Full wwPDB X-ray Structure Validation Report (i)

Mar 5, 2024 – 02:32 PM EST

PDB ID	:	2ZUT
Title	:	Crystal structure of Galacto-N-biose/Lacto-N-biose I phosphorylase in complex with GalNAc
Authors	:	Hidaka, M.; Nishimoto, M.; Kitaoka, M.; Wakagi, T.; Shoun, H.; Fushinobu, S.
Deposited on	:	2008-10-28
Resolution	:	1.90 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 (i) 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 (i)) were used in the production of this report:

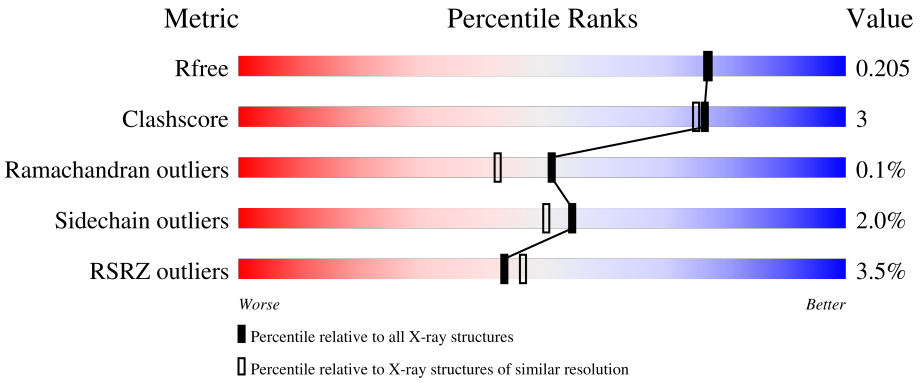
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 <=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	2% 92% 6% • •
1	B	759	6% 88% 8% • •
1	C	759	% 92% 5% • •
1	D	759	5% 91% 6% •

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 26811 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
			Total	C	N	O	S			
1	A	744	5920	3779	996	1129	16	0	0	0
1	B	735	5851	3734	985	1116	16	0	0	0
1	C	744	5920	3779	996	1129	16	0	0	0
1	D	739	5882	3756	989	1121	16	0	0	0

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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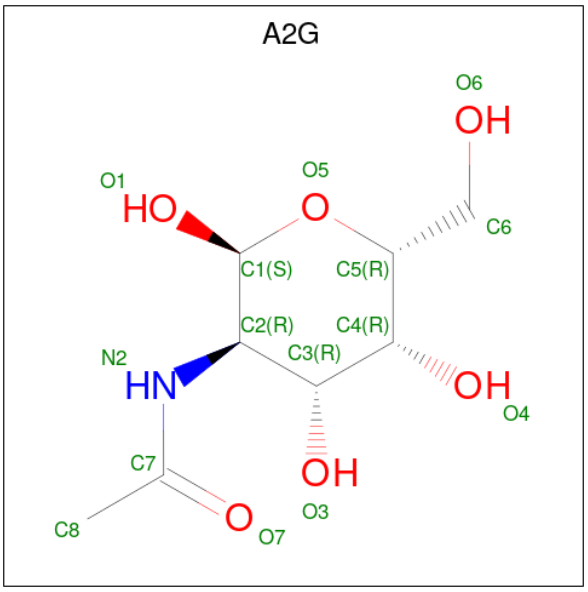
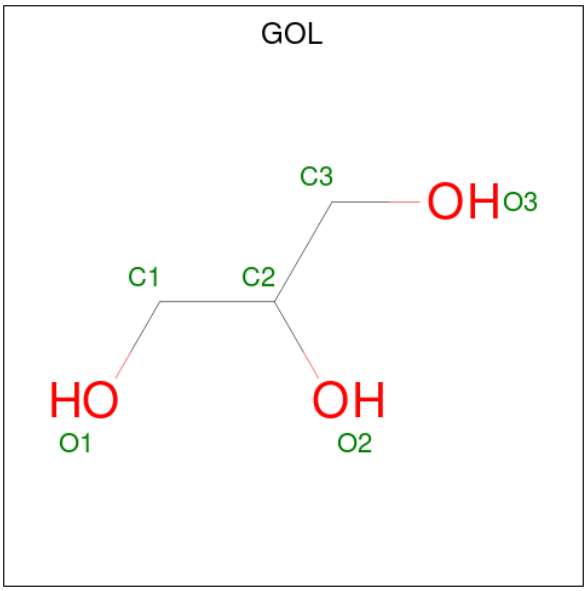
Chain	Residue	Modelled	Actual	Comment	Reference
C	757	HIS	-	expression tag	UNP Q5NU17
C	758	HIS	-	expression tag	UNP Q5NU17
C	759	HIS	-	expression tag	UNP Q5NU17
D	752	LEU	-	expression tag	UNP Q5NU17
D	753	GLU	-	expression tag	UNP Q5NU17
D	754	HIS	-	expression tag	UNP Q5NU17
D	755	HIS	-	expression tag	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-acetamido-2-deoxy-alpha-D-galactopyranose (three-letter code: A2G) (formula: $C_8H_{15}NO_6$).



