



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:08 PM UTC

PDB ID : 3AFJ / pdb_00003afj
Title : Crystal Structure of Cellvibrio gilvus Cellobiose Phosphorylase triple mutant
Authors : Hidaka, M.; Ogawa, N.; Fushinobu, S.
Deposited on : 2010-03-04
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

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>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

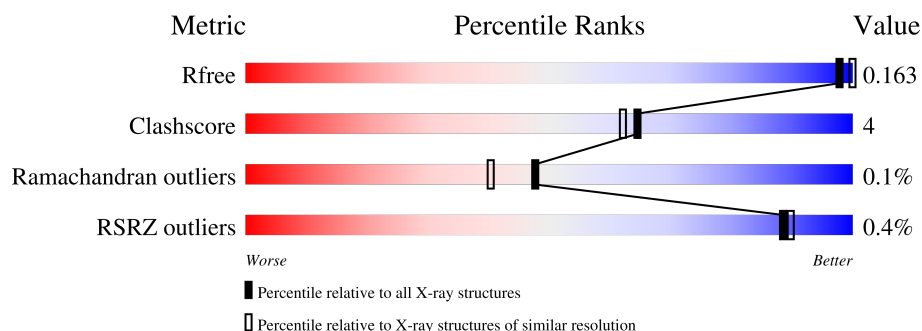
1 Overall quality at a glance

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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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 ≥ 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	842	
1	B	842	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15056 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 Cellobiose Phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	822	Total	C	N	O	S	0	0	0
			6424	4065	1100	1245	14			
1	B	822	Total	C	N	O	S	0	0	0
			6424	4065	1100	1245	14			

There are 46 discrepancies between the modelled and reference sequences:

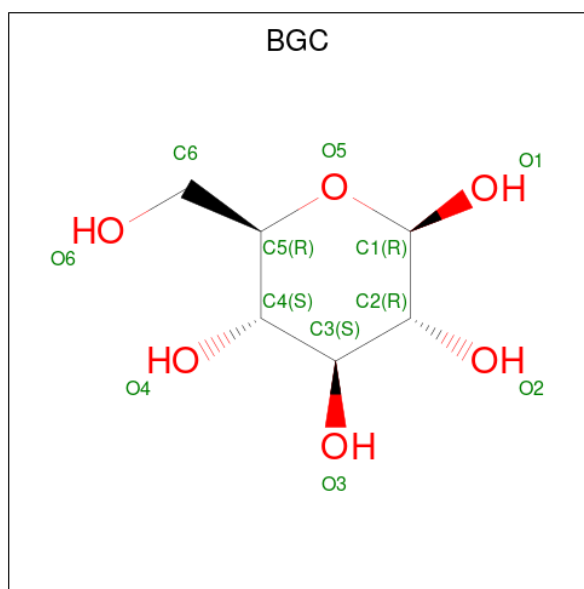
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP O66264
A	-18	GLY	-	expression tag	UNP O66264
A	-17	SER	-	expression tag	UNP O66264
A	-16	SER	-	expression tag	UNP O66264
A	-15	HIS	-	expression tag	UNP O66264
A	-14	HIS	-	expression tag	UNP O66264
A	-13	HIS	-	expression tag	UNP O66264
A	-12	HIS	-	expression tag	UNP O66264
A	-11	HIS	-	expression tag	UNP O66264
A	-10	HIS	-	expression tag	UNP O66264
A	-9	SER	-	expression tag	UNP O66264
A	-8	SER	-	expression tag	UNP O66264
A	-7	GLY	-	expression tag	UNP O66264
A	-6	LEU	-	expression tag	UNP O66264
A	-5	VAL	-	expression tag	UNP O66264
A	-4	PRO	-	expression tag	UNP O66264
A	-3	ARG	-	expression tag	UNP O66264
A	-2	GLY	-	expression tag	UNP O66264
A	-1	SER	-	expression tag	UNP O66264
A	0	HIS	-	expression tag	UNP O66264
A	508	ILE	THR	engineered mutation	UNP O66264
A	666	ASN	HIS	engineered mutation	UNP O66264
A	667	ALA	ASN	engineered mutation	UNP O66264
B	-19	MET	-	expression tag	UNP O66264
B	-18	GLY	-	expression tag	UNP O66264

