



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:40 AM UTC

PDB ID : 3ACT / pdb_00003act
Title : Crystal Structure of Cellvibrio gilvus Cellobiose Phosphorylase Histidine mutant
Authors : Hidaka, M.; Hayashi, M.A.; Fushinobu, S.
Deposited on : 2010-01-08
Resolution : 1.85 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

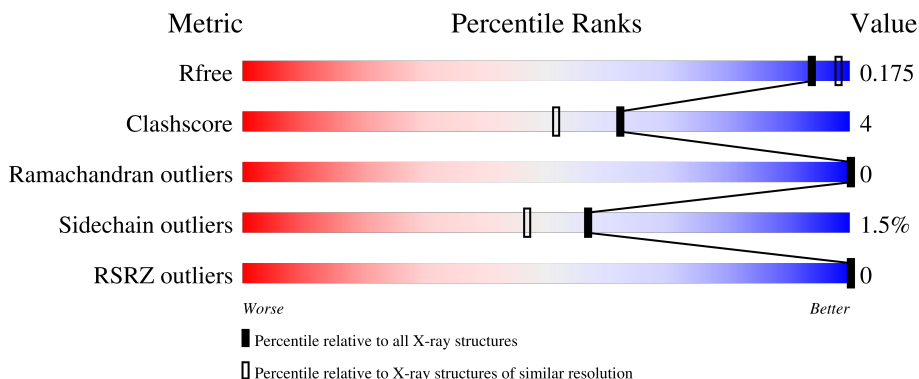
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

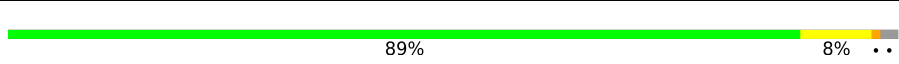

The reported resolution of this entry is 1.85 Å.

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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	 89% 8% ..
1	B	842	 88% 9% .

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 15120 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
			Total	C	N	O	S			
1	A	822	6426	4064	1101	1247	14	0	0	0
1	B	822	6426	4064	1101	1247	14	0	0	0

There are 42 discrepancies between the modelled and reference sequences:

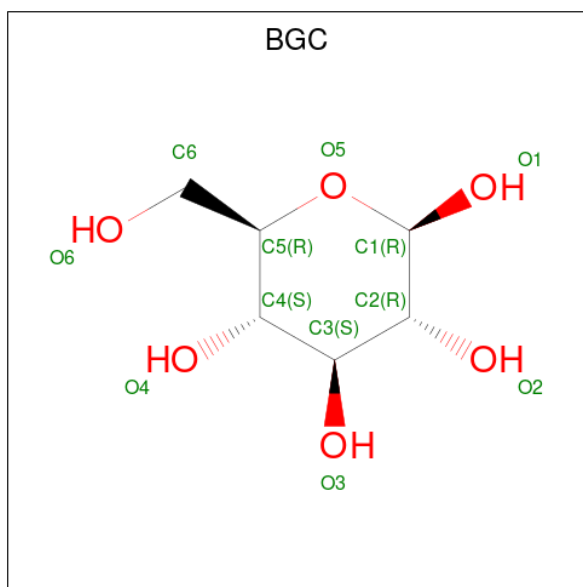
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP O66264
A	-18	GLY	-	expression tag	UNP O66264
A	-17	SER	-	expression tag	UNP O66264
A	-16	SER	-	expression tag	UNP O66264
A	-15	HIS	-	expression tag	UNP O66264
A	-14	HIS	-	expression tag	UNP O66264
A	-13	HIS	-	expression tag	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	666	ASN	HIS	engineered mutation	UNP O66264
B	-19	MET	-	expression tag	UNP O66264
B	-18	GLY	-	expression tag	UNP O66264
B	-17	SER	-	expression tag	UNP O66264
B	-16	SER	-	expression tag	UNP O66264

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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	666	ASN	HIS	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		
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 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0

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

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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 6 is water.

