Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:20 AM GMT

PDB ID	:	3AFJ
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

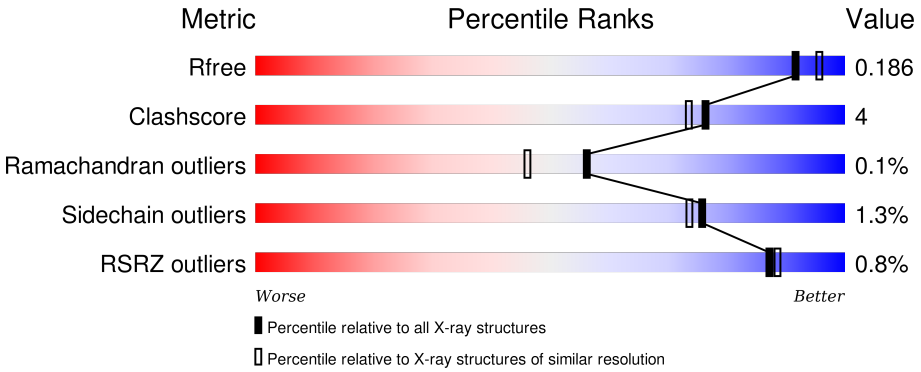
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (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 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 <=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	% 87% 10% • •
1	B	842	% 89% 8% • •

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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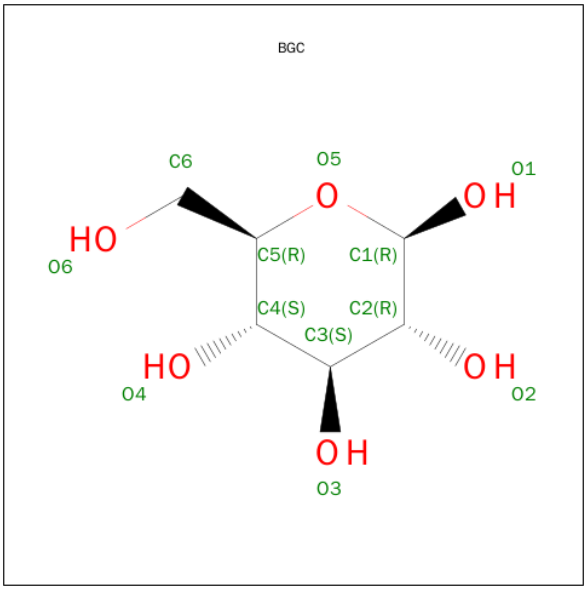
Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	SER	-	EXPRESSION TAG	UNP O66264
B	-16	SER	-	EXPRESSION TAG	UNP O66264
B	-15	HIS	-	EXPRESSION TAG	UNP O66264
B	-14	HIS	-	EXPRESSION TAG	UNP O66264
B	-13	HIS	-	EXPRESSION TAG	UNP O66264
B	-12	HIS	-	EXPRESSION TAG	UNP O66264
B	-11	HIS	-	EXPRESSION TAG	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 SUGAR (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		

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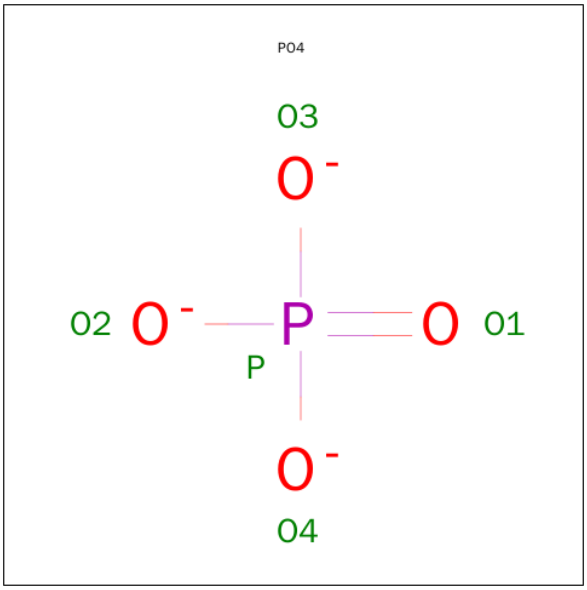
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 12 6 6	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

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

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

- Molecule 5 is water.

