Full wwPDB X-ray Structure Validation Report (i)

Jan 5, 2024 – 12:13 am GMT

PDB ID	:	5A8R
Title	:	METHYL-COENZYME M REDUCTASE II FROM METHANOTHERMOBACTER MARBURGENSIS AT 2.15 A RESOLUTION
Authors	:	Wagner, T.; Ermler, U.
Deposited on	:	2015-07-16
Resolution	:	2.15 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 (i) 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 (i)) were used in the production of this report:

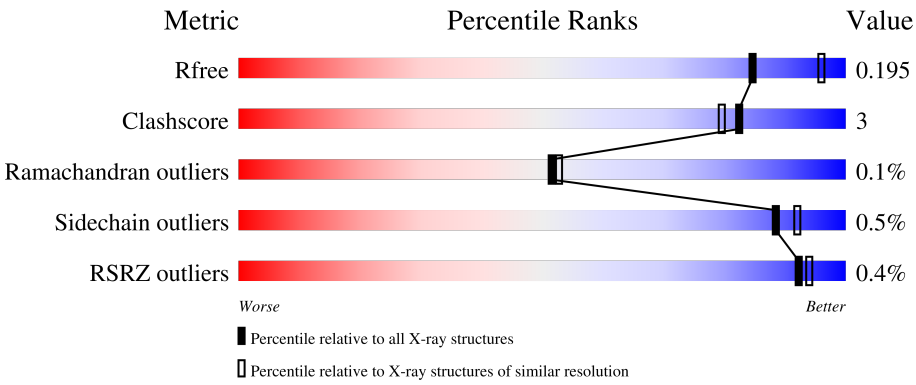
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	553	93% 6% ••
1	D	553	92% 7% •
1	G	553	90% 8% •
1	J	553	92% 7% •
2	B	443	.% 93% 7%

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Mol	Chain	Length	Quality of chain
2	E	443	94% 5%
2	H	443	92% 8%
2	K	443	95% 5%
3	C	265	% 92% 7%
3	F	265	89% 9%
3	I	265	% 92% 7%
3	L	265	% 92% 7%

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
4	COM	G	601	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 40798 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 METHYL-COENZYME M REDUCTASE II SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	548	4235	2676	714	822	23	0	0	0
1	D	548	4235	2676	714	822	23	0	0	0
1	G	548	4235	2676	714	822	23	0	0	0
1	J	548	4238	2678	714	823	23	0	1	0

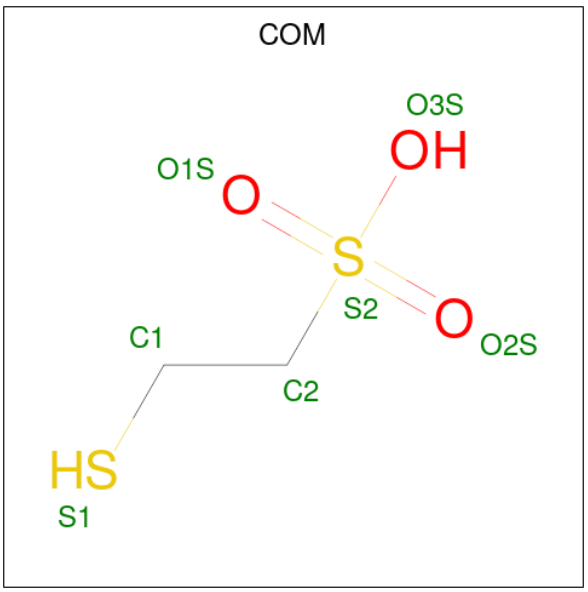
- Molecule 2 is a protein called METHYL-COENZYME M REDUCTASE II SUBUNIT GAMMA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	442	3296	2087	557	639	13	0	0	0
2	E	442	3296	2087	557	639	13	0	0	0
2	H	442	3296	2087	557	639	13	0	0	0
2	K	442	3296	2087	557	639	13	0	0	0

- Molecule 3 is a protein called METHYL-COENZYME M REDUCTASE II, SUBUNIT BETA.

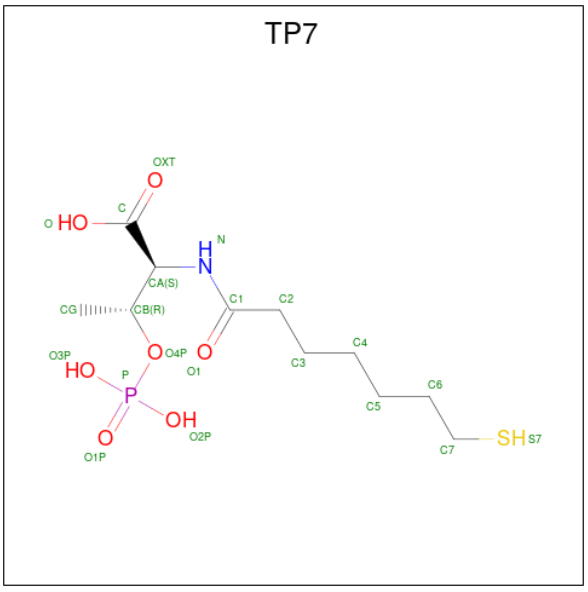
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	262	2122	1321	376	415	10	0	0	0
3	F	261	2114	1317	375	412	10	0	0	0
3	I	262	2120	1320	376	414	10	0	0	0
3	L	263	2128	1324	377	417	10	0	0	0

- Molecule 4 is 1-THIOETHANESULFONIC ACID (three-letter code: COM) (formula: $C_2H_6O_3S_2$).



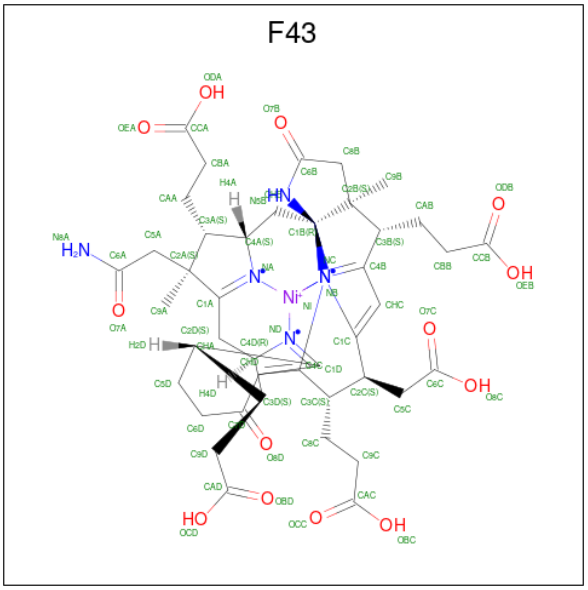
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
4	A	1	7	2	3	2	0	0
4	D	1	7	2	3	2	0	0
4	G	1	7	2	3	2	0	0
4	J	1	7	2	3	2	0	0

- Molecule 5 is Coenzyme B (three-letter code: TP7) (formula: $C_{11}H_{22}NO_7PS$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
5	A	1	21	11	1	7	1	1	0	0
5	D	1	21	11	1	7	1	1	0	0
5	G	1	21	11	1	7	1	1	0	0
5	J	1	21	11	1	7	1	1	0	0

- Molecule 6 is FACTOR 430 (three-letter code: F43) (formula: $C_{42}H_{51}N_6NiO_{13}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	Ni	O		
6	A	1	62	42	6	1	13	0	0
6	D	1	62	42	6	1	13	0	0
6	G	1	62	42	6	1	13	0	0
6	J	1	62	42	6	1	13	0	0

- Molecule 7 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
7	A	1	1	1	0	0
7	D	2	2	2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
7	G	1	1	1	0	0
			Total	K		
7	J	3	3	3	0	0

- Molecule 8 is water.

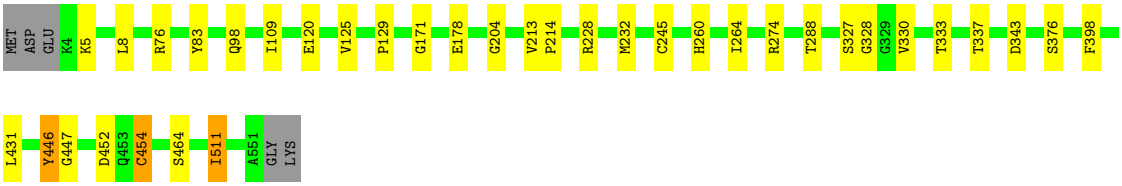
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	297	297	297	0	0
			Total	O		
8	B	146	146	146	0	0
			Total	O		
8	C	72	72	72	0	0
			Total	O		
8	D	208	208	208	0	0
			Total	O		
8	E	110	110	110	0	0
			Total	O		
8	F	71	71	71	0	0
			Total	O		
8	G	260	260	260	0	0
			Total	O		
8	H	158	158	158	0	0
			Total	O		
8	I	45	45	45	0	0
			Total	O		
8	J	220	220	220	0	0
			Total	O		
8	K	137	137	137	0	0
			Total	O		
8	L	96	96	96	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.