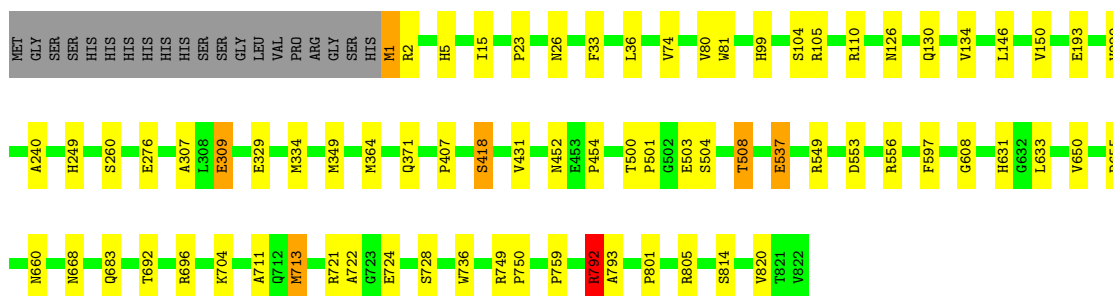
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1093	Total O 1093 1093	0	0
6	B	1109	Total O 1109 1109	0	0

3 Residue-property plots [i](#)


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.

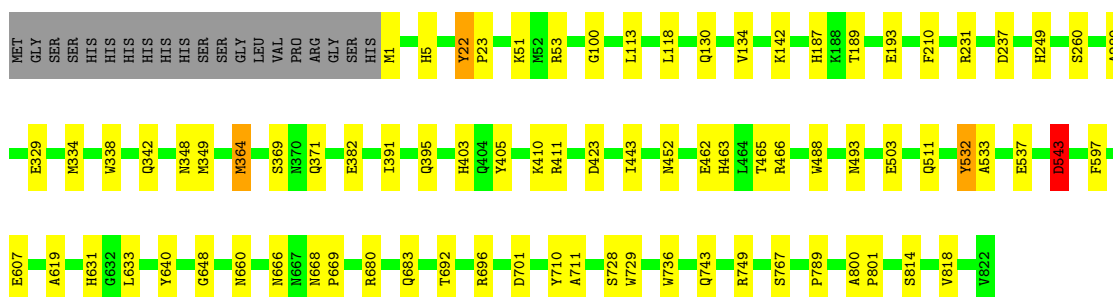
- Molecule 1: Cellobiose Phosphorylase

Chain A:  89% 8% ..



- Molecule 1: Cellobiose Phosphorylase

Chain B:  88% 9% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.36Å 98.31Å 104.33Å 90.00° 102.72° 90.00°	Depositor
Resolution (Å)	50.00 – 1.85 50.00 – 1.85	Depositor EDS
% Data completeness (in resolution range)	97.6 (50.00-1.85) 97.6 (50.00-1.85)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 1.85Å)	Xtrriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.128 , 0.176 0.129 , 0.175	Depositor DCC
R_{free} test set	6955 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	13.4	Xtrriage
Anisotropy	0.058	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15120	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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, GOL, 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	1.31	11/6601 (0.2%)	1.11	9/9005 (0.1%)
1	B	1.31	9/6601 (0.1%)	1.10	4/9005 (0.0%)
All	All	1.31	20/13202 (0.2%)	1.10	13/18010 (0.1%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	289	ALA	CA-CB	8.57	1.61	1.54
1	B	349	MET	SD-CE	-7.11	1.61	1.79
1	B	818	VAL	CA-CB	6.51	1.61	1.54
1	A	307	ALA	C-O	6.23	1.31	1.24
1	B	619	ALA	N-CA	6.16	1.53	1.46
1	A	349	MET	SD-CE	-6.07	1.64	1.79
1	A	240	ALA	CA-CB	5.97	1.63	1.53
1	A	150	VAL	C-O	-5.88	1.18	1.23
1	A	15	ILE	CA-CB	5.84	1.60	1.54
1	B	53	ARG	CZ-NH1	5.53	1.40	1.32
1	B	543	ASP	CB-CG	5.51	1.65	1.52
1	A	820	VAL	CA-CB	5.43	1.60	1.54
1	A	500	THR	CA-C	-5.34	1.46	1.52
1	A	814	SER	C-O	5.34	1.30	1.23
1	A	537	GLU	CG-CD	5.32	1.65	1.52
1	B	100	GLY	N-CA	5.27	1.48	1.44
1	B	532	TYR	CA-C	5.16	1.59	1.52
1	A	431	VAL	CA-CB	5.12	1.61	1.54
1	B	814	SER	C-O	5.03	1.30	1.23
1	A	309	GLU	CD-OE2	5.01	1.34	1.25

