Full wwPDB X-ray Structure Validation Report ⓘ

Dec 1, 2022 – 12:27 am GMT

PDB ID	:	6S99
Title	:	Dimethylated fusion protein of RSL and trimeric coiled coil in complex with cucurbit[7]uril
Authors	:	Ramberg, K.; Engilberge, S.; Crowley, P.B.
Deposited on	:	2019-07-11
Resolution	:	2.65 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 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:

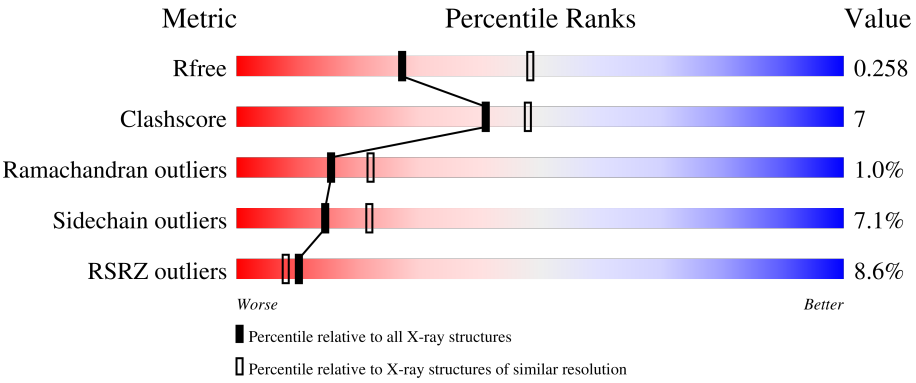
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.65 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	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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

Mol	Chain	Length	Quality of chain
1	A	114	7% 83% 15% ••
1	B	114	5% 79% 18% •••
1	C	114	6% 81% 18% •
1	D	114	11% 84% 13% ••
1	E	114	9% 85% 14% •

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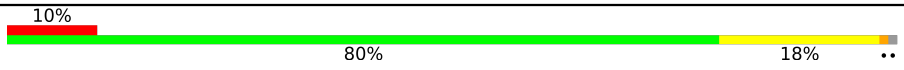
Mol	Chain	Length	Quality of chain
1	F	114	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	SNM	A	204	-	-	-	X
1	SNM	B	204	-	-	-	X
1	MLY	B	219	-	-	-	X
1	MLY	C	219	-	-	-	X
1	SNM	D	204	-	-	-	X
1	SNM	E	204	-	-	-	X
1	SNM	F	204	-	-	-	X
1	MLY	F	211	-	-	-	X
3	QQ7	A	403	X	-	-	-
3	QQ7	B	403	X	-	-	-
3	QQ7	C	403	X	-	-	-
3	QQ7	D	403	X	-	-	-
3	QQ7	E	403	X	-	-	-
3	QQ7	F	403	X	-	-	-

2 Entry composition

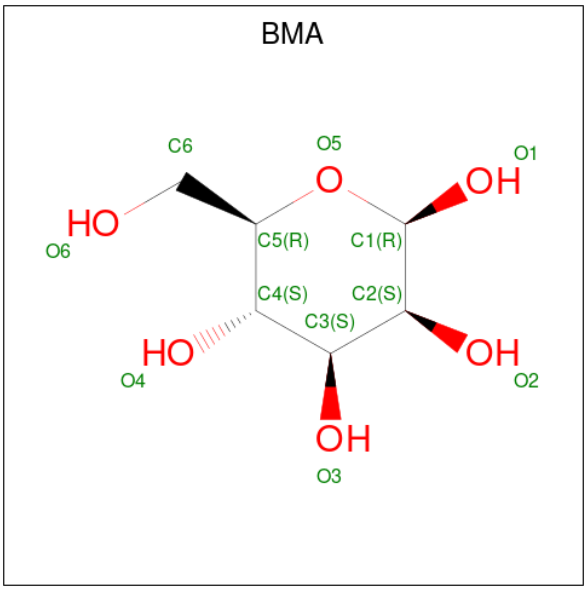
There are 4 unique types of molecules in this entry. The entry contains 5590 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 4dzn-RSL,Fucose-binding lectin protein,Fucose-binding lectin protein.

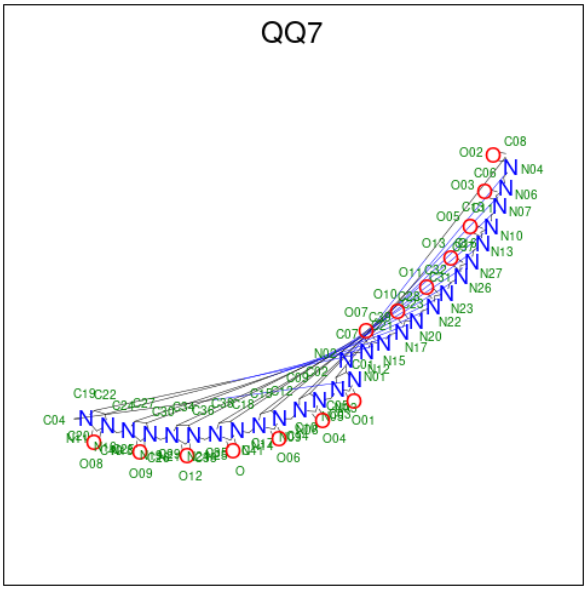
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	113	Total	C	N	O	S	0	0	0
			805	506	140	157	2			
1	B	113	Total	C	N	O	S	0	0	0
			805	506	140	157	2			
1	C	113	Total	C	N	O	S	0	0	0
			805	506	140	157	2			
1	D	113	Total	C	N	O	S	0	0	0
			805	506	140	157	2			
1	E	113	Total	C	N	O	S	0	0	0
			805	506	140	157	2			
1	F	113	Total	C	N	O	S	0	0	0
			805	506	140	157	2			

- Molecule 2 is beta-D-mannopyranose (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 12 6 6	0	0
2	A	1	Total C O 12 6 6	0	0
2	B	1	Total C O 12 6 6	0	0
2	B	1	Total C O 12 6 6	0	0
2	C	1	Total C O 12 6 6	0	0
2	C	1	Total C O 12 6 6	0	0
2	D	1	Total C O 12 6 6	0	0
2	D	1	Total C O 12 6 6	0	0
2	E	1	Total C O 12 6 6	0	0
2	E	1	Total C O 12 6 6	0	0
2	F	1	Total C O 12 6 6	0	0
2	F	1	Total C O 12 6 6	0	0

- Molecule 3 is cucurbit[7]uril (three-letter code: QQ7) (formula: $C_{42}H_{42}N_{28}O_{14}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			84	42	28	14		
3	B	1	Total	C	N	O	0	0
			84	42	28	14		
3	C	1	Total	C	N	O	0	0
			84	42	28	14		
3	D	1	Total	C	N	O	0	0
			84	42	28	14		
3	E	1	Total	C	N	O	0	0
			84	42	28	14		
3	F	1	Total	C	N	O	0	0
			84	42	28	14		

- Molecule 4 is water.

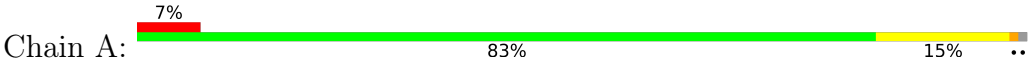
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	18	Total	O	0	0
			18	18		
4	B	21	Total	O	0	0
			21	21		
4	C	21	Total	O	0	0
			21	21		
4	D	12	Total	O	0	0
			12	12		
4	E	18	Total	O	0	0
			18	18		
4	F	22	Total	O	0	0
			22	22		

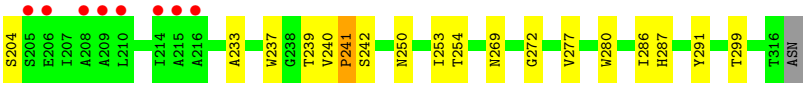
3 Residue-property plots (i)

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: 4dzn-RSL,Fucose-binding lectin protein,Fucose-binding lectin protein

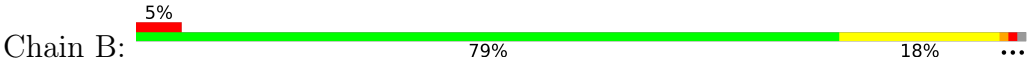
Chain A:

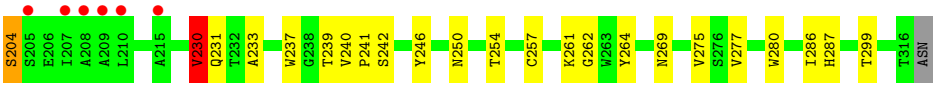




• Molecule 1: 4dzn-RSL,Fucose-binding lectin protein,Fucose-binding lectin protein

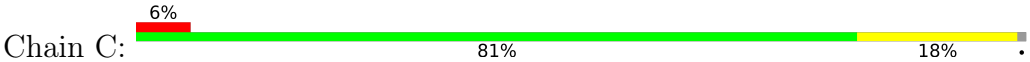
Chain B:

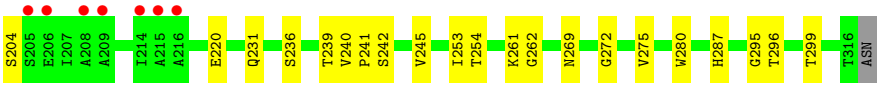




• Molecule 1: 4dzn-RSL,Fucose-binding lectin protein,Fucose-binding lectin protein

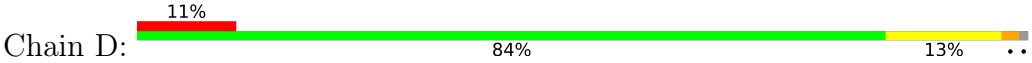
Chain C:

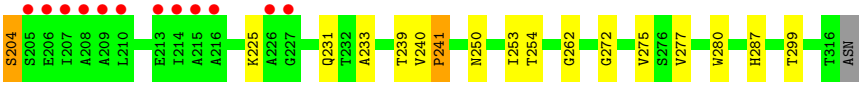




• Molecule 1: 4dzn-RSL,Fucose-binding lectin protein,Fucose-binding lectin protein

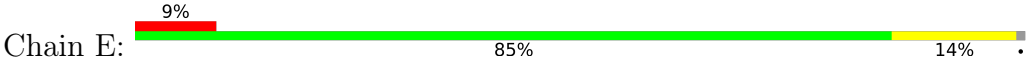
Chain D:

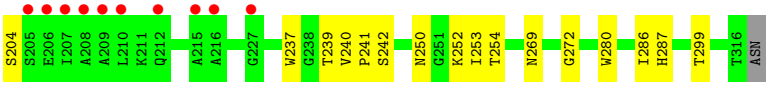




• Molecule 1: 4dzn-RSL,Fucose-binding lectin protein,Fucose-binding lectin protein

