



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 06:00 am BST

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 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

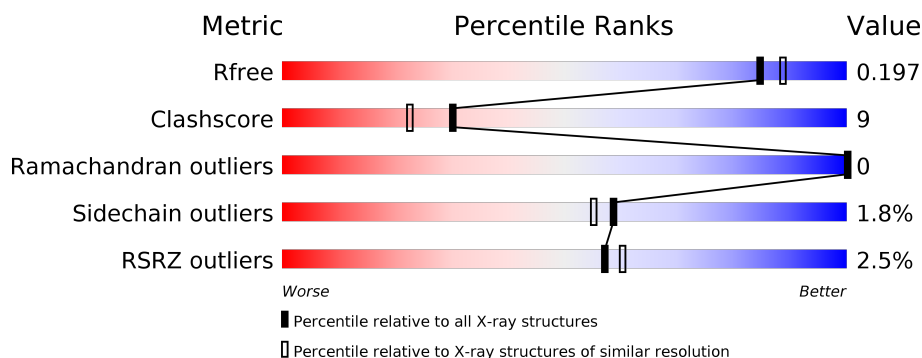
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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 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	1	237	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>12%</div> </div> <div>.</div> </div>
1	2	237	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>18%</div> </div> <div>.</div> </div>
1	3	237	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>19%</div> </div> <div>.</div> </div>
1	4	237	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>14%</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 crite-

ria:

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

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.

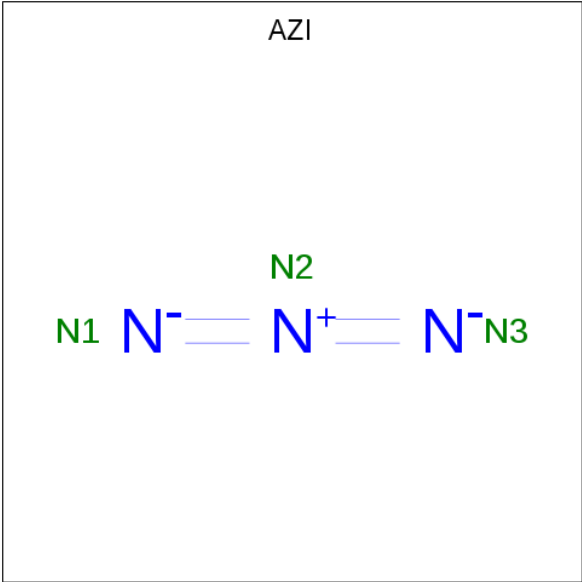
- Molecule 1 is a protein called concanavalin A.

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: N₃).



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	0	0
			3	3		
2	4	1	Total	N	0	0
			3	3		

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

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

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

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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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

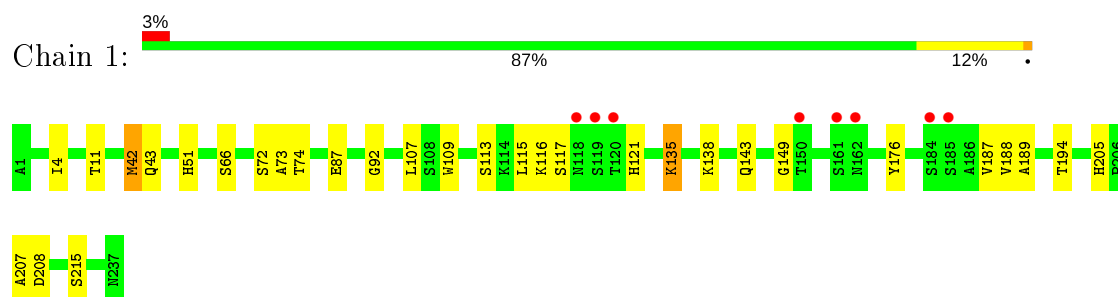
- Molecule 6 is water.

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

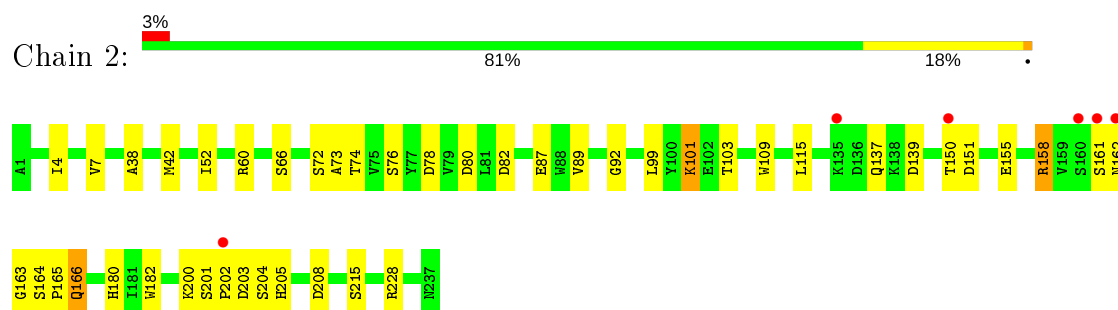
3 Residue-property plots [i](#)

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.