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	SER	-	expression tag	UNP O66264
B	-16	SER	-	expression tag	UNP O66264
B	-15	HIS	-	expression tag	UNP O66264
B	-14	HIS	-	expression tag	UNP O66264
B	-13	HIS	-	expression tag	UNP O66264
B	-12	HIS	-	expression tag	UNP O66264
B	-11	HIS	-	expression tag	UNP O66264
B	-10	HIS	-	expression tag	UNP O66264
B	-9	SER	-	expression tag	UNP O66264
B	-8	SER	-	expression tag	UNP O66264
B	-7	GLY	-	expression tag	UNP O66264
B	-6	LEU	-	expression tag	UNP O66264
B	-5	VAL	-	expression tag	UNP O66264
B	-4	PRO	-	expression tag	UNP O66264
B	-3	ARG	-	expression tag	UNP O66264
B	-2	GLY	-	expression tag	UNP O66264
B	-1	SER	-	expression tag	UNP O66264
B	0	HIS	-	expression tag	UNP O66264
B	508	ILE	THR	engineered mutation	UNP O66264
B	666	ASN	HIS	engineered mutation	UNP O66264
B	667	ALA	ASN	engineered mutation	UNP O66264

- Molecule 2 is beta-D-glucopyranose (CCD ID: BGC) (formula: C₆H₁₂O₆).



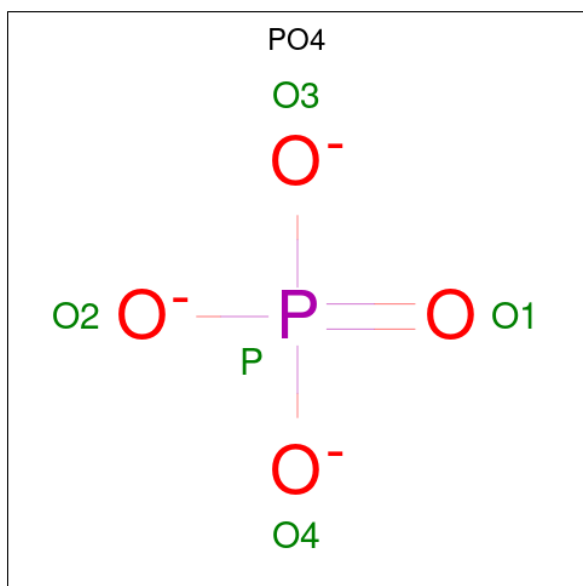
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		

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

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 5 is water.

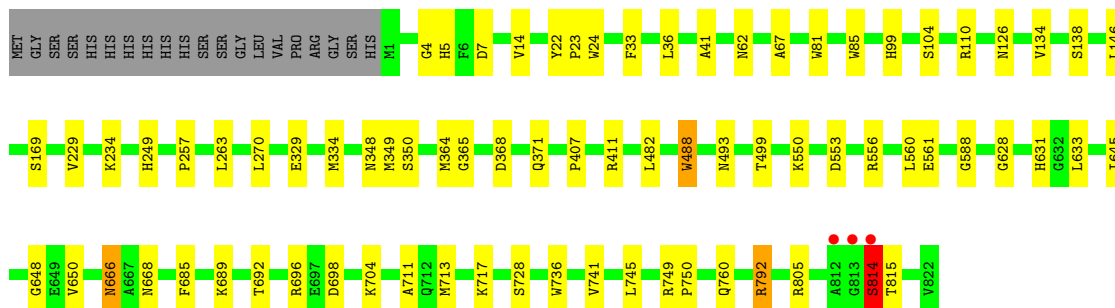
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1047	Total	O	0	0
			1047	1047		
5	B	1125	Total	O	0	0
			1125	1125		

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.

