



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 08:35 am BST

PDB ID : 4XN7
Title : Crystal Structure of E. coli Aminopeptidase N in complex with L-2,3-Diaminopropionic acid
Authors : Addlagatta, A.; Gumpena, R.
Deposited on : 2015-01-15
Resolution : 2.22 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 ⓘ symbol.

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 : 2.11
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) : 2.11

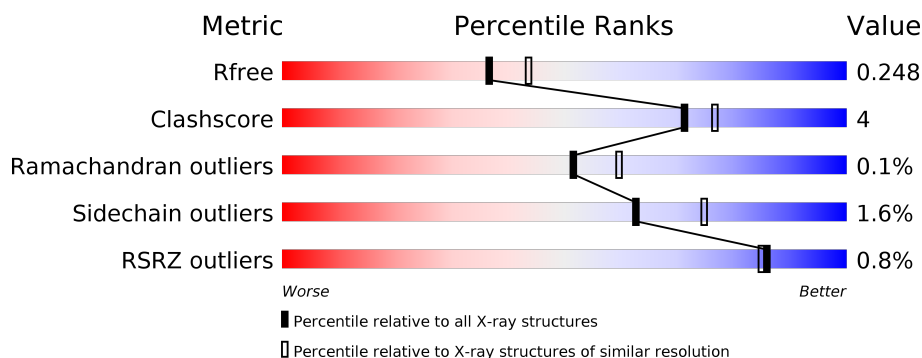
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 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	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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 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	866	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; left: 0; top: 0; width: 100%; height: 100%; background: linear-gradient(to right, red, orange, yellow, green);"></div> <div style="position: absolute; left: 0; top: 0; width: 10%; height: 100%; background-color: red;"></div> <div style="position: absolute; left: 90%; top: 0; width: 10%; height: 100%; background-color: yellow;"></div> <div style="position: absolute; left: 90%; top: 0; width: 10%; height: 100%; background-color: green;"></div> </div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 92% 7% </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
5	GOL	A	920	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7679 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.

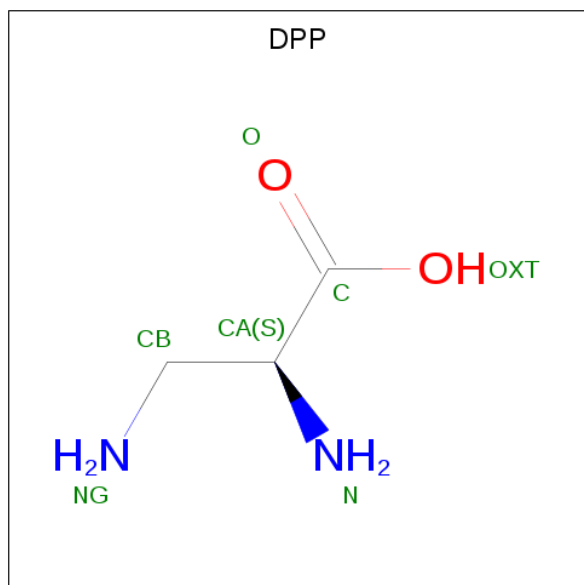
- Molecule 1 is a protein called Aminopeptidase N.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	866	Total	C	N	O	S	0	5	0
			6979	4419	1212	1320	28			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is DIAMINOPROPANOIC ACID (three-letter code: DPP) (formula: C₃H₈N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			7	3	2	2		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total	Na	0	0
			4	4		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

- Molecule 6 is MALONATE ION (three-letter code: MLI) (formula: C₃H₂O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	3	4		
6	A	1	Total	C	O	0	0
			7	3	4		

