



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:20 AM GMT

PDB ID : 3ACT
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
<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

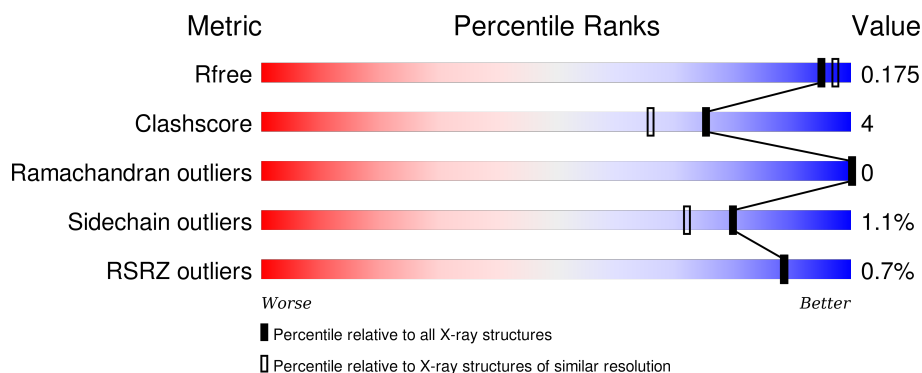
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	1745 (1.86-1.86)
Clashscore	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)
RSRZ outliers	91569	1747 (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 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	842	<div> <div></div> <div>88% 9% .</div> </div>
1	B	842	<div> <div></div> <div>87% 10% .</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
5	GOL	B	2905	-	-	-	X

2 Entry composition

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
1	A	822	Total	C	N	O	S	0	0	0
			6426	4064	1101	1247	14			
1	B	822	Total	C	N	O	S	0	0	0
			6426	4064	1101	1247	14			

There are 42 discrepancies between the modelled and reference sequences:

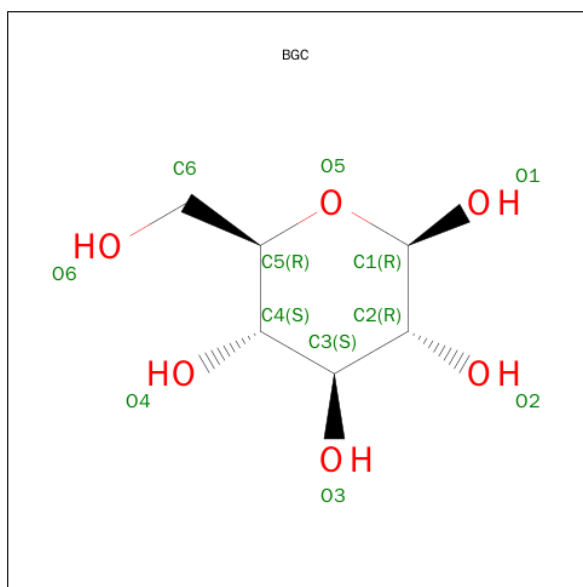
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP O66264
A	-18	GLY	-	EXPRESSION TAG	UNP O66264
A	-17	SER	-	EXPRESSION TAG	UNP O66264
A	-16	SER	-	EXPRESSION TAG	UNP O66264
A	-15	HIS	-	EXPRESSION TAG	UNP O66264
A	-14	HIS	-	EXPRESSION TAG	UNP O66264
A	-13	HIS	-	EXPRESSION TAG	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 SUGAR (BETA-D-GLUCOSE) (three-letter code: 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 (three-letter code: 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 (three-letter code: K) (formula: K).

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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

