



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2017 – 03:37 PM EDT

PDB ID : 3D4K
Title : Concanavalin A Complexed to a Synthetic Analog of the Trimannoside
Authors : Kadirvelraj, R.; Foley, B.L.; Dyekjaer, J.D.; Woods, R.J.
Deposited on : unknown
Resolution : 1.80 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

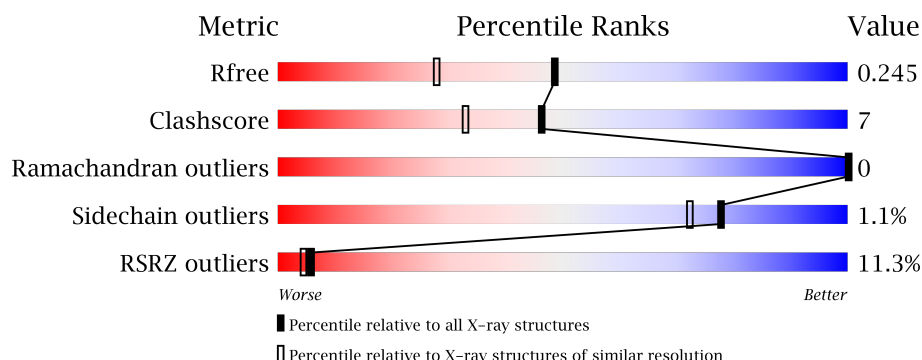
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	4827 (1.80-1.80)
Clashscore	112137	5742 (1.80-1.80)
Ramachandran outliers	110173	5676 (1.80-1.80)
Sidechain outliers	110143	5675 (1.80-1.80)
RSRZ outliers	101464	4906 (1.80-1.80)

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. 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	237	<div> <div>12%</div> <div>86%</div> <div>14%</div> </div>
1	B	237	<div> <div>11%</div> <div>86%</div> <div>14%</div> </div>
1	C	237	<div> <div>10%</div> <div>84%</div> <div>15%</div> </div>
1	D	237	<div> <div>12%</div> <div>86%</div> <div>14%</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
5	H1M	C	241	-	-	-	X
6	GOL	D	900	-	-	-	X

2 Entry composition [i](#)

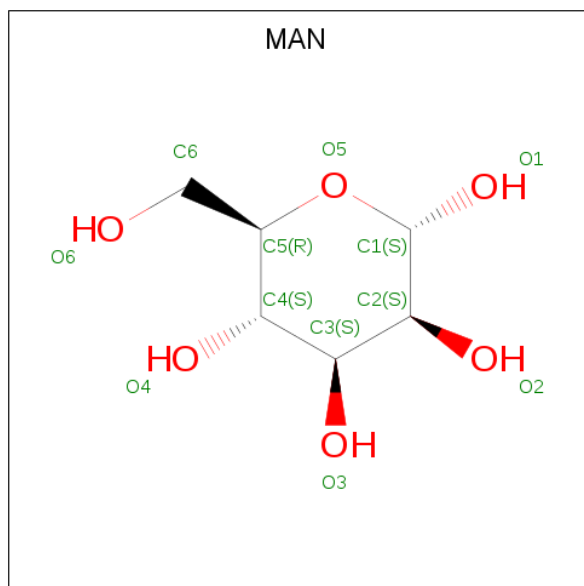
There are 7 unique types of molecules in this entry. The entry contains 7988 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	A	237	Total	C	N	O	S	0	0	0
			1809	1141	302	364	2			
1	B	237	Total	C	N	O	S	0	0	0
			1809	1141	302	364	2			
1	C	237	Total	C	N	O	S	0	0	0
			1809	1141	302	364	2			
1	D	237	Total	C	N	O	S	0	0	0
			1809	1141	302	364	2			

- Molecule 2 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			11	6	5		
2	A	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			11	6	5		
2	B	1	Total	C	O	0	0
			11	6	5		
2	C	1	Total	C	O	0	0
			11	6	5		
2	C	1	Total	C	O	0	0
			11	6	5		
2	D	1	Total	C	O	0	0
			11	6	5		
2	D	1	Total	C	O	0	0
			11	6	5		

