CD	2.74	0.50
1:A:724:ASP:HB2	6:A:1290:HOH:O	2.11	0.50
1:B:728:HIS:HB3	1:B:733:GLN:HB2	1.93	0.50
1:A:21:TYR:O	1:B:172:ASN:HB2	2.10	0.50
1:A:246:ILE:HD13	1:B:239:LEU:CD1	2.41	0.50
1:B:115:LEU:HB2	2:B:997:GLC:H4	1.93	0.49
1:A:329:TRP:CZ3	1:A:373:GLU:HG2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:723:PHE:HB2	1:B:727:LEU:HD22	1.93	0.49
1:A:691:TYR:CE2	1:A:739:LEU:HD22	2.47	0.49
1:B:560:GLN:HB3	6:B:2283:HOH:O	2.12	0.49
1:B:97:ASN:ND2	1:B:100:ASP:H	2.10	0.49
1:B:667:LYS:HE2	1:B:777:MET:SD	2.53	0.48
1:B:220:TRP:CD2	1:B:278:CYS:HB3	2.49	0.48
1:B:35:TRP:CZ2	1:B:105:GLU:HG3	2.49	0.48
1:B:43:ALA:O	1:B:47:ARG:HG3	2.14	0.48
1:B:659:GLY:O	6:B:2130:HOH:O	2.20	0.47
1:B:529:ASP:OD1	1:B:629:GLU:OE2	2.32	0.47
1:B:676:PHE:CE2	1:B:747:TYR:HB2	2.49	0.47
1:A:346:THR:HG23	6:A:1313:HOH:O	2.14	0.47
1:A:47:ARG:HD2	1:A:170:ARG:HD3	1.97	0.47
1:A:488:LYS:HG2	6:A:1270:HOH:O	2.15	0.47
1:B:492:ASP:OD1	1:B:492:ASP:C	2.54	0.46
1:B:354:ARG:HD2	1:B:403:GLN:NE2	2.30	0.46
1:B:185:VAL:HG23	1:B:365:PRO:HB2	1.97	0.46
3:A:999:VO4:O2	3:A:999:VO4:O4	2.33	0.46
1:A:66:MET:HG3	1:A:309:HIS:HB3	1.99	0.45
1:B:266:LYS:HG3	1:B:359:LEU:HD11	1.97	0.45
1:B:47:ARG:HD2	1:B:170:ARG:HD3	1.98	0.45
1:B:645:LYS:NZ	4:B:900:PLP:O3	2.49	0.44
1:A:7:ASP:O	1:A:11:GLN:HG2	2.17	0.44
1:A:97:ASN:ND2	1:A:100:ASP:H	2.14	0.44
1:B:591:VAL:O	1:B:592:ALA:C	2.55	0.44
3:B:1999:VO4:O4	3:B:1999:VO4:O2	2.36	0.44
1:A:601:VAL:O	1:A:604:LYS:HB2	2.18	0.44
1:B:309:HIS:N	1:B:310:PRO:CD	2.80	0.43
1:A:536:HIS:HB3	1:A:539:LYS:HG2	1.98	0.43
1:A:53:LYS:HE3	1:A:53:LYS:HB3	1.87	0.43
1:A:354:ARG:HD2	1:A:403:GLN:NE2	2.34	0.43
1:B:557:GLU:O	1:B:558:ASN:CB	2.54	0.43
1:A:529:ASP:OD1	1:A:629:GLU:OE2	2.36	0.43
5:A:990:TRS:H32	6:A:1108:HOH:O	2.18	0.43
1:B:270:MET:CG	1:B:363:LEU:HD21	2.48	0.43
1:B:295:HIS:CD2	1:B:296:GLU:CG	3.00	0.42
1:B:451:ILE:HG21	1:B:645:LYS:HG3	2.00	0.42
1:B:601:VAL:O	1:B:604:LYS:HB2	2.19	0.42
3:A:999:VO4:O3	3:A:999:VO4:O4	2.37	0.42
3:B:1999:VO4:O4	3:B:1999:VO4:O3	2.37	0.42
1:A:250:LYS:NZ	6:A:1085:HOH:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:536:HIS:HB3	1:B:539:LYS:HG2	2.02	0.42
1:A:544:ASN:HD22	1:A:544:ASN:C	2.22	0.42
1:A:536:HIS:HD1	1:A:538:TYR:H	1.68	0.41
1:B:53:LYS:HE3	1:B:53:LYS:HB3	1.83	0.41
1:B:6:ASN:HB3	1:B:9:GLN:HE21	1.85	0.41
1:B:287:HIS:CE1	1:B:297:LEU:HA	2.56	0.41
1:A:692:ASP:HA	1:A:693:PRO:HD2	1.92	0.41
1:A:270:MET:CG	1:A:363:LEU:HD21	2.51	0.41
1:B:309:HIS:HB2	1:B:310:PRO:HD3	2.03	0.41
1:A:590:LYS:HD2	1:A:590:LYS:HA	1.97	0.41
1:B:84:TYR:CD1	1:B:84:TYR:C	2.94	0.41
1:A:115:LEU:HB2	2:A:997:GLC:H4	2.03	0.40
1:B:590:LYS:HD2	1:B:590:LYS:HA	1.84	0.40
1:B:266:LYS:O	1:B:270:MET:HG3	2.22	0.40
1:A:551:LEU:O	1:A:555:ILE:HG23	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%)	772 (97%)	21 (3%)	1 (0%)	56	57
1	B	794/796 (100%)	758 (96%)	32 (4%)	4 (0%)	34	26
All	All	1588/1592 (100%)	1530 (96%)	53 (3%)	5 (0%)	46	42

