



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 16, 2023 – 09:18 AM EST

PDB ID : 2004  
Title : Structure of LNR-HD (Negative Regulatory Region) from human Notch 2  
Authors : Gordon, W.R.; Vardar-Ulu, D.; Histen, G.; Sanchez-Irizarry, C.; Aster, J.C.; Blacklow, S.C.  
Deposited on : 2007-01-25  
Resolution : 2.00 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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

MolProbity : 4.02b-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

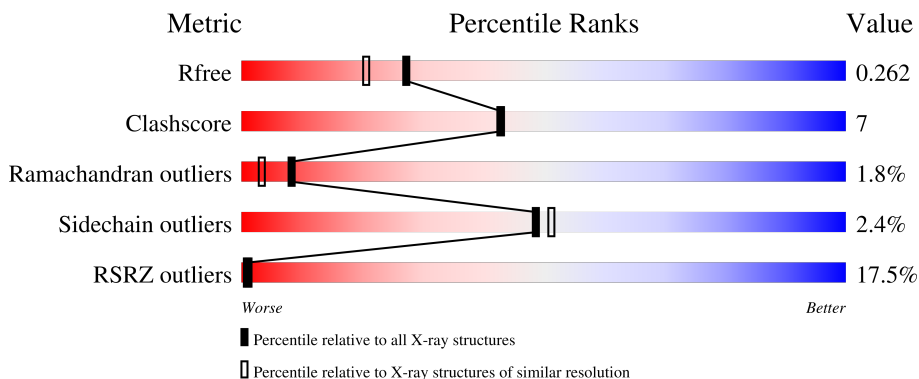
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	234	
1	B	234	

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
4	GOL	A	7007	-	-	X	-
4	GOL	B	7005	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3642 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 Neurogenic locus notch homolog protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	226	1724	1058	292	351	23	0	0	0
1	B	226	1687	1032	289	343	23	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1422	GLY	-	expression tag	UNP Q04721
A	1519	ASN	ASP	conflict	UNP Q04721
A	?	-	GLU	deletion	UNP Q04721
A	?	-	LYS	deletion	UNP Q04721
A	?	-	SER	deletion	UNP Q04721
A	?	-	ALA	deletion	UNP Q04721
A	?	-	ALA	deletion	UNP Q04721
A	?	-	MET	deletion	UNP Q04721
A	?	-	LYS	deletion	UNP Q04721
A	?	-	LYS	deletion	UNP Q04721
A	?	-	GLN	deletion	UNP Q04721
A	?	-	ARG	deletion	UNP Q04721
A	?	-	MET	deletion	UNP Q04721
A	?	-	THR	deletion	UNP Q04721
A	?	-	ARG	deletion	UNP Q04721
A	?	-	ARG	deletion	UNP Q04721
A	?	-	SER	deletion	UNP Q04721
A	?	-	LEU	deletion	UNP Q04721
A	?	-	PRO	deletion	UNP Q04721
A	?	-	GLY	deletion	UNP Q04721
A	?	-	GLU	deletion	UNP Q04721
A	?	-	GLN	deletion	UNP Q04721
A	?	-	GLU	deletion	UNP Q04721
A	?	-	GLN	deletion	UNP Q04721
B	1422	GLY	-	expression tag	UNP Q04721

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1519	ASN	ASP	conflict	UNP Q04721
B	?	-	GLU	deletion	UNP Q04721
B	?	-	LYS	deletion	UNP Q04721
B	?	-	SER	deletion	UNP Q04721
B	?	-	ALA	deletion	UNP Q04721
B	?	-	ALA	deletion	UNP Q04721
B	?	-	MET	deletion	UNP Q04721
B	?	-	LYS	deletion	UNP Q04721
B	?	-	LYS	deletion	UNP Q04721
B	?	-	GLN	deletion	UNP Q04721
B	?	-	ARG	deletion	UNP Q04721
B	?	-	MET	deletion	UNP Q04721
B	?	-	THR	deletion	UNP Q04721
B	?	-	ARG	deletion	UNP Q04721
B	?	-	ARG	deletion	UNP Q04721
B	?	-	SER	deletion	UNP Q04721
B	?	-	LEU	deletion	UNP Q04721
B	?	-	PRO	deletion	UNP Q04721
B	?	-	GLY	deletion	UNP Q04721
B	?	-	GLU	deletion	UNP Q04721
B	?	-	GLN	deletion	UNP Q04721
B	?	-	GLU	deletion	UNP Q04721
B	?	-	GLN	deletion	UNP Q04721