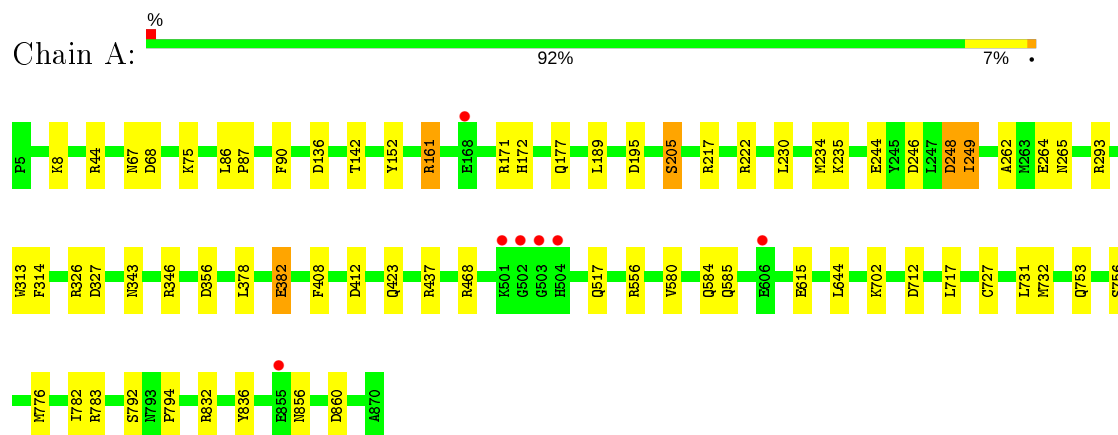
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	506	Total	O	0	0
			506	506		

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: Aminopeptidase N



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	120.69Å 120.69Å 170.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.25 – 2.22 49.25 – 2.22	Depositor EDS
% Data completeness (in resolution range)	98.3 (49.25-2.22) 98.3 (49.25-2.22)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.22Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.199 , 0.246 0.205 , 0.248	Depositor DCC
R_{free} test set	3535 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	19.4	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.033 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7679	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, MLI, NA, DPP

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	0.69	2/7146 (0.0%)	0.81	5/9701 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	382	GLU	CD-OE2	-5.80	1.19	1.25
1	A	205	SER	CB-OG	-5.31	1.35	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	248	ASP	CB-CG-OD2	-7.72	111.35	118.30
1	A	293	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	A	136	ASP	CB-CG-OD1	5.89	123.60	118.30
1	A	437	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	644	LEU	CA-CB-CG	5.02	126.84	115.30

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	6979	0	6829	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
3	A	7	0	7	2	0
4	A	4	0	0	0	0
5	A	168	0	223	18	0
6	A	14	0	4	1	0
7	A	506	0	0	11	0
All	All	7679	0	7063	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 4.

