



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 02:18 PM BST

PDB ID : 3QFZ  
Title : Crystal Structure of Cellvibrio gilvus Cellobiose Phosphorylase Complexed with Sulfate and 1-Deoxynojirimycin  
Authors : Fushinobu, S.; Hidaka, M.; Hayashi, A.M.; Wakagi, T.; Shoun, H.; Kitaoka, M.  
Deposited on : 2011-01-24  
Resolution : 2.39 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

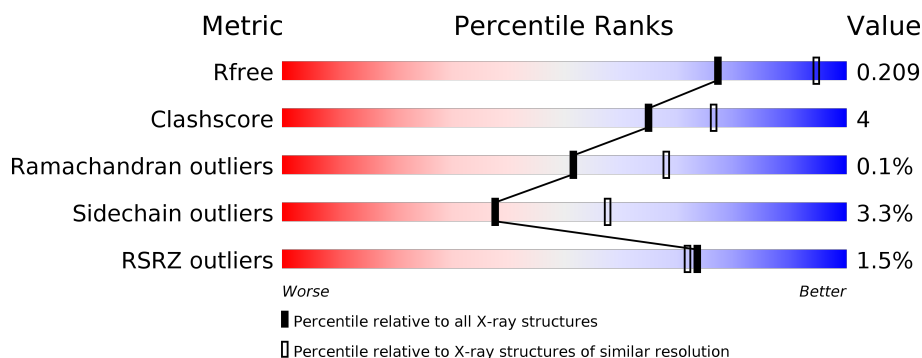
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.39 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div>..</div> </div> </div>
1	B	842	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>12%</div> <div>..</div> </div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13721 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:

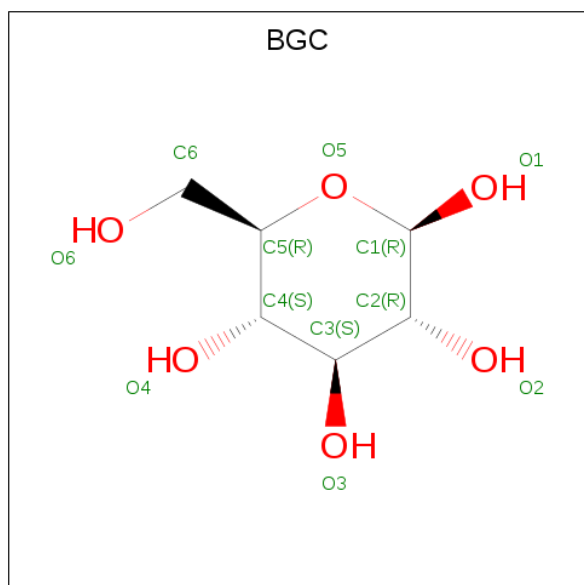
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP O66264
A	-18	GLY	-	expression tag	UNP O66264
A	-17	SER	-	expression tag	UNP O66264
A	-16	SER	-	expression tag	UNP O66264
A	-15	HIS	-	expression tag	UNP O66264
A	-14	HIS	-	expression tag	UNP O66264
A	-13	HIS	-	expression tag	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:  $C_6H_{12}O_6$ ).



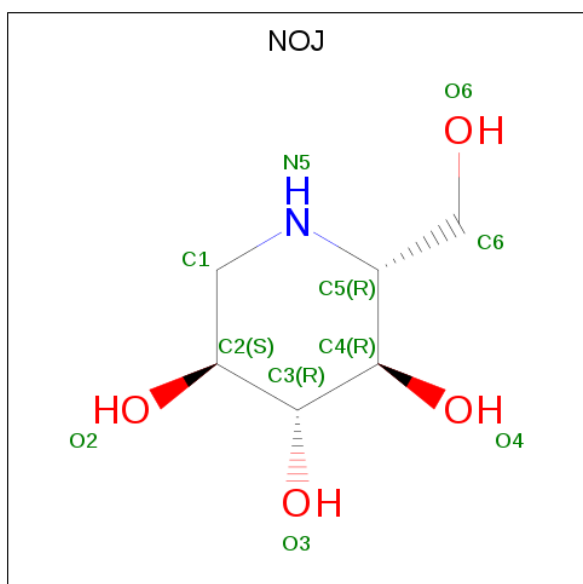
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



