



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 06:42 am BST

PDB ID : 4P9W
Title : Structure of ConA/Rh3Man
Authors : Sakai, F.; Weiss, M.S.; Jiang, M.
Deposited on : 2014-04-06
Resolution : 2.11 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
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

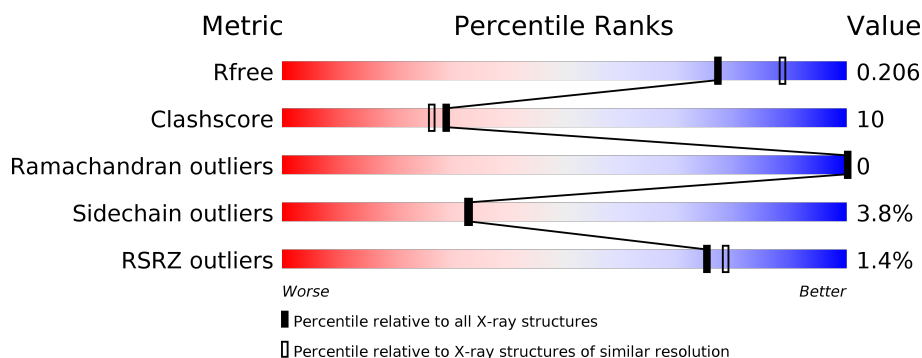
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.11 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	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	237	<div> <div>2%</div> <div>84%</div> <div>14%</div> <div>•</div> </div>
1	B	237	<div> <div>2%</div> <div>82%</div> <div>15%</div> <div>•</div> </div>
1	C	237	<div> <div>83%</div> <div>14%</div> <div>•</div> </div>
1	D	237	<div> <div>2%</div> <div>84%</div> <div>14%</div> <div>•</div> </div>

2 Entry composition [i](#)

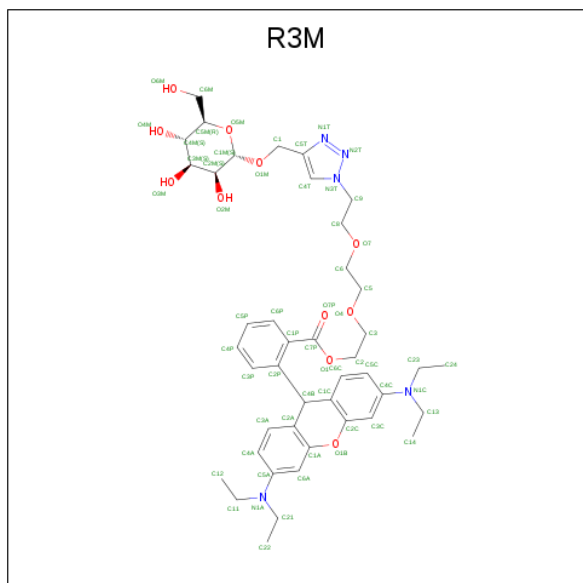
There are 5 unique types of molecules in this entry. The entry contains 7690 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	1	0
			1819	1147	305	365	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 2-[2-(2-{4-[(alpha-D-mannopyranosyloxy)methyl]-1H-1,2,3-triazol-1-yl}ethoxy)ethoxy]ethyl 2-[3,6-bis(diethylamino)-9H-xanthen-9-yl]benzoate (three-letter code: R3M) (formula: C₄₃H₅₇N₅O₁₁).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			59	43	5	11		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			59	43	5	11		
2	C	1	Total	C	N	O	0	0
			59	43	5	11		
2	D	1	Total	C	N	O	0	0
			59	43	5	11		

- 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		

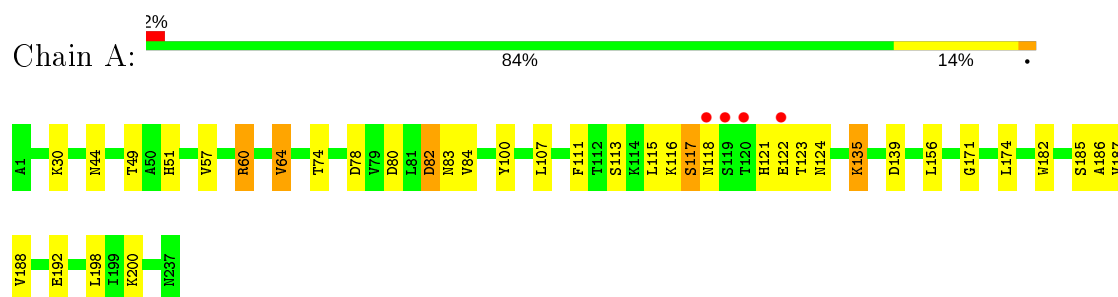
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	59	Total	O	0	0
			59	59		
5	B	46	Total	O	0	0
			46	46		
5	C	54	Total	O	0	0
			54	54		
5	D	41	Total	O	0	0
			41	41		

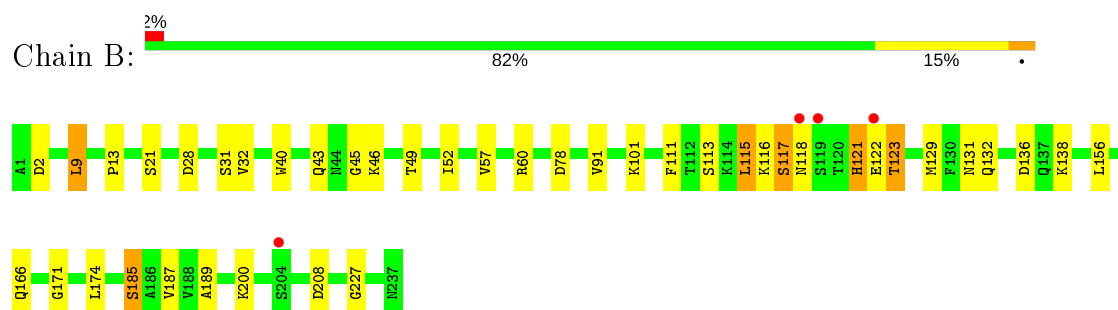
3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). 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.

