



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 04:12 PM UTC

PDB ID : 3QG0 / pdb_00003qg0
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

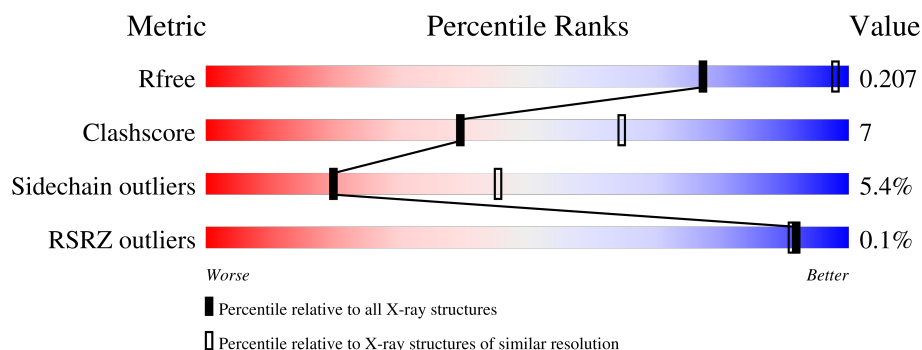
1 Overall quality at a glance

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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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:

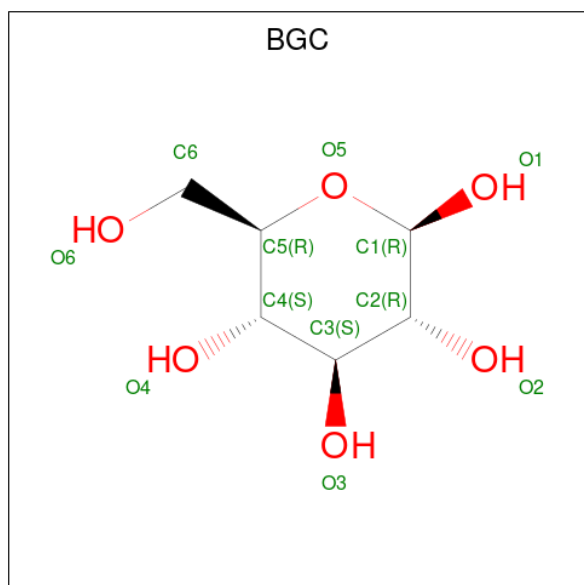
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP O66264
A	-18	GLY	-	expression tag	UNP O66264
A	-17	SER	-	expression tag	UNP O66264
A	-16	SER	-	expression tag	UNP O66264
A	-15	HIS	-	expression tag	UNP O66264
A	-14	HIS	-	expression tag	UNP O66264
A	-13	HIS	-	expression tag	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 (CCD ID: BGC) (formula: C₆H₁₂O₆).



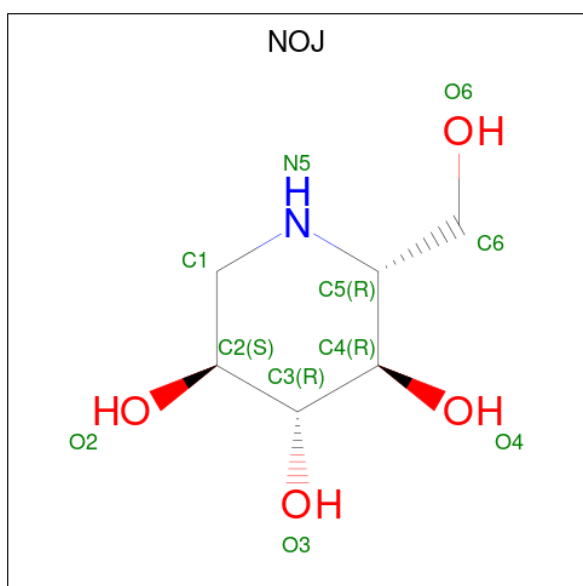
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 4 is 1-DEOXYNOJIRIMYCIN (CCD ID: 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		