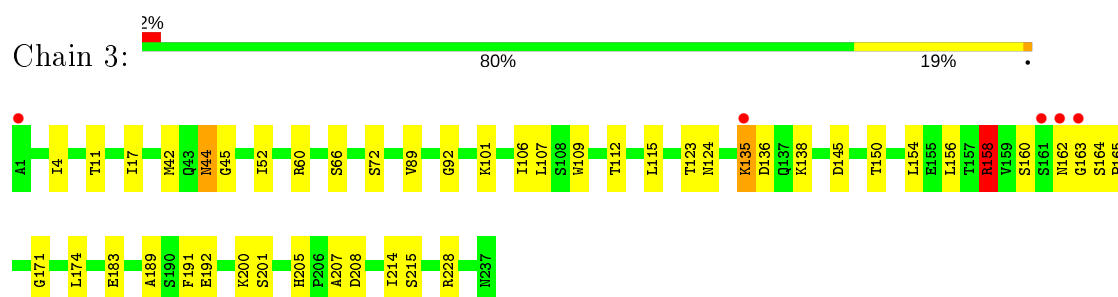
• Molecule 1: concanavalin A



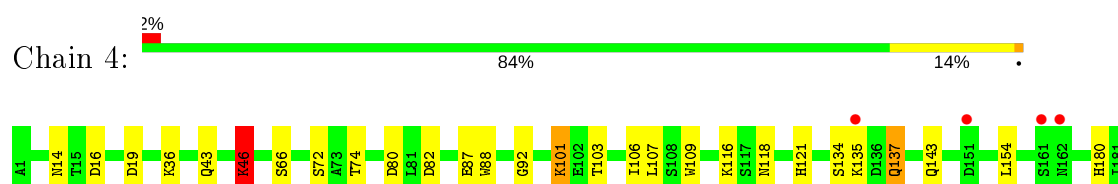
• Molecule 1: concanavalin A



• Molecule 1: concanavalin A



• Molecule 1: concanavalin A





4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	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.*

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: 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

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	101	LYS	O-C-N	-5.83	113.36	122.70
1	3	163	GLY	O-C-N	5.76	131.91	122.70
1	4	135	LYS	N-CA-CB	5.61	120.69	110.60
1	4	137	GLN	CA-CB-CG	5.55	125.61	113.40
1	2	74	THR	O-C-N	-5.48	113.93	122.70
1	4	204	SER	CB-CA-C	5.45	120.46	110.10
1	2	201	SER	N-CA-CB	5.22	118.33	110.50
1	3	163	GLY	CA-C-N	-5.12	105.94	117.20