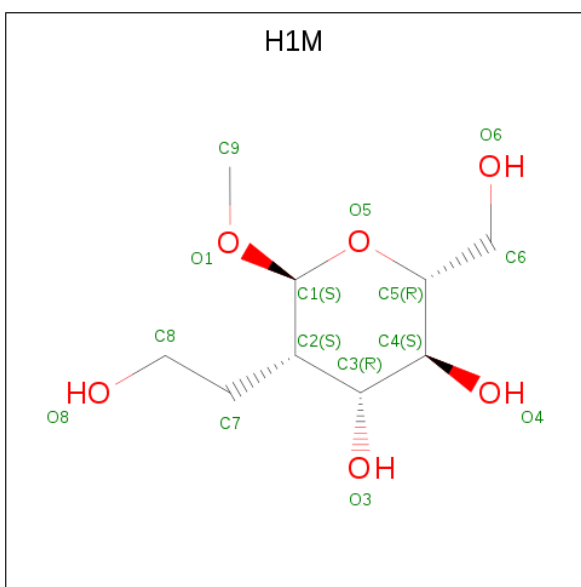
- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mn	0	0
			1	1		
3	A	1	Total	Mn	0	0
			1	1		
3	D	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	A	1	Total	Ca	0	0
			1	1		
4	D	1	Total	Ca	0	0
			1	1		
4	C	1	Total	Ca	0	0
			1	1		

- Molecule 5 is methyl 2-deoxy-2-(2-hydroxyethyl)-alpha-D-mannopyranoside (three-letter code: H1M) (formula: C₉H₁₈O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			15	9	6		
5	B	1	Total	C	O	0	0
			15	9	6		
5	C	1	Total	C	O	0	0
			15	9	6		
5	D	1	Total	C	O	0	0
			15	9	6		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

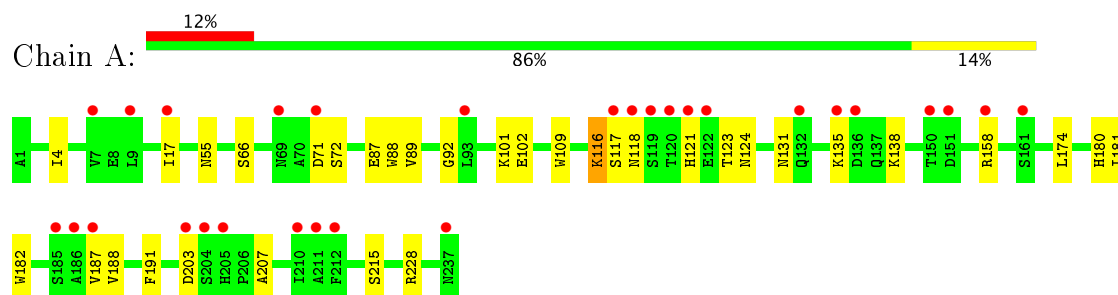
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	145	Total	O	0	0
			145	145		
7	B	144	Total	O	0	0
			144	144		
7	C	134	Total	O	0	0
			134	134		
7	D	149	Total	O	0	0
			149	149		

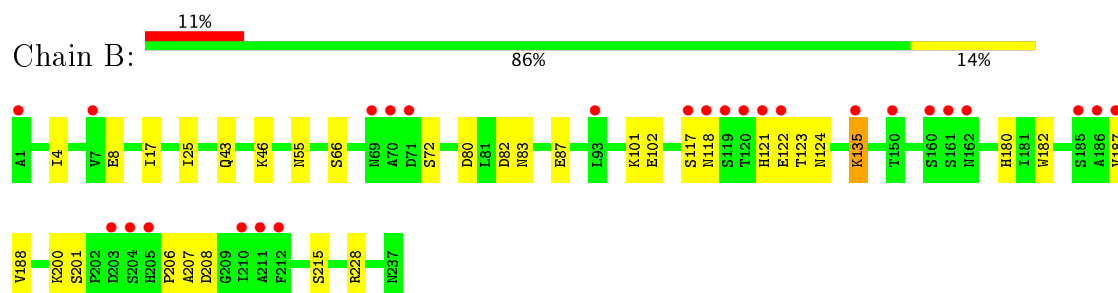
3 Residue-property plots [i](#)

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.