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total Ca 3 3	0	0
2	B	3	Total Ca 3 3	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

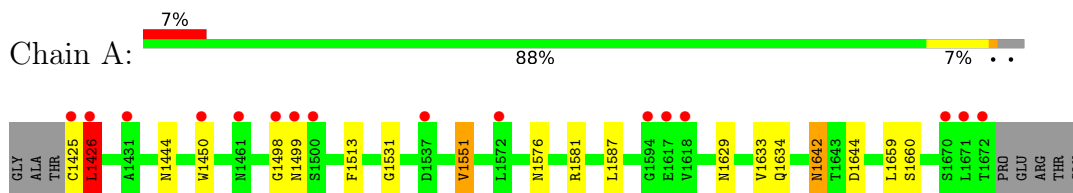
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	99	Total O 99 99	0	0
5	B	65	Total O 65 65	0	0

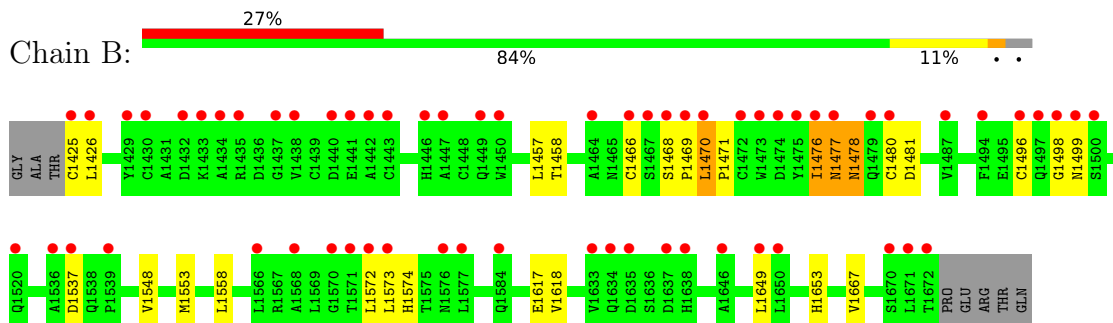
### 3 Residue-property plots [i](#)

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: Neurogenic locus notch homolog protein 2



- Molecule 1: Neurogenic locus notch homolog protein 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	45.37Å 74.71Å 139.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 26.65 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.1 (30.00-2.00) 97.1 (26.65-2.00)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.31 (at 2.01Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.226 , 0.268 0.227 , 0.262	Depositor DCC
$R_{free}$ test set	1603 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.4	Xtrriage
Anisotropy	0.143	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 56.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3642	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% 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: GOL, ZN, CA

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	0.51	1/1759 (0.1%)	0.64	3/2393 (0.1%)
1	B	0.38	0/1720	0.55	0/2343
All	All	0.45	1/3479 (0.0%)	0.60	3/4736 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1426	LEU	CG-CD2	11.06	1.92	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1426	LEU	CB-CG-CD2	-10.48	93.18	111.00
1	A	1426	LEU	CB-CG-CD1	8.01	124.62	111.00
1	A	1551	VAL	CB-CA-C	-5.16	101.60	111.40

