



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:15 PM GMT

PDB ID : 3WIR  
Title : Crystal structure of kojibiose phosphorylase complexed with glucose  
Authors : Okada, S.; Yamamoto, T.; Watanabe, H.; Nishimoto, T.; Chaen, H.; Fukuda, S.; Wakagi, T.; Fushinobu, S.  
Deposited on : 2013-09-24  
Resolution : 2.05 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

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

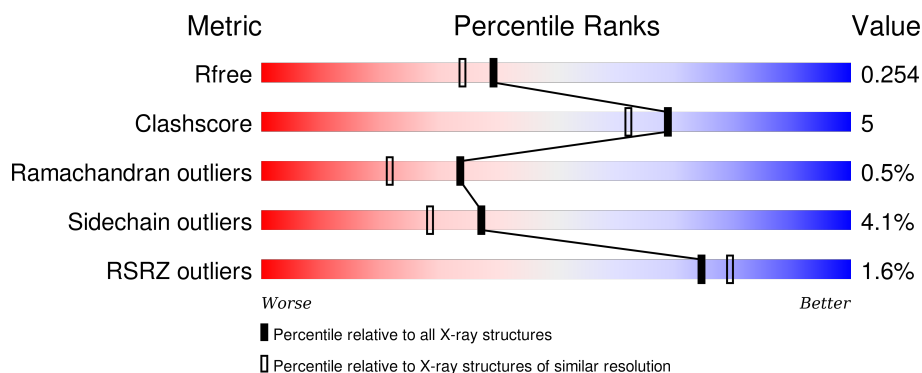
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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  $\geq 3$ , 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	764	<div> <div>2%</div> <div>86%</div> <div>12%</div> <div>..</div> </div>
1	B	764	<div> <div>2%</div> <div>86%</div> <div>11%</div> <div>..</div> </div>
1	C	764	<div> <div>%</div> <div>85%</div> <div>12%</div> <div>..</div> </div>
1	D	764	<div> <div>2%</div> <div>84%</div> <div>13%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	804	-	-	-	X
3	GOL	C	803	-	-	-	X
3	GOL	D	803	-	-	-	X
3	GOL	D	804	-	-	-	X
3	GOL	D	806	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26306 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 Kojibiose phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	756	Total	C	N	O	S	0	0	0
			6187	3985	1019	1162	21			
1	B	756	Total	C	N	O	S	0	0	0
			6187	3985	1019	1162	21			
1	C	756	Total	C	N	O	S	0	0	0
			6187	3985	1019	1162	21			
1	D	756	Total	C	N	O	S	0	0	0
			6187	3985	1019	1162	21			

There are 32 discrepancies between the modelled and reference sequences:

