



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 24, 2024 – 09:56 AM EST

PDB ID : 5CNA  
Title : REFINED STRUCTURE OF CONCAVALIN A COMPLEXED WITH A LPHA-METHYL-D-MANNOPYRANOSIDE AT 2.0 ANGSTROMS RESOLUTION AND COMPARISON WITH THE SACCHARIDE-FREE STRUCTURE  
Authors : Naismith, J.H.; Emmerich, C.; Habash, J.; Harrop, S.J.; Helliwell, J.R.; Hunter, W.N.; Raftery, J.; Kalb(Gilboa), A.J.; Yariv, J.  
Deposited on : 1994-02-11  
Resolution : 2.00 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

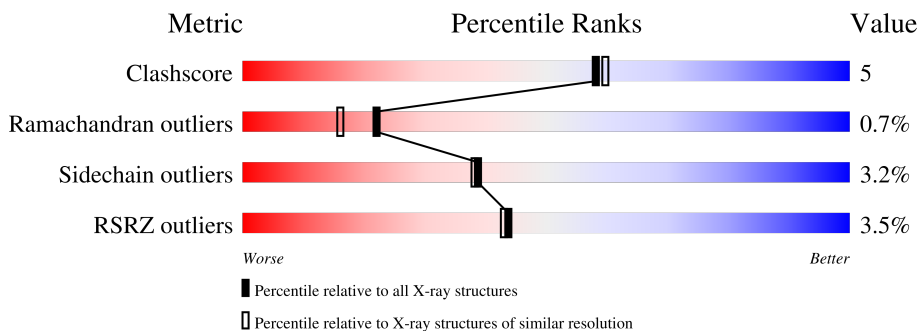
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

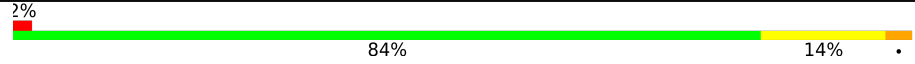


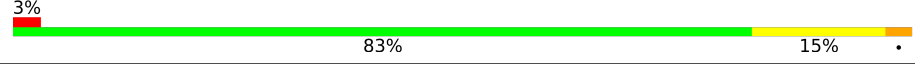
The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	237	
1	B	237	
1	C	237	
1	D	237	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7830 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.

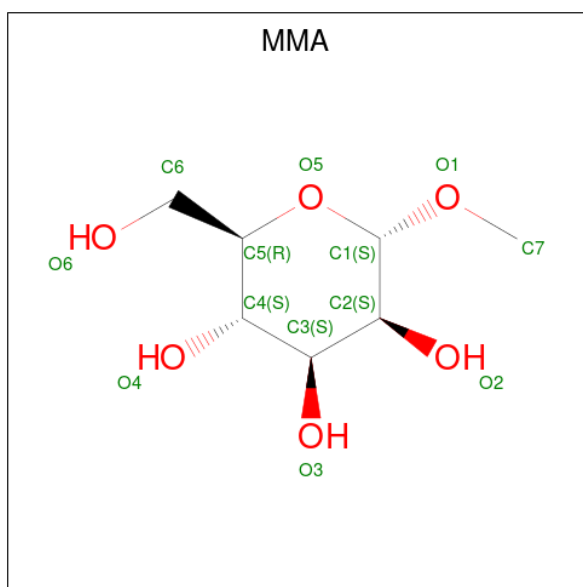
- Molecule 1 is a protein called CONCANAVALIN A.

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

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	151	ASP	GLU	conflict	UNP P02866
A	155	GLU	ARG	conflict	UNP P02866
B	151	ASP	GLU	conflict	UNP P02866
B	155	GLU	ARG	conflict	UNP P02866
C	151	ASP	GLU	conflict	UNP P02866
C	155	GLU	ARG	conflict	UNP P02866
D	151	ASP	GLU	conflict	UNP P02866
D	155	GLU	ARG	conflict	UNP P02866

- Molecule 2 is methyl alpha-D-mannopyranoside (three-letter code: MMA) (formula: C<sub>7</sub>H<sub>14</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 13 7 6	0	0
2	B	1	Total C O 13 7 6	0	0
2	C	1	Total C O 13 7 6	0	0
2	D	1	Total C O 13 7 6	0	0

