



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2017 – 09:05 AM EDT

PDB ID : 2ZUV  
Title : Crystal structure of Galacto-N-biose/Lacto-N-biose I phosphorylase in complex with GlcNAc, Ethylene glycol, and nitrate  
Authors : Hidaka, M.; Nishimoto, M.; Kitaoka, M.; Wakagi, T.; Shoun, H.; Fushinobu, S.  
Deposited on : unknown  
Resolution : 1.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<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

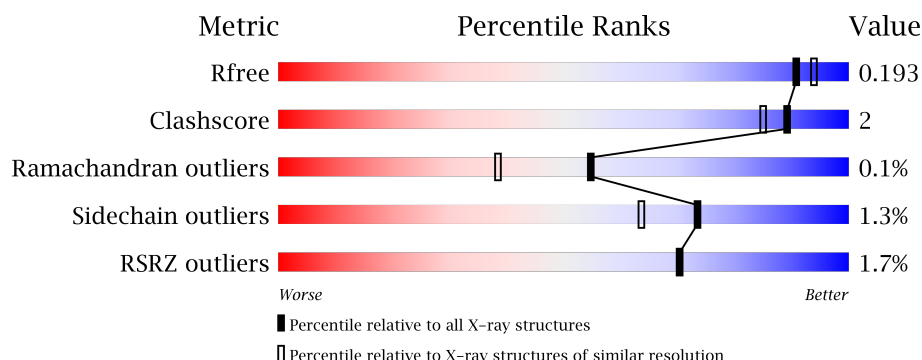
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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	1923 (1.86-1.86)
Clashscore	112137	2083 (1.86-1.86)
Ramachandran outliers	110173	2060 (1.86-1.86)
Sidechain outliers	110143	2060 (1.86-1.86)
RSRZ outliers	101464	1932 (1.86-1.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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>%</div> <div>94%</div> <div>.</div> <div>.</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NO3	A	2004	-	-	-	X
3	NO3	B	2006	-	-	-	X
4	EDO	A	2010	-	-	-	X
4	EDO	A	2011	-	-	-	X
4	EDO	B	2013	-	-	-	X
4	EDO	B	2015	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13707 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.

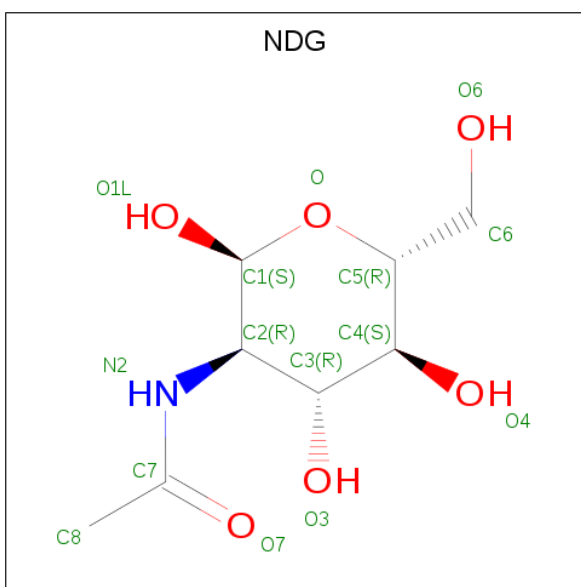
- Molecule 1 is a protein called Lacto-N-biose phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	741	Total	C	N	O	S	0	1	0
			5900	3766	994	1124	16			
1	B	740	Total	C	N	O	S	0	0	0
			5887	3759	990	1122	16			

There are 16 discrepancies between the modelled and reference sequences:

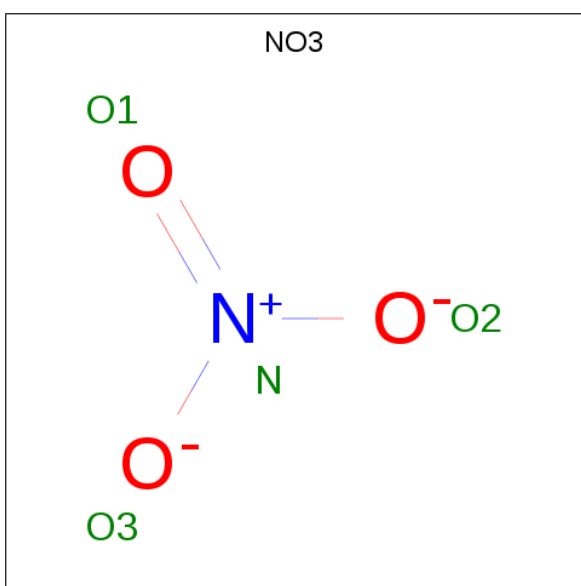
Chain	Residue	Modelled	Actual	Comment	Reference
A	752	LEU	-	EXPRESSION TAG	UNP Q5NU17
A	753	GLU	-	EXPRESSION TAG	UNP Q5NU17
A	754	HIS	-	EXPRESSION TAG	UNP Q5NU17
A	755	HIS	-	EXPRESSION TAG	UNP Q5NU17
A	756	HIS	-	EXPRESSION TAG	UNP Q5NU17
A	757	HIS	-	EXPRESSION TAG	UNP Q5NU17
A	758	HIS	-	EXPRESSION TAG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

- Molecule 2 is 2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE (three-letter code: NDG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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		

- Molecule 3 is NITRATE ION (three-letter code: NO3) (formula: NO<sub>3</sub>).



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

*Continued on next page...*

*Continued from previous page...*

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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	5	Total	Mg	0	0
			5	5		
5	A	3	Total	Mg	0	0
			3	3		

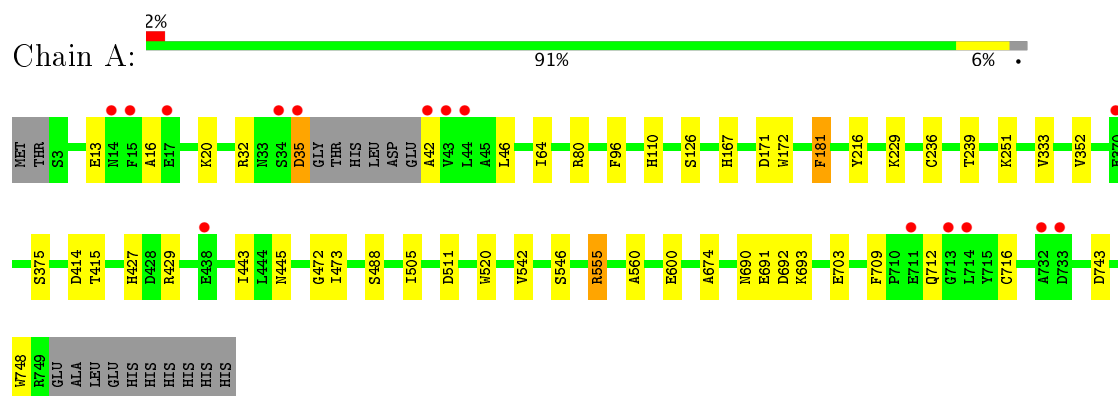
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	878	Total	O	3	0
			878	878		
6	B	948	Total	O	1	0
			948	948		

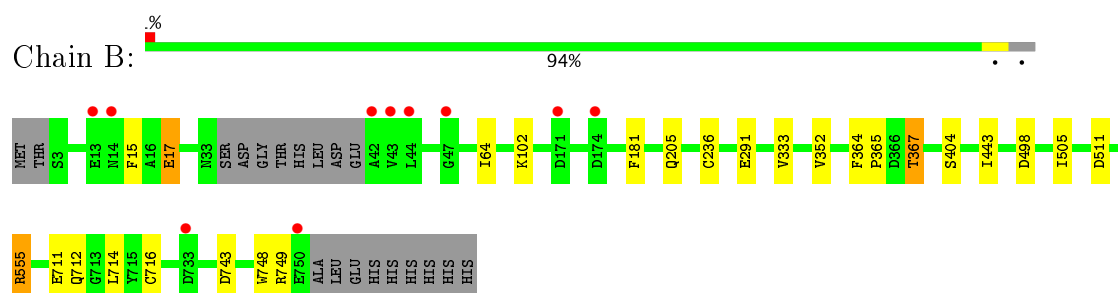
### 3 Residue-property plots [i](#)

