



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 01:57 PM BST

PDB ID : 3QG0  
Title : Crystal Structure of Cellvibrio gilvus Cellobiose Phosphorylase Complexed with Phosphate and 1-Deoxynojirimycin  
Authors : Fushinobu, S.; Hidaka, M.; Hayashi, A.M.; Wakagi, T.; Shoun, H.; Kitaoka, M.  
Deposited on : 2011-01-24  
Resolution : 2.70 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

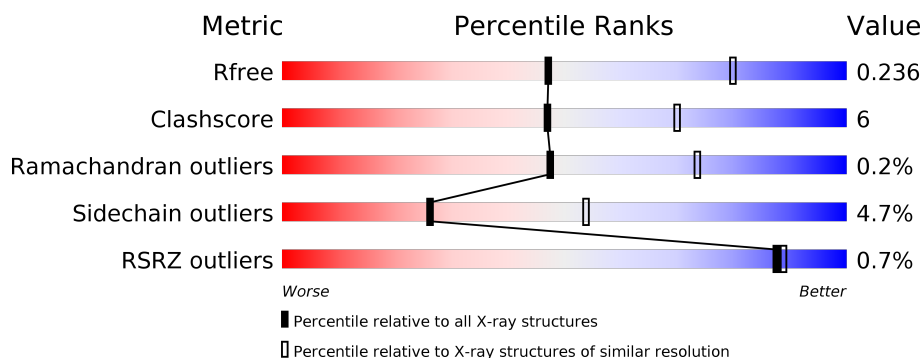
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	
1	B	842	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13264 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:

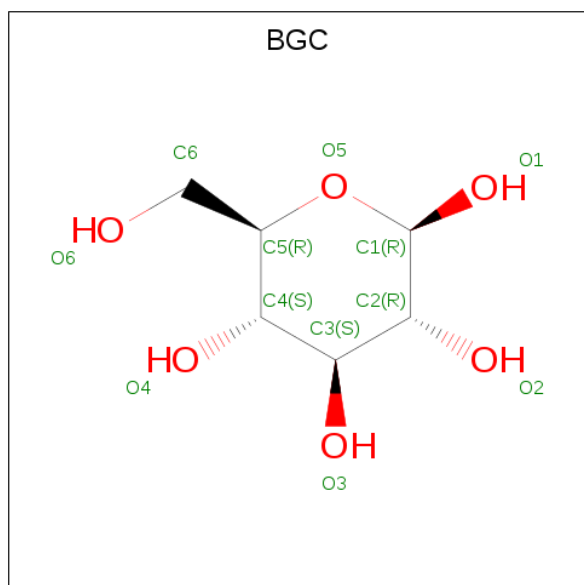
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP O66264
A	-18	GLY	-	expression tag	UNP O66264
A	-17	SER	-	expression tag	UNP O66264
A	-16	SER	-	expression tag	UNP O66264
A	-15	HIS	-	expression tag	UNP O66264
A	-14	HIS	-	expression tag	UNP O66264
A	-13	HIS	-	expression tag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



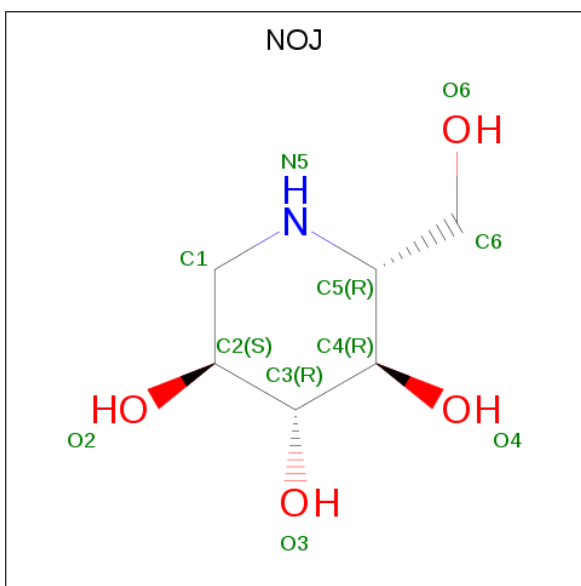
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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 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		

