



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2017 – 09:10 AM EDT

PDB ID : 2ZUW
Title : Crystal structure of Galacto-N-biose/Lacto-N-biose I phosphorylase in complex with GlcNAc and sulfate
Authors : Hidaka, M.; Nishimoto, M.; Kitaoka, M.; Wakagi, T.; Shoun, H.; Fushinobu, S.
Deposited on : unknown
Resolution : 2.11 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

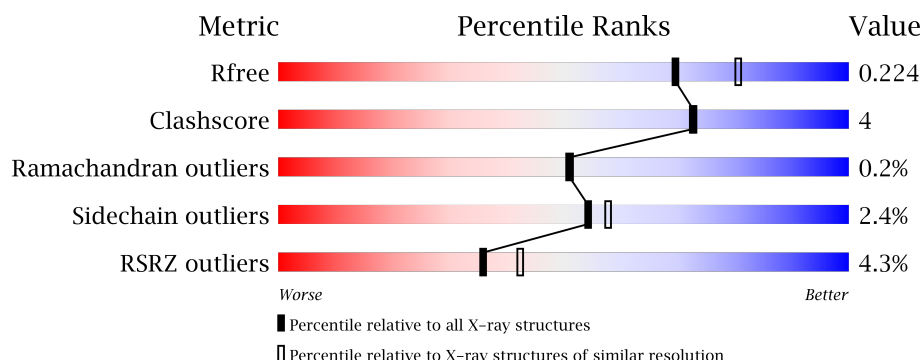
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.11 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}	100719	4988 (2.14-2.10)
Clashscore	112137	5557 (2.14-2.10)
Ramachandran outliers	110173	5504 (2.14-2.10)
Sidechain outliers	110143	5505 (2.14-2.10)
RSRZ outliers	101464	5021 (2.14-2.10)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	759	<div> <div>2%</div> <div>91%</div> <div>6%</div> <div>••</div> </div>
1	B	759	<div> <div>6%</div> <div>87%</div> <div>8%</div> <div>••</div> </div>
1	C	759	<div> <div>2%</div> <div>92%</div> <div>6%</div> <div>•</div> </div>
1	D	759	<div> <div>7%</div> <div>81%</div> <div>11%</div> <div>• 6%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	B	4006	-	-	-	X
3	GOL	D	4009	-	-	-	X
3	GOL	D	4010	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 25782 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 Lacto-N-biose phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	745	Total	C	N	O	S	0	0	0
			5926	3782	995	1133	16			
1	B	734	Total	C	N	O	S	0	0	0
			5833	3723	983	1111	16			
1	C	748	Total	C	N	O	S	0	0	0
			5950	3795	1000	1139	16			
1	D	713	Total	C	N	O	S	0	0	0
			5686	3635	957	1078	16			

There are 32 discrepancies between the modelled and reference sequences:

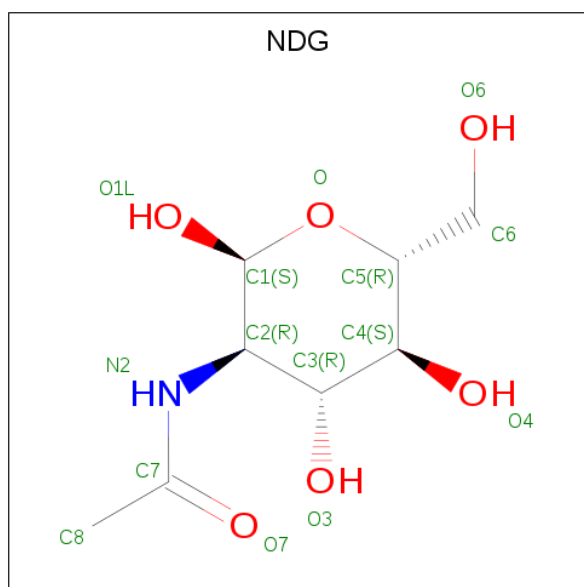
Chain	Residue	Modelled	Actual	Comment	Reference
A	752	LEU	-	EXPRESSION TAG	UNP Q5NU17
A	753	GLU	-	EXPRESSION TAG	UNP Q5NU17
A	754	HIS	-	EXPRESSION TAG	UNP Q5NU17
A	755	HIS	-	EXPRESSION TAG	UNP Q5NU17
A	756	HIS	-	EXPRESSION TAG	UNP Q5NU17
A	757	HIS	-	EXPRESSION TAG	UNP Q5NU17
A	758	HIS	-	EXPRESSION TAG	UNP Q5NU17
A	759	HIS	-	EXPRESSION TAG	UNP Q5NU17
B	752	LEU	-	EXPRESSION TAG	UNP Q5NU17
B	753	GLU	-	EXPRESSION TAG	UNP Q5NU17
B	754	HIS	-	EXPRESSION TAG	UNP Q5NU17
B	755	HIS	-	EXPRESSION TAG	UNP Q5NU17
B	756	HIS	-	EXPRESSION TAG	UNP Q5NU17
B	757	HIS	-	EXPRESSION TAG	UNP Q5NU17
B	758	HIS	-	EXPRESSION TAG	UNP Q5NU17
B	759	HIS	-	EXPRESSION TAG	UNP Q5NU17
C	752	LEU	-	EXPRESSION TAG	UNP Q5NU17
C	753	GLU	-	EXPRESSION TAG	UNP Q5NU17
C	754	HIS	-	EXPRESSION TAG	UNP Q5NU17
C	755	HIS	-	EXPRESSION TAG	UNP Q5NU17
C	756	HIS	-	EXPRESSION TAG	UNP Q5NU17

