wwPDB X-ray Structure Validation Summary Report (i)

Aug 7, 2023 – 11:02 PM EDT

PDB ID	:	1NXD
Title	:	Crystal structure of MnMn Concanavalin A
Authors	:	Lopez-Jaramillo, F.J.; Gonzalez-Ramirez, L.A.; Albert, A.; Santoyo-Gonzalez, F.; Vargas-Berenguel, A.; Otalora, F.
Deposited on	:	2003-02-10
Resolution	:	1.90 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

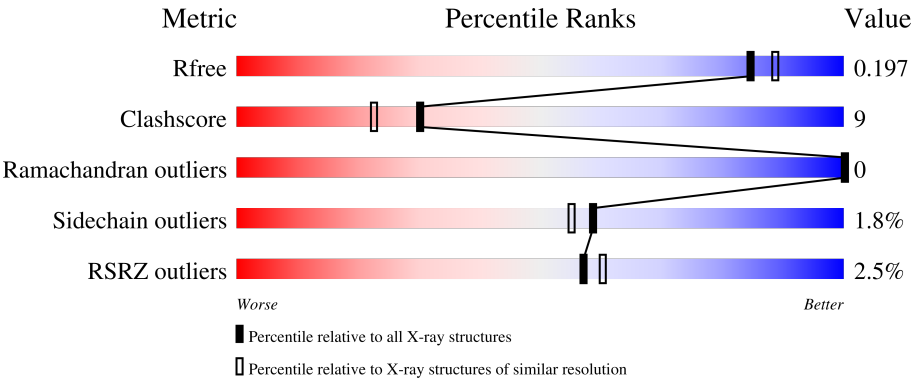
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	237	3% 87% 12%
1	2	237	3% 81% 18%
1	3	237	2% 80% 19%
1	4	237	2% 84% 14%

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
2	AZI	2	913	-	-	X	-
2	AZI	2	915	-	-	X	-
2	AZI	3	901	-	-	X	-
2	AZI	3	909	-	-	-	X
2	AZI	4	903	-	-	X	-
5	GOL	1	804	-	X	-	-
5	GOL	1	806	-	X	-	-
5	GOL	1	807	-	X	-	-
5	GOL	1	812	-	X	-	-
5	GOL	1	821	-	X	-	-
5	GOL	1	822	-	X	-	-
5	GOL	1	823	-	X	X	-
5	GOL	1	824	-	X	-	-
5	GOL	2	809	-	X	-	-
5	GOL	2	811	-	X	X	-
5	GOL	2	814	-	X	-	-
5	GOL	2	815	-	X	-	-
5	GOL	2	818	-	X	-	-
5	GOL	2	820	-	X	-	-
5	GOL	3	802	-	X	-	-
5	GOL	3	803	-	X	-	-
5	GOL	3	808	-	X	-	-
5	GOL	3	816	-	X	-	-
5	GOL	3	825	-	X	-	X
5	GOL	4	801	-	X	-	-
5	GOL	4	805	-	X	-	-
5	GOL	4	810	-	X	-	-
5	GOL	4	813	-	X	-	-
5	GOL	4	817	-	X	-	-
5	GOL	4	819	-	X	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8210 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.

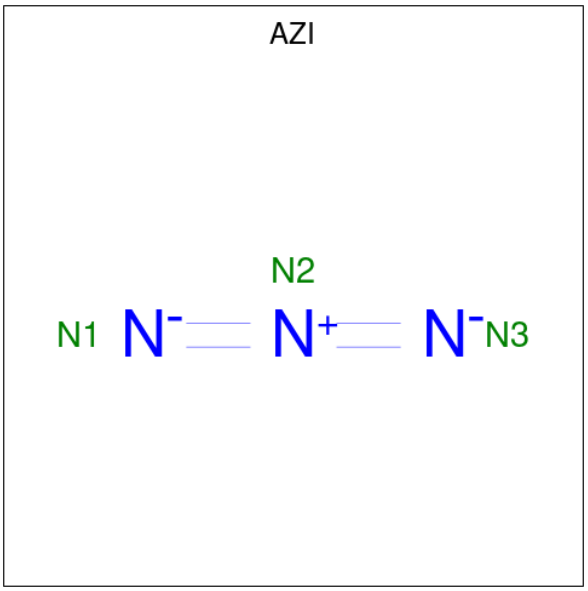
- Molecule 1 is a protein called concanavalin A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	237	Total	C	N	O	S	0	0	0
			1809	1141	302	364	2			
1	2	237	Total	C	N	O	S	0	0	0
			1809	1141	302	364	2			
1	3	237	Total	C	N	O	S	0	0	0
			1809	1141	302	364	2			
1	4	237	Total	C	N	O	S	0	0	0
			1809	1141	302	364	2			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	151	ASP	GLU	conflict	UNP P02866
1	155	GLU	ARG	conflict	UNP P02866
2	151	ASP	GLU	conflict	UNP P02866
2	155	GLU	ARG	conflict	UNP P02866
3	151	ASP	GLU	conflict	UNP P02866
3	155	GLU	ARG	conflict	UNP P02866
4	151	ASP	GLU	conflict	UNP P02866
4	155	GLU	ARG	conflict	UNP P02866