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	1724	0	1556	27	0
1	B	1687	0	1499	18	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	1	0	0	0	0
4	A	48	0	64	12	0
4	B	12	0	16	2	0
5	A	99	0	0	2	0
5	B	65	0	0	1	0
All	All	3642	0	3135	45	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (45) 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:1426:LEU:CG	1:A:1426:LEU:CD2	1.92	1.45
1:A:1576:ASN:OD1	4:A:7007:GOL:H12	1.58	1.03
1:A:1513:PHE:HZ	4:A:7007:GOL:H2	1.33	0.93
1:B:1476:ILE:N	1:B:1477:ASN:HB2	1.87	0.88
1:B:1469:PRO:HA	1:B:1470:LEU:C	1.96	0.85
1:A:1426:LEU:CD2	1:A:1426:LEU:CB	2.59	0.80
1:A:1634:GLN:NE2	4:B:7004:GOL:H31	1.95	0.80
1:A:1513:PHE:CZ	4:A:7007:GOL:H2	2.19	0.76
1:A:1634:GLN:HE22	4:B:7004:GOL:H31	1.52	0.72
1:A:1531:GLY:HA2	4:A:7007:GOL:H11	1.70	0.72
1:A:1425:CYS:SG	1:A:1426:LEU:N	2.63	0.71
1:B:1469:PRO:HA	1:B:1470:LEU:O	1.93	0.67
1:A:1513:PHE:HZ	4:A:7007:GOL:C2	2.06	0.66
1:A:1642:ASN:ND2	1:A:1644:ASP:H	1.93	0.66
1:A:1581:ARG:HE	4:A:7006:GOL:H32	1.67	0.60
1:B:1458:THR:HG21	5:B:74:HOH:O	2.03	0.58
1:A:1513:PHE:CZ	4:A:7007:GOL:H11	2.42	0.55
1:B:1477:ASN:O	1:B:1478:ASN:HB2	2.09	0.52
1:A:1426:LEU:CD2	1:A:1426:LEU:HB3	2.37	0.51
1:B:1548:VAL:HB	1:B:1667:VAL:HG22	1.93	0.51
1:A:1642:ASN:HD21	1:A:1644:ASP:HB2	1.75	0.51
1:B:1480:CYS:HB2	1:B:1496:CYS:HA	1.92	0.50
1:B:1468:SER:N	1:B:1469:PRO:HD3	2.28	0.49
1:A:1587:LEU:O	4:A:7001:GOL:H11	2.14	0.48
1:A:1642:ASN:HD21	1:A:1644:ASP:CB	2.27	0.48
1:B:1553:MET:HE3	1:B:1558:LEU:HD13	1.96	0.46

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1425:CYS:HA	1:B:1426:LEU:HA	1.58	0.46
1:B:1498:GLY:O	1:B:1574:HIS:NE2	2.49	0.45
1:A:1444:ASN:OD1	1:A:1450:TRP:HD1	2.00	0.45
1:B:1477:ASN:HB3	1:B:1478:ASN:H	1.55	0.44
1:A:1629:ASN:HB3	1:A:1633:VAL:HG13	1.99	0.43
1:B:1476:ILE:CA	1:B:1477:ASN:HB2	2.48	0.43
1:A:1642:ASN:ND2	5:A:36:HOH:O	2.51	0.43
1:B:1573:LEU:HD23	1:B:1649:LEU:HD23	2.02	0.42
1:A:1426:LEU:CD2	1:A:1426:LEU:CD1	2.87	0.42
1:A:1513:PHE:CZ	4:A:7007:GOL:C2	2.93	0.42
1:A:1513:PHE:HZ	4:A:7007:GOL:C1	2.32	0.42
1:A:1660:SER:HB2	5:A:23:HOH:O	2.20	0.41
1:B:1553:MET:CE	1:B:1558:LEU:HD13	2.50	0.41
1:A:1642:ASN:ND2	1:A:1642:ASN:C	2.73	0.41
1:B:1477:ASN:O	1:B:1478:ASN:CB	2.69	0.41
1:A:1581:ARG:HD2	4:A:7006:GOL:H12	2.04	0.40
1:B:1457:LEU:O	1:B:1458:THR:HB	2.21	0.40
1:B:1572:LEU:HD22	1:B:1653:HIS:CE1	2.56	0.40
1:A:1513:PHE:CZ	4:A:7007:GOL:C1	3.03	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	224/234 (96%)	218 (97%)	4 (2%)	2 (1%)	17	11
1	B	224/234 (96%)	199 (89%)	19 (8%)	6 (3%)	5	1
All	All	448/468 (96%)	417 (93%)	23 (5%)	8 (2%)	8	3

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1478	ASN
1	B	1499	ASN
1	A	1498	GLY
1	A	1499	ASN
1	B	1466	CYS
1	B	1477	ASN
1	B	1618	VAL
1	B	1471	PRO