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	713	MET	CA-CB-CG	6.78	127.66	114.10
1	A	549	ARG	CG-CD-NE	-6.72	97.21	112.00
1	B	53	ARG	NE-CZ-NH2	-6.38	113.46	119.20
1	A	418	SER	CA-CB-OG	-6.30	98.49	111.10
1	A	792	ARG	CG-CD-NE	-5.81	99.22	112.00
1	B	22	TYR	N-CA-C	-5.68	103.11	108.22
1	A	537	GLU	CB-CG-CD	5.54	122.02	112.60
1	A	608	GLY	CA-C-N	5.50	125.33	119.28
1	A	608	GLY	C-N-CA	5.50	125.33	119.28
1	B	348	ASN	N-CA-C	5.24	117.07	111.36
1	A	105	ARG	NE-CZ-NH1	-5.20	116.30	121.50
1	A	549	ARG	NE-CZ-NH1	-5.03	116.47	121.50
1	B	338	TRP	CA-CB-CG	-5.01	104.07	113.60

There are no chirality outliers.

There are no planarity outliers.

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	6426	0	6070	42	0
1	B	6426	0	6070	60	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	6	0	8	0	0
5	B	24	0	32	0	0
6	A	1093	0	0	15	0
6	B	1109	0	0	24	0
All	All	15120	0	12204	102	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 (102) 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:543:ASP:HB3	6:B:977:HOH:O	1.49	1.12
1:B:329:GLU:HG2	6:B:1308:HOH:O	1.58	1.01
1:B:511:GLN:HG3	6:B:1267:HOH:O	1.63	0.99
1:B:382:GLU:CG	6:B:1246:HOH:O	2.19	0.90
1:B:403:HIS:HD2	1:B:423:ASP:OD2	1.56	0.88
1:B:631:HIS:HD2	1:B:696:ARG:HH12	1.23	0.86
1:B:51:LYS:HE2	6:B:1905:HOH:O	1.76	0.84
1:B:465:THR:HG21	6:B:1147:HOH:O	1.78	0.82
1:B:640:TYR:H	1:B:660:ASN:HD21	1.26	0.81
1:A:633:LEU:H	1:A:668:ASN:HD21	1.26	0.81
1:A:537:GLU:HG3	6:A:1018:HOH:O	1.81	0.80
1:B:342:GLN:HE22	1:B:710:TYR:H	1.27	0.80
1:A:631:HIS:HD2	1:A:696:ARG:HH12	1.30	0.78
1:B:633:LEU:H	1:B:668:ASN:HD21	1.29	0.78
1:A:329:GLU:HG3	6:A:981:HOH:O	1.82	0.78
1:B:371:GLN:HE21	1:B:736:TRP:HE1	1.33	0.76
1:B:382:GLU:HG3	6:B:1246:HOH:O	1.82	0.76
1:B:465:THR:HG22	1:B:532:TYR:OH	1.87	0.74
1:B:411:ARG:HE	1:B:452:ASN:ND2	1.85	0.73
1:B:382:GLU:CD	6:B:1246:HOH:O	2.32	0.71
1:A:371:GLN:HE21	1:A:736:TRP:HE1	1.40	0.70
1:B:5:HIS:HD2	6:B:913:HOH:O	1.75	0.70
1:B:631:HIS:CD2	1:B:696:ARG:HH12	2.07	0.69
1:A:329:GLU:HG3	6:A:1497:HOH:O	1.93	0.69
1:A:631:HIS:CD2	1:A:696:ARG:HH12	2.14	0.66
1:A:99:HIS:HD2	1:A:104:SER:OG	1.80	0.64
1:B:249:HIS:HD2	6:B:835:HOH:O	1.82	0.63
1:A:134:VAL:HG21	1:A:146:LEU:HD11	1.80	0.63
1:B:411:ARG:HE	1:B:452:ASN:HD22	1.49	0.59
1:B:403:HIS:HE1	6:B:866:HOH:O	1.84	0.59
1:A:1:MET:CB	6:A:1205:HOH:O	2.51	0.58
1:B:1:MET:HG2	1:B:701:ASP:HB3	1.84	0.58
1:A:1:MET:HB2	6:A:1205:HOH:O	2.03	0.58
1:A:249:HIS:HD2	6:A:837:HOH:O	1.87	0.57
1:A:1:MET:CA	6:A:1205:HOH:O	2.53	0.57
1:A:329:GLU:CG	6:A:981:HOH:O	2.48	0.57
1:B:187:HIS:HD2	6:B:849:HOH:O	1.88	0.56
1:B:249:HIS:HE1	6:B:869:HOH:O	1.88	0.56
1:B:118:LEU:O	1:B:130:GLN:HA	2.06	0.56
1:A:5:HIS:HD2	6:A:1588:HOH:O	1.88	0.55
1:A:249:HIS:HE1	6:A:955:HOH:O	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:792:ARG:HG2	1:A:805:ARG:CZ	2.37	0.54
1:B:371:GLN:HE21	1:B:736:TRP:NE1	2.03	0.54