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Chain	Residue	Modelled	Actual	Comment	Reference
C	757	HIS	-	EXPRESSION TAG	UNP Q5NU17
C	758	HIS	-	EXPRESSION TAG	UNP Q5NU17
C	759	HIS	-	EXPRESSION TAG	UNP Q5NU17
D	752	LEU	-	EXPRESSION TAG	UNP Q5NU17
D	753	GLU	-	EXPRESSION TAG	UNP Q5NU17
D	754	HIS	-	EXPRESSION TAG	UNP Q5NU17
D	755	HIS	-	EXPRESSION TAG	UNP Q5NU17
D	756	HIS	-	EXPRESSION TAG	UNP Q5NU17
D	757	HIS	-	EXPRESSION TAG	UNP Q5NU17
D	758	HIS	-	EXPRESSION TAG	UNP Q5NU17
D	759	HIS	-	EXPRESSION TAG	UNP Q5NU17

- Molecule 2 is 2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).



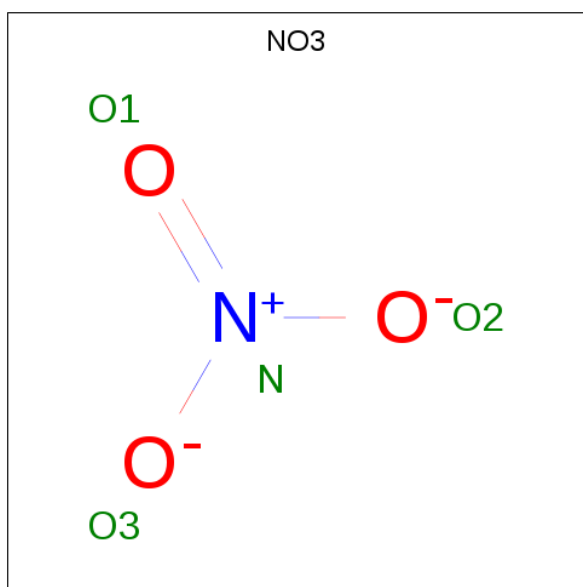
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	B	1	Total	C	N	O	0	0
			15	8	1	6		
2	C	1	Total	C	N	O	0	0
			15	8	1	6		
2	D	1	Total	C	N	O	0	0
			15	8	1	6		

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



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

- Molecule 4 is NITRATE ION (three-letter code: NO3) (formula: NO₃).

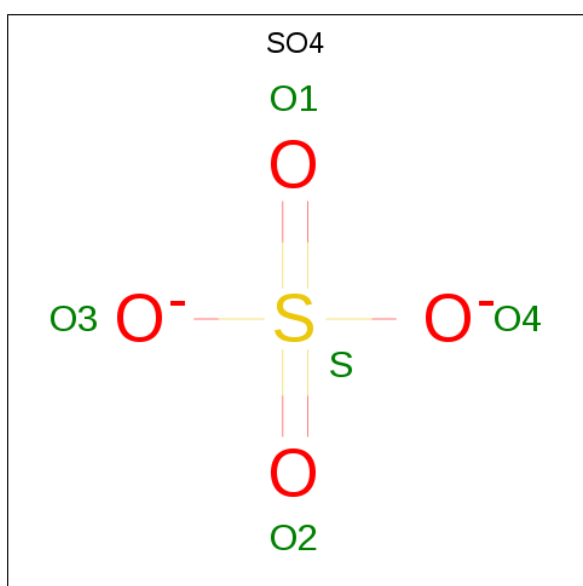


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	N	O	0	0
			4	1	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	O	S	0	0
			5	4	1		

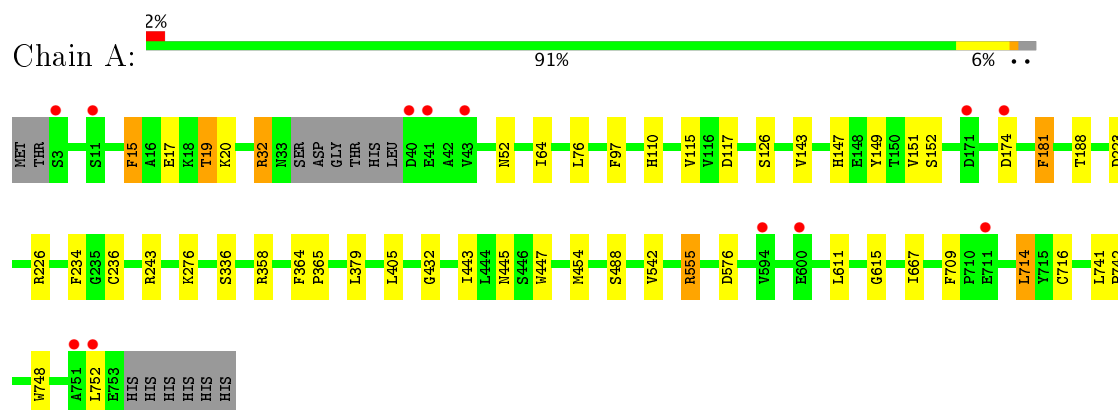
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	627	Total	O	0	0
			627	627		
7	B	533	Total	O	2	0
			533	533		
7	C	601	Total	O	1	0
			601	601		
7	D	520	Total	O	0	0
			520	520		

