Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:11 AM GMT

PDB ID	:	2ZUU
Title	:	Crystal structure of Galacto-N-biose/Lacto-N-biose I phosphorylase in complex with GlcNAc
Authors	:	Hidaka, M.; Nishimoto, M.; Kitaoka, M.; Wakagi, T.; Shoun, H.; Fushinobu, S.
Deposited on	:	2008-10-28
Resolution	:	2.30 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

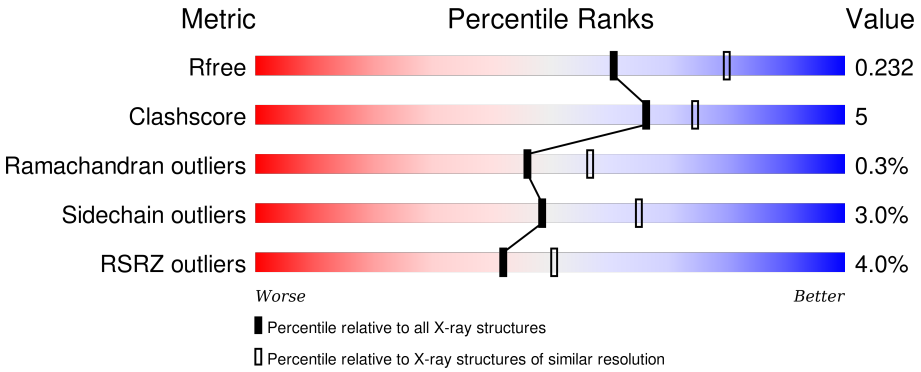
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.30 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 <=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% 89% 9%
1	B	759	6% 80% 14%
1	C	759	% 90% 7%
1	D	759	6% 84% 12%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	D	4008	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 25272 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	746	Total	C	N	O	S	0	0	0
			5934	3787	998	1133	16			
1	B	731	Total	C	N	O	S	0	0	0
			5813	3708	981	1108	16			
1	C	744	Total	C	N	O	S	0	0	0
			5920	3779	996	1129	16			
1	D	739	Total	C	N	O	S	0	0	0
			5882	3756	989	1121	16			

There are 32 discrepancies between the modelled and reference sequences:

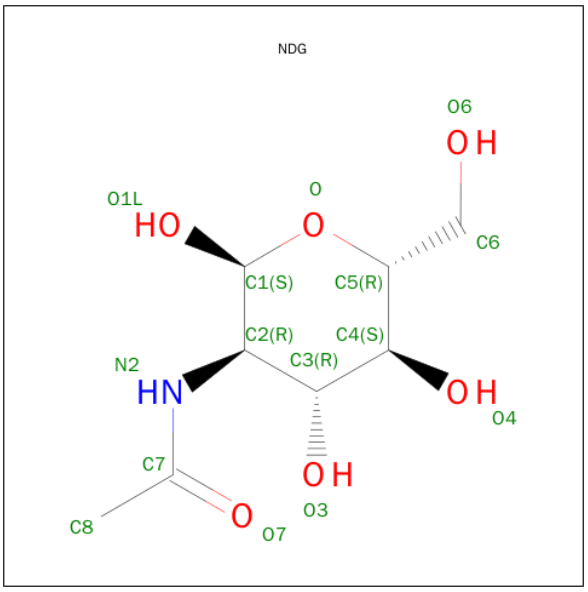
Chain	Residue	Modelled	Actual	Comment	Reference
A	752	LEU	-	EXPRESSION TAG	UNP Q5NU17
A	753	GLU	-	EXPRESSION TAG	UNP Q5NU17
A	754	HIS	-	EXPRESSION TAG	UNP Q5NU17
A	755	HIS	-	EXPRESSION TAG	UNP Q5NU17
A	756	HIS	-	EXPRESSION TAG	UNP Q5NU17
A	757	HIS	-	EXPRESSION TAG	UNP Q5NU17
A	758	HIS	-	EXPRESSION TAG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

Continued on next page...

Continued from previous page...

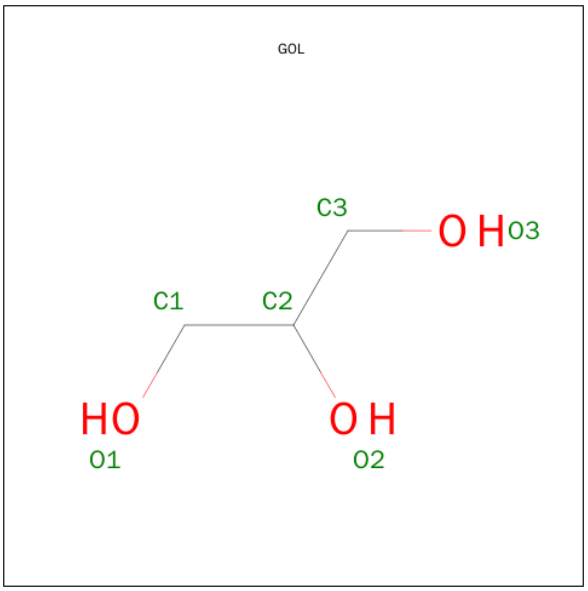
Chain	Residue	Modelled	Actual	Comment	Reference
C	757	HIS	-	EXPRESSION TAG	UNP Q5NU17
C	758	HIS	-	EXPRESSION TAG	UNP Q5NU17
C	759	HIS	-	EXPRESSION TAG	UNP Q5NU17
D	752	LEU	-	EXPRESSION TAG	UNP Q5NU17
D	753	GLU	-	EXPRESSION TAG	UNP Q5NU17
D	754	HIS	-	EXPRESSION TAG	UNP Q5NU17
D	755	HIS	-	EXPRESSION TAG	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 SUGAR (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 15 8 1 6	0	0
2	B	1	Total C N O 15 8 1 6	0	0
2	C	1	Total C N O 15 8 1 6	0	0
2	D	1	Total C N O 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
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is water.