- Molecule 2 is AZIDE ION (three-letter code: AZI) (formula: N_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	1	1	Total N 3 3	0	0
2	1	1	Total N 3 3	0	0
2	1	1	Total N 3 3	0	0
2	2	1	Total N 3 3	0	0
2	2	1	Total N 3 3	0	0
2	2	1	Total N 3 3	0	0
2	2	1	Total N 3 3	0	0
2	2	1	Total N 3 3	0	0
2	3	1	Total N 3 3	0	0
2	3	1	Total N 3 3	0	0
2	3	1	Total N 3 3	0	0
2	3	1	Total N 3 3	0	0
2	4	1	Total N 3 3	0	0
2	4	1	Total N 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	4	1	Total N 3 3	0	0
2	4	1	Total N 3 3	0	0

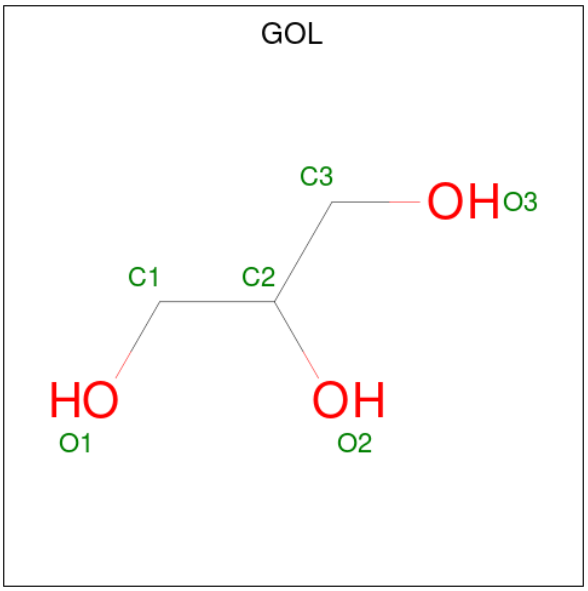
- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	1	2	Total Mn 2 2	0	0
3	2	2	Total Mn 2 2	0	0
3	3	2	Total Mn 2 2	0	0
3	4	2	Total Mn 2 2	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	1	1	Total Na 1 1	0	0
4	2	1	Total Na 1 1	0	0
4	3	1	Total Na 1 1	0	0
4	4	1	Total Na 1 1	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	1	1	Total C O 6 3 3	0	0
5	1	1	Total C O 6 3 3	0	0
5	1	1	Total C O 6 3 3	0	0
5	1	1	Total C O 6 3 3	0	0
5	1	1	Total C O 6 3 3	0	0
5	1	1	Total C O 6 3 3	0	0
5	1	1	Total C O 6 3 3	0	0
5	1	1	Total C O 6 3 3	0	0
5	2	1	Total C O 6 3 3	0	0
5	2	1	Total C O 6 3 3	0	0
5	2	1	Total C O 6 3 3	0	0
5	2	1	Total C O 6 3 3	0	0
5	2	1	Total C O 6 3 3	0	0
5	2	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	3	1	Total C O 6 3 3	0	0
5	3	1	Total C O 6 3 3	0	0
5	3	1	Total C O 6 3 3	0	0
5	3	1	Total C O 6 3 3	0	0
5	3	1	Total C O 6 3 3	0	0
5	4	1	Total C O 6 3 3	0	0
5	4	1	Total C O 6 3 3	0	0
5	4	1	Total C O 6 3 3	0	0
5	4	1	Total C O 6 3 3	0	0
5	4	1	Total C O 6 3 3	0	0
5	4	1	Total C O 6 3 3	0	0

- Molecule 6 is water.