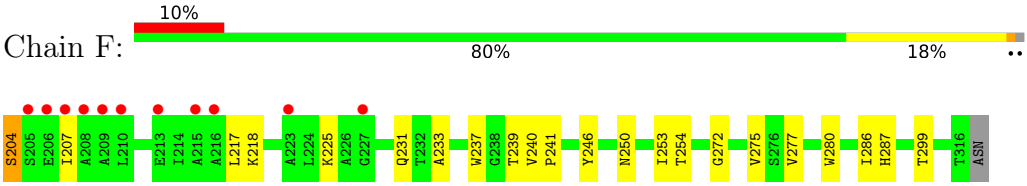
Chain E:





• Molecule 1: 4dzn-RSL,Fucose-binding lectin protein,Fucose-binding lectin protein

Chain F:


10%
80%
18%
S204
S205
E206
I207
A208
A209
L210
E213
I214
A215
A216
L217
K218
A223
L224
K225
A226
G227
Q231
T232
A233
W237
G238
T239
V240
P241
Y246
N250
I253
T254
G272
V275
S276
V277
W280
I286
H287
T299
T316
ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	51.22Å 51.24Å 111.28Å 76.80° 89.88° 60.05°	Depositor
Resolution (Å)	42.84 – 2.65 42.84 – 2.65	Depositor EDS
% Data completeness (in resolution range)	97.3 (42.84-2.65) 96.0 (42.84-2.65)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.65 (at 2.65Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.225 , 0.257 0.226 , 0.258	Depositor DCC
R_{free} test set	1410 reflections (5.26%)	wwPDB-VP
Wilson B-factor (Å^2)	62.4	Xtriage
Anisotropy	0.678	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.427 for -h+k,-h,-k+l 0.427 for -k,h-k,h-k+l 0.368 for h,h-k,-l 0.368 for -h+k,k,k-l 0.359 for -k,-h,-h+k-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5590	wwPDB-VP
Average B, all atoms (Å^2)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.70% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SNM, BMA, QQ7, MLY

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	0.67	0/766	0.57	0/1059
1	B	0.67	0/766	0.57	0/1059
1	C	0.67	0/766	0.57	0/1059
1	D	0.67	0/766	0.57	0/1059
1	E	0.68	0/766	0.57	0/1059
1	F	0.68	0/766	0.57	0/1059
All	All	0.67	0/4596	0.57	0/6354

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	B	0	1
1	D	0	1
1	F	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	204	SNM	Mainchain
1	D	204	SNM	Mainchain
1	F	204	SNM	Mainchain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	805	0	703	12	0
1	B	805	0	702	16	0
1	C	805	0	702	12	0
1	D	805	0	702	10	0
1	E	805	0	702	11	0
1	F	805	0	701	13	0
2	A	24	0	24	0	0
2	B	24	0	24	0	0
2	C	24	0	24	0	0
2	D	24	0	24	0	0
2	E	24	0	24	0	0
2	F	24	0	24	0	0
3	A	84	0	42	0	0
3	B	84	0	42	2	0
3	C	84	0	42	2	0
3	D	84	0	42	1	0
3	E	84	0	42	0	0
3	F	84	0	42	0	0
4	A	18	0	0	0	0
4	B	21	0	0	0	0
4	C	21	0	0	0	0
4	D	12	0	0	0	0
4	E	18	0	0	0	0
4	F	22	0	0	0	0
All	All	5590	0	4608	72	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 (72) 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:E:240:VAL:N	1:E:241:PRO:HA	2.05	0.72
1:B:240:VAL:N	1:B:241:PRO:HA	2.05	0.70
1:D:240:VAL:N	1:D:241:PRO:HA	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:240:VAL:N	1:C:241:PRO:HA	2.08	0.69
1:A:240:VAL:N	1:A:241:PRO:HA	2.08	0.68
1:F:240:VAL:N	1:F:241:PRO:HA	2.10	0.65
1:F:204:SNM:C2	1:F:207:ILE:CB	2.76	0.64
1:C:240:VAL:H	1:C:241:PRO:HA	1.66	0.60
1:E:240:VAL:H	1:E:241:PRO:HA	1.67	0.60
1:B:240:VAL:H	1:B:241:PRO:HA	1.65	0.59
1:D:240:VAL:HG12	1:D:241:PRO:O	2.03	0.58
1:D:240:VAL:H	1:D:241:PRO:HA	1.71	0.56
1:F:233:ALA:HB1	1:F:277:VAL:HG12	1.88	0.56
1:D:204:SNM:C2	1:D:204:SNM:O	2.55	0.55
1:A:240:VAL:H	1:A:241:PRO:HA	1.73	0.53
1:F:204:SNM:C2	1:F:204:SNM:O	2.57	0.53
1:B:204:SNM:O	1:B:204:SNM:C2	2.57	0.53
1:A:280:TRP:CE2	1:A:287:HIS:HB2	2.44	0.52
1:F:240:VAL:H	1:F:241:PRO:HA	1.75	0.52
1:E:204:SNM:C2	1:E:204:SNM:O	2.57	0.52
1:C:240:VAL:HG12	1:C:241:PRO:O	2.10	0.51
1:F:240:VAL:HG12	1:F:241:PRO:O	2.12	0.49
1:A:204:SNM:O	1:A:204:SNM:C2	2.59	0.49
1:F:237:TRP:CG	1:F:286:ILE:HD13	2.47	0.49
1:F:253:ILE:HD11	1:F:272:GLY:HA3	1.94	0.49
1:D:253:ILE:HD11	1:D:272:GLY:HA3	1.94	0.49
1:E:253:ILE:HD11	1:E:272:GLY:HA3	1.95	0.49
1:E:240:VAL:HG12	1:E:241:PRO:O	2.13	0.48
1:B:280:TRP:CE2	1:B:287:HIS:HB2	2.49	0.48
1:D:231:GLN:OE1	1:D:275:VAL:HG12	2.14	0.48
1:A:233:ALA:HB1	1:A:277:VAL:HG12	1.95	0.47
1:C:231:GLN:OE1	1:C:275:VAL:HG12	2.15	0.46
1:B:233:ALA:HB1	1:B:277:VAL:HG12	1.98	0.46
1:B:246:TYR:CE1	1:B:277:VAL:HG21	2.50	0.46
1:B:237:TRP:CG	1:B:286:ILE:HD13	2.51	0.46
1:B:240:VAL:HG12	1:B:241:PRO:O	2.16	0.46
1:B:257:CYS:HB2	1:B:264:TYR:CZ	2.51	0.45
1:C:204:SNM:O	1:C:204:SNM:C2	2.64	0.45
1:B:240:VAL:HB	1:B:241:PRO:C	2.38	0.45
1:A:240:VAL:HG12	1:A:241:PRO:O	2.17	0.44
1:C:261:MLY:CH2	3:C:403:QQ7:C37	2.96	0.44
1:C:262:GLY:HA3	3:C:403:QQ7:O12	2.18	0.44
1:B:230:VAL:HG22	1:C:296:THR:HA	2.00	0.44
1:C:280:TRP:CE2	1:C:287:HIS:HB2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:TRP:CE2	1:A:242:SER:HB2	2.53	0.43
1:A:237:TRP:CG	1:A:286:ILE:HD13	2.54	0.43
1:A:291:TYR:CE2	1:C:245:VAL:HG21	2.54	0.43
1:D:262:GLY:HA3	3:D:403:QQ7:O12	2.19	0.43
1:F:280:TRP:CE2	1:F:287:HIS:HB2	2.54	0.43
1:F:240:VAL:HB	1:F:241:PRO:C	2.39	0.42
1:E:240:VAL:HB	1:E:241:PRO:C	2.39	0.42
1:E:240:VAL:N	1:E:241:PRO:CA	2.80	0.42
1:F:231:GLN:OE1	1:F:275:VAL:HG12	2.19	0.42
1:B:237:TRP:CE2	1:B:242:SER:HB2	2.55	0.42
1:A:253:ILE:HD11	1:A:272:GLY:HA3	2.02	0.42
1:E:252:MLY:HB2	1:E:252:MLY:HE2	1.93	0.42
1:D:233:ALA:HB1	1:D:277:VAL:HG12	2.01	0.42
1:E:280:TRP:CE2	1:E:287:HIS:HB2	2.54	0.42
1:B:231:GLN:OE1	1:B:275:VAL:HG12	2.20	0.42
1:F:240:VAL:HB	1:F:241:PRO:CA	2.50	0.42
1:B:240:VAL:N	1:B:241:PRO:CA	2.79	0.41
1:D:280:TRP:CE2	1:D:287:HIS:HB2	2.55	0.41
1:E:237:TRP:CG	1:E:286:ILE:HD13	2.54	0.41
1:F:246:TYR:CE1	1:F:277:VAL:HG21	2.55	0.41
1:B:261:MLY:HH21	3:B:403:QQ7:C37	2.50	0.41
1:C:236:SER:HA	1:C:242:SER:O	2.19	0.41
1:D:240:VAL:CG1	1:D:241:PRO:O	2.69	0.41
1:A:240:VAL:HB	1:A:241:PRO:C	2.41	0.41
1:B:262:GLY:HA3	3:B:403:QQ7:O12	2.20	0.41
1:C:253:ILE:HD11	1:C:272:GLY:HA3	2.03	0.41
1:E:237:TRP:CE2	1:E:242:SER:HB2	2.56	0.41
1:A:240:VAL:HB	1:A:241:PRO:CA	2.51	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	104/114 (91%)	96 (92%)	7 (7%)	1 (1%)	15 22
1	B	104/114 (91%)	96 (92%)	7 (7%)	1 (1%)	15 22
1	C	104/114 (91%)	95 (91%)	7 (7%)	2 (2%)	8 10
1	D	104/114 (91%)	97 (93%)	6 (6%)	1 (1%)	15 22
1	E	104/114 (91%)	97 (93%)	7 (7%)	0	100 100
1	F	104/114 (91%)	93 (89%)	10 (10%)	1 (1%)	15 22
All	All	624/684 (91%)	574 (92%)	44 (7%)	6 (1%)	15 22

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	220	GLU
1	F	217	LEU
1	B	230	VAL
1	C	295	GLY
1	D	241	PRO
1	A	241	PRO

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	66/78 (85%)	61 (92%)	5 (8%)	13 20
1	B	66/78 (85%)	60 (91%)	6 (9%)	9 13
1	C	66/78 (85%)	62 (94%)	4 (6%)	18 29
1	D	66/78 (85%)	62 (94%)	4 (6%)	18 29
1	E	66/78 (85%)	61 (92%)	5 (8%)	13 20
1	F	66/78 (85%)	62 (94%)	4 (6%)	18 29
All	All	396/468 (85%)	368 (93%)	28 (7%)	14 22