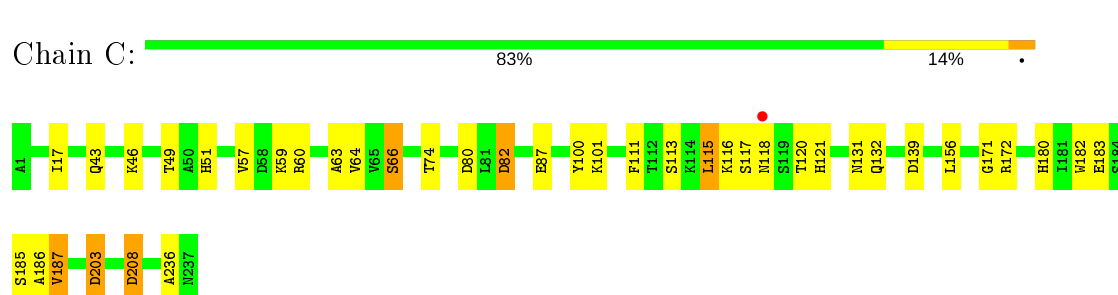
- Molecule 1: Concanavalin-A



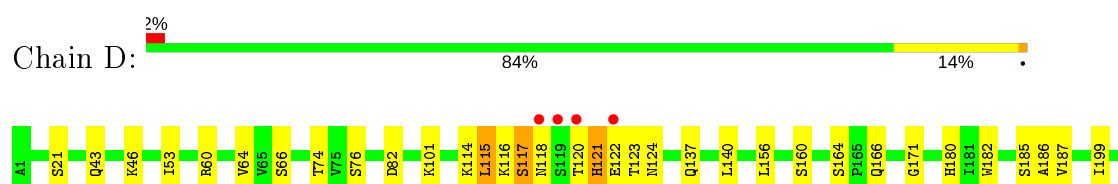
- Molecule 1: Concanavalin-A



- 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	84.00Å 116.03Å 84.10Å 90.00° 95.03° 90.00°	Depositor
Resolution (Å)	39.40 – 2.11 39.36 – 2.11	Depositor EDS
% Data completeness (in resolution range)	95.5 (39.40-2.11) 95.5 (39.36-2.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.173 , 0.202 0.177 , 0.206	Depositor DCC
R_{free} test set	1777 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å ²)	28.5	Xtriage
Anisotropy	0.283	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 18.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.428 for l,-k,h	Xtriage
Reported twinning fraction	0.630 for H, K, L 0.370 for L, -K, H	Depositor
Outliers	1 of 88321 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7690	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.73% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: R3M, CA, MN

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	0.90	0/1862	1.00	4/2537 (0.2%)
1	B	0.80	0/1851	0.91	3/2522 (0.1%)
1	C	0.97	1/1851 (0.1%)	1.02	4/2522 (0.2%)
1	D	0.90	0/1851	0.96	2/2522 (0.1%)
All	All	0.89	1/7415 (0.0%)	0.97	13/10103 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	100	TYR	CG-CD2	5.80	1.46	1.39

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	82	ASP	CB-CG-OD2	7.24	124.82	118.30
1	B	115	LEU	CA-CB-CG	7.10	131.63	115.30
1	A	115	LEU	CA-CB-CG	6.45	130.13	115.30
1	C	139	ASP	CB-CG-OD1	6.07	123.77	118.30
1	B	115	LEU	CB-CG-CD1	-6.03	100.76	111.00
1	C	172	ARG	NE-CZ-NH2	5.91	123.26	120.30
1	A	82	ASP	CB-CG-OD2	5.90	123.61	118.30
1	A	82	ASP	N-CA-CB	5.66	120.80	110.60
1	B	2	ASP	CB-CG-OD1	5.37	123.14	118.30
1	D	115	LEU	CA-CB-CG	5.22	127.32	115.30
1	D	82	ASP	CB-CA-C	-5.20	100.01	110.40
1	C	208	ASP	CB-CG-OD2	-5.07	113.73	118.30
1	A	139	ASP	CB-CG-OD1	5.03	122.82	118.30

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	1819	0	1761	52	0
1	B	1809	0	1755	26	0
1	C	1809	0	1755	59	0
1	D	1809	0	1755	25	0
2	A	59	0	56	3	0
2	B	59	0	56	2	0
2	C	59	0	56	3	0
2	D	59	0	56	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	59	0	0	2	0
5	B	46	0	0	3	0
5	C	54	0	0	2	0
5	D	41	0	0	1	0
All	All	7690	0	7250	141	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 10.