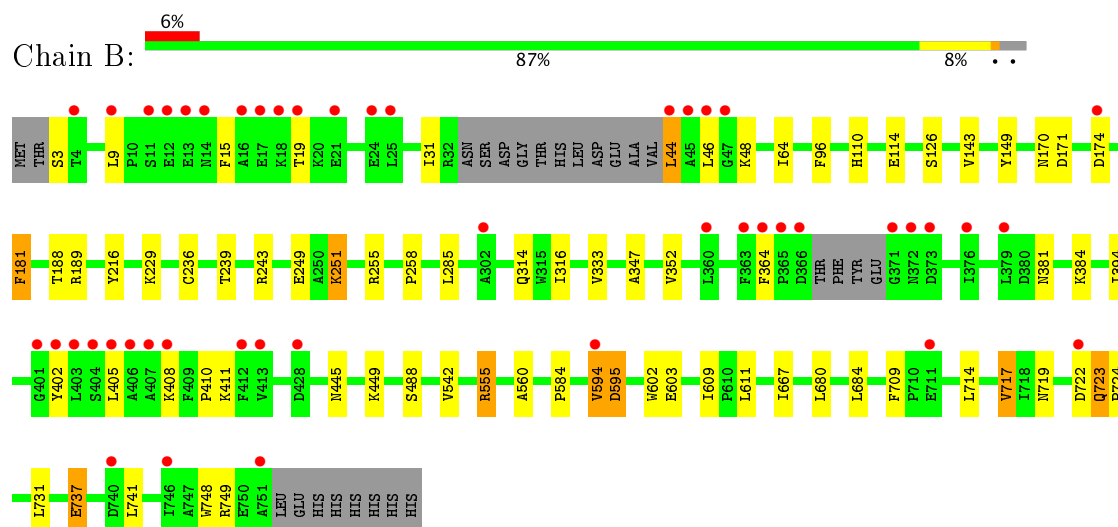
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

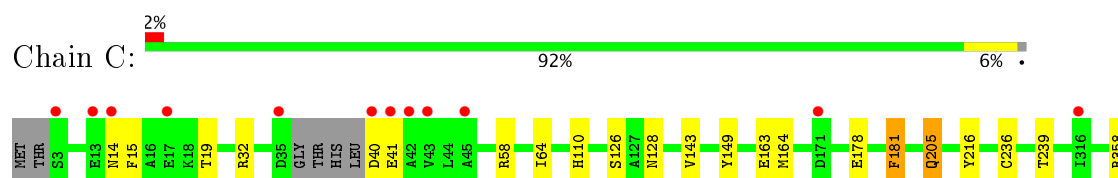
• Molecule 1: Lacto-N-biose phosphorylase

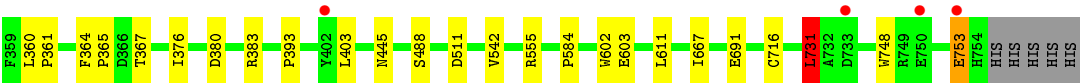


• Molecule 1: Lacto-N-biose phosphorylase

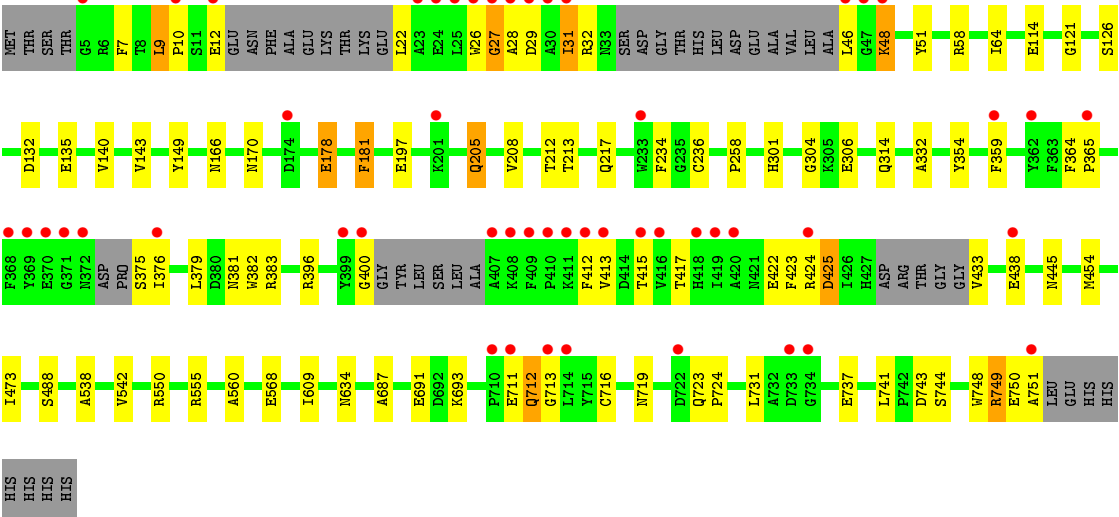
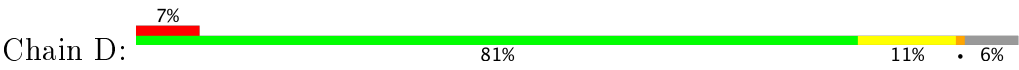


• Molecule 1: Lacto-N-biose phosphorylase





● Molecule 1: Lacto-N-biose phosphorylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	67.91Å 112.04Å 118.66Å 105.21° 90.43° 107.32°	Depositor
Resolution (Å)	41.07 – 2.11 40.88 – 2.11	Depositor EDS
% Data completeness (in resolution range)	97.4 (41.07-2.11) 88.5 (40.88-2.11)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 2.12Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.169 , 0.225 0.169 , 0.224	Depositor DCC
R_{free} test set	8997 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	22.2	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.025 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	25782	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, SO4, NDG, NO3