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	239	THR
1	A	250	ASN
1	A	254	THR
1	A	269	ASN
1	A	299	THR
1	B	230	VAL
1	B	239	THR
1	B	250	ASN
1	B	254	THR
1	B	269	ASN
1	B	299	THR
1	C	239	THR
1	C	254	THR
1	C	269	ASN
1	C	299	THR
1	D	239	THR
1	D	250	ASN
1	D	254	THR
1	D	299	THR
1	E	239	THR
1	E	250	ASN
1	E	254	THR
1	E	269	ASN
1	E	299	THR
1	F	239	THR
1	F	250	ASN
1	F	254	THR
1	F	299	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	274	ASN
1	F	274	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

48 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
1	MLY	D	218	1	3,4,11	0.81	0	2,4,13	1.35	0
1	SNM	F	204	1	4,6,8	1.23	0	5,7,10	0.88	0
1	MLY	E	252	1	9,10,11	0.50	0	6,11,13	0.06	0
1	MLY	B	219	1	3,4,11	0.81	0	2,4,13	1.36	0
1	MLY	D	219	1	3,4,11	0.81	0	2,4,13	1.41	0
1	MLY	B	225	1	3,4,11	0.83	0	2,4,13	1.41	0
1	MLY	D	310	1	9,10,11	0.49	0	6,11,13	0.05	0
1	MLY	D	211	1	3,4,11	0.81	0	2,4,13	1.35	0
1	MLY	F	219	1	3,4,11	0.82	0	2,4,13	1.38	0
1	MLY	C	252	1	9,10,11	0.49	0	6,11,13	0.06	0
1	MLY	E	211	1	3,4,11	0.81	0	2,4,13	1.36	0
1	MLY	B	310	1	9,10,11	0.50	0	6,11,13	0.05	0
1	MLY	C	225	1	3,4,11	0.81	0	2,4,13	1.35	0
1	SNM	E	204	1	4,6,8	1.24	0	5,7,10	0.89	0
1	MLY	C	310	1	9,10,11	0.49	0	6,11,13	0.06	0
1	SNM	A	204	1	4,6,8	1.22	0	5,7,10	0.89	0
1	MLY	F	310	1	9,10,11	0.50	0	6,11,13	0.05	0
1	SNM	D	204	1	4,6,8	1.24	0	5,7,10	0.88	0
1	SNM	B	204	1	4,6,8	1.24	0	5,7,10	0.89	0
1	MLY	E	261	1	9,10,11	0.49	0	6,11,13	0.06	0
1	MLY	C	211	1	3,4,11	0.82	0	2,4,13	1.34	0
1	MLY	A	252	1	9,10,11	0.50	0	6,11,13	0.05	0
1	MLY	B	252	1	9,10,11	0.49	0	6,11,13	0.06	0
1	MLY	A	225	1	3,4,11	0.82	0	2,4,13	1.38	0
1	MLY	E	225	1	3,4,11	0.82	0	2,4,13	1.39	0
1	MLY	E	218	1	3,4,11	0.82	0	2,4,13	1.35	0
1	MLY	A	219	1	3,4,11	0.80	0	2,4,13	1.34	0
1	SNM	C	204	1	4,6,8	1.22	0	5,7,10	0.88	0
1	MLY	A	218	1	3,4,11	0.82	0	2,4,13	1.40	0
1	MLY	E	219	1	3,4,11	0.81	0	2,4,13	1.37	0
1	MLY	E	310	1	9,10,11	0.49	0	6,11,13	0.05	0
1	MLY	C	261	1	9,10,11	0.50	0	6,11,13	0.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	MLY	F	252	1	9,10,11	0.49	0	6,11,13	0.05	0
1	MLY	B	218	1	3,4,11	0.82	0	2,4,13	1.39	0
1	MLY	A	211	1	3,4,11	0.81	0	2,4,13	1.35	0
1	MLY	F	261	1	9,10,11	0.50	0	6,11,13	0.06	0
1	MLY	C	219	1	3,4,11	0.83	0	2,4,13	1.35	0
1	MLY	F	225	1	3,4,11	0.81	0	2,4,13	1.43	1 (50%)
1	MLY	B	211	1	3,4,11	0.82	0	2,4,13	1.35	0
1	MLY	D	252	1	9,10,11	0.50	0	6,11,13	0.06	0
1	MLY	F	211	1	3,4,11	0.81	0	2,4,13	1.39	0
1	MLY	F	218	1	3,4,11	0.80	0	2,4,13	1.42	1 (50%)
1	MLY	C	218	1	3,4,11	0.81	0	2,4,13	1.39	0
1	MLY	A	310	1	9,10,11	0.50	0	6,11,13	0.05	0
1	MLY	A	261	1	9,10,11	0.50	0	6,11,13	0.06	0
1	MLY	B	261	1	9,10,11	0.49	0	6,11,13	0.06	0
1	MLY	D	261	1	9,10,11	0.50	0	6,11,13	0.06	0
1	MLY	D	225	1	3,4,11	0.82	0	2,4,13	1.43	1 (50%)

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
1	MLY	D	218	1	-	0/0/2/11	-
1	SNM	F	204	1	-	0/4/6/10	-
1	MLY	E	252	1	-	4/8/9/11	-
1	MLY	B	219	1	-	0/0/2/11	-
1	MLY	D	219	1	-	0/0/2/11	-
1	MLY	B	225	1	-	0/0/2/11	-
1	MLY	D	310	1	-	6/8/9/11	-
1	MLY	D	211	1	-	0/0/2/11	-
1	MLY	F	219	1	-	0/0/2/11	-
1	MLY	C	252	1	-	1/8/9/11	-
1	MLY	E	211	1	-	0/0/2/11	-
1	MLY	B	310	1	-	5/8/9/11	-
1	MLY	C	225	1	-	0/0/2/11	-
1	SNM	E	204	1	-	0/4/6/10	-
1	MLY	C	310	1	-	5/8/9/11	-
1	SNM	A	204	1	-	0/4/6/10	-
1	MLY	F	310	1	-	6/8/9/11	-
1	SNM	D	204	1	-	0/4/6/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SNM	B	204	1	-	0/4/6/10	-
1	MLY	E	261	1	-	4/8/9/11	-
1	MLY	C	211	1	-	0/0/2/11	-
1	MLY	A	252	1	-	1/8/9/11	-
1	MLY	B	252	1	-	1/8/9/11	-
1	MLY	A	225	1	-	0/0/2/11	-
1	MLY	E	225	1	-	0/0/2/11	-
1	MLY	E	218	1	-	0/0/2/11	-
1	MLY	A	219	1	-	0/0/2/11	-
1	SNM	C	204	1	-	0/4/6/10	-
1	MLY	A	218	1	-	0/0/2/11	-
1	MLY	E	219	1	-	0/0/2/11	-
1	MLY	E	310	1	-	5/8/9/11	-
1	MLY	C	261	1	-	2/8/9/11	-
1	MLY	F	252	1	-	1/8/9/11	-
1	MLY	B	218	1	-	0/0/2/11	-
1	MLY	A	211	1	-	0/0/2/11	-
1	MLY	F	261	1	-	4/8/9/11	-
1	MLY	C	219	1	-	0/0/2/11	-
1	MLY	F	225	1	-	0/0/2/11	-
1	MLY	B	211	1	-	0/0/2/11	-
1	MLY	D	252	1	-	1/8/9/11	-
1	MLY	F	211	1	-	0/0/2/11	-
1	MLY	F	218	1	-	0/0/2/11	-
1	MLY	C	218	1	-	0/0/2/11	-
1	MLY	A	310	1	-	5/8/9/11	-
1	MLY	A	261	1	-	4/8/9/11	-
1	MLY	B	261	1	-	3/8/9/11	-
1	MLY	D	261	1	-	3/8/9/11	-
1	MLY	D	225	1	-	0/0/2/11	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	225	MLY	O-C-CA	-2.01	117.91	124.28
1	D	225	MLY	O-C-CA	-2.01	117.92	124.28
1	F	218	MLY	O-C-CA	-2.01	117.93	124.28

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	310	MLY	N-CA-CB-CG
1	A	310	MLY	C-CA-CB-CG
1	B	310	MLY	N-CA-CB-CG
1	B	310	MLY	C-CA-CB-CG
1	C	310	MLY	N-CA-CB-CG
1	C	310	MLY	C-CA-CB-CG
1	D	310	MLY	N-CA-CB-CG
1	D	310	MLY	C-CA-CB-CG
1	D	310	MLY	O-C-CA-CB
1	E	310	MLY	N-CA-CB-CG
1	E	310	MLY	C-CA-CB-CG
1	F	310	MLY	N-CA-CB-CG
1	F	310	MLY	C-CA-CB-CG
1	F	310	MLY	O-C-CA-CB
1	A	261	MLY	CD-CE-NZ-CH1
1	A	310	MLY	CD-CE-NZ-CH1
1	A	310	MLY	CD-CE-NZ-CH2
1	B	261	MLY	CD-CE-NZ-CH1
1	B	261	MLY	CD-CE-NZ-CH2
1	B	310	MLY	CD-CE-NZ-CH1
1	B	310	MLY	CD-CE-NZ-CH2
1	C	310	MLY	CD-CE-NZ-CH1
1	C	310	MLY	CD-CE-NZ-CH2
1	D	310	MLY	CD-CE-NZ-CH1
1	D	310	MLY	CD-CE-NZ-CH2
1	E	252	MLY	CD-CE-NZ-CH1
1	E	252	MLY	CD-CE-NZ-CH2
1	E	261	MLY	CD-CE-NZ-CH2
1	E	310	MLY	CD-CE-NZ-CH1
1	E	310	MLY	CD-CE-NZ-CH2
1	F	310	MLY	CD-CE-NZ-CH1
1	F	310	MLY	CD-CE-NZ-CH2
1	A	252	MLY	CG-CD-CE-NZ
1	F	252	MLY	CG-CD-CE-NZ
1	B	252	MLY	CG-CD-CE-NZ
1	C	252	MLY	CG-CD-CE-NZ
1	D	252	MLY	CG-CD-CE-NZ
1	E	252	MLY	CG-CD-CE-NZ
1	F	261	MLY	CG-CD-CE-NZ
1	A	261	MLY	CD-CE-NZ-CH2
1	D	261	MLY	CD-CE-NZ-CH1
1	D	261	MLY	CD-CE-NZ-CH2

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Mol	Chain	Res	Type	Atoms
1	E	261	MLY	CD-CE-NZ-CH1
1	F	261	MLY	CD-CE-NZ-CH1
1	F	261	MLY	CD-CE-NZ-CH2
1	C	261	MLY	CG-CD-CE-NZ
1	F	310	MLY	CG-CD-CE-NZ
1	D	310	MLY	CG-CD-CE-NZ
1	E	310	MLY	CG-CD-CE-NZ
1	C	310	MLY	CG-CD-CE-NZ
1	B	310	MLY	CG-CD-CE-NZ
1	A	310	MLY	CG-CD-CE-NZ
1	B	261	MLY	CE-CD-CG-CB
1	A	261	MLY	CE-CD-CG-CB
1	C	261	MLY	CE-CD-CG-CB
1	E	261	MLY	CE-CD-CG-CB
1	F	261	MLY	CE-CD-CG-CB
1	D	261	MLY	CE-CD-CG-CB
1	E	252	MLY	CE-CD-CG-CB
1	A	261	MLY	CG-CD-CE-NZ
1	E	261	MLY	CG-CD-CE-NZ

There are no ring outliers.