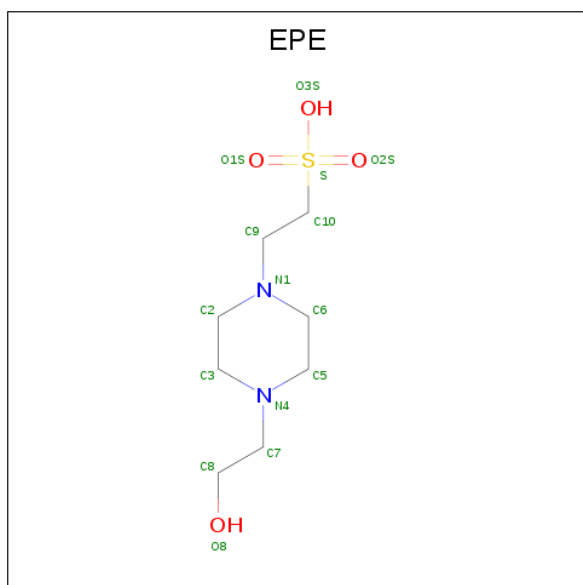
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 1-DEOXYNOJIRIMYCIN (three-letter code: NOJ) (formula:  $C_6H_{13}NO_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			11	6	1	4		
4	B	1	Total	C	N	O	0	0
			11	6	1	4		

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



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

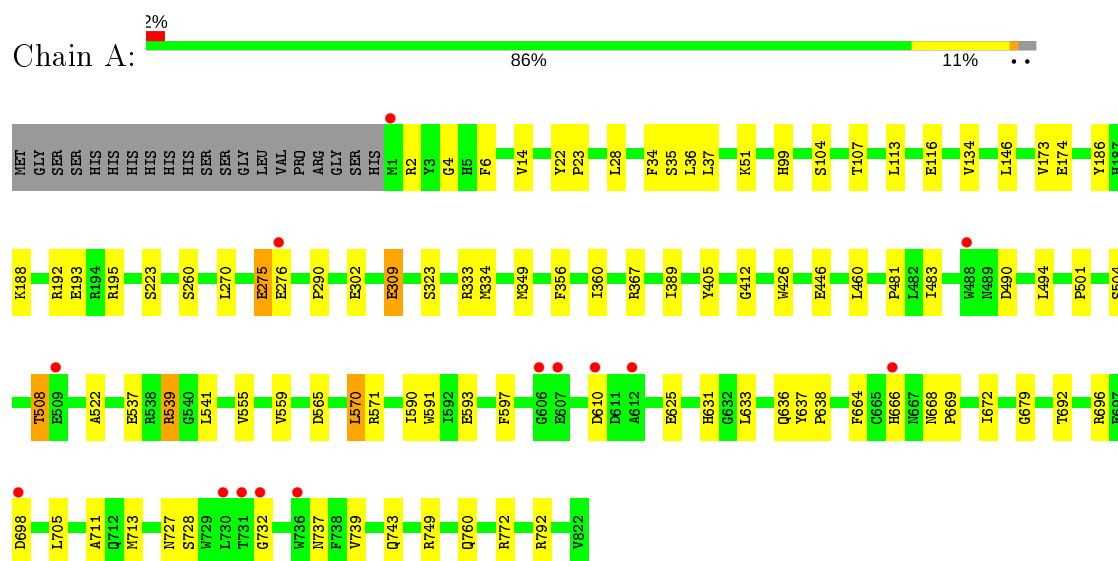
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	398	Total	O	0	0
			398	398		
6	B	381	Total	O	0	0
			381	381		