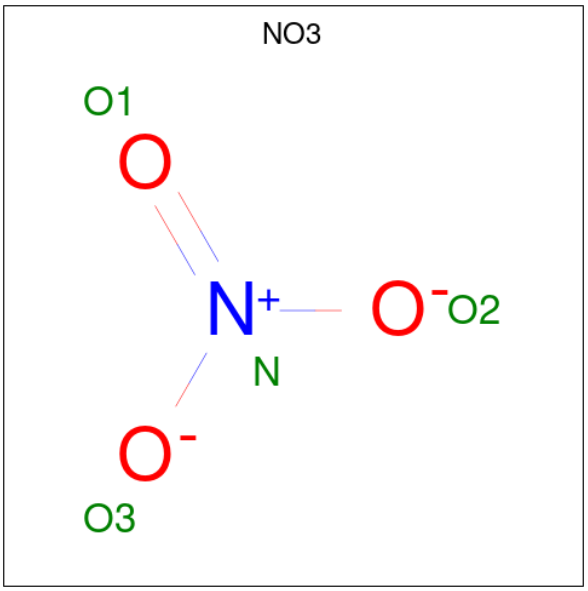
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	15	8	1	6	0	0
			Total	C	N	O		
2	B	1	15	8	1	6	0	0
			Total	C	N	O		
2	C	1	15	8	1	6	0	0
			Total	C	N	O		
2	D	1	15	8	1	6	0	0

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



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

- Molecule 4 is NITRATE ION (three-letter code: NO3) (formula: NO_3).



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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
5	A	1	1	1	0	0
5	B	2	2	2	0	0
5	C	1	1	1	0	0
5	D	2	2	2	0	0

- Molecule 6 is water.

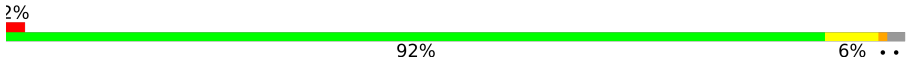
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	825	825	825	0	0
6	B	687	687	687	0	0
6	C	874	874	874	0	0
6	D	728	728	728	1	0

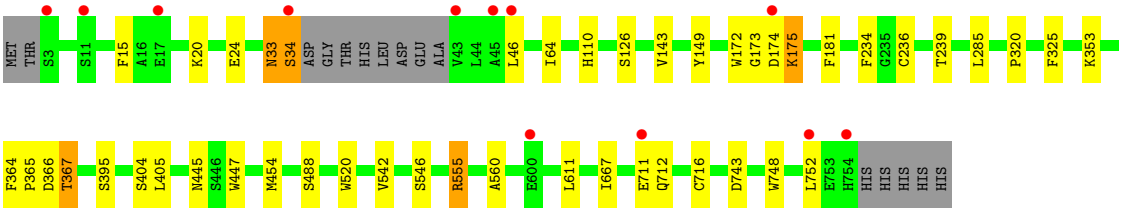
3 Residue-property plots (i)

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: Lacto-N-biose phosphorylase

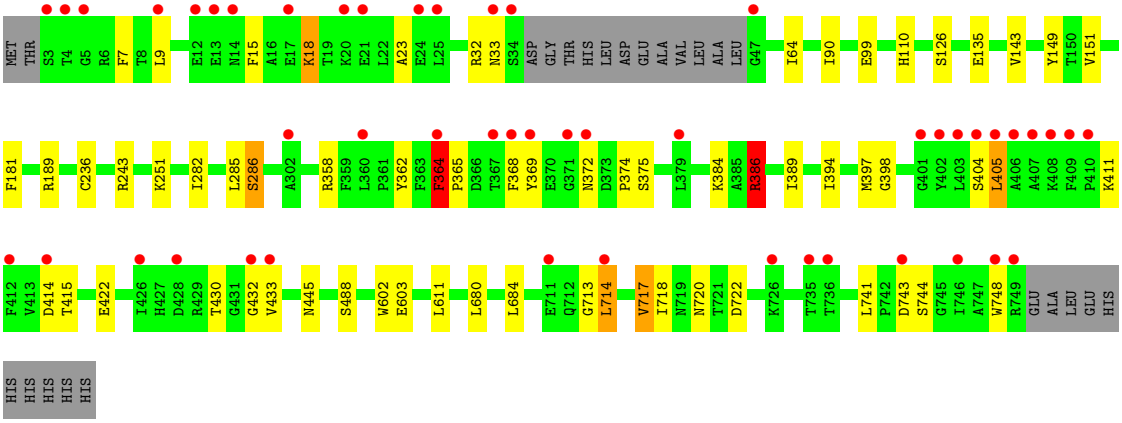
Chain A:





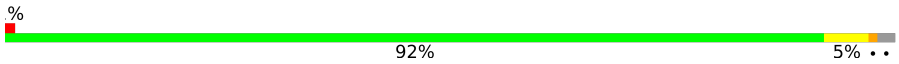
• Molecule 1: Lacto-N-biose phosphorylase

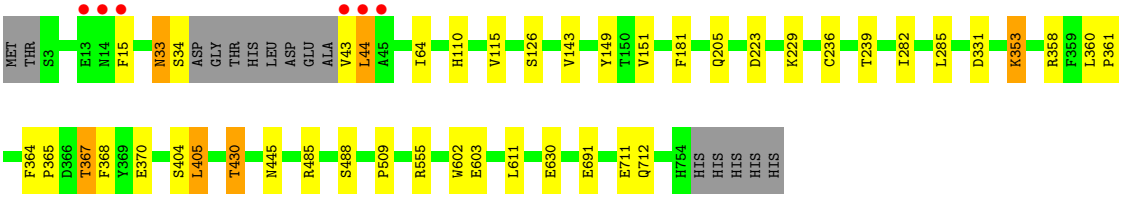
Chain B:



• Molecule 1: Lacto-N-biose phosphorylase

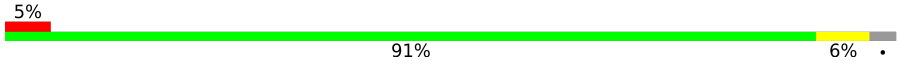
Chain C:

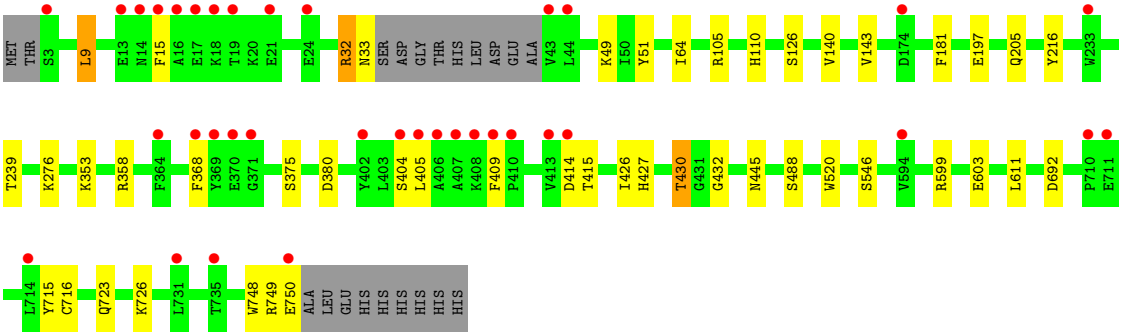




• Molecule 1: Lacto-N-biose phosphorylase

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	67.86Å 111.66Å 118.66Å 105.20° 90.48° 107.27°	Depositor
Resolution (Å)	44.81 – 1.90 44.81 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.7 (44.81-1.90) 96.7 (44.81-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.99 (at 1.89Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.161 , 0.204 0.161 , 0.205	Depositor DCC
R_{free} test set	12254 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	23.7	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 51.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.039 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	26811	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: A2G, NO3, GOL, MG

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	0.72	1/6088 (0.0%)	0.69	0/8292
1	B	0.68	1/6018 (0.0%)	0.69	3/8196 (0.0%)
1	C	0.71	1/6088 (0.0%)	0.70	3/8292 (0.0%)
1	D	0.68	0/6049	0.67	2/8239 (0.0%)
All	All	0.70	3/24243 (0.0%)	0.69	8/33019 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	236	CYS	CB-SG	-7.28	1.69	1.82
1	C	236	CYS	CB-SG	-6.77	1.70	1.82
1	B	236	CYS	CB-SG	-5.21	1.73	1.81

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	555	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	B	386	ARG	NE-CZ-NH2	5.63	123.12	120.30
1	C	485	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	D	9	LEU	CA-CB-CG	5.40	127.73	115.30
1	B	364	PHE	CB-CA-C	5.18	120.75	110.40
1	C	555	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	B	386	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	D	105	ARG	NE-CZ-NH2	-5.06	117.77	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	5920	0	5612	28	0
1	B	5851	0	5541	53	0
1	C	5920	0	5612	33	0
1	D	5882	0	5578	23	0
2	A	15	0	12	0	0
2	B	15	0	12	0	0
2	C	15	0	12	0	0
2	D	15	0	12	0	0
3	A	18	0	24	1	0
3	B	12	0	16	0	0
3	C	12	0	16	0	0
3	D	12	0	16	0	0
4	A	4	0	0	0	0
5	A	1	0	0	0	0
5	B	2	0	0	0	0
5	C	1	0	0	0	0
5	D	2	0	0	0	0
6	A	825	0	0	3	0
6	B	687	0	0	12	0
6	C	874	0	0	10	0
6	D	728	0	0	6	0
All	All	26811	0	22463	137	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 3.