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 ⓘ

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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:H	1:1:135:LYS:HZ1	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
1:3:44:ASN:HD21	1:3:201:SER:H	1.28	0.79
1:1:194:THR:HG23	2:1:912:AZI:N3	1.98	0.79
1:2:38:ALA:HB1	5:2:809:GOL:H12	1.64	0.78
1:1:135:LYS:N	1:1:135:LYS:HZ1	1.82	0.77
1:1:74:THR:HG22	5:1:823:GOL:C3	2.16	0.76
1:2:200:LYS:HE2	2:2:915:AZI:N1	2.00	0.76
2:3:901:AZI:N1	6:3:1175:HOH:O	2.19	0.73
1:1:138:LYS:HA	5:1:824:GOL:H12	1.71	0.72
1:3:192:GLU:HG3	2:3:901:AZI:N1	2.05	0.72
5:2:820:GOL:O2	6:2:1132:HOH:O	2.07	0.71
1:3:158:ARG:NH1	6:3:1142:HOH:O	2.22	0.71
1:4:43:GLN:HB3	1:4:46:LYS:HG3	1.72	0.70
1:2:158:ARG:HD2	6:2:1173:HOH:O	1.91	0.70
1:3:135:LYS:HD2	1:3:136:ASP:N	2.07	0.68
1:3:138:LYS:HA	5:3:825:GOL:H12	1.75	0.68
1:2:87:GLU:OE1	6:2:1183:HOH:O	2.12	0.68
1:2:150:THR:CG2	6:2:1136:HOH:O	2.42	0.67
1:2:60:ARG:HD2	1:2:76:SER:HB3	1.75	0.67
1:1:42:MET:HE2	1:1:43:GLN:N	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:180:HIS:H	5:2:811:GOL:C1	2.10	0.64
1:4:134:SER:H	1:4:137:GLN:HE21	1.46	0.64
1:4:234:PRO:HG3	5:4:801:GOL:H11	1.80	0.63
1:1:113:SER:OG	5:1:812:GOL:H12	1.99	0.62
1:2:158:ARG:CD	6:2:1173:HOH:O	2.49	0.60
1:1:74:THR:HG22	5:1:823:GOL:C2	2.31	0.60
1:1:11:THR:O	1:1:205:HIS:HE1	1.85	0.60
1:2:150:THR:HG23	6:2:1136:HOH:O	2.01	0.59
1:1:42:MET:HG2	6:1:1069:HOH:O	2.02	0.59
1:1:73:ALA:HA	5:1:823:GOL:H12	1.86	0.58
1:4:143:GLN:HB3	5:4:819:GOL:C2	2.34	0.57
1:3:115:LEU:HD12	1:3:189:ALA:HB2	1.87	0.57
1:3:44:ASN:ND2	1:3:200:LYS:HA	2.20	0.57
1:2:73:ALA:HA	5:2:809:GOL:H11	1.86	0.56
1:4:200:LYS:HE2	6:4:1124:HOH:O	2.05	0.56
5:2:814:GOL:O2	5:2:815:GOL:H11	2.04	0.56
1:2:87:GLU:HG3	1:2:182:TRP:O	2.05	0.56
5:1:812:GOL:C3	2:2:913:AZI:N3	2.70	0.55
1:4:218:ASP:O	2:4:903:AZI:N1	2.40	0.55
1:2:137:GLN:NE2	2:2:913:AZI:N2	2.55	0.55
1:4:116:LYS:HE3	1:4:121:HIS:O	2.07	0.54
1:1:107:LEU:HD12	1:1:107:LEU:N	2.22	0.54
1:4:143:GLN:CD	5:4:819:GOL:H12	2.28	0.54
1:2:115:LEU:HD13	5:2:811:GOL:O3	2.08	0.54
1:4:143:GLN:NE2	5:4:819:GOL:H12	2.23	0.53
1:1:115:LEU:HD12	1:1:189:ALA:HB2	1.89	0.53
1:4:134:SER:H	1:4:137:GLN:NE2	2.04	0.53
1:4:143:GLN:CG	5:4:819:GOL:H12	2.38	0.53
5:3:825:GOL:C1	6:3:1125:HOH:O	2.56	0.52
1:2:205:HIS:HD2	6:2:1068:HOH:O	1.93	0.52
1:4:88:TRP:HB3	1:4:217:ILE:HD11	1.92	0.52
1:3:150:THR:HB	6:3:1153:HOH:O	2.10	0.51
1:2:103:THR:OG1	1:2:200:LYS:HG2	2.11	0.51
1:2:180:HIS:N	5:2:811:GOL:H12	2.21	0.51
1:3:66:SER:HB3	1:3:72:SER:CB	2.41	0.51
1:4:234:PRO:CG	5:4:801:GOL:H11	2.41	0.50
1:3:89:VAL:HB	1:3:215:SER:O	2.11	0.50
1:4:92:GLY:HA2	1:4:109:TRP:CH2	2.46	0.50
1:2:208:ASP:OD1	5:2:814:GOL:O3	2.20	0.50
1:1:143:GLN:HB3	5:1:822:GOL:C2	2.41	0.50
1:1:66:SER:HB3	1:1:72:SER:CB	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:66:SER:HB3	1:4:72:SER:CB	2.40	0.49
1:1:87:GLU:OE1	6:1:1223:HOH:O	2.20	0.49
1:4:87:GLU:HG2	1:4:180:HIS:CD2	2.47	0.49
5:2:811:GOL:O1	6:2:1024:HOH:O	1.85	0.49
1:3:92:GLY:HA2	1:3:109:TRP:CH2	2.47	0.49
1:2:155:GLU:OE2	2:2:915:AZI:N3	2.45	0.49
1:1:135:LYS:H	1:1:135:LYS:CE	2.25	0.49
1:2:92:GLY:HA2	1:2:109:TRP:CH2	2.49	0.48
1:3:115:LEU:HD21	1:3:183:GLU:HB2	1.95	0.48
1:2:66:SER:HB3	1:2:72:SER:CB	2.44	0.48
1:2:80:ASP:OD1	1:2:82:ASP:HB2	2.15	0.47
1:3:44:ASN:HD22	1:3:45:GLY:N	2.12	0.47
1:4:87:GLU:HG2	1:4:180:HIS:NE2	2.29	0.47
1:1:51:HIS:CD2	1:1:194:THR:HG22	2.50	0.47
1:2:228:ARG:HB3	5:2:814:GOL:O1	2.14	0.47
1:1:92:GLY:HA2	1:1:109:TRP:CH2	2.49	0.47
1:4:87:GLU:HG2	1:4:180:HIS:HE2	1.80	0.47
1:1:208:ASP:OD2	5:1:807:GOL:O2	2.33	0.47
1:3:11:THR:O	1:3:205:HIS:HE1	1.98	0.47
1:2:99:LEU:HB3	5:2:815:GOL:O2	2.15	0.46
1:3:44:ASN:ND2	1:3:201:SER:H	2.06	0.46
1:4:80:ASP:OD1	1:4:82:ASP:HB2	2.16	0.46
1:2:87:GLU:HG2	1:2:180:HIS:CD2	2.50	0.46
1:3:107:LEU:HD12	1:3:107:LEU:N	2.31	0.46
1:4:16:ASP:HB3	5:4:810:GOL:O3	2.16	0.45
1:2:101:LYS:N	1:2:101:LYS:HD3	2.32	0.45
1:4:103:THR:OG1	1:4:200:LYS:HG2	2.17	0.45
1:3:207:ALA:HA	1:3:208:ASP:HA	1.79	0.45
1:3:112:THR:O	1:3:191:PHE:HA	2.16	0.45
1:3:106:ILE:HB	1:3:154:LEU:HB3	1.98	0.45
1:3:4:ILE:HD13	1:3:215:SER:HB3	1.98	0.45
1:3:17:ILE:HD13	1:3:228:ARG:HD2	1.99	0.44
1:2:4:ILE:HD13	1:2:215:SER:HB3	2.00	0.44
1:1:187:VAL:HG22	1:1:188:VAL:HG23	2.00	0.44
1:1:51:HIS:HD2	1:1:194:THR:HG22	1.82	0.44
1:2:89:VAL:HB	1:2:215:SER:O	2.17	0.44
1:4:187:VAL:HG13	1:4:188:VAL:HG23	1.98	0.44
1:4:87:GLU:HG3	1:4:182:TRP:O	2.18	0.44
1:1:207:ALA:HA	1:1:208:ASP:HA	1.81	0.44
1:4:74:THR:HG22	6:4:1168:HOH:O	2.17	0.44
1:3:52:ILE:O	1:3:192:GLU:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:89:VAL:HG21	1:3:214:ILE:CG2	2.48	0.43
1:3:174:LEU:HD12	1:3:174:LEU:N	2.33	0.43
1:1:4:ILE:HD13	1:1:215:SER:HB3	2.01	0.43
1:2:60:ARG:HD3	1:2:78:ASP:OD1	2.18	0.43
1:3:145:ASP:HB3	1:3:158:ARG:HG2	2.01	0.43
1:1:117:SER:O	1:1:121:HIS:HA	2.18	0.42
1:3:101:LYS:HD2	1:3:165:PRO:O	2.19	0.42
1:4:36:LYS:HB2	1:4:36:LYS:HE2	1.91	0.42
1:2:7:VAL:HG21	1:2:52:ILE:HG12	2.02	0.42
1:4:106:ILE:HB	1:4:154:LEU:HB3	2.01	0.42
1:4:14:ASN:O	1:4:19:ASP:HB2	2.19	0.42
1:1:135:LYS:HG3	1:1:149:GLY:HA3	2.01	0.42
1:3:115:LEU:HD23	6:3:1071:HOH:O	2.20	0.42
1:1:116:LYS:HE3	1:1:187:VAL:CG1	2.50	0.42
1:4:43:GLN:CB	1:4:46:LYS:HG3	2.48	0.42
1:2:87:GLU:HG2	1:2:180:HIS:NE2	2.35	0.41
1:3:123:THR:HG22	1:3:124:ASN:N	2.34	0.41
1:3:44:ASN:HD21	1:3:201:SER:N	2.06	0.41
1:3:42:MET:HG2	6:3:1026:HOH:O	2.21	0.41
1:4:143:GLN:HG2	5:4:819:GOL:H12	2.01	0.41
1:4:107:LEU:N	1:4:107:LEU:HD12	2.35	0.41
1:1:176:TYR:HE2	5:1:824:GOL:C3	2.34	0.41
1:4:220:SER:OG	2:4:903:AZI:N2	2.53	0.41
1:2:150:THR:O	1:2:151:ASP:HB2	2.21	0.41
1:2:164:SER:HA	1:2:165:PRO:HD2	1.77	0.40
1:2:137:GLN:HG3	1:2:139:ASP:OD1	2.21	0.40
1:1:74:THR:HG22	5:1:823:GOL:C1	2.51	0.40
1:3:156:LEU:O	1:3:171:GLY:HA3	2.22	0.40