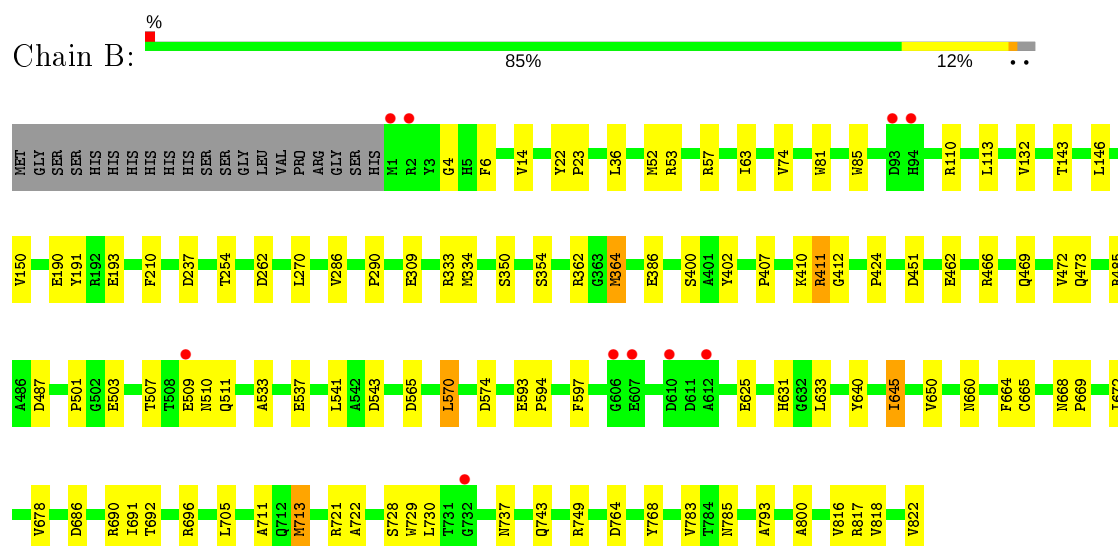
### 3 Residue-property plots [i](#)

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



#### • Molecule 1: Cellobiose Phosphorylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.91Å 98.13Å 104.78Å 90.00° 102.53° 90.00°	Depositor
Resolution (Å)	36.27 – 2.39 37.59 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.3 (36.27-2.39) 99.5 (37.59-2.39)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.10 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.141 , 0.208 0.146 , 0.209	Depositor DCC
$R_{free}$ test set	3338 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.5	Xtriage
Anisotropy	0.701	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 36.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	13721	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BGC, EPE, SO4, NOJ