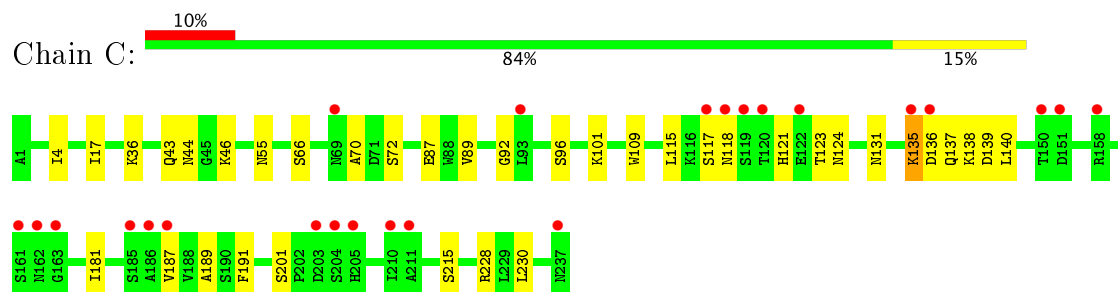
• Molecule 1: Concanavalin-A



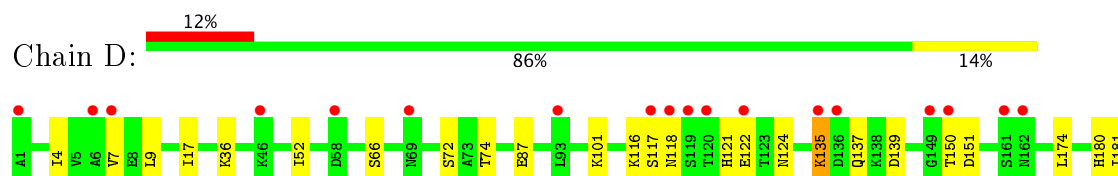
• Molecule 1: Concanavalin-A

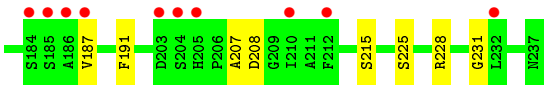


• Molecule 1: Concanavalin-A



• Molecule 1: Concanavalin-A





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.02Å 63.55Å 126.22Å 90.00° 86.91° 90.00°	Depositor
Resolution (Å)	30.00 – 1.80 29.96 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.0 (30.00-1.80) 99.0 (29.96-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.94 (at 1.80Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.205 , 0.238 0.212 , 0.245	Depositor DCC
R_{free} test set	8749 reflections (10.02%)	DCC
Wilson B-factor (Å ²)	19.1	Xtriage
Anisotropy	0.528	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 53.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7988	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.16% 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, CA, MN, H1M, MAN

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	0.33	0/1851	0.69	0/2522
1	B	0.33	0/1851	0.69	0/2522
1	C	0.32	0/1851	0.69	0/2522
1	D	0.34	0/1851	0.70	1/2522 (0.0%)
All	All	0.33	0/7404	0.69	1/10088 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	9	LEU	N-CA-C	-5.21	96.93	111.00