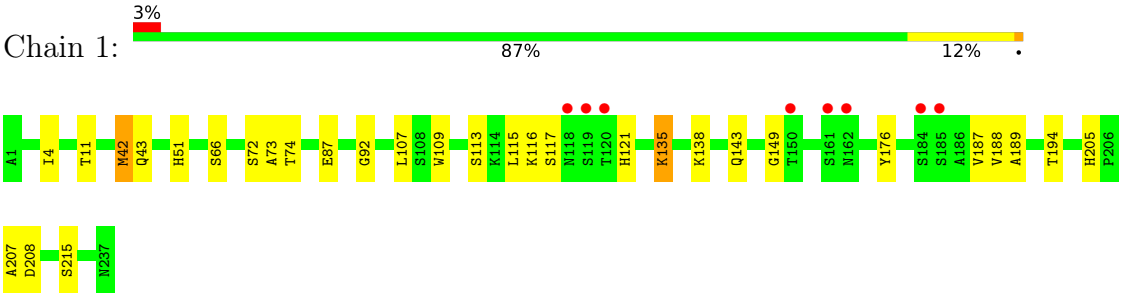
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	1	214	Total O 214 214	0	0
6	2	183	Total O 183 183	0	0
6	3	165	Total O 165 165	0	0
6	4	202	Total O 202 202	0	0

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.

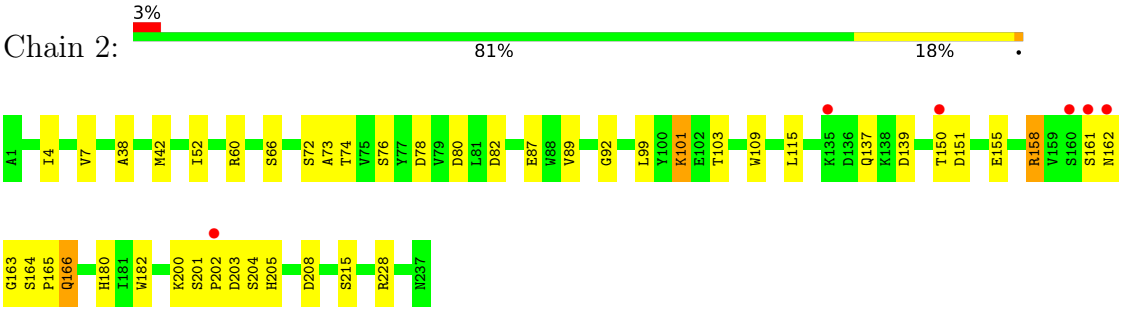
• Molecule 1: concanavalin A

Chain 1:



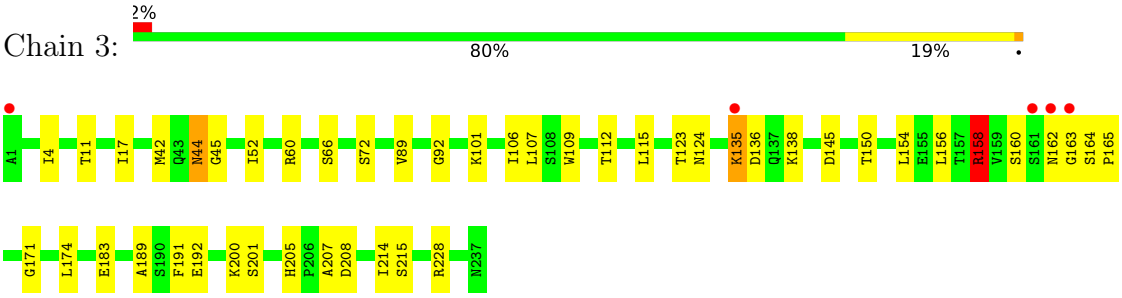
• Molecule 1: concanavalin A

Chain 2:



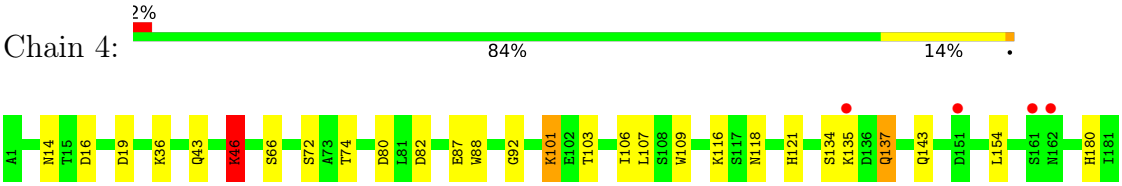
• Molecule 1: concanavalin A

Chain 3:



• Molecule 1: concanavalin A

Chain 4:




W182
E183
S184
V187
V188
K200
S204
I217
D218
S219
S220
P234
N237

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	101.30Å 118.00Å 249.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.00 – 1.90 19.61 – 1.84	Depositor EDS
% Data completeness (in resolution range)	95.0 (19.00-1.90) 94.2 (19.61-1.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.02	Depositor
$< I/\sigma(I) >$ [1]	10.52 (at 1.85Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.184 , 0.201 0.180 , 0.197	Depositor DCC
R_{free} test set	11146 reflections (9.23%)	wwPDB-VP
Wilson B-factor (Å^2)	15.0	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 53.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8210	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AZI, GOL, MN, NA

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	1	0.34	0/1851	0.70	0/2522
1	2	0.44	0/1851	0.83	4/2522 (0.2%)
1	3	0.46	2/1851 (0.1%)	0.79	3/2522 (0.1%)
1	4	0.43	0/1851	0.80	6/2522 (0.2%)
All	All	0.42	2/7404 (0.0%)	0.78	13/10088 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	2	0	2
1	3	0	2
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	3	164	SER	CB-OG	-6.23	1.34	1.42
1	3	158	ARG	C-O	-6.18	1.11	1.23

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	3	158	ARG	CD-NE-CZ	11.34	139.48	123.60
1	2	201	SER	C-N-CD	10.76	151.00	128.40
1	2	202	PRO	CA-N-CD	-6.78	102.00	111.50
1	4	46	LYS	CB-CA-C	-6.61	97.18	110.40
1	4	118	ASN	CB-CA-C	-6.36	97.67	110.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2	163	GLY	Mainchain
1	2	203	ASP	Mainchain
1	3	160	SER	Mainchain
1	3	162	ASN	Mainchain

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	1	1809	0	1755	30	0
1	2	1809	0	1755	35	0
1	3	1809	0	1755	31	1
1	4	1809	0	1755	31	0
2	1	9	0	0	1	0
2	2	15	0	0	4	0
2	3	12	0	0	2	0
2	4	12	0	0	2	0
3	1	2	0	0	0	0
3	2	2	0	0	0	0
3	3	2	0	0	0	0
3	4	2	0	0	0	0
4	1	1	0	0	0	0
4	2	1	0	0	0	0
4	3	1	0	0	0	0
4	4	1	0	0	0	0
5	1	48	0	32	10	0
5	2	36	0	24	13	0
5	3	30	0	20	2	1
5	4	36	0	24	8	1
6	1	214	0	0	2	0
6	2	183	0	0	9	0
6	3	165	0	0	6	1
6	4	202	0	0	2	1
All	All	8210	0	7120	134	3

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 9.

The worst 5 of 134 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)
5:2:809:GOL:O2	6:2:1192:HOH:O	1.67	1.10
1:2:158:ARG:HB3	1:2:166:GLN:HG2	1.46	0.97
1:1:135:LYS:HZ1	1:1:135:LYS:H	1.07	0.94
1:1:135:LYS:H	1:1:135:LYS:NZ	1.73	0.85
1:2:180:HIS:H	5:2:811:GOL:H12	1.46	0.80

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:60:ARG:NH2	1:3:60:ARG:NH2[4_565]	1.68	0.52
5:3:802:GOL:O2	6:4:1149:HOH:O[5_555]	2.17	0.03
5:4:813:GOL:C1	6:3:1147:HOH:O[5_445]	2.18	0.02

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	1	235/237 (99%)	224 (95%)	11 (5%)	0	100	100
1	2	235/237 (99%)	225 (96%)	10 (4%)	0	100	100
1	3	235/237 (99%)	225 (96%)	10 (4%)	0	100	100
1	4	235/237 (99%)	220 (94%)	15 (6%)	0	100	100
All	All	940/948 (99%)	894 (95%)	46 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	1	203/203 (100%)	201 (99%)	2 (1%)	76	76
1	2	203/203 (100%)	196 (97%)	7 (3%)	37	28
1	3	203/203 (100%)	200 (98%)	3 (2%)	65	62
1	4	203/203 (100%)	200 (98%)	3 (2%)	65	62
All	All	812/812 (100%)	797 (98%)	15 (2%)	59	55