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	0.91	4/6604 (0.1%)	0.82	1/9009 (0.0%)
1	B	0.93	3/6604 (0.0%)	0.84	4/9009 (0.0%)
All	All	0.92	7/13208 (0.1%)	0.83	5/18018 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	625	GLU	CG-CD	6.73	1.62	1.51
1	B	309	GLU	CG-CD	6.55	1.61	1.51
1	A	537	GLU	CG-CD	6.19	1.61	1.51
1	B	386	GLU	CG-CD	6.14	1.61	1.51
1	A	302	GLU	CG-CD	6.10	1.61	1.51
1	A	275	GLU	CG-CD	5.97	1.60	1.51
1	A	309	GLU	CG-CD	5.55	1.60	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	713	MET	CA-CB-CG	6.00	123.49	113.30
1	B	57	ARG	NE-CZ-NH2	5.78	123.19	120.30
1	B	487	ASP	CB-CG-OD1	5.72	123.45	118.30
1	A	192	ARG	NE-CZ-NH1	-5.09	117.75	120.30
1	B	817	ARG	NE-CZ-NH1	5.02	122.81	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	50	0
1	B	6428	0	6071	53	0
2	A	12	0	12	1	0
2	B	12	0	12	0	0
3	A	15	0	0	0	0
3	B	10	0	0	0	0
4	A	11	0	13	0	0
4	B	11	0	13	0	0
5	A	15	0	17	1	0
6	A	398	0	0	3	0
6	B	381	0	0	4	0
All	All	13721	0	12209	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:631:HIS:HD2	1:B:696:ARG:HH12	1.12	0.97
1:B:631:HIS:CD2	1:B:696:ARG:HH12	1.96	0.84
1:B:640:TYR:H	1:B:660:ASN:HD21	1.33	0.76
1:A:539:ARG:HG3	1:A:539:ARG:HH21	1.50	0.76
1:B:633:LEU:H	1:B:668:ASN:HD21	1.31	0.75
1:A:633:LEU:H	1:A:668:ASN:HD21	1.35	0.74
1:B:533:ALA:O	1:B:537:GLU:HG3	1.88	0.74
1:A:631:HIS:HD2	1:A:696:ARG:HH12	1.37	0.69
1:A:539:ARG:CG	1:A:539:ARG:HH21	2.04	0.69
1:B:743:GLN:HB3	1:B:749:ARG:HB3	1.75	0.68
1:A:99:HIS:HD2	1:A:104:SER:OG	1.81	0.64
1:A:28:LEU:HB2	1:A:35:SER:HB2	1.78	0.63
1:A:631:HIS:CD2	1:A:696:ARG:HH12	2.16	0.63
1:B:728:SER:O	1:B:729:TRP:HB2	1.98	0.62
1:B:334:MET:HG3	1:B:692:THR:CG2	2.30	0.62
1:A:539:ARG:HG3	1:A:539:ARG:NH2	2.13	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:PHE:O	1:B:237:ASP:HA	2.00	0.61
1:B:633:LEU:H	1:B:668:ASN:ND2	1.99	0.60
1:B:469:GLN:HA	1:B:472:VAL:HG13	1.83	0.59
1:B:645:ILE:HG22	6:B:881:HOH:O	2.03	0.58
5:A:3001:EPE:H81	6:A:1142:HOH:O	2.03	0.58
1:B:631:HIS:HD2	1:B:696:ARG:NH1	1.92	0.56
1:A:174:GLU:HG3	1:A:188:LYS:HE2	1.87	0.56
1:A:711:ALA:HA	1:A:728:SER:HA	1.86	0.55
1:B:143:THR:HG22	1:B:254:THR:HG22	1.88	0.54
1:A:504:SER:O	1:A:508:THR:HB	2.08	0.54
1:B:800:ALA:HB3	6:B:1013:HOH:O	2.07	0.54
1:A:134:VAL:HG21	1:A:146:LEU:HD11	1.91	0.52
1:A:666:HIS:O	1:A:669:PRO:HD2	2.08	0.52
1:B:650:VAL:O	1:B:660:ASN:HB2	2.10	0.52
1:B:686:ASP:O	1:B:690:ARG:HG3	2.10	0.52
1:B:485:ARG:HA	1:B:510:ASN:ND2	2.25	0.51
1:A:270:LEU:HD12	1:A:290:PRO:HB2	1.92	0.51
1:A:6:PHE:CD1	1:A:333:ARG:HD3	2.45	0.51
1:B:711:ALA:HA	1:B:728:SER:HA	1.91	0.51
1:A:34:PHE:CG	1:A:349:MET:HE1	2.46	0.51
1:B:472:VAL:HG22	1:B:473:GLN:HG3	1.93	0.51
1:B:462:GLU:O	1:B:466:ARG:HG2	2.11	0.51
1:B:36:LEU:HD12	1:B:36:LEU:N	2.27	0.50
1:B:565:ASP:HB2	1:B:570:LEU:HD13	1.93	0.50
1:A:22:TYR:CG	1:A:23:PRO:HD2	2.48	0.49
1:B:22:TYR:CD2	1:B:23:PRO:HD2	2.48	0.49