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

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

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

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

*Continued on next page...*

*Continued from previous page...*

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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0

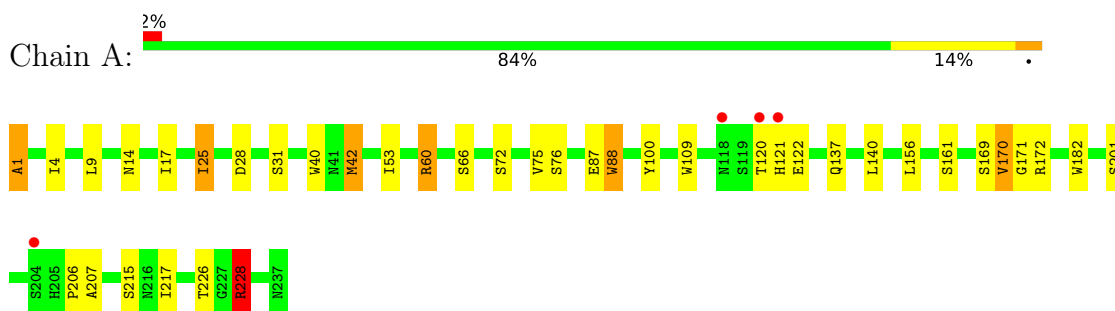
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	148	Total O 148 148	0	0
6	B	153	Total O 153 153	0	0
6	C	101	Total O 101 101	0	0
6	D	131	Total O 131 131	0	0

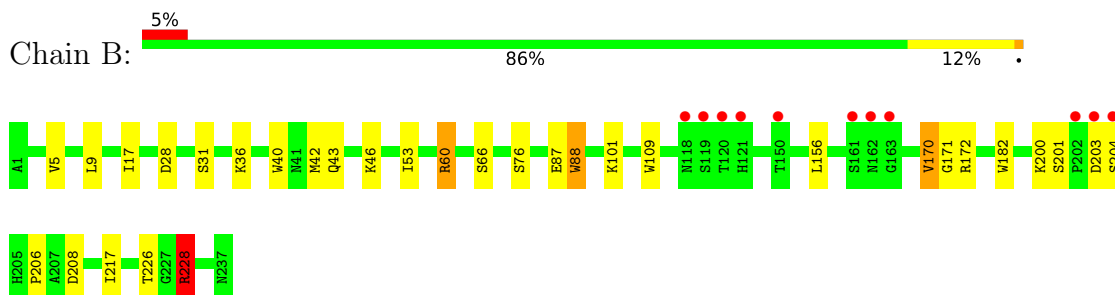
### 3 Residue-property plots [i](#)

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.