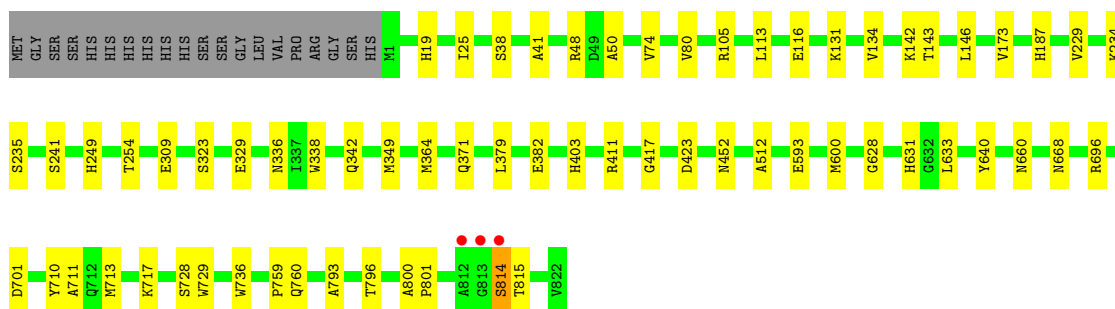
• Molecule 1: Cellobiose Phosphorylase

Chain A: 



• Molecule 1: Cellobiose Phosphorylase

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.14Å 97.96Å 104.23Å 90.00° 102.67° 90.00°	Depositor
Resolution (Å)	27.87 – 1.90 27.87 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (27.87-1.90) 99.6 (27.87-1.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.15 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.133 , 0.186 (Not available) , 0.163	Depositor DCC
R_{free} test set	6513 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	11.0	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15056	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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, 0.333 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: K, PO4, BGC

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	1.32	10/6599 (0.2%)	1.11	7/9002 (0.1%)
1	B	1.32	11/6599 (0.2%)	1.11	6/9002 (0.1%)
All	All	1.32	21/13198 (0.2%)	1.11	13/18004 (0.1%)

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 (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	229	VAL	CA-CB	8.05	1.58	1.54
1	A	229	VAL	CA-CB	7.84	1.58	1.54
1	A	814	SER	C-O	7.58	1.33	1.23
1	B	349	MET	SD-CE	-6.27	1.63	1.79
1	A	41	ALA	CA-CB	6.17	1.63	1.53
1	A	349	MET	SD-CE	-5.85	1.65	1.79
1	B	235	SER	N-CA	5.81	1.53	1.45
1	B	173	VAL	N-CA	5.71	1.52	1.46
1	A	650	VAL	CA-CB	5.59	1.60	1.54
1	B	379	LEU	CA-C	-5.59	1.46	1.52
1	B	41	ALA	CA-CB	5.51	1.61	1.53
1	B	241	SER	CA-C	5.40	1.58	1.53
1	A	7	ASP	C-O	5.38	1.29	1.23
1	A	588	GLY	C-O	-5.24	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	131	LYS	C-O	5.17	1.30	1.24
1	B	512	ALA	CA-CB	5.15	1.61	1.53
1	A	350	SER	C-O	-5.12	1.19	1.24
1	A	270	LEU	CA-C	-5.12	1.46	1.52
1	A	488	TRP	CA-CB	5.09	1.61	1.53
1	B	50	ALA	CA-CB	5.05	1.62	1.53
1	B	417	GLY	C-O	5.00	1.28	1.23