1:B:22:TYR:CG	1:B:23:PRO:HD2	2.48	0.48
1:B:191:TYR:CE2	1:B:286:VAL:HG12	2.49	0.48
1:B:270:LEU:HD12	1:B:290:PRO:HB2	1.95	0.48
1:A:739:VAL:O	1:A:743:GLN:HB2	2.13	0.47
1:A:2:ARG:HD3	1:A:698:ASP:OD1	2.14	0.47
1:B:4:GLY:HA3	1:B:14:VAL:O	2.15	0.47
1:A:37:LEU:HD23	1:A:104:SER:HB2	1.96	0.47
1:B:132:VAL:O	1:B:262:ASP:HA	2.15	0.47
1:B:6:PHE:CD1	1:B:333:ARG:HD3	2.50	0.47
1:A:389:ILE:CD1	1:A:446:GLU:HG2	2.45	0.47
1:B:793:ALA:HB2	1:B:822:VAL:HG22	1.98	0.46
1:A:481:PRO:HD2	1:A:522:ALA:HB2	1.97	0.46
1:A:323:SER:HB3	6:A:968:HOH:O	2.16	0.46
1:A:134:VAL:O	1:A:260:SER:HA	2.16	0.45
1:B:669:PRO:HA	1:B:672:ILE:HD12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:GLY:HA3	1:A:14:VAL:O	2.16	0.45
1:B:768:TYR:CE1	1:B:783:VAL:HG21	2.51	0.45
1:A:669:PRO:HA	1:A:672:ILE:HD12	1.99	0.45
1:B:364:MET:HE3	1:B:407:PRO:HG3	1.99	0.45
1:A:637:TYR:CD1	1:A:638:PRO:HA	2.52	0.44
1:B:354:SER:HB3	1:B:730:LEU:HG	1.99	0.44
1:A:99:HIS:CD2	1:A:104:SER:OG	2.67	0.44
1:A:483:ILE:HG21	1:A:494:LEU:HD12	2.00	0.44
1:B:665:CYS:O	1:B:669:PRO:HD3	2.18	0.44
1:A:501:PRO:HG2	6:B:1108:HOH:O	2.17	0.44
1:A:555:VAL:O	1:A:559:VAL:HG23	2.18	0.44
1:A:490:ASP:OD2	2:A:1901:BGC:O4	2.27	0.43
1:B:400:SER:HA	1:B:424:PRO:HG3	2.00	0.43
1:B:574:ASP:HB2	6:B:839:HOH:O	2.17	0.43
1:A:405:TYR:HA	1:A:412:GLY:HA2	2.00	0.43
1:B:668:ASN:N	1:B:669:PRO:CD	2.82	0.43
1:B:411:ARG:NH2	1:B:451:ASP:OD1	2.52	0.43
1:B:691:ILE:HD11	1:B:737:ASN:HD21	1.84	0.43
1:B:485:ARG:HA	1:B:510:ASN:HD21	1.84	0.43
1:B:402:TYR:CD2	1:B:412:GLY:HA3	2.55	0.42
1:B:743:GLN:CB	1:B:749:ARG:HB3	2.47	0.42
1:A:334:MET:HG3	1:A:692:THR:CG2	2.50	0.42
1:B:52:MET:O	1:B:53:ARG:HD3	2.19	0.42
6:A:885:HOH:O	1:B:190:GLU:HA	2.19	0.42
1:A:571:ARG:HE	1:A:593:GLU:CD	2.23	0.42
1:A:173:VAL:HA	1:A:186:TYR:O	2.19	0.42
1:A:356:PHE:HB3	1:A:727:ASN:ND2	2.35	0.42
1:A:571:ARG:HG2	1:A:591:TRP:CD2	2.55	0.42
1:A:223:SER:HA	1:B:63:ILE:HG22	2.00	0.42
1:A:107:THR:OG1	1:A:116:GLU:HG3	2.20	0.41
1:B:593:GLU:N	1:B:594:PRO:HD2	2.34	0.41
1:A:356:PHE:CB	1:A:727:ASN:HD22	2.34	0.41
1:A:666:HIS:ND1	1:A:732:GLY:HA3	2.34	0.41
1:B:81:TRP:CG	1:B:110:ARG:HD3	2.55	0.41
1:A:590:ILE:O	1:A:636:GLN:HA	2.21	0.41
1:A:195:ARG:HG2	1:B:501:PRO:HB3	2.02	0.41
1:A:367:ARG:HB2	1:A:426:TRP:CD1	2.56	0.41
1:A:51:LYS:HG3	1:A:360:ILE:HA	2.03	0.41
1:A:743:GLN:HB3	1:A:749:ARG:HB3	2.03	0.41
1:B:721:ARG:O	1:B:722:ALA:C	2.58	0.41
1:A:679:GLY:HA2	1:A:760:GLN:NE2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:640:TYR:N	1:B:660:ASN:HD21	2.10	0.40
1:A:565:ASP:HB2	1:A:570:LEU:HD13	2.04	0.40
1:A:36:LEU:N	1:A:36:LEU:HD12	2.36	0.40
1:B:74:VAL:HG22	1:B:146:LEU:HD22	2.03	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%)	785 (96%)	35 (4%)	0	100	100
1	B	820/842 (97%)	776 (95%)	43 (5%)	1 (0%)	51	68
All	All	1640/1684 (97%)	1561 (95%)	78 (5%)	1 (0%)	51	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	85	TRP

