



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 09:00 AM BST

PDB ID : 3QFY  
Title : Crystal Structure of Cellvibrio gilvus Cellobiose Phosphorylase Complexed with Sulfate and Isofagomine  
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Deposited on : 2011-01-24  
Resolution : 2.30 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](mailto: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.

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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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

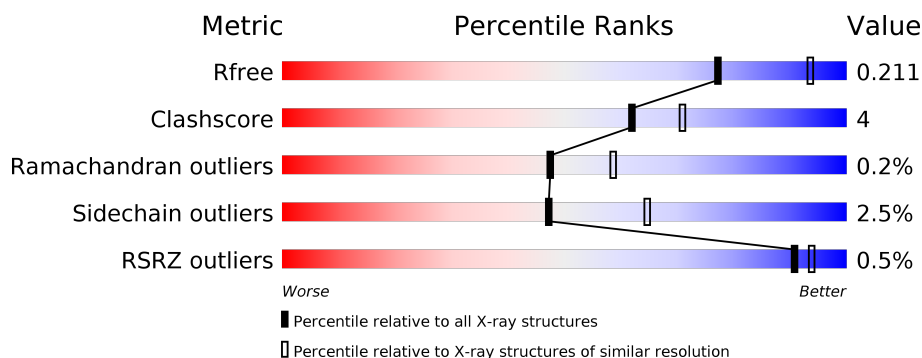
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 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	 87% 10% .
1	B	842	 86% 11% ..

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14083 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
			6428	4066	1102	1246	14			
1	B	822	Total	C	N	O	S	0	0	0
			6428	4066	1102	1246	14			

There are 40 discrepancies between the modelled and reference sequences:

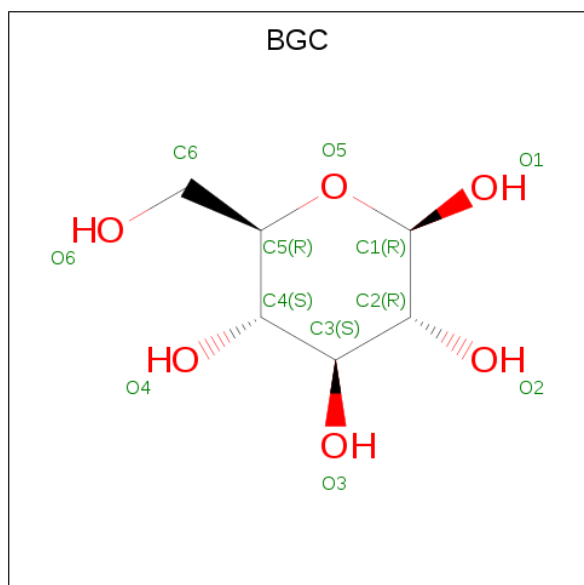
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP O66264
A	-18	GLY	-	expression tag	UNP O66264
A	-17	SER	-	expression tag	UNP O66264
A	-16	SER	-	expression tag	UNP O66264
A	-15	HIS	-	expression tag	UNP O66264
A	-14	HIS	-	expression tag	UNP O66264
A	-13	HIS	-	expression tag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

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Chain	Residue	Modelled	Actual	Comment	Reference
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

- Molecule 2 is beta-D-glucopyranose (three-letter code: BGC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



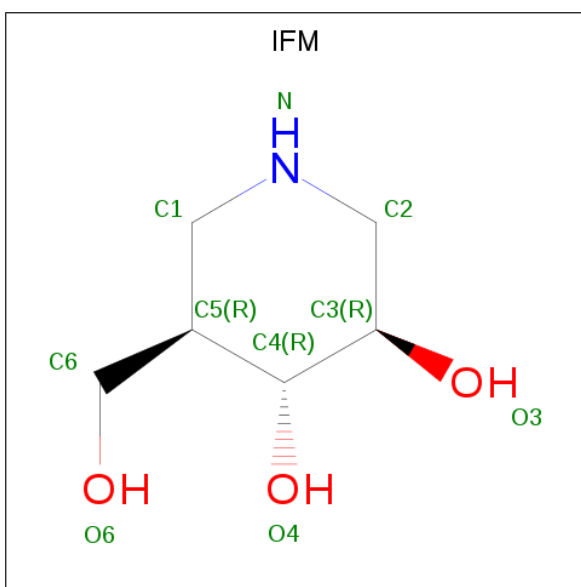
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