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	1809	0	1755	28	0
1	B	1809	0	1755	23	0
1	C	1809	0	1755	30	0
1	D	1809	0	1755	26	0
2	A	22	0	20	0	0
2	B	22	0	20	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	22	0	20	0	0
2	D	22	0	20	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	15	0	16	0	0
5	B	15	0	16	0	0
5	C	15	0	16	0	0
5	D	15	0	16	0	0
6	A	6	0	8	2	0
6	B	6	0	8	2	0
6	C	6	0	8	0	0
6	D	6	0	8	3	0
7	A	145	0	0	3	0
7	B	144	0	0	3	0
7	C	134	0	0	5	0
7	D	149	0	0	5	0
All	All	7988	0	7196	105	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 (105) 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:B:118:ASN:HA	1:B:187:VAL:HG23	1.65	0.77
1:D:4:ILE:HD13	1:D:215:SER:HB3	1.66	0.76
1:D:74:THR:HG23	7:D:487:HOH:O	1.88	0.73
1:D:118:ASN:HA	1:D:187:VAL:HG23	1.72	0.71
1:A:135:LYS:H	1:A:135:LYS:HD3	1.57	0.68
1:D:116:LYS:HD2	1:D:121:HIS:C	2.14	0.67
1:C:43:GLN:HE21	1:C:46:LYS:HD3	1.59	0.66
1:C:118:ASN:HA	1:C:187:VAL:HG23	1.77	0.66
1:A:17:ILE:HD13	1:A:228:ARG:HD2	1.79	0.64
1:C:135:LYS:HD3	1:C:136:ASP:H	1.64	0.63
1:A:118:ASN:HA	1:A:187:VAL:HG23	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ASN:HB3	6:A:900:GOL:H12	1.82	0.60
1:D:116:LYS:HD2	1:D:121:HIS:O	2.02	0.60
1:C:118:ASN:HA	1:C:187:VAL:CG2	2.32	0.60
1:D:87:GLU:HG2	7:D:400:HOH:O	2.02	0.58
1:A:116:LYS:HG3	1:A:123:THR:OG1	2.04	0.58
1:C:17:ILE:HD13	1:C:228:ARG:HD2	1.84	0.57
1:C:55:ASN:HB3	7:C:734:HOH:O	2.03	0.57
1:B:17:ILE:HD13	1:B:228:ARG:HD2	1.86	0.57
1:B:66:SER:HB3	1:B:72:SER:CB	2.36	0.56
1:A:87:GLU:HG3	1:A:182:TRP:O	2.05	0.56
1:C:43:GLN:NE2	1:C:46:LYS:HD3	2.21	0.55
1:B:4:ILE:HD13	1:B:215:SER:HB3	1.89	0.55
1:D:135:LYS:H	1:D:135:LYS:HD3	1.72	0.54
1:B:123:THR:HG22	7:B:465:HOH:O	2.06	0.54
1:C:66:SER:HB3	1:C:72:SER:HB3	1.89	0.54
1:B:55:ASN:HB3	7:B:801:HOH:O	2.07	0.53
1:A:135:LYS:N	1:A:135:LYS:HD3	2.24	0.53
1:B:124:ASN:HB3	6:B:900:GOL:H12	1.90	0.53