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	449	ASN
1	B	558	ASN
1	B	348	MET

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Mol	Chain	Res	Type
1	A	348	MET
1	B	639	SER

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%)	626 (94%)	41 (6%)	23	17
1	B	667/667 (100%)	623 (93%)	44 (7%)	21	14
All	All	1334/1334 (100%)	1249 (94%)	85 (6%)	22	15

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LYS
1	A	66	MET
1	A	97	ASN
1	A	139	ASN
1	A	165	ASN
1	A	181	ILE
1	A	194	GLU
1	A	237	ASP
1	A	346	THR
1	A	347	LEU
1	A	350	GLU
1	A	391	LYS
1	A	392	VAL
1	A	402	LYS
1	A	423	LEU
1	A	426	ASP
1	A	427	LEU
1	A	429	VAL
1	A	454	ARG
1	A	458	LYS
1	A	494	LYS

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Mol	Chain	Res	Type
1	A	515	LYS
1	A	533	LYS
1	A	535	LEU
1	A	542	HIS
1	A	544	ASN
1	A	555	ILE
1	A	564	VAL
1	A	600	LEU
1	A	609	PHE
1	A	643	ASN
1	A	663	GLU
1	A	670	GLU
1	A	727	LEU
1	A	732	LYS
1	A	739	LEU
1	A	749	GLU
1	A	755	ASP
1	A	785	ARG
1	A	795	LYS
1	A	796	ARG
1	B	8	LYS
1	B	92	LYS
1	B	107	ASP
1	B	165	ASN
1	B	181	ILE
1	B	188	ASP
1	B	190	ARG
1	B	194	GLU
1	B	237	ASP
1	B	346	THR
1	B	347	LEU
1	B	391	LYS
1	B	392	VAL
1	B	402	LYS
1	B	423	LEU
1	B	426	ASP
1	B	427	LEU
1	B	429	VAL
1	B	458	LYS
1	B	494	LYS
1	B	515	LYS
1	B	533	LYS

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Mol	Chain	Res	Type
1	B	535	LEU
1	B	542	HIS
1	B	544	ASN
1	B	555	ILE
1	B	560	GLN
1	B	564	VAL
1	B	578	TYR
1	B	600	LEU
1	B	609	PHE
1	B	643	ASN
1	B	663	GLU
1	B	670	GLU
1	B	712	SER
1	B	717	ASP
1	B	727	LEU
1	B	732	LYS
1	B	739	LEU
1	B	749	GLU
1	B	755	ASP
1	B	785	ARG
1	B	795	LYS
1	B	796	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	9	GLN
1	A	97	ASN
1	A	112	ASN
1	A	139	ASN
1	A	221	GLN
1	A	260	ASN
1	A	403	GLN
1	A	446	ASN
1	A	459	GLN
1	A	498	GLN
1	A	531	GLN
1	A	544	ASN
1	B	9	GLN
1	B	97	ASN
1	B	112	ASN