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:836:TYR:OH	5:A:927:GOL:H12	1.80	0.81
1:A:585:GLN:HG3	5:A:919:GOL:O1	1.86	0.74
5:A:912:GOL:O3	5:A:913:GOL:H2	1.87	0.73
1:A:580:VAL:O	1:A:584:GLN:HG3	1.90	0.72
1:A:171:ARG:NE	7:A:1002:HOH:O	2.23	0.71
1:A:712:ASP:OD2	5:A:928:GOL:H11	1.96	0.65
1:A:468:ARG:HD3	7:A:1427:HOH:O	1.99	0.63
1:A:152:TYR:HE2	5:A:920:GOL:C3	2.13	0.60
1:A:517:GLN:HB2	7:A:1185:HOH:O	1.99	0.60
1:A:264:GLU:OE1	3:A:902:DPP:HB2	2.02	0.60
1:A:205:SER:HB2	1:A:244:GLU:OE2	2.03	0.59
1:A:195:ASP:OD1	1:A:217:ARG:NH1	2.38	0.57
1:A:776:MET:O	1:A:782:ILE:HD11	2.05	0.56
1:A:161:ARG:NH1	7:A:1008:HOH:O	2.38	0.56
1:A:152:TYR:HE2	5:A:920:GOL:H32	1.71	0.55
1:A:44:ARG:NH1	1:A:86:LEU:O	2.41	0.53
1:A:230:LEU:O	1:A:234:MET:HG3	2.09	0.52
1:A:87:PRO:HG2	1:A:90:PHE:HB3	1.91	0.52
1:A:152:TYR:CE2	5:A:920:GOL:H32	2.45	0.51
1:A:346[B]:ARG:NH2	1:A:615:GLU:OE1	2.43	0.50
1:A:152:TYR:HE2	5:A:920:GOL:H31	1.78	0.49
1:A:792:SER:C	1:A:794:PRO:HD3	2.33	0.49
6:A:936:MLI:O7	6:A:936:MLI:O9	2.26	0.49
1:A:783:ARG:NH1	7:A:1005:HOH:O	2.34	0.48
1:A:727:CYS:O	1:A:731:LEU:HG	2.14	0.48
1:A:152:TYR:CE2	5:A:920:GOL:C3	2.96	0.48
1:A:314:PHE:CE2	5:A:921:GOL:H31	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:756:SER:CB	5:A:931:GOL:H11	2.44	0.47
1:A:142:THR:HG22	1:A:177:GLN:HG3	1.96	0.47
1:A:313:TRP:HB2	5:A:921:GOL:H32	1.97	0.47
1:A:75:LYS:NZ	7:A:1022:HOH:O	2.49	0.46
5:A:920:GOL:O2	7:A:1001:HOH:O	2.09	0.46
1:A:556:ARG:NH1	7:A:1021:HOH:O	2.47	0.46
1:A:249:ILE:HD11	7:A:1394:HOH:O	2.16	0.46
1:A:326:ARG:HG2	1:A:326:ARG:HH11	1.81	0.45
5:A:930:GOL:H31	7:A:1456:HOH:O	2.17	0.45
1:A:832:ARG:HB2	5:A:927:GOL:H11	1.99	0.45
1:A:262:ALA:O	3:A:902:DPP:N	2.49	0.45
1:A:67:ASN:O	1:A:68:ASP:HB2	2.18	0.44
1:A:717:LEU:HD11	1:A:732:MET:SD	2.57	0.44
5:A:925:GOL:O3	5:A:925:GOL:O1	2.32	0.44
1:A:343:ASN:OD1	1:A:346[B]:ARG:NH1	2.50	0.44
1:A:189:LEU:C	1:A:189:LEU:HD23	2.39	0.43
1:A:246:ASP:HB3	5:A:932:GOL:H11	2.01	0.41
1:A:378:LEU:O	1:A:382:GLU:HB2	2.21	0.41
1:A:152:TYR:CE2	5:A:920:GOL:H31	2.56	0.40
1:A:408:PHE:O	1:A:412:ASP:HB2	2.21	0.40
1:A:8:LYS:HG3	7:A:1273:HOH:O	2.22	0.40
1:A:264:GLU:O	1:A:265:ASN:C	2.59	0.40
1:A:346[B]:ARG:NH1	1:A:615:GLU:OE1	2.52	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	869/866 (100%)	849 (98%)	19 (2%)	1 (0%)	51 60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	856	ASN

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	746/741 (101%)	732 (98%)	14 (2%)	57 69