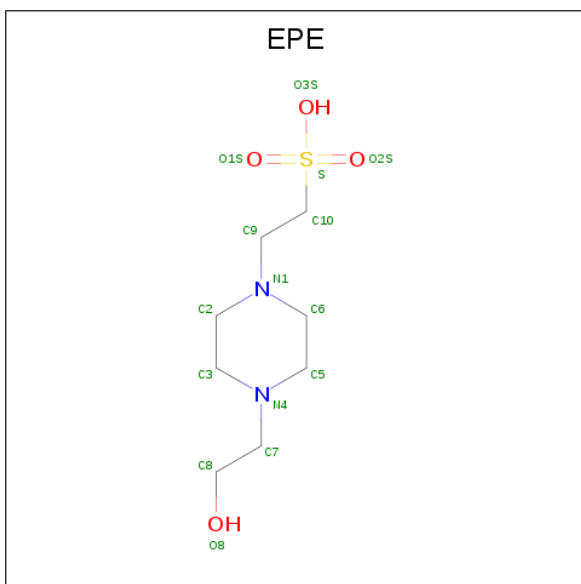
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 5-HYDROXYMETHYL-3,4-DIHYDROXYPIPERIDINE (three-letter code: IFM) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 10	C 6	N 1	O 3	0	0
4	B	1	Total 10	C 6	N 1	O 3	0	0

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula:  $C_8H_{18}N_2O_4S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

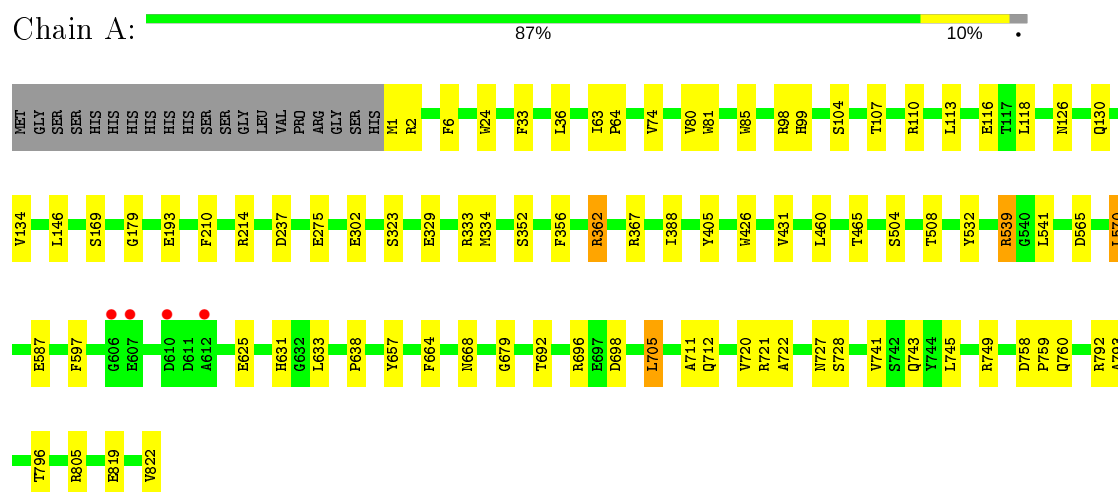
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	558	Total 558	O 558	0	0
6	B	585	Total 585	O 585	0	0