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

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	42	MET
1	1	135	LYS

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Mol	Chain	Res	Type
1	2	42	MET
1	2	101	LYS
1	2	158	ARG
1	2	161	SER
1	2	162	ASN
1	2	166	GLN
1	2	204	SER
1	3	44	ASN
1	3	135	LYS
1	3	158	ARG
1	4	46	LYS
1	4	101	LYS
1	4	204	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	51	HIS
1	1	83	ASN
1	1	237	ASN
1	2	44	ASN
1	2	51	HIS
1	2	69	ASN
1	2	83	ASN
1	2	118	ASN
1	2	205	HIS
1	2	237	ASN
1	3	44	ASN
1	3	69	ASN
1	3	83	ASN
1	3	237	ASN
1	4	51	HIS
1	4	69	ASN
1	4	83	ASN
1	4	118	ASN
1	4	137	GLN
1	4	237	ASN

5.3.3 RNA ⓘ

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 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	817	-	5,5,5	4.54	5 (100%)	5,5,5	5.78	3 (60%)
2	AZI	4	916	-	0,2,2	0.00	-	0,1,1	0.00	-
2	AZI	4	903	-	0,2,2	0.00	-	0,1,1	0.00	-
2	AZI	4	906	-	0,2,2	0.00	-	0,1,1	0.00	-
2	AZI	4	911	-	0,2,2	0.00	-	0,1,1	0.00	-
5	GOL	3	808	-	5,5,5	4.54	5 (100%)	5,5,5	5.77	3 (60%)
2	AZI	2	915	-	0,2,2	0.00	-	0,1,1	0.00	-
5	GOL	4	819	-	5,5,5	4.54	5 (100%)	5,5,5	5.78	3 (60%)
5	GOL	2	814	-	5,5,5	4.53	5 (100%)	5,5,5	3.69	3 (60%)
5	GOL	2	818	-	5,5,5	4.54	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	804	-	5,5,5	4.53	5 (100%)	5,5,5	5.78	3 (60%)
5	GOL	3	803	-	5,5,5	4.53	5 (100%)	5,5,5	5.78	3 (60%)
5	GOL	4	805	-	5,5,5	4.53	5 (100%)	5,5,5	5.77	3 (60%)
5	GOL	4	801	-	5,5,5	4.54	5 (100%)	5,5,5	5.77	3 (60%)
5	GOL	2	811	-	5,5,5	4.52	5 (100%)	5,5,5	5.77	3 (60%)
2	AZI	2	902	-	0,2,2	0.00	-	0,1,1	0.00	-
5	GOL	2	815	-	5,5,5	4.53	5 (100%)	5,5,5	5.78	3 (60%)
5	GOL	3	816	-	5,5,5	4.53	5 (100%)	5,5,5	5.77	3 (60%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	1	821	-	5,5,5	4.53	5 (100%)	5,5,5	5.78	3 (60%)
5	GOL	1	806	-	5,5,5	4.53	5 (100%)	5,5,5	5.78	3 (60%)
2	AZI	3	904	-	0,2,2	0.00	-	0,1,1	0.00	-
5	GOL	4	813	1	5,5,5	4.53	5 (100%)	5,5,5	5.79	3 (60%)
2	AZI	3	901	-	0,2,2	0.00	-	0,1,1	0.00	-
5	GOL	1	807	-	5,5,5	4.52	5 (100%)	5,5,5	5.77	3 (60%)
2	AZI	2	913	-	0,2,2	0.00	-	0,1,1	0.00	-
5	GOL	1	824	-	5,5,5	4.53	5 (100%)	5,5,5	5.78	3 (60%)
5	GOL	2	809	-	5,5,5	4.54	5 (100%)	5,5,5	5.78	3 (60%)
5	GOL	1	812	-	5,5,5	4.53	5 (100%)	5,5,5	5.78	3 (60%)
2	AZI	2	908	-	0,2,2	0.00	-	0,1,1	0.00	-
2	AZI	2	905	-	0,2,2	0.00	-	0,1,1	0.00	-
5	GOL	1	823	-	5,5,5	4.54	5 (100%)	5,5,5	5.78	3 (60%)
2	AZI	1	907	-	0,2,2	0.00	-	0,1,1	0.00	-
2	AZI	3	909	-	0,2,2	0.00	-	0,1,1	0.00	-
5	GOL	1	822	-	5,5,5	4.53	5 (100%)	5,5,5	5.78	3 (60%)
5	GOL	3	825	-	5,5,5	4.53	5 (100%)	5,5,5	5.78	3 (60%)
2	AZI	3	914	-	0,2,2	0.00	-	0,1,1	0.00	-
5	GOL	2	820	-	5,5,5	4.53	5 (100%)	5,5,5	5.78	3 (60%)
2	AZI	1	910	-	0,2,2	0.00	-	0,1,1	0.00	-
2	AZI	1	912	-	0,2,2	0.00	-	0,1,1	0.00	-
5	GOL	4	810	-	5,5,5	4.52	5 (100%)	5,5,5	5.77	3 (60%)