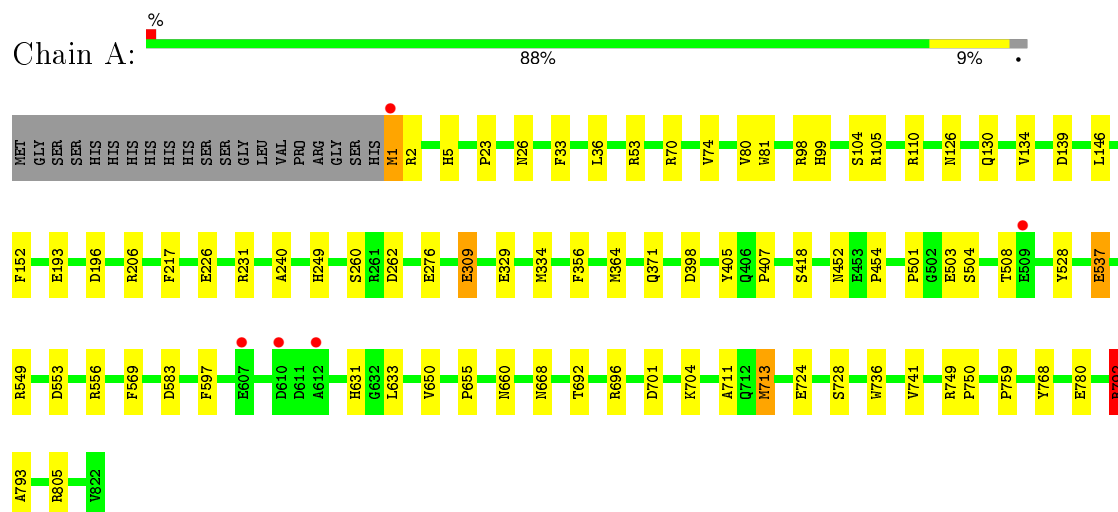
- Molecule 6 is water.

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

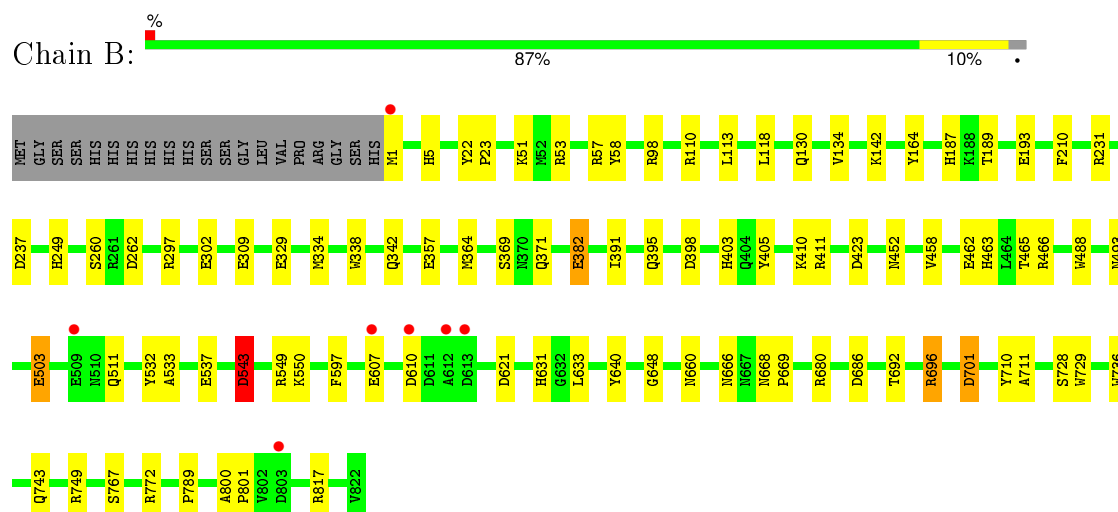
3 Residue-property plots

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: Cellobiose Phosphorylase



• Molecule 1: Cellobiose Phosphorylase



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 38.19 – 1.85	Depositor EDS
% Data completeness (in resolution range)	97.6 (50.00-1.85) 97.6 (38.19-1.85)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 1.85Å)	Xtriage
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 (5.30%)	DCC
Wilson B-factor (Å ²)	13.4	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 51.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 138200 reflections (0.001%)	Xtriage
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

Xtriage'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, 0.375 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: GOL, 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	1.19	15/6601 (0.2%)	0.98	20/9005 (0.2%)
1	B	1.18	12/6601 (0.2%)	0.97	19/9005 (0.2%)
All	All	1.18	27/13202 (0.2%)	0.97	39/18010 (0.2%)