1:D:180:HIS:HB3	6:D:900:GOL:H11	1.90	0.53
1:D:17:ILE:HD13	1:D:228:ARG:HD2	1.92	0.52
1:C:87:GLU:HG2	7:C:583:HOH:O	2.09	0.52
1:A:180:HIS:HB3	6:A:900:GOL:H2	1.92	0.52
1:A:117:SER:O	1:A:121:HIS:HA	2.10	0.51
1:A:4:ILE:HD13	1:A:215:SER:HB3	1.91	0.51
1:D:150:THR:HG22	1:D:151:ASP:OD2	2.10	0.51
1:C:181:ILE:HD11	1:C:191:PHE:CD2	2.46	0.51
1:C:117:SER:O	1:C:121:HIS:HA	2.11	0.51
1:D:135:LYS:N	1:D:135:LYS:HD3	2.25	0.51
1:B:187:VAL:HG12	1:B:188:VAL:HG23	1.93	0.50
1:A:118:ASN:HA	1:A:187:VAL:CG2	2.42	0.50
1:B:180:HIS:HB3	6:B:900:GOL:H2	1.95	0.49
1:C:43:GLN:HE22	1:C:46:LYS:NZ	2.10	0.48
1:D:118:ASN:HA	1:D:187:VAL:CG2	2.43	0.48
1:D:36:LYS:HD2	7:D:395:HOH:O	2.14	0.48
1:A:92:GLY:HA2	1:A:109:TRP:CH2	2.48	0.48
1:D:66:SER:HB3	1:D:72:SER:HB3	1.95	0.48
1:C:4:ILE:HD13	1:C:215:SER:HB3	1.95	0.48
1:B:118:ASN:HA	1:B:187:VAL:CG2	2.39	0.47
1:D:124:ASN:HB3	6:D:900:GOL:H32	1.96	0.47
1:C:189:ALA:CB	7:C:459:HOH:O	2.61	0.47
1:A:187:VAL:HG12	1:A:188:VAL:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:GLU:HG2	1:A:207:ALA:O	2.15	0.47
1:C:66:SER:HB3	1:C:72:SER:CB	2.44	0.46
1:A:131:ASN:HB3	1:D:122:GLU:HB3	1.97	0.46
1:D:66:SER:HB3	1:D:72:SER:CB	2.46	0.46
1:B:200:LYS:NZ	1:B:200:LYS:HB3	2.31	0.45
1:D:87:GLU:H	1:D:87:GLU:CD	2.20	0.45
1:C:92:GLY:HA2	1:C:109:TRP:CH2	2.52	0.45
1:A:135:LYS:H	1:A:135:LYS:CD	2.27	0.45
1:D:181:ILE:HD11	1:D:191:PHE:CD2	2.51	0.45
1:B:80:ASP:OD1	1:B:82:ASP:HB2	2.17	0.44
1:D:137:GLN:HG3	1:D:139:ASP:OD1	2.18	0.44
1:A:203:ASP:HB3	7:A:691:HOH:O	2.16	0.44
1:A:89:VAL:HB	1:A:215:SER:O	2.17	0.44
1:C:36:LYS:HE3	7:C:641:HOH:O	2.17	0.44
1:A:55:ASN:HB3	7:A:666:HOH:O	2.16	0.44
1:C:70:ALA:HB2	7:C:745:HOH:O	2.18	0.44
1:B:135:LYS:N	1:B:135:LYS:HD3	2.33	0.43
1:C:135:LYS:HD3	1:C:135:LYS:N	2.33	0.43
1:A:87:GLU:HG2	1:A:180:HIS:CD2	2.53	0.43
1:C:135:LYS:HD3	1:C:136:ASP:N	2.30	0.43
1:C:87:GLU:H	1:C:87:GLU:HG2	1.59	0.43