All (141) 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:129:MET:HG3	5:B:418:HOH:O	1.70	0.91
1:D:66:SER:HB2	5:D:422:HOH:O	1.69	0.91
1:B:122:GLU:OE2	1:B:123:THR:HG22	1.72	0.89
1:A:51[A]:HIS:HE1	1:C:116:LYS:CE	1.88	0.87
5:B:432:HOH:O	1:D:114:LYS:HD3	1.76	0.85
1:A:51[A]:HIS:CE1	1:C:116:LYS:HE2	2.15	0.82
1:A:51[A]:HIS:CE1	1:C:116:LYS:CE	2.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:VAL:HG13	1:D:74:THR:HG22	1.65	0.79
1:A:135:LYS:H	1:A:135:LYS:CE	1.96	0.77
1:A:135:LYS:H	1:A:135:LYS:HE2	1.50	0.77
1:A:64:VAL:HG13	1:A:74:THR:HG22	1.65	0.77
1:D:118:ASN:N	1:D:185:SER:O	2.16	0.77
1:C:59:LYS:NZ	1:C:80:ASP:CG	2.39	0.76
1:A:51[A]:HIS:HE1	1:C:116:LYS:HE3	1.50	0.76
1:A:118:ASN:N	1:A:185:SER:O	2.19	0.75
1:C:131:ASN:H	1:D:124:ASN:ND2	1.84	0.75
1:B:118:ASN:N	1:B:185:SER:O	2.16	0.74
1:C:118:ASN:N	1:C:185:SER:O	2.20	0.73
1:A:60:ARG:HD2	1:A:78:ASP:OD1	1.89	0.72
1:A:51[B]:HIS:NE2	1:A:192:GLU:OE2	2.23	0.71
1:A:116:LYS:HE3	1:C:49:THR:HG21	1.71	0.71
1:A:135:LYS:H	1:A:135:LYS:CD	2.02	0.71
1:A:117:SER:HA	1:A:186:ALA:HA	1.71	0.71
1:A:51[B]:HIS:CE1	1:A:192:GLU:OE2	2.43	0.71
1:C:115:LEU:CD1	1:C:186:ALA:HB2	2.23	0.69
1:B:115:LEU:HD23	1:B:189:ALA:HB2	1.76	0.68
1:C:64:VAL:HG22	1:C:74:THR:HG22	1.75	0.68
1:C:59:LYS:HZ2	1:C:80:ASP:CG	1.98	0.65
1:C:116:LYS:NZ	1:C:121:HIS:CG	2.64	0.65
1:A:80:ASP:OD2	5:A:423:HOH:O	2.14	0.65
1:A:51[A]:HIS:HE1	1:C:116:LYS:HE2	1.57	0.65
1:A:57:VAL:HG22	1:C:64:VAL:HG21	1.78	0.64
1:A:60:ARG:HH21	1:C:60:ARG:HH21	1.46	0.64
1:C:116:LYS:NZ	1:C:121:HIS:HA	2.14	0.63
1:C:115:LEU:HD11	1:C:186:ALA:HB2	1.80	0.62
1:D:43:GLN:HE22	1:D:46:LYS:NZ	1.98	0.61
1:C:17:ILE:HG21	1:C:236:ALA:HB1	1.81	0.60
1:A:135:LYS:CD	1:A:135:LYS:N	2.66	0.59
1:A:135:LYS:N	1:A:135:LYS:HD3	2.18	0.59
1:C:116:LYS:HZ2	1:C:121:HIS:HA	1.67	0.59
1:C:116:LYS:HZ3	1:C:121:HIS:CB	2.16	0.58
1:C:59:LYS:HZ1	1:C:80:ASP:CG	2.05	0.58
1:D:199:ILE:HD11	1:D:210:ILE:HD12	1.86	0.58
1:B:136:ASP:OD2	1:B:138:LYS:HE2	2.03	0.58
1:A:116:LYS:CB	1:A:123:THR:HG22	2.34	0.58
1:B:111:PHE:CE2	1:B:113:SER:HB2	2.39	0.58
1:A:156:LEU:O	1:A:171:GLY:HA3	2.05	0.57
1:D:60:ARG:HE	1:D:76:SER:HB3	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:LYS:HG2	1:C:187:VAL:HG13	1.87	0.56
1:A:116:LYS:HB2	1:A:123:THR:HG22	1.88	0.56
1:A:80:ASP:HB3	1:A:83:ASN:ND2	2.20	0.56
1:A:30:LYS:HD2	1:A:84:VAL:HG13	1.88	0.56
1:A:49:THR:HG21	1:C:116:LYS:HE2	1.88	0.56
1:D:160:SER:OG	1:D:166:GLN:NE2	2.39	0.55
1:C:59:LYS:NZ	1:C:80:ASP:OD1	2.39	0.55
1:A:121:HIS:NE2	1:C:66:SER:OG	2.39	0.55
1:D:117:SER:HA	1:D:186:ALA:HA	1.89	0.55
1:B:60:ARG:NH2	1:D:60:ARG:HH21	2.05	0.55
1:A:82:ASP:HB3	1:A:182:TRP:CG	2.41	0.55
1:C:115:LEU:HD13	1:C:186:ALA:HB2	1.89	0.54
1:A:135:LYS:H	1:A:135:LYS:HD3	1.72	0.54
1:B:208:ASP:OD2	1:B:227:GLY:HA2	2.07	0.54
1:A:121:HIS:CE1	1:C:66:SER:HG	2.25	0.54
1:B:9:LEU:HB3	1:B:40:TRP:CZ3	2.43	0.53
1:C:116:LYS:HZ1	1:C:121:HIS:CG	2.26	0.53
1:C:120:THR:O	1:C:121:HIS:HB2	2.08	0.53
1:A:57:VAL:CG2	1:C:64:VAL:HG21	2.38	0.53
1:B:122:GLU:HA	1:B:122:GLU:OE2	2.09	0.53
1:D:137:GLN:HG2	1:D:140:LEU:HD12	1.90	0.52
2:A:301:R3M:H7	5:A:426:HOH:O	2.09	0.52
1:B:28:ASP:HB3	1:B:31:SER:O	2.10	0.52
1:D:180:HIS:CD2	1:D:182:TRP:O	2.63	0.52
1:B:49:THR:OG1	1:D:121:HIS:HD2	1.93	0.52
1:A:124:ASN:ND2	1:B:131:ASN:H	2.09	0.51
1:B:156:LEU:O	1:B:171:GLY:HA3	2.11	0.51
1:C:116:LYS:NZ	1:C:121:HIS:CB	2.72	0.51
1:A:111:PHE:CE2	1:A:113:SER:HB2	2.46	0.51
1:C:82:ASP:HB3	1:C:182:TRP:CG	2.46	0.51
1:B:57:VAL:HG21	1:D:64:VAL:HG22	1.91	0.51
2:C:301:R3M:H3	2:C:301:R3M:H13	1.93	0.51
1:C:116:LYS:HZ3	1:C:121:HIS:CA	2.25	0.50
1:D:115:LEU:O	1:D:123:THR:HA	2.12	0.50
1:A:107:LEU:N	1:A:107:LEU:HD12	2.26	0.50
1:C:116:LYS:NZ	1:C:121:HIS:CA	2.75	0.49
1:C:43:GLN:HE22	1:C:46:LYS:NZ	2.10	0.49
1:A:82:ASP:HB3	1:A:182:TRP:CD2	2.48	0.49
1:B:45:GLY:HA2	1:B:200:LYS:HG3	1.93	0.49
1:C:115:LEU:HD11	1:C:183:GLU:HB3	1.95	0.49
1:C:117:SER:HA	1:C:186:ALA:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:LYS:HD3	1:C:51:HIS:NE2	2.28	0.48
1:A:117:SER:O	1:A:121:HIS:HA	2.13	0.48
1:B:115:LEU:HD23	1:B:189:ALA:CB	2.43	0.48
1:C:115:LEU:HD13	1:C:186:ALA:CB	2.44	0.48
1:B:60:ARG:HG3	1:B:78:ASP:OD1	2.14	0.47
1:C:156:LEU:O	1:C:171:GLY:HA3	2.14	0.47
1:C:59:LYS:NZ	1:C:80:ASP:OD2	2.42	0.47
1:A:57:VAL:CG2	1:C:64:VAL:CG2	2.93	0.47
1:A:44:ASN:OD1	1:A:200:LYS:HA	2.15	0.47
1:A:57:VAL:HG22	1:C:64:VAL:CG2	2.44	0.47
1:C:80:ASP:OD1	1:C:82:ASP:OD1	2.33	0.47
1:B:174:LEU:N	1:B:174:LEU:HD12	2.30	0.46
1:D:43:GLN:HE22	1:D:46:LYS:HZ1	1.63	0.46
1:C:203:ASP:HB3	5:C:427:HOH:O	2.15	0.46
1:A:174:LEU:N	1:A:174:LEU:HD12	2.31	0.45
1:C:111:PHE:CE2	1:C:113:SER:HB2	2.52	0.45
1:A:124:ASN:HD21	1:B:132:GLN:H	1.64	0.45
1:C:116:LYS:HZ3	1:C:121:HIS:HB3	1.82	0.45
2:A:301:R3M:H44	2:A:301:R3M:H40	1.53	0.44
1:D:120:THR:O	1:D:121:HIS:HB2	2.17	0.44
1:B:121:HIS:HE1	5:B:427:HOH:O	2.01	0.44
1:A:60:ARG:HH21	1:C:60:ARG:NH2	2.13	0.43
1:A:51[A]:HIS:CE1	1:C:116:LYS:HE3	2.37	0.43
1:C:116:LYS:NZ	1:C:121:HIS:CD2	2.86	0.43
1:D:156:LEU:O	1:D:171:GLY:HA3	2.18	0.43
1:A:64:VAL:HG22	1:C:57:VAL:HG21	2.00	0.43
1:C:87:GLU:CG	1:C:180:HIS:HE2	2.31	0.43
1:B:117:SER:O	1:B:121:HIS:HA	2.19	0.43
1:A:122:GLU:HA	1:A:122:GLU:OE2	2.18	0.43
1:C:131:ASN:H	1:D:124:ASN:HD21	1.65	0.43
1:C:182:TRP:HB3	5:C:428:HOH:O	2.19	0.43
1:A:100:TYR:CE1	2:A:301:R3M:H45	2.53	0.42
1:A:187:VAL:HG23	1:A:188:VAL:HG12	2.00	0.42
1:D:207:ALA:HA	1:D:208:ASP:HA	1.87	0.42
1:B:91:VAL:HG11	1:B:111:PHE:CE1	2.54	0.42
1:C:17:ILE:CG2	1:C:236:ALA:HB1	2.48	0.42
1:C:117:SER:O	1:C:121:HIS:HA	2.20	0.42
2:B:301:R3M:H35	2:B:301:R3M:H33	1.72	0.42
1:A:116:LYS:CG	1:A:123:THR:HG22	2.50	0.42
2:C:301:R3M:O7P	2:C:301:R3M:C4B	2.68	0.41
1:A:44:ASN:OD1	1:A:200:LYS:HD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:VAL:HG21	1:D:64:VAL:CG2	2.50	0.41
1:C:51:HIS:O	1:C:63:ALA:HA	2.21	0.41
1:D:122:GLU:OE2	1:D:122:GLU:HA	2.20	0.41
1:A:64:VAL:CG2	1:C:57:VAL:HG21	2.50	0.41
1:A:49:THR:HG1	1:C:121:HIS:HD1	1.65	0.41
1:B:43:GLN:NE2	1:B:46:LYS:HD2	2.36	0.41
1:D:64:VAL:HG13	1:D:74:THR:CG2	2.45	0.41
2:C:301:R3M:H44	2:C:301:R3M:H40	1.79	0.41
1:B:52:ILE:HD12	1:B:52:ILE:N	2.35	0.41
1:D:116:LYS:HD2	1:D:121:HIS:O	2.21	0.40
2:B:301:R3M:H38	2:B:301:R3M:H39	1.93	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	236/237 (100%)	231 (98%)	5 (2%)	0	100	100
1	B	235/237 (99%)	223 (95%)	12 (5%)	0	100	100
1	C	235/237 (99%)	225 (96%)	10 (4%)	0	100	100
1	D	235/237 (99%)	227 (97%)	8 (3%)	0	100	100
All	All	941/948 (99%)	906 (96%)	35 (4%)	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	A	204/203 (100%)	199 (98%)	5 (2%)	47	50
1	B	203/203 (100%)	191 (94%)	12 (6%)	19	16
1	C	203/203 (100%)	196 (97%)	7 (3%)	37	38
1	D	203/203 (100%)	196 (97%)	7 (3%)	37	38
All	All	813/812 (100%)	782 (96%)	31 (4%)	33	33