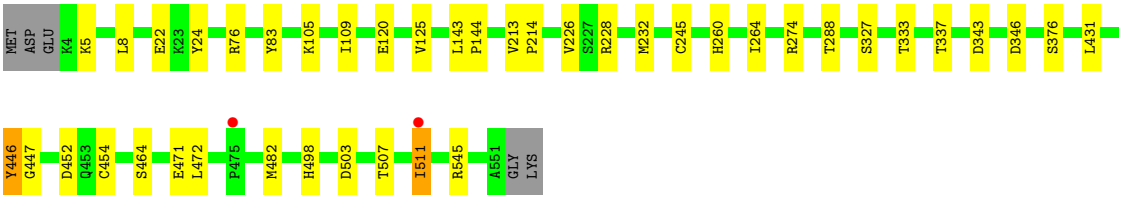
• Molecule 1: METHYL-COENZYME M REDUCTASE II SUBUNIT ALPHA

Chain A:



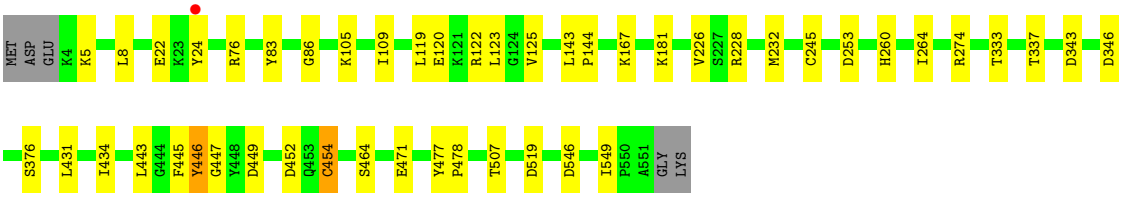
• Molecule 1: METHYL-COENZYME M REDUCTASE II SUBUNIT ALPHA

Chain D:



• Molecule 1: METHYL-COENZYME M REDUCTASE II SUBUNIT ALPHA

Chain G:

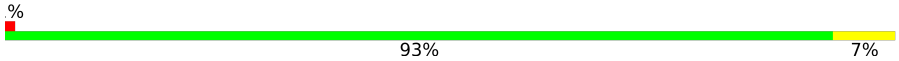


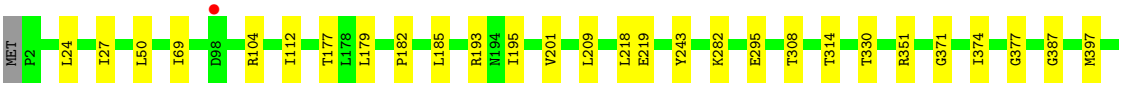
• Molecule 1: METHYL-COENZYME M REDUCTASE II SUBUNIT ALPHA

Chain J:

• Molecule 2: METHYL-COENZYME M REDUCTASE II SUBUNIT GAMMA

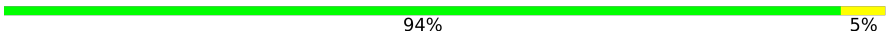
Chain B:

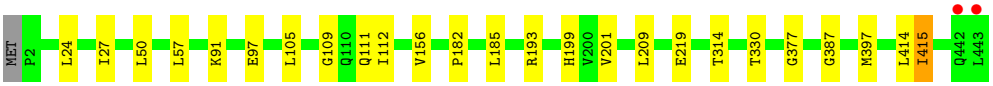




• Molecule 2: METHYL-COENZYME M REDUCTASE II SUBUNIT GAMMA

Chain E:



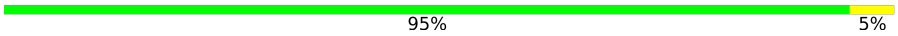


• Molecule 2: METHYL-COENZYME M REDUCTASE II SUBUNIT GAMMA

Chain H:

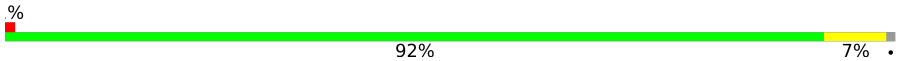
• Molecule 2: METHYL-COENZYME M REDUCTASE II SUBUNIT GAMMA

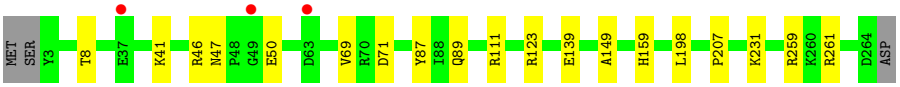
Chain K:



• Molecule 3: METHYL-COENZYME M REDUCTASE II, SUBUNIT BETA

Chain C:



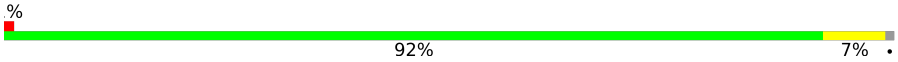


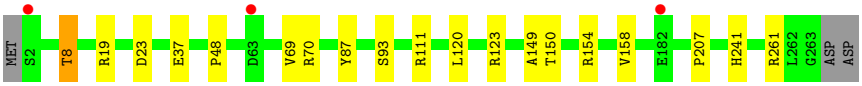
• Molecule 3: METHYL-COENZYME M REDUCTASE II, SUBUNIT BETA

Chain F:

• Molecule 3: METHYL-COENZYME M REDUCTASE II, SUBUNIT BETA

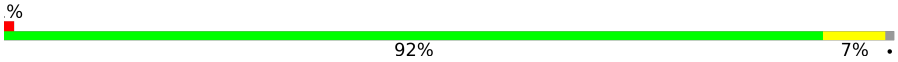
Chain I:

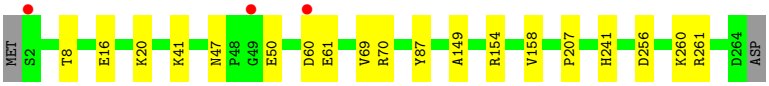




• Molecule 3: METHYL-COENZYME M REDUCTASE II, SUBUNIT BETA

Chain L:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	216.66Å 246.61Å 103.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.36 – 2.15 65.48 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.9 (55.36-2.15) 99.9 (65.48-2.15)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.02 (at 2.14Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.156 , 0.196 0.158 , 0.195	Depositor DCC
R_{free} test set	15160 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	25.7	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 43.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	40798	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: COM, MHS, TP7, AGM, F43, GL3, K, SMC, MGN, DYA

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	0.31	0/4270	0.50	0/5779
1	D	0.31	0/4270	0.49	0/5779
1	G	0.30	0/4270	0.49	0/5779
1	J	0.31	0/4276	0.49	0/5787
2	B	0.29	0/3350	0.51	0/4552
2	E	0.29	0/3350	0.51	0/4552
2	H	0.30	0/3350	0.50	0/4552
2	K	0.30	0/3350	0.51	0/4552
3	C	0.28	0/2162	0.51	0/2913
3	F	0.29	0/2154	0.51	0/2902
3	I	0.27	0/2160	0.50	0/2910
3	L	0.29	0/2168	0.50	0/2921
All	All	0.30	0/39130	0.50	0/52978

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4235	0	4075	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4235	0	4075	21	0
1	G	4235	0	4075	26	0
1	J	4238	0	4080	22	0
2	B	3296	0	3299	17	0
2	E	3296	0	3299	14	0
2	H	3296	0	3299	23	0
2	K	3296	0	3299	15	0
3	C	2122	0	2058	12	0
3	F	2114	0	2054	15	0
3	I	2120	0	2059	12	0
3	L	2128	0	2063	11	0
4	A	7	0	6	2	0
4	D	7	0	6	3	0
4	G	7	0	6	5	0
4	J	7	0	6	3	0
5	A	21	0	19	1	0
5	D	21	0	19	0	0
5	G	21	0	19	0	0
5	J	21	0	19	0	0
6	A	62	0	43	2	0
6	D	62	0	43	2	0
6	G	62	0	43	3	0
6	J	62	0	43	3	0
7	A	1	0	0	0	0
7	D	2	0	0	0	0
7	G	1	0	0	0	0
7	J	3	0	0	0	0
8	A	297	0	0	0	0
8	B	146	0	0	0	0
8	C	72	0	0	2	0
8	D	208	0	0	0	0
8	E	110	0	0	0	0
8	F	71	0	0	1	0
8	G	260	0	0	1	0
8	H	158	0	0	1	0
8	I	45	0	0	0	0
8	J	220	0	0	3	0
8	K	137	0	0	0	1
8	L	96	0	0	1	0
All	All	40798	0	38007	194	1

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 3.