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	0.65	0/6093	0.66	1/8299 (0.0%)
1	B	0.58	0/5997	0.62	0/8166
1	C	0.63	1/6118 (0.0%)	0.65	1/8333 (0.0%)
1	D	0.63	1/5846 (0.0%)	0.65	0/7958
All	All	0.62	2/24054 (0.0%)	0.64	2/32756 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	236	CYS	CB-SG	-7.78	1.69	1.82
1	C	236	CYS	CB-SG	-6.72	1.70	1.82

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	731	LEU	CA-CB-CG	5.50	127.95	115.30
1	A	223	ASP	CB-CG-OD1	5.10	122.89	118.30

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	5926	0	5615	30	0
1	B	5833	0	5536	52	0
1	C	5950	0	5631	32	0
1	D	5686	0	5386	64	0
2	A	15	0	15	0	0
2	B	15	0	15	0	0
2	C	15	0	15	0	0
2	D	15	0	15	0	0
3	A	6	0	8	1	0
3	B	6	0	8	2	0
3	C	12	0	16	0	0
3	D	12	0	16	1	0
4	A	4	0	0	0	0
5	B	1	0	0	0	0
6	D	5	0	0	0	0
7	A	627	0	0	7	0
7	B	533	0	0	12	0
7	C	601	0	0	7	0
7	D	520	0	0	11	0
All	All	25782	0	22276	177	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 (177) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:359:PHE:HD1	7:D:831:HOH:O	1.37	1.04
1:B:251:LYS:HE2	7:B:961:HOH:O	1.58	1.00
1:C:691:GLU:HG2	7:C:964:HOH:O	1.67	0.93
1:D:412:PHE:HA	1:D:415:THR:HG22	1.52	0.92
1:D:121:GLY:O	3:D:4010:GOL:H12	1.69	0.91
1:B:449:LYS:HB3	3:B:4006:GOL:H32	1.56	0.86
1:A:110:HIS:HD2	1:A:126:SER:HB2	1.41	0.83
1:A:20:LYS:HE2	7:A:2060:HOH:O	1.77	0.83
1:B:110:HIS:HD2	1:B:126:SER:HB2	1.42	0.82
1:D:412:PHE:HA	1:D:415:THR:CG2	2.10	0.81
1:C:15:PHE:O	1:C:19:THR:HG23	1.83	0.77
1:D:7:PHE:HB2	7:D:1375:HOH:O	1.83	0.77
1:C:163:GLU:HG2	7:C:1001:HOH:O	1.86	0.73
1:B:46:LEU:HD12	7:B:1962:HOH:O	1.88	0.73
1:B:737:GLU:HG2	7:B:2233:HOH:O	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:ASN:HA	1:B:384:LYS:CE	2.20	0.71
1:D:26:TRP:O	1:D:28:ALA:N	2.24	0.70
1:D:32:ARG:HB3	1:D:51:TYR:HB2	1.74	0.70
1:B:44:LEU:N	7:B:1962:HOH:O	2.25	0.69
1:B:722:ASP:OD1	1:B:723:GLN:NE2	2.26	0.69
1:C:110:HIS:HD2	1:C:126:SER:HB2	1.56	0.69
1:D:375:SER:CB	1:D:415:THR:HG21	2.22	0.68
1:A:110:HIS:CD2	1:A:126:SER:HB2	2.27	0.66
1:B:594:VAL:HG23	1:B:595:ASP:H	1.60	0.66
1:D:711:GLU:C	1:D:713:GLY:H	1.99	0.66
1:D:691:GLU:HG2	7:D:1234:HOH:O	1.98	0.64
1:B:249:GLU:OE1	1:B:255:ARG:NH1	2.31	0.63
1:B:64:ILE:HD13	1:B:181:PHE:HB3	1.78	0.63
1:B:236:CYS:HB3	1:B:316:ILE:HG21	1.79	0.63
1:B:555:ARG:HD2	7:B:1757:HOH:O	1.98	0.63
1:B:110:HIS:CD2	1:B:126:SER:HB2	2.30	0.63
1:A:709:PHE:HB2	1:A:714:LEU:HD12	1.82	0.62
1:D:412:PHE:CA	1:D:415:THR:HG22	2.27	0.62
1:D:724:PRO:HA	1:D:741:LEU:O	2.00	0.61
1:B:717:VAL:HG22	1:B:741:LEU:HD11	1.83	0.61
1:A:17:GLU:OE2	1:A:17:GLU:HA	2.01	0.61
1:D:731:LEU:HD11	1:D:737:GLU:HG3	1.82	0.61
1:B:381:ASN:HA	1:B:384:LYS:HE2	1.82	0.60
1:D:140:VAL:HG12	1:D:143:VAL:CG1	2.31	0.60
1:D:375:SER:HB3	1:D:415:THR:HG21	1.82	0.60
1:C:110:HIS:CD2	1:C:126:SER:HB2	2.37	0.60
1:B:381:ASN:HA	1:B:384:LYS:HE3	1.83	0.59
1:D:29:ASP:HB3	1:D:396:ARG:HH22	1.66	0.59
1:C:376:ILE:HD12	7:C:1002:HOH:O	2.02	0.58
1:D:48:LYS:HB2	7:D:811:HOH:O	2.03	0.58