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	815	THR	N-CA-CB	6.10	120.36	110.42
1	B	336	ASN	N-CA-C	6.00	118.78	111.82
1	B	593	GLU	CA-C-N	-5.86	113.64	119.56
1	B	593	GLU	C-N-CA	-5.86	113.64	119.56
1	B	815	THR	N-CA-CB	5.75	119.58	110.55
1	A	666	ASN	N-CA-C	-5.54	105.39	111.82
1	A	348	ASN	N-CA-C	5.52	117.38	111.36
1	A	792	ARG	CG-CD-NE	-5.48	99.94	112.00
1	B	713	MET	CA-CB-CG	5.41	124.93	114.10
1	A	36	LEU	N-CA-C	-5.34	100.03	108.73
1	B	338	TRP	CA-CB-CG	-5.17	103.78	113.60
1	A	169	SER	CA-C-N	-5.00	115.86	122.16
1	A	169	SER	C-N-CA	-5.00	115.86	122.16

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	814	SER	Peptide
1	B	814	SER	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	6424	0	6073	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	6424	0	6073	45	0
2	A	12	0	12	0	0
2	B	12	0	12	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	1047	0	0	20	0
5	B	1125	0	0	21	0
All	All	15056	0	12170	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)
1:A:717:LYS:HE3	5:A:1031:HOH:O	1.37	1.25
1:B:814:SER:HA	5:B:983:HOH:O	1.44	1.16
1:A:560:LEU:HD12	5:A:970:HOH:O	1.63	0.95
1:B:640:TYR:H	1:B:660:ASN:HD21	1.16	0.88
1:B:403:HIS:HD2	1:B:423:ASP:OD2	1.57	0.87
1:B:633:LEU:H	1:B:668:ASN:HD21	1.23	0.86
1:B:631:HIS:HD2	1:B:696:ARG:HH12	1.23	0.86
1:A:633:LEU:H	1:A:668:ASN:HD21	1.24	0.86
1:A:631:HIS:HD2	1:A:696:ARG:HH12	1.23	0.84
1:A:329:GLU:HG3	5:A:2138:HOH:O	1.79	0.81
1:A:561:GLU:HG3	5:A:1877:HOH:O	1.79	0.79
1:B:48:ARG:HD2	5:B:1424:HOH:O	1.83	0.77
1:B:342:GLN:HE22	1:B:710:TYR:H	1.31	0.76
1:B:382:GLU:HG3	5:B:1712:HOH:O	1.86	0.76
1:B:631:HIS:CD2	1:B:696:ARG:HH12	2.05	0.75
1:B:371:GLN:HE21	1:B:736:TRP:HE1	1.37	0.73
1:A:499:THR:HG22	1:A:645:ILE:CD1	2.19	0.73
1:A:371:GLN:HE21	1:A:736:TRP:HE1	1.38	0.71
1:B:309:GLU:HG2	5:B:1550:HOH:O	1.90	0.71
1:A:814:SER:HA	5:A:1448:HOH:O	1.91	0.70
1:A:631:HIS:CD2	1:A:696:ARG:HH12	2.09	0.67
1:A:134:VAL:HG21	1:A:146:LEU:HD11	1.78	0.66
1:A:249:HIS:HD2	5:A:837:HOH:O	1.79	0.65
1:B:411:ARG:HE	1:B:452:ASN:ND2	1.94	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:382:GLU:CG	5:B:1712:HOH:O	2.43	0.63
1:B:187:HIS:HD2	5:B:911:HOH:O	1.83	0.61
1:B:701:ASP:HB2	5:B:876:HOH:O	2.00	0.61
1:B:329:GLU:CG	5:B:2066:HOH:O	2.49	0.60
1:B:249:HIS:HD2	5:B:825:HOH:O	1.85	0.60
1:B:249:HIS:HE1	5:B:888:HOH:O	1.84	0.59
1:A:628:GLY:HA2	1:A:633:LEU:HD23	1.83	0.59
1:B:800:ALA:HB3	5:B:1317:HOH:O	2.02	0.59
1:A:499:THR:CG2	1:A:645:ILE:CD1	2.81	0.59
1:A:493:ASN:HB2	1:A:648:GLY:HA3	1.84	0.59
1:A:234:LYS:HD2	5:A:1331:HOH:O	2.03	0.58
1:A:99:HIS:HD2	1:A:104:SER:OG	1.87	0.57
1:A:329:GLU:CG	5:A:2138:HOH:O	2.44	0.56
1:A:698:ASP:CB	5:A:1259:HOH:O	2.53	0.56
1:B:48:ARG:CD	5:B:1424:HOH:O	2.47	0.56