All (194) 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)
3:F:47:ASN:N	3:F:50:GLU:OE2	2.05	0.87
2:K:91:LYS:NZ	2:K:97:GLU:OE2	2.09	0.86
3:L:256:ASP:OD1	3:L:260:LYS:NZ	2.15	0.79
3:F:46:ARG:HB2	3:F:50:GLU:OE2	1.83	0.77
2:H:281:VAL:HG21	2:H:344:LEU:HD11	1.73	0.70
2:E:91:LYS:NZ	2:E:97:GLU:OE2	2.24	0.69
2:H:209:LEU:HG	3:I:69:VAL:HG21	1.76	0.67
1:J:388:GLU:OE2	8:J:2160:HOH:O	2.12	0.67
1:G:22:GLU:HG3	1:G:24:TYR:H	1.60	0.67
3:C:46:ARG:HB2	3:C:50:GLU:OE2	1.94	0.67
3:I:23:ASP:O	3:I:111:ARG:NH2	2.32	0.63
3:C:71:ASP:OD2	8:C:2016:HOH:O	2.15	0.62
1:D:5:LYS:HB2	1:D:8:LEU:HG	1.81	0.62
2:K:209:LEU:HG	3:L:69:VAL:HG21	1.80	0.61
3:C:47:ASN:N	3:C:50:GLU:OE2	2.26	0.61
3:F:47:ASN:O	3:F:50:GLU:HG2	2.00	0.61
3:L:149:ALA:HB2	3:L:207:PRO:HB3	1.83	0.60
2:B:209:LEU:HG	3:C:69:VAL:HG21	1.84	0.60
1:A:5:LYS:HB2	1:A:8:LEU:HG	1.82	0.59
2:B:282:LYS:NZ	2:B:295:GLU:OE2	2.36	0.59
1:A:288:THR:HG23	1:A:511:ILE:HD12	1.85	0.59
3:C:47:ASN:O	3:C:50:GLU:HG2	2.04	0.58
2:K:50:LEU:HD11	2:K:112:ILE:HD11	1.86	0.57
2:B:50:LEU:HD11	2:B:112:ILE:HD11	1.87	0.56
1:G:434:ILE:HD11	3:I:241:HIS:HB2	1.88	0.56
1:J:76:ARG:NH1	1:J:343:ASP:OD2	2.38	0.56
3:C:231:LYS:NZ	8:C:2067:HOH:O	2.30	0.56
3:I:87:TYR:CZ	1:J:245:CYS:HB2	2.41	0.56
2:E:111:GLN:HG2	2:E:414:LEU:HD11	1.88	0.56
1:J:122:ARG:NH1	1:J:253:ASP:OD2	2.40	0.55
2:E:209:LEU:HG	3:F:69:VAL:HG21	1.89	0.54
1:D:288:THR:HG23	1:D:511:ILE:HD12	1.88	0.54
2:K:314:THR:HA	2:K:330:THR:HG21	1.90	0.54
1:J:5:LYS:HB2	1:J:8:LEU:HG	1.90	0.54
1:D:228:ARG:O	1:D:232:MET:HG2	2.08	0.53
2:H:182:PRO:HB2	2:K:182:PRO:HB2	1.91	0.53
2:B:182:PRO:HA	2:B:185:LEU:HG	1.90	0.53
2:H:104:ARG:NH2	2:H:421:GLU:HG3	2.24	0.52
2:H:416:GLY:O	2:H:420:SER:OG	2.20	0.52
1:A:76:ARG:NH1	1:A:343:ASP:OD2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:109:ILE:HB	1:G:264:ILE:HB	1.92	0.52
1:A:109:ILE:HB	1:A:264:ILE:HB	1.91	0.52
2:B:314:THR:HA	2:B:330:THR:HG21	1.92	0.52
4:G:601:COM:H22	6:G:603:F43:C6B	2.40	0.51
2:E:50:LEU:HD11	2:E:112:ILE:HD11	1.92	0.51
3:C:41:LYS:HG2	3:C:198:LEU:HD22	1.93	0.51
1:G:5:LYS:HB2	1:G:8:LEU:HG	1.93	0.50
2:H:24:LEU:O	2:H:27:ILE:HG13	2.12	0.50
1:J:446:TYR:HB2	4:J:601:COM:O1S	2.12	0.50
4:J:601:COM:H22	6:J:603:F43:N5B	2.28	0.49
1:G:120:GLU:HG2	1:G:125:VAL:O	2.13	0.49
3:L:47:ASN:O	3:L:50:GLU:HG2	2.12	0.49
4:J:601:COM:H22	6:J:603:F43:C6B	2.42	0.49
3:F:149:ALA:HB2	3:F:207:PRO:HB3	1.95	0.49
2:B:219:GLU:HB3	2:B:387:GLY:HA2	1.95	0.49
2:E:314:THR:HA	2:E:330:THR:HG21	1.93	0.49
1:D:76:ARG:NH1	1:D:343:ASP:OD2	2.46	0.49
1:A:76:ARG:HB2	1:A:83:TYR:CE2	2.48	0.49
2:B:104:ARG:NH1	2:B:421:GLU:HG3	2.28	0.48
1:D:446:TYR:HB2	4:D:601:COM:O2S	2.13	0.48
1:D:76:ARG:HB2	1:D:83:TYR:CE2	2.48	0.48
4:G:601:COM:H22	6:G:603:F43:N5B	2.29	0.48
2:K:57:LEU:HD21	2:K:156:VAL:HA	1.95	0.48
1:D:471:GLU:HB3	1:D:507:THR:HG22	1.96	0.48
3:F:154:ARG:HD3	3:F:158:VAL:HA	1.95	0.48
1:J:20:PRO:O	8:J:2008:HOH:O	2.20	0.48
1:D:22:GLU:HG3	1:D:24:TYR:H	1.79	0.48
2:H:50:LEU:HD11	2:H:112:ILE:HD11	1.95	0.48
1:G:76:ARG:HB2	1:G:83:TYR:CE2	2.49	0.48
2:H:439:VAL:O	2:H:442:GLN:HG2	2.13	0.48
2:E:57:LEU:HD21	2:E:156:VAL:HA	1.96	0.47
1:G:181:LYS:HE2	8:G:2090:HOH:O	2.14	0.47
2:H:322:ARG:NH2	3:I:70:ARG:HD2	2.29	0.47
3:I:87:TYR:CE1	1:J:245:CYS:HB2	2.50	0.47
1:A:333:THR:O	1:A:337:THR:HG23	2.14	0.47
3:C:87:TYR:CZ	1:D:245:CYS:HB2	2.49	0.47
3:I:8:THR:HG22	3:I:19:ARG:HG3	1.96	0.47
1:A:245:CYS:HB2	3:F:87:TYR:CZ	2.49	0.47
1:G:228:ARG:O	1:G:232:MET:HG2	2.14	0.47
2:E:105:LEU:HD22	2:E:109:GLY:HA2	1.97	0.47
3:F:170:LEU:HD11	3:F:180:PHE:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:TYR:HB2	4:A:601:COM:O3S	2.15	0.46
6:A:603:F43:CHC	4:D:601:COM:H12	2.45	0.46
2:H:7:ARG:NE	8:H:2007:HOH:O	2.45	0.46
3:I:149:ALA:HB2	3:I:207:PRO:HB3	1.98	0.46
1:J:109:ILE:HB	1:J:264:ILE:HB	1.96	0.46
1:J:434:ILE:HD11	3:L:241:HIS:HB2	1.97	0.46
1:G:376:SER:HB3	1:G:431:LEU:HD23	1.98	0.46
3:L:60:ASP:OD1	3:L:61:GLU:HG3	2.15	0.46
4:G:601:COM:H12	6:G:603:F43:CHC	2.46	0.46
2:B:195:ILE:HD12	2:B:218:LEU:HD13	1.98	0.46
3:C:149:ALA:HB2	3:C:207:PRO:HB3	1.97	0.46
2:E:182:PRO:HA	2:E:185:LEU:HG	1.98	0.46
2:H:104:ARG:HH22	2:H:421:GLU:HG3	1.79	0.46
1:J:120:GLU:HG2	1:J:125:VAL:O	2.16	0.46
1:A:228:ARG:O	1:A:232:MET:HG2	2.16	0.46
2:H:199:HIS:CG	2:H:415:ILE:HD12	2.51	0.46
1:A:376:SER:HB3	1:A:431:LEU:HD23	1.97	0.45
2:E:219:GLU:HB3	2:E:387:GLY:HA2	1.98	0.45
3:F:222:LYS:HA	3:F:226:ALA:HB2	1.96	0.45
2:B:182:PRO:HB2	2:E:182:PRO:HB2	1.98	0.45
1:G:333:THR:O	1:G:337:THR:HG23	2.15	0.45
1:G:443:LEU:HD23	1:G:449:ASP:HB3	1.99	0.45
2:B:193:ARG:HB3	2:B:377:GLY:HA3	1.98	0.45
2:H:286:GLU:HG2	2:H:292:LYS:HG2	1.99	0.45
2:K:201:VAL:HG21	2:K:397:MET:HB2	1.99	0.45
1:A:213:VAL:HG13	1:A:214:PRO:HD2	1.99	0.45
1:J:105:LYS:O	1:J:226:VAL:HG21	2.16	0.45
1:D:109:ILE:HB	1:D:264:ILE:HB	1.99	0.45
1:G:245:CYS:HB2	3:L:87:TYR:CZ	2.52	0.44
1:A:454:SMC:SG	2:B:351:ARG:HA	2.57	0.44
2:B:201:VAL:HG21	2:B:397:MET:HB2	1.98	0.44
1:A:327:SER:OG	1:A:328:GLY:N	2.49	0.44
2:H:132:LEU:HD13	2:K:226:THR:HA	1.99	0.44
2:H:203:ILE:CG2	2:H:425:PHE:HB3	2.48	0.44
2:H:47:ALA:HB2	2:H:418:VAL:HG11	2.00	0.44
3:F:81:GLU:O	8:F:2024:HOH:O	2.21	0.44
1:D:120:GLU:HG2	1:D:125:VAL:O	2.18	0.44
1:D:213:VAL:HG13	1:D:214:PRO:HD2	1.98	0.44
2:E:24:LEU:O	2:E:27:ILE:HG13	2.17	0.44
1:G:105:LYS:O	1:G:226:VAL:HG21	2.18	0.44
2:H:7:ARG:HD3	2:H:21:ASP:OD1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:LEU:O	2:B:27:ILE:HG13	2.18	0.43
2:K:203:ILE:CG2	2:K:425:PHE:HB3	2.48	0.43
1:D:333:THR:O	1:D:337:THR:HG23	2.18	0.43
2:B:243:TYR:HB3	2:B:308:THR:OG1	2.18	0.43
1:G:76:ARG:NH1	1:G:343:ASP:OD2	2.51	0.43
1:G:446:TYR:HB2	4:G:601:COM:O2S	2.18	0.43
1:J:76:ARG:HB2	1:J:83:TYR:CE2	2.53	0.43
1:J:471:GLU:HB3	1:J:507:THR:HG22	2.01	0.43
1:J:19:ASP:HA	1:J:20:PRO:HD3	1.85	0.43
1:J:33:TRP:HZ3	1:J:40:LYS:HG2	1.83	0.43
1:G:471:GLU:HB3	1:G:507:THR:CG2	2.48	0.43
2:E:193:ARG:HB3	2:E:377:GLY:HA3	2.01	0.43
1:G:471:GLU:HB3	1:G:507:THR:HG22	1.99	0.43
3:F:93:SER:HB3	3:F:150:THR:HB	2.01	0.43
3:F:259:ARG:HD3	3:F:259:ARG:HA	1.62	0.43
3:C:89:GLN:OE1	3:C:123:ARG:HD2	2.19	0.43
2:K:193:ARG:HB3	2:K:377:GLY:HA3	2.01	0.43
1:G:167:LYS:NZ	1:G:519:ASP:OD2	2.41	0.42
1:A:120:GLU:HG2	1:A:125:VAL:O	2.19	0.42
1:G:122:ARG:NH1	1:G:253:ASP:OD2	2.50	0.42
1:G:445:PHE:HB2	4:G:601:COM:O2S	2.19	0.42
2:H:339:GLU:HG2	2:H:344:LEU:O	2.19	0.42
3:I:120:LEU:HD13	3:I:123:ARG:HG3	2.01	0.42
1:J:213:VAL:HG13	1:J:214:PRO:HD2	2.00	0.42
2:K:182:PRO:HA	2:K:185:LEU:HG	2.01	0.42
1:J:228:ARG:O	1:J:232:MET:HG2	2.19	0.42
3:L:154:ARG:HD3	3:L:158:VAL:HA	2.01	0.42
2:E:199:HIS:CD2	2:E:415:ILE:HD12	2.54	0.42
3:I:37:GLU:HG3	3:I:48:PRO:HG2	2.01	0.42
1:D:471:GLU:HB3	1:D:507:THR:CG2	2.50	0.42
3:I:154:ARG:HD3	3:I:158:VAL:HA	2.01	0.42
2:K:104:ARG:HE	2:K:104:ARG:HB3	1.50	0.42
1:D:498:HIS:HB3	1:D:503:ASP:HB2	2.02	0.42
1:A:330:VAL:HB	6:D:603:F43:H9A1	2.00	0.42
2:H:196:MET:HA	2:H:376:HIS:HB3	2.02	0.42
3:L:41:LYS:HE3	8:L:2077:HOH:O	2.19	0.42
1:A:171:GLY:HA3	1:A:204:GLY:O	2.19	0.41
1:D:376:SER:HB3	1:D:431:LEU:HD23	2.02	0.41
2:K:63:GLY:HA2	2:K:163:ARG:HG3	2.02	0.41
1:G:119:LEU:HD23	1:G:123:LEU:HD12	2.02	0.41
1:G:546:ASP:HA	1:G:549:ILE:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:371:GLY:O	2:B:374:ILE:HG13	2.20	0.41
1:D:105:LYS:O	1:D:226:VAL:HG21	2.20	0.41
1:D:143:LEU:HB3	1:D:144:PRO:HD3	2.03	0.41
2:K:390:LEU:HD13	2:K:390:LEU:HA	1.88	0.41
5:A:602:TP7:H32C	1:D:482:MET:O	2.20	0.41
3:F:23:ASP:O	3:F:111:ARG:NH2	2.53	0.41
1:G:143:LEU:HB3	1:G:144:PRO:HD3	2.02	0.41
2:B:69:ILE:HD11	1:D:472:LEU:HD13	2.03	0.41
1:G:477:TYR:HA	1:G:478:PRO:HD3	1.96	0.41
2:H:182:PRO:HA	2:H:185:LEU:HG	2.02	0.41
3:I:93:SER:HB3	3:I:150:THR:HB	2.03	0.41
1:A:98:GLN:OE1	1:D:545:ARG:HD3	2.21	0.41
3:F:89:GLN:OE1	3:F:123:ARG:HD2	2.20	0.41
3:C:111:ARG:NE	3:C:139:GLU:OE2	2.54	0.41
1:G:86:GLY:HA3	1:J:154:VAL:HG11	2.03	0.41
2:H:193:ARG:HB3	2:H:377:GLY:HA3	2.03	0.40
2:K:322:ARG:NH2	3:L:70:ARG:HD2	2.37	0.40
1:A:398:PHE:CD1	3:C:159:HIS:HE1	2.40	0.40
4:A:601:COM:H12	6:D:603:F43:C1C	2.51	0.40
2:B:177:THR:OG1	2:B:179:LEU:O	2.37	0.40
3:F:108:TYR:CZ	3:F:126:ILE:HD11	2.57	0.40
1:J:9:LYS:HE3	1:J:9:LYS:HB2	1.77	0.40
1:J:181:LYS:NZ	8:J:2070:HOH:O	2.53	0.40
6:J:603:F43:HN5	6:J:603:F43:H4A	1.75	0.40
6:A:603:F43:C6B	4:D:601:COM:H22	2.51	0.40
2:H:197:ALA:O	2:H:201:VAL:HG23	2.21	0.40
1:J:471:GLU:HB3	1:J:507:THR:CG2	2.52	0.40
3:L:16:GLU:O	3:L:20:LYS:HG3	2.21	0.40
1:A:129:PRO:HG2	1:A:178:GLU:OE1	2.20	0.40
2:E:201:VAL:HG21	2:E:397:MET:HB2	2.03	0.40
1:G:454:SMC:SG	2:H:351:ARG:HA	2.61	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:K:2104:HOH:O	8:K:2104:HOH:O[2_555]	2.04	0.16