1:D:400:GLY:C	7:D:894:HOH:O	2.40	0.58
1:C:380:ASP:HB3	1:C:383:ARG:NH2	2.19	0.58
1:B:609:ILE:N	1:B:609:ILE:HD12	2.18	0.57
1:A:15:PHE:O	1:A:19:THR:HG23	2.04	0.57
1:A:64:ILE:HD13	1:A:181:PHE:HB3	1.87	0.57
1:D:413:VAL:CG2	7:D:2109:HOH:O	2.53	0.57
1:D:413:VAL:HG23	7:D:2109:HOH:O	2.05	0.57
1:B:449:LYS:CB	3:B:4006:GOL:H32	2.32	0.56
1:C:364:PHE:CD2	1:C:365:PRO:HD2	2.40	0.56
1:B:251:LYS:CE	7:B:961:HOH:O	2.34	0.56
1:D:64:ILE:HD13	1:D:181:PHE:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:VAL:HB	1:A:149:TYR:OH	2.06	0.55
1:A:447:TRP:O	3:A:4005:GOL:H31	2.07	0.55
1:A:181:PHE:HB2	1:A:188:THR:HG21	1.89	0.55
1:B:719:ASN:ND2	1:B:723:GLN:O	2.36	0.55
1:C:511:ASP:OD2	1:D:550:ARG:HD3	2.07	0.54
1:D:26:TRP:O	1:D:27:GLY:C	2.45	0.54
1:C:19:THR:HG22	1:C:403:LEU:HD23	1.90	0.53
1:C:64:ILE:HD13	1:C:181:PHE:HB3	1.91	0.53
1:D:750:GLU:O	1:D:751:ALA:C	2.44	0.53
1:D:473:ILE:HD11	1:D:542:VAL:HG11	1.89	0.53
1:C:205:GLN:H	1:C:205:GLN:CD	2.11	0.53
1:C:542:VAL:HA	1:C:667:ILE:O	2.09	0.53
1:D:140:VAL:HG12	1:D:143:VAL:HG11	1.90	0.53
1:D:58:ARG:HD2	1:D:178:GLU:HG2	1.90	0.53
1:D:205:GLN:H	1:D:205:GLN:CD	2.13	0.52
1:D:379:LEU:HG	1:D:383:ARG:HH12	1.74	0.52
1:B:15:PHE:O	1:B:19:THR:HG23	2.08	0.52
1:B:9:LEU:O	1:B:31:ILE:HA	2.09	0.52
1:C:32:ARG:HD3	7:C:1575:HOH:O	2.10	0.52
1:C:364:PHE:CG	1:C:365:PRO:HD2	2.45	0.52
1:D:445:ASN:O	1:D:488:SER:HA	2.10	0.52
1:D:438:GLU:HB3	1:D:693:LYS:NZ	2.24	0.51
1:A:234:PHE:CZ	1:A:454:MET:HB3	2.46	0.51
1:B:555:ARG:HD3	1:B:560:ALA:HB3	1.93	0.51
1:B:609:ILE:HD11	7:B:1404:HOH:O	2.11	0.51
1:A:32:ARG:HD3	7:A:887:HOH:O	2.10	0.50
1:D:422:GLU:HA	1:D:425:ASP:OD2	2.11	0.50
1:D:711:GLU:C	1:D:713:GLY:N	2.65	0.50
1:A:110:HIS:HE1	7:A:807:HOH:O	1.95	0.49
1:B:709:PHE:HB2	1:B:714:LEU:HD12	1.94	0.49
1:A:445:ASN:O	1:A:488:SER:HA	2.11	0.49
1:C:205:GLN:HB3	7:C:919:HOH:O	2.13	0.49
1:D:9:LEU:HA	7:D:1809:HOH:O	2.12	0.49
1:D:31:ILE:HG13	1:D:32:ARG:N	2.27	0.49
1:C:584:PRO:HD2	7:C:901:HOH:O	2.12	0.49
1:B:402:TYR:HB2	1:B:405:LEU:HD13	1.95	0.48
1:A:97:PHE:CE1	1:A:226:ARG:HD2	2.49	0.48
1:B:181:PHE:HB2	1:B:188:THR:HG21	1.96	0.48
1:D:711:GLU:O	1:D:713:GLY:N	2.47	0.48
1:D:383:ARG:NH1	1:D:744:SER:OG	2.47	0.48
1:C:602:TRP:CE3	1:C:603:GLU:HG3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:749:ARG:NH2	7:D:2064:HOH:O	2.47	0.47
1:B:410:PRO:HA	7:B:1449:HOH:O	2.13	0.47
1:D:170:ASN:ND2	1:D:365:PRO:HD3	2.30	0.47
1:D:140:VAL:CG1	1:D:143:VAL:HG11	2.45	0.47
1:D:413:VAL:O	1:D:417:THR:HG23	2.15	0.47
1:C:143:VAL:HB	1:C:149:TYR:CZ	2.50	0.47
1:C:393:PRO:HB3	7:C:992:HOH:O	2.15	0.47
1:D:379:LEU:HG	1:D:383:ARG:NH1	2.30	0.46
1:D:234:PHE:CZ	1:D:454:MET:HB3	2.49	0.46
1:C:380:ASP:HB3	1:C:383:ARG:HH22	1.79	0.46
1:D:359:PHE:CD1	7:D:831:HOH:O	2.27	0.46
1:C:216:TYR:HB3	1:C:239:THR:HG22	1.98	0.46
1:C:555:ARG:HE	1:C:555:ARG:HA	1.80	0.46
1:D:132:ASP:HB3	1:D:135:GLU:O	2.16	0.46
1:B:114:GLU:HB2	1:B:258:PRO:HG2	1.98	0.46
1:D:555:ARG:HD2	1:D:560:ALA:HB3	1.97	0.46
1:B:555:ARG:HE	1:B:555:ARG:HA	1.80	0.46