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Mol	Chain	Res	Type
1	B	139	ASN
1	B	178	GLN
1	B	221	GLN
1	B	260	ASN
1	B	295	HIS
1	B	403	GLN
1	B	446	ASN
1	B	504	GLN
1	B	531	GLN
1	B	544	ASN
1	B	678	HIS

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 ⓘ

8 carbohydrates 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	BGC	A	994	2	12,12,12	0.70	0	17,17,17	1.41	3 (17%)
2	GLC	A	995	2	11,11,12	0.86	0	14,15,17	1.89	5 (35%)
2	GLC	A	996	2	11,11,12	0.73	0	14,15,17	1.19	1 (7%)
2	GLC	A	997	2	11,11,12	0.99	1 (9%)	14,15,17	2.50	4 (28%)
2	BGC	B	994	2	12,12,12	0.62	0	17,17,17	1.70	7 (41%)
2	GLC	B	995	2	11,11,12	1.12	1 (9%)	14,15,17	1.89	4 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	B	996	2	11,11,12	0.77	0	14,15,17	1.50	3 (21%)
2	GLC	B	997	2	11,11,12	0.92	1 (9%)	14,15,17	2.42	5 (35%)

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	BGC	A	994	2	-	0/2/22/22	0/1/1/1
2	GLC	A	995	2	-	0/2/19/22	0/1/1/1
2	GLC	A	996	2	-	0/2/19/22	0/1/1/1
2	GLC	A	997	2	-	0/2/19/22	0/1/1/1
2	BGC	B	994	2	-	0/2/22/22	0/1/1/1
2	GLC	B	995	2	-	0/2/19/22	0/1/1/1
2	GLC	B	996	2	-	0/2/19/22	0/1/1/1
2	GLC	B	997	2	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	997	GLC	C2-C3	2.17	1.55	1.52
2	B	995	GLC	C4-C5	2.30	1.58	1.53
2	A	997	GLC	C2-C3	2.77	1.56	1.52

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	996	GLC	O2-C2-C1	-2.48	104.24	109.21
2	A	994	BGC	C1-O5-C5	-2.42	109.00	113.47
2	B	994	BGC	O2-C2-C3	-2.38	104.98	110.34
2	B	995	GLC	C2-C3-C4	-2.31	107.11	111.04
2	A	994	BGC	O2-C2-C3	-2.25	105.26	110.34
2	B	994	BGC	O5-C1-C2	-2.24	106.22	109.80
2	A	995	GLC	C2-C3-C4	-2.23	107.26	111.04
2	B	994	BGC	C1-O5-C5	-2.11	109.58	113.47
2	B	995	GLC	O5-C1-C2	2.04	114.16	110.86
2	A	995	GLC	C1-C2-C3	2.09	112.01	109.54
2	B	994	BGC	O1-C1-C2	2.09	114.81	109.21
2	B	994	BGC	O5-C5-C4	2.12	113.66	109.68
2	A	997	GLC	C1-C2-C3	2.20	112.15	109.54
2	A	995	GLC	O3-C3-C2	2.21	114.00	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	995	GLC	O2-C2-C3	2.25	114.64	110.12
2	B	996	GLC	O3-C3-C2	2.29	114.13	110.00
2	B	997	GLC	O6-C6-C5	2.29	118.89	111.33
2	B	997	GLC	O2-C2-C3	2.34	114.82	110.12
2	B	997	GLC	C1-C2-C3	2.34	112.31	109.54
2	B	994	BGC	O2-C2-C1	2.63	115.61	109.82
2	B	997	GLC	O5-C1-C2	2.79	115.38	110.86
2	A	994	BGC	C3-C4-C5	2.87	115.20	110.20
2	B	996	GLC	O2-C2-C3	2.88	115.91	110.12
2	A	997	GLC	O5-C1-C2	2.89	115.55	110.86
2	A	996	GLC	C1-C2-C3	2.94	113.02	109.54
2	B	995	GLC	O3-C3-C2	2.98	115.37	110.00
2	B	994	BGC	C3-C4-C5	3.33	116.00	110.20
2	A	997	GLC	O2-C2-C3	3.96	118.07	110.12
2	B	995	GLC	C1-O5-C5	5.06	118.67	112.25
2	A	995	GLC	C1-O5-C5	5.14	118.78	112.25
2	A	997	GLC	C1-O5-C5	6.99	121.12	112.25
2	B	997	GLC	C1-O5-C5	7.21	121.40	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	997	GLC	3	0
2	B	996	GLC	1	0
2	B	997	GLC	3	0