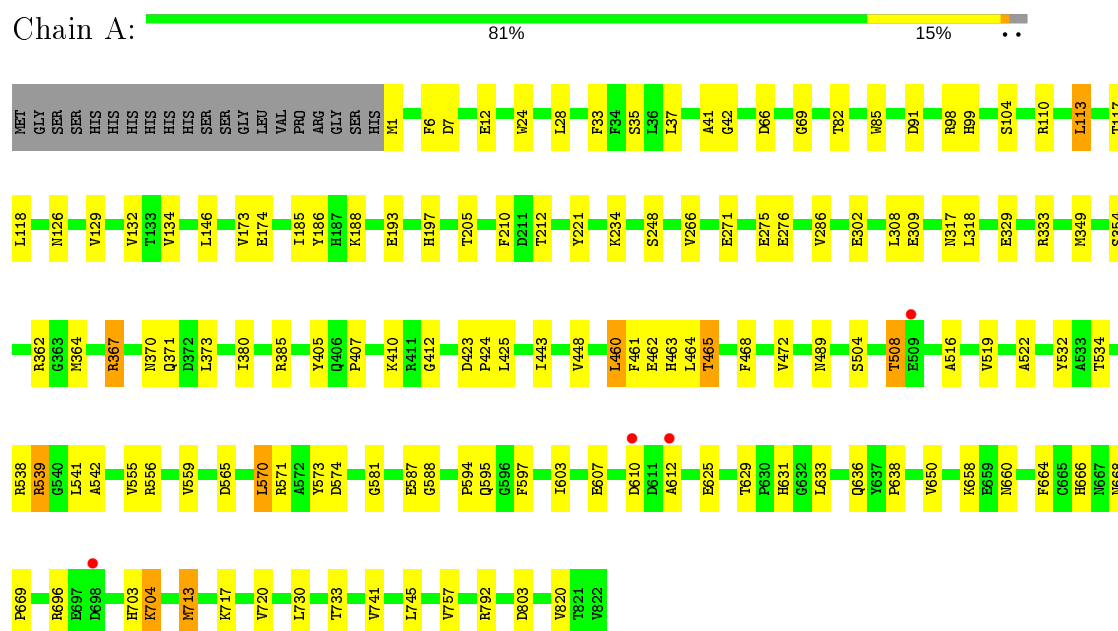
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	179	Total 179	O 179	0	0
5	B	173	Total 173	O 173	0	0