All (137) 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:99:GLU:HG3	6:B:787:HOH:O	1.65	0.97
1:B:364:PHE:HD1	1:B:365:PRO:HD2	1.40	0.85
1:A:110:HIS:HD2	1:A:126:SER:HB2	1.40	0.85
1:A:33:ASN:HD22	1:A:34:SER:H	1.22	0.83
1:B:411:LYS:HD3	6:B:2332:HOH:O	1.78	0.83
1:B:251:LYS:HD3	6:B:2358:HOH:O	1.77	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:VAL:HG13	1:C:44:LEU:H	1.41	0.83
1:B:64:ILE:HD13	1:B:181:PHE:HB3	1.63	0.80
1:D:426:ILE:O	1:D:430:THR:HB	1.83	0.79
1:D:110:HIS:HD2	1:D:126:SER:HB2	1.50	0.76
1:C:711:GLU:HG2	6:C:1929:HOH:O	1.87	0.75
1:B:110:HIS:HD2	1:B:126:SER:HB2	1.51	0.74
1:C:430:THR:CG2	6:C:1923:HOH:O	2.34	0.74
1:C:331:ASP:HA	1:C:353:LYS:HD3	1.70	0.73
1:A:711:GLU:HG2	6:A:883:HOH:O	1.90	0.72
1:A:367:THR:HG23	6:A:2044:HOH:O	1.92	0.70
1:B:432:GLY:HA2	6:B:2800:HOH:O	1.90	0.70
1:B:374:PRO:HD2	6:B:2547:HOH:O	1.91	0.69
1:C:691:GLU:HG2	6:C:2527:HOH:O	1.93	0.68
1:A:172:TRP:O	1:A:174:ASP:N	2.29	0.66
1:C:430:THR:HG21	6:C:1923:HOH:O	1.94	0.66
1:B:720:ASN:HB2	6:B:2483:HOH:O	1.96	0.64
1:A:33:ASN:HD22	1:A:34:SER:N	1.92	0.64
1:C:110:HIS:HD2	1:C:126:SER:HB2	1.64	0.63
1:B:99:GLU:CG	6:B:787:HOH:O	2.32	0.63
1:C:367:THR:HG23	6:C:2563:HOH:O	1.97	0.62
1:C:603:GLU:HG2	6:C:1117:HOH:O	1.98	0.62
1:B:384:LYS:HD2	6:B:1403:HOH:O	2.00	0.61
1:A:110:HIS:CD2	1:A:126:SER:HB2	2.30	0.61
1:D:110:HIS:CD2	1:D:126:SER:HB2	2.36	0.60
1:B:251:LYS:HB2	1:B:251:LYS:NZ	2.17	0.60
1:D:430:THR:HG22	1:D:432:GLY:H	1.65	0.60
1:B:282:ILE:O	1:B:286:SER:HB2	2.00	0.60
1:A:20:LYS:HG3	1:A:46:LEU:HD21	1.83	0.59
1:B:714:LEU:CD1	1:B:748:TRP:HE3	2.14	0.59
1:B:110:HIS:CD2	1:B:126:SER:HB2	2.35	0.57
1:B:714:LEU:HD12	1:B:748:TRP:HE3	1.70	0.57
1:D:276:LYS:HD3	6:D:766:HOH:O	2.05	0.56
1:A:15:PHE:CZ	1:A:404:SER:HA	2.40	0.56
1:C:364:PHE:CD2	1:C:365:PRO:HD2	2.40	0.56
1:B:386:ARG:HG2	1:B:386:ARG:HH21	1.71	0.56
1:A:447:TRP:O	3:A:4005:GOL:H12	2.06	0.55
1:D:380:ASP:HB2	6:D:2333:HOH:O	2.05	0.55
1:D:15:PHE:CZ	1:D:404:SER:HA	2.41	0.55
1:B:430:THR:HG22	1:B:433:VAL:H	1.72	0.55
1:A:555:ARG:HD2	1:A:560:ALA:HB3	1.87	0.54
1:A:364:PHE:CD2	1:A:365:PRO:HD2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:711:GLU:HG3	1:C:712:GLN:NE2	2.23	0.53
1:B:358:ARG:O	1:B:358:ARG:NH1	2.41	0.53
1:B:718:ILE:HD12	1:B:720:ASN:HD21	1.73	0.53
1:C:34:SER:C	6:C:2356:HOH:O	2.46	0.53
1:B:368:PHE:HB2	1:B:405:LEU:HD23	1.90	0.53
1:A:711:GLU:HG3	1:A:712:GLN:NE2	2.23	0.53
1:C:43:VAL:CG1	1:C:44:LEU:H	2.18	0.53
1:D:368:PHE:HB2	1:D:405:LEU:HD23	1.91	0.53
1:B:386:ARG:HH21	1:B:386:ARG:CG	2.22	0.53
1:D:599:ARG:O	1:D:603:GLU:HG3	2.09	0.53
1:B:99:GLU:CD	6:B:787:HOH:O	2.47	0.52
1:C:43:VAL:HG13	1:C:44:LEU:N	2.20	0.52
1:B:430:THR:CG2	1:B:433:VAL:O	2.58	0.51
1:B:189:ARG:HD2	6:B:3055:HOH:O	2.11	0.51
1:D:445:ASN:O	1:D:488:SER:HA	2.11	0.50
1:C:331:ASP:HA	1:C:353:LYS:CD	2.40	0.50
1:B:15:PHE:CZ	1:B:404:SER:HA	2.47	0.49
1:C:143:VAL:HB	1:C:149:TYR:CZ	2.47	0.49
1:A:64:ILE:HD13	1:A:181:PHE:HB3	1.95	0.49
1:B:362:TYR:HD2	1:B:364:PHE:HD2	1.60	0.49
1:A:143:VAL:HB	1:A:149:TYR:CZ	2.48	0.48
1:B:143:VAL:HB	1:B:149:TYR:OH	2.14	0.48
1:D:380:ASP:CB	6:D:2333:HOH:O	2.61	0.48
1:A:716:CYS:HB3	1:A:748:TRP:CE3	2.49	0.47
1:B:445:ASN:O	1:B:488:SER:HA	2.14	0.47
1:C:15:PHE:CZ	1:C:404:SER:HA	2.50	0.47