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	817	-	-	2/4/4/4	-
5	GOL	3	808	-	-	2/4/4/4	-
5	GOL	3	816	-	-	2/4/4/4	-
5	GOL	2	814	-	-	2/4/4/4	-
5	GOL	2	818	-	-	2/4/4/4	-
5	GOL	1	822	-	-	2/4/4/4	-
5	GOL	3	803	-	-	2/4/4/4	-
5	GOL	4	805	-	-	2/4/4/4	-
5	GOL	4	801	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	2	811	-	-	2/4/4/4	-
5	GOL	2	815	-	-	2/4/4/4	-
5	GOL	1	821	-	-	2/4/4/4	-
5	GOL	4	813	1	-	2/4/4/4	-
5	GOL	1	807	-	-	2/4/4/4	-
5	GOL	1	824	-	-	2/4/4/4	-
5	GOL	1	812	-	-	2/4/4/4	-
5	GOL	4	819	-	-	2/4/4/4	-
5	GOL	1	823	-	-	2/4/4/4	-
5	GOL	4	810	-	-	2/4/4/4	-
5	GOL	2	809	-	-	2/4/4/4	-
5	GOL	1	804	-	-	2/4/4/4	-
5	GOL	3	825	-	-	2/4/4/4	-
5	GOL	3	802	-	-	2/4/4/4	-
5	GOL	2	820	-	-	2/4/4/4	-
5	GOL	1	806	-	-	2/4/4/4	-