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2	166	GLN
1	4	101	LYS
1	2	204	SER
1	4	204	SER
1	3	158	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	4	51	HIS
1	4	118	ASN
1	4	237	ASN
1	4	137	GLN
1	2	83	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 53 ligands modelled in this entry, 12 are monoatomic - leaving 41 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	4	805	-	5,5,5	4.53	5 (100%)	5,5,5	5.77	3 (60%)
5	GOL	4	810	-	5,5,5	4.52	5 (100%)	5,5,5	5.77	3 (60%)
2	AZI	2	908	-	0,2,2	-	-	0,1,1	-	-
2	AZI	1	910	-	0,2,2	-	-	0,1,1	-	-
2	AZI	3	904	-	0,2,2	-	-	0,1,1	-	-
5	GOL	1	821	-	5,5,5	4.53	5 (100%)	5,5,5	5.78	3 (60%)
2	AZI	4	903	-	0,2,2	-	-	0,1,1	-	-
5	GOL	2	814	-	5,5,5	4.53	5 (100%)	5,5,5	3.69	3 (60%)
5	GOL	3	816	-	5,5,5	4.53	5 (100%)	5,5,5	5.77	3 (60%)
5	GOL	2	818	-	5,5,5	4.54	5 (100%)	5,5,5	5.78	3 (60%)
2	AZI	4	906	-	0,2,2	-	-	0,1,1	-	-
5	GOL	1	807	-	5,5,5	4.52	5 (100%)	5,5,5	5.77	3 (60%)
5	GOL	4	813	1	5,5,5	4.53	5 (100%)	5,5,5	5.79	3 (60%)
5	GOL	3	808	-	5,5,5	4.54	5 (100%)	5,5,5	5.77	3 (60%)
2	AZI	2	902	-	0,2,2	-	-	0,1,1	-	-
2	AZI	4	911	-	0,2,2	-	-	0,1,1	-	-
5	GOL	1	804	-	5,5,5	4.53	5 (100%)	5,5,5	5.78	3 (60%)
5	GOL	2	815	-	5,5,5	4.53	5 (100%)	5,5,5	5.78	3 (60%)
5	GOL	1	822	-	5,5,5	4.53	5 (100%)	5,5,5	5.78	3 (60%)
5	GOL	3	802	-	5,5,5	4.54	5 (100%)	5,5,5	5.77	3 (60%)
5	GOL	1	823	-	5,5,5	4.54	5 (100%)	5,5,5	5.78	3 (60%)
2	AZI	3	909	-	0,2,2	-	-	0,1,1	-	-
5	GOL	4	817	-	5,5,5	4.54	5 (100%)	5,5,5	5.78	3 (60%)
2	AZI	3	901	-	0,2,2	-	-	0,1,1	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	GOL	2	811	-	5,5,5	4.52	5 (100%)	5,5,5	5.77	3 (60%)
5	GOL	1	824	-	5,5,5	4.53	5 (100%)	5,5,5	5.78	3 (60%)
5	GOL	4	819	-	5,5,5	4.54	5 (100%)	5,5,5	5.78	3 (60%)
2	AZI	2	905	-	0,2,2	-	-	0,1,1	-	-
2	AZI	4	916	-	0,2,2	-	-	0,1,1	-	-
5	GOL	2	809	-	5,5,5	4.54	5 (100%)	5,5,5	5.78	3 (60%)
5	GOL	4	801	-	5,5,5	4.54	5 (100%)	5,5,5	5.77	3 (60%)
5	GOL	1	812	-	5,5,5	4.53	5 (100%)	5,5,5	5.78	3 (60%)
2	AZI	1	912	-	0,2,2	-	-	0,1,1	-	-
5	GOL	1	806	-	5,5,5	4.53	5 (100%)	5,5,5	5.78	3 (60%)
2	AZI	3	914	-	0,2,2	-	-	0,1,1	-	-
5	GOL	3	803	-	5,5,5	4.53	5 (100%)	5,5,5	5.78	3 (60%)
2	AZI	2	913	-	0,2,2	-	-	0,1,1	-	-
5	GOL	3	825	-	5,5,5	4.53	5 (100%)	5,5,5	5.78	3 (60%)
2	AZI	2	915	-	0,2,2	-	-	0,1,1	-	-
5	GOL	2	820	-	5,5,5	4.53	5 (100%)	5,5,5	5.78	3 (60%)
2	AZI	1	907	-	0,2,2	-	-	0,1,1	-	-