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





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	204.04Å 68.02Å 116.05Å 90.00° 108.79° 90.00°	Depositor
Resolution (Å)	35.14 – 1.85 35.13 – 1.85	Depositor EDS
% Data completeness (in resolution range)	98.4 (35.14-1.85) 98.4 (35.13-1.85)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.03 (at 1.85Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.149 , 0.192 0.149 , 0.193	Depositor DCC
$R_{free}$ test set	6359 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.0	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 50.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	13707	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, EDO, 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	0.67	1/6070 (0.0%)	0.68	1/8267 (0.0%)
1	B	0.66	1/6054 (0.0%)	0.67	0/8246
All	All	0.67	2/12124 (0.0%)	0.67	1/16513 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	236	CYS	CB-SG	-7.53	1.69	1.82
1	A	236	CYS	CB-SG	-5.16	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	ARG	NE-CZ-NH1	-5.48	117.56	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	5900	0	5599	31	0
1	B	5887	0	5583	19	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
3	A	12	0	0	1	0
3	B	8	0	0	0	0
4	A	20	0	30	0	0
4	B	16	0	24	0	0
5	A	3	0	0	0	0
5	B	5	0	0	0	0
6	A	878	0	0	5	0
6	B	948	0	0	7	0
All	All	13707	0	11266	50	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 2.

All (50) 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:A:691:GLU:HG2	6:A:1690:HOH:O	1.81	0.80
1:A:110:HIS:HD2	1:A:126:SER:HB2	1.48	0.78
1:B:711:GLU:HG2	1:B:712:GLN:H	1.57	0.68
1:A:427:HIS:ND1	6:A:1643:HOH:O	2.27	0.68
1:B:711:GLU:HG2	1:B:712:GLN:N	2.10	0.67
1:A:692:ASP:HB3	6:A:1749:HOH:O	1.96	0.65
1:A:600:GLU:HG3	6:A:1706:HOH:O	2.02	0.59
1:A:64:ILE:HD13	1:A:181:PHE:HB3	1.83	0.59
1:B:364:PHE:CD1	1:B:365:PRO:HD2	2.38	0.58
1:A:716:CYS:HB3	1:A:748:TRP:CE3	2.39	0.57
1:B:367:THR:HG23	6:B:1229:HOH:O	2.05	0.56
1:B:716:CYS:HB3	1:B:748:TRP:CE3	2.41	0.55
1:B:17:GLU:HG3	6:B:1421:HOH:O	2.06	0.55
1:A:110:HIS:CD2	1:A:126:SER:HB2	2.36	0.54
1:B:443:ILE:HD13	1:B:505:ILE:HB	1.90	0.53
1:B:15:PHE:CZ	1:B:404:SER:HA	2.44	0.53
1:A:20:LYS:HG2	1:A:46:LEU:HD11	1.93	0.50
1:B:712:GLN:CG	6:B:1351:HOH:O	2.60	0.49
1:B:712:GLN:NE2	6:B:1692:HOH:O	2.46	0.49
1:B:712:GLN:HG3	6:B:1351:HOH:O	2.13	0.48
1:A:20:LYS:HD3	1:A:42:ALA:HB1	1.95	0.48
1:A:690:ASN:HD22	1:A:693:LYS:HD3	1.78	0.48
1:A:473:ILE:HD11	1:A:542:VAL:HG11	1.96	0.47
1:B:291:GLU:OE1	6:B:1668:HOH:O	2.20	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:ILE:HD13	1:A:505:ILE:HB	1.95	0.47
1:A:709:PHE:HB3	1:A:712:GLN:OE1	2.14	0.47
1:A:555:ARG:HD2	1:A:560:ALA:HB3	1.96	0.47
1:B:64:ILE:HD13	1:B:181:PHE:HB3	1.97	0.47
1:A:445:ASN:O	1:A:488:SER:HA	2.14	0.47
1:A:16:ALA:O	1:A:20:LYS:HG3	2.16	0.46
1:A:167:HIS:HA	1:A:172:TRP:CE3	2.51	0.46
1:A:375:SER:HB2	1:A:415:THR:OG1	2.17	0.44
1:A:555:ARG:HA	1:A:555:ARG:HD3	1.74	0.44
1:A:690:ASN:ND2	1:A:693:LYS:HD3	2.32	0.44
1:B:555:ARG:HD3	1:B:555:ARG:HA	1.60	0.43
1:A:429:ARG:HD2	1:A:748:TRP:CE2	2.54	0.43
1:A:333:VAL:HG23	1:A:352:VAL:HG11	2.01	0.42
1:A:674:ALA:HB1	1:A:703:GLU:HA	2.01	0.42
1:A:216:TYR:HB3	1:A:239:THR:HG22	2.01	0.42
1:B:333:VAL:HG23	1:B:352:VAL:HG11	2.03	0.41
1:A:96:PHE:CE1	1:A:229:LYS:HE2	2.56	0.41
1:A:110:HIS:HE1	6:A:1302:HOH:O	2.02	0.41
1:B:102:LYS:NZ	6:B:1603:HOH:O	2.52	0.41
1:A:35:ASP:OD1	1:A:35:ASP:N	2.54	0.40
1:B:714:LEU:HD12	1:B:749:ARG:O	2.20	0.40
1:A:472:GLY:HA2	3:A:2004:NO3:O2	2.21	0.40
1:B:711:GLU:CG	1:B:712:GLN:H	2.30	0.40
1:A:520:TRP:CE2	1:A:546:SER:HA	2.56	0.40
1:A:429:ARG:HD2	1:A:748:TRP:CD2	2.57	0.40
1:B:711:GLU:CG	1:B:712:GLN:N	2.83	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	738/759 (97%)	716 (97%)	22 (3%)	0	100	100
1	B	736/759 (97%)	709 (96%)	26 (4%)	1 (0%)	55	38
All	All	1474/1518 (97%)	1425 (97%)	48 (3%)	1 (0%)	55	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	743	ASP