1:A:704:LYS:HE2	1:A:724:GLU:CD	2.34	0.53
1:B:789:PRO:CB	6:B:1421:HOH:O	2.57	0.52
1:A:2:ARG:CZ	6:A:2195:HOH:O	2.57	0.52
1:B:403:HIS:CD2	1:B:423:ASP:OD2	2.49	0.52
1:B:187:HIS:CE1	1:B:189:THR:OG1	2.64	0.51
1:B:411:ARG:NE	1:B:452:ASN:ND2	2.58	0.50
1:B:364:MET:HA	1:B:364:MET:HE2	1.93	0.49
1:A:2:ARG:NH2	6:A:1646:HOH:O	2.45	0.49
1:A:2:ARG:NH1	6:A:2195:HOH:O	2.45	0.49
1:B:767:SER:HB2	6:B:1352:HOH:O	2.13	0.49
1:B:1:MET:CE	6:B:1371:HOH:O	2.61	0.48
1:A:33:PHE:HB2	1:A:126:ASN:HD22	1.79	0.48
1:A:503:GLU:HG2	1:A:508:THR:OG1	2.14	0.48
1:B:187:HIS:HE1	1:B:189:THR:OG1	1.97	0.47
1:A:309:GLU:HG3	6:A:1840:HOH:O	2.14	0.47
1:A:36:LEU:N	1:A:36:LEU:HD12	2.29	0.47
1:A:553:ASP:OD1	1:A:556:ARG:NH2	2.47	0.47
1:A:650:VAL:O	1:A:660:ASN:HB2	2.15	0.47
1:B:789:PRO:HB2	6:B:1421:HOH:O	2.15	0.47
1:A:501:PRO:HG3	6:B:1143:HOH:O	2.16	0.46
1:B:743:GLN:HB3	1:B:749:ARG:HB3	1.98	0.46
1:B:462:GLU:O	1:B:466:ARG:HG2	2.15	0.46
1:B:488:TRP:HE1	1:B:666:ASN:ND2	2.14	0.46
1:A:74:VAL:O	1:A:80:VAL:HA	2.15	0.46
1:B:493:ASN:HB2	1:B:648:GLY:HA3	1.97	0.46
1:A:99:HIS:CD2	1:A:104:SER:OG	2.64	0.46
1:A:749:ARG:HA	1:A:750:PRO:HD3	1.82	0.46
1:B:395:GLN:HE22	1:B:463:HIS:HB3	1.81	0.45
1:B:1:MET:HE1	6:B:1371:HOH:O	2.16	0.45
1:B:543:ASP:CA	6:B:977:HOH:O	2.62	0.45
1:A:26:ASN:HB2	1:A:99:HIS:CD2	2.51	0.45
1:A:504:SER:O	1:A:508:THR:HB	2.17	0.45
1:B:711:ALA:HA	1:B:728:SER:HA	1.99	0.45
1:B:728:SER:O	1:B:729:TRP:HB2	2.17	0.44
1:B:503:GLU:HB2	6:B:1966:HOH:O	2.17	0.44
1:B:113:LEU:HG	1:B:142:LYS:HE2	2.00	0.44
1:A:81:TRP:CG	1:A:110:ARG:HD3	2.53	0.44
1:B:1:MET:HE2	1:B:1:MET:HB2	1.53	0.44
1:A:134:VAL:O	1:A:260:SER:HA	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:711:ALA:HA	1:A:728:SER:HA	2.01	0.43
1:B:231:ARG:NH2	6:B:1095:HOH:O	2.48	0.43
1:B:364:MET:HE2	1:B:364:MET:CA	2.48	0.43
1:B:134:VAL:O	1:B:260:SER:HA	2.18	0.43
1:B:334:MET:HG3	1:B:692:THR:CG2	2.49	0.42
1:A:364:MET:HG2	1:A:407:PRO:HG3	2.01	0.42
1:A:721:ARG:O	1:A:722:ALA:C	2.61	0.42
1:B:631:HIS:HE1	6:B:881:HOH:O	2.02	0.42
1:B:405:TYR:CD1	1:B:410:LYS:HA	2.54	0.42
1:B:22:TYR:CD2	1:B:23:PRO:HD2	2.55	0.42
1:B:369:SER:HB3	1:B:391:ILE:HD11	2.02	0.42
1:B:668:ASN:N	1:B:669:PRO:CD	2.83	0.41
1:B:680:ARG:HB3	6:B:1113:HOH:O	2.20	0.41
1:A:334:MET:HG3	1:A:692:THR:CG2	2.50	0.41
1:A:452:ASN:O	1:A:454:PRO:HD3	2.20	0.41
1:A:759:PRO:HD2	1:A:793:ALA:HB2	2.02	0.41
1:B:800:ALA:HA	1:B:801:PRO:HD3	1.95	0.41
1:B:210:PHE:O	1:B:237:ASP:HA	2.21	0.41
1:B:533:ALA:O	1:B:537:GLU:HG3	2.22	0.40
1:A:130:GLN:NE2	6:A:1239:HOH:O	2.52	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%)	31 (4%)	0	100	100
1	B	820/842 (97%)	789 (96%)	31 (4%)	0	100	100
All	All	1640/1684 (97%)	1578 (96%)	62 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	665/682 (98%)	652 (98%)	13 (2%)	48 36
1	B	665/682 (98%)	658 (99%)	7 (1%)	65 57
All	All	1330/1364 (98%)	1310 (98%)	20 (2%)	57 47