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	540/553 (98%)	521 (96%)	18 (3%)	1 (0%)	47	46
1	D	540/553 (98%)	521 (96%)	17 (3%)	2 (0%)	34	29
1	G	540/553 (98%)	521 (96%)	18 (3%)	1 (0%)	47	46
1	J	541/553 (98%)	522 (96%)	18 (3%)	1 (0%)	47	46
2	B	440/443 (99%)	433 (98%)	7 (2%)	0	100	100
2	E	440/443 (99%)	432 (98%)	8 (2%)	0	100	100
2	H	440/443 (99%)	432 (98%)	8 (2%)	0	100	100
2	K	440/443 (99%)	431 (98%)	9 (2%)	0	100	100
3	C	260/265 (98%)	253 (97%)	7 (3%)	0	100	100
3	F	259/265 (98%)	252 (97%)	7 (3%)	0	100	100
3	I	260/265 (98%)	253 (97%)	7 (3%)	0	100	100
3	L	261/265 (98%)	254 (97%)	7 (3%)	0	100	100
All	All	4961/5044 (98%)	4825 (97%)	131 (3%)	5 (0%)	51	53

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	464	SER
1	D	464	SER
1	G	464	SER
1	J	464	SER
1	D	327	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	430/434 (99%)	428 (100%)	2 (0%)	88	92
1	D	430/434 (99%)	427 (99%)	3 (1%)	84	89
1	G	430/434 (99%)	428 (100%)	2 (0%)	88	92
1	J	431/434 (99%)	429 (100%)	2 (0%)	88	92
2	B	344/345 (100%)	344 (100%)	0	100	100
2	E	344/345 (100%)	343 (100%)	1 (0%)	92	95
2	H	344/345 (100%)	343 (100%)	1 (0%)	92	95
2	K	344/345 (100%)	343 (100%)	1 (0%)	92	95
3	C	228/231 (99%)	225 (99%)	3 (1%)	69	74
3	F	227/231 (98%)	225 (99%)	2 (1%)	78	83
3	I	228/231 (99%)	226 (99%)	2 (1%)	78	83
3	L	229/231 (99%)	227 (99%)	2 (1%)	78	83
All	All	4009/4040 (99%)	3988 (100%)	21 (0%)	88	92

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	446	TYR
1	A	511	ILE
3	C	8	THR
3	C	259	ARG
3	C	261	ARG
1	D	346	ASP
1	D	446	TYR
1	D	511	ILE
2	E	415	ILE
3	F	8	THR
3	F	261	ARG
1	G	346	ASP
1	G	446	TYR
2	H	415	ILE
3	I	8	THR
3	I	261	ARG
1	J	346	ASP
1	J	446	TYR
2	K	390	LEU

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Mol	Chain	Res	Type
3	L	8	THR
3	L	261	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

24 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	GL3	A	447	1	2,3,4	5.53	1 (50%)	1,2,4	0.26	0
1	SMC	G	454	1	5,6,7	1.25	1 (20%)	2,6,8	1.16	0
1	MGN	G	402	1	6,9,10	0.88	0	5,12,14	0.74	0
1	MHS	G	260	1	7,11,12	1.19	0	6,14,16	1.60	2 (33%)
1	SMC	D	454	1	5,6,7	1.41	1 (20%)	2,6,8	1.76	1 (50%)
1	DYA	G	452	1	7,7,8	1.50	1 (14%)	5,8,10	2.47	2 (40%)
1	MGN	J	402	1	6,9,10	0.87	0	5,12,14	0.95	0
1	MHS	D	260	1	7,11,12	1.20	0	6,14,16	1.29	2 (33%)
1	SMC	J	454	1	5,6,7	1.18	1 (20%)	2,6,8	0.87	0
1	DYA	A	452	1	7,7,8	1.45	1 (14%)	5,8,10	2.52	2 (40%)
1	MHS	J	260	1	7,11,12	1.21	0	6,14,16	1.31	2 (33%)
1	GL3	D	447	1	2,3,4	4.98	1 (50%)	1,2,4	0.13	0
1	MHS	A	260	1	7,11,12	1.21	0	6,14,16	1.21	1 (16%)
1	AGM	G	274	1	10,11,12	1.37	1 (10%)	6,13,15	1.06	0
1	MGN	D	402	1	6,9,10	0.92	0	5,12,14	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	AGM	J	274	1	10,11,12	1.25	1 (10%)	6,13,15	1.07	0
1	DYA	D	452	1	7,7,8	1.51	1 (14%)	5,8,10	2.58	2 (40%)
1	MGN	A	402	1	6,9,10	0.87	0	5,12,14	0.98	0
1	DYA	J	452	1	7,7,8	1.51	2 (28%)	5,8,10	2.30	2 (40%)
1	AGM	A	274	1	10,11,12	1.29	1 (10%)	6,13,15	0.79	0
1	SMC	A	454	1	5,6,7	1.52	1 (20%)	2,6,8	2.59	1 (50%)
1	GL3	G	447	1	2,3,4	5.79	1 (50%)	1,2,4	0.11	0
1	GL3	J	447	1	2,3,4	4.80	1 (50%)	1,2,4	0.30	0
1	AGM	D	274	1	10,11,12	1.27	1 (10%)	6,13,15	0.92	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
1	GL3	A	447	1	-	1/1/1/2	-
1	SMC	G	454	1	-	1/3/5/7	-
1	MGN	G	402	1	-	0/7/9/12	-
1	MHS	G	260	1	-	0/5/6/8	0/1/1/1
1	SMC	D	454	1	-	1/3/5/7	-
1	DYA	G	452	1	-	3/4/6/8	-
1	MGN	J	402	1	-	0/7/9/12	-
1	MHS	D	260	1	-	0/5/6/8	0/1/1/1
1	SMC	J	454	1	-	1/3/5/7	-
1	DYA	A	452	1	-	3/4/6/8	-
1	MHS	J	260	1	-	0/5/6/8	0/1/1/1
1	GL3	D	447	1	-	1/1/1/2	-
1	MHS	A	260	1	-	0/5/6/8	0/1/1/1
1	AGM	G	274	1	-	2/10/11/13	-
1	MGN	D	402	1	-	0/7/9/12	-
1	AGM	J	274	1	-	1/10/11/13	-
1	DYA	D	452	1	-	3/4/6/8	-
1	MGN	A	402	1	-	0/7/9/12	-
1	DYA	J	452	1	-	3/4/6/8	-
1	AGM	A	274	1	-	0/10/11/13	-
1	SMC	A	454	1	-	1/3/5/7	-
1	GL3	G	447	1	-	1/1/1/2	-
1	GL3	J	447	1	-	1/1/1/2	-
1	AGM	D	274	1	-	1/10/11/13	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	447	GL3	C-S	-8.19	1.52	1.80
1	A	447	GL3	C-S	-7.81	1.53	1.80
1	D	447	GL3	C-S	-7.05	1.56	1.80
1	J	447	GL3	C-S	-6.79	1.57	1.80
1	G	274	AGM	CZ-NE1	3.29	1.38	1.33
1	A	454	SMC	CB-SG	-3.07	1.76	1.80
1	J	274	AGM	CZ-NE1	2.94	1.38	1.33
1	D	274	AGM	CZ-NE1	2.92	1.38	1.33
1	A	274	AGM	CZ-NE1	2.91	1.38	1.33
1	G	452	DYA	CA-N	2.82	1.42	1.35
1	J	452	DYA	CA-N	2.79	1.42	1.35
1	D	452	DYA	CA-N	2.79	1.42	1.35
1	D	454	SMC	CB-SG	-2.71	1.77	1.80
1	A	452	DYA	CA-N	2.52	1.41	1.35
1	G	454	SMC	CB-SG	-2.34	1.77	1.80
1	J	452	DYA	OD1-CG	-2.06	1.25	1.30
1	J	454	SMC	CB-SG	-2.03	1.78	1.80