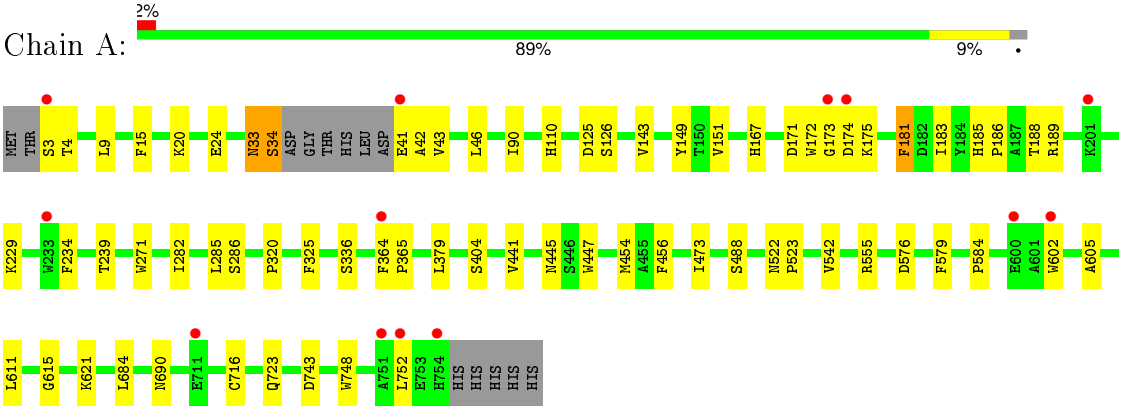
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	427	Total O 427 427	0	0
5	B	368	Total O 368 368	0	0
5	C	454	Total O 454 454	0	0
5	D	389	Total O 389 389	0	0

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 errors 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.

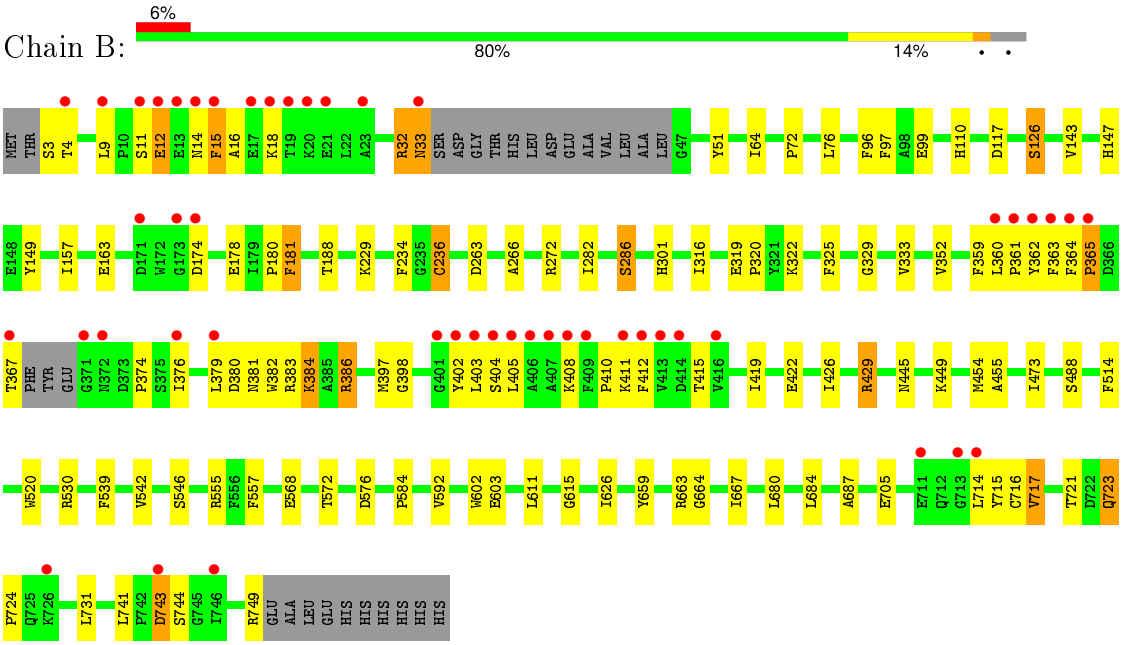
- Molecule 1: Lacto-N-biose phosphorylase

Chain A:



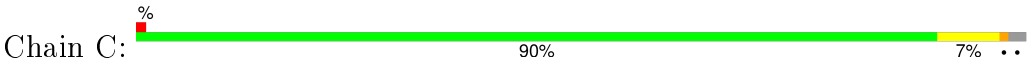
- Molecule 1: Lacto-N-biose phosphorylase