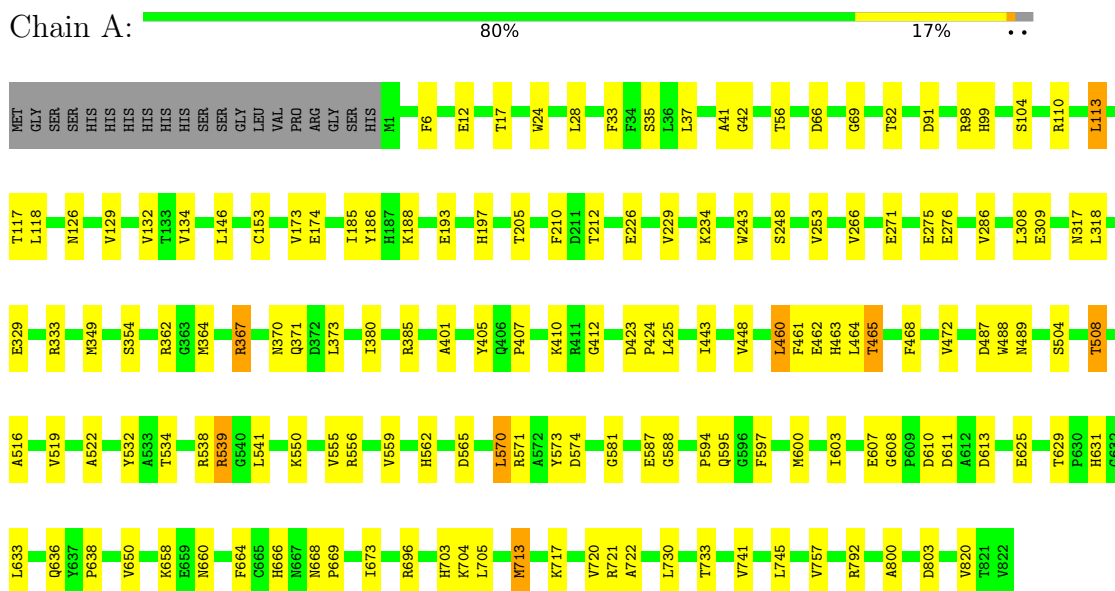
- Molecule 5 is water.