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	452	DYA	O-C-CA	-4.12	120.15	125.39
1	G	452	DYA	O-C-CA	-3.93	120.39	125.39
1	A	452	DYA	CA-CB-CG	-3.80	117.59	126.82
1	A	454	SMC	CA-CB-SG	-3.65	108.14	114.04
1	J	452	DYA	O-C-CA	-3.45	121.01	125.39
1	A	452	DYA	O-C-CA	-3.18	121.34	125.39
1	G	452	DYA	CA-CB-CG	-3.17	119.12	126.82
1	G	260	MHS	CB-CA-C	-3.16	105.55	111.47
1	D	452	DYA	CA-CB-CG	-3.15	119.16	126.82
1	J	452	DYA	CA-CB-CG	-2.99	119.55	126.82
1	D	454	SMC	CA-CB-SG	-2.47	110.04	114.04
1	A	260	MHS	CM-ND1-CG	2.40	127.63	124.44
1	J	260	MHS	CM-ND1-CG	2.26	127.44	124.44
1	D	260	MHS	CM-ND1-CG	2.21	127.39	124.44
1	G	260	MHS	CM-ND1-CG	2.11	127.25	124.44
1	J	260	MHS	CB-CA-C	-2.07	107.60	111.47
1	D	260	MHS	CB-CA-C	-2.00	107.71	111.47

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	452	DYA	O-C-CA-CB
1	A	452	DYA	CA-CB-CG-OD2
1	A	454	SMC	CA-CB-SG-CS
1	D	452	DYA	O-C-CA-CB
1	D	452	DYA	CA-CB-CG-OD1
1	D	454	SMC	CA-CB-SG-CS
1	G	452	DYA	O-C-CA-CB
1	G	452	DYA	CA-CB-CG-OD1
1	G	452	DYA	CA-CB-CG-OD2
1	G	454	SMC	CA-CB-SG-CS
1	J	452	DYA	O-C-CA-CB
1	J	452	DYA	CA-CB-CG-OD1
1	J	454	SMC	CA-CB-SG-CS
1	A	452	DYA	CA-CB-CG-OD1
1	D	452	DYA	CA-CB-CG-OD2
1	J	452	DYA	CA-CB-CG-OD2
1	G	447	GL3	S-C-CA-N
1	A	447	GL3	S-C-CA-N
1	D	447	GL3	S-C-CA-N
1	D	274	AGM	NE1-CD-CG-CB
1	J	447	GL3	S-C-CA-N
1	G	274	AGM	NE1-CD-CG-CB
1	G	274	AGM	N-CA-CB-CG
1	J	274	AGM	N-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	454	SMC	1	0
1	A	454	SMC	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 7 are monoatomic - leaving 12 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	$\#\|Z\| > 2$
6	F43	D	603	1	61,71,71	2.08	5 (8%)	64,118,118	1.35	9 (14%)
6	F43	G	603	1	61,71,71	2.04	5 (8%)	64,118,118	1.34	11 (17%)
5	TP7	J	602	-	19,20,20	0.66	0	24,26,26	0.88	1 (4%)
6	F43	J	603	1	61,71,71	2.05	6 (9%)	64,118,118	1.41	9 (14%)
4	COM	D	601	-	6,6,6	1.40	2 (33%)	7,8,8	2.66	3 (42%)
5	TP7	D	602	-	19,20,20	0.65	0	24,26,26	0.93	0
6	F43	A	603	1	61,71,71	2.09	5 (8%)	64,118,118	1.40	11 (17%)
5	TP7	A	602	-	19,20,20	0.64	0	24,26,26	0.91	1 (4%)
4	COM	G	601	-	6,6,6	1.37	2 (33%)	7,8,8	2.97	3 (42%)
4	COM	J	601	-	6,6,6	1.31	2 (33%)	7,8,8	2.81	4 (57%)
4	COM	A	601	-	6,6,6	1.42	2 (33%)	7,8,8	2.67	4 (57%)
5	TP7	G	602	-	19,20,20	0.63	0	24,26,26	1.00	1 (4%)

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
6	F43	D	603	1	-	6/28/185/185	-
6	F43	G	603	1	-	5/28/185/185	-
5	TP7	J	602	-	-	1/24/24/24	-
6	F43	J	603	1	-	8/28/185/185	-
4	COM	D	601	-	-	0/4/4/4	-
5	TP7	D	602	-	-	1/24/24/24	-
6	F43	A	603	1	-	8/28/185/185	-
5	TP7	A	602	-	-	1/24/24/24	-
4	COM	G	601	-	-	0/4/4/4	-
4	COM	J	601	-	-	1/4/4/4	-
4	COM	A	601	-	-	0/4/4/4	-
5	TP7	G	602	-	-	3/24/24/24	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	603	F43	NI-NA	7.82	2.06	1.89
6	D	603	F43	NI-NA	7.78	2.06	1.89
6	G	603	F43	NI-NA	7.69	2.06	1.89
6	J	603	F43	NI-NA	7.50	2.05	1.89
6	A	603	F43	NI-NB	7.50	2.05	1.89
6	D	603	F43	NI-NB	7.49	2.05	1.89
6	J	603	F43	NI-NB	7.28	2.05	1.89
6	G	603	F43	NI-NB	7.02	2.04	1.89
6	A	603	F43	NI-ND	6.90	2.04	1.89
6	J	603	F43	CHD-C1D	-6.72	1.34	1.43
6	A	603	F43	CHD-C1D	-6.70	1.34	1.43
6	G	603	F43	NI-ND	6.68	2.03	1.89
6	D	603	F43	CHD-C1D	-6.56	1.34	1.43
6	D	603	F43	NI-ND	6.47	2.03	1.89
6	G	603	F43	CHD-C1D	-6.47	1.34	1.43
6	J	603	F43	NI-ND	6.10	2.02	1.89
6	A	603	F43	CHC-C4B	2.94	1.47	1.39
6	D	603	F43	CHC-C4B	2.87	1.47	1.39
6	J	603	F43	CHC-C4B	2.85	1.47	1.39
6	G	603	F43	CHC-C4B	2.73	1.46	1.39
4	A	601	COM	O1S-S2	2.47	1.52	1.45
6	J	603	F43	CHB-C1B	-2.18	1.51	1.53
4	G	601	COM	O1S-S2	2.14	1.51	1.45
4	D	601	COM	O2S-S2	2.14	1.51	1.45
4	D	601	COM	O1S-S2	2.10	1.51	1.45
4	A	601	COM	O2S-S2	2.08	1.51	1.45
4	G	601	COM	O2S-S2	2.05	1.51	1.45
4	J	601	COM	O2S-S2	2.04	1.51	1.45
4	J	601	COM	O1S-S2	2.03	1.51	1.45