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	4	805	-	-	2/4/4/4	-
5	GOL	4	810	-	-	2/4/4/4	-
5	GOL	1	821	-	-	2/4/4/4	-
5	GOL	2	814	-	-	2/4/4/4	-
5	GOL	3	816	-	-	2/4/4/4	-
5	GOL	2	818	-	-	2/4/4/4	-
5	GOL	1	807	-	-	2/4/4/4	-
5	GOL	4	813	1	-	2/4/4/4	-
5	GOL	3	808	-	-	2/4/4/4	-
5	GOL	1	804	-	-	2/4/4/4	-
5	GOL	2	815	-	-	2/4/4/4	-
5	GOL	1	822	-	-	2/4/4/4	-
5	GOL	3	802	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	1	823	-	-	2/4/4/4	-
5	GOL	4	817	-	-	2/4/4/4	-
5	GOL	2	811	-	-	2/4/4/4	-
5	GOL	1	824	-	-	2/4/4/4	-
5	GOL	4	819	-	-	2/4/4/4	-
5	GOL	2	809	-	-	2/4/4/4	-
5	GOL	4	801	-	-	2/4/4/4	-
5	GOL	1	812	-	-	2/4/4/4	-
5	GOL	1	806	-	-	2/4/4/4	-
5	GOL	3	803	-	-	2/4/4/4	-
5	GOL	3	825	-	-	2/4/4/4	-
5	GOL	2	820	-	-	2/4/4/4	-

The worst 5 of 125 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	2	818	GOL	C3-C2	-7.43	1.21	1.51
5	4	817	GOL	C3-C2	-7.42	1.21	1.51
5	1	823	GOL	C3-C2	-7.42	1.21	1.51
5	3	802	GOL	C3-C2	-7.42	1.21	1.51
5	1	804	GOL	C3-C2	-7.42	1.21	1.51

The worst 5 of 75 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	4	813	GOL	O3-C3-C2	10.48	160.47	110.20
5	2	809	GOL	O3-C3-C2	10.48	160.46	110.20
5	1	824	GOL	O3-C3-C2	10.48	160.45	110.20
5	1	823	GOL	O3-C3-C2	10.48	160.45	110.20
5	1	812	GOL	O3-C3-C2	10.48	160.44	110.20

There are no chirality outliers.

5 of 50 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	1	804	GOL	O1-C1-C2-C3
5	1	804	GOL	C1-C2-C3-O3
5	1	806	GOL	O1-C1-C2-C3
5	1	806	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
5	1	807	GOL	O1-C1-C2-C3

There are no ring outliers.

21 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	4	810	GOL	1	0
2	4	903	AZI	2	0
5	2	814	GOL	3	0
5	1	807	GOL	1	0
5	4	813	GOL	0	1
5	2	815	GOL	2	0
5	1	822	GOL	1	0
5	3	802	GOL	0	1
5	1	823	GOL	4	0
2	3	901	AZI	2	0
5	2	811	GOL	5	0
5	1	824	GOL	2	0
5	4	819	GOL	5	0
5	2	809	GOL	3	0
5	4	801	GOL	2	0
5	1	812	GOL	2	0
2	1	912	AZI	1	0
2	2	913	AZI	2	0
5	3	825	GOL	2	0
2	2	915	AZI	2	0
5	2	820	GOL	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	1	237/237 (100%)	-0.26	8 (3%)	45	48	7, 13, 31, 45	0
1	2	237/237 (100%)	-0.18	6 (2%)	57	60	9, 16, 32, 50	0
1	3	237/237 (100%)	-0.16	5 (2%)	63	66	10, 18, 31, 49	0
1	4	237/237 (100%)	-0.31	5 (2%)	63	66	8, 14, 29, 47	0
All	All	948/948 (100%)	-0.23	24 (2%)	57	60	7, 15, 31, 50	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	2	161	SER	4.4
1	2	162	ASN	4.2
1	1	161	SER	3.8
1	3	162	ASN	3.5
1	4	162	ASN	3.4