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	665/682 (98%)	646 (97%)	19 (3%)	42	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	665/682 (98%)	640 (96%)	25 (4%)	33 51
All	All	1330/1364 (98%)	1286 (97%)	44 (3%)	38 57

All (44) 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	276	GLU
1	A	309	GLU
1	A	460	LEU
1	A	508	THR
1	A	539	ARG
1	A	541	LEU
1	A	570	LEU
1	A	597	PHE
1	A	610	ASP
1	A	625	GLU
1	A	664	PHE
1	A	705	LEU
1	A	713	MET
1	A	737	ASN
1	A	772	ARG
1	A	792	ARG
1	B	113	LEU
1	B	150	VAL
1	B	193	GLU
1	B	350	SER
1	B	362	ARG
1	B	364	MET
1	B	410	LYS
1	B	411	ARG
1	B	503	GLU
1	B	507	THR
1	B	509	GLU
1	B	511	GLN
1	B	541	LEU
1	B	543	ASP
1	B	570	LEU
1	B	597	PHE
1	B	645	ILE

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Mol	Chain	Res	Type
1	B	664	PHE
1	B	678	VAL
1	B	705	LEU
1	B	713	MET
1	B	764	ASP
1	B	785	ASN
1	B	816	VAL
1	B	818	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	HIS
1	A	126	ASN
1	A	130	GLN
1	A	256	GLN
1	A	339	ASN
1	A	562	HIS
1	A	624	ASN
1	A	631	HIS
1	A	668	ASN
1	A	727	ASN
1	A	737	ASN
1	A	760	GLN
1	B	19	HIS
1	B	32	GLN
1	B	126	ASN
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
1	B	511	GLN
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	$\# Z  > 2$
3	SO4	A	3004	-	4,4,4	0.25	0	6,6,6	0.51	0
4	NOJ	B	2903	-	11,11,11	0.94	1 (9%)	13,15,15	1.13	1 (7%)
3	SO4	A	1902	-	4,4,4	0.29	0	6,6,6	0.66	0
2	BGC	A	1901	-	12,12,12	0.79	0	17,17,17	1.35	2 (11%)
3	SO4	B	3002	-	4,4,4	0.07	0	6,6,6	0.37	0
3	SO4	B	2902	-	4,4,4	0.25	0	6,6,6	0.34	0
2	BGC	B	2901	-	12,12,12	0.81	0	17,17,17	1.58	4 (23%)
5	EPE	A	3001	-	15,15,15	0.86	1 (6%)	18,20,20	2.75	9 (50%)
4	NOJ	A	1903	-	11,11,11	1.04	1 (9%)	13,15,15	1.90	3 (23%)
3	SO4	A	3003	-	4,4,4	0.26	0	6,6,6	0.53	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	NOJ	B	2903	-	-	0/2/19/19	0/1/1/1
2	BGC	B	2901	-	-	0/2/22/22	0/1/1/1
4	NOJ	A	1903	-	-	0/2/19/19	0/1/1/1
2	BGC	A	1901	-	-	0/2/22/22	0/1/1/1
5	EPE	A	3001	-	-	3/9/19/19	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	2.76	1.81	1.77
4	A	1903	NOJ	C2-C3	2.36	1.56	1.52
4	B	2903	NOJ	C1-C2	2.20	1.54	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	3001	EPE	O3S-S-C10	6.93	116.97	105.77
5	A	3001	EPE	C5-N4-C3	5.14	120.41	108.83
4	A	1903	NOJ	C1-N5-C5	4.63	119.62	109.61
5	A	3001	EPE	C6-N1-C2	3.60	116.94	108.83
2	B	2901	BGC	O5-C1-C2	-3.31	104.38	110.28
5	A	3001	EPE	C7-N4-C3	3.11	119.19	111.23
2	A	1901	BGC	O5-C1-C2	-3.08	104.80	110.28
5	A	3001	EPE	C2-C3-N4	2.96	116.72	110.64
4	A	1903	NOJ	C1-C2-C3	2.93	113.77	110.33
2	B	2901	BGC	O5-C5-C4	-2.87	104.49	109.69
5	A	3001	EPE	C7-N4-C5	2.84	118.49	111.23
4	A	1903	NOJ	O4-C4-C3	-2.78	103.92	110.35
2	A	1901	BGC	O1-C1-O5	-2.61	102.54	110.38
5	A	3001	EPE	C3-C2-N1	2.34	115.44	110.64
5	A	3001	EPE	O2S-S-C10	-2.21	104.26	106.92
5	A	3001	EPE	C9-N1-C6	-2.19	105.64	111.23
4	B	2903	NOJ	O3-C3-C2	-2.13	105.92	109.99
2	B	2901	BGC	O1-C1-C2	2.07	114.85	109.03
2	B	2901	BGC	O1-C1-O5	-2.01	104.35	110.38