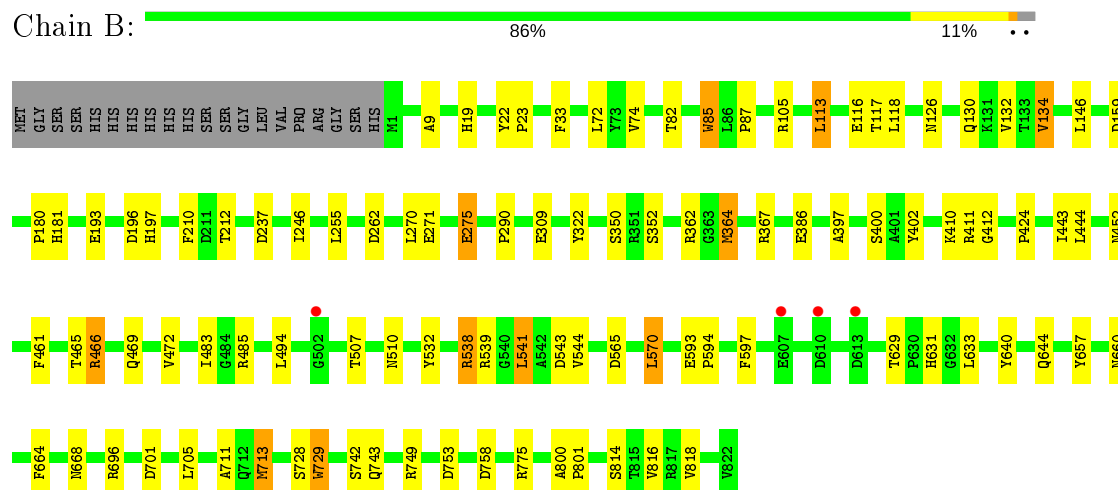
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Cellobiose Phosphorylase



#### • Molecule 1: Cellobiose Phosphorylase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.71Å 98.25Å 104.45Å 90.00° 102.73° 90.00°	Depositor
Resolution (Å)	38.32 – 2.30 42.23 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (38.32-2.30) 99.8 (42.23-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.68 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.138 , 0.208 0.141 , 0.211	Depositor DCC
$R_{free}$ test set	3731 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.5	Xtriage
Anisotropy	0.438	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 38.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14083	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, 0.333 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: BGC, IFM, EPE, SO4

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	1.01	4/6604 (0.1%)	0.87	7/9009 (0.1%)
1	B	0.98	5/6604 (0.1%)	0.86	9/9009 (0.1%)
All	All	1.00	9/13208 (0.1%)	0.86	16/18018 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	275	GLU	CG-CD	6.38	1.61	1.51
1	A	329	GLU	CG-CD	6.23	1.61	1.51
1	B	386	GLU	CG-CD	5.70	1.60	1.51
1	A	302	GLU	CG-CD	5.52	1.60	1.51
1	B	309	GLU	CG-CD	5.49	1.60	1.51
1	B	701	ASP	CB-CG	5.40	1.63	1.51
1	B	9	ALA	CA-CB	5.37	1.63	1.52
1	A	405	TYR	CD2-CE2	5.27	1.47	1.39
1	A	657	TYR	CD2-CE2	5.09	1.47	1.39

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	701	ASP	CB-CG-OD1	8.42	125.88	118.30
1	A	805	ARG	NE-CZ-NH1	-7.88	116.36	120.30
1	A	705	LEU	CB-CG-CD1	6.54	122.12	111.00
1	A	362	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	B	466	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	B	713	MET	CG-SD-CE	-6.04	90.54	100.20
1	A	98	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	B	701	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	B	113	LEU	CB-CG-CD1	5.53	120.41	111.00
1	B	113	LEU	CA-CB-CG	5.49	127.94	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	758	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	A	362	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	805	ARG	NE-CZ-NH2	5.20	122.90	120.30
1	B	196	ASP	CB-CG-OD1	5.20	122.98	118.30
1	B	159	ASP	CB-CG-OD1	-5.09	113.72	118.30
1	A	214	ARG	NE-CZ-NH2	-5.07	117.76	120.30