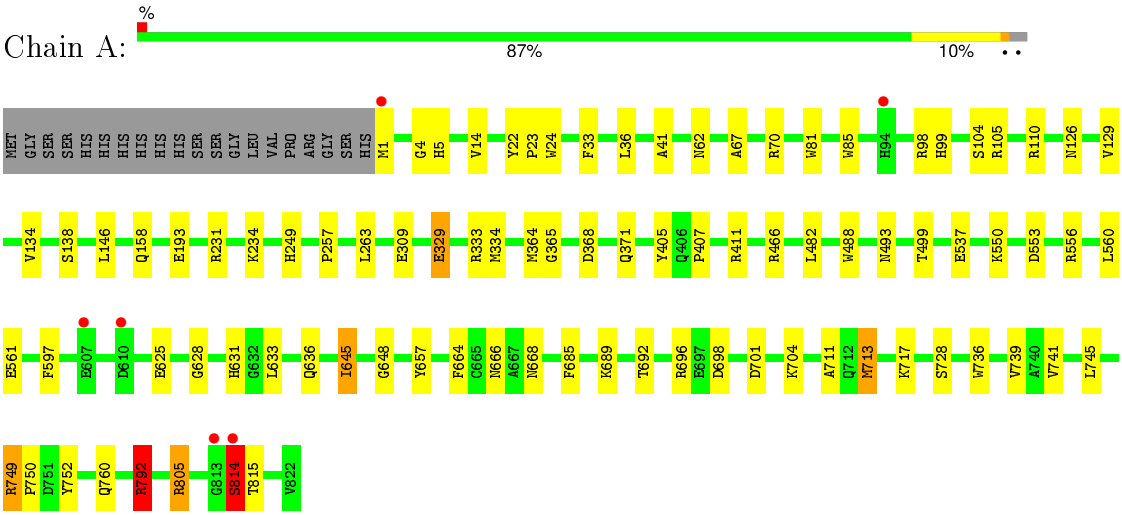
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1047	Total O 1047 1047	0	0
5	B	1125	Total O 1125 1125	0	0

3 Residue-property plots (i)

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 (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.

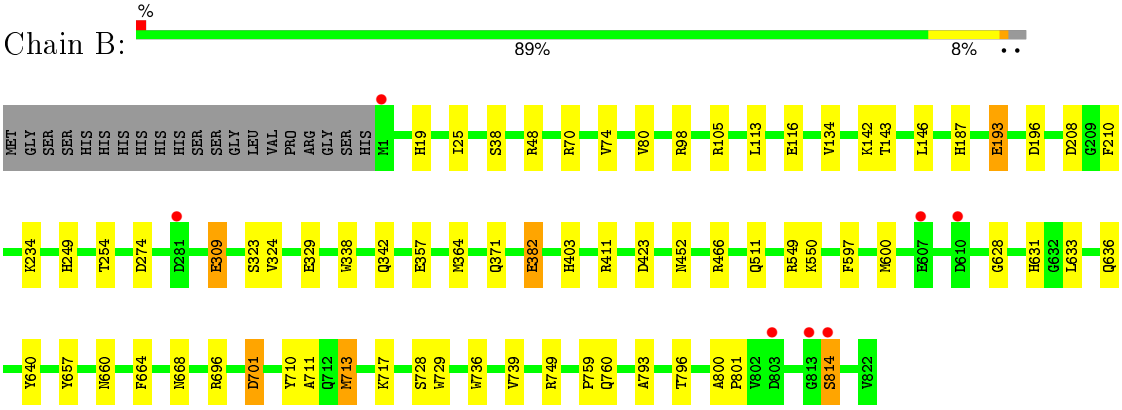
- Molecule 1: Cellobiose Phosphorylase

Chain A:



- Molecule 1: Cellobiose Phosphorylase

Chain B:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	3.15 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.133 , 0.186 0.135 , 0.186	Depositor DCC
R_{free} test set	6511 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	11.0	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 49.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 129386 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: K, BGC, PO4