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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^{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	B-factors(Å^2)	Q<0.9
2	AZI	3	909	3/3	0.01	0.48	56,56,57,58	0
2	AZI	3	914	3/3	0.29	0.35	45,45,45,47	0
2	AZI	1	912	3/3	0.42	0.31	37,37,40,41	0
2	AZI	4	903	3/3	0.47	0.26	29,29,35,35	0
4	NA	3	1011	1/1	0.53	0.24	35,35,35,35	0
2	AZI	4	916	3/3	0.54	0.31	42,42,43,45	0
2	AZI	2	902	3/3	0.57	0.28	45,45,46,47	0
2	AZI	2	913	3/3	0.64	0.29	35,35,37,38	0
5	GOL	1	823	6/6	0.64	0.36	36,38,40,40	0
5	GOL	2	811	6/6	0.65	0.32	34,36,37,38	0
4	NA	4	1010	1/1	0.66	0.17	34,34,34,34	0
4	NA	2	1009	1/1	0.68	0.19	38,38,38,38	0
5	GOL	2	818	6/6	0.69	0.36	28,31,33,33	0
5	GOL	2	814	6/6	0.70	0.30	29,31,33,34	0
5	GOL	2	820	6/6	0.70	0.33	38,39,39,39	0
5	GOL	4	819	6/6	0.70	0.30	22,27,28,29	0
5	GOL	3	825	6/6	0.71	0.42	45,46,46,46	0
2	AZI	2	915	3/3	0.71	0.31	33,33,34,36	0
2	AZI	4	906	3/3	0.72	0.25	36,36,36,39	0
5	GOL	3	802	6/6	0.73	0.22	30,31,34,34	0
5	GOL	4	810	6/6	0.74	0.21	33,37,39,40	0
2	AZI	2	908	3/3	0.75	0.29	34,34,34,37	0
5	GOL	3	816	6/6	0.76	0.21	37,39,39,42	0
5	GOL	2	809	6/6	0.76	0.33	29,34,35,37	0
5	GOL	3	808	6/6	0.77	0.37	35,39,40,41	0
5	GOL	4	801	6/6	0.77	0.29	29,35,36,37	0
5	GOL	2	815	6/6	0.78	0.32	42,42,43,43	0
5	GOL	1	822	6/6	0.78	0.32	15,28,30,33	0
5	GOL	4	817	6/6	0.79	0.24	43,44,45,45	0
5	GOL	1	812	6/6	0.80	0.23	29,32,34,37	0
5	GOL	4	813	6/6	0.80	0.30	34,37,40,41	0
2	AZI	3	904	3/3	0.81	0.23	43,43,44,44	0
2	AZI	1	907	3/3	0.83	0.20	31,31,34,35	0
2	AZI	4	911	3/3	0.84	0.27	31,31,34,34	0
5	GOL	1	804	6/6	0.84	0.20	34,34,35,35	0
5	GOL	1	807	6/6	0.84	0.19	16,19,23,28	0
5	GOL	1	806	6/6	0.85	0.32	30,32,33,33	0
5	GOL	1	821	6/6	0.85	0.27	33,36,36,36	0
5	GOL	1	824	6/6	0.85	0.35	40,42,43,43	0
5	GOL	3	803	6/6	0.86	0.13	28,28,30,30	0
5	GOL	4	805	6/6	0.86	0.17	16,19,21,21	0
2	AZI	3	901	3/3	0.87	0.32	38,38,39,41	0
2	AZI	2	905	3/3	0.88	0.20	35,35,37,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	AZI	1	910	3/3	0.88	0.18	33,33,35,36	0
4	NA	1	1012	1/1	0.90	0.16	30,30,30,30	0
3	MN	3	1005	1/1	0.92	0.11	24,24,24,24	0
3	MN	4	1007	1/1	0.98	0.07	18,18,18,18	0
3	MN	2	1004	1/1	0.99	0.05	12,12,12,12	0
3	MN	3	1006	1/1	0.99	0.05	15,15,15,15	0
3	MN	2	1003	1/1	1.00	0.03	18,18,18,18	0
3	MN	1	1001	1/1	1.00	0.02	16,16,16,16	0
3	MN	4	1008	1/1	1.00	0.04	11,11,11,11	0
3	MN	1	1002	1/1	1.00	0.05	10,10,10,10	0

6.5 Other polymers (i)

There are no such residues in this entry.