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	6428	0	6071	49	0
1	B	6428	0	6071	61	0
2	A	12	0	12	0	0
2	B	12	0	12	0	0
3	A	15	0	0	0	0
3	B	10	0	0	0	0
4	A	10	0	13	0	0
4	B	10	0	13	1	0
5	A	15	0	17	1	0
6	A	558	0	0	5	0
6	B	585	0	0	3	0
All	All	14083	0	12209	110	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 (110) 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:796:THR:HG23	1:A:819:GLU:HB3	1.38	1.04
1:A:539:ARG:HG3	1:A:539:ARG:HH21	1.32	0.94
1:B:631:HIS:HD2	1:B:696:ARG:HH12	1.16	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:796:THR:CG2	1:A:819:GLU:HB3	2.02	0.89
1:A:539:ARG:CG	1:A:539:ARG:HH21	1.91	0.84
1:B:631:HIS:CD2	1:B:696:ARG:HH12	1.97	0.82
1:A:631:HIS:HD2	1:A:696:ARG:HH12	1.27	0.82
1:A:633:LEU:H	1:A:668:ASN:HD21	1.32	0.77
1:B:465:THR:HG22	1:B:532:TYR:OH	1.85	0.76
1:A:743:GLN:HB3	1:A:749:ARG:HB3	1.68	0.76
1:B:633:LEU:H	1:B:668:ASN:HD21	1.37	0.71
1:A:539:ARG:HG3	1:A:539:ARG:NH2	2.01	0.69
1:A:134:VAL:HG21	1:A:146:LEU:HD11	1.75	0.69
1:A:631:HIS:CD2	1:A:696:ARG:HH12	2.11	0.68
1:B:465:THR:HG21	6:B:1076:HOH:O	1.94	0.67
1:B:640:TYR:H	1:B:660:ASN:HD21	1.41	0.66
1:A:99:HIS:HD2	1:A:104:SER:OG	1.78	0.65
1:B:134:VAL:HG22	1:B:255:LEU:HD11	1.79	0.65
1:B:350:SER:CB	1:B:364:MET:HE2	2.26	0.65
1:B:364:MET:HE2	1:B:364:MET:HA	1.79	0.65
1:B:711:ALA:HA	1:B:728:SER:HA	1.82	0.62
1:A:565:ASP:HB2	1:A:570:LEU:HD13	1.80	0.62
1:B:350:SER:HB3	1:B:364:MET:HE2	1.80	0.61
1:B:465:THR:HG22	1:B:532:TYR:CE1	2.37	0.60
1:A:6:PHE:CD1	1:A:333:ARG:HD3	2.38	0.58
1:B:270:LEU:HD12	1:B:290:PRO:HB2	1.85	0.58
1:B:465:THR:HG22	1:B:532:TYR:CZ	2.41	0.56
5:A:3001:EPE:H81	6:A:951:HOH:O	2.05	0.56
1:A:352:SER:HA	1:A:362:ARG:HB2	1.90	0.54
1:B:367:ARG:HD2	4:B:2903:IFM:O3	2.08	0.54
1:A:711:ALA:HA	1:A:728:SER:HA	1.91	0.53
1:A:99:HIS:CD2	1:A:104:SER:OG	2.61	0.53
1:B:631:HIS:HD2	1:B:696:ARG:NH1	1.95	0.53
1:B:483:ILE:HG21	1:B:494:LEU:HD12	1.91	0.53
1:A:504:SER:O	1:A:508:THR:HB	2.09	0.53
1:B:465:THR:CG2	1:B:532:TYR:OH	2.56	0.53
1:B:538:ARG:HH11	1:B:538:ARG:HG3	1.75	0.52
1:B:322:TYR:CE1	1:B:742:SER:HB2	2.44	0.52
1:A:720:VAL:HG23	6:A:1067:HOH:O	2.11	0.51
1:A:334:MET:HG3	1:A:692:THR:CG2	2.41	0.51
1:A:1:MET:HG3	1:A:2:ARG:N	2.25	0.50
1:B:22:TYR:CD2	1:B:23:PRO:HD2	2.47	0.50
1:A:741:VAL:HA	1:A:745:LEU:HB2	1.94	0.50
1:B:402:TYR:CD2	1:B:412:GLY:HA3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:SER:HB2	1:B:364:MET:HE2	1.93	0.49
1:B:350:SER:CB	1:B:364:MET:CE	2.91	0.48
1:B:469:GLN:HA	1:B:472:VAL:HG13	1.96	0.48
1:A:33:PHE:HB2	1:A:126:ASN:HD22	1.78	0.48
1:B:728:SER:O	1:B:729:TRP:HB2	2.12	0.48
1:B:593:GLU:N	1:B:594:PRO:HD2	2.28	0.48
1:B:352:SER:HA	1:B:362:ARG:HB2	1.96	0.48
1:B:105:ARG:HD3	1:B:116:GLU:OE2	2.15	0.47