5.6 Ligand geometry

6 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	PLP	A	900	1	15,15,16	1.28	3 (20%)	21,22,23	1.49	4 (19%)
5	TRS	A	990	-	7,7,7	1.37	1 (14%)	9,9,9	2.23	4 (44%)
3	VO4	A	999	-	1,4,4	1.96	0	0,6,6	0.00	-
5	TRS	B	1990	-	7,7,7	0.73	0	9,9,9	2.43	4 (44%)
3	VO4	B	1999	-	1,4,4	2.01	1 (100%)	0,6,6	0.00	-
4	PLP	B	900	1	15,15,16	1.19	2 (13%)	21,22,23	1.21	3 (14%)

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	PLP	A	900	1	-	0/6/6/8	0/1/1/1
5	TRS	A	990	-	-	0/9/9/9	0/0/0/0
3	VO4	A	999	-	-	0/0/0/0	0/0/0/0
5	TRS	B	1990	-	-	0/9/9/9	0/0/0/0
3	VO4	B	1999	-	-	0/0/0/0	0/0/0/0
4	PLP	B	900	1	-	0/6/6/8	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	990	TRS	C-N	-3.11	1.46	1.50
4	A	900	PLP	O3-C3	-2.20	1.31	1.37
3	B	1999	VO4	O1-V	-2.01	1.49	1.63
4	B	900	PLP	P-O2P	-2.01	1.47	1.54
4	B	900	PLP	C2-N1	2.23	1.38	1.34
4	A	900	PLP	C2-N1	2.36	1.39	1.34
4	A	900	PLP	C6-N1	2.50	1.39	1.34