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	537	GLU	CG-CD	8.93	1.65	1.51
1	A	309	GLU	CD-OE2	8.39	1.34	1.25
1	A	152	PHE	CE1-CZ	8.10	1.52	1.37
1	A	537	GLU	CD-OE1	7.89	1.34	1.25
1	B	543	ASP	CB-CG	6.70	1.65	1.51
1	B	309	GLU	CD-OE2	6.66	1.32	1.25
1	A	741	VAL	CB-CG1	6.38	1.66	1.52
1	B	53	ARG	CZ-NH1	5.73	1.40	1.33
1	B	701	ASP	CB-CG	5.72	1.63	1.51
1	A	356	PHE	CE1-CZ	5.71	1.48	1.37
1	A	537	GLU	CB-CG	5.68	1.62	1.52
1	B	357	GLU	CG-CD	5.66	1.60	1.51
1	A	780	GLU	CD-OE2	5.65	1.31	1.25
1	B	458	VAL	CB-CG1	5.51	1.64	1.52
1	A	217	PHE	CE2-CZ	5.49	1.47	1.37
1	B	503	GLU	CG-CD	5.45	1.60	1.51
1	B	302	GLU	CG-CD	5.42	1.60	1.51
1	A	405	TYR	CD2-CE2	5.27	1.47	1.39
1	B	550	LYS	CD-CE	5.27	1.64	1.51
1	B	58	TYR	CD2-CE2	5.26	1.47	1.39
1	A	768	TYR	CD1-CE1	5.19	1.47	1.39
1	B	164	TYR	CD1-CE1	5.17	1.47	1.39
1	A	226	GLU	CD-OE1	-5.15	1.20	1.25
1	A	240	ALA	CA-CB	5.13	1.63	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	569	PHE	CE2-CZ	5.13	1.47	1.37
1	A	528	TYR	CE2-CZ	5.02	1.45	1.38
1	B	382	GLU	CD-OE1	5.00	1.31	1.25

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	53	ARG	NE-CZ-NH2	-13.68	113.46	120.30
1	A	53	ARG	NE-CZ-NH2	-9.75	115.43	120.30
1	B	701	ASP	CB-CG-OD1	9.69	127.02	118.30
1	A	231	ARG	NE-CZ-NH2	-9.44	115.58	120.30
1	A	231	ARG	NE-CZ-NH1	8.71	124.66	120.30
1	A	713	MET	CA-CB-CG	8.45	127.66	113.30
1	A	98	ARG	NE-CZ-NH1	8.32	124.46	120.30
1	A	105	ARG	NE-CZ-NH1	-7.99	116.30	120.30
1	B	53	ARG	NE-CZ-NH1	7.97	124.28	120.30
1	B	297	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	A	701	ASP	CB-CG-OD1	7.72	125.25	118.30
1	A	549	ARG	NE-CZ-NH1	-7.66	116.47	120.30
1	B	772	ARG	NE-CZ-NH1	7.41	124.00	120.30
1	B	98	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	B	262	ASP	CB-CG-OD2	7.24	124.82	118.30
1	A	549	ARG	CG-CD-NE	-6.95	97.21	111.80
1	B	772	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	B	686	ASP	CB-CG-OD1	6.52	124.17	118.30
1	A	713	MET	CG-SD-CE	-6.17	90.33	100.20
1	B	549	ARG	NE-CZ-NH2	6.17	123.38	120.30
1	A	262	ASP	CB-CG-OD2	6.10	123.79	118.30
1	A	98	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	A	792	ARG	CG-CD-NE	-5.99	99.22	111.80
1	B	110	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	A	139	ASP	CB-CG-OD2	5.74	123.47	118.30
1	B	57	ARG	NE-CZ-NH2	5.64	123.12	120.30
1	A	792	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	196	ASP	CB-CG-OD1	5.63	123.37	118.30
1	B	98	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	B	696	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	398	ASP	CB-CG-OD1	5.42	123.18	118.30
1	A	53	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	A	583	ASP	CB-CG-OD2	5.26	123.03	118.30
1	B	621	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	206	ARG	NE-CZ-NH2	-5.17	117.72	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	338	TRP	CA-CB-CG	-5.07	104.07	113.70
1	B	817	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	B	610	ASP	CB-CG-OD1	5.01	122.81	118.30
1	B	398	ASP	CB-CG-OD1	5.00	122.80	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6426	0	6070	41	0
1	B	6426	0	6070	58	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	99	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 (99) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:382:GLU:CD	6:B:1246:HOH:O	2.32	0.67
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:329:GLU:CG	6:A:981:HOH:O	2.48	0.57
1:A:1:MET:CA	6:A:1205:HOH:O	2.53	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
1:A:792:ARG:HG2	1:A:805:ARG:CZ	2.37	0.54
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:364:MET:HE2	1:B:364:MET:HA	1.94	0.48
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:704:LYS:HE2	1:A:724:GLU:CD	2.34	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:B:493:ASN:HB2	1:B:648:GLY:HA3	1.97	0.46
1:A:74:VAL:O	1:A:80:VAL:HA	2.15	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: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:1:MET:HE1	6:B:1371:HOH:O	2.16	0.44
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:A:134:VAL:O	1:A:260:SER:HA	2.18	0.43
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: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:B:631:HIS:HE1	6:B:881:HOH:O	2.02	0.42
1:A:364:MET:HG2	1:A:407:PRO:HG3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:364:MET:CA	1:B:364:MET:HE2	2.49	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%)	655 (98%)	10 (2%)	72	60
1	B	665/682 (98%)	661 (99%)	4 (1%)	90	87
All	All	1330/1364 (98%)	1316 (99%)	14 (1%)	80	72