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	23	PRO
1	A	193	GLU
1	A	229	VAL
1	A	276	GLU
1	A	418	SER
1	A	508	THR
1	A	597	PHE
1	A	655	PRO
1	A	683	GLN
1	A	713	MET
1	A	792	ARG
1	A	801	PRO
1	B	193	GLU
1	B	364	MET
1	B	443	ILE
1	B	543	ASP
1	B	597	PHE
1	B	607	GLU
1	B	683	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	HIS
1	A	99	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	126	ASN
1	A	130	GLN
1	A	249	HIS
1	A	312	ASN
1	A	371	GLN
1	A	567	GLN
1	A	578	ASN
1	A	631	HIS
1	A	644	GLN
1	A	666	ASN
1	A	668	ASN
1	A	727	ASN
1	A	737	ASN
1	A	760	GLN
1	B	5	HIS
1	B	19	HIS
1	B	32	GLN
1	B	126	ASN
1	B	158	GLN
1	B	177	GLN
1	B	187	HIS
1	B	249	HIS
1	B	342	GLN
1	B	371	GLN
1	B	395	GLN
1	B	403	HIS
1	B	414	ASN
1	B	452	ASN
1	B	469	GLN
1	B	473	GLN
1	B	506	GLN
1	B	567	GLN
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 [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 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	GOL	A	2904	-	5,5,5	0.20	0	5,5,5	0.95	0
2	BGC	A	2901	-	12,12,12	0.83	0	17,17,17	1.08	1 (5%)
5	GOL	B	3904	-	5,5,5	0.61	0	5,5,5	1.01	0
5	GOL	B	2905	-	5,5,5	0.55	0	5,5,5	1.15	0
3	PO4	A	2902	-	4,4,4	1.15	0	6,6,6	1.61	1 (16%)
2	BGC	B	3901	-	12,12,12	0.91	0	17,17,17	1.11	1 (5%)
5	GOL	B	3906	-	5,5,5	0.56	0	5,5,5	0.65	0
3	PO4	B	3902	-	4,4,4	1.92	1 (25%)	6,6,6	1.87	1 (16%)
5	GOL	B	3905	-	5,5,5	0.59	0	5,5,5	1.24	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
5	GOL	A	2904	-	-	1/4/4/4	-
2	BGC	A	2901	-	-	0/2/22/22	0/1/1/1
5	GOL	B	3904	-	-	0/4/4/4	-
5	GOL	B	2905	-	-	0/4/4/4	-
2	BGC	B	3901	-	-	0/2/22/22	0/1/1/1
5	GOL	B	3906	-	-	0/4/4/4	-
5	GOL	B	3905	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	3902	PO4	P-O1	3.21	1.58	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2901	BGC	O4-C4-C5	-2.88	102.24	109.32
3	B	3902	PO4	O2-P-O1	-2.72	101.33	110.95
2	B	3901	BGC	O5-C5-C4	-2.49	105.21	109.70
3	A	2902	PO4	O3-P-O2	2.10	114.43	107.91