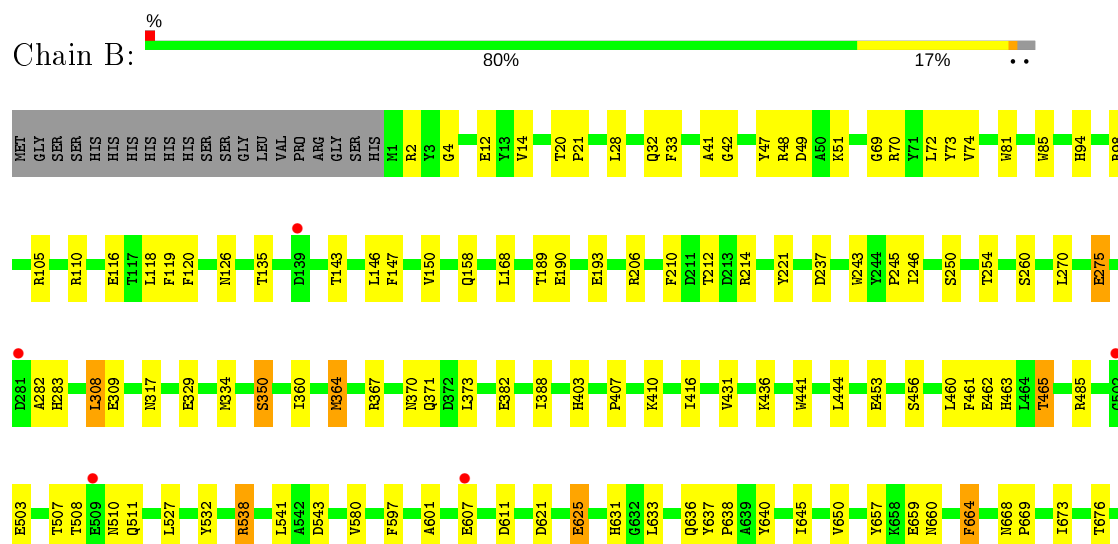
### 3 Residue-property plots

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, $\alpha$ , $\beta$ , $\gamma$	85.14Å 97.88Å 104.93Å 90.00° 102.56° 90.00°	Depositor
Resolution (Å)	36.37 – 2.70 37.56 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.3 (36.37-2.70) 99.5 (37.56-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.39 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.150 , 0.232 0.155 , 0.236	Depositor DCC
$R_{free}$ test set	2344 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.4	Xtriage
Anisotropy	0.563	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 33.5	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	0.95	EDS
Total number of atoms	13264	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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: PO4, BGC, 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	0.70	2/6604 (0.0%)	0.76	1/9009 (0.0%)
1	B	0.72	3/6604 (0.0%)	0.77	3/9009 (0.0%)
All	All	0.71	5/13208 (0.0%)	0.76	4/18018 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	275	GLU	CG-CD	5.76	1.60	1.51
1	B	309	GLU	CG-CD	5.42	1.60	1.51
1	A	302	GLU	CG-CD	5.09	1.59	1.51
1	A	309	GLU	CG-CD	5.07	1.59	1.51
1	B	275	GLU	CB-CG	5.06	1.61	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	206	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	A	7	ASP	CB-CG-OD1	6.11	123.80	118.30
1	B	580	VAL	CB-CA-C	-5.47	101.00	111.40
1	B	206	ARG	NE-CZ-NH2	-5.35	117.63	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6428	0	6071	69	0
1	B	6428	0	6071	86	0
2	A	12	0	12	0	0
2	B	12	0	12	1	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	11	0	13	0	0
4	B	11	0	13	3	0
5	A	179	0	0	0	0
5	B	173	0	0	3	0
All	All	13264	0	12192	156	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 6.