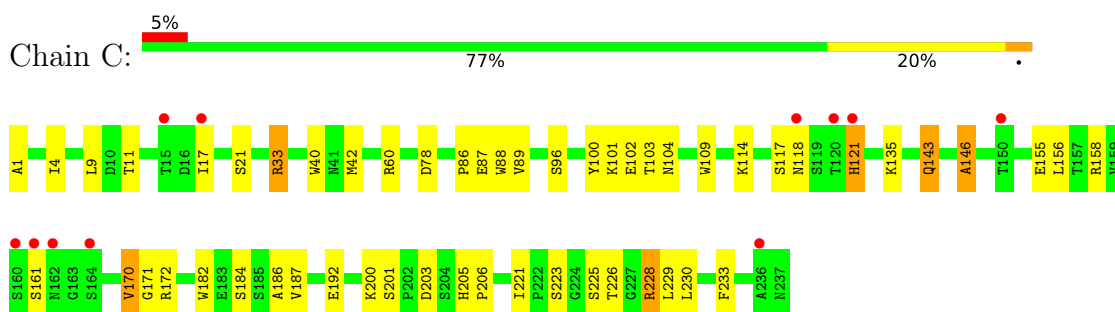
- Molecule 1: CONCANAVALIN A



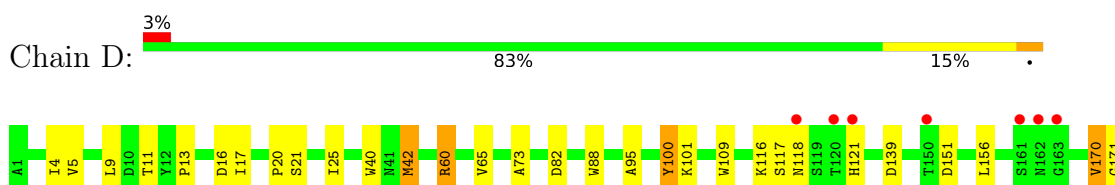
- Molecule 1: CONCANAVALIN A



- Molecule 1: CONCANAVALIN A



- Molecule 1: CONCANAVALIN A





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	123.70Å 128.60Å 67.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.00 39.26 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.00) 81.5 (39.26-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.67 (at 2.00Å)	Xtrriage
Refinement program	X-PLOR 2.1	Depositor
R, $R_{free}$	0.199 , (Not available) 0.187 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.3	Xtrriage
Anisotropy	0.339	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 86.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.000 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7830	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.25 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.7280e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

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



## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MN, CL, MMA, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.80	0/1851	1.48	24/2522 (1.0%)
1	B	0.81	0/1851	1.45	20/2522 (0.8%)
1	C	0.76	0/1851	1.45	21/2522 (0.8%)
1	D	0.78	0/1851	1.45	22/2522 (0.9%)
All	All	0.79	0/7404	1.46	87/10088 (0.9%)

There are no bond length outliers.

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	ARG	NE-CZ-NH2	-11.38	114.61	120.30
1	D	170	VAL	CG1-CB-CG2	-10.75	93.70	110.90
1	C	228	ARG	NE-CZ-NH1	9.63	125.12	120.30
1	A	228	ARG	NE-CZ-NH1	9.06	124.83	120.30
1	B	88	TRP	CD1-CG-CD2	8.82	113.36	106.30
1	D	182	TRP	CD1-CG-CD2	8.41	113.03	106.30
1	B	170	VAL	CG1-CB-CG2	-8.40	97.45	110.90
1	C	40	TRP	CD1-CG-CD2	8.37	113.00	106.30
1	A	182	TRP	CD1-CG-CD2	7.94	112.65	106.30
1	A	88	TRP	CD1-CG-CD2	7.90	112.62	106.30
1	D	88	TRP	CD1-CG-CD2	7.83	112.56	106.30
1	A	172	ARG	NE-CZ-NH1	7.81	124.20	120.30
1	B	182	TRP	CD1-CG-CD2	7.79	112.53	106.30
1	D	182	TRP	CE2-CD2-CG	-7.66	101.17	107.30
1	C	170	VAL	CG1-CB-CG2	-7.60	98.74	110.90
1	B	228	ARG	NE-CZ-NH1	7.59	124.09	120.30
1	B	88	TRP	CE2-CD2-CG	-7.58	101.24	107.30
1	C	87	GLU	CA-CB-CG	7.51	129.92	113.40
1	C	182	TRP	CD1-CG-CD2	7.45	112.26	106.30
1	A	25	ILE	CG1-CB-CG2	-7.36	95.20	111.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	109	TRP	CD1-CG-CD2	7.35	112.18	106.30
1	A	40	TRP	CD1-CG-CD2	7.33	112.16	106.30
1	C	40	TRP	CE2-CD2-CG	-7.29	101.47	107.30
1	C	182	TRP	CE2-CD2-CG	-7.11	101.61	107.30
1	B	40	TRP	CE2-CD2-CG	-7.07	101.65	107.30
1	C	109	TRP	CD1-CG-CD2	7.05	111.94	106.30
1	B	182	TRP	CE2-CD2-CG	-7.00	101.70	107.30
1	D	88	TRP	CE2-CD2-CG	-6.97	101.72	107.30
1	C	109	TRP	CE2-CD2-CG	-6.96	101.74	107.30
1	A	87	GLU	CA-CB-CG	6.85	128.47	113.40
1	A	88	TRP	CE2-CD2-CG	-6.84	101.83	107.30
1	D	40	TRP	CE2-CD2-CG	-6.78	101.87	107.30
1	B	40	TRP	CD1-CG-CD2	6.78	111.72	106.30
1	D	40	TRP	CD1-CG-CD2	6.76	111.71	106.30
1	A	40	TRP	CE2-CD2-CG	-6.62	102.00	107.30
1	B	172	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	B	172	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	A	172	ARG	CB-CG-CD	-6.47	94.78	111.60
1	A	182	TRP	CE2-CD2-CG	-6.43	102.16	107.30
1	A	109	TRP	CE2-CD2-CG	-6.39	102.19	107.30
1	D	109	TRP	CE2-CD2-CG	-6.39	102.19	107.30
1	C	172	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	B	172	ARG	CB-CG-CD	-6.23	95.41	111.60
1	B	109	TRP	CD1-CG-CD2	6.21	111.27	106.30
1	D	109	TRP	CD1-CG-CD2	6.16	111.23	106.30
1	B	60	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	B	109	TRP	CE2-CD2-CG	-6.12	102.41	107.30
1	C	172	ARG	CB-CG-CD	-5.96	96.11	111.60
1	C	88	TRP	CE2-CD2-CG	-5.94	102.55	107.30
1	D	182	TRP	CG-CD1-NE1	-5.93	104.17	110.10
1	A	161	SER	N-CA-CB	-5.88	101.68	110.50
1	A	169	SER	N-CA-CB	-5.84	101.73	110.50
1	D	9	LEU	N-CA-C	-5.84	95.23	111.00
1	D	139	ASP	CB-CG-OD1	5.82	123.54	118.30
1	A	228	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	C	88	TRP	CD1-CG-CD2	5.67	110.83	106.30
1	D	182	TRP	CB-CG-CD1	-5.59	119.73	127.00
1	D	182	TRP	CG-CD2-CE3	5.59	138.94	133.90
1	B	88	TRP	CG-CD1-NE1	-5.59	104.51	110.10
1	A	1	ALA	N-CA-C	-5.59	95.91	111.00
1	B	9	LEU	N-CA-C	-5.57	95.97	111.00
1	B	228	ARG	NE-CZ-NH2	-5.56	117.52	120.30