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	1.17	12/6599 (0.2%)	0.95	15/9002 (0.2%)
1	B	1.17	9/6599 (0.1%)	0.95	11/9002 (0.1%)
All	All	1.17	21/13198 (0.2%)	0.95	26/18004 (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	309	GLU	CD-OE2	8.01	1.34	1.25
1	A	309	GLU	CG-CD	6.90	1.62	1.51
1	A	739	VAL	CB-CG2	6.24	1.66	1.52
1	A	657	TYR	CD1-CE1	6.19	1.48	1.39
1	A	329	GLU	CG-CD	6.12	1.61	1.51
1	A	537	GLU	CD-OE1	5.90	1.32	1.25
1	A	752	TYR	CD1-CE1	5.86	1.48	1.39
1	A	309	GLU	CD-OE2	5.83	1.32	1.25
1	B	210	PHE	CG-CD1	5.75	1.47	1.38
1	A	625	GLU	CG-CD	5.75	1.60	1.51
1	A	405	TYR	CD2-CE2	5.70	1.47	1.39
1	B	193	GLU	CB-CG	5.47	1.62	1.52
1	A	814	SER	C-O	5.33	1.33	1.23
1	B	382	GLU	CD-OE1	5.19	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	309	GLU	CG-CD	5.17	1.59	1.51
1	B	324	VAL	CB-CG2	5.14	1.63	1.52
1	B	739	VAL	CB-CG2	5.09	1.63	1.52
1	A	41	ALA	CA-CB	5.08	1.63	1.52
1	B	357	GLU	CD-OE2	5.07	1.31	1.25
1	B	657	TYR	CD1-CE1	5.07	1.47	1.39
1	A	129	VAL	CB-CG2	5.03	1.63	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	701	ASP	CB-CG-OD1	8.53	125.98	118.30
1	B	196	ASP	CB-CG-OD1	8.20	125.68	118.30
1	A	333	ARG	NE-CZ-NH2	-7.75	116.42	120.30
1	A	466	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	A	231	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	A	333	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	B	713	MET	CA-CB-CG	6.84	124.93	113.30
1	B	98	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	B	749	ARG	NE-CZ-NH1	6.37	123.49	120.30
1	A	98	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	B	466	ARG	NE-CZ-NH1	6.27	123.43	120.30
1	B	549	ARG	NE-CZ-NH2	6.26	123.43	120.30
1	A	749	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	A	231	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	A	792	ARG	CG-CD-NE	-5.64	99.94	111.80
1	A	749	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	B	274	ASP	CB-CG-OD1	5.42	123.17	118.30
1	B	550	LYS	CD-CE-NZ	5.40	124.12	111.70
1	A	815	THR	N-CA-CB	5.29	120.36	110.30
1	A	701	ASP	CB-CG-OD1	5.28	123.05	118.30
1	B	208	ASP	CB-CG-OD1	-5.27	113.56	118.30
1	A	36	LEU	CB-CG-CD2	-5.25	102.08	111.00
1	B	338	TRP	CA-CB-CG	-5.22	103.78	113.70
1	A	805	ARG	NE-CZ-NH2	5.21	122.90	120.30
1	A	98	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	105	ARG	NE-CZ-NH1	-5.09	117.75	120.30

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6424	0	6073	51	0
1	B	6424	0	6073	44	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	95	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 (95) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:48:ARG:CD	5:B:1424:HOH:O	2.47	0.56
1:A:698:ASP:CB	5:A:1259:HOH:O	2.53	0.56
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:LEU:HD23	5:A:1107:HOH:O	2.13	0.49
1:A:22:TYR:CG	1:A:23:PRO:HD2	2.48	0.48
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: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
1:B:600:MET:HE2	5:B:2065:HOH:O	2.15	0.45
1:A:711:ALA:HA	1:A:728:SER:HA	1.97	0.45
1:B:364:MET:HE2	1:B:364:MET:HA	1.98	0.45
1:A:499:THR:HG22	1:A:645:ILE:HD13	1.97	0.45
1:A:334:MET:HG3	1:A:692:THR:CG2	2.46	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:382:GLU:CD	5:B:1712:HOH:O	2.54	0.44
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:713:MET:HE3	1:A:713:MET:HB2	1.91	0.42
1:B:728:SER:O	1:B:729:TRP:HB2	2.20	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: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:792:ARG:HG2	1:A:805:ARG:CZ	2.51	0.40
1:A:4:GLY:HA3	1:A:14:VAL:O	2.21	0.40
1:B:796:THR:HG22	1:B:801:PRO:HA	2.04	0.40
1:B:364:MET:CA	1:B:364:MET:HE2	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:GLY:HA3	1:A:368:ASP:OD2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	820/842 (97%)	789 (96%)	30 (4%)	1 (0%)	56 46
1	B	820/842 (97%)	791 (96%)	29 (4%)	0	100 100
All	All	1640/1684 (97%)	1580 (96%)	59 (4%)	1 (0%)	56 46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	TRP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	664/681 (98%)	654 (98%)	10 (2%)	72 69
1	B	664/681 (98%)	657 (99%)	7 (1%)	80 79
All	All	1328/1362 (98%)	1311 (99%)	17 (1%)	76 73