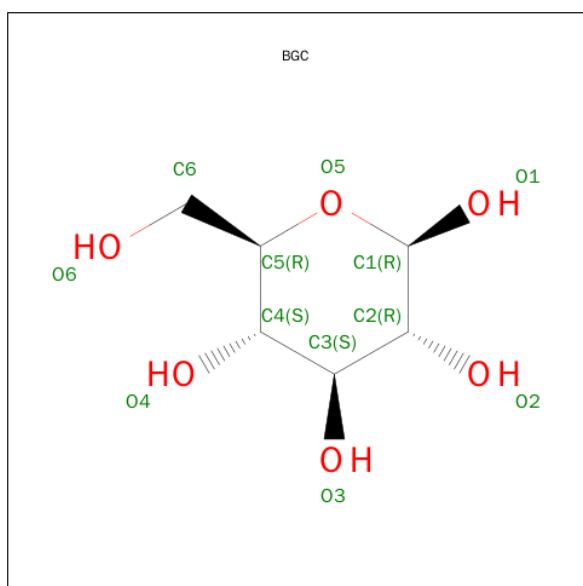
Chain	Residue	Modelled	Actual	Comment	Reference
A	757	GLY	-	EXPRESSION TAG	UNP A4XGP2
A	758	SER	-	EXPRESSION TAG	UNP A4XGP2
A	759	HIS	-	EXPRESSION TAG	UNP A4XGP2
A	760	HIS	-	EXPRESSION TAG	UNP A4XGP2
A	761	HIS	-	EXPRESSION TAG	UNP A4XGP2
A	762	HIS	-	EXPRESSION TAG	UNP A4XGP2
A	763	HIS	-	EXPRESSION TAG	UNP A4XGP2
A	764	HIS	-	EXPRESSION TAG	UNP A4XGP2
B	757	GLY	-	EXPRESSION TAG	UNP A4XGP2
B	758	SER	-	EXPRESSION TAG	UNP A4XGP2
B	759	HIS	-	EXPRESSION TAG	UNP A4XGP2
B	760	HIS	-	EXPRESSION TAG	UNP A4XGP2
B	761	HIS	-	EXPRESSION TAG	UNP A4XGP2
B	762	HIS	-	EXPRESSION TAG	UNP A4XGP2
B	763	HIS	-	EXPRESSION TAG	UNP A4XGP2
B	764	HIS	-	EXPRESSION TAG	UNP A4XGP2
C	757	GLY	-	EXPRESSION TAG	UNP A4XGP2
C	758	SER	-	EXPRESSION TAG	UNP A4XGP2
C	759	HIS	-	EXPRESSION TAG	UNP A4XGP2
C	760	HIS	-	EXPRESSION TAG	UNP A4XGP2
C	761	HIS	-	EXPRESSION TAG	UNP A4XGP2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	762	HIS	-	EXPRESSION TAG	UNP A4XGP2
C	763	HIS	-	EXPRESSION TAG	UNP A4XGP2
C	764	HIS	-	EXPRESSION TAG	UNP A4XGP2
D	757	GLY	-	EXPRESSION TAG	UNP A4XGP2
D	758	SER	-	EXPRESSION TAG	UNP A4XGP2
D	759	HIS	-	EXPRESSION TAG	UNP A4XGP2
D	760	HIS	-	EXPRESSION TAG	UNP A4XGP2
D	761	HIS	-	EXPRESSION TAG	UNP A4XGP2
D	762	HIS	-	EXPRESSION TAG	UNP A4XGP2
D	763	HIS	-	EXPRESSION TAG	UNP A4XGP2
D	764	HIS	-	EXPRESSION TAG	UNP A4XGP2

- Molecule 2 is SUGAR (BETA-D-GLUCOSE) (three-letter code: BGC) (formula:  $C_6H_{12}O_6$ ).



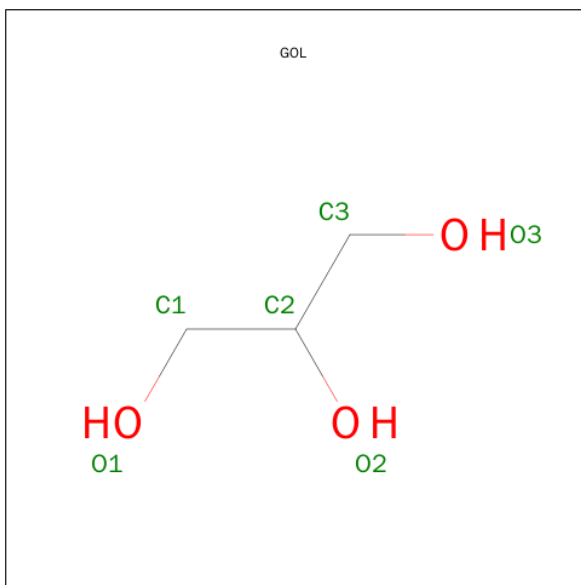
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 12 6 6	0	0
2	A	1	Total C O 12 6 6	0	0
2	B	1	Total C O 12 6 6	0	0
2	B	1	Total C O 12 6 6	0	0
2	C	1	Total C O 12 6 6	0	0
2	C	1	Total C O 12 6 6	0	0

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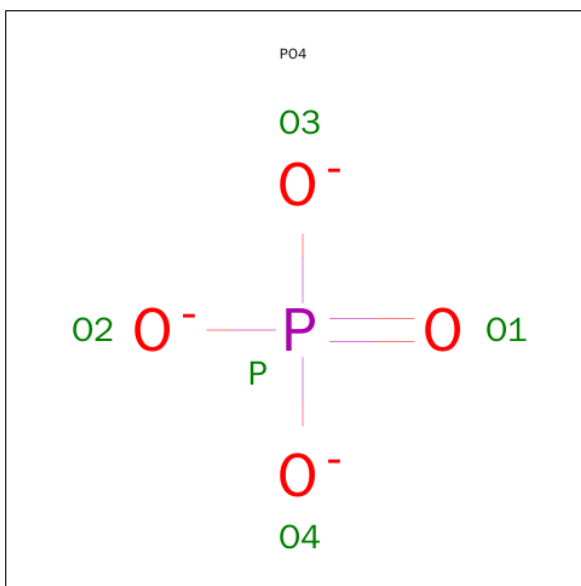
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			12	6	6		
2	D	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