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	ARG
1	A	64	VAL
1	A	117	SER
1	A	135	LYS
1	A	198	LEU
1	B	9	LEU
1	B	13	PRO
1	B	21	SER
1	B	32	VAL
1	B	101	LYS
1	B	116	LYS
1	B	117	SER
1	B	121	HIS
1	B	123	THR
1	B	166	GLN
1	B	185	SER
1	B	187	VAL
1	C	66	SER
1	C	101	LYS
1	C	115	LEU
1	C	132	GLN
1	C	187	VAL
1	C	203	ASP
1	C	208	ASP
1	D	21	SER
1	D	53	ILE
1	D	101	LYS
1	D	117	SER
1	D	121	HIS
1	D	164	SER

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Mol	Chain	Res	Type
1	D	187	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	118	ASN
1	A	124	ASN
1	A	132	GLN
1	A	166	GLN
1	A	237	ASN
1	B	43	GLN
1	B	121	HIS
1	B	237	ASN
1	C	43	GLN
1	C	69	ASN
1	C	118	ASN
1	C	237	ASN
1	D	43	GLN
1	D	118	ASN
1	D	121	HIS
1	D	124	ASN
1	D	166	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 12 ligands modelled in this entry, 8 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	R3M	D	301	-	64,64,64	1.99	11 (17%)	81,88,88	1.90	23 (28%)
2	R3M	A	301	-	64,64,64	2.26	8 (12%)	81,88,88	1.92	22 (27%)
2	R3M	C	301	-	64,64,64	2.18	9 (14%)	81,88,88	1.95	19 (23%)
2	R3M	B	301	-	64,64,64	2.01	9 (14%)	81,88,88	2.03	22 (27%)

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	R3M	D	301	-	-	2/41/75/75	0/6/6/6
2	R3M	A	301	-	-	7/41/75/75	0/6/6/6
2	R3M	C	301	-	-	9/41/75/75	0/6/6/6
2	R3M	B	301	-	-	9/41/75/75	0/6/6/6

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	R3M	O1B-C2C	-8.48	1.25	1.38
2	A	301	R3M	O1B-C1A	-8.43	1.25	1.38
2	C	301	R3M	C2A-C4B	-8.15	1.38	1.52
2	A	301	R3M	C1C-C4B	-7.66	1.39	1.52
2	B	301	R3M	C1C-C4B	-7.66	1.39	1.52
2	D	301	R3M	C1C-C4B	-7.30	1.39	1.52
2	A	301	R3M	O1B-C2C	-7.18	1.27	1.38
2	B	301	R3M	C2A-C4B	-7.06	1.40	1.52
2	C	301	R3M	C1C-C4B	-6.90	1.40	1.52
2	A	301	R3M	C2A-C4B	-6.69	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	R3M	O1B-C1A	-6.57	1.28	1.38
2	D	301	R3M	C2A-C4B	-6.16	1.41	1.52
2	B	301	R3M	O1B-C1A	-5.91	1.29	1.38
2	C	301	R3M	O1B-C1A	-5.56	1.30	1.38
2	D	301	R3M	O1B-C2C	-5.37	1.30	1.38
2	B	301	R3M	O1B-C2C	-5.13	1.30	1.38
2	A	301	R3M	O1-C7P	4.85	1.45	1.33
2	B	301	R3M	O1-C7P	4.54	1.45	1.33
2	C	301	R3M	O1-C7P	4.37	1.44	1.33
2	A	301	R3M	N1T-N2T	4.01	1.41	1.34
2	D	301	R3M	N2T-N3T	3.77	1.41	1.34
2	B	301	R3M	N2T-N3T	3.41	1.41	1.34
2	C	301	R3M	N1T-N2T	3.14	1.40	1.34
2	A	301	R3M	C2P-C4B	-3.07	1.49	1.53
2	C	301	R3M	O1M-C1M	3.07	1.45	1.40
2	B	301	R3M	N1T-N2T	2.95	1.39	1.34
2	D	301	R3M	C4T-C5T	2.81	1.40	1.36
2	B	301	R3M	C2P-C4B	-2.71	1.49	1.53
2	D	301	R3M	C1A-C2A	2.61	1.44	1.39
2	D	301	R3M	O1M-C1M	2.51	1.44	1.40
2	D	301	R3M	N1T-N2T	2.46	1.38	1.34
2	D	301	R3M	O1-C7P	2.40	1.39	1.33
2	C	301	R3M	C2P-C4B	-2.27	1.50	1.53
2	A	301	R3M	N2T-N3T	2.23	1.38	1.34
2	B	301	R3M	C9-N3T	-2.13	1.44	1.47
2	D	301	R3M	C1P-C7P	-2.08	1.45	1.50
2	C	301	R3M	C4T-C5T	2.05	1.39	1.36