9 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	F	204	SNM	2	0
1	E	252	MLY	1	0
1	E	204	SNM	1	0
1	A	204	SNM	1	0
1	D	204	SNM	1	0
1	B	204	SNM	1	0
1	C	204	SNM	1	0
1	C	261	MLY	1	0
1	B	261	MLY	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

18 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
3	QQ7	D	403	-	105,105,105	0.12	0	182,182,182	0.20	0
3	QQ7	E	403	-	105,105,105	0.12	0	182,182,182	0.20	0
2	BMA	A	402	-	12,12,12	0.45	0	17,17,17	0.50	0
2	BMA	E	401	-	12,12,12	0.45	0	17,17,17	0.55	0
3	QQ7	A	403	-	105,105,105	0.12	0	182,182,182	0.20	0
2	BMA	D	402	-	12,12,12	0.45	0	17,17,17	0.50	0
2	BMA	F	402	-	12,12,12	0.45	0	17,17,17	0.50	0
2	BMA	D	401	-	12,12,12	0.45	0	17,17,17	0.53	0
3	QQ7	B	403	-	105,105,105	0.12	0	182,182,182	0.20	0
3	QQ7	C	403	-	105,105,105	0.12	0	182,182,182	0.20	0
2	BMA	E	402	-	12,12,12	0.46	0	17,17,17	0.50	0
3	QQ7	F	403	-	105,105,105	0.12	0	182,182,182	0.21	0
2	BMA	C	401	-	12,12,12	0.45	0	17,17,17	0.53	0
2	BMA	A	401	-	12,12,12	0.45	0	17,17,17	0.54	0
2	BMA	C	402	-	12,12,12	0.46	0	17,17,17	0.51	0
2	BMA	F	401	-	12,12,12	0.46	0	17,17,17	0.54	0
2	BMA	B	402	-	12,12,12	0.44	0	17,17,17	0.51	0
2	BMA	B	401	-	12,12,12	0.46	0	17,17,17	0.53	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
3	QQ7	D	403	-	14/14/56/56	-	-
3	QQ7	E	403	-	14/14/56/56	-	-
3	QQ7	A	403	-	14/14/56/56	-	-
2	BMA	A	402	-	-	0/2/22/22	0/1/1/1
2	BMA	E	401	-	-	0/2/22/22	0/1/1/1
2	BMA	D	402	-	-	0/2/22/22	0/1/1/1
3	QQ7	B	403	-	14/14/56/56	-	-
3	QQ7	C	403	-	14/14/56/56	-	-
2	BMA	D	401	-	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BMA	F	402	-	-	0/2/22/22	0/1/1/1
2	BMA	E	402	-	-	0/2/22/22	0/1/1/1
3	QQ7	F	403	-	14/14/56/56	-	-
2	BMA	C	401	-	-	0/2/22/22	0/1/1/1
2	BMA	A	401	-	-	0/2/22/22	0/1/1/1
2	BMA	C	402	-	-	0/2/22/22	0/1/1/1
2	BMA	F	401	-	-	0/2/22/22	0/1/1/1
2	BMA	B	402	-	-	0/2/22/22	0/1/1/1
2	BMA	B	401	-	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

All (84) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	403	QQ7	N18
3	A	403	QQ7	N19
3	A	403	QQ7	N01
3	A	403	QQ7	N14
3	A	403	QQ7	N16
3	A	403	QQ7	N11
3	A	403	QQ7	N21
3	A	403	QQ7	N25
3	A	403	QQ7	N
3	A	403	QQ7	N24
3	A	403	QQ7	N05
3	A	403	QQ7	N08
3	A	403	QQ7	N09
3	A	403	QQ7	N03
3	B	403	QQ7	N18
3	B	403	QQ7	N19
3	B	403	QQ7	N01
3	B	403	QQ7	N14
3	B	403	QQ7	N16
3	B	403	QQ7	N11
3	B	403	QQ7	N21
3	B	403	QQ7	N25
3	B	403	QQ7	N
3	B	403	QQ7	N24
3	B	403	QQ7	N05
3	B	403	QQ7	N08

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Mol	Chain	Res	Type	Atom
3	B	403	QQ7	N09
3	B	403	QQ7	N03
3	C	403	QQ7	N18
3	C	403	QQ7	N19
3	C	403	QQ7	N01
3	C	403	QQ7	N14
3	C	403	QQ7	N16
3	C	403	QQ7	N11
3	C	403	QQ7	N21
3	C	403	QQ7	N25
3	C	403	QQ7	N
3	C	403	QQ7	N24
3	C	403	QQ7	N05
3	C	403	QQ7	N08
3	C	403	QQ7	N09
3	C	403	QQ7	N03
3	D	403	QQ7	N18
3	D	403	QQ7	N19
3	D	403	QQ7	N01
3	D	403	QQ7	N14
3	D	403	QQ7	N16
3	D	403	QQ7	N11
3	D	403	QQ7	N21
3	D	403	QQ7	N25
3	D	403	QQ7	N
3	D	403	QQ7	N24
3	D	403	QQ7	N05
3	D	403	QQ7	N08
3	D	403	QQ7	N09
3	D	403	QQ7	N03
3	E	403	QQ7	N18
3	E	403	QQ7	N19
3	E	403	QQ7	N01
3	E	403	QQ7	N14
3	E	403	QQ7	N16
3	E	403	QQ7	N11
3	E	403	QQ7	N21
3	E	403	QQ7	N25
3	E	403	QQ7	N
3	E	403	QQ7	N24
3	E	403	QQ7	N05
3	E	403	QQ7	N08

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Mol	Chain	Res	Type	Atom
3	E	403	QQ7	N09
3	E	403	QQ7	N03
3	F	403	QQ7	N18
3	F	403	QQ7	N19
3	F	403	QQ7	N01
3	F	403	QQ7	N14
3	F	403	QQ7	N16
3	F	403	QQ7	N11
3	F	403	QQ7	N21
3	F	403	QQ7	N25
3	F	403	QQ7	N
3	F	403	QQ7	N24
3	F	403	QQ7	N05
3	F	403	QQ7	N08
3	F	403	QQ7	N09
3	F	403	QQ7	N03

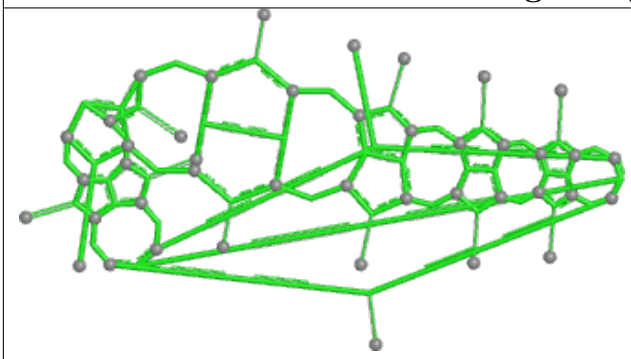
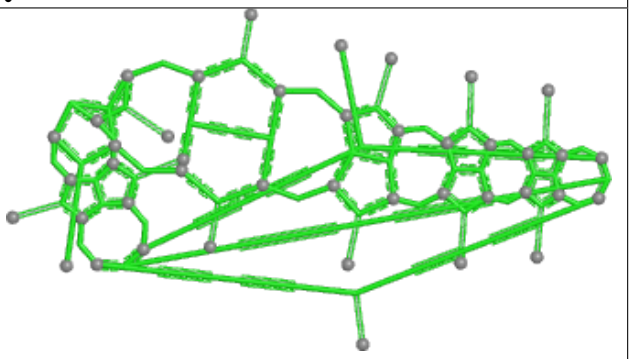
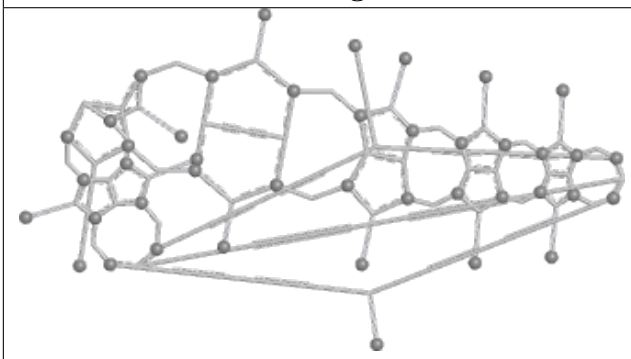
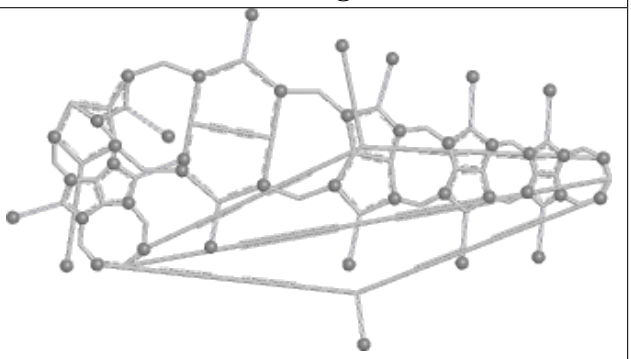
There are no torsion outliers.