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	TRP	CG-CD1-NE1	-5.49	104.61	110.10
1	A	9	LEU	N-CA-C	-5.46	96.25	111.00
1	A	42	MET	CA-CB-CG	5.46	122.59	113.30
1	A	182	TRP	CG-CD1-NE1	-5.45	104.65	110.10
1	A	60	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	C	40	TRP	CG-CD1-NE1	-5.36	104.74	110.10
1	D	82	ASP	CA-CB-CG	5.34	125.15	113.40
1	D	42	MET	CA-CB-CG	5.33	122.36	113.30
1	B	5	VAL	N-CA-C	-5.32	96.65	111.00
1	C	143	GLN	CA-C-N	5.21	126.61	116.20
1	C	33	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	C	182	TRP	CG-CD1-NE1	-5.19	104.91	110.10
1	C	9	LEU	N-CA-C	-5.17	97.03	111.00
1	B	87	GLU	CA-CB-CG	5.10	124.63	113.40
1	D	172	ARG	CB-CG-CD	-5.10	98.33	111.60
1	B	182	TRP	CA-CB-CG	5.09	123.37	113.70
1	D	100	TYR	CB-CG-CD1	-5.08	117.95	121.00
1	D	60	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	D	5	VAL	N-CA-C	-5.08	97.29	111.00
1	C	158	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	C	146	ALA	CB-CA-C	-5.06	102.51	110.10
1	A	170	VAL	CB-CA-C	-5.05	101.80	111.40
1	C	146	ALA	N-CA-CB	5.05	117.18	110.10
1	D	73	ALA	N-CA-C	-5.04	97.40	111.00
1	D	212	PHE	N-CA-C	-5.02	97.44	111.00

There are no chirality outliers.

There are no planarity outliers.