1:C:445:ASN:O	1:C:488:SER:HA	2.16	0.46
1:D:10:PRO:HA	1:D:32:ARG:O	2.16	0.45
1:D:716:CYS:HB3	1:D:748:TRP:CE3	2.50	0.45
1:D:719:ASN:ND2	1:D:723:GLN:O	2.38	0.45
1:C:731:LEU:HD23	1:C:731:LEU:N	2.31	0.45
1:D:375:SER:HB2	1:D:415:THR:HG21	1.99	0.45
1:B:724:PRO:HA	1:B:741:LEU:O	2.17	0.45
1:A:716:CYS:HB3	1:A:748:TRP:CE3	2.52	0.45
1:B:243:ARG:HA	1:B:243:ARG:HD2	1.44	0.44
1:B:408:LYS:O	1:B:410:PRO:HD3	2.18	0.44
1:B:609:ILE:CD1	7:B:1404:HOH:O	2.64	0.44
1:B:555:ARG:CD	7:B:1757:HOH:O	2.61	0.44
1:A:143:VAL:HB	1:A:149:TYR:CZ	2.52	0.44
1:B:542:VAL:HA	1:B:667:ILE:O	2.17	0.44
1:B:748:TRP:O	1:B:749:ARG:NH1	2.50	0.44
1:C:128:ASN:N	1:C:128:ASN:HD22	2.15	0.44
1:A:143:VAL:HG12	7:A:2021:HOH:O	2.16	0.44
1:A:576:ASP:HB3	1:A:615:GLY:HA2	2.00	0.44
1:C:58:ARG:HD2	1:C:178:GLU:OE1	2.18	0.44
1:A:432:GLY:HA2	7:A:1535:HOH:O	2.17	0.44
1:B:584:PRO:HD2	7:B:815:HOH:O	2.17	0.44
1:C:716:CYS:HB3	1:C:748:TRP:CE3	2.53	0.43
1:D:166:ASN:ND2	1:D:364:PHE:HE2	2.16	0.43
1:D:217:GLN:HA	1:D:314:GLN:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:GLU:HG3	7:D:1792:HOH:O	2.18	0.43
1:D:301:HIS:O	1:D:304:GLY:N	2.39	0.43
1:A:276:LYS:HE2	7:A:1055:HOH:O	2.18	0.43
1:B:445:ASN:O	1:B:488:SER:HA	2.18	0.43
1:B:189:ARG:HD2	7:B:1674:HOH:O	2.18	0.43
1:B:333:VAL:HG23	1:B:352:VAL:HG11	2.01	0.43
1:A:555:ARG:HD3	7:A:1008:HOH:O	2.19	0.43
1:D:538:ALA:HB1	1:D:687:ALA:HB1	2.00	0.42
1:B:216:TYR:O	1:B:314:GLN:HA	2.19	0.42
1:B:402:TYR:CB	1:B:405:LEU:HD13	2.49	0.42
1:B:143:VAL:HB	1:B:149:TYR:OH	2.20	0.42
1:B:680:LEU:O	1:B:684:LEU:HG	2.19	0.42
1:A:234:PHE:CE1	1:A:454:MET:HB3	2.55	0.42
1:A:117:ASP:OD2	1:A:147:HIS:ND1	2.53	0.42
1:A:741:LEU:HA	1:A:742:PRO:HD3	1.93	0.42
1:C:164:MET:HE2	1:C:164:MET:HB3	1.96	0.42
1:D:114:GLU:HB2	1:D:258:PRO:HG2	2.01	0.42
1:A:542:VAL:HA	1:A:667:ILE:O	2.20	0.41
1:B:170:ASN:HD21	1:B:364:PHE:HZ	1.64	0.41
1:C:602:TRP:CZ3	1:C:603:GLU:HG3	2.55	0.41
1:D:332:ALA:HA	1:D:354:TYR:O	2.19	0.41
1:D:438:GLU:HB3	1:D:693:LYS:HZ3	1.85	0.41
1:A:115:VAL:HG22	1:A:151:VAL:HG22	2.02	0.41
1:C:753:GLU:HG2	1:C:753:GLU:H	1.71	0.41
1:D:212:THR:N	1:D:213:THR:HA	2.35	0.41
1:B:143:VAL:HB	1:B:149:TYR:CZ	2.55	0.41
1:A:364:PHE:CD2	1:A:365:PRO:HD2	2.56	0.41
1:C:360:LEU:HB3	1:C:361:PRO:HA	2.03	0.41
1:B:602:TRP:CE3	1:B:603:GLU:HG3	2.55	0.41
1:D:22:LEU:O	1:D:26:TRP:HB2	2.20	0.41
1:B:96:PHE:CE1	1:B:229:LYS:HE2	2.56	0.41
1:D:143:VAL:HB	1:D:149:TYR:CZ	2.56	0.41
1:D:9:LEU:O	1:D:31:ILE:HD12	2.21	0.41
1:A:97:PHE:CZ	1:A:226:ARG:HD2	2.56	0.40
1:B:239:THR:HG21	1:B:285:LEU:HD21	2.02	0.40
1:B:347:ALA:HB2	1:B:394:ILE:CG2	2.51	0.40
1:D:568:GLU:HB3	1:D:634:ASN:HB3	2.02	0.40
1:A:76:LEU:O	1:A:152:SER:HA	2.21	0.40
1:D:208:VAL:HG22	1:D:306:GLU:HB2	2.04	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	741/759 (98%)	711 (96%)	30 (4%)	0	100	100
1	B	728/759 (96%)	694 (95%)	32 (4%)	2 (0%)	44	43
1	C	744/759 (98%)	718 (96%)	25 (3%)	1 (0%)	55	56
1	D	701/759 (92%)	663 (95%)	34 (5%)	4 (1%)	28	23
All	All	2914/3036 (96%)	2786 (96%)	121 (4%)	7 (0%)	51	51