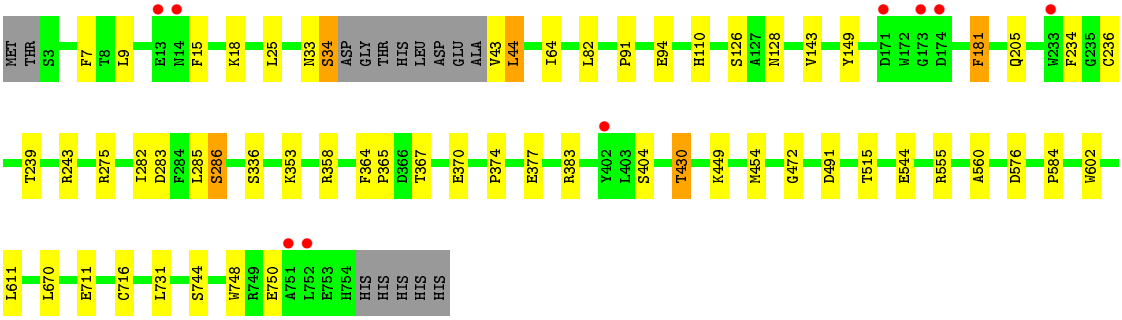
Chain B:



- Molecule 1: Lacto-N-biose phosphorylase

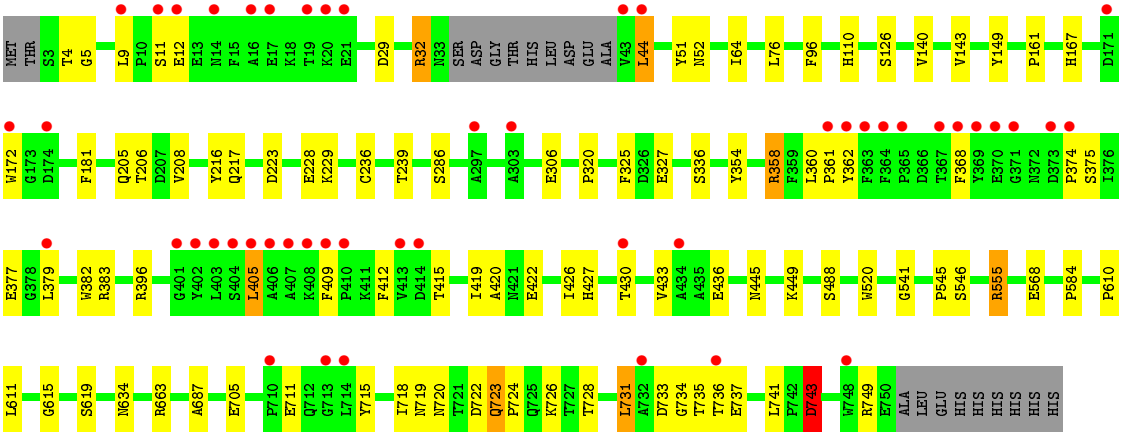
Chain C:





- 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	67.78Å 111.48Å 118.43Å 105.19° 90.48° 107.35°	Depositor
Resolution (Å)	40.68 – 2.30 40.68 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.1 (40.68-2.30) 87.9 (40.68-2.30)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0044	Depositor
R, R_{free}	0.170 , 0.231 0.171 , 0.232	Depositor DCC
R_{free} test set	6869 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	31.2	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 44.0	EDS
Estimated twinning fraction	0.027 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 137184 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	25272	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, MG, NDG

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	0.54	0/6102	0.61	0/8311
1	B	0.52	0/5977	0.61	0/8139
1	C	0.55	1/6088 (0.0%)	0.61	0/8292
1	D	0.53	1/6049 (0.0%)	0.59	0/8239
All	All	0.53	2/24216 (0.0%)	0.61	0/32981

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	236	CYS	CB-SG	-7.47	1.69	1.82
1	C	236	CYS	CB-SG	-6.68	1.70	1.82

There are no bond angle outliers.

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	5934	0	5623	40	0
1	B	5813	0	5511	80	0
1	C	5920	0	5612	40	0
1	D	5882	0	5578	68	0
2	A	15	0	15	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1	0
3	C	6	0	8	3	0
3	D	6	0	8	4	0
4	B	1	0	0	0	0
5	A	427	0	0	8	0
5	B	368	0	0	3	0
5	C	454	0	0	8	0
5	D	389	0	0	12	0
All	All	25272	0	22416	227	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 5.