## 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	A	1809	0	1755	17	0
1	B	1809	0	1755	14	0
1	C	1809	0	1755	25	0
1	D	1809	0	1755	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	13	0	14	0	0
2	B	13	0	14	1	0
2	C	13	0	14	0	0
2	D	13	0	14	1	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	1	0	0	0	0
6	A	148	0	0	4	0
6	B	153	0	0	1	0
6	C	101	0	0	2	0
6	D	131	0	0	0	0
All	All	7830	0	7076	69	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 5.

All (69) 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:170:VAL:HG23	1:B:226:THR:HG22	1.73	0.71
1:B:43:GLN:HE21	1:B:46:LYS:HG3	1.57	0.70
1:A:17:ILE:HD13	1:A:228:ARG:HD3	1.75	0.68
1:C:117:SER:HA	1:C:186:ALA:HA	1.77	0.65
1:D:117:SER:HA	1:D:186:ALA:HA	1.78	0.64
1:C:170:VAL:HG12	1:C:221:ILE:HD13	1.80	0.64
1:A:201:SER:HB2	1:A:206:PRO:HB3	1.80	0.63
1:A:14:ASN:HA	6:A:303:HOH:O	1.99	0.60
1:B:201:SER:HB2	1:B:206:PRO:HB3	1.82	0.59
1:C:96:SER:OG	1:C:230:LEU:HA	2.02	0.59
1:C:201:SER:HB2	1:C:206:PRO:HB3	1.84	0.59
1:A:170:VAL:HG23	1:A:226:THR:HG22	1.86	0.58
1:D:4:ILE:HD13	1:D:215:SER:HB3	1.84	0.58
1:B:36:LYS:HD2	1:B:76:SER:O	2.05	0.57
1:D:201:SER:HB2	1:D:206:PRO:HB3	1.85	0.56
1:B:60:ARG:HD3	1:B:76:SER:HB3	1.90	0.53

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:SER:HA	6:B:336:HOH:O	2.08	0.53
1:B:17:ILE:HD13	1:B:228:ARG:HD3	1.90	0.52
1:C:170:VAL:CG2	1:C:226:THR:HA	2.40	0.51
1:B:42:MET:HE1	1:B:206:PRO:HG3	1.92	0.51
1:D:13:PRO:HB3	1:D:20:PRO:O	2.11	0.51
1:A:60:ARG:HD3	1:A:76:SER:HB3	1.93	0.49
1:C:143:GLN:O	1:C:221:ILE:HD11	2.12	0.49
1:C:102:GLU:HG3	1:C:104:ASN:ND2	2.27	0.48
1:D:170:VAL:CG2	1:D:226:THR:HA	2.42	0.48
1:B:88:TRP:HB3	1:B:217:ILE:HD11	1.94	0.48
1:C:96:SER:HB3	1:C:170:VAL:HG22	1.96	0.48
1:A:66:SER:HB3	1:A:72:SER:HB3	1.95	0.47
1:D:170:VAL:HG23	1:D:226:THR:HG22	1.95	0.47
1:A:28:ASP:HB3	1:A:31:SER:O	2.14	0.47
1:C:11:THR:HG22	1:C:42:MET:HG3	1.96	0.47
1:A:1:ALA:HB1	6:A:296:HOH:O	2.15	0.47
1:A:60:ARG:NH2	1:C:60:ARG:HH21	2.13	0.47
1:D:170:VAL:HG23	1:D:226:THR:HA	1.97	0.46
1:A:100:TYR:HB2	1:A:207:ALA:HB3	1.98	0.46
1:C:118:ASN:HA	1:C:187:VAL:HG23	1.97	0.46
1:A:42:MET:HE2	6:A:301:HOH:O	2.16	0.46
1:C:17:ILE:HG22	1:C:33:ARG:NH2	2.30	0.46
1:D:11:THR:HG22	1:D:42:MET:HG3	1.97	0.46
1:A:156:LEU:O	1:A:171:GLY:HA3	2.15	0.46
1:D:17:ILE:HD13	1:D:228:ARG:HD3	1.97	0.46
1:C:114:LYS:HE3	1:C:114:LYS:HB2	1.59	0.45
1:C:100:TYR:HB3	1:C:205:HIS:O	2.16	0.45
1:C:156:LEU:O	1:C:171:GLY:HA3	2.17	0.45
1:A:228:ARG:HD2	6:A:288:HOH:O	2.16	0.45
1:D:156:LEU:O	1:D:171:GLY:HA3	2.16	0.45
1:A:4:ILE:HD13	1:A:215:SER:HB3	2.00	0.44
1:C:86:PRO:HG2	1:C:89:VAL:HG12	1.99	0.44
1:A:25:ILE:HG22	1:A:75:VAL:HG11	2.00	0.44
1:B:28:ASP:HB3	1:B:31:SER:O	2.17	0.44
1:A:88:TRP:HB3	1:A:217:ILE:HD11	2.00	0.43
1:B:156:LEU:O	1:B:171:GLY:HA3	2.18	0.43
1:C:225:SER:HB3	1:C:233:PHE:O	2.18	0.43
1:C:1:ALA:N	6:C:278:HOH:O	2.52	0.43
1:B:228:ARG:HG2	2:B:238:MMA:O3	2.18	0.43
1:C:170:VAL:HG23	1:C:226:THR:HG22	2.00	0.43
1:B:60:ARG:NH2	1:D:60:ARG:HH21	2.17	0.43