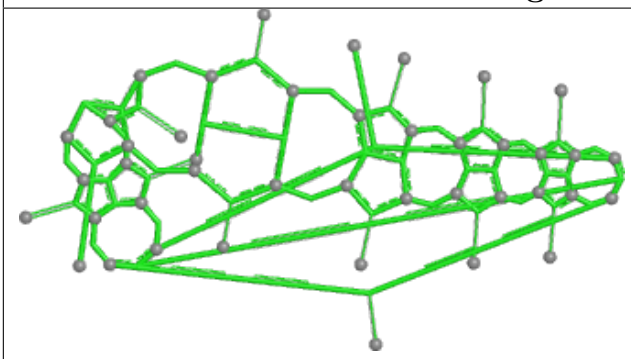
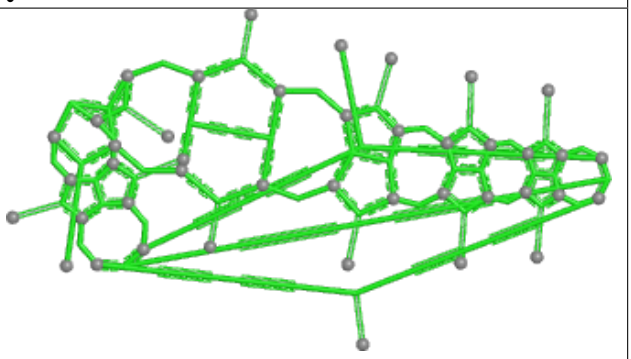
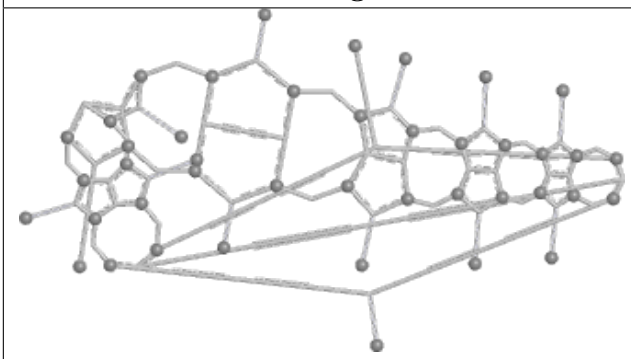
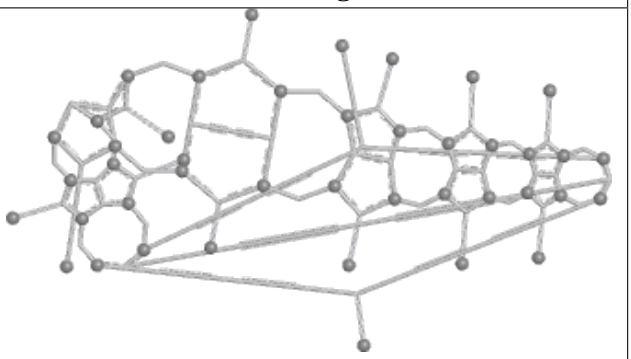
There are no ring outliers.

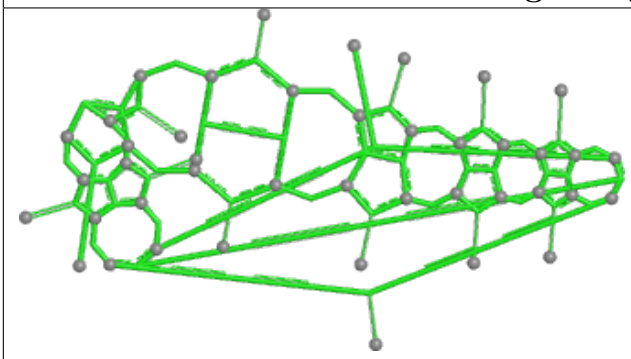
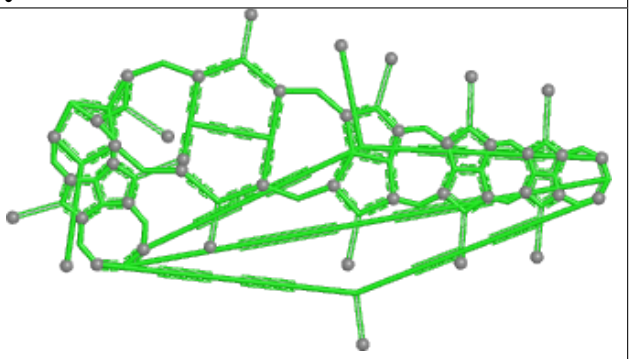
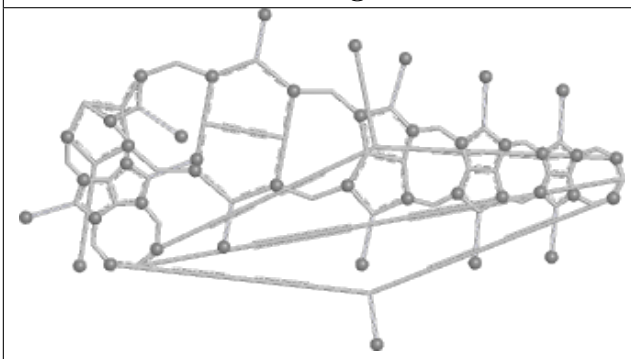
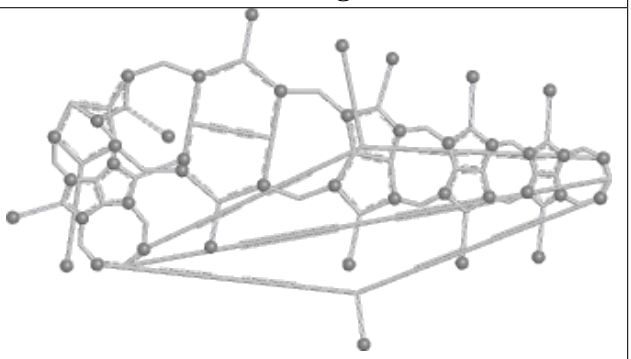
3 monomers are involved in 5 short contacts:

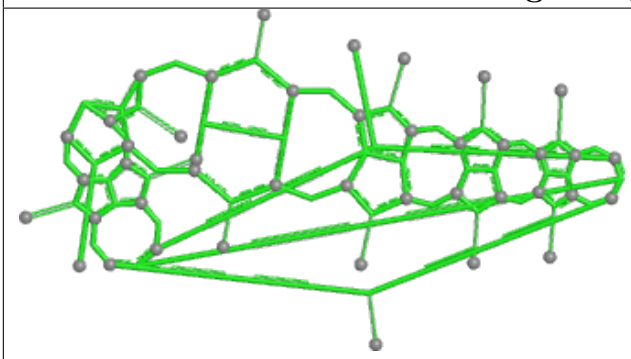
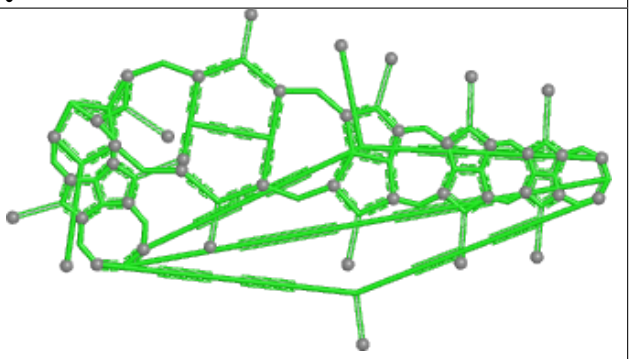
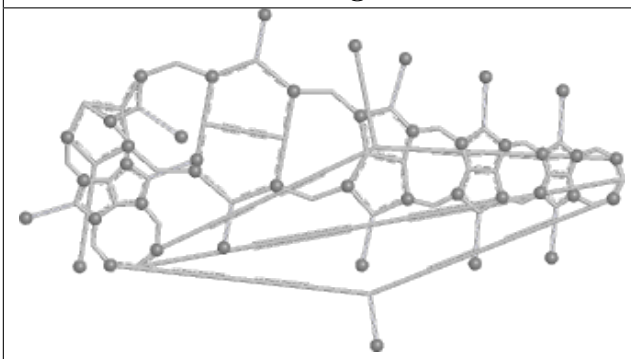
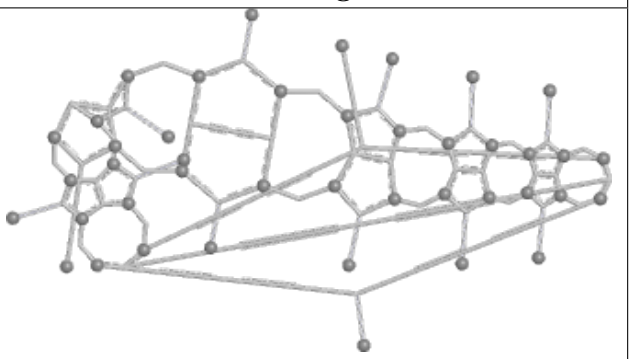
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	403	QQ7	1	0
3	B	403	QQ7	2	0
3	C	403	QQ7	2	0

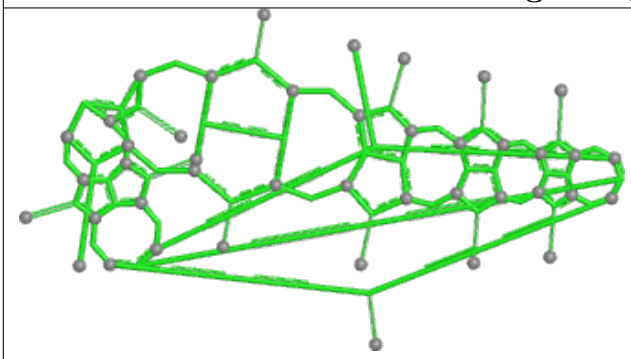
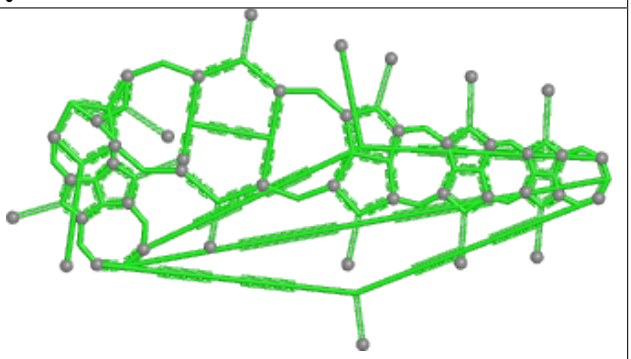
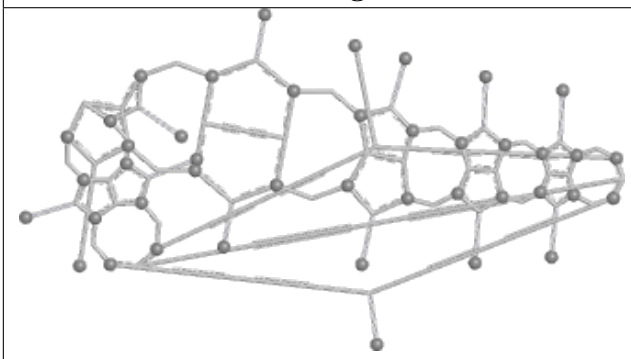
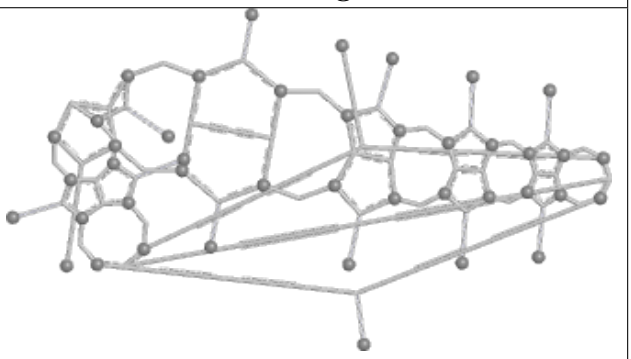
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