1:C:110:HIS:CD2	1:C:126:SER:HB2	2.47	0.46
1:B:251:LYS:HB2	1:B:251:LYS:HZ3	1.80	0.46
1:C:239:THR:HG21	1:C:285:LEU:HD21	1.96	0.46
1:D:375:SER:HB2	1:D:415:THR:OG1	2.16	0.46
1:B:397:MET:HG2	1:B:398:GLY:N	2.30	0.46
1:A:172:TRP:CE3	1:A:175:LYS:HE3	2.50	0.46
1:C:64:ILE:HD13	1:C:181:PHE:HB3	1.98	0.45
1:D:64:ILE:HD13	1:D:181:PHE:HB3	1.99	0.45
1:C:602:TRP:CE3	1:C:603:GLU:HG3	2.52	0.45
1:A:445:ASN:O	1:A:488:SER:HA	2.16	0.45
1:B:362:TYR:HB3	6:B:3032:HOH:O	2.15	0.45
1:B:422:GLU:OE1	6:B:860:HOH:O	2.21	0.45
1:B:364:PHE:HD1	1:B:365:PRO:CD	2.20	0.45
1:A:239:THR:HG21	1:A:285:LEU:HD21	1.99	0.44
1:B:717:VAL:HG22	1:B:741:LEU:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:715:TYR:CE2	1:D:749:ARG:HB2	2.52	0.44
1:A:110:HIS:HD2	1:A:126:SER:CB	2.22	0.44
1:B:680:LEU:O	1:B:684:LEU:HG	2.16	0.44
1:C:43:VAL:HG12	6:C:2431:HOH:O	2.17	0.44
1:C:33:ASN:HD22	1:C:34:SER:N	2.15	0.44
1:D:368:PHE:HB2	1:D:405:LEU:CD2	2.48	0.44
1:D:716:CYS:HB3	1:D:748:TRP:CE3	2.51	0.44
1:B:90:ILE:HG21	1:B:151:VAL:HG23	2.00	0.44
1:B:364:PHE:CD1	1:B:365:PRO:HD2	2.32	0.44
1:C:445:ASN:O	1:C:488:SER:HA	2.18	0.44
1:D:32:ARG:HA	1:D:51:TYR:HB2	1.99	0.44
1:B:7:PHE:HA	1:B:397:MET:O	2.18	0.43
1:B:714:LEU:HD12	1:B:748:TRP:CE3	2.53	0.43
1:A:367:THR:CG2	6:A:2044:HOH:O	2.60	0.43
1:A:234:PHE:CZ	1:A:454:MET:HB3	2.53	0.43
1:C:360:LEU:HB3	1:C:361:PRO:HA	1.99	0.43
1:B:722:ASP:HA	1:B:743:ASP:OD1	2.19	0.43
1:C:143:VAL:HB	1:C:149:TYR:OH	2.19	0.43
1:B:9:LEU:HD12	1:B:23:ALA:HB2	2.01	0.43
1:B:718:ILE:HD12	1:B:720:ASN:ND2	2.34	0.42
1:B:369:TYR:CE1	1:B:372:ASN:HB2	2.54	0.42
1:A:364:PHE:HB3	1:A:366:ASP:OD1	2.19	0.42
1:B:372:ASN:O	1:B:374:PRO:HD3	2.19	0.42
1:B:714:LEU:HD11	1:B:748:TRP:HE3	1.84	0.42
1:D:216:TYR:HB3	1:D:239:THR:HG22	2.02	0.42
1:A:542:VAL:HA	1:A:667:ILE:O	2.20	0.42
1:C:115:VAL:HG22	1:C:151:VAL:HG22	2.01	0.42
1:D:140:VAL:HG12	1:D:143:VAL:CG1	2.50	0.42
1:B:430:THR:HG22	1:B:433:VAL:N	2.35	0.42
1:D:197:GLU:HG3	6:D:2979:HOH:O	2.19	0.42
1:D:520:TRP:CE2	1:D:546:SER:HA	2.54	0.42
1:D:692:ASP:HB3	6:D:2893:HOH:O	2.19	0.42
1:A:172:TRP:CD2	1:A:175:LYS:HE3	2.55	0.42
1:B:602:TRP:CE3	1:B:603:GLU:HG3	2.55	0.41
1:C:430:THR:HG23	6:C:1923:HOH:O	2.11	0.41
1:A:520:TRP:CE2	1:A:546:SER:HA	2.55	0.41
1:C:368:PHE:HB2	1:C:405:LEU:HG	2.03	0.41
1:B:389:ILE:HG12	1:B:394:ILE:HG12	2.02	0.41
1:C:223:ASP:HB3	1:C:229:LYS:HB2	2.02	0.41
1:D:409:PHE:HB3	6:D:2359:HOH:O	2.20	0.41
1:B:143:VAL:HB	1:B:149:TYR:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:282:ILE:HD13	1:C:282:ILE:HA	1.93	0.41
1:B:364:PHE:HA	1:B:365:PRO:HD3	1.97	0.41
1:A:555:ARG:HA	1:A:555:ARG:HD3	1.77	0.40
1:C:630:GLU:OE2	6:C:2210:HOH:O	2.22	0.40
1:B:18:LYS:NZ	1:B:18:LYS:HB3	2.36	0.40
1:C:44:LEU:HD21	1:C:205:GLN:HB2	2.04	0.40
1:A:320:PRO:HA	1:A:325:PHE:CD1	2.57	0.40
1:B:375:SER:HB2	1:B:415:THR:OG1	2.21	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	740/759 (98%)	716 (97%)	22 (3%)	2 (0%)	41	31
1	B	731/759 (96%)	703 (96%)	27 (4%)	1 (0%)	51	42
1	C	740/759 (98%)	718 (97%)	22 (3%)	0	100	100
1	D	735/759 (97%)	709 (96%)	26 (4%)	0	100	100
All	All	2946/3036 (97%)	2846 (97%)	97 (3%)	3 (0%)	51	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	173	GLY
1	A	743	ASP
1	B	713	GLY