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	601	COM	O1S-S2-C2	5.97	114.10	106.92
4	A	601	COM	O2S-S2-C2	4.86	112.77	106.92
4	J	601	COM	O2S-S2-C2	4.84	112.74	106.92
4	D	601	COM	O1S-S2-C2	4.74	112.62	106.92
6	J	603	F43	O7B-C6B-C8B	-4.15	121.53	126.59
6	D	603	F43	O7B-C6B-C8B	-3.83	121.91	126.59
6	G	603	F43	O7B-C6B-C8B	-3.75	122.01	126.59
4	D	601	COM	O2S-S2-O1S	-3.67	101.25	113.95
6	D	603	F43	CAB-C3B-C2B	-3.64	111.39	119.09
6	A	603	F43	O7B-C6B-C8B	-3.63	122.16	126.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	601	COM	O2S-S2-O1S	-3.59	101.53	113.95
6	J	603	F43	CAB-C3B-C2B	-3.51	111.67	119.09
6	A	603	F43	O8D-C7D-C6D	-3.43	115.24	120.86
4	J	601	COM	O3S-S2-O1S	-3.40	102.97	111.27
6	J	603	F43	O8D-C7D-C6D	-3.37	115.34	120.86
4	A	601	COM	O2S-S2-O1S	-3.17	102.98	113.95
6	A	603	F43	CAB-C3B-C2B	-3.16	112.41	119.09
4	J	601	COM	O1S-S2-C2	3.15	110.71	106.92
6	G	603	F43	CAB-C3B-C2B	-3.05	112.63	119.09
4	D	601	COM	O2S-S2-C2	3.01	110.54	106.92
6	D	603	F43	O8D-C7D-C6D	-2.96	116.02	120.86
6	A	603	F43	C6D-C5D-C2D	-2.87	105.67	111.46
4	A	601	COM	O3S-S2-C2	2.84	110.36	105.77
6	G	603	F43	O8D-C7D-C6D	-2.78	116.30	120.86
6	A	603	F43	C9A-C2A-C3A	2.74	117.03	112.98
4	G	601	COM	O3S-S2-C2	2.60	109.97	105.77
6	G	603	F43	C4D-ND-C1D	2.57	111.89	108.51
6	D	603	F43	C2B-C1B-NB	2.55	105.65	101.84
6	J	603	F43	C4D-ND-C1D	2.47	111.77	108.51
6	D	603	F43	C9A-C2A-C3A	2.44	116.58	112.98
6	G	603	F43	C9A-C2A-C3A	2.37	116.48	112.98
4	J	601	COM	O3S-S2-C2	2.37	109.60	105.77
6	D	603	F43	ODA-CCA-CBA	2.33	121.53	114.03
6	J	603	F43	C9A-C2A-C3A	2.28	116.35	112.98
6	D	603	F43	C4D-ND-C1D	2.26	111.48	108.51
6	A	603	F43	C4D-ND-C1D	2.25	111.47	108.51
6	J	603	F43	C6D-C7D-CHD	2.22	121.12	116.95
6	G	603	F43	ODA-CCA-CBA	2.20	121.11	114.03
6	A	603	F43	OEA-CCA-CBA	-2.16	116.13	123.08
6	G	603	F43	C6D-C5D-C2D	-2.16	107.10	111.46
6	D	603	F43	C5D-C6D-C7D	-2.15	107.90	113.55
6	D	603	F43	OEA-CCA-CBA	-2.13	116.22	123.08
6	A	603	F43	ODA-CCA-CBA	2.13	120.87	114.03
6	J	603	F43	ODA-CCA-CBA	2.13	120.87	114.03
6	A	603	F43	C1B-C2B-C3B	2.12	104.65	101.51
6	J	603	F43	C2B-C1B-NB	2.11	105.00	101.84
6	J	603	F43	C1B-C2B-C3B	2.10	104.62	101.51
6	A	603	F43	C2B-C1B-NB	2.10	104.98	101.84
6	G	603	F43	OBC-CAC-C9C	2.10	120.78	114.03
5	A	602	TP7	O3P-P-O2P	2.09	115.63	107.64
4	A	601	COM	O1S-S2-C2	2.09	109.43	106.92
6	G	603	F43	C5D-C6D-C7D	-2.07	108.11	113.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	G	603	F43	OEA-CCA-CBA	-2.05	116.48	123.08
5	J	602	TP7	O4P-P-O1P	-2.03	101.55	109.39
6	G	603	F43	C2B-C1B-NB	2.02	104.87	101.84
5	G	602	TP7	O4P-P-O1P	-2.01	101.64	109.39
6	A	603	F43	OCD-CAD-C9D	2.00	120.49	114.07

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	602	TP7	C2-C3-C4-C5
5	D	602	TP7	C2-C3-C4-C5
4	J	601	COM	C1-C2-S2-O3S
6	G	603	F43	C2C-C5C-C6C-O7C
6	G	603	F43	C2C-C5C-C6C-O8C
5	G	602	TP7	O1-C1-N-CA
5	J	602	TP7	C2-C3-C4-C5
6	J	603	F43	C2C-C5C-C6C-O7C
6	J	603	F43	C2C-C5C-C6C-O8C
6	J	603	F43	CAB-CBB-CCB-OEB
6	A	603	F43	C8C-C9C-CAC-OBC
6	J	603	F43	CAB-CBB-CCB-ODB
6	A	603	F43	CAB-CBB-CCB-OEB
6	A	603	F43	C8C-C9C-CAC-OCC
6	A	603	F43	CAB-CBB-CCB-ODB
6	A	603	F43	C3A-CAA-CBA-CCA
6	D	603	F43	CAB-CBB-CCB-OEB
6	J	603	F43	C8C-C9C-CAC-OBC
6	G	603	F43	CAB-CBB-CCB-OEB
6	D	603	F43	CAB-CBB-CCB-ODB
6	G	603	F43	CAB-CBB-CCB-ODB
6	J	603	F43	C8C-C9C-CAC-OCC
6	A	603	F43	CAA-CBA-CCA-ODA
6	D	603	F43	C3D-C9D-CAD-OCD
6	J	603	F43	C3D-C9D-CAD-OCD
5	G	602	TP7	C2-C3-C4-C5
6	A	603	F43	CAA-CBA-CCA-OEA
6	A	603	F43	C3D-C9D-CAD-OBD
6	D	603	F43	C3D-C9D-CAD-OBD
6	J	603	F43	C3D-C9D-CAD-OBD
5	G	602	TP7	C2-C1-N-CA
6	D	603	F43	CAA-CBA-CCA-ODA

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Mol	Chain	Res	Type	Atoms
6	D	603	F43	CAA-CBA-CCA-OEA
6	G	603	F43	C8C-C9C-CAC-OBC

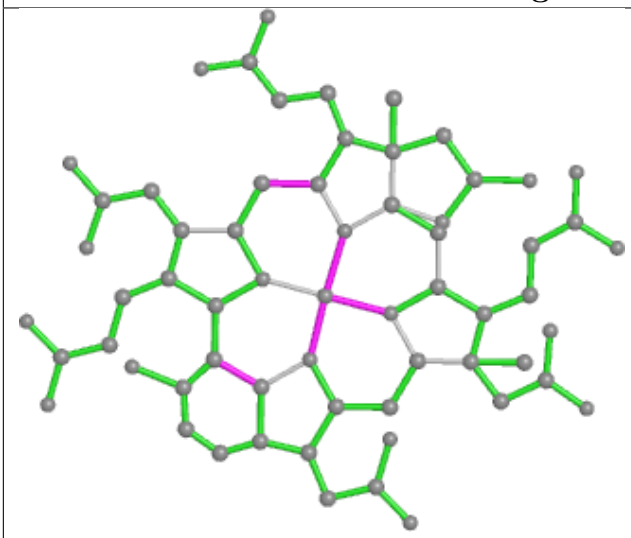
There are no ring outliers.

9 monomers are involved in 16 short contacts:

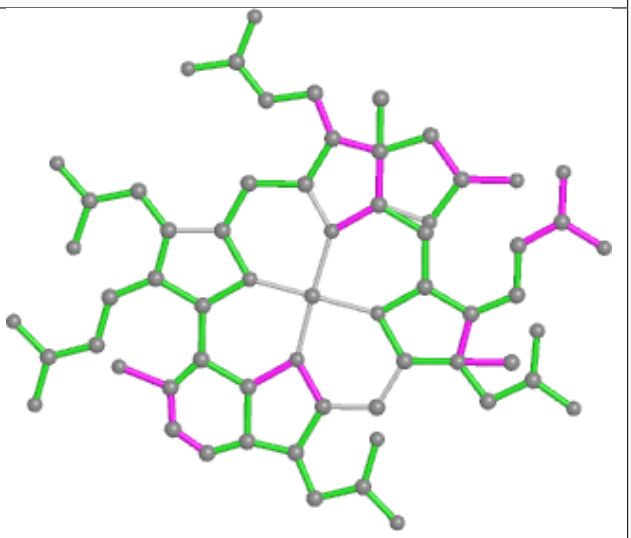
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	603	F43	2	0
6	G	603	F43	3	0
6	J	603	F43	3	0
4	D	601	COM	3	0
6	A	603	F43	2	0
5	A	602	TP7	1	0
4	G	601	COM	5	0
4	J	601	COM	3	0
4	A	601	COM	2	0

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.