1:A:169:SER:HB3	1:B:657:TYR:HB3	1.97	0.47
1:A:179:GLY:HA3	6:A:1128:HOH:O	2.12	0.47
1:A:465:THR:HG22	1:A:532:TYR:OH	2.13	0.47
1:A:367:ARG:HB2	1:A:426:TRP:CD1	2.50	0.47
1:A:81:TRP:CG	1:A:110:ARG:HD3	2.50	0.47
1:B:210:PHE:O	1:B:237:ASP:HA	2.15	0.46
1:B:743:GLN:HB3	1:B:749:ARG:HB3	1.97	0.46
1:A:210:PHE:O	1:A:237:ASP:HA	2.16	0.46
1:A:587:GLU:HA	1:A:638:PRO:HD2	1.96	0.46
1:A:74:VAL:O	1:A:80:VAL:HA	2.16	0.46
1:B:350:SER:HB2	1:B:364:MET:CE	2.46	0.46
1:A:793:ALA:HB2	1:A:822:VAL:HG22	1.97	0.45
1:B:33:PHE:HB2	1:B:126:ASN:HD22	1.82	0.45
1:B:538:ARG:NH1	1:B:538:ARG:HG3	2.31	0.45
1:B:485:ARG:HA	1:B:510:ASN:ND2	2.31	0.45
1:B:565:ASP:HB2	1:B:570:LEU:HD13	1.98	0.45
1:B:350:SER:HB3	1:B:364:MET:CE	2.46	0.45
1:B:461:PHE:O	1:B:465:THR:HG23	2.17	0.45
1:A:36:LEU:N	1:A:36:LEU:HD12	2.31	0.44
1:A:356:PHE:CB	1:A:727:ASN:HD22	2.30	0.44
1:A:721:ARG:O	1:A:722:ALA:C	2.55	0.44
1:B:74:VAL:HG22	1:B:146:LEU:HD22	2.00	0.44
1:B:72:LEU:HD21	1:B:146:LEU:HD13	2.00	0.44
1:B:411:ARG:HE	1:B:452:ASN:ND2	2.16	0.44
1:B:485:ARG:HA	1:B:510:ASN:HD21	1.81	0.44
1:A:633:LEU:H	1:A:668:ASN:ND2	2.09	0.44
1:B:118:LEU:O	1:B:130:GLN:HA	2.18	0.44
1:B:775:ARG:HA	6:B:1323:HOH:O	2.19	0.43
1:B:132:VAL:O	1:B:262:ASP:HA	2.18	0.43
1:B:541:LEU:HB3	1:B:544:VAL:HB	2.00	0.43
1:A:356:PHE:HB3	1:A:727:ASN:ND2	2.33	0.43
1:A:63:ILE:HA	1:A:64:PRO:HA	1.82	0.43
1:A:760:GLN:NE2	6:A:975:HOH:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:HIS:HB3	1:B:271:GLU:HG2	2.01	0.42
1:B:402:TYR:CG	1:B:412:GLY:HA3	2.53	0.42
1:B:105:ARG:HA	1:B:117:THR:O	2.19	0.42
1:B:19:HIS:HD2	6:B:1399:HOH:O	2.02	0.42
1:A:323:SER:HB3	6:A:990:HOH:O	2.19	0.42
1:B:800:ALA:HA	1:B:801:PRO:HD3	1.94	0.42
1:B:444:LEU:HD13	1:B:539:ARG:HD2	2.01	0.42
1:A:388:ILE:HG21	1:A:431:VAL:HG22	2.02	0.42
1:A:539:ARG:CB	1:A:539:ARG:HH21	2.33	0.42
1:B:180:PRO:HB2	1:B:181:HIS:CD2	2.55	0.42
1:B:397:ALA:O	1:B:466:ARG:HD2	2.20	0.42
1:A:24:TRP:O	1:A:99:HIS:HE1	2.02	0.42
1:A:741:VAL:HA	1:A:745:LEU:HD12	2.02	0.42
1:A:758:ASP:N	1:A:759:PRO:HD3	2.35	0.41
1:B:212:THR:HA	1:B:246:ILE:O	2.20	0.41
1:B:19:HIS:HE1	1:B:85:TRP:CZ2	2.39	0.41
1:B:400:SER:HA	1:B:424:PRO:HG3	2.03	0.41
1:B:640:TYR:CD1	1:B:644:GLN:HG3	2.55	0.41
1:B:82:THR:HG21	1:B:87:PRO:HD2	2.03	0.41
1:A:2:ARG:HD3	1:A:698:ASP:OD1	2.20	0.41
1:B:465:THR:HG22	1:B:532:TYR:HE1	1.85	0.40
1:A:118:LEU:O	1:A:130:GLN:HA	2.21	0.40
1:A:679:GLY:HA2	1:A:760:GLN:NE2	2.36	0.40
1:A:712:GLN:HB3	1:A:727:ASN:HB2	2.03	0.40
1:A:107:THR:OG1	1:A:116:GLU:HG3	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	820/842 (97%)	786 (96%)	33 (4%)	1 (0%)	51 64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	820/842 (97%)	783 (96%)	35 (4%)	2 (0%)	47 58
All	All	1640/1684 (97%)	1569 (96%)	68 (4%)	3 (0%)	47 58