All (227) 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:420:ALA:HB3	5:D:1553:HOH:O	1.59	1.00
1:C:449:LYS:HB3	3:C:4007:GOL:H11	1.48	0.96
1:B:449:LYS:HB3	3:B:4006:GOL:H11	1.51	0.93
1:B:429:ARG:HH11	1:B:429:ARG:HG2	1.33	0.90
1:B:32:ARG:HD2	1:B:33:ASN:H	1.45	0.81
1:B:374:PRO:HG2	1:B:412:PHE:HB2	1.64	0.79
1:B:163:GLU:HG3	1:B:178:GLU:HG3	1.64	0.79
1:C:430:THR:HG21	5:C:1552:HOH:O	1.82	0.79
1:A:33:ASN:HD22	1:A:34:SER:N	1.83	0.77
1:C:430:THR:CG2	5:C:1552:HOH:O	2.34	0.75
1:D:449:LYS:N	3:D:4008:GOL:H11	2.02	0.74
1:D:64:ILE:HD13	1:D:181:PHE:HB3	1.70	0.74
1:B:386:ARG:HH21	1:B:386:ARG:CG	2.01	0.72
1:D:32:ARG:HB2	1:D:51:TYR:HB2	1.71	0.72
1:C:110:HIS:HD2	1:C:126:SER:HB2	1.57	0.69
1:C:44:LEU:HD11	1:C:205:GLN:HG3	1.75	0.69
1:D:555:ARG:HG2	5:D:1544:HOH:O	1.93	0.67
1:D:718:ILE:HD12	1:D:720:ASN:HD21	1.60	0.65
1:B:429:ARG:NH1	1:B:429:ARG:HG2	2.10	0.65
1:D:449:LYS:H	3:D:4008:GOL:H11	1.62	0.65
1:D:430:THR:HG22	1:D:433:VAL:H	1.63	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:TRP:O	1:A:174:ASP:N	2.31	0.64
1:A:34:SER:HB2	5:A:1487:HOH:O	1.96	0.64
1:B:97:PHE:CE1	1:B:99:GLU:HG3	2.33	0.63
1:C:283:ASP:HB3	5:C:1250:HOH:O	1.97	0.63
1:C:91:PRO:HB2	1:C:94:GLU:HG3	1.81	0.62
1:B:724:PRO:HA	1:B:741:LEU:O	2.01	0.61
1:B:15:PHE:CE2	1:B:18:LYS:HB2	2.36	0.61
1:C:64:ILE:HD13	1:C:181:PHE:HB3	1.82	0.61
1:B:15:PHE:HD2	5:B:1554:HOH:O	1.83	0.60
1:D:449:LYS:HB3	3:D:4008:GOL:H12	1.84	0.59
1:B:359:PHE:CD2	1:B:397:MET:HG3	2.37	0.59
1:A:15:PHE:CZ	1:A:404:SER:HA	2.37	0.59
1:D:362:TYR:HB2	5:D:1309:HOH:O	2.02	0.59
1:D:445:ASN:O	1:D:488:SER:HA	2.02	0.59
1:D:724:PRO:HA	1:D:741:LEU:O	2.02	0.59
1:A:605:ALA:HB2	1:A:621:LYS:HD2	1.84	0.59
1:B:110:HIS:HD2	1:B:126:SER:HB2	1.67	0.58
1:B:266:ALA:HB1	1:B:272:ARG:HD2	1.85	0.58
1:B:72:PRO:HB2	1:B:157:ILE:HD12	1.85	0.58
1:B:364:PHE:CD1	1:B:365:PRO:HD2	2.38	0.58
1:A:42:ALA:HA	5:A:1469:HOH:O	2.03	0.58
1:B:282:ILE:O	1:B:286:SER:HB2	2.04	0.58
1:C:275:ARG:HD2	5:C:1550:HOH:O	2.04	0.57
1:D:382:TRP:CZ2	1:D:422:GLU:HG2	2.40	0.57
1:D:110:HIS:HD2	1:D:126:SER:HB2	1.68	0.57
1:B:266:ALA:CB	1:B:272:ARG:HD2	2.35	0.57
1:D:430:THR:CG2	1:D:433:VAL:O	2.52	0.56
1:B:362:TYR:HD2	1:B:364:PHE:HB3	1.71	0.56
1:A:473:ILE:HD11	1:A:542:VAL:HG11	1.88	0.56
1:B:163:GLU:CG	1:B:178:GLU:HG3	2.36	0.56
1:B:64:ILE:HD13	1:B:181:PHE:HB3	1.88	0.56
1:D:715:TYR:CE2	1:D:749:ARG:HB2	2.41	0.56
1:D:44:LEU:HD12	1:D:44:LEU:H	1.72	0.56
1:D:430:THR:HG22	1:D:433:VAL:N	2.20	0.55
1:B:397:MET:HG2	1:B:398:GLY:N	2.20	0.55
1:B:14:ASN:O	1:B:16:ALA:N	2.34	0.55
1:A:364:PHE:CD2	1:A:365:PRO:HD2	2.41	0.55
1:A:33:ASN:HD22	1:A:34:SER:H	1.54	0.55
1:C:377:GLU:HB2	5:C:782:HOH:O	2.08	0.54
1:D:374:PRO:HG2	1:D:412:PHE:HB2	1.87	0.54
1:A:3:SER:HA	5:A:1521:HOH:O	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:520:TRP:CE2	1:D:546:SER:HA	2.42	0.54
1:C:234:PHE:CZ	1:C:454:MET:HB3	2.43	0.54
1:D:110:HIS:CD2	1:D:126:SER:HB2	2.43	0.53
1:B:96:PHE:CE1	1:B:229:LYS:HE2	2.43	0.53
1:B:379:LEU:O	1:B:383:ARG:HG3	2.09	0.53
1:B:14:ASN:C	1:B:16:ALA:H	2.10	0.53
1:B:32:ARG:HA	1:B:51:TYR:HB2	1.90	0.53
1:A:716:CYS:HB3	1:A:748:TRP:CE3	2.44	0.53
1:D:12:GLU:HB2	5:D:1583:HOH:O	2.08	0.52
1:A:576:ASP:HB3	1:A:615:GLY:HA2	1.91	0.52
1:D:719:ASN:ND2	1:D:723:GLN:O	2.40	0.52
1:D:449:LYS:HB3	3:D:4008:GOL:C1	2.40	0.52
1:B:143:VAL:HB	1:B:149:TYR:OH	2.09	0.52
1:C:15:PHE:CZ	1:C:404:SER:HA	2.44	0.52
1:D:52:ASN:HD22	1:D:206:THR:HG23	1.74	0.52