All (156) 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:465:THR:HB	1:B:532:TYR:OH	1.66	0.94
1:A:99:HIS:HD2	1:A:104:SER:OG	1.54	0.90
2:B:2901:BGC:O4	4:B:2903:NOJ:H12	1.72	0.89
1:A:465:THR:HB	1:A:532:TYR:OH	1.74	0.86
1:A:633:LEU:H	1:A:668:ASN:HD21	1.24	0.86
1:B:538:ARG:HH11	1:B:538:ARG:CG	1.91	0.83
1:A:631:HIS:HD2	1:A:696:ARG:HH12	1.27	0.79
1:B:118:LEU:HD21	1:B:308:LEU:HD13	1.64	0.79
1:B:538:ARG:HH11	1:B:538:ARG:HG3	1.50	0.77
1:A:539:ARG:CB	1:A:539:ARG:HH21	1.97	0.76
1:A:631:HIS:CD2	1:A:696:ARG:HH12	2.04	0.76
1:B:607:GLU:HB2	1:B:611:ASP:HB2	1.69	0.73
1:B:118:LEU:HD21	1:B:308:LEU:CD1	2.20	0.70
1:A:367:ARG:HG3	1:A:371:GLN:HE21	1.55	0.70
1:B:631:HIS:HD2	1:B:696:ARG:HH12	1.40	0.70
1:B:650:VAL:O	1:B:660:ASN:HB2	1.91	0.69
1:B:485:ARG:HA	1:B:510:ASN:HD21	1.57	0.68
1:B:640:TYR:H	1:B:660:ASN:HD21	1.42	0.67
1:B:73:TYR:HB2	1:B:147:PHE:HB2	1.74	0.67
1:A:99:HIS:CD2	1:A:104:SER:OG	2.44	0.67
1:A:354:SER:HB3	1:A:730:LEU:HD12	1.77	0.66
1:B:2:ARG:HD2	1:B:697:GLU:CD	2.16	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:ARG:HG3	1:A:443:ILE:HD12	1.78	0.66
1:B:462:GLU:HA	1:B:465:THR:HG23	1.79	0.65
1:A:741:VAL:HG23	1:A:745:LEU:HD12	1.79	0.64
1:A:539:ARG:HB3	1:A:539:ARG:HH21	1.63	0.64
1:A:539:ARG:CG	1:A:539:ARG:HH21	2.09	0.64
1:B:465:THR:HB	1:B:532:TYR:HH	1.60	0.63
1:A:367:ARG:HG3	1:A:371:GLN:NE2	2.14	0.63
1:A:468:PHE:O	1:A:472:VAL:HG23	1.99	0.62
1:A:117:THR:HG23	1:A:132:VAL:HG22	1.81	0.62
1:A:666:HIS:O	1:A:669:PRO:HD2	2.00	0.61
1:A:462:GLU:HA	1:A:465:THR:HG23	1.83	0.60
1:B:444:LEU:HB3	1:B:461:PHE:HB2	1.83	0.59
1:B:143:THR:HG22	1:B:254:THR:HG22	1.85	0.59
1:B:282:ALA:O	1:B:283:HIS:HB2	2.03	0.58
1:A:703:HIS:O	1:A:704:LYS:HB2	2.03	0.58
1:B:334:MET:HG3	1:B:692:THR:CG2	2.35	0.57
1:B:669:PRO:HG3	1:B:737:ASN:ND2	2.21	0.56
1:B:538:ARG:NH1	1:B:538:ARG:CG	2.59	0.56
1:A:587:GLU:HA	1:A:638:PRO:HD2	1.86	0.56
1:B:135:THR:OG1	1:B:260:SER:HB3	2.06	0.56
1:B:631:HIS:CD2	1:B:696:ARG:HH12	2.22	0.56
1:A:555:VAL:O	1:A:559:VAL:HG23	2.06	0.55
1:B:33:PHE:HB2	1:B:126:ASN:HD22	1.72	0.54
1:B:633:LEU:H	1:B:668:ASN:ND2	2.06	0.54
1:B:633:LEU:H	1:B:668:ASN:HD21	1.56	0.53
1:A:134:VAL:HG21	1:A:146:LEU:HD11	1.90	0.53
1:B:41:ALA:O	1:B:69:GLY:HA3	2.09	0.53
1:B:728:SER:O	1:B:729:TRP:HB2	2.08	0.52
1:A:539:ARG:HB3	1:A:539:ARG:NH2	2.23	0.52
1:B:743:GLN:HB3	1:B:749:ARG:HB3	1.90	0.52
1:A:28:LEU:HB2	1:A:35:SER:HB2	1.91	0.52
1:A:37:LEU:HD23	1:A:104:SER:HB2	1.92	0.52
1:A:581:GLY:HA2	1:A:588:GLY:O	2.09	0.52
1:A:6:PHE:CD1	1:A:333:ARG:HD3	2.44	0.51
1:A:556:ARG:HG3	1:A:603:ILE:HG12	1.92	0.51
1:A:370:ASN:O	1:A:373:LEU:HB2	2.10	0.51
1:A:574:ASP:OD1	1:A:574:ASP:C	2.49	0.51
1:B:527:LEU:HB2	1:B:601:ALA:HB2	1.92	0.51
1:B:657:TYR:CZ	1:B:719:ALA:HB1	2.46	0.51
1:A:91:ASP:O	1:A:110:ARG:HD2	2.12	0.50
1:A:174:GLU:HG3	1:A:188:LYS:HE2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:HIS:HB3	1:A:271:GLU:HG2	1.94	0.50
1:A:534:THR:O	1:A:538:ARG:HG2	2.12	0.50
1:A:516:ALA:HA	1:A:573:TYR:O	2.12	0.50
1:B:364:MET:HE3	1:B:407:PRO:HG3	1.94	0.50
1:A:631:HIS:HD2	1:A:696:ARG:NH1	2.04	0.49
1:B:441:TRP:CH2	1:B:538:ARG:HG2	2.47	0.49
1:B:664:PHE:HE1	4:B:2903:NOJ:HN5	1.59	0.49
1:A:633:LEU:N	1:A:668:ASN:HD21	2.03	0.49
1:B:105:ARG:HD3	1:B:116:GLU:OE2	2.13	0.49
1:A:519:VAL:O	1:A:522:ALA:HB3	2.13	0.49
1:B:403:HIS:HD2	1:B:416:ILE:HD12	1.77	0.49
1:B:212:THR:HA	1:B:246:ILE:O	2.13	0.48
1:A:349:MET:HE2	1:A:349:MET:HA	1.95	0.48
1:B:693:PRO:HA	5:B:945:HOH:O	2.13	0.48
1:B:382:GLU:CD	1:B:382:GLU:H	2.17	0.48
1:B:74:VAL:HG22	1:B:146:LEU:HD22	1.95	0.48