1:B:600:MET:HE3	5:B:2065:HOH:O	2.05	0.55
1:A:704:LYS:HD3	5:A:2068:HOH:O	2.05	0.55
1:B:403:HIS:HE1	5:B:1164:HOH:O	1.88	0.54
1:B:329:GLU:HG2	5:B:2066:HOH:O	2.07	0.54
1:B:717:LYS:HE3	5:B:1862:HOH:O	2.07	0.54
1:A:698:ASP:HB2	5:A:1259:HOH:O	2.07	0.54
1:B:19:HIS:HD2	5:B:969:HOH:O	1.90	0.54
1:A:249:HIS:HE1	5:A:849:HOH:O	1.92	0.53
1:B:134:VAL:HG21	1:B:146:LEU:HD11	1.90	0.52
1:A:411:ARG:NH2	5:A:2137:HOH:O	2.42	0.52
1:A:62:ASN:ND2	1:A:67:ALA:HB3	2.24	0.51
1:B:113:LEU:HG	1:B:142:LYS:HE2	1.92	0.51
1:A:5:HIS:HD2	5:A:1097:HOH:O	1.94	0.50
1:B:382:GLU:CD	5:B:1712:HOH:O	2.54	0.50
1:A:24:TRP:O	1:A:99:HIS:HE1	1.94	0.50
1:A:81:TRP:CG	1:A:110:ARG:HD3	2.47	0.49
1:A:263:LEU:HD23	5:A:1107:HOH:O	2.13	0.49
1:A:371:GLN:HE21	1:A:736:TRP:NE1	2.10	0.48
1:A:22:TYR:CG	1:A:23:PRO:HD2	2.48	0.48
1:B:371:GLN:HE21	1:B:736:TRP:NE1	2.06	0.47
1:A:550:LYS:HE2	1:A:550:LYS:HB3	1.76	0.47
1:B:640:TYR:N	1:B:660:ASN:HD21	1.98	0.46
1:A:33:PHE:HB2	1:A:126:ASN:HD22	1.81	0.46
1:A:713:MET:HB2	1:A:713:MET:HE3	1.57	0.46
1:B:105:ARG:HD3	1:B:116:GLU:OE2	2.16	0.46
1:B:711:ALA:HA	1:B:728:SER:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:711:ALA:HA	1:A:728:SER:HA	1.97	0.45
1:A:334:MET:HG3	1:A:692:THR:CG2	2.46	0.45
1:A:499:THR:HG22	1:A:645:ILE:HD13	1.97	0.45
1:B:234:LYS:HD2	5:B:1944:HOH:O	2.16	0.45
1:A:749:ARG:HA	1:A:750:PRO:HD3	1.81	0.45
1:A:488:TRP:HE1	1:A:666:ASN:ND2	2.16	0.44
1:A:556:ARG:HD3	5:A:1747:HOH:O	2.18	0.44
1:B:628:GLY:HA2	1:B:633:LEU:HD23	2.00	0.44
1:B:364:MET:HA	1:B:364:MET:HE2	2.00	0.43
1:A:364:MET:HG2	1:A:407:PRO:HG3	1.99	0.43
1:B:631:HIS:HD2	1:B:696:ARG:NH1	2.03	0.43
1:B:323:SER:HB3	5:B:1131:HOH:O	2.19	0.43
1:A:760:GLN:NE2	5:A:1227:HOH:O	2.51	0.43
1:A:550:LYS:NZ	5:A:1970:HOH:O	2.52	0.42
1:B:760:GLN:NE2	5:B:1660:HOH:O	2.52	0.42
1:A:553:ASP:OD1	1:A:556:ARG:NH2	2.53	0.42
1:B:143:THR:HG22	1:B:254:THR:HG22	2.02	0.42
1:B:728:SER:O	1:B:729:TRP:HB2	2.20	0.42
1:B:759:PRO:HD2	1:B:793:ALA:HB2	2.02	0.42
1:A:22:TYR:CD2	1:A:23:PRO:HD2	2.55	0.41
1:A:482:LEU:HD22	5:A:1660:HOH:O	2.19	0.41
1:A:685:PHE:CD2	1:A:689:LYS:HE2	2.54	0.41
1:B:74:VAL:O	1:B:80:VAL:HA	2.20	0.41
1:A:698:ASP:HB3	5:A:1259:HOH:O	2.18	0.41
1:A:741:VAL:HA	1:A:745:LEU:HD12	2.02	0.41
1:A:138:SER:O	1:A:257:PRO:HB3	2.20	0.41
1:B:25:ILE:HA	1:B:38:SER:HA	2.03	0.41
1:A:4:GLY:HA3	1:A:14:VAL:O	2.21	0.40
1:A:792:ARG:HG2	1:A:805:ARG:CZ	2.51	0.40
1:B:796:THR:HG22	1:B:801:PRO:HA	2.04	0.40
1:A:365:GLY:HA3	1:A:368:ASP:OD2	2.21	0.40
1:B:364:MET:HE3	1:B:364:MET:HB2	1.96	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	687/842 (82%)	662 (96%)	24 (4%)	1 (0%)	48	40
1	B	507/842 (60%)	488 (96%)	19 (4%)	0	100	100
All	All	1194/1684 (71%)	1150 (96%)	43 (4%)	1 (0%)	48	40