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	R3M	C1C-C4B-C2A	8.93	119.15	105.83
2	A	301	R3M	C1C-C4B-C2A	8.47	118.46	105.83
2	B	301	R3M	C1C-C4B-C2A	7.93	117.65	105.83
2	D	301	R3M	C1C-C4B-C2A	6.75	115.90	105.83
2	B	301	R3M	N1T-N2T-N3T	-6.23	102.62	107.31
2	D	301	R3M	O1-C7P-C1P	5.11	122.32	112.21
2	B	301	R3M	C2-O1-C7P	4.73	126.41	116.43
2	C	301	R3M	C1A-C2A-C4B	-4.55	116.73	121.53
2	A	301	R3M	C2C-C1C-C4B	-4.33	116.97	121.53
2	C	301	R3M	O1B-C1A-C6A	4.18	121.39	115.20
2	B	301	R3M	O1B-C2C-C3C	4.05	121.20	115.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	R3M	C3A-C2A-C1A	4.00	122.26	117.75
2	D	301	R3M	O1B-C2C-C3C	3.91	120.98	115.20
2	B	301	R3M	C3A-C2A-C4B	-3.72	120.23	126.14
2	D	301	R3M	C6C-C1C-C4B	-3.70	120.27	126.14
2	C	301	R3M	C9-N3T-C4T	3.62	138.33	129.82
2	A	301	R3M	C11-N1A-C21	3.62	123.28	116.34
2	B	301	R3M	C6C-C1C-C4B	-3.61	120.42	126.14
2	B	301	R3M	O1-C7P-C1P	3.59	119.32	112.21
2	A	301	R3M	C11-N1A-C5A	-3.58	116.11	121.39
2	C	301	R3M	C3C-C4C-N1C	-3.47	117.60	121.33
2	D	301	R3M	C3C-C2C-C1C	-3.43	116.68	121.85
2	C	301	R3M	C3A-C2A-C4B	-3.26	120.96	126.14
2	B	301	R3M	O1B-C1A-C6A	3.26	120.03	115.20
2	B	301	R3M	C3C-C2C-C1C	-3.24	116.97	121.85
2	C	301	R3M	C2C-C1C-C4B	-3.20	118.15	121.53
2	A	301	R3M	C1A-C2A-C4B	-3.18	118.18	121.53
2	D	301	R3M	C6P-C1P-C2P	3.15	123.19	119.60
2	C	301	R3M	C2P-C4B-C2A	3.13	123.73	113.32
2	B	301	R3M	C3A-C2A-C1A	3.13	121.28	117.75
2	D	301	R3M	O1B-C1A-C6A	3.13	119.83	115.20
2	A	301	R3M	O1B-C1A-C6A	3.04	119.71	115.20
2	A	301	R3M	O3M-C3M-C2M	-3.03	103.34	110.35
2	A	301	R3M	C2C-O1B-C1A	2.98	125.10	118.58
2	C	301	R3M	O1B-C2C-C3C	2.95	119.57	115.20
2	D	301	R3M	O1-C7P-O7P	-2.94	117.72	123.67
2	D	301	R3M	O1M-C1M-C2M	2.93	112.88	108.30
2	A	301	R3M	C6M-C5M-C4M	2.90	119.79	113.00
2	D	301	R3M	C9-N3T-C4T	2.89	136.61	129.82
2	B	301	R3M	C1A-C2A-C4B	-2.89	118.49	121.53
2	B	301	R3M	C6A-C1A-C2A	-2.89	117.50	121.85
2	D	301	R3M	C2P-C4B-C2A	2.80	122.65	113.32
2	A	301	R3M	O1-C7P-C1P	2.79	117.73	112.21
2	A	301	R3M	O1-C7P-O7P	-2.78	118.03	123.67
2	B	301	R3M	C3P-C2P-C4B	-2.74	115.40	121.49
2	B	301	R3M	C6C-C1C-C2C	2.71	120.81	117.75
2	C	301	R3M	C6A-C1A-C2A	-2.65	117.85	121.85
2	D	301	R3M	C3P-C2P-C1P	-2.63	115.78	118.83
2	B	301	R3M	C2C-C1C-C4B	-2.62	118.77	121.53
2	A	301	R3M	C3A-C2A-C4B	-2.60	122.01	126.14
2	B	301	R3M	C2P-C4B-C2A	2.55	121.81	113.32
2	D	301	R3M	C3A-C2A-C4B	-2.55	122.10	126.14
2	C	301	R3M	C2C-O1B-C1A	2.51	124.08	118.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	R3M	C4M-C3M-C2M	2.49	115.18	110.82
2	A	301	R3M	C3P-C2P-C4B	-2.48	115.97	121.49
2	A	301	R3M	C6C-C1C-C2C	2.48	120.54	117.75
2	C	301	R3M	C4T-C5T-N1T	-2.45	107.69	111.34
2	C	301	R3M	C5C-C4C-N1C	2.45	124.75	121.38
2	A	301	R3M	C1-C5T-C4T	-2.44	123.85	128.45
2	B	301	R3M	O1-C2-C3	-2.41	101.49	108.61
2	D	301	R3M	C2P-C4B-C1C	2.41	121.34	113.32
2	A	301	R3M	C2-O1-C7P	2.40	121.50	116.43
2	D	301	R3M	N1T-N2T-N3T	-2.40	105.51	107.31
2	B	301	R3M	C4C-C3C-C2C	2.34	124.06	120.46
2	D	301	R3M	C6C-C1C-C2C	2.31	120.36	117.75
2	A	301	R3M	C2P-C4B-C2A	2.31	120.99	113.32
2	A	301	R3M	C5P-C4P-C3P	-2.31	116.68	120.19
2	A	301	R3M	C6C-C1C-C4B	-2.30	122.49	126.14
2	D	301	R3M	C3C-C4C-N1C	-2.29	118.87	121.33
2	A	301	R3M	O1B-C2C-C3C	2.28	118.58	115.20
2	C	301	R3M	C2-O1-C7P	2.22	121.10	116.43
2	B	301	R3M	O1-C7P-O7P	-2.20	119.21	123.67
2	B	301	R3M	O5M-C1M-O1M	-2.19	104.78	109.97
2	A	301	R3M	C2P-C4B-C1C	2.15	120.46	113.32
2	B	301	R3M	C2P-C4B-C1C	2.14	120.43	113.32
2	D	301	R3M	O2M-C2M-C1M	-2.14	104.86	110.05
2	C	301	R3M	C4C-C3C-C2C	2.13	123.75	120.46
2	D	301	R3M	C21-N1A-C5A	2.12	124.52	121.39
2	D	301	R3M	C2C-C1C-C4B	-2.06	119.36	121.53
2	A	301	R3M	C23-N1C-C4C	2.05	124.42	121.39
2	B	301	R3M	C8-O7-C6	-2.04	104.46	113.29
2	C	301	R3M	C3P-C2P-C4B	-2.03	116.97	121.49
2	D	301	R3M	C4C-C3C-C2C	2.03	123.59	120.46
2	C	301	R3M	O1-C2-C3	-2.02	102.64	108.61
2	D	301	R3M	O4M-C4M-C3M	-2.02	105.69	110.35
2	D	301	R3M	O7-C8-C9	-2.01	102.29	109.92

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	301	R3M	O4-C5-C6-O7
2	B	301	R3M	C22-C21-N1A-C11
2	B	301	R3M	C22-C21-N1A-C5A
2	B	301	R3M	O7-C8-C9-N3T