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

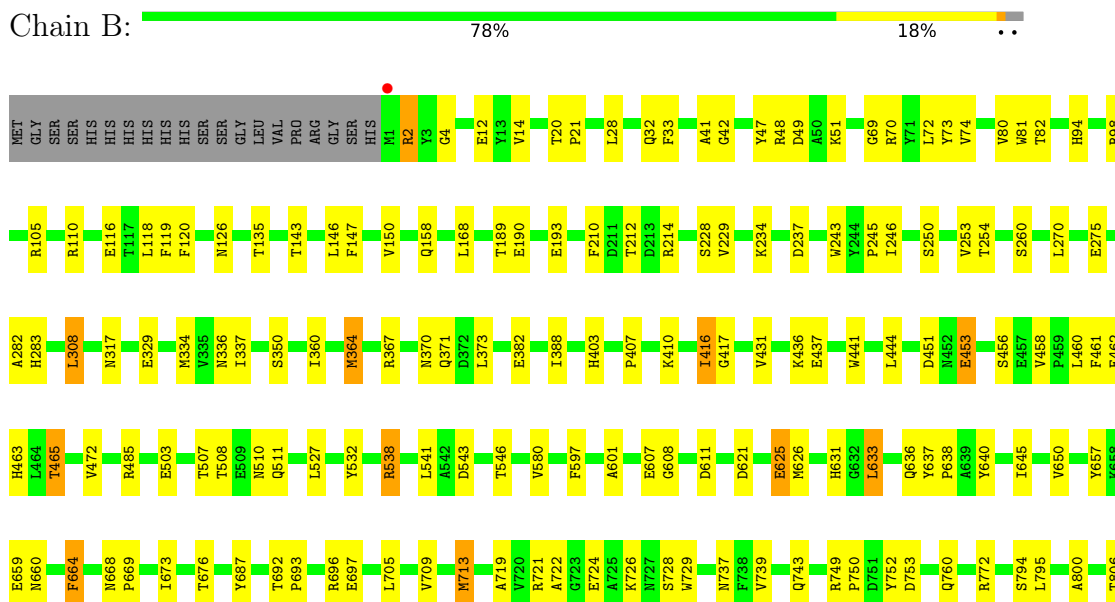
3 Residue-property plots

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, α , β , γ	85.14Å 97.88Å 104.93Å 90.00° 102.56° 90.00°	Depositor
Resolution (Å)	36.37 – 2.70 36.37 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.3 (36.37-2.70) 99.5 (36.37-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.150 , 0.232 (Not available) , 0.207	Depositor DCC
R_{free} test set	2344 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	25.4	Xtriage
Anisotropy	0.563	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 29.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: PO4, NOJ, 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	0.84	1/6604 (0.0%)	1.02	8/9009 (0.1%)
1	B	0.85	2/6604 (0.0%)	1.04	13/9009 (0.1%)
All	All	0.85	3/13208 (0.0%)	1.03	21/18018 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	229	VAL	CA-CB	6.65	1.57	1.54
1	B	229	VAL	CA-CB	5.86	1.57	1.54
1	B	818	VAL	CA-CB	5.25	1.60	1.54

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	458	VAL	CA-C-N	-9.83	109.92	119.85
1	B	458	VAL	C-N-CA	-9.83	109.92	119.85
1	B	580	VAL	CB-CA-C	-6.51	101.00	110.63
1	A	800	ALA	CA-C-N	6.46	126.22	119.76
1	A	800	ALA	C-N-CA	6.46	126.22	119.76
1	B	228	SER	N-CA-C	6.25	117.78	110.97
1	B	453	GLU	CA-C-N	-6.18	113.41	119.90
1	B	453	GLU	C-N-CA	-6.18	113.41	119.90
1	A	608	GLY	CA-C-N	6.00	125.70	119.82
1	A	608	GLY	C-N-CA	6.00	125.70	119.82
1	B	417	GLY	N-CA-C	5.81	117.96	112.04
1	A	17	THR	CA-C-N	-5.60	113.99	120.04
1	A	17	THR	C-N-CA	-5.60	113.99	120.04
1	B	80	VAL	N-CA-C	5.52	116.26	108.36
1	A	401	ALA	N-CA-C	5.44	117.34	109.07
1	B	608	GLY	CA-C-N	5.31	126.47	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	608	GLY	C-N-CA	5.31	126.47	119.84
1	A	243	TRP	N-CA-C	5.30	116.37	108.31
1	B	800	ALA	N-CA-C	5.29	117.08	109.04
1	B	2	ARG	N-CA-C	5.25	118.12	109.72
1	B	437	GLU	N-CA-C	5.14	116.57	111.07

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	76	0
1	B	6428	0	6071	92	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	169	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 7.