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	161	ARG
1	A	172	HIS
1	A	222[A]	ARG
1	A	222[B]	ARG
1	A	235	LYS
1	A	248	ASP
1	A	249	ILE
1	A	327	ASP
1	A	356	ASP
1	A	423[A]	GLN
1	A	423[B]	GLN
1	A	702	LYS
1	A	753	GLN
1	A	860	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	753	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 36 ligands modelled in this entry, 5 are monoatomic - leaving 31 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	$\# Z > 2$
5	GOL	A	908	-	5,5,5	0.25	0	5,5,5	0.44	0
5	GOL	A	911	-	5,5,5	0.47	0	5,5,5	0.54	0
5	GOL	A	914	-	5,5,5	0.46	0	5,5,5	0.32	0
6	MLI	A	935	-	0,6,6	0.00	-	0,7,7	0.00	-
5	GOL	A	925	-	5,5,5	0.19	0	5,5,5	0.27	0
5	GOL	A	929	-	5,5,5	0.72	0	5,5,5	0.49	0
5	GOL	A	916	-	5,5,5	0.50	0	5,5,5	0.29	0
5	GOL	A	920	-	5,5,5	1.22	0	5,5,5	1.71	2 (40%)
5	GOL	A	927	-	5,5,5	1.09	0	5,5,5	1.68	2 (40%)
5	GOL	A	931	-	5,5,5	0.71	0	5,5,5	0.73	0
5	GOL	A	930	-	5,5,5	0.89	0	5,5,5	0.89	0
5	GOL	A	922	-	5,5,5	0.75	0	5,5,5	0.46	0
5	GOL	A	926	-	5,5,5	0.74	0	5,5,5	1.41	0
5	GOL	A	933	-	5,5,5	0.27	0	5,5,5	0.23	0
5	GOL	A	932	-	5,5,5	0.40	0	5,5,5	1.22	0
5	GOL	A	934	-	5,5,5	0.15	0	5,5,5	0.42	0
5	GOL	A	924	4	5,5,5	0.71	0	5,5,5	0.34	0
5	GOL	A	907	-	5,5,5	0.52	0	5,5,5	0.60	0
5	GOL	A	928	-	5,5,5	0.46	0	5,5,5	0.77	0
5	GOL	A	921	-	5,5,5	0.79	0	5,5,5	1.30	0
5	GOL	A	919	-	5,5,5	0.31	0	5,5,5	0.25	0
5	GOL	A	910	-	5,5,5	0.41	0	5,5,5	0.98	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MLI	A	936	-	0,6,6	0.00	-	0,7,7	0.00	-
5	GOL	A	923	-	5,5,5	0.45	0	5,5,5	0.70	0
5	GOL	A	915	-	5,5,5	0.34	0	5,5,5	1.39	0
5	GOL	A	912	-	5,5,5	0.79	0	5,5,5	1.28	1 (20%)
5	GOL	A	909	-	5,5,5	0.53	0	5,5,5	0.37	0
3	DPP	A	902	2	2,6,6	1.50	0	1,7,7	0.62	0
5	GOL	A	917	-	5,5,5	0.63	0	5,5,5	0.59	0
5	GOL	A	913	-	5,5,5	0.98	0	5,5,5	1.48	2 (40%)
5	GOL	A	918	-	5,5,5	0.75	0	5,5,5	0.90	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
5	GOL	A	908	-	-	0/4/4/4	-
5	GOL	A	911	-	-	2/4/4/4	-
5	GOL	A	914	-	-	2/4/4/4	-
6	MLI	A	935	-	-	0/0/4/4	-
5	GOL	A	925	-	-	0/4/4/4	-
5	GOL	A	929	-	-	2/4/4/4	-
5	GOL	A	916	-	-	1/4/4/4	-
5	GOL	A	920	-	-	0/4/4/4	-
5	GOL	A	927	-	-	2/4/4/4	-
5	GOL	A	931	-	-	2/4/4/4	-
5	GOL	A	930	-	-	2/4/4/4	-
5	GOL	A	922	-	-	2/4/4/4	-
5	GOL	A	926	-	-	0/4/4/4	-
5	GOL	A	933	-	-	2/4/4/4	-
5	GOL	A	932	-	-	2/4/4/4	-
5	GOL	A	934	-	-	2/4/4/4	-
5	GOL	A	924	4	-	2/4/4/4	-
5	GOL	A	907	-	-	2/4/4/4	-
5	GOL	A	928	-	-	1/4/4/4	-
5	GOL	A	921	-	-	2/4/4/4	-
5	GOL	A	919	-	-	0/4/4/4	-
5	GOL	A	910	-	-	0/4/4/4	-
6	MLI	A	936	-	-	0/0/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	923	-	-	4/4/4/4	-
5	GOL	A	915	-	-	2/4/4/4	-
5	GOL	A	912	-	-	4/4/4/4	-
5	GOL	A	909	-	-	4/4/4/4	-
3	DPP	A	902	2	-	0/2/6/6	-
5	GOL	A	917	-	-	4/4/4/4	-
5	GOL	A	913	-	-	2/4/4/4	-
5	GOL	A	918	-	-	4/4/4/4	-