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	3905	GOL	O1-C1-C2-C3
5	B	3905	GOL	O1-C1-C2-O2
5	A	2904	GOL	O2-C2-C3-O3

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%)	-0.92	0 100 100	6, 11, 22, 37	0
1	B	822/842 (97%)	-0.93	0 100 100	7, 11, 21, 38	0
All	All	1644/1684 (97%)	-0.93	0 100 100	6, 11, 22, 38	0

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
5	GOL	B	2905	6/6	0.86	0.11	23,33,36,37	0
5	GOL	A	2904	6/6	0.94	0.07	19,22,26,26	0
5	GOL	B	3905	6/6	0.94	0.07	16,21,28,28	0
5	GOL	B	3906	6/6	0.96	0.06	14,15,18,18	0
5	GOL	B	3904	6/6	0.97	0.06	13,22,25,27	0
4	K	B	3903	1/1	0.98	0.09	22,22,22,22	0
3	PO4	B	3902	5/5	0.99	0.03	8,9,9,12	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	K	A	2903	1/1	0.99	0.05	21,21,21,21	0
2	BGC	A	2901	12/12	0.99	0.03	7,9,10,10	0
2	BGC	B	3901	12/12	0.99	0.03	8,10,13,13	0
3	PO4	A	2902	5/5	1.00	0.02	7,8,12,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.