All (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
5	3	825	GOL	C3-C2	-7.42	1.21	1.51
5	4	813	GOL	C3-C2	-7.41	1.21	1.51
5	4	819	GOL	C3-C2	-7.41	1.21	1.51
5	4	805	GOL	C3-C2	-7.41	1.21	1.51
5	1	822	GOL	C3-C2	-7.41	1.21	1.51
5	2	820	GOL	C3-C2	-7.41	1.21	1.51
5	3	808	GOL	C3-C2	-7.40	1.21	1.51
5	2	809	GOL	C3-C2	-7.40	1.21	1.51
5	2	814	GOL	C3-C2	-7.40	1.21	1.51
5	3	816	GOL	C3-C2	-7.40	1.21	1.51
5	3	803	GOL	C3-C2	-7.40	1.21	1.51
5	4	801	GOL	C3-C2	-7.40	1.21	1.51
5	1	824	GOL	C3-C2	-7.40	1.21	1.51
5	1	821	GOL	C3-C2	-7.40	1.21	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	1	812	GOL	C3-C2	-7.40	1.21	1.51
5	4	810	GOL	C3-C2	-7.39	1.21	1.51
5	2	815	GOL	C3-C2	-7.39	1.21	1.51
5	1	807	GOL	C3-C2	-7.39	1.21	1.51
5	1	806	GOL	C3-C2	-7.38	1.21	1.51
5	2	811	GOL	C3-C2	-7.38	1.21	1.51
5	2	809	GOL	O1-C1	4.53	1.61	1.42
5	3	808	GOL	O1-C1	4.53	1.61	1.42
5	3	803	GOL	O1-C1	4.53	1.61	1.42
5	1	822	GOL	O1-C1	4.52	1.61	1.42
5	4	801	GOL	O1-C1	4.52	1.61	1.42
5	4	819	GOL	O1-C1	4.52	1.61	1.42
5	2	820	GOL	O1-C1	4.52	1.61	1.42
5	1	823	GOL	O1-C1	4.52	1.61	1.42
5	2	815	GOL	O1-C1	4.52	1.61	1.42
5	3	825	GOL	O1-C1	4.51	1.61	1.42
5	1	806	GOL	O1-C1	4.51	1.61	1.42
5	1	812	GOL	O1-C1	4.51	1.61	1.42
5	1	824	GOL	O1-C1	4.51	1.61	1.42
5	1	807	GOL	O1-C1	4.51	1.61	1.42
5	3	816	GOL	O1-C1	4.51	1.61	1.42
5	4	805	GOL	O1-C1	4.51	1.61	1.42
5	1	804	GOL	O1-C1	4.51	1.61	1.42
5	2	814	GOL	O1-C1	4.50	1.61	1.42
5	4	810	GOL	O1-C1	4.50	1.61	1.42
5	2	818	GOL	O1-C1	4.50	1.61	1.42
5	2	811	GOL	O1-C1	4.50	1.61	1.42
5	3	802	GOL	O1-C1	4.50	1.61	1.42
5	1	821	GOL	O1-C1	4.50	1.61	1.42
5	4	813	GOL	O1-C1	4.50	1.61	1.42
5	4	817	GOL	O1-C1	4.49	1.61	1.42
5	4	817	GOL	O3-C3	3.43	1.56	1.42
5	1	823	GOL	O3-C3	3.42	1.56	1.42
5	4	813	GOL	O3-C3	3.41	1.56	1.42
5	3	802	GOL	O3-C3	3.41	1.56	1.42
5	2	818	GOL	O3-C3	3.41	1.56	1.42
5	2	809	GOL	O3-C3	3.40	1.56	1.42
5	1	824	GOL	O3-C3	3.40	1.56	1.42
5	2	814	GOL	O3-C3	3.40	1.56	1.42
5	4	805	GOL	O3-C3	3.40	1.56	1.42
5	4	819	GOL	O3-C3	3.40	1.56	1.42
5	3	808	GOL	O3-C3	3.40	1.56	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	3	825	GOL	O3-C3	3.40	1.56	1.42
5	1	822	GOL	O3-C3	3.40	1.56	1.42
5	1	812	GOL	O3-C3	3.40	1.56	1.42
5	4	801	GOL	O3-C3	3.40	1.56	1.42
5	3	816	GOL	O3-C3	3.40	1.56	1.42
5	1	821	GOL	O3-C3	3.40	1.56	1.42
5	1	804	GOL	O3-C3	3.40	1.56	1.42
5	3	803	GOL	O3-C3	3.39	1.56	1.42
5	4	810	GOL	O3-C3	3.39	1.56	1.42
5	2	815	GOL	O3-C3	3.39	1.56	1.42
5	1	806	GOL	O3-C3	3.38	1.56	1.42
5	2	811	GOL	O3-C3	3.38	1.56	1.42
5	1	807	GOL	O3-C3	3.37	1.56	1.42
5	2	820	GOL	O3-C3	3.37	1.56	1.42
5	3	808	GOL	C1-C2	-2.86	1.39	1.51
5	1	806	GOL	O2-C2	-2.85	1.34	1.43
5	4	801	GOL	C1-C2	-2.85	1.40	1.51
5	2	809	GOL	C1-C2	-2.85	1.40	1.51
5	1	824	GOL	O2-C2	-2.85	1.34	1.43
5	1	821	GOL	C1-C2	-2.85	1.40	1.51
5	2	820	GOL	C1-C2	-2.85	1.40	1.51
5	1	812	GOL	O2-C2	-2.85	1.34	1.43
5	4	805	GOL	C1-C2	-2.84	1.40	1.51
5	3	802	GOL	O2-C2	-2.84	1.34	1.43
5	3	802	GOL	C1-C2	-2.84	1.40	1.51
5	3	808	GOL	O2-C2	-2.84	1.34	1.43
5	2	815	GOL	O2-C2	-2.84	1.34	1.43
5	4	801	GOL	O2-C2	-2.84	1.34	1.43
5	4	819	GOL	O2-C2	-2.84	1.34	1.43
5	1	807	GOL	C1-C2	-2.84	1.40	1.51
5	1	823	GOL	C1-C2	-2.84	1.40	1.51
5	3	803	GOL	C1-C2	-2.83	1.40	1.51
5	1	822	GOL	O2-C2	-2.83	1.34	1.43
5	1	806	GOL	C1-C2	-2.83	1.40	1.51
5	4	817	GOL	C1-C2	-2.83	1.40	1.51
5	2	811	GOL	C1-C2	-2.83	1.40	1.51
5	3	816	GOL	O2-C2	-2.83	1.34	1.43
5	1	807	GOL	O2-C2	-2.83	1.34	1.43
5	1	821	GOL	O2-C2	-2.82	1.35	1.43
5	2	814	GOL	C1-C2	-2.82	1.40	1.51
5	4	813	GOL	O2-C2	-2.82	1.35	1.43
5	2	815	GOL	C1-C2	-2.82	1.40	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	3	803	GOL	O2-C2	-2.82	1.35	1.43
5	2	818	GOL	C1-C2	-2.82	1.40	1.51
5	3	816	GOL	C1-C2	-2.82	1.40	1.51
5	1	812	GOL	C1-C2	-2.82	1.40	1.51
5	1	824	GOL	C1-C2	-2.82	1.40	1.51
5	4	810	GOL	C1-C2	-2.82	1.40	1.51
5	4	813	GOL	C1-C2	-2.82	1.40	1.51
5	1	804	GOL	C1-C2	-2.82	1.40	1.51
5	2	811	GOL	O2-C2	-2.81	1.35	1.43
5	1	804	GOL	O2-C2	-2.81	1.35	1.43
5	3	825	GOL	O2-C2	-2.81	1.35	1.43
5	4	810	GOL	O2-C2	-2.81	1.35	1.43
5	4	817	GOL	O2-C2	-2.81	1.35	1.43
5	4	805	GOL	O2-C2	-2.81	1.35	1.43
5	3	825	GOL	C1-C2	-2.81	1.40	1.51
5	4	819	GOL	C1-C2	-2.81	1.40	1.51
5	2	820	GOL	O2-C2	-2.81	1.35	1.43
5	2	818	GOL	O2-C2	-2.81	1.35	1.43
5	1	822	GOL	C1-C2	-2.80	1.40	1.51
5	2	809	GOL	O2-C2	-2.80	1.35	1.43
5	2	814	GOL	O2-C2	-2.80	1.35	1.43
5	1	823	GOL	O2-C2	-2.78	1.35	1.43