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	23	PRO
1	A	70	ARG
1	A	193	GLU
1	A	276	GLU
1	A	418	SER
1	A	597	PHE
1	A	655	PRO
1	A	713	MET
1	A	792	ARG
1	B	193	GLU
1	B	543	ASP
1	B	597	PHE
1	B	607	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) 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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	760	GLN
1	B	5	HIS
1	B	19	HIS
1	B	126	ASN
1	B	130	GLN
1	B	187	HIS
1	B	249	HIS
1	B	284	GLN
1	B	339	ASN
1	B	342	GLN
1	B	371	GLN
1	B	395	GLN
1	B	403	HIS
1	B	452	ASN
1	B	469	GLN
1	B	473	GLN
1	B	506	GLN
1	B	631	HIS
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 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	$\# Z > 2$
2	BGC	A	2901	-	12,12,12	0.82	0	17,17,17	1.08	1 (5%)
3	PO4	A	2902	-	4,4,4	0.74	0	6,6,6	0.32	0
5	GOL	A	2904	-	5,5,5	0.18	0	5,5,5	0.95	0
5	GOL	B	2905	-	5,5,5	0.49	0	5,5,5	1.03	0
2	BGC	B	3901	-	12,12,12	0.91	0	17,17,17	1.12	1 (5%)
3	PO4	B	3902	-	4,4,4	0.91	0	6,6,6	0.40	0
5	GOL	B	3904	-	5,5,5	0.56	0	5,5,5	0.90	0
5	GOL	B	3905	-	5,5,5	0.52	0	5,5,5	1.18	0
5	GOL	B	3906	-	5,5,5	0.51	0	5,5,5	0.57	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
5	GOL	A	2904	-	-	0/4/4/4	0/0/0/0
5	GOL	B	2905	-	-	0/4/4/4	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
5	GOL	B	3904	-	-	0/4/4/4	0/0/0/0
5	GOL	B	3905	-	-	0/4/4/4	0/0/0/0
5	GOL	B	3906	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2901	BGC	O4-C4-C5	-2.64	102.24	109.24
2	B	3901	BGC	O5-C5-C4	-2.38	105.21	109.68

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 [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%)	-0.73	5 (0%) 90 90	6, 11, 22, 37	0
1	B	822/842 (97%)	-0.72	7 (0%) 85 85	7, 11, 21, 38	0
All	All	1644/1684 (97%)	-0.72	12 (0%) 89 88	6, 11, 22, 38	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	3.0
1	B	509	GLU	2.9
1	B	607	GLU	2.7
1	A	612	ALA	2.6
1	B	803	ASP	2.5
1	A	607	GLU	2.3
1	B	612	ALA	2.2
1	A	610	ASP	2.2
1	A	509	GLU	2.1
1	B	610	ASP	2.1
1	B	1	MET	2.0
1	B	613	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](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
5	GOL	B	2905	6/6	0.92	0.10	2.49	23,33,36,37	0
5	GOL	B	3905	6/6	0.94	0.09	1.62	16,21,28,28	0
5	GOL	A	2904	6/6	0.94	0.08	1.37	19,22,26,26	0
5	GOL	B	3904	6/6	0.96	0.14	0.89	13,22,25,27	0
5	GOL	B	3906	6/6	0.97	0.07	0.61	14,15,18,18	0
2	BGC	A	2901	12/12	0.99	0.07	-0.67	7,9,10,10	0
3	PO4	A	2902	5/5	1.00	0.11	-0.80	7,8,12,12	0
3	PO4	B	3902	5/5	0.99	0.08	-1.03	8,9,9,12	0
2	BGC	B	3901	12/12	0.99	0.05	-1.08	8,10,13,13	0
4	K	A	2903	1/1	0.99	0.07	-1.60	21,21,21,21	0
4	K	B	3903	1/1	0.99	0.04	-	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.