### 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	190/201 (94%)	186 (98%)	4 (2%)	53	57
1	B	181/201 (90%)	176 (97%)	5 (3%)	43	44
All	All	371/402 (92%)	362 (98%)	9 (2%)	49	51

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1426	LEU
1	A	1551	VAL
1	A	1642	ASN
1	A	1659	LEU
1	B	1470	LEU
1	B	1476	ILE
1	B	1481	ASP
1	B	1537	ASP
1	B	1617	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1629	ASN
1	A	1634	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1642	ASN
1	B	1629	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 17 ligands modelled in this entry, 7 are monoatomic - leaving 10 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
4	GOL	A	7008	-	5,5,5	0.42	0	5,5,5	0.22	0
4	GOL	A	7007	-	5,5,5	0.70	0	5,5,5	0.89	0
4	GOL	A	7001	-	5,5,5	0.41	0	5,5,5	0.32	0
4	GOL	A	7006	-	5,5,5	0.36	0	5,5,5	0.31	0
4	GOL	A	7002	-	5,5,5	0.37	0	5,5,5	0.23	0
4	GOL	B	7004	-	5,5,5	0.35	0	5,5,5	0.54	0
4	GOL	A	7010	-	5,5,5	0.36	0	5,5,5	0.28	0
4	GOL	A	7009	-	5,5,5	0.35	0	5,5,5	0.26	0
4	GOL	A	7003	-	5,5,5	0.39	0	5,5,5	0.24	0
4	GOL	B	7005	-	5,5,5	0.35	0	5,5,5	0.27	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
4	GOL	A	7008	-	-	1/4/4/4	-
4	GOL	A	7007	-	-	4/4/4/4	-
4	GOL	A	7001	-	-	4/4/4/4	-
4	GOL	A	7006	-	-	0/4/4/4	-
4	GOL	A	7002	-	-	3/4/4/4	-
4	GOL	B	7004	-	-	2/4/4/4	-
4	GOL	A	7010	-	-	0/4/4/4	-
4	GOL	A	7009	-	-	2/4/4/4	-
4	GOL	A	7003	-	-	2/4/4/4	-
4	GOL	B	7005	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	7002	GOL	C1-C2-C3-O3
4	A	7007	GOL	C1-C2-C3-O3
4	A	7007	GOL	O2-C2-C3-O3
4	A	7009	GOL	O1-C1-C2-C3
4	B	7005	GOL	C1-C2-C3-O3
4	A	7001	GOL	O1-C1-C2-C3
4	A	7001	GOL	C1-C2-C3-O3
4	A	7002	GOL	O1-C1-C2-C3
4	A	7003	GOL	C1-C2-C3-O3
4	A	7008	GOL	C1-C2-C3-O3
4	B	7004	GOL	O1-C1-C2-C3
4	A	7001	GOL	O1-C1-C2-O2
4	A	7009	GOL	O1-C1-C2-O2
4	B	7004	GOL	O1-C1-C2-O2
4	B	7005	GOL	O2-C2-C3-O3
4	A	7001	GOL	O2-C2-C3-O3
4	A	7002	GOL	O2-C2-C3-O3
4	A	7007	GOL	O1-C1-C2-O2
4	A	7003	GOL	O2-C2-C3-O3
4	A	7007	GOL	O1-C1-C2-C3

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	7007	GOL	9	0
4	A	7001	GOL	1	0
4	A	7006	GOL	2	0
4	B	7004	GOL	2	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	226/234 (96%)	0.52	16 (7%) <span style="border: 1px solid red; padding: 0 2px;">16</span> <span style="border: 1px solid red; padding: 0 2px;">15</span>	25, 41, 64, 90	0
1	B	226/234 (96%)	1.41	63 (27%) <span style="border: 1px solid red; padding: 0 2px;">0</span> <span style="border: 1px solid red; padding: 0 2px;">0</span>	28, 57, 102, 120	0
All	All	452/468 (96%)	0.97	79 (17%) <span style="border: 1px solid red; padding: 0 2px;">1</span> <span style="border: 1px solid red; padding: 0 2px;">1</span>	25, 49, 92, 120	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1500	SER	10.3
1	A	1426	LEU	9.3
1	B	1425	CYS	8.8
1	B	1476	ILE	8.6
1	B	1672	THR	8.1
1	B	1447	ALA	8.0
1	B	1437	GLY	7.8
1	A	1499	ASN	6.7
1	A	1594	GLY	6.2
1	A	1425	CYS	6.1
1	B	1467	SER	5.5
1	B	1499	ASN	5.5
1	B	1438	VAL	5.3
1	B	1498	GLY	5.3
1	A	1498	GLY	5.1
1	B	1671	LEU	5.1
1	B	1470	LEU	5.0
1	A	1672	THR	5.0
1	B	1475	TYR	4.9
1	B	1480	CYS	4.7
1	B	1670	SER	4.5
1	B	1573	LEU	4.4
1	B	1634	GLN	4.2
1	A	1671	LEU	4.2