1:B:333:VAL:HG23	1:B:352:VAL:HG11	1.91	0.52
1:B:263:ASP:OD2	1:B:272:ARG:HD3	2.10	0.51
1:D:377:GLU:HG3	5:D:1421:HOH:O	2.09	0.51
1:C:239:THR:HG21	1:C:285:LEU:HD21	1.92	0.51
1:A:320:PRO:HA	1:A:325:PHE:CD1	2.46	0.51
1:A:690:ASN:ND2	5:A:951:HOH:O	2.41	0.51
1:D:728:THR:CG2	1:D:736:THR:HB	2.40	0.51
1:B:382:TRP:NE1	1:B:422:GLU:OE2	2.34	0.51
1:B:381:ASN:HA	1:B:384:LYS:HE2	1.93	0.50
1:B:568:GLU:OE1	1:B:572:THR:OG1	2.26	0.50
1:D:619:SER:HB3	5:D:1348:HOH:O	2.11	0.50
1:D:216:TYR:HB3	1:D:239:THR:HG22	1.93	0.50
1:B:364:PHE:HD1	1:B:365:PRO:HD2	1.77	0.50
1:D:382:TRP:HZ2	1:D:422:GLU:HG2	1.76	0.50
1:B:473:ILE:HD11	1:B:542:VAL:HG11	1.94	0.50
1:B:236:CYS:HB3	1:B:316:ILE:HG21	1.94	0.50
1:A:584:PRO:HG3	1:A:602:TRP:CH2	2.47	0.49
1:B:11:SER:HB3	1:B:32:ARG:O	2.12	0.49
1:D:419:ILE:O	1:D:422:GLU:HB3	2.12	0.49
1:A:271:TRP:CZ2	1:A:456:PHE:HA	2.47	0.49
1:C:491:ASP:OD1	3:C:4007:GOL:H32	2.12	0.49
1:D:32:ARG:HB2	1:D:51:TYR:CB	2.42	0.49
1:C:33:ASN:HD22	1:C:34:SER:N	2.11	0.49
1:B:680:LEU:O	1:B:684:LEU:HG	2.13	0.49
1:B:386:ARG:HG2	1:B:386:ARG:HH21	1.75	0.49
1:B:415:THR:O	1:B:419:ILE:HG13	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:429:ARG:HH11	1:B:429:ARG:CG	2.15	0.49
1:B:181:PHE:HB2	1:B:188:THR:HG21	1.94	0.48
1:A:234:PHE:CE1	1:A:454:MET:HB3	2.47	0.48
1:B:403:LEU:HD23	5:B:1554:HOH:O	2.13	0.48
1:D:44:LEU:HD11	5:D:1628:HOH:O	2.13	0.48
1:C:364:PHE:CG	1:C:365:PRO:HD2	2.48	0.48
1:A:172:TRP:CD2	1:A:175:LYS:HE3	2.48	0.48
1:D:320:PRO:HA	1:D:325:PHE:CD1	2.49	0.48
1:C:44:LEU:HD21	1:C:205:GLN:HB2	1.94	0.48
1:B:717:VAL:HG22	1:B:741:LEU:HD11	1.94	0.48
1:B:386:ARG:HG3	1:B:386:ARG:HH21	1.75	0.48
1:D:375:SER:HB2	1:D:415:THR:OG1	2.14	0.48
1:D:358:ARG:O	1:D:358:ARG:NH1	2.47	0.48
1:B:422:GLU:O	1:B:426:ILE:HG13	2.14	0.48
1:D:733:ASP:OD1	1:D:734:GLY:N	2.43	0.48
1:D:379:LEU:HB2	5:D:841:HOH:O	2.13	0.48
1:B:301:HIS:HE1	1:B:329:GLY:O	1.97	0.48
1:D:208:VAL:HG22	1:D:306:GLU:HB2	1.96	0.48
1:D:368:PHE:HB2	1:D:405:LEU:CD2	2.44	0.47
1:B:445:ASN:O	1:B:488:SER:HA	2.14	0.47
1:C:711:GLU:HG2	5:C:773:HOH:O	2.14	0.47
1:D:143:VAL:HB	1:D:149:TYR:CZ	2.48	0.47
1:C:143:VAL:HB	1:C:149:TYR:CZ	2.49	0.47
1:B:542:VAL:HA	1:B:667:ILE:O	2.14	0.47
1:C:472:GLY:HA3	1:C:670:LEU:O	2.14	0.47
1:C:449:LYS:CB	3:C:4007:GOL:H11	2.34	0.47
1:A:41:GLU:C	1:A:43:VAL:H	2.16	0.47
1:B:383:ARG:HD3	1:B:744:SER:HB3	1.96	0.47
1:D:731:LEU:CD2	1:D:731:LEU:N	2.78	0.47
1:D:368:PHE:HB3	1:D:405:LEU:HD23	1.98	0.46
1:C:110:HIS:CD2	1:C:126:SER:HB2	2.45	0.46
1:A:42:ALA:CA	5:A:1469:HOH:O	2.63	0.46
1:B:408:LYS:O	1:B:410:PRO:HD3	2.16	0.46
1:B:320:PRO:HA	1:B:325:PHE:CD1	2.50	0.46
1:A:90:ILE:HG21	1:A:151:VAL:HG23	1.98	0.46
1:B:520:TRP:CE2	1:B:546:SER:HA	2.50	0.46
1:B:555:ARG:HD2	1:B:557:PHE:O	2.15	0.46
1:D:722:ASP:O	1:D:743:ASP:HB2	2.15	0.46
1:D:555:ARG:HE	1:D:555:ARG:HA	1.80	0.45
1:B:743:ASP:C	1:B:743:ASP:OD1	2.53	0.45
1:B:234:PHE:CE1	1:B:454:MET:HB3	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:383:ARG:HB3	5:D:1520:HOH:O	2.16	0.45
1:B:9:LEU:HD21	1:B:403:LEU:HD22	1.99	0.45
1:B:530:ARG:HD3	1:B:659:TYR:OH	2.17	0.45
1:C:82:LEU:HB2	5:D:944:HOH:O	2.17	0.44
1:A:555:ARG:HA	1:A:555:ARG:HD3	1.67	0.44
1:B:12:GLU:HG3	1:B:404:SER:H	1.82	0.44
1:C:43:VAL:HG13	1:C:44:LEU:H	1.82	0.44
1:B:363:PHE:O	1:B:402:TYR:HD2	2.01	0.44
1:D:541:GLY:HA3	1:D:545:PRO:HG3	1.98	0.44
1:B:723:GLN:HB3	1:B:724:PRO:CD	2.48	0.44
1:D:412:PHE:O	1:D:415:THR:HB	2.16	0.44