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:ASN:HA	1:C:187:VAL:CG2	2.49	0.42
1:C:78:ASP:HB3	6:C:289:HOH:O	2.20	0.42
1:B:200:LYS:HB3	1:B:200:LYS:HE2	1.77	0.42
1:A:137:GLN:HG2	1:A:140:LEU:HD12	2.01	0.41
1:C:225:SER:HA	1:C:229:LEU:HD12	2.03	0.41
1:C:170:VAL:HG21	1:C:226:THR:HA	2.03	0.41
1:D:95:ALA:HB3	1:D:156:LEU:HB3	2.03	0.40
1:C:146:ALA:HA	1:C:155:GLU:O	2.21	0.40
1:D:100:TYR:CD1	1:D:205:HIS:HB2	2.56	0.40
1:D:25:ILE:HG21	1:D:65:VAL:HG21	2.03	0.40
1:C:103:THR:OG1	1:C:200:LYS:HG2	2.21	0.40
1:D:228:ARG:HG2	2:D:238:MMA:O3	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	235/237 (99%)	221 (94%)	12 (5%)	2 (1%)	17	11
1	B	235/237 (99%)	222 (94%)	11 (5%)	2 (1%)	17	11
1	C	235/237 (99%)	216 (92%)	17 (7%)	2 (1%)	17	11
1	D	235/237 (99%)	219 (93%)	15 (6%)	1 (0%)	34	30
All	All	940/948 (99%)	878 (93%)	55 (6%)	7 (1%)	22	16

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	120	THR
1	C	121	HIS
1	A	121	HIS

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	204	SER
1	D	21	SER
1	B	203	ASP
1	C	21	SER

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	203/203 (100%)	200 (98%)	3 (2%)	65	69
1	B	203/203 (100%)	199 (98%)	4 (2%)	55	58
1	C	203/203 (100%)	193 (95%)	10 (5%)	25	21
1	D	203/203 (100%)	194 (96%)	9 (4%)	28	25
All	All	812/812 (100%)	786 (97%)	26 (3%)	39	38

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ILE
1	A	122	GLU
1	A	228	ARG
1	B	53	ILE
1	B	101	LYS
1	B	208	ASP
1	B	228	ARG
1	C	4	ILE
1	C	101	LYS
1	C	121	HIS
1	C	135	LYS
1	C	161	SER
1	C	184	SER
1	C	192	GLU
1	C	203	ASP
1	C	223	SER
1	C	228	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	16	ASP
1	D	101	LYS
1	D	116	LYS
1	D	118	ASN
1	D	121	HIS
1	D	151	ASP
1	D	198	LEU
1	D	226	THR
1	D	228	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	237	ASN
1	B	43	GLN
1	B	237	ASN
1	C	43	GLN

### 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 13 ligands modelled in this entry, 9 are monoatomic - leaving 4 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	MMA	A	238	-	13,13,13	1.25	1 (7%)	18,18,18	1.03	1 (5%)
2	MMA	B	238	-	13,13,13	0.69	0	18,18,18	1.02	2 (11%)
2	MMA	C	238	-	13,13,13	1.24	1 (7%)	18,18,18	1.00	0
2	MMA	D	238	-	13,13,13	1.13	1 (7%)	18,18,18	1.37	3 (16%)