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
5	1	806	GOL	O3-C3-C2	10.48	160.43	110.20
5	1	821	GOL	O3-C3-C2	10.48	160.43	110.20
5	3	803	GOL	O3-C3-C2	10.48	160.43	110.20
5	2	820	GOL	O3-C3-C2	10.47	160.42	110.20
5	3	802	GOL	O3-C3-C2	10.47	160.41	110.20
5	2	818	GOL	O3-C3-C2	10.47	160.41	110.20
5	1	804	GOL	O3-C3-C2	10.47	160.41	110.20
5	1	822	GOL	O3-C3-C2	10.47	160.41	110.20
5	4	817	GOL	O3-C3-C2	10.47	160.41	110.20
5	1	807	GOL	O3-C3-C2	10.47	160.41	110.20
5	3	825	GOL	O3-C3-C2	10.47	160.40	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	2	815	GOL	O3-C3-C2	10.47	160.40	110.20
5	3	816	GOL	O3-C3-C2	10.47	160.40	110.20
5	4	819	GOL	O3-C3-C2	10.47	160.39	110.20
5	4	801	GOL	O3-C3-C2	10.47	160.38	110.20
5	4	810	GOL	O3-C3-C2	10.46	160.37	110.20
5	3	808	GOL	O3-C3-C2	10.46	160.34	110.20
5	4	805	GOL	O3-C3-C2	10.46	160.34	110.20
5	2	811	GOL	O3-C3-C2	10.46	160.33	110.20
5	4	813	GOL	O2-C2-C3	6.81	139.10	109.12
5	1	812	GOL	O2-C2-C3	6.80	139.08	109.12
5	2	809	GOL	O2-C2-C3	6.80	139.07	109.12
5	1	824	GOL	O2-C2-C3	6.80	139.06	109.12
5	1	806	GOL	O2-C2-C3	6.80	139.06	109.12
5	1	823	GOL	O2-C2-C3	6.80	139.05	109.12
5	1	822	GOL	O2-C2-C3	6.79	139.05	109.12
5	2	820	GOL	O2-C2-C3	6.79	139.05	109.12
5	2	815	GOL	O2-C2-C3	6.79	139.04	109.12
5	4	819	GOL	O2-C2-C3	6.79	139.04	109.12
5	3	803	GOL	O2-C2-C3	6.79	139.04	109.12
5	2	818	GOL	O2-C2-C3	6.79	139.04	109.12
5	3	825	GOL	O2-C2-C3	6.79	139.03	109.12
5	1	804	GOL	O2-C2-C3	6.79	139.02	109.12
5	4	817	GOL	O2-C2-C3	6.79	139.02	109.12
5	1	807	GOL	O2-C2-C3	6.79	139.01	109.12
5	3	816	GOL	O2-C2-C3	6.79	139.01	109.12
5	4	801	GOL	O2-C2-C3	6.79	139.01	109.12
5	4	810	GOL	O2-C2-C3	6.78	139.00	109.12
5	1	821	GOL	O2-C2-C3	6.78	139.00	109.12
5	2	814	GOL	O2-C2-C3	6.78	138.98	109.12
5	3	802	GOL	O2-C2-C3	6.78	138.97	109.12
5	3	808	GOL	O2-C2-C3	6.77	138.96	109.12
5	2	811	GOL	O2-C2-C3	6.77	138.94	109.12
5	4	805	GOL	O2-C2-C3	6.77	138.94	109.12
5	2	814	GOL	O3-C3-C2	3.35	126.26	110.20
5	4	813	GOL	O1-C1-C2	3.25	125.80	110.20
5	2	818	GOL	O1-C1-C2	3.25	125.78	110.20
5	1	821	GOL	O1-C1-C2	3.24	125.74	110.20
5	2	811	GOL	O1-C1-C2	3.24	125.74	110.20
5	2	820	GOL	O1-C1-C2	3.24	125.74	110.20
5	4	819	GOL	O1-C1-C2	3.24	125.73	110.20
5	2	814	GOL	O1-C1-C2	3.24	125.73	110.20
5	3	825	GOL	O1-C1-C2	3.24	125.73	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	4	805	GOL	O1-C1-C2	3.24	125.72	110.20
5	3	808	GOL	O1-C1-C2	3.24	125.72	110.20
5	3	816	GOL	O1-C1-C2	3.24	125.72	110.20
5	1	824	GOL	O1-C1-C2	3.24	125.72	110.20
5	4	801	GOL	O1-C1-C2	3.24	125.72	110.20
5	2	815	GOL	O1-C1-C2	3.24	125.72	110.20
5	1	812	GOL	O1-C1-C2	3.24	125.71	110.20
5	1	823	GOL	O1-C1-C2	3.23	125.71	110.20
5	4	817	GOL	O1-C1-C2	3.23	125.71	110.20
5	3	803	GOL	O1-C1-C2	3.23	125.70	110.20
5	1	807	GOL	O1-C1-C2	3.23	125.69	110.20
5	1	822	GOL	O1-C1-C2	3.23	125.68	110.20
5	1	806	GOL	O1-C1-C2	3.23	125.68	110.20
5	2	809	GOL	O1-C1-C2	3.23	125.68	110.20
5	3	802	GOL	O1-C1-C2	3.23	125.68	110.20
5	1	804	GOL	O1-C1-C2	3.23	125.67	110.20
5	4	810	GOL	O1-C1-C2	3.23	125.67	110.20