1:C:716:CYS:HB3	1:C:748:TRP:CE3	2.53	0.44
1:C:128:ASN:N	1:C:128:ASN:HD22	2.15	0.44
1:B:319:GLU:HG3	1:B:322:LYS:HD2	2.00	0.44
1:B:455:ALA:HA	1:B:514:PHE:CE1	2.52	0.44
1:D:663:ARG:HB2	1:D:687:ALA:O	2.18	0.44
1:C:576:ASP:OD2	1:D:228:GLU:OE2	2.36	0.44
1:C:584:PRO:HG3	1:C:602:TRP:CH2	2.53	0.43
1:A:447:TRP:O	3:A:4005:GOL:H12	2.19	0.43
1:C:43:VAL:HG13	1:C:44:LEU:N	2.34	0.43
1:D:520:TRP:NE1	1:D:546:SER:HA	2.32	0.43
1:B:584:PRO:HD2	5:B:1350:HOH:O	2.18	0.43
1:B:592:VAL:HG21	1:B:626:ILE:HD11	2.00	0.43
1:C:15:PHE:CE2	1:C:18:LYS:HB3	2.54	0.43
1:B:386:ARG:CG	1:B:386:ARG:NH2	2.70	0.43
1:A:282:ILE:O	1:A:286:SER:HB2	2.19	0.43
1:B:663:ARG:HB2	1:B:687:ALA:O	2.19	0.43
1:A:181:PHE:HB2	1:A:188:THR:HG21	2.00	0.43
1:D:426:ILE:O	1:D:430:THR:OG1	2.32	0.43
1:D:223:ASP:HB3	1:D:229:LYS:HB2	2.00	0.43
1:B:715:TYR:CE2	1:B:749:ARG:HB2	2.54	0.43
1:B:117:ASP:OD2	1:B:147:HIS:ND1	2.52	0.43
1:B:386:ARG:HG2	1:B:386:ARG:NH2	2.33	0.43
1:B:72:PRO:HD2	1:B:180:PRO:HG2	2.01	0.42
1:A:185:HIS:HA	1:A:186:PRO:HD2	1.77	0.42
1:A:20:LYS:HG3	1:A:46:LEU:HD21	2.01	0.42
1:B:360:LEU:HB3	1:B:361:PRO:HA	2.02	0.42
1:C:555:ARG:HD3	1:C:560:ALA:HB3	2.01	0.42
1:D:409:PHE:HB3	5:D:1295:HOH:O	2.19	0.42
1:C:584:PRO:HD2	5:C:1186:HOH:O	2.18	0.42
1:A:143:VAL:HB	1:A:149:TYR:CZ	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:ASN:O	1:A:488:SER:HA	2.19	0.42
1:D:161:PRO:HG2	1:D:217:GLN:HG2	2.00	0.42
1:A:110:HIS:HD2	1:A:126:SER:OG	2.03	0.42
1:B:723:GLN:HB3	1:B:724:PRO:HD2	2.02	0.42
1:D:584:PRO:HD2	5:D:1364:HOH:O	2.20	0.42
1:A:441:VAL:HG21	1:A:684:LEU:HD13	2.01	0.42
1:C:44:LEU:HD11	1:C:205:GLN:CG	2.47	0.42
1:A:167:HIS:HA	1:A:172:TRP:CE3	2.55	0.42
1:A:584:PRO:HD2	5:A:970:HOH:O	2.19	0.42
1:C:374:PRO:HD2	5:C:1303:HOH:O	2.20	0.41
1:A:183:ILE:O	1:A:189:ARG:HB2	2.20	0.41
1:A:239:THR:HB	1:A:285:LEU:HD21	2.01	0.41
1:D:610:PRO:HA	1:D:615:GLY:O	2.20	0.41
1:D:5:GLY:HA2	1:D:29:ASP:CG	2.41	0.41
1:B:76:LEU:HB3	1:B:96:PHE:CZ	2.54	0.41
1:D:110:HIS:HD2	1:D:126:SER:CB	2.32	0.41
1:D:368:PHE:HB2	1:D:405:LEU:HD22	2.03	0.41
1:C:383:ARG:HD3	1:C:744:SER:OG	2.21	0.41
1:C:33:ASN:ND2	1:C:34:SER:N	2.69	0.41
1:D:568:GLU:HB3	1:D:634:ASN:HB3	2.01	0.41
1:B:539:PHE:O	1:B:664:GLY:HA2	2.21	0.41
1:D:140:VAL:HG12	1:D:143:VAL:CG1	2.51	0.41
1:A:41:GLU:O	1:A:43:VAL:N	2.37	0.41
1:C:243:ARG:HD2	1:C:243:ARG:HA	1.69	0.41
1:D:167:HIS:HA	1:D:172:TRP:CE3	2.56	0.41
1:B:602:TRP:CE3	1:B:603:GLU:HG3	2.56	0.41
1:B:576:ASP:HB3	1:B:615:GLY:HA2	2.03	0.41
1:A:723:GLN:HG3	5:A:1431:HOH:O	2.21	0.41
1:B:234:PHE:CZ	1:B:454:MET:HB3	2.56	0.40
1:D:360:LEU:HB3	1:D:361:PRO:HA	2.02	0.40
1:D:354:TYR:CE1	1:D:396:ARG:HD3	2.56	0.40
1:A:522:ASN:HA	1:A:523:PRO:HD2	1.92	0.40
1:D:76:LEU:HB3	1:D:96:PHE:CZ	2.56	0.40
1:B:429:ARG:NH1	1:B:429:ARG:CG	2.78	0.40
1:D:718:ILE:HD12	1:D:720:ASN:ND2	2.33	0.40
1:D:5:GLY:HA2	1:D:29:ASP:HB3	2.03	0.40
1:C:515:THR:HG21	1:C:544:GLU:O	2.22	0.40
1:C:282:ILE:O	1:C:286:SER:HB3	2.20	0.40
1:A:229:LYS:NZ	5:A:1399:HOH:O	2.54	0.40
1:A:110:HIS:CD2	1:A:126:SER:OG	2.75	0.40
1:C:7:PHE:C	1:C:7:PHE:CD2	2.94	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:ILE:H	1:B:376:ILE:HG12	1.79	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	742/759 (98%)	714 (96%)	26 (4%)	2 (0%)	46	57
1	B	725/759 (96%)	686 (95%)	35 (5%)	4 (1%)	30	36
1	C	740/759 (98%)	712 (96%)	28 (4%)	0	100	100
1	D	735/759 (97%)	698 (95%)	35 (5%)	2 (0%)	46	57
All	All	2942/3036 (97%)	2810 (96%)	124 (4%)	8 (0%)	46	57