1:B:453:GLU:HB2	1:B:456:SER:OG	2.13	0.48
1:A:460:LEU:O	1:A:463:HIS:HB2	2.14	0.48
1:A:173:VAL:HA	1:A:186:TYR:O	2.14	0.48
1:B:538:ARG:NH2	1:B:753:ASP:OD2	2.46	0.48
1:B:388:ILE:HD13	1:B:431:VAL:HG22	1.96	0.47
1:B:538:ARG:HH11	1:B:538:ARG:HG2	1.75	0.47
1:A:489:ASN:HB2	1:A:571:ARG:HH21	1.80	0.47
1:A:443:ILE:HG12	1:A:460:LEU:HD12	1.96	0.47
1:A:658:LYS:HD2	1:A:713:MET:HG2	1.95	0.47
1:B:637:TYR:CD1	1:B:638:PRO:HA	2.50	0.47
1:B:721:ARG:O	1:B:722:ALA:C	2.52	0.47
1:A:364:MET:HG2	1:A:407:PRO:HG3	1.97	0.46
1:B:146:LEU:O	1:B:250:SER:HA	2.16	0.46
1:A:405:TYR:HA	1:A:412:GLY:HA2	1.98	0.46
1:B:633:LEU:HD21	1:B:687:TYR:CE1	2.51	0.45
1:A:28:LEU:HD11	1:A:37:LEU:HD22	1.97	0.45
1:B:42:GLY:HA2	1:B:69:GLY:HA3	1.98	0.45
1:A:448:VAL:HG12	1:A:463:HIS:NE2	2.32	0.45
1:A:504:SER:O	1:A:508:THR:HB	2.17	0.45
1:B:721:ARG:O	1:B:724:GLU:HG3	2.17	0.45
1:B:20:THR:HB	1:B:21:PRO:HD2	1.99	0.44
1:B:51:LYS:HD2	1:B:360:ILE:O	2.17	0.44
1:B:12:GLU:OE1	1:B:98:ARG:HD3	2.17	0.44
1:B:243:TRP:O	1:B:245:PRO:HD3	2.17	0.44
1:B:503:GLU:CG	1:B:508:THR:HB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:750:PRO:HD3	1:B:772:ARG:NH1	2.32	0.44
1:A:185:ILE:HD13	1:A:212:THR:HG22	1.99	0.44
1:B:436:LYS:HE3	1:B:752:TYR:CZ	2.53	0.44
1:A:423:ASP:HB2	1:A:424:PRO:HD3	1.99	0.44
1:A:594:PRO:HG2	1:A:595:GLN:NE2	2.32	0.44
1:A:425:LEU:HA	1:A:425:LEU:HD23	1.86	0.44
1:B:669:PRO:O	1:B:673:ILE:HG13	2.18	0.44
1:A:210:PHE:HA	1:A:248:SER:O	2.17	0.43
1:A:461:PHE:O	1:A:464:LEU:HB2	2.18	0.43
1:B:47:TYR:O	1:B:49:ASP:N	2.49	0.43
1:B:20:THR:HB	1:B:21:PRO:CD	2.48	0.43
1:B:32:GLN:HB3	1:B:48:ARG:HG2	2.00	0.43
1:B:81:TRP:CG	1:B:110:ARG:HD3	2.54	0.43
1:B:28:LEU:HD13	1:B:120:PHE:HA	2.00	0.43
1:B:94:HIS:HD2	5:B:994:HOH:O	2.01	0.43
1:B:538:ARG:NH1	1:B:538:ARG:HG2	2.32	0.43
1:B:370:ASN:O	1:B:373:LEU:HB2	2.19	0.42
1:B:676:THR:HB	1:B:760:GLN:HB3	2.01	0.42
1:B:270:LEU:N	1:B:270:LEU:HD22	2.35	0.42
1:A:129:VAL:HG22	1:A:266:VAL:HG22	2.02	0.42
1:B:189:THR:HG22	1:B:190:GLU:HG3	2.00	0.42
1:B:214:ARG:HA	1:B:246:ILE:HD13	2.01	0.42
1:A:113:LEU:HA	1:A:113:LEU:HD12	1.90	0.42
1:A:118:LEU:HD21	1:A:308:LEU:HD13	2.02	0.42
1:B:636:GLN:N	1:B:636:GLN:OE1	2.53	0.42
1:B:168:LEU:HA	1:B:168:LEU:HD23	1.71	0.42
1:A:757:VAL:HG11	1:A:820:VAL:HG21	2.01	0.42
1:B:659:GLU:OE2	4:B:2903:NOJ:H61	2.20	0.42
1:B:462:GLU:HA	1:B:465:THR:CG2	2.46	0.42
1:B:460:LEU:O	1:B:463:HIS:HB2	2.20	0.42
1:B:739:VAL:O	1:B:743:GLN:HB2	2.19	0.42
1:A:462:GLU:HA	1:A:465:THR:CG2	2.50	0.42
1:A:42:GLY:HA3	1:A:66:ASP:OD1	2.20	0.41
1:B:158:GLN:NE2	5:B:912:HOH:O	2.52	0.41
1:A:650:VAL:O	1:A:660:ASN:HB2	2.20	0.41
1:B:119:PHE:O	1:B:120:PHE:HB3	2.19	0.41
1:B:436:LYS:HE3	1:B:752:TYR:CE2	2.55	0.41
1:B:334:MET:HG3	1:B:692:THR:HG21	2.02	0.41
1:B:4:GLY:HA3	1:B:14:VAL:O	2.20	0.41
1:A:318:LEU:HD21	1:A:380:ILE:HD11	2.01	0.41
1:A:405:TYR:CD1	1:A:410:LYS:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:565:ASP:HB2	1:A:570:LEU:HD13	2.02	0.41
1:A:33:PHE:HB2	1:A:126:ASN:HD22	1.84	0.41
1:A:24:TRP:O	1:A:99:HIS:HE1	2.04	0.41
1:A:41:ALA:O	1:A:69:GLY:HA3	2.21	0.41
1:B:210:PHE:O	1:B:237:ASP:HA	2.21	0.41
1:B:503:GLU:HG3	1:B:508:THR:HB	2.02	0.41
1:B:350:SER:HB2	1:B:364:MET:HE2	2.03	0.41
1:B:621:ASP:O	1:B:625:GLU:HG3	2.21	0.41
1:B:538:ARG:HH22	1:B:753:ASP:CG	2.22	0.40
1:B:367:ARG:HG2	1:B:371:GLN:HE21	1.86	0.40
1:A:12:GLU:OE1	1:A:98:ARG:NH1	2.49	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%)	774 (94%)	43 (5%)	3 (0%)	34	60
1	B	820/842 (97%)	769 (94%)	50 (6%)	1 (0%)	51	78
All	All	1640/1684 (97%)	1543 (94%)	93 (6%)	4 (0%)	47	73