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	927	GOL	O1-C1-C2	2.71	123.22	110.20
5	A	920	GOL	O3-C3-C2	2.55	122.41	110.20
5	A	920	GOL	O1-C1-C2	2.50	122.17	110.20
5	A	927	GOL	O3-C3-C2	2.20	120.73	110.20
5	A	912	GOL	O3-C3-C2	2.14	120.47	110.20
5	A	913	GOL	O3-C3-C2	2.09	120.23	110.20
5	A	913	GOL	O1-C1-C2	2.09	120.22	110.20

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	929	GOL	C1-C2-C3-O3
5	A	927	GOL	C1-C2-C3-O3
5	A	931	GOL	O1-C1-C2-C3
5	A	930	GOL	C1-C2-C3-O3
5	A	922	GOL	O1-C1-C2-C3
5	A	933	GOL	C1-C2-C3-O3
5	A	932	GOL	O1-C1-C2-C3
5	A	924	GOL	C1-C2-C3-O3
5	A	923	GOL	O1-C1-C2-C3
5	A	915	GOL	O1-C1-C2-C3
5	A	912	GOL	O1-C1-C2-O2
5	A	912	GOL	C1-C2-C3-O3
5	A	909	GOL	O1-C1-C2-C3
5	A	917	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	A	917	GOL	O1-C1-C2-C3
5	A	918	GOL	C1-C2-C3-O3
5	A	914	GOL	O1-C1-C2-O2
5	A	924	GOL	O2-C2-C3-O3
5	A	915	GOL	O1-C1-C2-O2
5	A	909	GOL	O1-C1-C2-O2
5	A	918	GOL	O2-C2-C3-O3
5	A	911	GOL	C1-C2-C3-O3
5	A	914	GOL	O1-C1-C2-C3
5	A	934	GOL	O1-C1-C2-C3
5	A	907	GOL	C1-C2-C3-O3
5	A	921	GOL	C1-C2-C3-O3
5	A	923	GOL	C1-C2-C3-O3
5	A	912	GOL	O1-C1-C2-C3
5	A	913	GOL	O1-C1-C2-C3
5	A	918	GOL	O1-C1-C2-C3
5	A	929	GOL	O2-C2-C3-O3
5	A	927	GOL	O2-C2-C3-O3
5	A	931	GOL	O1-C1-C2-O2
5	A	922	GOL	O1-C1-C2-O2
5	A	932	GOL	O1-C1-C2-O2
5	A	923	GOL	O2-C2-C3-O3
5	A	913	GOL	O1-C1-C2-O2
5	A	918	GOL	O1-C1-C2-O2
5	A	930	GOL	O2-C2-C3-O3
5	A	923	GOL	O1-C1-C2-O2
5	A	916	GOL	O2-C2-C3-O3
5	A	933	GOL	O2-C2-C3-O3
5	A	912	GOL	O2-C2-C3-O3
5	A	934	GOL	O1-C1-C2-O2
5	A	921	GOL	O2-C2-C3-O3
5	A	909	GOL	O2-C2-C3-O3
5	A	911	GOL	O2-C2-C3-O3
5	A	928	GOL	C1-C2-C3-O3
5	A	909	GOL	C1-C2-C3-O3
5	A	917	GOL	C1-C2-C3-O3
5	A	917	GOL	O2-C2-C3-O3
5	A	907	GOL	O2-C2-C3-O3

There are no ring outliers.