All (169) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:538:ARG:CG	1:B:538:ARG:HH11	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:2:ARG:HD2	1:B:697:GLU:CD	2.16	0.70
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: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:HH21	1:A:539:ARG:HB3	1.63	0.64
1:A:539:ARG:HH21	1:A:539:ARG:CG	2.09	0.64
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:A:703:HIS:O	1:A:704:LYS:HB2	2.03	0.58
1:B:282:ALA:O	1:B:283:HIS:HB2	2.03	0.57
1:B:334:MET:HG3	1:B:692:THR:CG2	2.35	0.57
1:B:538:ARG:CG	1:B:538:ARG:NH1	2.59	0.56
1:B:669:PRO:HG3	1:B:737:ASN:ND2	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:VAL:HG21	1:A:146:LEU:HD11	1.90	0.53
1:A:574:ASP:OD1	1:A:574:ASP:C	2.49	0.53
1:B:41:ALA:O	1:B:69:GLY:HA3	2.09	0.53
1:B:382:GLU:H	1:B:382:GLU:CD	2.17	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:B:721:ARG:O	1:B:722:ALA:C	2.52	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: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:349:MET:HA	1:A:349:MET:HE2	1.93	0.50
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
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:B:693:PRO:HA	5:B:945:HOH:O	2.13	0.48
1:B:713:MET:HE3	1:B:726:LYS:HD2	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:538:ARG:HH22	1:B:753:ASP:CG	2.22	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:A:600:MET:HE3	1:A:673:ILE:HG21	2.00	0.44
1:B:12:GLU:OE1	1:B:98:ARG:HD3	2.17	0.44
1:B:51:LYS:HD2	1:B:360:ILE:O	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
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:A:460:LEU:O	1:A:461:PHE:C	2.59	0.44
1:A:562:HIS:O	1:A:573:TYR:OH	2.33	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:HD23	1:A:425:LEU:HA	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:A:611:ASP:C	1:A:613:ASP:H	2.26	0.43
1:A:721:ARG:O	1:A:722:ALA:C	2.60	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:451:ASP:O	1:B:451:ASP:CG	2.62	0.43
1:B:28:LEU:HD13	1:B:120:PHE:HA	2.00	0.43
1:B:538:ARG:NH2	1:B:753:ASP:CG	2.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:ASN:O	1:B:373:LEU:HB2	2.19	0.42
1:B:47:TYR:C	1:B:49:ASP:H	2.27	0.42
1:B:676:THR:HB	1:B:760:GLN:HB3	2.01	0.42
1:B:270:LEU:HD22	1:B:270:LEU:N	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:B:626:MET:HE2	1:B:637:TYR:HD2	1.84	0.42
1:A:113:LEU:HD12	1:A:113:LEU:HA	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:HD23	1:B:168:LEU:HA	1.71	0.42
1:B:669:PRO:HG3	1:B:737:ASN:CG	2.45	0.42
1:A:757:VAL:HG11	1:A:820:VAL:HG21	2.01	0.42
1:B:462:GLU:HA	1:B:465:THR:CG2	2.46	0.42
1:B:659:GLU:OE2	4:B:2903:NOJ:H61	2.20	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:A:56:THR:C	1:A:153:CYS:HB2	2.45	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:336:ASN:C	1:B:337:ILE:HG13	2.45	0.41
1:B:436:LYS:HE3	1:B:752:TYR:CE2	2.55	0.41
1:B:4:GLY:HA3	1:B:14:VAL:O	2.20	0.41
1:B:334:MET:HG3	1:B:692:THR:HG21	2.02	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
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:A:487:ASP:O	1:A:488:TRP:C	2.64	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: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](#)

There are no protein backbone outliers to report in this entry.

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%)	629 (95%)	36 (5%)	20	45
1	B	665/682 (98%)	629 (95%)	36 (5%)	20	45
All	All	1330/1364 (98%)	1258 (95%)	72 (5%)	20	45

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	THR
1	A	113	LEU
1	A	193	GLU
1	A	205	THR
1	A	226	GLU
1	A	234	LYS
1	A	253	VAL
1	A	275	GLU
1	A	276	GLU
1	A	286	VAL
1	A	309	GLU
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

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Mol	Chain	Res	Type
1	A	539	ARG
1	A	541	LEU
1	A	550	LYS
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
1	A	705	LEU
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	82	THR
1	B	150	VAL
1	B	193	GLU
1	B	234	LYS
1	B	253	VAL
1	B	275	GLU
1	B	308	LEU
1	B	317	ASN
1	B	329	GLU
1	B	364	MET
1	B	410	LYS
1	B	416	ILE
1	B	465	THR
1	B	472	VAL
1	B	507	THR
1	B	511	GLN
1	B	538	ARG
1	B	541	LEU
1	B	543	ASP
1	B	546	THR
1	B	597	PHE
1	B	625	GLU