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	621/634 (98%)	610 (98%)	11 (2%)	59	55
1	B	614/634 (97%)	599 (98%)	15 (2%)	49	43
1	C	621/634 (98%)	611 (98%)	10 (2%)	62	60
1	D	617/634 (97%)	603 (98%)	14 (2%)	50	45
All	All	2473/2536 (98%)	2423 (98%)	50 (2%)	55	51

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	GLU
1	A	33	ASN
1	A	34	SER
1	A	175	LYS
1	A	353	LYS
1	A	367	THR
1	A	395	SER
1	A	405	LEU
1	A	555	ARG
1	A	611	LEU
1	A	752	LEU
1	B	18	LYS
1	B	32	ARG
1	B	33	ASN
1	B	135	GLU
1	B	243	ARG
1	B	285	LEU
1	B	286	SER
1	B	364	PHE
1	B	386	ARG
1	B	405	LEU
1	B	414	ASP
1	B	611	LEU
1	B	714	LEU

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Mol	Chain	Res	Type
1	B	717	VAL
1	B	744	SER
1	C	33	ASN
1	C	44	LEU
1	C	353	LYS
1	C	358	ARG
1	C	367	THR
1	C	370	GLU
1	C	405	LEU
1	C	430	THR
1	C	509	PRO
1	C	611	LEU
1	D	9	LEU
1	D	32	ARG
1	D	33	ASN
1	D	49	LYS
1	D	205	GLN
1	D	353	LYS
1	D	358	ARG
1	D	414	ASP
1	D	427	HIS
1	D	430	THR
1	D	611	LEU
1	D	723	GLN
1	D	726	LYS
1	D	750	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	52	ASN
1	A	110	HIS
1	A	128	ASN
1	A	170	ASN
1	A	690	ASN
1	A	720	ASN
1	B	33	ASN
1	B	52	ASN
1	B	166	ASN
1	B	641	ASN
1	B	690	ASN