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	TRP

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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
3	PO4	A	2902	-	4,4,4	1.46	1 (25%)	6,6,6	0.76	0
3	PO4	B	3902	-	4,4,4	1.70	2 (50%)	6,6,6	1.25	0
2	BGC	B	3901	-	12,12,12	0.68	0	17,17,17	1.34	2 (11%)
2	BGC	A	2901	-	12,12,12	0.58	0	17,17,17	0.95	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	B	3901	-	-	0/2/22/22	0/1/1/1
2	BGC	A	2901	-	-	0/2/22/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	3902	PO4	P-O4	-2.16	1.48	1.54
3	B	3902	PO4	P-O1	2.15	1.55	1.50
3	A	2902	PO4	P-O3	-2.14	1.48	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3901	BGC	O4-C4-C3	-2.92	103.48	110.38
2	B	3901	BGC	O4-C4-C5	2.08	114.45	109.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	822/842 (97%)	-0.86	3 (0%) 88 90	4, 9, 21, 38	0
1	B	822/842 (97%)	-0.88	3 (0%) 88 90	4, 9, 19, 41	0
All	All	1644/1684 (97%)	-0.87	6 (0%) 88 90	4, 9, 20, 41	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	814	SER	4.0
1	B	814	SER	3.1
1	B	813	GLY	3.1
1	A	813	GLY	3.0
1	A	812	ALA	2.6
1	B	812	ALA	2.2

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 oligosaccharides 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, 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	B-factors($\text{\AA}^2$)	Q<0.9
4	K	B	3903	1/1	0.93	0.08	28,28,28,28	0
4	K	A	2903	1/1	0.96	0.09	26,26,26,26	0
2	BGC	B	3901	12/12	0.98	0.03	4,8,8,9	0
3	PO4	B	3902	5/5	0.99	0.04	6,7,10,11	0
2	BGC	A	2901	12/12	0.99	0.03	5,8,9,13	0
3	PO4	A	2902	5/5	0.99	0.03	7,8,9,10	0

6.5 Other polymers [i](#)

There are no such residues in this entry.