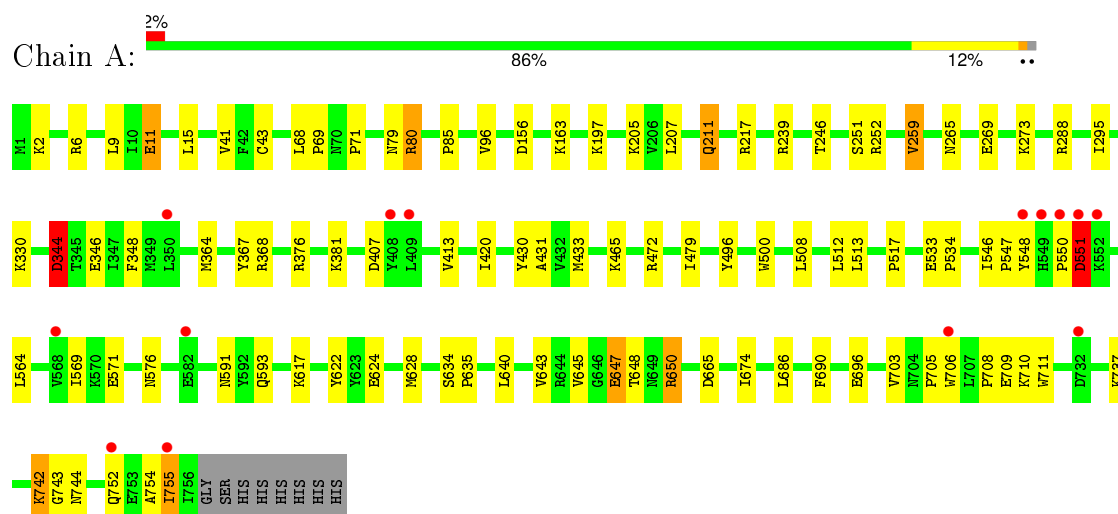
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	371	Total	O	0	0
			371	371		
5	B	387	Total	O		
			387	387		
5	C	299	Total	O	0	0
			299	299		
5	D	321	Total	O		
			321	321		

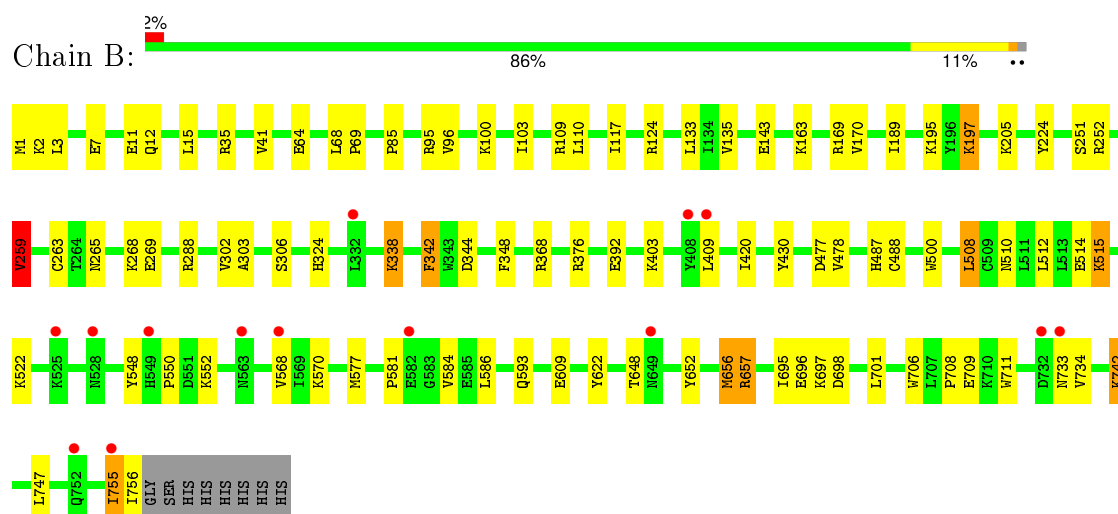
### 3 Residue-property plots

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 ( $RSRZ > 2$ ). 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.