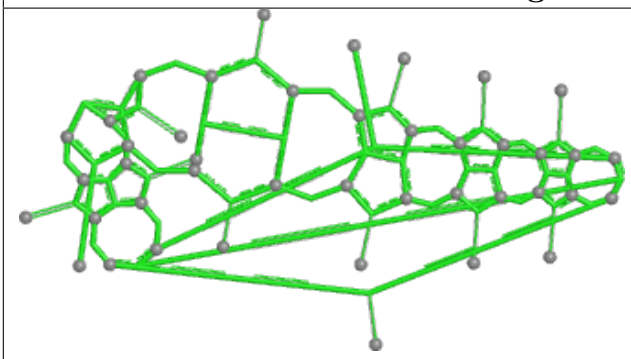
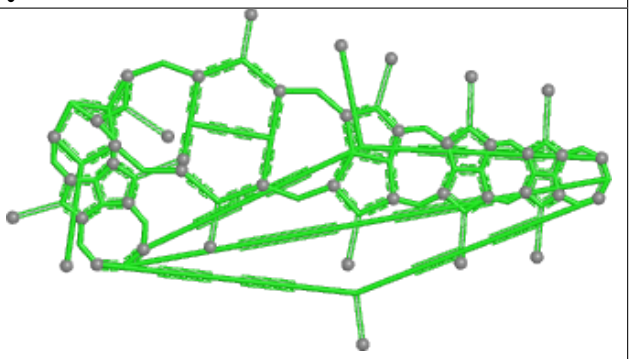
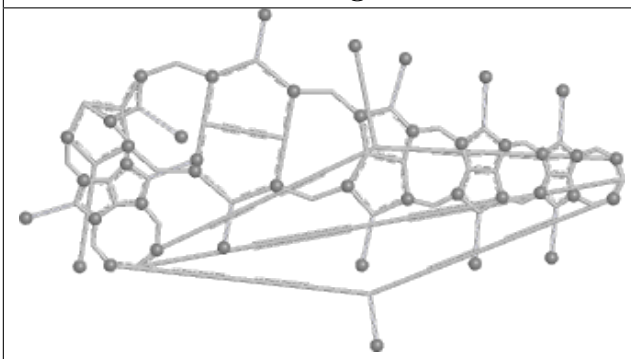
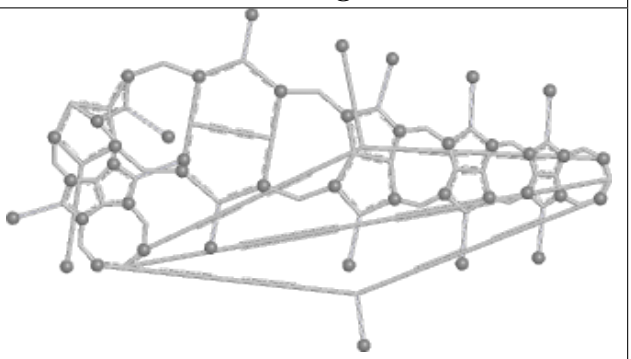
Ligand QQ7 D 403	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand QQ7 E 403	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand QQ7 A 403	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand QQ7 B 403	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand QQ7 C 403	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand QQ7 F 403	
	
Bond lengths	Bond angles
	
Torsions	Rings

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	105/114 (92%)	-0.02	8 (7%) 13 10	35, 65, 344, 556	0
1	B	105/114 (92%)	0.10	6 (5%) 23 21	39, 65, 331, 423	0
1	C	105/114 (92%)	0.08	7 (6%) 17 15	38, 66, 322, 522	0
1	D	105/114 (92%)	0.53	12 (11%) 5 3	41, 69, 365, 566	0
1	E	105/114 (92%)	0.25	10 (9%) 8 6	38, 68, 386, 525	0
1	F	105/114 (92%)	0.26	11 (10%) 6 4	41, 69, 359, 519	0
All	All	630/684 (92%)	0.20	54 (8%) 10 8	35, 68, 359, 566	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	205	SER	14.9
1	B	205	SER	14.2
1	D	205	SER	13.7
1	B	208	ALA	13.6
1	D	209	ALA	13.4
1	F	205	SER	13.1
1	E	208	ALA	12.5
1	D	210	LEU	12.3
1	C	209	ALA	12.0
1	D	208	ALA	11.6
1	D	207	ILE	11.6
1	E	207	ILE	11.0
1	E	206	GLU	10.9
1	A	205	SER	10.3
1	F	216	ALA	10.0
1	F	207	ILE	9.5
1	D	206	GLU	9.2
1	A	208	ALA	9.2
1	F	208	ALA	9.1

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Mol	Chain	Res	Type	RSRZ
1	C	208	ALA	8.5
1	C	215	ALA	8.2
1	D	215	ALA	7.8
1	B	215	ALA	7.0
1	F	206	GLU	6.9
1	E	209	ALA	6.9
1	A	209	ALA	6.7
1	A	206	GLU	6.6
1	D	216	ALA	6.5
1	B	209	ALA	6.2
1	E	216	ALA	6.0
1	F	210	LEU	5.9
1	C	216	ALA	5.3
1	A	210	LEU	5.2
1	F	209	ALA	5.2
1	A	215	ALA	5.2
1	C	205	SER	5.1
1	F	215	ALA	4.9
1	E	212	GLN	4.6
1	D	213	GLU	4.1
1	A	216	ALA	3.6
1	B	207	ILE	3.0
1	E	215	ALA	3.0
1	C	206	GLU	2.9
1	D	227	GLY	2.8
1	F	227	GLY	2.7
1	E	210	LEU	2.7
1	A	214	ILE	2.6
1	D	214	ILE	2.5
1	B	210	LEU	2.4
1	F	223	ALA	2.4
1	E	227	GLY	2.2
1	F	213	GLU	2.2
1	D	226	ALA	2.1
1	C	214	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	SNM	B	204	7/9	0.37	0.66	236,239,242,244	0
1	MLY	A	211	5/12	0.42	0.29	238,243,245,248	0
1	MLY	F	211	5/12	0.43	0.43	197,202,208,213	0
1	MLY	C	219	5/12	0.47	0.80	574,574,583,585	0
1	MLY	F	218	5/12	0.49	0.22	213,217,226,226	0
1	MLY	A	218	5/12	0.53	0.17	206,208,215,216	0
1	MLY	D	218	5/12	0.54	0.29	275,278,286,287	0
1	MLY	B	225	5/12	0.55	0.15	153,155,161,162	0
1	MLY	C	211	5/12	0.58	0.30	199,204,206,210	0
1	MLY	B	218	5/12	0.58	0.22	229,232,237,240	0
1	SNM	E	204	7/9	0.59	1.30	364,368,371,374	0
1	SNM	A	204	7/9	0.61	0.58	256,259,263,265	0
1	MLY	D	211	5/12	0.66	0.32	175,180,181,185	0
1	MLY	B	211	5/12	0.66	0.24	160,165,168,170	0
1	MLY	C	218	5/12	0.67	0.22	337,340,347,348	0
1	MLY	E	211	5/12	0.69	0.33	185,190,193,198	0
1	SNM	F	204	7/9	0.74	1.05	276,279,284,284	0
1	SNM	D	204	7/9	0.75	1.05	222,226,229,231	0
1	MLY	B	219	5/12	0.76	0.71	485,488,495,497	0
1	MLY	E	219	5/12	0.81	0.38	195,199,202,207	0
1	MLY	E	218	5/12	0.81	0.25	196,200,203,205	0
1	MLY	D	219	5/12	0.83	0.33	197,200,209,210	0
1	MLY	E	225	5/12	0.84	0.11	149,151,157,158	0
1	MLY	C	225	5/12	0.85	0.11	124,126,130,132	0
1	MLY	D	225	5/12	0.85	0.13	146,149,154,155	0
1	SNM	C	204	7/9	0.85	0.74	209,212,214,216	0
1	MLY	A	219	5/12	0.86	0.61	534,537,543,547	0
1	MLY	F	219	5/12	0.86	0.23	300,304,313,316	0
1	MLY	F	225	5/12	0.87	0.12	173,175,180,181	0
1	MLY	A	310	11/12	0.88	0.26	65,71,89,89	0
1	MLY	B	252	11/12	0.89	0.33	83,94,105,109	0
1	MLY	A	252	11/12	0.89	0.22	102,112,126,131	0
1	MLY	D	252	11/12	0.90	0.21	109,119,131,135	0
1	MLY	A	225	5/12	0.91	0.08	145,147,153,154	0
1	MLY	C	310	11/12	0.91	0.20	68,73,92,93	0
1	MLY	F	252	11/12	0.91	0.26	88,100,112,117	0
1	MLY	D	261	11/12	0.92	0.17	67,77,97,98	0
1	MLY	C	261	11/12	0.93	0.14	59,67,86,90	0
1	MLY	F	310	11/12	0.93	0.30	65,71,88,91	0
1	MLY	C	252	11/12	0.93	0.15	78,90,103,108	0
1	MLY	D	310	11/12	0.93	0.24	70,74,90,92	0
1	MLY	E	261	11/12	0.94	0.14	66,76,96,98	0
1	MLY	B	261	11/12	0.94	0.15	53,63,81,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	MLY	B	310	11/12	0.94	0.17	74,81,98,100	0
1	MLY	E	252	11/12	0.95	0.15	104,116,128,132	0
1	MLY	A	261	11/12	0.95	0.13	58,66,89,92	0
1	MLY	F	261	11/12	0.96	0.16	71,80,102,102	0
1	MLY	E	310	11/12	0.96	0.20	65,70,88,89	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