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1990	TRS	O3-C3-C	-4.94	101.18	111.18
5	A	990	TRS	O3-C3-C	-3.92	103.26	111.18
5	A	990	TRS	O2-C2-C	-2.86	105.40	111.18
5	A	990	TRS	O1-C1-C	-2.81	105.49	111.18
4	A	900	PLP	C4A-C4-C3	-2.59	115.67	120.36
4	B	900	PLP	C4A-C4-C3	-2.27	116.25	120.36
5	B	1990	TRS	O2-C2-C	-2.12	106.89	111.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1990	TRS	O1-C1-C	-2.08	106.98	111.18
4	B	900	PLP	O3-C3-C2	2.03	121.19	117.66
4	A	900	PLP	O2P-P-O1P	2.07	117.23	110.58
4	A	900	PLP	C2A-C2-N1	2.26	122.95	117.95
4	A	900	PLP	C4A-C4-C5	2.83	123.83	120.88
5	A	990	TRS	C1-C-N	3.05	113.63	108.09
4	B	900	PLP	C3-C4-C5	3.12	122.19	118.78
5	B	1990	TRS	C1-C-N	3.82	115.04	108.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	990	TRS	1	0
3	A	999	VO4	7	0
5	B	1990	TRS	1	0
3	B	1999	VO4	8	0
4	B	900	PLP	1	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, 95th 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 ²)	Q<0.9
1	A	796/796 (100%)	0.14	35 (4%)	38 49	22, 37, 59, 74	0
1	B	796/796 (100%)	0.21	51 (6%)	23 32	22, 37, 60, 76	0
All	All	1592/1592 (100%)	0.17	86 (5%)	29 40	22, 37, 60, 76	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	559	PRO	5.6
1	B	562	ASP	5.4
1	B	560	GLN	5.0
1	B	702	VAL	4.8
1	B	561	ALA	4.8
1	A	351	ALA	4.1
1	B	599	PRO	3.9
1	B	689	LYS	3.8
1	A	262	PHE	3.8
1	A	423	LEU	3.7
1	B	187	LYS	3.6
1	B	579	TYR	3.5
1	A	57	ASN	3.4
1	B	190	ARG	3.4
1	B	717	ASP	3.4
1	B	391	LYS	3.4
1	B	188	ASP	3.2
1	A	559	PRO	3.2
1	B	521	GLU	3.1
1	B	687	LEU	3.1
1	B	597	ASN	3.0
1	B	718	GLY	3.0
1	A	390	GLU	3.0
1	B	53	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	600	LEU	2.9
1	A	732	LYS	2.9
1	B	50	PRO	2.9
1	B	721	HIS	2.8
1	A	545	LEU	2.8
1	A	710	LEU	2.8
1	B	57	ASN	2.8
1	A	546	LEU	2.7
1	B	1	SER	2.7
1	A	688	ALA	2.7
1	A	260	ASN	2.7
1	B	289	LEU	2.7
1	B	388	GLY	2.7
1	A	51	PHE	2.7
1	B	2	GLN	2.6
1	A	348	MET	2.6
1	B	51	PHE	2.6
1	A	772	THR	2.6
1	A	441	PRO	2.6
1	A	442	ASN	2.5
1	B	732	LYS	2.5
1	A	599	PRO	2.5
1	A	289	LEU	2.5
1	B	497	GLN	2.5
1	B	56	ALA	2.4
1	A	648	LEU	2.4
1	B	595	ILE	2.4
1	B	603	ASP	2.4
1	A	382	VAL	2.4
1	B	350	GLU	2.4
1	A	387	PRO	2.3
1	A	56	ALA	2.3
1	B	351	ALA	2.3
1	B	648	LEU	2.3
1	A	426	ASP	2.3
1	B	602	GLY	2.3
1	A	733	GLN	2.3
1	A	740	VAL	2.2
1	A	473	GLN	2.2
1	B	186	THR	2.2
1	B	691	TYR	2.2
1	B	685	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	688	ALA	2.2
1	A	730	ILE	2.1
1	B	390	GLU	2.1
1	B	769	ILE	2.1
1	B	347	LEU	2.1
1	B	745	ALA	2.1
1	B	759	ARG	2.1
1	A	698	LYS	2.1
1	B	151	ASP	2.1
1	A	402	LYS	2.1
1	A	769	ILE	2.1
1	B	349	PRO	2.1
1	A	795	LYS	2.1
1	B	701	LYS	2.1
1	B	712	SER	2.1
1	A	430	LYS	2.0
1	B	150	VAL	2.0
1	A	386	TRP	2.0
1	A	670	GLU	2.0
1	B	593	ASP	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](#)

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, 95th 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 ²)	Q<0.9
2	GLC	B	997	11/12	0.51	0.39	18.74	73,77,79,79	0
2	GLC	A	997	11/12	0.67	0.28	10.08	73,77,78,78	0
2	GLC	B	995	11/12	0.58	0.41	4.97	74,76,77,77	0
2	GLC	B	996	11/12	0.81	0.19	4.77	71,73,75,77	0
2	GLC	A	996	11/12	0.84	0.16	1.64	70,73,75,77	0
2	GLC	A	995	11/12	0.57	0.24	1.49	73,76,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	BGC	A	994	12/12	0.83	0.19	-	77,79,79,81	0
2	BGC	B	994	12/12	0.80	0.38	-	77,79,80,81	0

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, 95th 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(\AA^2)	Q<0.9
3	VO4	A	999	5/5	0.91	0.23	9.33	75,75,77,82	0
3	VO4	B	1999	5/5	0.88	0.29	9.09	75,76,77,83	0
5	TRS	A	990	8/8	0.87	0.19	4.23	47,49,50,55	0
5	TRS	B	1990	8/8	0.89	0.17	2.12	48,49,50,53	0
4	PLP	B	900	15/16	0.96	0.09	-0.83	25,29,40,42	0
4	PLP	A	900	15/16	0.97	0.08	-2.27	20,26,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.