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

Mol	Chain	Res	Type
1	A	1	MET
1	A	70	ARG
1	A	158	GLN
1	A	193	GLU
1	A	597	PHE
1	A	636	GLN
1	A	645	ILE
1	A	664	PHE
1	A	713	MET
1	A	792	ARG
1	B	70	ARG
1	B	193	GLU
1	B	511	GLN
1	B	597	PHE
1	B	636	GLN
1	B	664	PHE
1	B	713	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	HIS
1	A	99	HIS
1	A	126	ASN
1	A	130	GLN
1	A	249	HIS
1	A	284	GLN
1	A	339	ASN
1	A	371	GLN
1	A	578	ASN
1	A	631	HIS
1	A	666	ASN
1	A	668	ASN
1	A	727	ASN
1	A	760	GLN
1	B	19	HIS
1	B	126	ASN
1	B	130	GLN
1	B	187	HIS
1	B	249	HIS
1	B	284	GLN

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Mol	Chain	Res	Type
1	B	339	ASN
1	B	342	GLN
1	B	371	GLN
1	B	395	GLN
1	B	403	HIS
1	B	406	GLN
1	B	452	ASN
1	B	469	GLN
1	B	473	GLN
1	B	506	GLN
1	B	578	ASN
1	B	631	HIS
1	B	644	GLN
1	B	660	ASN
1	B	666	ASN
1	B	668	ASN
1	B	737	ASN
1	B	760	GLN

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

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	$\#\|Z\| > 2$
2	BGC	A	2901	-	12,12,12	0.56	0	17,17,17	1.07	2 (11%)
3	PO4	A	2902	-	4,4,4	1.01	0	6,6,6	0.27	0
2	BGC	B	3901	-	12,12,12	0.67	0	17,17,17	1.41	3 (17%)
3	PO4	B	3902	-	4,4,4	0.92	0	6,6,6	0.34	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	A	2901	-	-	0/2/22/22	0/1/1/1
3	PO4	A	2902	-	-	0/0/0/0	0/0/0/0
2	BGC	B	3901	-	-	0/2/22/22	0/1/1/1
3	PO4	B	3902	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	3901	BGC	O4-C4-C3	-3.04	103.48	110.34
2	A	2901	BGC	C1-C2-C3	-2.68	106.44	110.43
2	B	3901	BGC	C1-C2-C3	-2.26	107.06	110.43
2	A	2901	BGC	O1-C1-C2	-2.20	103.31	109.21
2	B	3901	BGC	O1-C1-O5	-2.05	104.64	110.25

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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%)	-0.70	6 (0%) 89 90	4, 9, 21, 38	0
1	B	822/842 (97%)	-0.72	7 (0%) 85 87	4, 9, 19, 41	0
All	All	1644/1684 (97%)	-0.71	13 (0%) 87 88	4, 9, 20, 41	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	4.2
1	B	813	GLY	4.1
1	A	814	SER	3.9
1	B	814	SER	3.8
1	B	803	ASP	3.7
1	A	1	MET	3.5
1	A	607	GLU	2.9
1	A	610	ASP	2.7
1	B	610	ASP	2.7
1	A	813	GLY	2.5
1	B	607	GLU	2.5
1	A	94	HIS	2.1
1	B	281	ASP	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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^{th} 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	BGC	B	3901	12/12	0.99	0.06	-0.02	4,8,8,9	0
2	BGC	A	2901	12/12	0.99	0.05	-0.59	5,8,9,13	0
3	PO4	B	3902	5/5	0.99	0.04	-1.54	6,7,10,11	0
3	PO4	A	2902	5/5	0.99	0.03	-3.05	7,8,9,10	0
4	K	A	2903	1/1	0.97	0.06	-	26,26,26,26	0
4	K	B	3903	1/1	0.97	0.07	-	28,28,28,28	0

6.5 Other polymers

There are no such residues in this entry.