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	TRP
1	A	542	ALA
1	A	612	ALA
1	B	85	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%)	631 (95%)	34 (5%)	24	50
1	B	665/682 (98%)	636 (96%)	29 (4%)	28	56
All	All	1330/1364 (98%)	1267 (95%)	63 (5%)	26	54

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	82	THR
1	A	113	LEU
1	A	193	GLU
1	A	205	THR
1	A	221	TYR
1	A	234	LYS
1	A	275	GLU
1	A	276	GLU
1	A	286	VAL
1	A	317	ASN
1	A	329	GLU
1	A	362	ARG
1	A	367	ARG
1	A	460	LEU
1	A	465	THR
1	A	508	THR
1	A	539	ARG
1	A	541	LEU
1	A	570	LEU
1	A	597	PHE
1	A	607	GLU
1	A	610	ASP
1	A	625	GLU
1	A	629	THR
1	A	636	GLN
1	A	664	PHE

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Mol	Chain	Res	Type
1	A	704	LYS
1	A	713	MET
1	A	717	LYS
1	A	720	VAL
1	A	733	THR
1	A	792	ARG
1	A	803	ASP
1	B	70	ARG
1	B	72	LEU
1	B	150	VAL
1	B	193	GLU
1	B	221	TYR
1	B	275	GLU
1	B	308	LEU
1	B	317	ASN
1	B	329	GLU
1	B	350	SER
1	B	364	MET
1	B	410	LYS
1	B	465	THR
1	B	507	THR
1	B	511	GLN
1	B	538	ARG
1	B	541	LEU
1	B	543	ASP
1	B	597	PHE
1	B	625	GLU
1	B	645	ILE
1	B	664	PHE
1	B	709	VAL
1	B	713	MET
1	B	794	SER
1	B	795	LEU
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