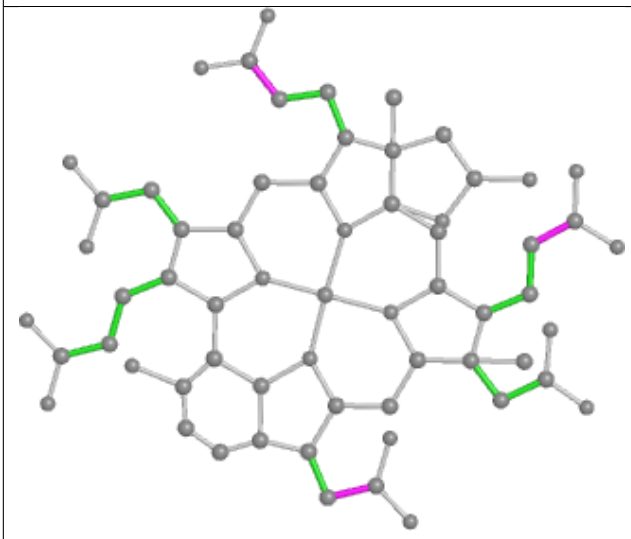
Ligand F43 D 603



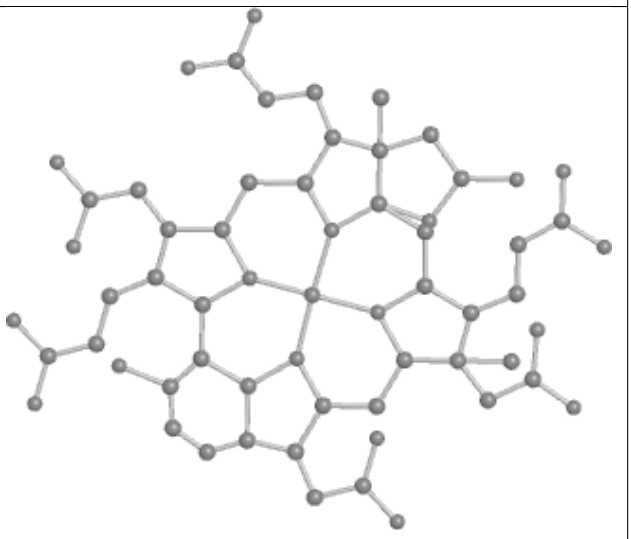
Bond lengths



Bond angles

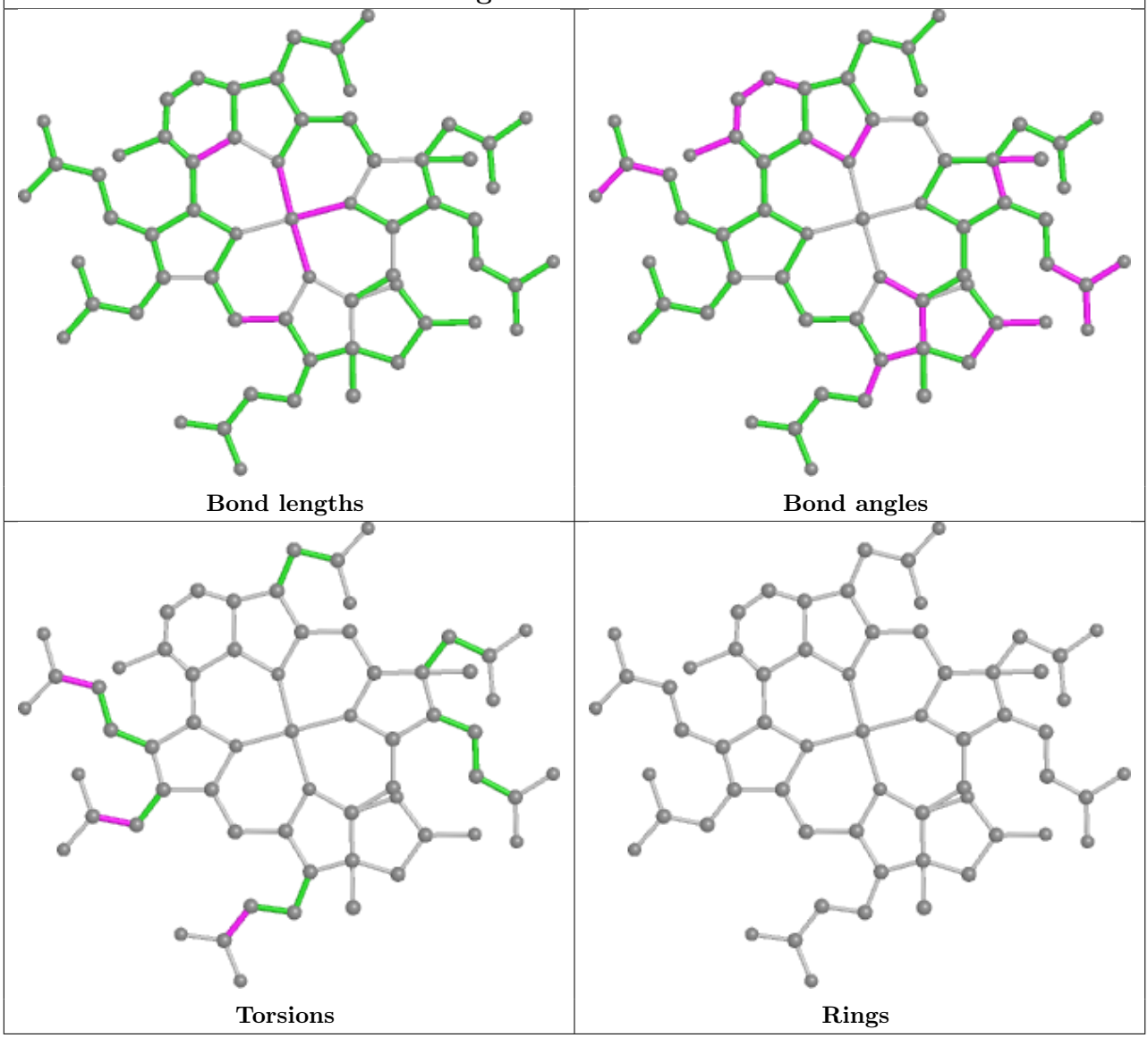


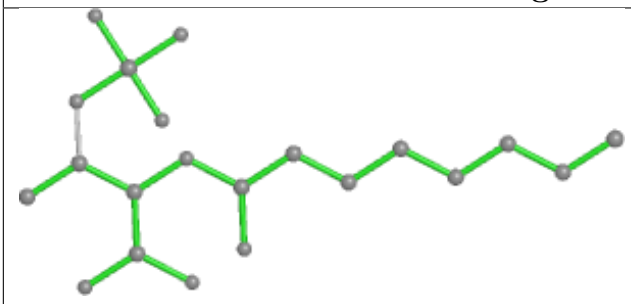
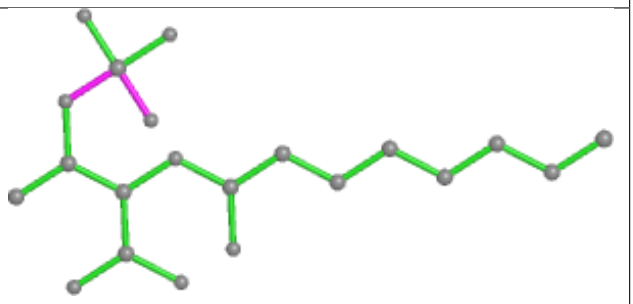
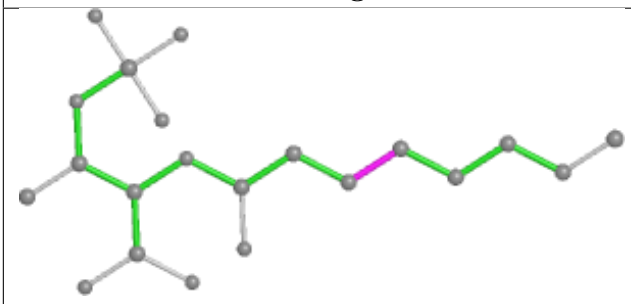
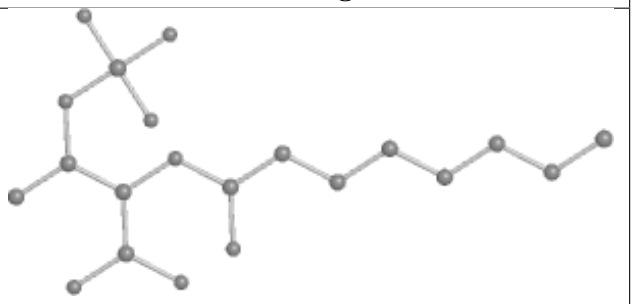
Torsions