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Mol	Chain	Res	Type	Atoms
2	C	301	R3M	C3-C2-O1-C7P
2	A	301	R3M	O1-C2-C3-O4
2	A	301	R3M	O4-C5-C6-O7
2	C	301	R3M	C12-C11-N1A-C5A
2	C	301	R3M	C8-C9-N3T-C4T
2	A	301	R3M	C12-C11-N1A-C5A
2	C	301	R3M	C12-C11-N1A-C21
2	B	301	R3M	O4-C5-C6-O7
2	A	301	R3M	C9-C8-O7-C6
2	B	301	R3M	C3P-C2P-C4B-C1C
2	B	301	R3M	C5-C6-O7-C8
2	C	301	R3M	C2-C3-O4-C5
2	B	301	R3M	C6-C5-O4-C3
2	B	301	R3M	C1P-C2P-C4B-C1C
2	B	301	R3M	C9-C8-O7-C6
2	A	301	R3M	C12-C11-N1A-C21
2	C	301	R3M	C5-C6-O7-C8
2	D	301	R3M	O1-C2-C3-O4
2	C	301	R3M	C3P-C2P-C4B-C1C
2	D	301	R3M	C1P-C2P-C4B-C2A
2	A	301	R3M	C1P-C2P-C4B-C1C
2	C	301	R3M	C1P-C2P-C4B-C1C
2	A	301	R3M	C6-C5-O4-C3

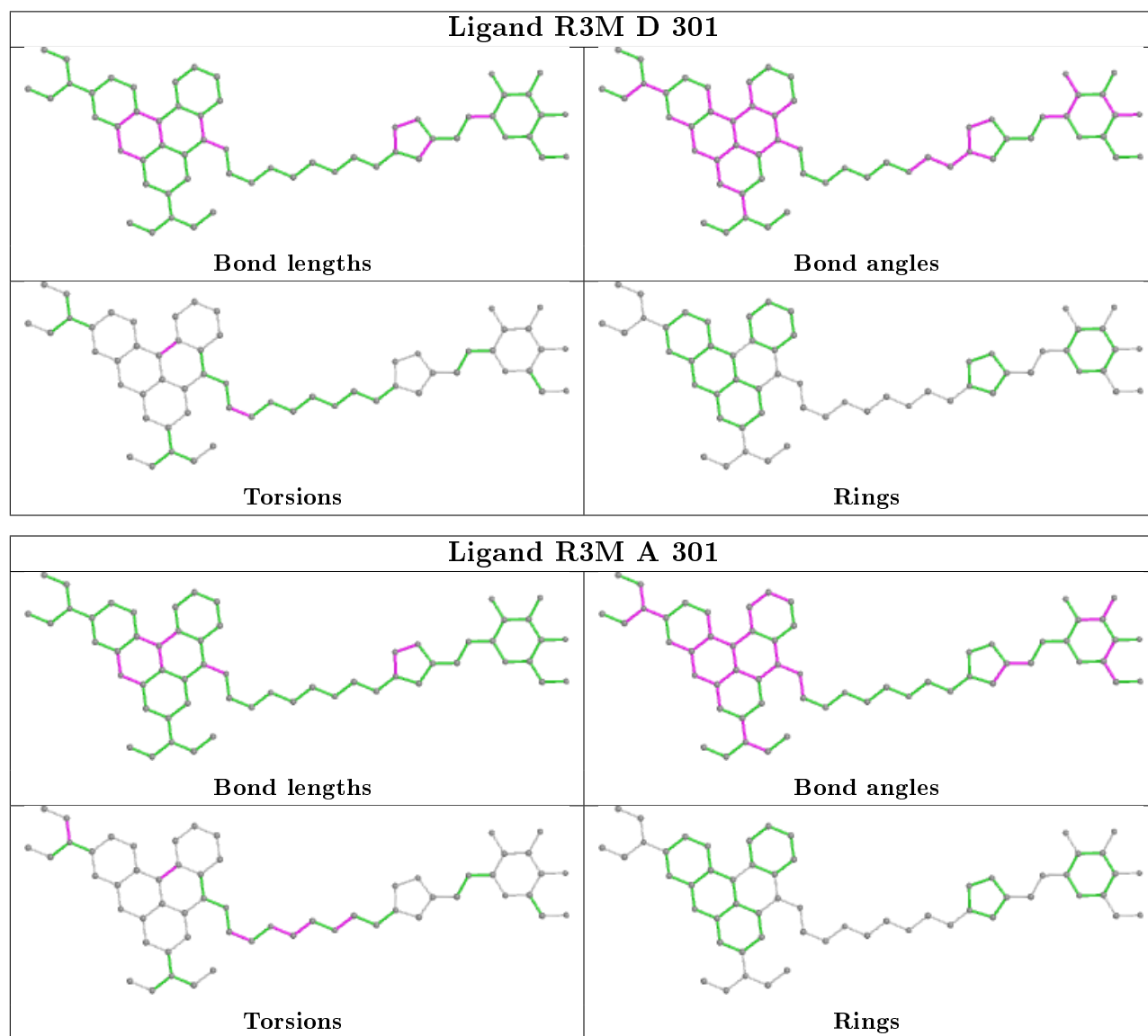
There are no ring outliers.

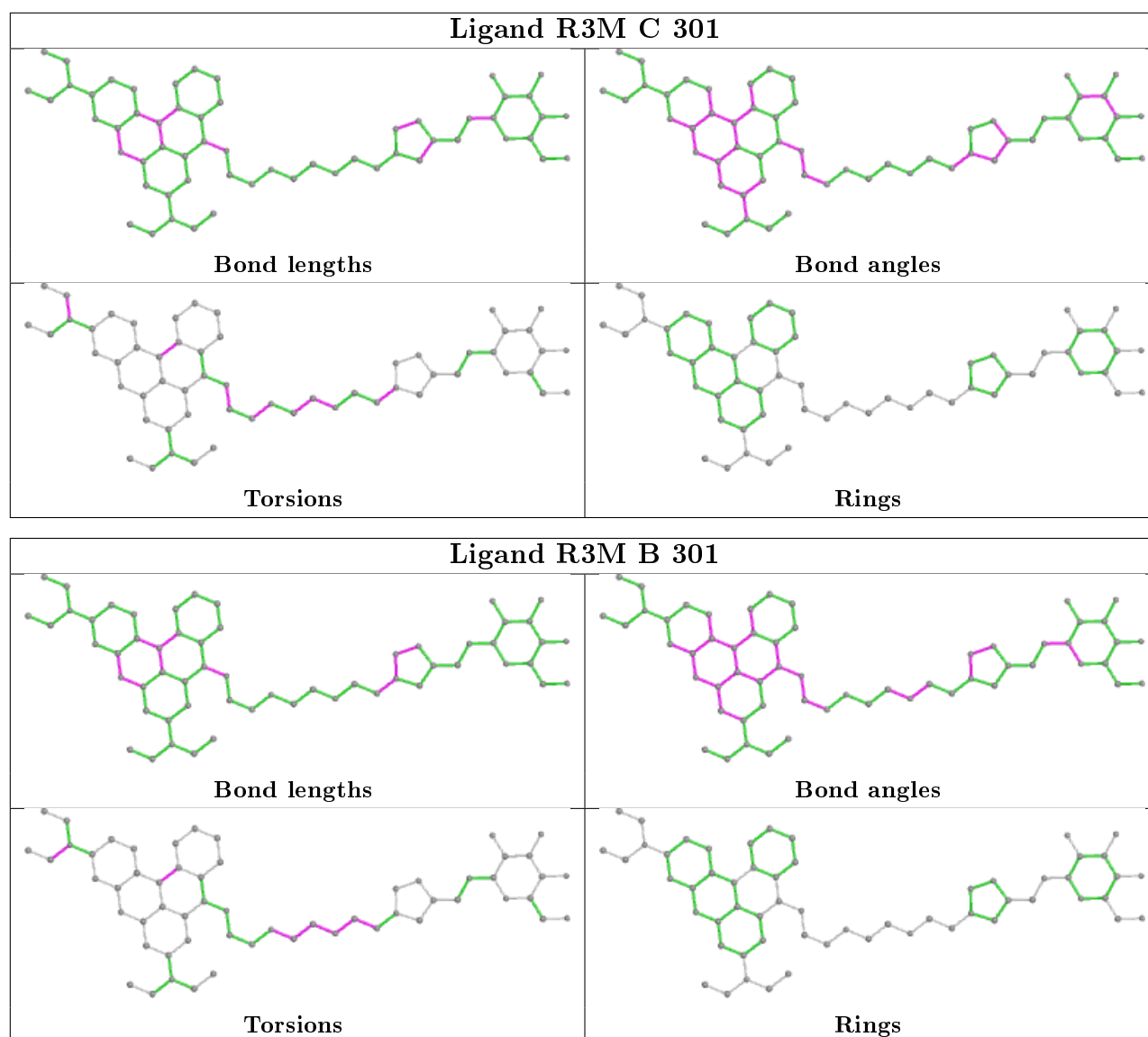
3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	R3M	3	0
2	C	301	R3M	3	0
2	B	301	R3M	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	A	237/237 (100%)	-0.30	4 (1%) 70 74	17, 26, 48, 72	0
1	B	237/237 (100%)	-0.26	4 (1%) 70 74	19, 31, 54, 69	0
1	C	237/237 (100%)	-0.30	1 (0%) 92 93	17, 25, 47, 61	0
1	D	237/237 (100%)	-0.25	4 (1%) 70 74	19, 27, 51, 72	0
All	All	948/948 (100%)	-0.28	13 (1%) 75 78	17, 27, 50, 72	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	119	SER	4.2
1	D	119	SER	4.0
1	B	204	SER	3.0
1	A	122	GLU	2.9
1	B	119	SER	2.8
1	A	120	THR	2.8
1	B	122	GLU	2.5
1	D	122	GLU	2.4
1	D	118	ASN	2.4
1	B	118	ASN	2.2
1	C	118	ASN	2.2
1	D	120	THR	2.1
1	A	118	ASN	2.1