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Mol	Chain	Res	Type
1	B	720	ASN
1	C	33	ASN
1	C	128	ASN
1	C	641	ASN
1	C	690	ASN
1	C	720	ASN
1	D	52	ASN
1	D	128	ASN
1	D	166	ASN
1	D	720	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)

Of 20 ligands modelled in this entry, 6 are monoatomic - leaving 14 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	A2G	B	4002	-	15,15,15	0.71	0	21,21,21	0.83	1 (4%)
3	GOL	B	4009	-	5,5,5	0.30	0	5,5,5	0.73	0
3	GOL	A	4005	-	5,5,5	0.31	0	5,5,5	0.79	0
3	GOL	D	4012	-	5,5,5	0.25	0	5,5,5	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GOL	D	4013	-	5,5,5	0.37	0	5,5,5	0.63	0
3	GOL	C	4011	-	5,5,5	0.31	0	5,5,5	0.62	0
3	GOL	A	4006	-	5,5,5	0.34	0	5,5,5	0.19	0
4	NO3	A	4014	-	1,3,3	3.93	1 (100%)	0,3,3	-	-
3	GOL	B	4008	-	5,5,5	0.32	0	5,5,5	0.82	0
3	GOL	C	4010	-	5,5,5	0.22	0	5,5,5	0.83	0
2	A2G	C	4003	-	15,15,15	0.49	0	21,21,21	0.85	2 (9%)
2	A2G	A	4001	-	15,15,15	0.60	0	21,21,21	0.78	0
3	GOL	A	4007	-	5,5,5	0.29	0	5,5,5	0.33	0
2	A2G	D	4004	-	15,15,15	0.75	0	21,21,21	0.81	1 (4%)

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	A2G	B	4002	-	-	0/6/26/26	0/1/1/1
3	GOL	B	4009	-	-	2/4/4/4	-
3	GOL	A	4005	-	-	3/4/4/4	-
3	GOL	D	4012	-	-	0/4/4/4	-
3	GOL	D	4013	-	-	0/4/4/4	-
3	GOL	C	4011	-	-	0/4/4/4	-
3	GOL	A	4006	-	-	3/4/4/4	-
3	GOL	B	4008	-	-	0/4/4/4	-
3	GOL	C	4010	-	-	0/4/4/4	-
2	A2G	C	4003	-	-	0/6/26/26	0/1/1/1
2	A2G	A	4001	-	-	0/6/26/26	0/1/1/1
3	GOL	A	4007	-	-	3/4/4/4	-
2	A2G	D	4004	-	-	0/6/26/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	4014	NO3	O1-N	3.93	1.42	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	4002	A2G	O5-C1-C2	2.34	111.87	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	4004	A2G	O5-C1-C2	2.24	111.76	109.52
2	C	4003	A2G	O5-C1-C2	2.05	111.58	109.52
2	C	4003	A2G	O3-C3-C4	2.02	115.01	110.35