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	85	TRP
1	A	85	TRP
1	B	729	TRP

### 5.3.2 Protein sidechains ⓘ

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%)	653 (98%)	12 (2%)	59 75
1	B	665/682 (98%)	644 (97%)	21 (3%)	39 54
All	All	1330/1364 (98%)	1297 (98%)	33 (2%)	47 65

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	LEU
1	A	193	GLU
1	A	275	GLU
1	A	460	LEU
1	A	539	ARG
1	A	541	LEU
1	A	570	LEU
1	A	597	PHE
1	A	625	GLU
1	A	664	PHE
1	A	705	LEU
1	A	792	ARG
1	B	113	LEU

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Mol	Chain	Res	Type
1	B	134	VAL
1	B	193	GLU
1	B	275	GLU
1	B	364	MET
1	B	410	LYS
1	B	443	ILE
1	B	507	THR
1	B	538	ARG
1	B	541	LEU
1	B	543	ASP
1	B	570	LEU
1	B	597	PHE
1	B	629	THR
1	B	664	PHE
1	B	705	LEU
1	B	713	MET
1	B	753	ASP
1	B	814	SER
1	B	816	VAL
1	B	818	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	HIS
1	A	126	ASN
1	A	339	ASN
1	A	631	HIS
1	A	668	ASN
1	A	727	ASN
1	A	760	GLN
1	B	19	HIS
1	B	94	HIS
1	B	126	ASN
1	B	130	GLN
1	B	161	GLN
1	B	339	ASN
1	B	406	GLN
1	B	452	ASN
1	B	469	GLN
1	B	473	GLN
1	B	510	ASN

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Mol	Chain	Res	Type
1	B	624	ASN
1	B	631	HIS
1	B	660	ASN
1	B	668	ASN
1	B	737	ASN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