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Mol	Chain	Res	Type
1	B	633	LEU
1	B	645	ILE
1	B	664	PHE
1	B	705	LEU
1	B	709	VAL
1	B	713	MET
1	B	794	SER
1	B	795	LEU
1	B	806	THR
1	B	814	SER
1	B	816	VAL
1	B	818	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
1	A	99	HIS
1	A	126	ASN
1	A	158	GLN
1	A	161	GLN
1	A	177	GLN
1	A	283	HIS
1	A	284	GLN
1	A	414	ASN
1	A	452	ASN
1	A	473	GLN
1	A	631	HIS
1	A	668	ASN
1	A	727	ASN
1	A	760	GLN
1	B	40	GLN
1	B	94	HIS
1	B	126	ASN
1	B	222	ASN
1	B	406	GLN
1	B	510	ASN
1	B	567	GLN
1	B	631	HIS
1	B	660	ASN
1	B	668	ASN
1	B	737	ASN

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Mol	Chain	Res	Type
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 oligosaccharides 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	B	2903	-	11,11,11	1.15	2 (18%)	13,15,15	2.53	5 (38%)
3	PO4	B	2902	-	4,4,4	1.03	0	6,6,6	1.28	1 (16%)
3	PO4	A	1902	-	4,4,4	1.15	0	6,6,6	0.61	0
2	BGC	A	1901	-	12,12,12	0.45	0	17,17,17	1.48	1 (5%)
4	NOJ	A	1903	-	11,11,11	0.81	0	13,15,15	1.30	1 (7%)
2	BGC	B	2901	-	12,12,12	0.71	0	17,17,17	1.28	3 (17%)

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	B	2901	-	-	0/2/22/22	0/1/1/1
2	BGC	A	1901	-	-	0/2/22/22	0/1/1/1
4	NOJ	B	2903	-	-	2/2/19/19	1/1/1/1
4	NOJ	A	1903	-	-	0/2/19/19	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	2.35	1.54	1.52
4	B	2903	NOJ	C1-N5	-2.23	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	6.08	123.07	109.71
2	A	1901	BGC	O5-C1-C2	-4.57	102.26	110.30
4	B	2903	NOJ	C1-C2-C3	4.52	115.78	110.25
4	A	1903	NOJ	C1-N5-C5	3.85	118.17	109.71
2	B	2901	BGC	O4-C4-C3	-2.60	104.24	110.38
4	B	2903	NOJ	C2-C3-C4	2.56	115.36	110.86
4	B	2903	NOJ	O6-C6-C5	-2.51	105.02	111.10
3	B	2902	PO4	O3-P-O2	2.47	115.60	107.91
4	B	2903	NOJ	C4-C5-N5	2.41	113.99	109.12
2	B	2901	BGC	O1-C1-C2	2.35	115.81	108.98
2	B	2901	BGC	O5-C1-C2	-2.21	106.41	110.30

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
4	B	2903	NOJ	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2901	BGC	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	822/842 (97%)	-0.72	0 100 100	9, 20, 33, 46	0
1	B	822/842 (97%)	-0.68	1 (0%) 92 91	10, 21, 33, 46	0
All	All	1644/1684 (97%)	-0.70	1 (0%) 92 91	9, 20, 33, 46	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	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 oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NOJ	B	2903	11/11	0.96	0.06	22,24,26,29	0
4	NOJ	A	1903	11/11	0.97	0.06	11,15,18,18	0
2	BGC	B	2901	12/12	0.97	0.06	16,20,22,22	0
2	BGC	A	1901	12/12	0.98	0.05	22,24,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PO4	A	1902	5/5	0.99	0.04	19,19,21,22	0
3	PO4	B	2902	5/5	0.99	0.04	22,22,23,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.