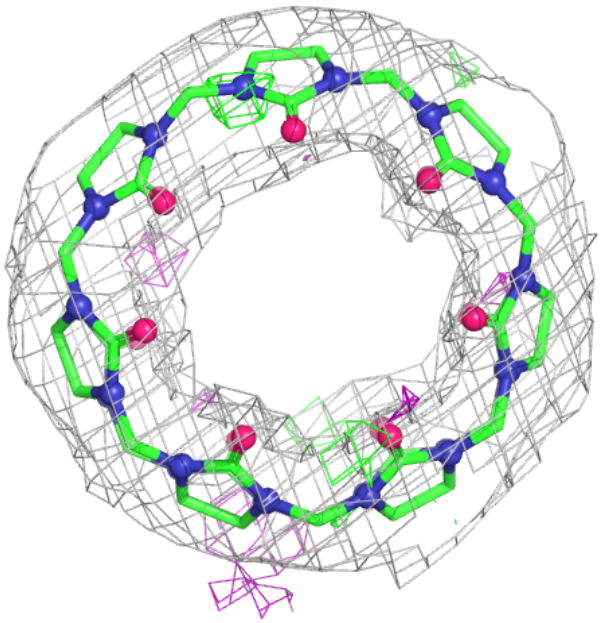
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

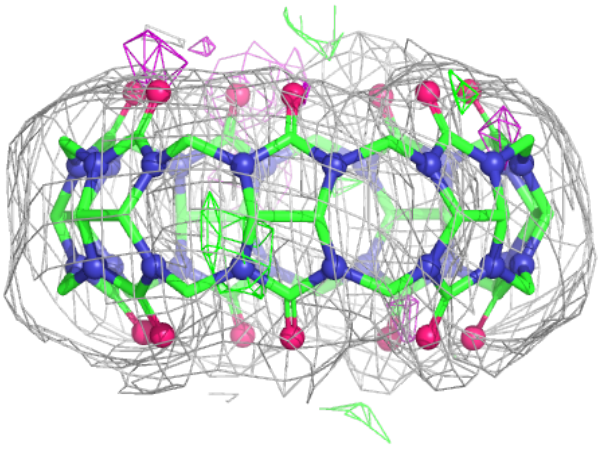
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BMA	E	401	12/12	0.89	0.26	58,71,74,79	0
3	QQ7	A	403	84/84	0.91	0.12	60,79,90,94	0
3	QQ7	D	403	84/84	0.91	0.11	64,80,87,91	0
3	QQ7	F	403	84/84	0.91	0.10	64,83,91,95	0
2	BMA	F	402	12/12	0.92	0.11	50,61,64,69	0
3	QQ7	B	403	84/84	0.92	0.11	61,75,85,89	0
2	BMA	D	401	12/12	0.93	0.14	59,69,70,71	0
2	BMA	A	402	12/12	0.93	0.11	46,58,61,66	0
2	BMA	F	401	12/12	0.93	0.15	61,73,77,82	0
2	BMA	C	402	12/12	0.93	0.13	54,60,63,69	0
2	BMA	C	401	12/12	0.94	0.14	58,67,70,71	0
3	QQ7	C	403	84/84	0.94	0.10	56,74,87,91	0
2	BMA	B	401	12/12	0.94	0.20	69,77,82,84	0
3	QQ7	E	403	84/84	0.94	0.09	60,77,87,90	0
2	BMA	E	402	12/12	0.94	0.12	49,60,65,71	0
2	BMA	A	401	12/12	0.95	0.12	59,73,76,77	0
2	BMA	B	402	12/12	0.96	0.09	49,56,58,63	0
2	BMA	D	402	12/12	0.96	0.10	47,58,61,68	0

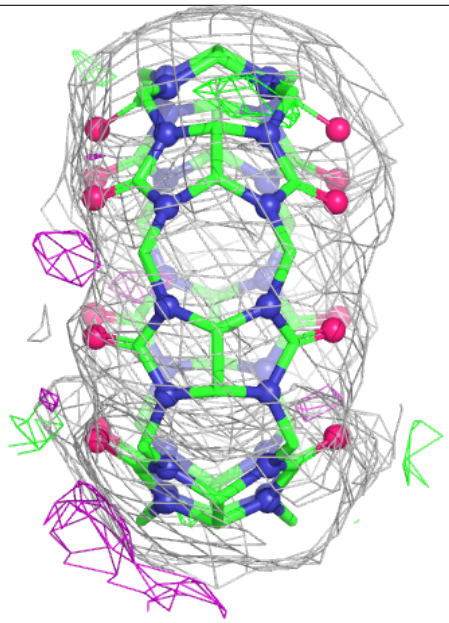
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around QQ7 A 403:

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

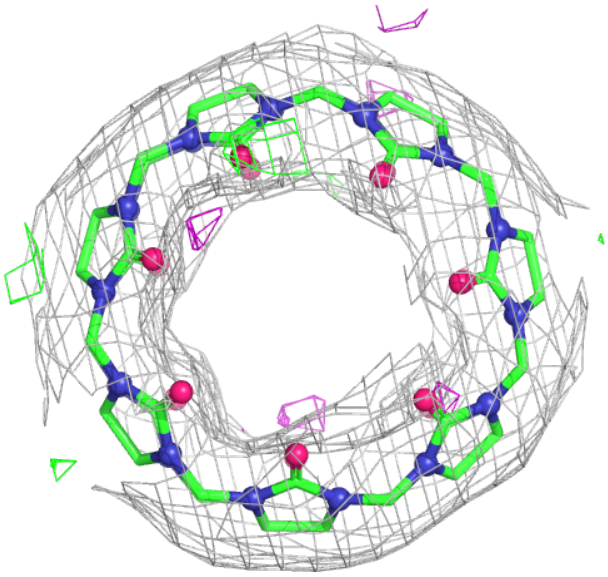


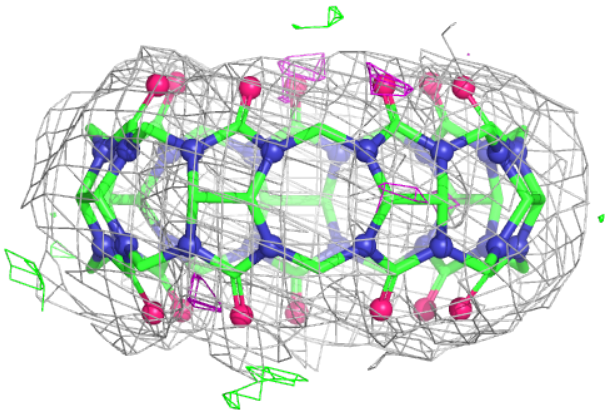


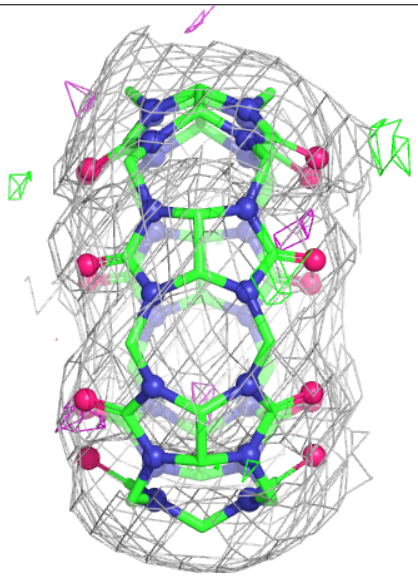


Electron density around QQ7 D 403:

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

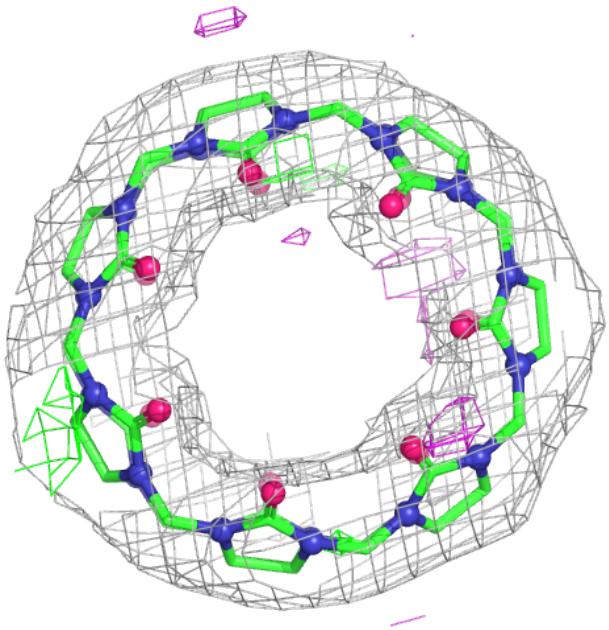


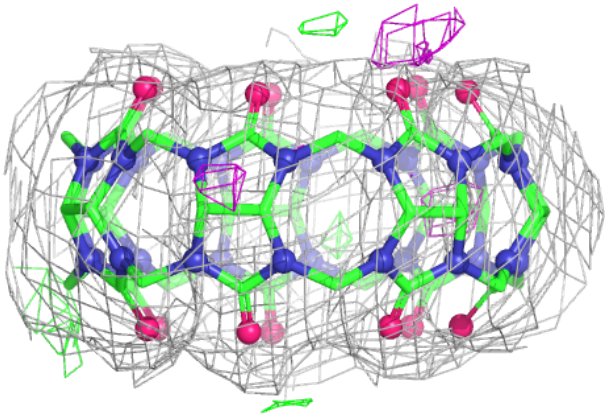


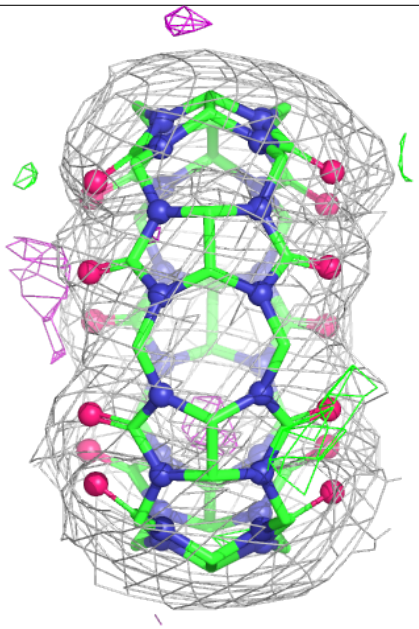


Electron density around QQ7 F 403:

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

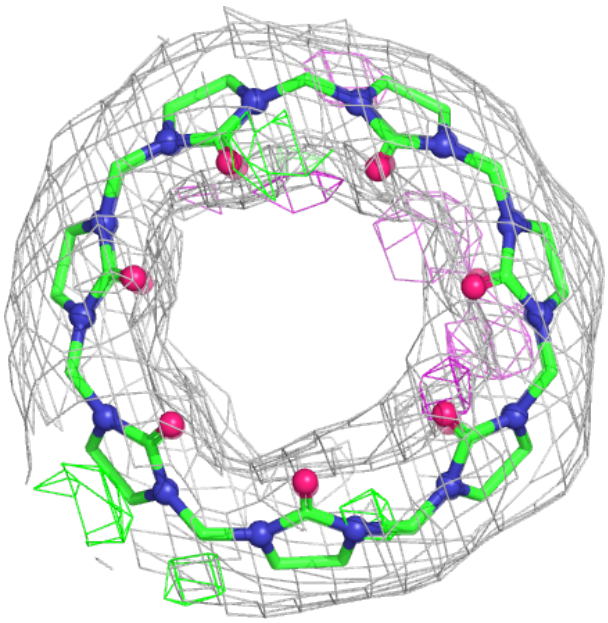


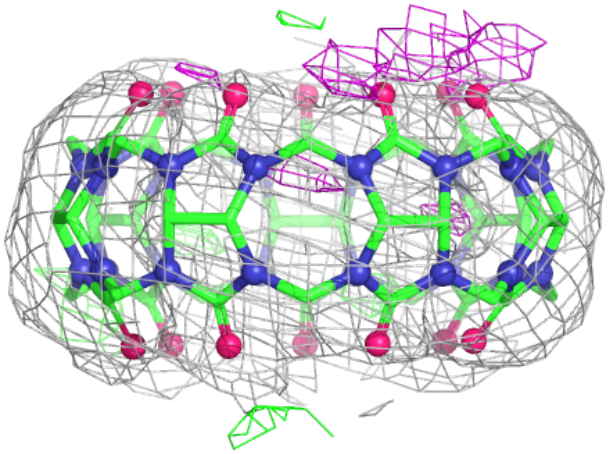


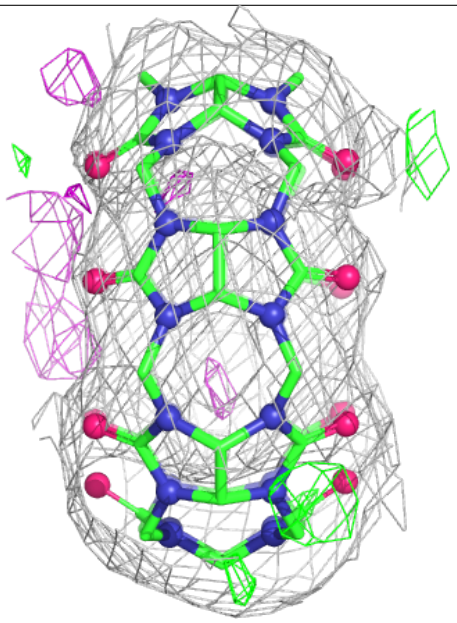


Electron density around QQ7 B 403:

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

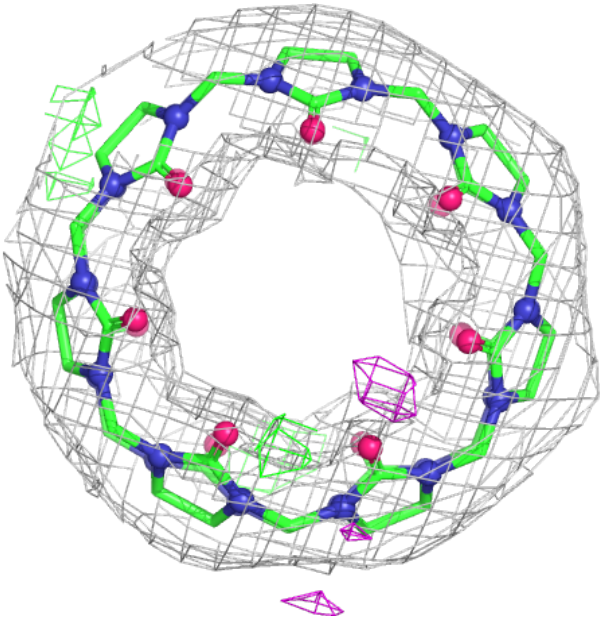


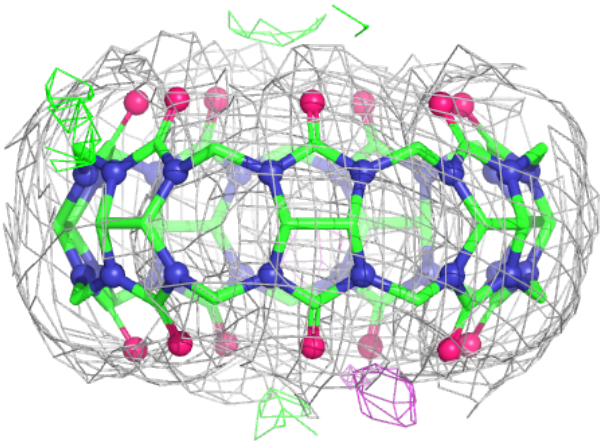


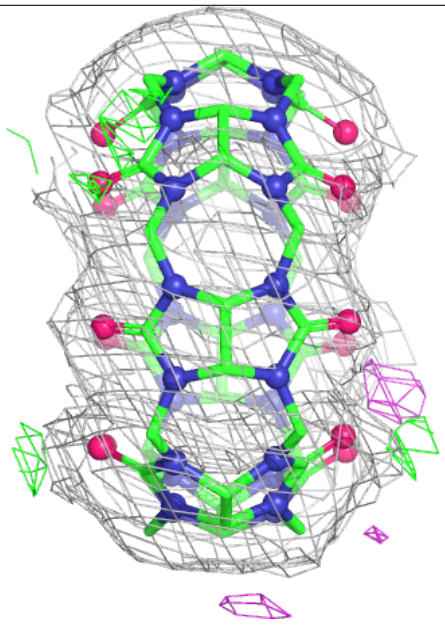


Electron density around QQ7 C 403:

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

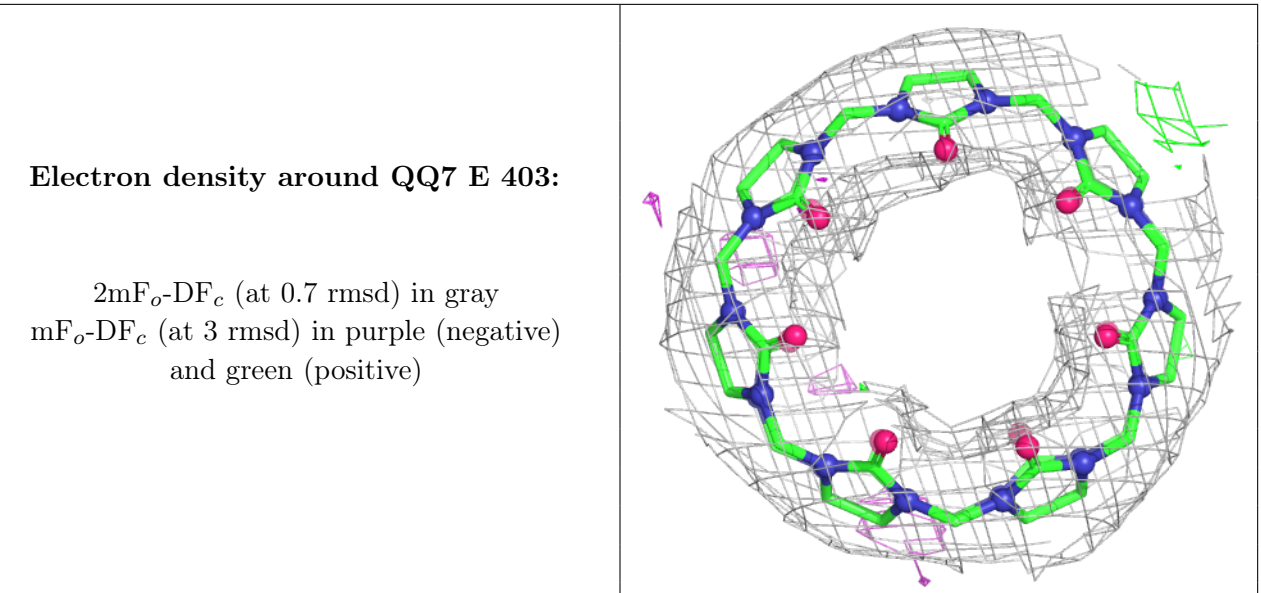


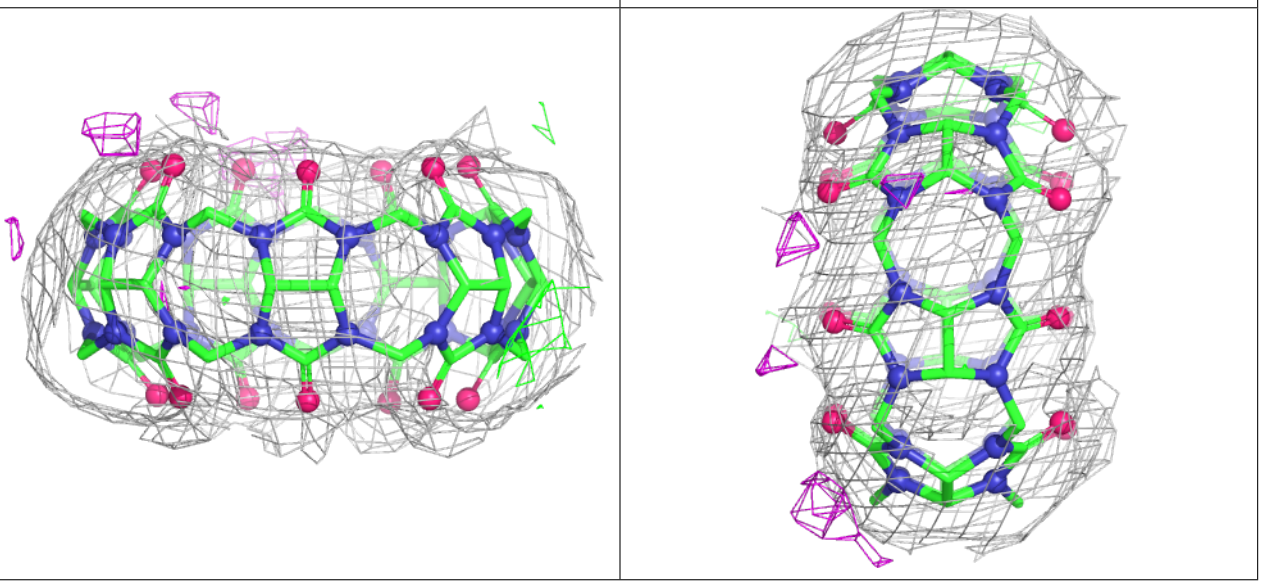




Electron density around QQ7 E 403:

$2mF_o$-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

There are no such residues in this entry.