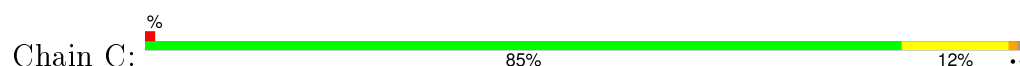
- Molecule 1: Kojibiose phosphorylase



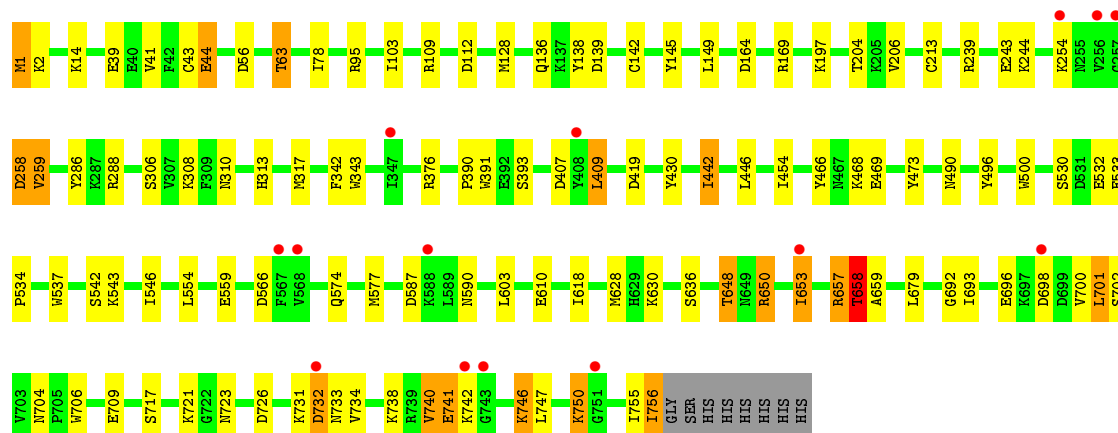
- Molecule 1: Kojibiose phosphorylase



- Molecule 1: Kojibiose phosphorylase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.58Å 104.46Å 124.16Å 68.83° 86.02° 90.06°	Depositor
Resolution (Å)	46.26 – 2.05 46.26 – 2.05	Depositor EDS
% Data completeness (in resolution range)	97.0 (46.26-2.05) 85.3 (46.26-2.05)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.29 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.191 , 0.251 0.196 , 0.254	Depositor DCC
$R_{free}$ test set	10233 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.3	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 47.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 203950 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	26306	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.80 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 8.0405e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.93	0/6328	0.94	12/8550 (0.1%)
1	B	0.91	1/6328 (0.0%)	0.95	12/8550 (0.1%)
1	C	0.81	0/6328	0.88	6/8550 (0.1%)
1	D	0.82	1/6328 (0.0%)	0.93	14/8550 (0.2%)
All	All	0.87	2/25312 (0.0%)	0.93	44/34200 (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	C	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	658	THR	CB-CG2	-5.97	1.32	1.52
1	B	488	CYS	CB-SG	-5.47	1.72	1.81

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	657	ARG	NE-CZ-NH1	11.81	126.21	120.30
1	D	95	ARG	NE-CZ-NH1	-9.29	115.65	120.30
1	B	657	ARG	NE-CZ-NH2	-8.81	115.89	120.30
1	D	95	ARG	NE-CZ-NH2	8.66	124.63	120.30
1	D	657	ARG	NE-CZ-NH1	8.03	124.32	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	551	ASP	Peptide
1	C	255	ASN	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	6187	0	6120	47	0
1	B	6187	0	6119	60	0
1	C	6187	0	6120	57	0
1	D	6187	0	6119	66	0
2	A	24	0	24	0	0
2	B	24	0	24	0	0
2	C	24	0	24	0	0
2	D	24	0	24	0	0
3	A	12	0	16	0	0
3	B	6	0	8	1	0
3	C	12	0	16	0	0
3	D	24	0	32	2	0
4	A	5	0	0	0	0
4	B	10	0	0	1	0
4	C	10	0	0	0	0
4	D	5	0	0	0	0
5	A	371	0	0	6	0
5	B	387	0	0	2	0
5	C	299	0	0	5	0
5	D	321	0	0	9	0
All	All	26306	0	24646	229	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 5.