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

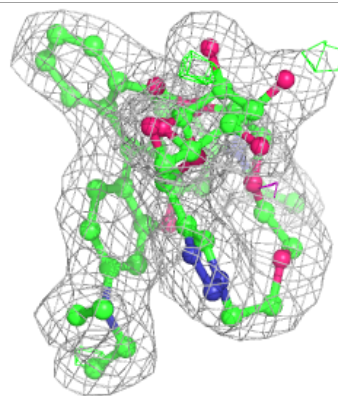
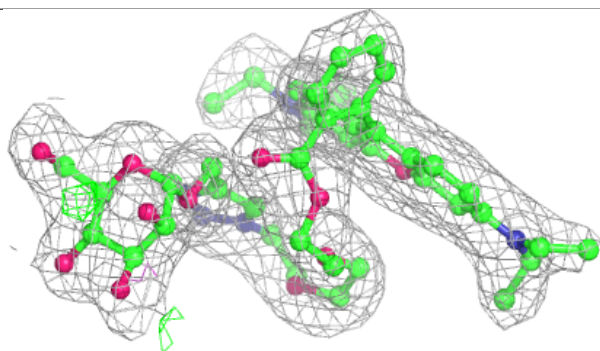
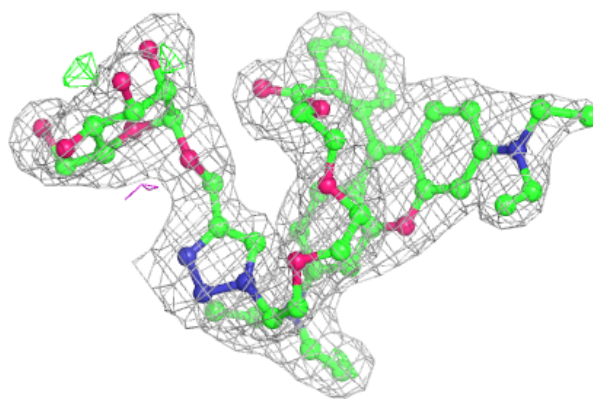
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	R3M	B	301	59/59	0.95	0.12	29,39,42,44	0
2	R3M	A	301	59/59	0.96	0.10	23,37,43,46	0
2	R3M	C	301	59/59	0.96	0.10	18,23,30,31	0
2	R3M	D	301	59/59	0.96	0.12	22,27,31,34	0
3	MN	B	302	1/1	0.98	0.10	35,35,35,35	0
4	CA	B	303	1/1	0.99	0.10	31,31,31,31	0
3	MN	D	302	1/1	0.99	0.08	25,25,25,25	0
4	CA	A	303	1/1	0.99	0.07	19,19,19,19	0
3	MN	C	302	1/1	0.99	0.12	22,22,22,22	0
3	MN	A	302	1/1	0.99	0.12	26,26,26,26	0
4	CA	C	303	1/1	0.99	0.07	18,18,18,18	0
4	CA	D	303	1/1	1.00	0.08	20,20,20,20	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

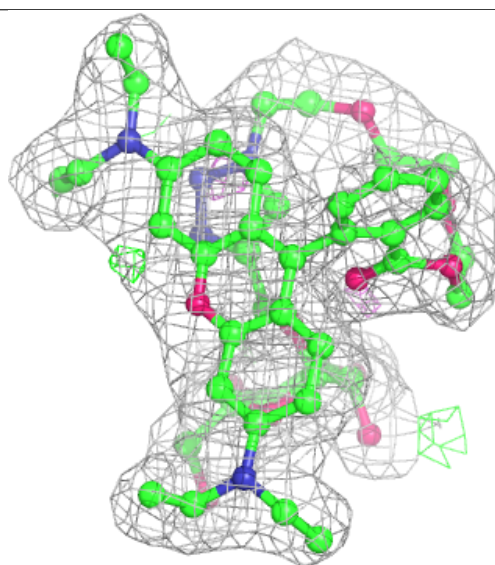
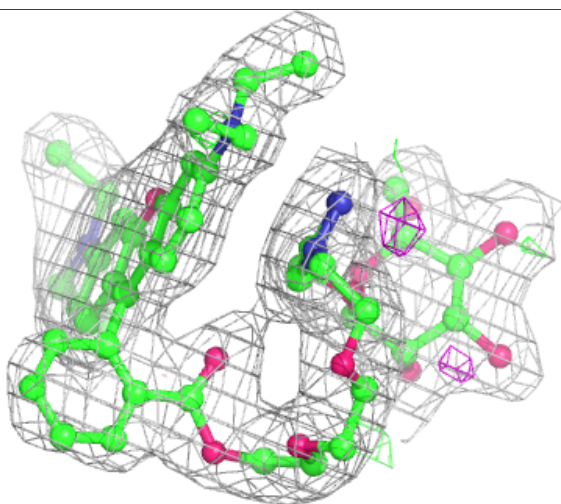
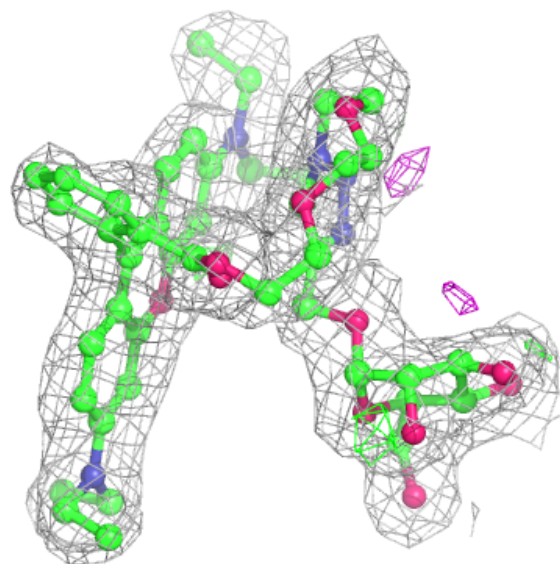
Electron density around R3M B 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