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	MMA	A	238	-	-	2/4/24/24	0/1/1/1
2	MMA	B	238	-	-	0/4/24/24	0/1/1/1
2	MMA	C	238	-	-	0/4/24/24	0/1/1/1
2	MMA	D	238	-	-	0/4/24/24	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	238	MMA	O1-C1	3.18	1.45	1.40
2	C	238	MMA	O1-C1	3.06	1.45	1.40
2	A	238	MMA	O1-C1	2.76	1.44	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	238	MMA	O4-C4-C3	-3.17	103.03	110.35
2	D	238	MMA	O1-C1-C2	2.67	111.28	108.15
2	D	238	MMA	C6-C5-C4	-2.54	107.05	113.00
2	B	238	MMA	O4-C4-C3	-2.42	104.76	110.35
2	B	238	MMA	C6-C5-C4	-2.31	107.60	113.00
2	A	238	MMA	O4-C4-C3	-2.28	105.07	110.35

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	238	MMA	O5-C5-C6-O6
2	A	238	MMA	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	238	MMA	1	0
2	D	238	MMA	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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	237/237 (100%)	-0.44	4 (1%) 70 68	12, 22, 61, 93	0
1	B	237/237 (100%)	-0.32	11 (4%) 32 31	11, 23, 60, 85	0
1	C	237/237 (100%)	0.16	11 (4%) 32 31	16, 39, 70, 99	0
1	D	237/237 (100%)	-0.29	7 (2%) 50 49	14, 26, 66, 97	0
All	All	948/948 (100%)	-0.22	33 (3%) 44 43	11, 27, 67, 99	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	120	THR	6.4
1	D	121	HIS	6.1
1	C	120	THR	5.5
1	D	120	THR	5.2
1	C	161	SER	4.7
1	C	160	SER	4.5
1	C	121	HIS	3.9
1	C	17	ILE	3.8
1	A	121	HIS	3.8
1	B	204	SER	3.7
1	B	163	GLY	3.7
1	A	120	THR	3.7
1	B	121	HIS	3.6
1	B	162	ASN	3.2
1	D	163	GLY	3.0
1	C	236	ALA	2.8
1	D	161	SER	2.8
1	B	203	ASP	2.7
1	A	118	ASN	2.7
1	D	162	ASN	2.7
1	C	150	THR	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	162	ASN	2.6
1	B	161	SER	2.5
1	C	118	ASN	2.5
1	B	119	SER	2.4
1	B	150	THR	2.3
1	D	118	ASN	2.3
1	A	204	SER	2.3
1	B	202	PRO	2.2
1	C	164	SER	2.2
1	B	118	ASN	2.1
1	D	150	THR	2.0
1	C	15	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MMA	C	238	13/13	0.88	0.13	45,51,57,59	0
3	MN	C	239	1/1	0.94	0.06	41,41,41,41	0
4	CA	C	240	1/1	0.94	0.04	39,39,39,39	0
2	MMA	D	238	13/13	0.96	0.09	22,30,36,36	0
2	MMA	A	238	13/13	0.98	0.12	16,19,23,25	0
2	MMA	B	238	13/13	0.98	0.11	16,23,28,28	0
5	CL	A	241	1/1	0.98	0.14	32,32,32,32	0
4	CA	B	240	1/1	0.99	0.09	19,19,19,19	0
3	MN	B	239	1/1	0.99	0.06	18,18,18,18	0
4	CA	D	240	1/1	0.99	0.05	23,23,23,23	0
3	MN	D	239	1/1	0.99	0.07	26,26,26,26	0

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Atoms</b>	<b>RSCC</b>	<b>RSR</b>	<b>B-factors(<math>\text{\AA}^2</math>)</b>	<b>Q&lt;0.9</b>
3	MN	A	239	1/1	1.00	0.06	19,19,19,19	0
4	CA	A	240	1/1	1.00	0.06	14,14,14,14	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.