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	3001	EPE	N4-C7-C8-O8
5	A	3001	EPE	S-C10-C9-N1

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Mol	Chain	Res	Type	Atoms
5	A	3001	EPE	C8-C7-N4-C3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1901	BGC	1	0
5	A	3001	EPE	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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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%)	-0.20	14 (1%) 70 68	17, 27, 41, 57	0
1	B	822/842 (97%)	-0.23	10 (1%) 79 77	19, 28, 42, 58	0
All	All	1644/1684 (97%)	-0.21	24 (1%) 73 72	17, 27, 41, 58	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	612	ALA	3.2
1	A	610	ASP	3.0
1	B	610	ASP	3.0
1	A	612	ALA	2.9
1	A	730	LEU	2.9
1	B	607	GLU	2.8
1	A	731	THR	2.6
1	B	1	MET	2.6
1	B	606	GLY	2.6
1	B	2	ARG	2.5
1	A	607	GLU	2.4
1	A	1	MET	2.3
1	A	736	TRP	2.3
1	B	94	HIS	2.3
1	B	93	ASP	2.2
1	A	606	GLY	2.2
1	B	732	GLY	2.2
1	B	509	GLU	2.1
1	A	488	TRP	2.1
1	A	732	GLY	2.1
1	A	509	GLU	2.1
1	A	276	GLU	2.0
1	A	666	HIS	2.0
1	A	698	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 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	0.82	0.25	86,86,88,89	0
5	EPE	A	3001	15/15	0.91	0.34	69,71,74,74	0
3	SO4	B	3002	5/5	0.96	0.25	59,59,60,60	0
4	NOJ	A	1903	11/11	0.96	0.27	26,32,34,35	0
3	SO4	A	3003	5/5	0.96	0.26	54,55,58,58	0
4	NOJ	B	2903	11/11	0.98	0.14	26,28,30,32	0
2	BGC	A	1901	12/12	0.99	0.13	23,24,27,27	0
3	SO4	A	1902	5/5	0.99	0.20	25,25,27,30	0
2	BGC	B	2901	12/12	0.99	0.10	17,21,24,25	0
3	SO4	B	2902	5/5	1.00	0.13	20,21,22,24	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.