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	594	VAL
1	D	27	GLY
1	D	712	GLN
1	B	595	ASP
1	C	41	GLU
1	D	382	TRP
1	D	423	PHE

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	621/634 (98%)	604 (97%)	17 (3%)	50	53
1	B	611/634 (96%)	597 (98%)	14 (2%)	56	59
1	C	624/634 (98%)	615 (99%)	9 (1%)	71	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	596/634 (94%)	578 (97%)	18 (3%)	46	48
All	All	2452/2536 (97%)	2394 (98%)	58 (2%)	54	58

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	PHE
1	A	19	THR
1	A	32	ARG
1	A	52	ASN
1	A	174	ASP
1	A	181	PHE
1	A	236	CYS
1	A	243	ARG
1	A	336	SER
1	A	358	ARG
1	A	379	LEU
1	A	405	LEU
1	A	443	ILE
1	A	555	ARG
1	A	611	LEU
1	A	714	LEU
1	A	752	LEU
1	B	3	SER
1	B	44	LEU
1	B	48	LYS
1	B	171	ASP
1	B	174	ASP
1	B	181	PHE
1	B	251	LYS
1	B	411	LYS
1	B	555	ARG
1	B	611	LEU
1	B	717	VAL
1	B	723	GLN
1	B	731	LEU
1	B	737	GLU
1	C	14	ASN
1	C	40	ASP
1	C	181	PHE
1	C	205	GLN
1	C	358	ARG

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Mol	Chain	Res	Type
1	C	367	THR
1	C	611	LEU
1	C	731	LEU
1	C	753	GLU
1	D	9	LEU
1	D	12	GLU
1	D	31	ILE
1	D	46	LEU
1	D	48	LYS
1	D	126	SER
1	D	178	GLU
1	D	181	PHE
1	D	205	GLN
1	D	376	ILE
1	D	381	ASN
1	D	424	ARG
1	D	425	ASP
1	D	433	VAL
1	D	609	ILE
1	D	712	GLN
1	D	743	ASP
1	D	749	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	HIS
1	A	128	ASN
1	A	170	ASN
1	A	690	ASN
1	A	720	ASN
1	B	52	ASN
1	B	128	ASN
1	B	690	ASN
1	B	720	ASN
1	C	110	HIS
1	C	128	ASN
1	C	170	ASN
1	C	641	ASN
1	C	690	ASN
1	C	720	ASN
1	D	128	ASN