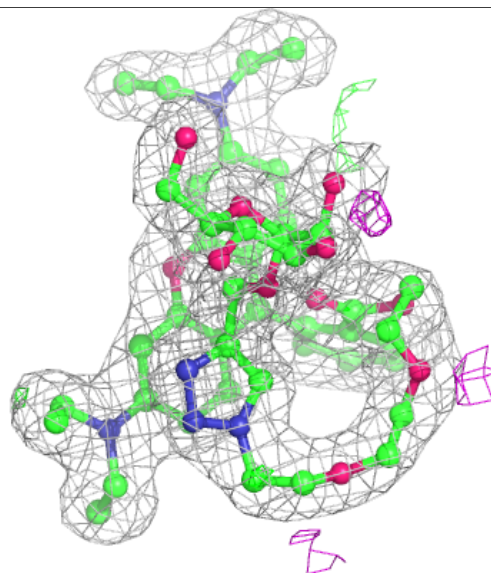
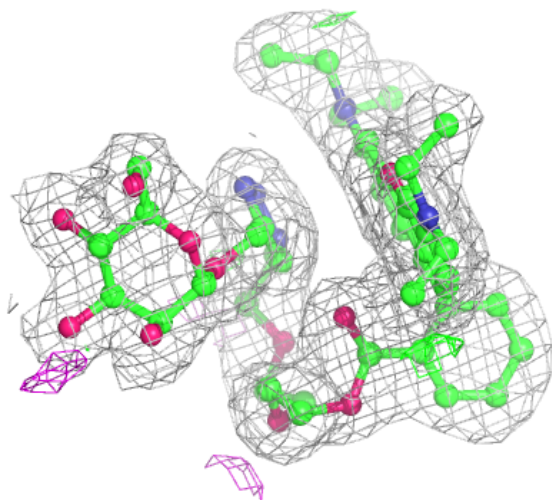
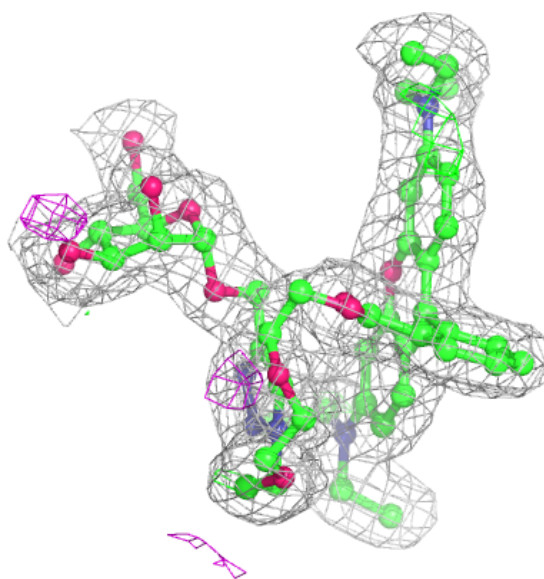
Electron density around R3M A 301:

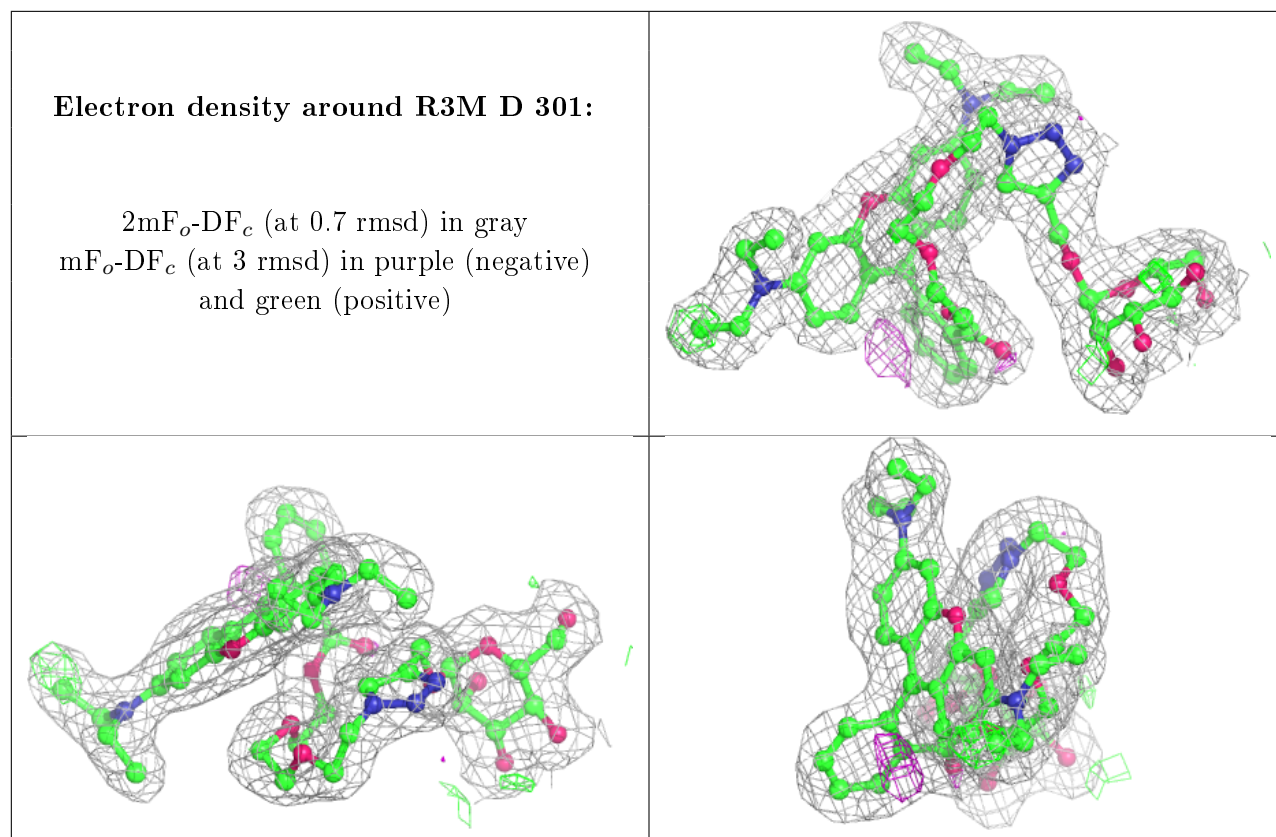
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around R3M C 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.