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	4	817	GOL	O1-C1-C2-C3
5	4	817	GOL	C1-C2-C3-O3
5	3	808	GOL	O1-C1-C2-C3
5	3	808	GOL	C1-C2-C3-O3
5	3	802	GOL	O1-C1-C2-C3
5	3	802	GOL	C1-C2-C3-O3
5	2	814	GOL	O1-C1-C2-C3
5	2	818	GOL	O1-C1-C2-C3
5	2	818	GOL	C1-C2-C3-O3
5	3	803	GOL	O1-C1-C2-C3
5	3	803	GOL	C1-C2-C3-O3
5	4	805	GOL	O1-C1-C2-C3
5	4	805	GOL	C1-C2-C3-O3
5	4	801	GOL	O1-C1-C2-C3
5	4	801	GOL	C1-C2-C3-O3
5	2	811	GOL	O1-C1-C2-C3
5	2	811	GOL	C1-C2-C3-O3
5	2	815	GOL	O1-C1-C2-C3
5	2	815	GOL	C1-C2-C3-O3
5	1	822	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
5	1	822	GOL	C1-C2-C3-O3
5	3	816	GOL	O1-C1-C2-C3
5	3	816	GOL	C1-C2-C3-O3
5	1	821	GOL	O1-C1-C2-C3
5	1	821	GOL	C1-C2-C3-O3
5	4	813	GOL	O1-C1-C2-C3
5	4	813	GOL	C1-C2-C3-O3
5	1	807	GOL	O1-C1-C2-C3
5	1	807	GOL	C1-C2-C3-O3
5	4	819	GOL	O1-C1-C2-C3
5	4	819	GOL	C1-C2-C3-O3
5	1	824	GOL	O1-C1-C2-C3
5	1	824	GOL	C1-C2-C3-O3
5	2	809	GOL	O1-C1-C2-C3
5	2	809	GOL	C1-C2-C3-O3
5	1	812	GOL	O1-C1-C2-C3
5	1	812	GOL	C1-C2-C3-O3
5	1	823	GOL	O1-C1-C2-C3
5	1	823	GOL	C1-C2-C3-O3
5	1	806	GOL	O1-C1-C2-C3
5	1	806	GOL	C1-C2-C3-O3
5	1	804	GOL	O1-C1-C2-C3
5	1	804	GOL	C1-C2-C3-O3
5	3	825	GOL	O1-C1-C2-C3
5	3	825	GOL	C1-C2-C3-O3
5	2	820	GOL	O1-C1-C2-C3
5	2	820	GOL	C1-C2-C3-O3
5	4	810	GOL	O1-C1-C2-C3
5	4	810	GOL	C1-C2-C3-O3
5	2	814	GOL	C1-C2-C3-O3

There are no ring outliers.

21 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	4	903	AZI	2	0
2	2	915	AZI	2	0
5	4	819	GOL	5	0
5	2	814	GOL	3	0
5	3	802	GOL	0	1
5	4	801	GOL	2	0
5	2	811	GOL	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	2	815	GOL	2	0
5	4	813	GOL	0	1
2	3	901	AZI	2	0
5	1	807	GOL	1	0
2	2	913	AZI	2	0
5	1	824	GOL	2	0
5	2	809	GOL	3	0
5	1	812	GOL	2	0
5	1	823	GOL	4	0
5	1	822	GOL	1	0
5	3	825	GOL	2	0
5	2	820	GOL	1	0
2	1	912	AZI	1	0
5	4	810	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 ⓘ

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, 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	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

All (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
1	3	161	SER	3.3
1	2	202	PRO	3.3
1	4	161	SER	3.2
1	1	162	ASN	3.2
1	1	184	SER	2.9
1	4	135	LYS	2.7
1	3	163	GLY	2.7
1	2	160	SER	2.7
1	3	1	ALA	2.6
1	3	135	LYS	2.5
1	1	150	THR	2.4
1	2	135	LYS	2.3
1	1	185	SER	2.2
1	1	120	THR	2.2
1	1	118	ASN	2.1
1	4	184	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	4	151	ASP	2.0
1	1	119	SER	2.0
1	2	150	THR	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. 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(\AA^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	4	819	6/6	0.70	0.30	22,27,28,29	0
5	GOL	2	820	6/6	0.70	0.33	38,39,39,39	0
2	AZI	2	915	3/3	0.71	0.31	33,33,34,36	0
5	GOL	3	825	6/6	0.71	0.42	45,46,46,46	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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
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	4	801	6/6	0.77	0.29	29,35,36,37	0
5	GOL	3	808	6/6	0.77	0.37	35,39,40,41	0
5	GOL	1	822	6/6	0.78	0.32	15,28,30,33	0
5	GOL	2	815	6/6	0.78	0.32	42,42,43,43	0
5	GOL	4	817	6/6	0.79	0.24	43,44,45,45	0
5	GOL	4	813	6/6	0.80	0.30	34,37,40,41	0
5	GOL	1	812	6/6	0.80	0.23	29,32,34,37	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
5	GOL	1	804	6/6	0.84	0.20	34,34,35,35	0
2	AZI	4	911	3/3	0.84	0.27	31,31,34,34	0
5	GOL	1	807	6/6	0.84	0.19	16,19,23,28	0
5	GOL	1	821	6/6	0.85	0.27	33,36,36,36	0
5	GOL	1	806	6/6	0.85	0.32	30,32,33,33	0
5	GOL	1	824	6/6	0.85	0.35	40,42,43,43	0
5	GOL	4	805	6/6	0.86	0.17	16,19,21,21	0
5	GOL	3	803	6/6	0.86	0.13	28,28,30,30	0
2	AZI	3	901	3/3	0.87	0.32	38,38,39,41	0
2	AZI	1	910	3/3	0.88	0.18	33,33,35,36	0
2	AZI	2	905	3/3	0.88	0.20	35,35,37,38	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	1	1002	1/1	1.00	0.05	10,10,10,10	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	2	1003	1/1	1.00	0.03	18,18,18,18	0

6.5 Other polymers ⓘ

There are no such residues in this entry.