The worst 5 of 229 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:D:636:SER:HB3	1:D:658:THR:HG21	1.54	0.87
1:B:303:ALA:HB2	1:B:656:MET:HE1	1.58	0.86
1:B:303:ALA:HB2	1:B:656:MET:CE	2.07	0.85
1:C:10:ILE:HD12	1:C:99:LEU:HD21	1.65	0.78
1:D:709:GLU:CD	1:D:709:GLU:H	1.88	0.76

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	754/764 (99%)	724 (96%)	27 (4%)	3 (0%)	39	28
1	B	754/764 (99%)	729 (97%)	23 (3%)	2 (0%)	46	36
1	C	754/764 (99%)	726 (96%)	23 (3%)	5 (1%)	26	15
1	D	754/764 (99%)	717 (95%)	33 (4%)	4 (0%)	34	22
All	All	3016/3056 (99%)	2896 (96%)	106 (4%)	14 (0%)	34	22

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	742	LYS
1	D	259	VAL
1	D	741	GLU
1	D	258	ASP
1	B	742	LYS

### 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	669/676 (99%)	645 (96%)	24 (4%)	42	34
1	B	669/676 (99%)	651 (97%)	18 (3%)	52	45
1	C	669/676 (99%)	638 (95%)	31 (5%)	33	24
1	D	669/676 (99%)	631 (94%)	38 (6%)	25	15
All	All	2676/2704 (99%)	2565 (96%)	111 (4%)	37	28

5 of 111 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	277	LYS
1	C	650	ARG
1	D	721	LYS
1	C	288	ARG
1	C	539	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	593	GLN
1	A	752	GLN
1	B	101	GLN
1	B	575	ASN

### 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

23 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	BGC	A	801	-	12,12,12	0.75	0	17,17,17	1.63	5 (29%)
2	BGC	A	802	-	12,12,12	0.64	0	17,17,17	2.00	5 (29%)
3	GOL	A	803	-	5,5,5	0.72	0	5,5,5	0.57	0
3	GOL	A	804	-	5,5,5	0.82	0	5,5,5	1.15	1 (20%)
4	PO4	A	805	-	4,4,4	0.45	0	6,6,6	0.31	0
2	BGC	B	801	-	12,12,12	1.26	2 (16%)	17,17,17	1.23	2 (11%)
2	BGC	B	802	-	12,12,12	0.57	0	17,17,17	1.35	2 (11%)
3	GOL	B	803	-	5,5,5	0.42	0	5,5,5	0.97	0
4	PO4	B	804	-	4,4,4	0.92	0	6,6,6	0.33	0
4	PO4	B	805	-	4,4,4	0.63	0	6,6,6	0.28	0
2	BGC	C	801	-	12,12,12	0.55	0	17,17,17	1.33	2 (11%)
2	BGC	C	802	-	12,12,12	0.98	1 (8%)	17,17,17	1.14	2 (11%)
3	GOL	C	803	-	5,5,5	0.64	0	5,5,5	0.49	0
3	GOL	C	804	-	5,5,5	0.38	0	5,5,5	0.28	0
4	PO4	C	805	-	4,4,4	0.76	0	6,6,6	0.33	0
4	PO4	C	806	-	4,4,4	0.55	0	6,6,6	0.29	0
2	BGC	D	801	-	12,12,12	0.68	0	17,17,17	1.01	1 (5%)
2	BGC	D	802	-	12,12,12	1.26	2 (16%)	17,17,17	1.88	6 (35%)
3	GOL	D	803	-	5,5,5	0.68	0	5,5,5	0.45	0
3	GOL	D	804	-	5,5,5	0.74	0	5,5,5	1.09	0
3	GOL	D	805	-	5,5,5	1.09	1 (20%)	5,5,5	0.96	0
3	GOL	D	806	-	5,5,5	0.58	0	5,5,5	0.48	0
4	PO4	D	807	-	4,4,4	0.66	0	6,6,6	0.31	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	801	-	-	0/2/22/22	0/1/1/1
2	BGC	A	802	-	-	0/2/22/22	0/1/1/1
3	GOL	A	803	-	-	0/4/4/4	0/0/0/0
3	GOL	A	804	-	-	0/4/4/4	0/0/0/0
4	PO4	A	805	-	-	0/0/0/0	0/0/0/0
2	BGC	B	801	-	-	0/2/22/22	0/1/1/1
2	BGC	B	802	-	-	0/2/22/22	0/1/1/1
3	GOL	B	803	-	-	0/4/4/4	0/0/0/0
4	PO4	B	804	-	-	0/0/0/0	0/0/0/0
4	PO4	B	805	-	-	0/0/0/0	0/0/0/0
2	BGC	C	801	-	-	0/2/22/22	0/1/1/1
2	BGC	C	802	-	-	0/2/22/22	0/1/1/1
3	GOL	C	803	-	-	0/4/4/4	0/0/0/0
3	GOL	C	804	-	-	0/4/4/4	0/0/0/0
4	PO4	C	805	-	-	0/0/0/0	0/0/0/0
4	PO4	C	806	-	-	0/0/0/0	0/0/0/0
2	BGC	D	801	-	-	0/2/22/22	0/1/1/1
2	BGC	D	802	-	-	0/2/22/22	0/1/1/1
3	GOL	D	803	-	-	0/4/4/4	0/0/0/0
3	GOL	D	804	-	-	0/4/4/4	0/0/0/0
3	GOL	D	805	-	-	0/4/4/4	0/0/0/0
3	GOL	D	806	-	-	0/4/4/4	0/0/0/0
4	PO4	D	807	-	-	0/0/0/0	0/0/0/0