10 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	$\# Z  > 2$
5	EPE	A	3001	-	15,15,15	0.80	1 (6%)	18,20,20	2.07	6 (33%)
4	IFM	A	1903	-	9,10,10	1.28	1 (11%)	9,13,13	1.74	3 (33%)
3	SO4	B	3002	-	4,4,4	0.16	0	6,6,6	0.53	0
2	BGC	A	1901	-	12,12,12	0.84	0	17,17,17	1.25	1 (5%)
2	BGC	B	2901	-	12,12,12	0.78	0	17,17,17	1.38	3 (17%)
3	SO4	A	3004	-	4,4,4	0.09	0	6,6,6	0.49	0
3	SO4	A	1902	-	4,4,4	0.27	0	6,6,6	0.53	0
4	IFM	B	2903	-	9,10,10	1.32	1 (11%)	9,13,13	1.92	2 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	B	2902	-	4,4,4	0.37	0	6,6,6	0.36	0
3	SO4	A	3003	-	4,4,4	0.25	0	6,6,6	0.37	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
4	IFM	B	2903	-	-	0/2/16/16	0/1/1/1
5	EPE	A	3001	-	-	1/9/19/19	0/1/1/1
2	BGC	A	1901	-	-	0/2/22/22	0/1/1/1
2	BGC	B	2901	-	-	1/2/22/22	0/1/1/1
4	IFM	A	1903	-	-	0/2/16/16	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	3001	EPE	C10-S	2.45	1.81	1.77
4	A	1903	IFM	C2-N	2.39	1.50	1.46
4	B	2903	IFM	C2-C3	2.09	1.54	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	3001	EPE	C5-N4-C3	4.63	119.24	108.83
4	B	2903	IFM	C1-N-C2	4.00	116.10	111.70
5	A	3001	EPE	O3S-S-C10	3.94	112.14	105.77
4	A	1903	IFM	O4-C4-C3	-3.21	103.85	109.99
5	A	3001	EPE	O2S-S-C10	3.00	110.52	106.92
5	A	3001	EPE	C7-N4-C5	2.81	118.41	111.23
2	B	2901	BGC	O5-C5-C6	-2.74	99.61	106.44
2	B	2901	BGC	O1-C1-O5	-2.40	103.18	110.38
4	B	2903	IFM	O3-C3-C4	-2.36	105.41	110.14
5	A	3001	EPE	C2-C3-N4	2.34	115.45	110.64
4	A	1903	IFM	C1-N-C2	2.31	114.24	111.70
5	A	3001	EPE	C7-N4-C3	2.28	117.05	111.23
2	A	1901	BGC	O5-C5-C6	2.27	112.08	106.44
4	A	1903	IFM	O4-C4-C5	2.23	113.85	110.08
2	B	2901	BGC	O5-C5-C4	-2.09	105.90	109.69

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	3001	EPE	C8-C7-N4-C3
2	B	2901	BGC	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	3001	EPE	1	0
4	B	2903	IFM	1	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	822/842 (97%)	-0.50	4 (0%) 91 94	12, 21, 33, 52	0
1	B	822/842 (97%)	-0.54	4 (0%) 91 94	13, 21, 34, 54	0
All	All	1644/1684 (97%)	-0.52	8 (0%) 91 94	12, 21, 34, 54	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	606	GLY	3.1
1	A	610	ASP	3.1
1	A	612	ALA	2.9
1	B	610	ASP	2.7
1	B	607	GLU	2.7
1	B	613	ASP	2.4
1	A	607	GLU	2.4
1	B	502	GLY	2.3

### 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 monosaccharides 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, 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	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	A	3004	5/5	0.89	0.22	74,75,77,77	0
5	EPE	A	3001	15/15	0.94	0.23	50,52,55,56	0
3	SO4	A	3003	5/5	0.96	0.23	52,54,54,56	0
4	IFM	B	2903	10/10	0.97	0.21	19,20,21,25	0
3	SO4	B	3002	5/5	0.97	0.19	53,53,53,54	0
4	IFM	A	1903	10/10	0.99	0.19	18,19,21,24	0
2	BGC	A	1901	12/12	0.99	0.12	15,17,19,20	0
3	SO4	B	2902	5/5	0.99	0.14	16,17,19,22	0
2	BGC	B	2901	12/12	0.99	0.13	14,19,22,22	0
3	SO4	A	1902	5/5	1.00	0.14	20,22,23,24	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.