1:C:115:LEU:HD23	1:C:189:ALA:HB2	2.00	0.43
1:A:66:SER:HB3	1:A:72:SER:HB3	2.00	0.43
1:C:89:VAL:HB	1:C:215:SER:O	2.19	0.43
1:B:43:GLN:HE21	1:B:46:LYS:HG3	1.83	0.43
1:A:158:ARG:HD2	7:A:786:HOH:O	2.19	0.43
1:B:117:SER:O	1:B:121:HIS:HA	2.19	0.42
1:A:174:LEU:N	1:A:174:LEU:HD12	2.34	0.42
1:B:102:GLU:HG2	1:B:207:ALA:O	2.19	0.42
1:C:44:ASN:HD21	1:C:201:SER:HB3	1.84	0.42
1:C:137:GLN:HG2	1:C:140:LEU:HD12	2.01	0.42
1:B:87:GLU:HG3	1:B:182:TRP:O	2.18	0.42
1:B:207:ALA:HA	1:B:208:ASP:HA	1.87	0.42
1:B:8:GLU:O	1:B:25:ILE:HA	2.19	0.42
1:B:122:GLU:HB3	1:C:131:ASN:HB3	2.00	0.42
1:A:181:ILE:HD11	1:A:191:PHE:CD2	2.55	0.42
1:D:174:LEU:N	1:D:174:LEU:HD12	2.34	0.42
1:D:7:VAL:HG21	1:D:52:ILE:HG12	2.01	0.42
1:D:207:ALA:HA	1:D:208:ASP:HA	1.90	0.42
1:A:88:TRP:HH2	1:D:137:GLN:NE2	2.17	0.42
1:A:138:LYS:HE3	7:D:766:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:SER:HB3	1:B:72:SER:HB3	2.01	0.41
1:C:137:GLN:HG3	1:C:139:ASP:OD1	2.20	0.41
1:A:87:GLU:HG2	1:A:180:HIS:NE2	2.34	0.41
6:D:900:GOL:H31	7:D:509:HOH:O	2.19	0.41
1:D:117:SER:O	1:D:121:HIS:HA	2.21	0.41
7:B:714:HOH:O	1:C:138:LYS:HE3	2.21	0.41
1:C:96:SER:OG	1:C:230:LEU:HA	2.21	0.41
1:B:201:SER:HB3	1:B:206:PRO:HB3	2.02	0.41
1:C:123:THR:HG22	1:C:124:ASN:N	2.36	0.41
1:A:66:SER:HB3	1:A:72:SER:CB	2.50	0.40
1:B:83:ASN:N	1:B:83:ASN:ND2	2.70	0.40
1:D:225:SER:OG	1:D:231:GLY:HA2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	235/237 (99%)	220 (94%)	15 (6%)	0	100	100
1	B	235/237 (99%)	223 (95%)	12 (5%)	0	100	100
1	C	235/237 (99%)	219 (93%)	16 (7%)	0	100	100
1	D	235/237 (99%)	222 (94%)	13 (6%)	0	100	100
All	All	940/948 (99%)	884 (94%)	56 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	203/203 (100%)	200 (98%)	3 (2%)	70	61
1	B	203/203 (100%)	201 (99%)	2 (1%)	80	75
1	C	203/203 (100%)	201 (99%)	2 (1%)	80	75
1	D	203/203 (100%)	201 (99%)	2 (1%)	80	75
All	All	812/812 (100%)	803 (99%)	9 (1%)	78	72