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	802	BGC	O5-C5	-3.03	1.36	1.44
2	D	802	BGC	O1-C1	2.05	1.46	1.39
2	C	802	BGC	O1-C1	2.20	1.47	1.39
2	B	801	BGC	O5-C1	2.21	1.47	1.43
3	D	805	GOL	O2-C2	2.34	1.50	1.43

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	802	BGC	O2-C2-C1	-3.97	101.07	109.82
2	B	802	BGC	O1-C1-O5	-3.45	100.82	110.25
2	D	802	BGC	O2-C2-C1	-3.44	102.24	109.82
2	C	801	BGC	C4-C3-C2	-2.93	105.33	110.79
2	A	801	BGC	C4-C3-C2	-2.76	105.63	110.79

There are no chirality outliers.



There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	803	GOL	1	0
4	B	805	PO4	1	0
3	D	805	GOL	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	756/764 (98%)	-0.04	14 (1%) 70 75	13, 27, 53, 93	0
1	B	756/764 (98%)	-0.05	14 (1%) 70 75	13, 26, 51, 69	0
1	C	756/764 (98%)	-0.12	5 (0%) 89 91	17, 30, 54, 72	0
1	D	756/764 (98%)	-0.03	14 (1%) 70 75	16, 30, 55, 75	0
All	All	3024/3056 (98%)	-0.06	47 (1%) 74 79	13, 29, 53, 93	0

The worst 5 of 47 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	257	GLY	4.7
1	D	743	GLY	4.4
1	A	550	PRO	4.3
1	A	568	VAL	4.1
1	B	568	VAL	3.9

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	GOL	A	804	6/6	0.84	0.25	4.12	33,35,40,41	0
3	GOL	D	803	6/6	0.72	0.17	3.90	44,54,61,61	0
3	GOL	D	804	6/6	0.77	0.28	3.41	55,57,60,64	0
3	GOL	C	803	6/6	0.81	0.18	3.34	46,55,59,62	0
3	GOL	D	806	6/6	0.81	0.12	2.76	46,47,49,49	0
2	BGC	A	802	12/12	0.92	0.13	1.47	21,26,29,32	0
2	BGC	B	802	12/12	0.93	0.14	0.67	19,26,29,31	0
3	GOL	D	805	6/6	0.85	0.13	0.53	27,36,38,50	0
2	BGC	C	802	12/12	0.94	0.10	0.06	20,25,29,30	0
2	BGC	D	802	12/12	0.94	0.12	-0.04	21,26,27,27	0
2	BGC	D	801	12/12	0.97	0.14	-0.11	21,24,25,25	0
2	BGC	B	801	12/12	0.96	0.14	-0.13	20,22,24,26	0
4	PO4	B	805	5/5	0.96	0.10	-0.18	42,43,47,47	0
2	BGC	A	801	12/12	0.95	0.11	-0.32	19,21,23,24	0
2	BGC	C	801	12/12	0.96	0.11	-0.45	19,24,25,25	0
3	GOL	C	804	6/6	0.90	0.11	-0.75	47,49,50,55	0
4	PO4	A	805	5/5	0.99	0.09	-1.25	20,20,23,24	0
4	PO4	B	804	5/5	0.99	0.11	-1.51	18,21,23,26	0
4	PO4	C	806	5/5	0.96	0.09	-1.98	45,46,46,50	0
4	PO4	D	807	5/5	0.99	0.07	-2.37	22,25,27,28	0
4	PO4	C	805	5/5	0.99	0.07	-2.57	22,24,26,27	0
3	GOL	A	803	6/6	0.88	0.14	-	29,41,45,47	0
3	GOL	B	803	6/6	0.91	0.22	-	30,40,42,42	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.