13 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	925	GOL	1	0
5	A	920	GOL	7	0
5	A	927	GOL	2	0
5	A	931	GOL	1	0
5	A	930	GOL	1	0
5	A	932	GOL	1	0
5	A	928	GOL	1	0
5	A	921	GOL	2	0
5	A	919	GOL	1	0
6	A	936	MLI	1	0
5	A	912	GOL	1	0
3	A	902	DPP	2	0
5	A	913	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	866/866 (100%)	-0.43	7 (0%) 86 85	10, 19, 34, 60	5 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	504	HIS	4.8
1	A	855[A]	GLU	3.3
1	A	503	GLY	2.4
1	A	168	GLU	2.3
1	A	501	LYS	2.2
1	A	606	GLU	2.1
1	A	502	GLY	2.1

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. 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	GOL	A	929	6/6	0.75	0.22	39,46,47,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	GOL	A	916	6/6	0.77	0.20	58,63,67,80	0
5	GOL	A	924	6/6	0.77	0.19	48,51,53,56	0
5	GOL	A	920	6/6	0.78	0.28	30,36,36,40	0
5	GOL	A	922	6/6	0.79	0.21	45,51,53,53	0
5	GOL	A	911	6/6	0.79	0.21	40,46,51,55	0
5	GOL	A	914	6/6	0.81	0.25	54,59,65,65	0
5	GOL	A	931	6/6	0.82	0.26	41,48,50,52	0
5	GOL	A	918	6/6	0.82	0.28	42,49,53,55	0
5	GOL	A	926	6/6	0.83	0.13	39,42,43,45	0
5	GOL	A	923	6/6	0.84	0.16	43,44,52,59	0
5	GOL	A	930	6/6	0.86	0.16	29,37,39,40	0
5	GOL	A	913	6/6	0.87	0.24	38,42,43,44	0
6	MLI	A	935	7/7	0.87	0.20	56,61,67,72	0
5	GOL	A	933	6/6	0.88	0.48	56,58,60,60	0
5	GOL	A	912	6/6	0.88	0.20	34,42,46,49	0
5	GOL	A	927	6/6	0.88	0.22	35,37,40,50	0
5	GOL	A	919	6/6	0.88	0.19	43,45,47,48	0
4	NA	A	905	1/1	0.89	0.21	38,38,38,38	0
5	GOL	A	934	6/6	0.90	0.15	42,43,45,46	0
6	MLI	A	936	7/7	0.90	0.19	37,45,51,57	0
5	GOL	A	921	6/6	0.90	0.15	22,26,26,30	0
5	GOL	A	928	6/6	0.91	0.20	35,39,41,49	0
5	GOL	A	932	6/6	0.91	0.32	4,4,4,4	6
5	GOL	A	925	6/6	0.92	0.16	49,51,52,54	0
5	GOL	A	917	6/6	0.92	0.14	37,41,41,42	0
5	GOL	A	907	6/6	0.93	0.13	26,29,31,31	0
5	GOL	A	909	6/6	0.94	0.14	35,36,37,38	0
4	NA	A	903	1/1	0.94	0.11	28,28,28,28	0
5	GOL	A	908	6/6	0.94	0.27	36,37,39,40	0
5	GOL	A	910	6/6	0.94	0.11	33,37,38,39	0
4	NA	A	904	1/1	0.95	0.14	31,31,31,31	0
5	GOL	A	915	6/6	0.95	0.10	19,21,23,26	0
3	DPP	A	902	7/7	0.95	0.17	23,26,28,32	0
2	ZN	A	901	1/1	0.97	0.04	33,33,33,33	0
4	NA	A	906	1/1	0.98	0.04	23,23,23,23	0

6.5 Other polymers

There are no such residues in this entry.