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	1472	CYS	4.2
1	B	1450	TRP	4.1
1	B	1434	ALA	4.1
1	B	1435	ARG	4.0
1	B	1537	ASP	4.0
1	B	1469	PRO	4.0
1	B	1577	LEU	3.9
1	B	1466	CYS	3.9
1	A	1500	SER	3.8
1	A	1617	GLU	3.8
1	A	1537	ASP	3.8
1	B	1426	LEU	3.6
1	B	1477	ASN	3.6
1	B	1442	ALA	3.5
1	B	1474	ASP	3.4
1	A	1670	SER	3.4
1	B	1496	CYS	3.4
1	B	1433	LYS	3.3
1	B	1487	VAL	3.3
1	B	1479	GLN	3.3
1	B	1473	TRP	3.2
1	B	1572	LEU	3.1
1	B	1520	GLN	3.0
1	B	1536	ALA	3.0
1	B	1539	PRO	2.9
1	B	1637	ASP	2.9
1	B	1440	ASP	2.9
1	B	1566	LEU	2.9
1	B	1633	VAL	2.8
1	B	1430	CYS	2.8
1	B	1468	SER	2.8
1	B	1646	ALA	2.7
1	B	1449	GLN	2.7
1	B	1570	GLY	2.7
1	A	1431	ALA	2.5
1	B	1464	ALA	2.5
1	B	1446	HIS	2.5
1	B	1576	ASN	2.5
1	B	1441	GLU	2.5
1	A	1461	ASN	2.4
1	A	1572	LEU	2.4
1	B	1432	ASP	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	1635	ASP	2.4
1	B	1650	LEU	2.3
1	B	1429	TYR	2.3
1	B	1497	GLN	2.3
1	B	1568	ALA	2.3
1	A	1450	TRP	2.2
1	A	1618	VAL	2.2
1	B	1649	LEU	2.2
1	B	1443	CYS	2.2
1	B	1494	PHE	2.2
1	B	1638	HIS	2.2
1	B	1571	THR	2.0
1	B	1584	GLN	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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
4	GOL	A	7006	6/6	0.58	0.25	88,88,88,88	0
4	GOL	B	7004	6/6	0.59	0.38	64,66,67,67	0
4	GOL	B	7005	6/6	0.69	0.42	93,93,94,94	0
4	GOL	A	7009	6/6	0.74	0.32	104,104,104,105	0
2	CA	B	5004	1/1	0.76	0.09	90,90,90,90	0
4	GOL	A	7007	6/6	0.77	0.32	33,36,38,43	0
4	GOL	A	7010	6/6	0.77	0.19	85,85,85,85	0
4	GOL	A	7008	6/6	0.79	0.28	73,74,75,76	0
4	GOL	A	7003	6/6	0.81	0.21	80,80,81,81	0
4	GOL	A	7002	6/6	0.83	0.18	74,74,74,75	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	GOL	A	7001	6/6	0.87	0.14	47,49,50,50	0
2	CA	B	5005	1/1	0.88	0.10	69,69,69,69	0
2	CA	A	5001	1/1	0.90	0.08	54,54,54,54	0
2	CA	B	5006	1/1	0.94	0.10	46,46,46,46	0
2	CA	A	5002	1/1	0.97	0.05	51,51,51,51	0
2	CA	A	5003	1/1	0.98	0.10	39,39,39,39	0
3	ZN	A	6001	1/1	0.99	0.08	51,51,51,51	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.