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Mol	Chain	Res	Type
1	A	161	GLN
1	A	283	HIS
1	A	511	GLN
1	A	631	HIS
1	A	668	ASN
1	A	727	ASN
1	A	760	GLN
1	B	62	ASN
1	B	94	HIS
1	B	126	ASN
1	B	158	GLN
1	B	312	ASN
1	B	406	GLN
1	B	452	ASN
1	B	510	ASN
1	B	624	ASN
1	B	631	HIS
1	B	660	ASN
1	B	668	ASN
1	B	737	ASN
1	B	760	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

6 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	$\# Z  > 2$
4	NOJ	A	1903	-	11,11,11	0.79	0	13,15,15	1.33	1 (7%)
3	PO4	B	2902	-	4,4,4	0.99	0	6,6,6	1.23	1 (16%)
2	BGC	B	2901	-	12,12,12	0.71	0	17,17,17	1.29	3 (17%)
3	PO4	A	1902	-	4,4,4	1.10	0	6,6,6	0.58	0
4	NOJ	B	2903	-	11,11,11	1.11	2 (18%)	13,15,15	2.58	5 (38%)
2	BGC	A	1901	-	12,12,12	0.45	0	17,17,17	1.47	1 (5%)

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	A	1903	-	-	0/2/19/19	0/1/1/1
2	BGC	B	2901	-	-	0/2/22/22	0/1/1/1
4	NOJ	B	2903	-	-	2/2/19/19	1/1/1/1
2	BGC	A	1901	-	-	0/2/22/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2903	NOJ	C1-C2	2.16	1.54	1.52
4	B	2903	NOJ	C1-N5	-2.13	1.44	1.47

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2903	NOJ	C1-N5-C5	6.22	123.07	109.61
4	B	2903	NOJ	C1-C2-C3	4.64	115.78	110.33
2	A	1901	BGC	O5-C1-C2	-4.50	102.26	110.28
4	A	1903	NOJ	C1-N5-C5	3.96	118.17	109.61
2	B	2901	BGC	O4-C4-C3	-2.64	104.24	110.35
4	B	2903	NOJ	C2-C3-C4	2.58	115.36	110.89
4	B	2903	NOJ	O6-C6-C5	-2.51	105.02	111.09
4	B	2903	NOJ	C4-C5-N5	2.42	113.99	109.14
2	B	2901	BGC	O1-C1-C2	2.41	115.81	109.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2902	PO4	O3-P-O2	2.38	115.60	107.97
2	B	2901	BGC	O5-C1-C2	-2.17	106.41	110.28

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	2903	NOJ	C4-C5-C6-O6
4	B	2903	NOJ	N5-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	2903	NOJ	C1-C2-C3-C4-C5-N5

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2901	BGC	1	0
4	B	2903	NOJ	3	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%)	-0.45	4 (0%) 91 92	9, 20, 33, 46	0
1	B	822/842 (97%)	-0.49	8 (0%) 82 83	10, 21, 33, 46	0
All	All	1644/1684 (97%)	-0.47	12 (0%) 87 89	9, 20, 33, 46	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	612	ALA	3.2
1	B	803	ASP	3.0
1	B	502	GLY	2.4
1	A	610	ASP	2.4
1	B	281	ASP	2.4
1	A	509	GLU	2.3
1	B	822	VAL	2.3
1	B	789	PRO	2.2
1	B	607	GLU	2.2
1	B	509	GLU	2.1
1	A	698	ASP	2.1
1	B	139	ASP	2.1

### 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
2	BGC	B	2901	12/12	0.96	0.13	16,20,22,22	0
4	NOJ	B	2903	11/11	0.97	0.17	22,24,26,29	0
4	NOJ	A	1903	11/11	0.98	0.27	11,15,18,18	0
2	BGC	A	1901	12/12	0.98	0.13	22,24,25,25	0
3	PO4	B	2902	5/5	0.99	0.16	22,22,23,24	0
3	PO4	A	1902	5/5	0.99	0.23	19,19,21,22	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.