### 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	619/634 (98%)	608 (98%)	11 (2%)	64	50
1	B	617/634 (97%)	611 (99%)	6 (1%)	80	74
All	All	1236/1268 (98%)	1219 (99%)	17 (1%)	73	61

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLU
1	A	32[A]	ARG
1	A	32[B]	ARG
1	A	35	ASP
1	A	171	ASP
1	A	181	PHE
1	A	251	LYS
1	A	414	ASP
1	A	511	ASP
1	A	555	ARG
1	A	743	ASP
1	B	17	GLU
1	B	205	GLN
1	B	367	THR
1	B	498	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	511	ASP
1	B	555	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	HIS
1	A	166	ASN
1	A	170	ASN
1	A	205	GLN
1	A	381	ASN
1	A	690	ASN
1	A	720	ASN
1	B	128	ASN
1	B	205	GLN
1	B	690	ASN
1	B	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 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 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	2001	-	15,15,15	0.53	0	21,21,21	1.38	2 (9%)
3	NO3	A	2003	-	1,3,3	4.19	1 (100%)	0,3,3	0.00	-
3	NO3	A	2004	-	1,3,3	4.07	1 (100%)	0,3,3	0.00	-
3	NO3	A	2005	-	1,3,3	4.14	1 (100%)	0,3,3	0.00	-
4	EDO	A	2008	-	3,3,3	0.53	0	2,2,2	0.51	0
4	EDO	A	2009	-	3,3,3	0.63	0	2,2,2	0.34	0
4	EDO	A	2010	-	3,3,3	0.47	0	2,2,2	0.73	0
4	EDO	A	2011	-	3,3,3	0.44	0	2,2,2	0.38	0
4	EDO	A	2012	-	3,3,3	0.38	0	2,2,2	0.61	0
2	NDG	B	2002	-	15,15,15	0.62	0	21,21,21	1.12	2 (9%)
3	NO3	B	2006	-	1,3,3	3.62	1 (100%)	0,3,3	0.00	-
3	NO3	B	2007	-	1,3,3	3.98	1 (100%)	0,3,3	0.00	-
4	EDO	B	2013	-	3,3,3	0.51	0	2,2,2	0.47	0
4	EDO	B	2014	-	3,3,3	0.58	0	2,2,2	0.30	0
4	EDO	B	2015	-	3,3,3	0.41	0	2,2,2	0.95	0
4	EDO	B	2016	-	3,3,3	0.47	0	2,2,2	0.55	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	2001	-	-	0/6/26/26	0/1/1/1
3	NO3	A	2003	-	-	0/0/0/0	0/0/0/0
3	NO3	A	2004	-	-	0/0/0/0	0/0/0/0
3	NO3	A	2005	-	-	0/0/0/0	0/0/0/0
4	EDO	A	2008	-	-	0/1/1/1	0/0/0/0
4	EDO	A	2009	-	-	0/1/1/1	0/0/0/0
4	EDO	A	2010	-	-	0/1/1/1	0/0/0/0
4	EDO	A	2011	-	-	0/1/1/1	0/0/0/0
4	EDO	A	2012	-	-	0/1/1/1	0/0/0/0
2	NDG	B	2002	-	-	0/6/26/26	0/1/1/1
3	NO3	B	2006	-	-	0/0/0/0	0/0/0/0
3	NO3	B	2007	-	-	0/0/0/0	0/0/0/0
4	EDO	B	2013	-	-	0/1/1/1	0/0/0/0
4	EDO	B	2014	-	-	0/1/1/1	0/0/0/0
4	EDO	B	2015	-	-	0/1/1/1	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	2016	-	-	0/1/1/1	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2006	NO3	O1-N	3.62	1.37	1.23
3	B	2007	NO3	O1-N	3.98	1.38	1.23
3	A	2004	NO3	O1-N	4.07	1.39	1.23
3	A	2005	NO3	O1-N	4.14	1.39	1.23