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Mol	Chain	Res	Type
1	D	166	ASN
1	D	170	ASN
1	D	381	ASN
1	D	690	ASN
1	D	720	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NDG	A	4001	-	15,15,15	0.62	0	21,21,21	1.09	1 (4%)
3	GOL	A	4005	-	5,5,5	0.28	0	5,5,5	0.73	0
4	NO3	A	4012	-	1,3,3	4.72	1 (100%)	0,3,3	0.00	-
2	NDG	B	4002	-	15,15,15	0.63	0	21,21,21	1.27	2 (9%)
3	GOL	B	4006	-	5,5,5	0.27	0	5,5,5	0.72	0
2	NDG	C	4003	-	15,15,15	0.66	0	21,21,21	1.06	1 (4%)
3	GOL	C	4007	-	5,5,5	0.21	0	5,5,5	0.64	0
3	GOL	C	4008	-	5,5,5	0.29	0	5,5,5	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NDG	D	4004	-	15,15,15	0.65	0	21,21,21	1.29	3 (14%)
3	GOL	D	4009	-	5,5,5	0.25	0	5,5,5	0.79	0
3	GOL	D	4010	-	5,5,5	0.37	0	5,5,5	0.50	0
6	SO4	D	4011	-	4,4,4	0.18	0	6,6,6	0.20	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NDG	A	4001	-	-	0/6/26/26	0/1/1/1
3	GOL	A	4005	-	-	0/4/4/4	0/0/0/0
4	NO3	A	4012	-	-	0/0/0/0	0/0/0/0
2	NDG	B	4002	-	-	0/6/26/26	0/1/1/1
3	GOL	B	4006	-	-	0/4/4/4	0/0/0/0
2	NDG	C	4003	-	-	0/6/26/26	0/1/1/1
3	GOL	C	4007	-	-	0/4/4/4	0/0/0/0
3	GOL	C	4008	-	-	0/4/4/4	0/0/0/0
2	NDG	D	4004	-	-	0/6/26/26	0/1/1/1
3	GOL	D	4009	-	-	0/4/4/4	0/0/0/0
3	GOL	D	4010	-	-	0/4/4/4	0/0/0/0
6	SO4	D	4011	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	4012	NO3	O1-N	4.72	1.41	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4002	NDG	C1-C2-N2	-4.54	105.47	110.73
2	A	4001	NDG	C1-C2-N2	-3.58	106.59	110.73
2	D	4004	NDG	C1-C2-N2	-3.54	106.62	110.73
2	C	4003	NDG	C1-C2-N2	-3.51	106.66	110.73
2	B	4002	NDG	O-C1-C2	2.04	111.56	109.52
2	D	4004	NDG	C3-C2-N2	2.13	114.69	110.61
2	D	4004	NDG	O-C1-C2	2.45	111.98	109.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4005	GOL	1	0
3	B	4006	GOL	2	0
3	D	4010	GOL	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, 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	745/759 (98%)	-0.25	12 (1%) 72 76	12, 21, 35, 66	0
1	B	734/759 (96%)	0.09	46 (6%) 21 26	13, 24, 55, 69	0
1	C	748/759 (98%)	-0.23	16 (2%) 64 68	11, 21, 38, 64	0
1	D	713/759 (93%)	0.11	51 (7%) 16 20	12, 23, 53, 64	0
All	All	2940/3036 (96%)	-0.07	125 (4%) 36 42	11, 22, 49, 69	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	406	ALA	7.5
1	D	24	GLU	6.1
1	D	371	GLY	6.0
1	D	25	LEU	6.0
1	B	594	VAL	5.9
1	B	45	ALA	5.4
1	D	710	PRO	5.2
1	D	376	ILE	5.1
1	D	365	PRO	5.0
1	D	47	GLY	4.9
1	D	412	PHE	4.8
1	B	44	LEU	4.7
1	B	407	ALA	4.7
1	D	415	THR	4.5
1	D	418	HIS	4.5
1	D	370	GLU	4.4
1	B	401	GLY	4.3
1	B	14	ASN	4.3
1	B	405	LEU	4.2
1	B	46	LEU	4.2
1	B	364	PHE	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	12	GLU	4.1
1	A	752	LEU	3.9
1	B	47	GLY	3.9
1	B	13	GLU	3.9
1	C	40	ASP	3.8
1	D	362	TYR	3.8
1	B	11	SER	3.7
1	D	408	LYS	3.5
1	D	5	GLY	3.5
1	B	25	LEU	3.5
1	D	713	GLY	3.5
1	C	13	GLU	3.4
1	D	23	ALA	3.4
1	D	413	VAL	3.4
1	C	14	ASN	3.4
1	B	404	SER	3.3
1	D	416	VAL	3.3
1	B	373	ASP	3.3
1	D	424	ARG	3.2
1	D	28	ALA	3.2
1	B	402	TYR	3.2
1	D	10	PRO	3.2
1	C	43	VAL	3.2
1	D	410	PRO	3.2
1	B	363	PHE	3.1
1	B	17	GLU	3.1
1	B	19	THR	3.1
1	D	29	ASP	3.1
1	A	41	GLU	3.1
1	B	403	LEU	3.1
1	B	379	LEU	3.0
1	D	46	LEU	3.0
1	D	407	ALA	3.0
1	B	413	VAL	3.0
1	D	372	ASN	3.0
1	D	174	ASP	3.0
1	D	411	LYS	3.0
1	C	42	ALA	3.0
1	B	371	GLY	2.9
1	C	35	ASP	2.9
1	D	419	ILE	2.9
1	D	30	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	4	THR	2.8
1	D	369	TYR	2.8
1	D	751	ALA	2.8
1	D	399	TYR	2.8
1	C	171	ASP	2.7
1	B	408	LYS	2.7
1	D	722	ASP	2.7
1	B	711	GLU	2.7
1	B	16	ALA	2.7
1	C	41	GLU	2.7
1	D	714	LEU	2.7
1	B	751	ALA	2.6
1	B	302	ALA	2.6
1	B	366	ASP	2.6
1	B	372	ASN	2.5
1	A	40	ASP	2.5
1	A	174	ASP	2.5
1	B	412	PHE	2.5
1	B	18	LYS	2.5
1	C	750	GLU	2.5
1	B	360	LEU	2.5
1	D	409	PHE	2.5
1	B	21	GLU	2.4
1	D	27	GLY	2.4
1	B	24	GLU	2.4
1	A	3	SER	2.4
1	D	26	TRP	2.4
1	D	12	GLU	2.4
1	A	751	ALA	2.4
1	A	600	GLU	2.4
1	A	171	ASP	2.4
1	C	3	SER	2.4
1	D	438	GLU	2.4
1	C	17	GLU	2.4
1	D	368	PHE	2.3
1	B	365	PRO	2.3
1	B	428	ASP	2.3
1	D	733	ASP	2.3
1	D	711	GLU	2.2
1	B	740	ASP	2.2
1	A	594	VAL	2.2
1	D	420	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	359	PHE	2.2
1	C	753	GLU	2.2
1	B	376	ILE	2.2
1	C	316	ILE	2.2
1	D	48	LYS	2.2
1	C	402	TYR	2.2
1	A	711	GLU	2.2
1	D	400	GLY	2.2
1	D	233	TRP	2.1
1	D	734	GLY	2.1
1	B	174	ASP	2.1
1	B	746	ILE	2.1
1	D	31	ILE	2.1
1	B	9	LEU	2.1
1	A	43	VAL	2.1
1	A	11	SER	2.0
1	C	733	ASP	2.0
1	C	45	ALA	2.0
1	B	722	ASP	2.0
1	D	201	LYS	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
3	GOL	D	4009	6/6	0.88	0.19	3.45	26,30,31,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	GOL	D	4010	6/6	0.83	0.18	2.06	50,51,52,52	0
3	GOL	B	4006	6/6	0.89	0.16	2.05	31,35,37,39	0
3	GOL	C	4008	6/6	0.93	0.13	1.18	35,39,40,42	0
3	GOL	A	4005	6/6	0.89	0.13	1.02	26,28,30,33	0
2	NDG	C	4003	15/15	0.96	0.14	0.54	18,19,22,25	0
2	NDG	D	4004	15/15	0.97	0.15	0.14	18,22,23,25	0
3	GOL	C	4007	6/6	0.91	0.10	0.00	19,22,24,26	0
2	NDG	A	4001	15/15	0.97	0.14	-0.04	13,18,21,23	0
2	NDG	B	4002	15/15	0.95	0.10	-0.57	17,22,25,25	0
6	SO4	D	4011	5/5	0.93	0.14	-0.73	70,71,71,71	0
4	NO3	A	4012	4/4	0.81	0.17	-	41,41,42,43	0
5	MG	B	4013	1/1	1.00	0.03	-	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.