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

Mol	Chain	Res	Type
1	A	71	ASP
1	A	101	LYS
1	A	116	LYS
1	B	101	LYS
1	B	135	LYS
1	C	101	LYS
1	C	135	LYS
1	D	101	LYS
1	D	135	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	HIS
1	A	237	ASN
1	B	43	GLN
1	B	51	HIS
1	B	69	ASN
1	B	83	ASN
1	B	166	GLN
1	C	43	GLN
1	C	51	HIS
1	C	121	HIS
1	C	237	ASN
1	D	43	GLN
1	D	237	ASN

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 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	MAN	A	240	5	11,11,12	0.50	0	13,15,17	0.74	0
5	H1M	A	241	2	15,15,15	0.69	0	14,20,20	1.05	1 (7%)
2	MAN	A	242	5	11,11,12	0.44	0	13,15,17	0.76	0
6	GOL	A	900	-	5,5,5	0.28	0	5,5,5	0.26	0
2	MAN	B	240	5	11,11,12	0.46	0	13,15,17	0.74	0
5	H1M	B	241	2	15,15,15	0.76	0	14,20,20	1.09	1 (7%)
2	MAN	B	242	5	11,11,12	0.54	0	13,15,17	0.78	0
6	GOL	B	900	-	5,5,5	0.31	0	5,5,5	0.27	0
2	MAN	C	240	5	11,11,12	0.53	0	13,15,17	0.73	0
5	H1M	C	241	2	15,15,15	0.77	0	14,20,20	0.99	1 (7%)
2	MAN	C	242	5	11,11,12	0.47	0	13,15,17	0.78	0
6	GOL	C	900	-	5,5,5	0.39	0	5,5,5	0.21	0
2	MAN	D	240	5	11,11,12	0.48	0	13,15,17	0.77	0
5	H1M	D	241	2	15,15,15	0.78	0	14,20,20	1.11	1 (7%)
2	MAN	D	242	5	11,11,12	0.52	0	13,15,17	0.75	0
6	GOL	D	900	-	5,5,5	0.31	0	5,5,5	0.29	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	A	240	5	-	0/2/19/22	0/1/1/1
5	H1M	A	241	2	-	0/7/27/27	0/1/1/1
2	MAN	A	242	5	-	0/2/19/22	0/1/1/1
6	GOL	A	900	-	-	0/4/4/4	0/0/0/0
2	MAN	B	240	5	-	0/2/19/22	0/1/1/1
5	H1M	B	241	2	-	0/7/27/27	0/1/1/1
2	MAN	B	242	5	-	0/2/19/22	0/1/1/1
6	GOL	B	900	-	-	0/4/4/4	0/0/0/0
2	MAN	C	240	5	-	0/2/19/22	0/1/1/1
5	H1M	C	241	2	-	0/7/27/27	0/1/1/1
2	MAN	C	242	5	-	0/2/19/22	0/1/1/1
6	GOL	C	900	-	-	0/4/4/4	0/0/0/0
2	MAN	D	240	5	-	0/2/19/22	0/1/1/1
5	H1M	D	241	2	-	0/7/27/27	0/1/1/1
2	MAN	D	242	5	-	0/2/19/22	0/1/1/1
6	GOL	D	900	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	241	H1M	C9-O1-C1	2.65	117.42	113.29
5	B	241	H1M	C9-O1-C1	2.78	117.63	113.29
5	A	241	H1M	C9-O1-C1	2.79	117.65	113.29
5	D	241	H1M	C9-O1-C1	2.85	117.74	113.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	900	GOL	2	0
6	B	900	GOL	2	0
6	D	900	GOL	3	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, 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	237/237 (100%)	0.58	29 (12%) 5 4	12, 21, 42, 53	0
1	B	237/237 (100%)	0.54	26 (10%) 6 5	12, 21, 40, 46	0
1	C	237/237 (100%)	0.63	24 (10%) 8 6	12, 22, 42, 53	0
1	D	237/237 (100%)	0.61	28 (11%) 5 4	11, 21, 42, 51	0
All	All	948/948 (100%)	0.59	107 (11%) 6 4	11, 21, 42, 53	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	119	SER	5.5
1	B	186	ALA	5.4
1	C	205	HIS	5.2
1	A	118	ASN	5.1
1	B	205	HIS	5.0
1	D	119	SER	5.0
1	C	118	ASN	5.0
1	A	119	SER	5.0
1	D	118	ASN	4.8
1	C	186	ALA	4.7
1	D	120	THR	4.7
1	D	150	THR	4.5
1	D	205	HIS	4.5
1	A	185	SER	4.5
1	B	119	SER	4.5
1	A	120	THR	4.4
1	C	117	SER	4.3