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	4006	GOL	C1-C2-C3-O3
3	A	4007	GOL	O1-C1-C2-C3
3	B	4009	GOL	O1-C1-C2-C3
3	A	4005	GOL	O1-C1-C2-C3
3	A	4006	GOL	O2-C2-C3-O3
3	B	4009	GOL	O1-C1-C2-O2
3	A	4007	GOL	O1-C1-C2-O2
3	A	4006	GOL	O1-C1-C2-C3
3	A	4007	GOL	O2-C2-C3-O3
3	A	4005	GOL	O2-C2-C3-O3
3	A	4005	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4005	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 (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	744/759 (98%)	-0.28	12 (1%)	72	74	15, 22, 39, 54	0
1	B	735/759 (96%)	-0.01	49 (6%)	17	20	16, 25, 57, 73	0
1	C	744/759 (98%)	-0.35	6 (0%)	86	87	15, 23, 38, 52	0
1	D	739/759 (97%)	-0.07	36 (4%)	29	33	16, 25, 48, 58	0
All	All	2962/3036 (97%)	-0.18	103 (3%)	44	47	15, 24, 48, 73	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	364	PHE	6.4
1	B	406	ALA	5.8
1	B	369	TYR	5.1
1	B	368	PHE	5.0
1	D	406	ALA	4.6
1	B	14	ASN	4.4
1	B	13	GLU	4.1
1	D	414	ASP	3.8
1	B	748	TRP	3.7
1	D	369	TYR	3.7
1	B	407	ALA	3.6
1	B	714	LEU	3.5
1	B	401	GLY	3.5
1	C	45	ALA	3.4
1	B	405	LEU	3.4
1	D	407	ALA	3.3
1	A	11	SER	3.3
1	B	3	SER	3.3
1	A	174	ASP	3.2
1	C	14	ASN	3.2
1	B	711	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	711	GLU	3.1
1	B	20	LYS	3.1
1	B	746	ILE	3.1
1	D	371	GLY	3.0
1	C	43	VAL	3.0
1	D	15	PHE	3.0
1	B	736	THR	3.0
1	D	368	PHE	2.9
1	D	174	ASP	2.9
1	B	9	LEU	2.9
1	D	43	VAL	2.9
1	D	44	LEU	2.8
1	D	370	GLU	2.8
1	D	14	ASN	2.8
1	B	47	GLY	2.8
1	B	5	GLY	2.8
1	B	408	LYS	2.8
1	B	735	THR	2.8
1	B	432	GLY	2.8
1	B	410	PRO	2.7
1	D	364	PHE	2.7
1	B	371	GLY	2.7
1	D	410	PRO	2.7
1	B	403	LEU	2.7
1	B	302	ALA	2.7
1	B	34	SER	2.7
1	D	24	GLU	2.7
1	B	21	GLU	2.6
1	C	44	LEU	2.6
1	D	3	SER	2.6
1	D	409	PHE	2.6
1	D	714	LEU	2.6
1	B	4	THR	2.6
1	D	413	VAL	2.6
1	D	594	VAL	2.5
1	B	402	TYR	2.5
1	A	711	GLU	2.5
1	B	404	SER	2.5
1	A	34	SER	2.5
1	D	16	ALA	2.5
1	D	233	TRP	2.5
1	B	12	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	19	THR	2.4
1	A	754	HIS	2.4
1	B	726	LYS	2.4
1	B	426	ILE	2.4
1	A	17	GLU	2.4
1	D	17	GLU	2.4
1	D	13	GLU	2.3
1	B	428	ASP	2.3
1	B	24	GLU	2.3
1	A	3	SER	2.3
1	D	18	LYS	2.3
1	B	749	ARG	2.3
1	A	43	VAL	2.3
1	A	45	ALA	2.3
1	B	379	LEU	2.3
1	D	750	GLU	2.3
1	B	17	GLU	2.2
1	A	46	LEU	2.2
1	D	404	SER	2.2
1	B	433	VAL	2.2
1	C	13	GLU	2.2
1	D	735	THR	2.2
1	B	409	PHE	2.2
1	B	25	LEU	2.2
1	A	600	GLU	2.2
1	C	15	PHE	2.2
1	D	21	GLU	2.1
1	B	414	ASP	2.1
1	A	752	LEU	2.1
1	D	402	TYR	2.1
1	B	412	PHE	2.1
1	B	367	THR	2.1
1	D	710	PRO	2.1
1	B	743	ASP	2.1
1	B	372	ASN	2.1
1	D	405	LEU	2.1
1	D	408	LYS	2.1
1	B	360	LEU	2.0
1	D	731	LEU	2.0
1	B	33	ASN	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, 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
5	MG	B	4015	1/1	0.81	0.10	47,47,47,47	0
4	NO3	A	4014	4/4	0.83	0.14	33,33,35,35	0
3	GOL	A	4007	6/6	0.83	0.13	53,53,53,54	0
3	GOL	B	4009	6/6	0.90	0.17	35,43,43,45	0
3	GOL	D	4013	6/6	0.92	0.19	29,41,42,44	0
3	GOL	A	4006	6/6	0.93	0.10	30,39,41,45	0
3	GOL	B	4008	6/6	0.93	0.10	26,30,32,34	0
3	GOL	C	4010	6/6	0.94	0.08	24,24,28,29	0
3	GOL	D	4012	6/6	0.95	0.09	26,28,29,32	0
3	GOL	C	4011	6/6	0.95	0.10	32,38,40,40	0
5	MG	C	4018	1/1	0.95	0.16	42,42,42,42	0
3	GOL	A	4005	6/6	0.96	0.08	23,26,28,31	0
2	A2G	B	4002	15/15	0.96	0.11	21,23,25,27	0
5	MG	A	4016	1/1	0.97	0.06	48,48,48,48	0
2	A2G	A	4001	15/15	0.97	0.12	20,21,23,24	0
2	A2G	D	4004	15/15	0.97	0.13	21,22,24,25	0
2	A2G	C	4003	15/15	0.98	0.13	19,20,23,23	0
5	MG	D	4020	1/1	0.98	0.10	43,43,43,43	0
5	MG	D	4017	1/1	0.99	0.03	25,25,25,25	0
5	MG	B	4019	1/1	0.99	0.10	31,31,31,31	0

6.5 Other polymers (i)

There are no such residues in this entry.