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	173	GLY
1	B	15	PHE
1	A	743	ASP
1	D	743	ASP
1	B	743	ASP
1	D	711	GLU
1	B	365	PRO
1	B	723	GLN

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	622/634 (98%)	609 (98%)	13 (2%)	61 78
1	B	610/634 (96%)	586 (96%)	24 (4%)	39 53
1	C	621/634 (98%)	606 (98%)	15 (2%)	57 74
1	D	617/634 (97%)	595 (96%)	22 (4%)	42 57
All	All	2470/2536 (97%)	2396 (97%)	74 (3%)	48 65

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	9	LEU
1	A	24	GLU
1	A	33	ASN
1	A	34	SER
1	A	125	ASP
1	A	171	ASP
1	A	181	PHE
1	A	336	SER
1	A	379	LEU
1	A	579	PHE
1	A	611	LEU
1	A	752	LEU
1	B	3	SER
1	B	4	THR
1	B	12	GLU
1	B	32	ARG
1	B	33	ASN
1	B	126	SER
1	B	174	ASP
1	B	181	PHE
1	B	236	CYS
1	B	286	SER
1	B	367	THR
1	B	380	ASP
1	B	384	LYS
1	B	386	ARG
1	B	405	LEU
1	B	411	LYS
1	B	429	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	611	LEU
1	B	705	GLU
1	B	714	LEU
1	B	716	CYS
1	B	717	VAL
1	B	721	THR
1	B	731	LEU
1	C	9	LEU
1	C	25	LEU
1	C	34	SER
1	C	44	LEU
1	C	181	PHE
1	C	286	SER
1	C	336	SER
1	C	353	LYS
1	C	358	ARG
1	C	367	THR
1	C	370	GLU
1	C	430	THR
1	C	611	LEU
1	C	731	LEU
1	C	750	GLU
1	D	4	THR
1	D	9	LEU
1	D	11	SER
1	D	32	ARG
1	D	44	LEU
1	D	205	GLN
1	D	286	SER
1	D	327	GLU
1	D	336	SER
1	D	358	ARG
1	D	405	LEU
1	D	427	HIS
1	D	436	GLU
1	D	555	ARG
1	D	611	LEU
1	D	705	GLU
1	D	723	GLN
1	D	726	LYS
1	D	731	LEU
1	D	735	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	737	GLU
1	D	743	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	110	HIS
1	A	128	ASN
1	A	170	ASN
1	A	185	HIS
1	A	198	GLN
1	A	690	ASN
1	A	720	ASN
1	B	33	ASN
1	B	198	GLN
1	B	690	ASN
1	B	720	ASN
1	C	33	ASN
1	C	128	ASN
1	C	690	ASN
1	C	720	ASN
1	D	52	ASN
1	D	128	ASN
1	D	166	ASN
1	D	170	ASN
1	D	205	GLN
1	D	641	ASN
1	D	689	HIS
1	D	690	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	0.58	0	17,21,21	0.84	0
3	GOL	A	4005	-	5,5,5	0.30	0	5,5,5	0.81	0
2	NDG	B	4002	-	15,15,15	0.70	0	17,21,21	0.91	0
3	GOL	B	4006	-	5,5,5	0.21	0	5,5,5	0.61	0
2	NDG	C	4003	-	15,15,15	0.61	0	17,21,21	0.72	0
3	GOL	C	4007	-	5,5,5	0.24	0	5,5,5	0.87	0
2	NDG	D	4004	-	15,15,15	0.50	0	17,21,21	0.94	0
3	GOL	D	4008	-	5,5,5	0.32	0	5,5,5	0.73	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
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
2	NDG	D	4004	-	-	0/6/26/26	0/1/1/1
3	GOL	D	4008	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4005	GOL	1	0
3	B	4006	GOL	1	0
3	C	4007	GOL	3	0
3	D	4008	GOL	4	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	746/759 (98%)	-0.20	13 (1%) 73 79	20, 30, 45, 73	0
1	B	731/759 (96%)	0.18	48 (6%) 22 29	22, 34, 71, 85	0
1	C	744/759 (98%)	-0.20	9 (1%) 81 85	20, 30, 46, 62	0
1	D	739/759 (97%)	0.19	49 (6%) 22 29	19, 33, 64, 71	0