1	A	205	HIS	4.3
1	B	204	SER	4.2
1	C	151	ASP	4.1
1	C	150	THR	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	135	LYS	4.1
1	D	186	ALA	4.0
1	B	118	ASN	3.9
1	B	120	THR	3.8
1	A	210	ILE	3.7
1	D	185	SER	3.7
1	A	117	SER	3.7
1	D	204	SER	3.7
1	C	120	THR	3.7
1	C	185	SER	3.6
1	B	69	ASN	3.5
1	B	161	SER	3.4
1	B	185	SER	3.4
1	C	161	SER	3.4
1	D	187	VAL	3.3
1	B	162	ASN	3.3
1	C	237	ASN	3.3
1	A	161	SER	3.2
1	B	210	ILE	3.2
1	A	136	ASP	3.2
1	C	162	ASN	3.2
1	B	150	THR	3.1
1	A	151	ASP	3.1
1	D	69	ASN	3.1
1	A	204	SER	3.1
1	A	121	HIS	3.0
1	A	187	VAL	3.0
1	C	163	GLY	3.0
1	B	117	SER	3.0
1	D	122	GLU	3.0
1	D	162	ASN	3.0
1	C	135	LYS	2.9
1	B	187	VAL	2.9
1	A	203	ASP	2.9
1	A	135	LYS	2.8
1	B	122	GLU	2.8
1	A	17	ILE	2.8
1	C	210	ILE	2.8
1	C	203	ASP	2.8
1	A	69	ASN	2.8
1	A	186	ALA	2.7
1	C	69	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	158	ARG	2.7
1	D	203	ASP	2.7
1	B	70	ALA	2.7
1	D	117	SER	2.7
1	D	149	GLY	2.7
1	C	211	ALA	2.6
1	B	212	PHE	2.5
1	C	158	ARG	2.5
1	A	71	ASP	2.5
1	A	93	LEU	2.5
1	B	203	ASP	2.5
1	D	58	ASP	2.5
1	D	46	LYS	2.4
1	C	204	SER	2.4
1	A	212	PHE	2.4
1	D	184	SER	2.4
1	A	150	THR	2.4
1	B	93	LEU	2.4
1	A	122	GLU	2.3
1	C	93	LEU	2.3
1	D	210	ILE	2.3
1	C	136	ASP	2.3
1	C	187	VAL	2.3
1	B	160	SER	2.3
1	A	237	ASN	2.3
1	A	7	VAL	2.3
1	D	7	VAL	2.3
1	A	211	ALA	2.3
1	B	211	ALA	2.2
1	B	121	HIS	2.2
1	B	71	ASP	2.2
1	D	136	ASP	2.2
1	C	122	GLU	2.2
1	D	161	SER	2.2
1	D	93	LEU	2.2
1	B	1	ALA	2.2
1	B	7	VAL	2.2
1	D	135	LYS	2.1
1	D	212	PHE	2.1
1	A	9	LEU	2.1
1	D	6	ALA	2.1
1	A	132	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	1	ALA	2.0
1	D	232	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
6	GOL	D	900	6/6	0.80	0.18	3.21	29,32,34,37	0
5	H1M	C	241	15/15	0.84	0.17	2.06	29,37,41,42	0
6	GOL	C	900	6/6	0.88	0.14	1.13	25,31,32,35	0
6	GOL	A	900	6/6	0.82	0.15	1.07	29,32,34,34	0
6	GOL	B	900	6/6	0.82	0.13	0.33	26,29,32,32	0
2	MAN	C	242	11/12	0.81	0.17	0.03	36,38,41,43	0
5	H1M	B	241	15/15	0.89	0.11	-0.30	22,28,30,31	0
2	MAN	B	240	11/12	0.96	0.08	-0.60	18,20,21,22	0
2	MAN	C	240	11/12	0.90	0.09	-0.75	23,25,26,26	0
2	MAN	A	240	11/12	0.94	0.09	-1.10	18,24,25,26	0
2	MAN	D	240	11/12	0.95	0.08	-1.58	17,19,19,20	0
3	MN	B	238	1/1	0.98	0.07	-1.93	18,18,18,18	0
4	CA	C	239	1/1	0.98	0.07	-2.12	20,20,20,20	0
4	CA	A	239	1/1	0.98	0.06	-2.41	20,20,20,20	0
4	CA	B	239	1/1	0.98	0.07	-2.73	18,18,18,18	0
3	MN	A	238	1/1	0.98	0.06	-2.76	18,18,18,18	0
3	MN	D	238	1/1	0.99	0.07	-2.93	16,16,16,16	0
4	CA	D	239	1/1	0.99	0.06	-3.10	17,17,17,17	0
3	MN	C	238	1/1	0.97	0.06	-3.14	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	H1M	D	241	15/15	0.92	0.09	-	21,28,30,31	0
5	H1M	A	241	15/15	0.88	0.17	-	28,36,38,38	0
2	MAN	D	242	11/12	0.91	0.12	-	29,30,32,34	0
2	MAN	B	242	11/12	0.88	0.16	-	28,30,33,37	0
2	MAN	A	242	11/12	0.82	0.18	-	38,39,40,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.