3	A	2003	NO3	O1-N	4.19	1.39	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	NDG	C1-C2-N2	-4.79	105.17	110.73
2	B	2002	NDG	C1-C2-N2	-3.43	106.76	110.73
2	B	2002	NDG	C3-C2-N2	2.26	114.94	110.61
2	A	2001	NDG	O-C1-C2	3.09	112.62	109.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2004	NO3	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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	741/759 (97%)	-0.46	15 (2%) 65 65	11, 18, 36, 51	0
1	B	740/759 (97%)	-0.55	10 (1%) 75 76	11, 19, 33, 53	0
All	All	1481/1518 (97%)	-0.50	25 (1%) 70 70	11, 18, 35, 53	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	47	GLY	4.0
1	A	43	VAL	3.6
1	B	42	ALA	3.6
1	A	713	GLY	3.5
1	A	34	SER	3.1
1	B	14	ASN	3.0
1	B	13	GLU	2.9
1	A	438	GLU	2.9
1	A	44	LEU	2.9
1	A	17	GLU	2.9
1	B	44	LEU	2.8
1	A	15	PHE	2.8
1	A	711	GLU	2.8
1	A	42	ALA	2.5
1	A	732	ALA	2.5
1	B	733	ASP	2.4
1	A	14	ASN	2.4
1	A	714	LEU	2.3
1	B	174	ASP	2.2
1	A	733	ASP	2.2
1	B	171	ASP	2.2
1	B	750	GLU	2.2
1	B	43	VAL	2.1
1	A	370	GLU	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	35	ASP	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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	NO3	B	2006	4/4	0.92	0.14	7.23	30,30,31,34	0
4	EDO	B	2013	4/4	0.98	0.18	4.39	19,24,25,26	0
4	EDO	A	2011	4/4	0.92	0.13	3.98	21,22,28,30	0
3	NO3	A	2004	4/4	0.96	0.13	3.55	22,24,25,26	0
4	EDO	A	2010	4/4	0.87	0.13	3.41	25,26,29,31	0
4	EDO	B	2015	4/4	0.96	0.11	2.98	21,21,22,24	0
4	EDO	A	2008	4/4	0.94	0.10	1.30	18,27,29,36	0
4	EDO	A	2009	4/4	0.92	0.12	1.03	21,25,26,26	0
2	NDG	B	2002	15/15	0.98	0.10	0.91	11,14,16,17	0
4	EDO	B	2016	4/4	0.95	0.09	0.49	30,32,32,34	0
3	NO3	B	2007	4/4	0.98	0.09	0.23	23,24,24,26	0
4	EDO	A	2012	4/4	0.95	0.09	-0.23	26,27,28,30	0
3	NO3	A	2005	4/4	0.97	0.07	-0.36	32,32,32,33	0
3	NO3	A	2003	4/4	0.97	0.06	-0.67	27,27,27,27	0
2	NDG	A	2001	15/15	0.98	0.07	-0.73	13,15,17,18	0
4	EDO	B	2014	4/4	0.99	0.04	-1.49	15,19,20,21	0
5	MG	B	2022	1/1	1.00	0.12	-	25,25,25,25	1
5	MG	B	2019	1/1	0.94	0.12	-	30,30,30,30	0
5	MG	A	2023	1/1	0.97	0.13	-	34,34,34,34	0
5	MG	B	2018	1/1	0.97	0.03	-	30,30,30,30	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MG	B	2020	1/1	0.98	0.11	-	34,34,34,34	0
5	MG	A	2021	1/1	0.97	0.04	-	34,34,34,34	0
5	MG	A	2017	1/1	0.98	0.03	-	24,24,24,24	0
5	MG	B	2024	1/1	0.89	0.07	-	37,37,37,37	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.