All	All	2960/3036 (97%)	-0.01	119 (4%) 42 51	19, 32, 61, 85	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	401	GLY	9.3
1	B	406	ALA	6.5
1	B	407	ALA	6.3
1	D	406	ALA	6.0
1	D	368	PHE	5.8
1	B	403	LEU	5.8
1	D	407	ALA	5.7
1	B	13	GLU	5.1
1	B	364	PHE	4.9
1	D	19	THR	4.7
1	B	15	PHE	4.7
1	B	19	THR	4.6
1	D	43	VAL	4.6
1	D	414	ASP	4.6
1	D	379	LEU	4.5
1	B	14	ASN	4.3
1	D	370	GLU	4.1
1	D	14	ASN	4.0
1	D	174	ASP	4.0
1	D	404	SER	4.0
1	D	402	TYR	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	11	SER	3.9
1	D	364	PHE	3.9
1	D	363	PHE	3.9
1	A	174	ASP	3.8
1	B	379	LEU	3.8
1	A	752	LEU	3.7
1	B	404	SER	3.7
1	A	751	ALA	3.7
1	D	369	TYR	3.7
1	D	409	PHE	3.7
1	D	403	LEU	3.6
1	D	9	LEU	3.6
1	C	174	ASP	3.5
1	B	17	GLU	3.5
1	D	20	LYS	3.3
1	D	297	ALA	3.3
1	B	363	PHE	3.2
1	C	751	ALA	3.1
1	C	13	GLU	3.1
1	D	12	GLU	3.1
1	A	41	GLU	3.1
1	B	18	LYS	3.1
1	D	413	VAL	3.1
1	C	14	ASN	3.0
1	D	371	GLY	3.0
1	D	11	SER	3.0
1	B	726	LYS	3.0
1	D	374	PRO	2.9
1	B	23	ALA	2.9
1	C	173	GLY	2.9
1	D	17	GLU	2.9
1	B	12	GLU	2.9
1	C	171	ASP	2.9
1	B	409	PHE	2.9
1	B	412	PHE	2.9
1	B	171	ASP	2.9
1	B	408	LYS	2.8
1	B	376	ILE	2.8
1	D	410	PRO	2.8
1	D	44	LEU	2.8
1	D	16	ALA	2.8
1	B	367	THR	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	405	LEU	2.8
1	B	743	ASP	2.8
1	D	361	PRO	2.7
1	B	405	LEU	2.7
1	B	713	GLY	2.7
1	B	365	PRO	2.6
1	C	752	LEU	2.6
1	B	4	THR	2.6
1	B	414	ASP	2.6
1	D	367	THR	2.6
1	B	174	ASP	2.6
1	B	9	LEU	2.6
1	B	714	LEU	2.6
1	D	408	LYS	2.5
1	D	714	LEU	2.5
1	A	754	HIS	2.5
1	B	416	VAL	2.5
1	D	171	ASP	2.5
1	D	21	GLU	2.5
1	A	173	GLY	2.4
1	B	371	GLY	2.4
1	D	401	GLY	2.4
1	D	373	ASP	2.4
1	B	33	ASN	2.4
1	D	365	PRO	2.4
1	B	21	GLU	2.4
1	D	172	TRP	2.3
1	B	360	LEU	2.3
1	B	411	LYS	2.3
1	B	362	TYR	2.3
1	B	372	ASN	2.3
1	D	732	ALA	2.3
1	B	711	GLU	2.3
1	D	362	TYR	2.3
1	A	233	TRP	2.3
1	B	361	PRO	2.2
1	D	736	THR	2.2
1	D	710	PRO	2.2
1	D	430	THR	2.2
1	A	3	SER	2.2
1	D	303	ALA	2.2
1	B	413	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	434	ALA	2.2
1	B	20	LYS	2.2
1	B	746	ILE	2.1
1	B	402	TYR	2.1
1	D	713	GLY	2.1
1	C	233	TRP	2.1
1	B	173	GLY	2.1
1	C	402	TYR	2.1
1	A	600	GLU	2.1
1	D	748	TRP	2.0
1	A	201	LYS	2.0
1	A	364	PHE	2.0
1	A	602	TRP	2.0
1	A	711	GLU	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, 95^{th} 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	A	4005	6/6	0.90	0.15	1.51	30,34,35,37	0
3	GOL	C	4007	6/6	0.89	0.16	1.51	36,39,41,41	0
3	GOL	B	4006	6/6	0.90	0.16	1.12	46,47,47,48	0
3	GOL	D	4008	6/6	0.91	0.13	0.93	39,42,42,43	0
2	NDG	C	4003	15/15	0.97	0.16	-0.01	27,28,31,31	0
2	NDG	A	4001	15/15	0.98	0.14	-0.21	23,26,29,30	0
2	NDG	B	4002	15/15	0.96	0.11	-0.67	28,32,33,34	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	NDG	D	4004	15/15	0.98	0.12	-0.75	27,30,32,33	0
4	MG	B	4009	1/1	0.92	0.06	-	36,36,36,36	0

6.5 Other polymers (i)

There are no such residues in this entry.