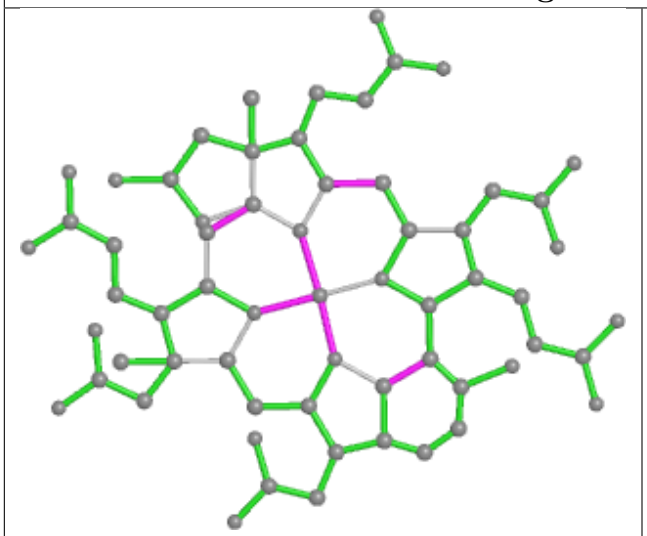
Rings

Ligand F43 G 603

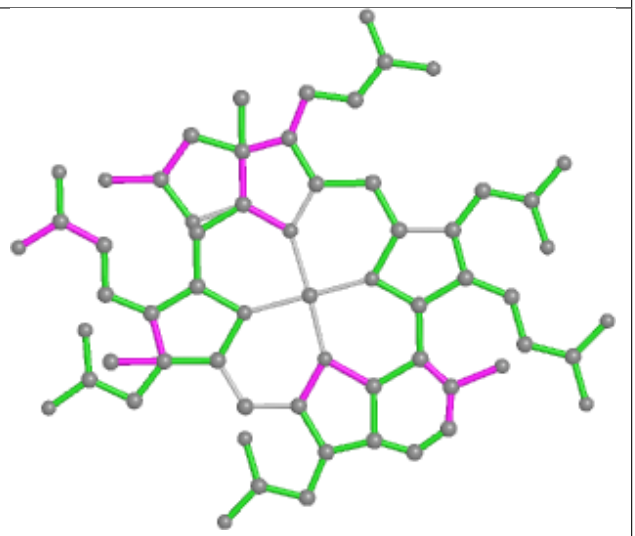


Ligand TP7 J 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

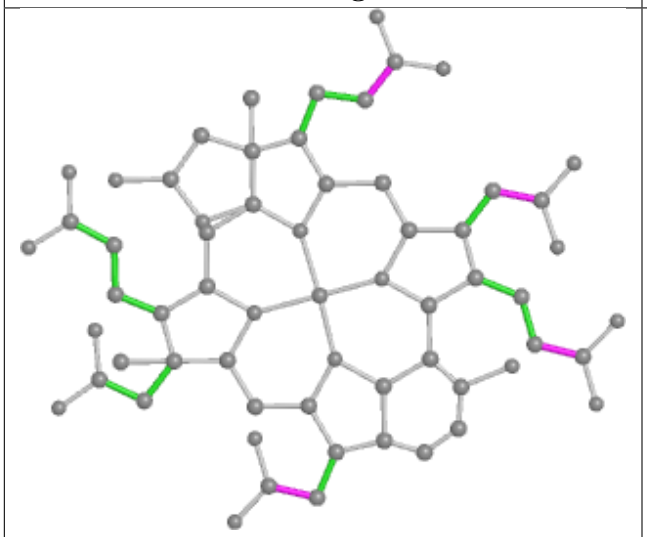
Ligand F43 J 603



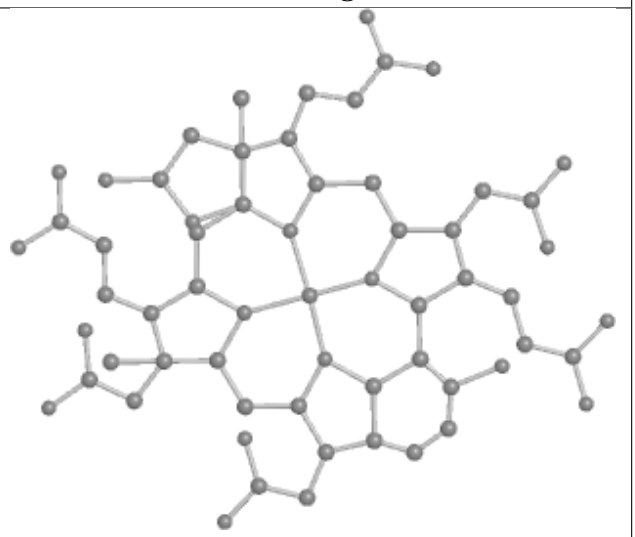
Bond lengths



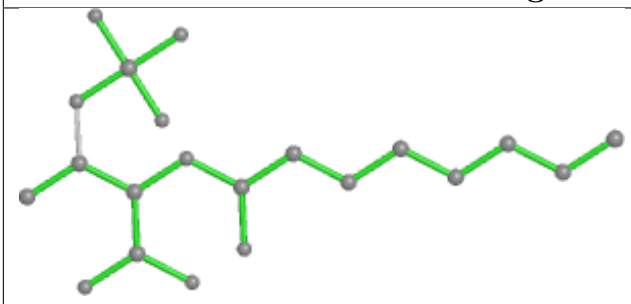
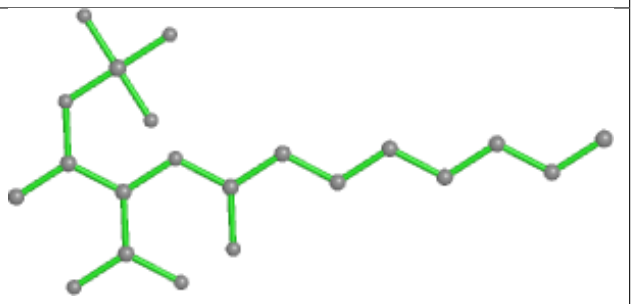
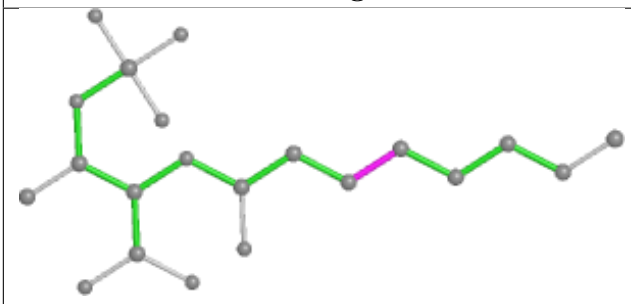
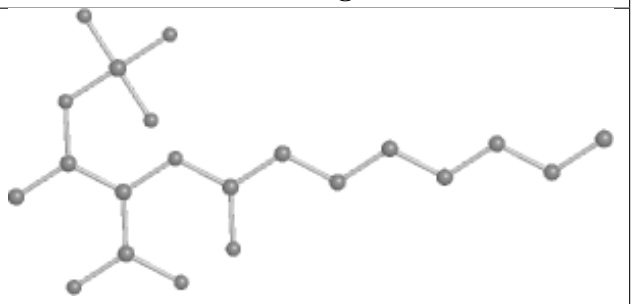
Bond angles



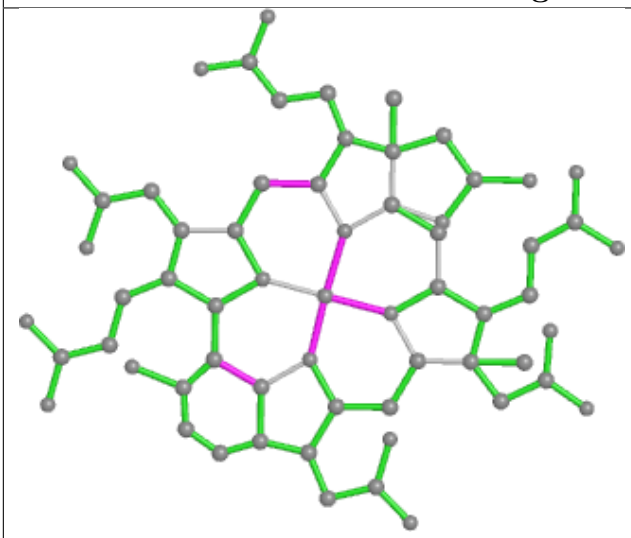
Torsions



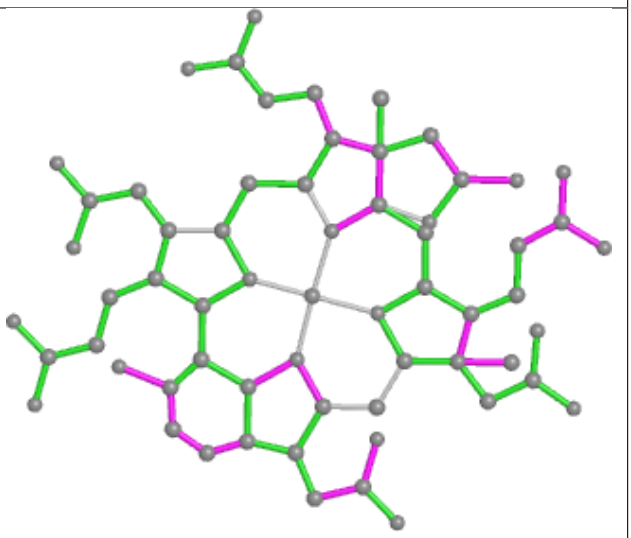
Rings

Ligand TP7 D 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

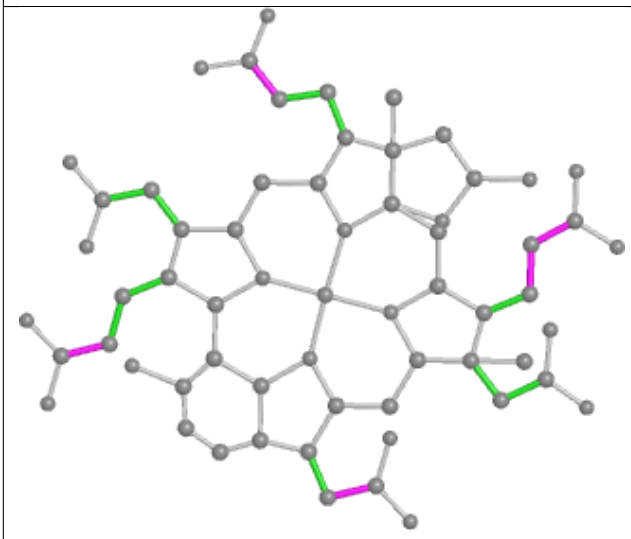
Ligand F43 A 603



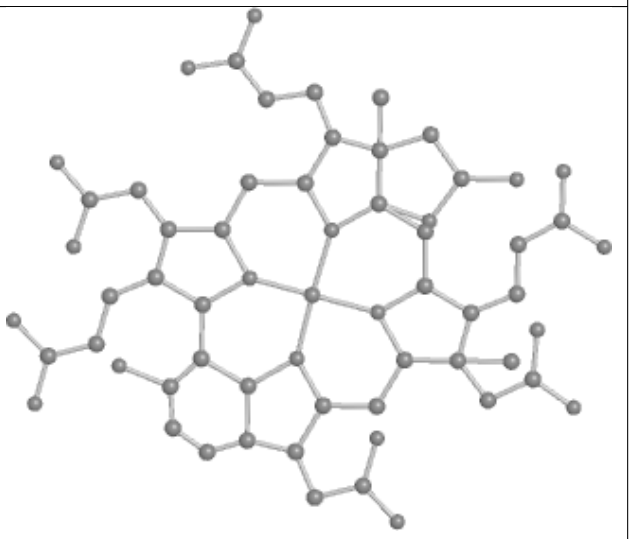
Bond lengths



Bond angles

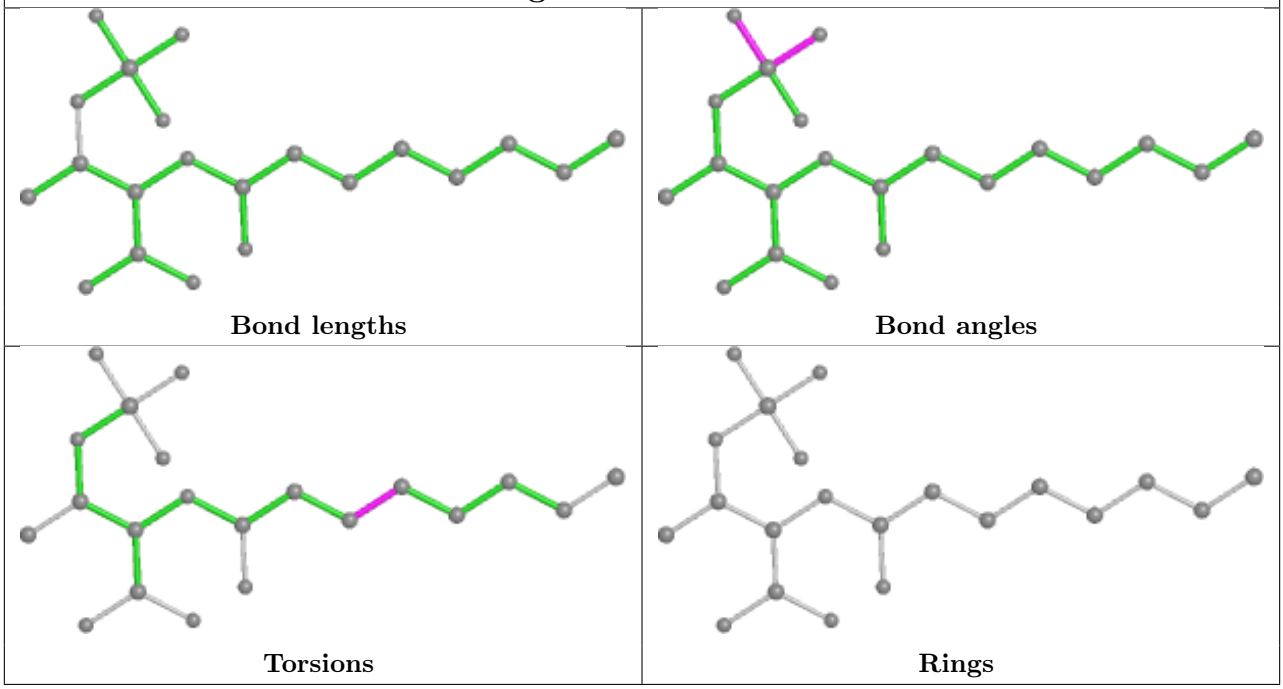


Torsions

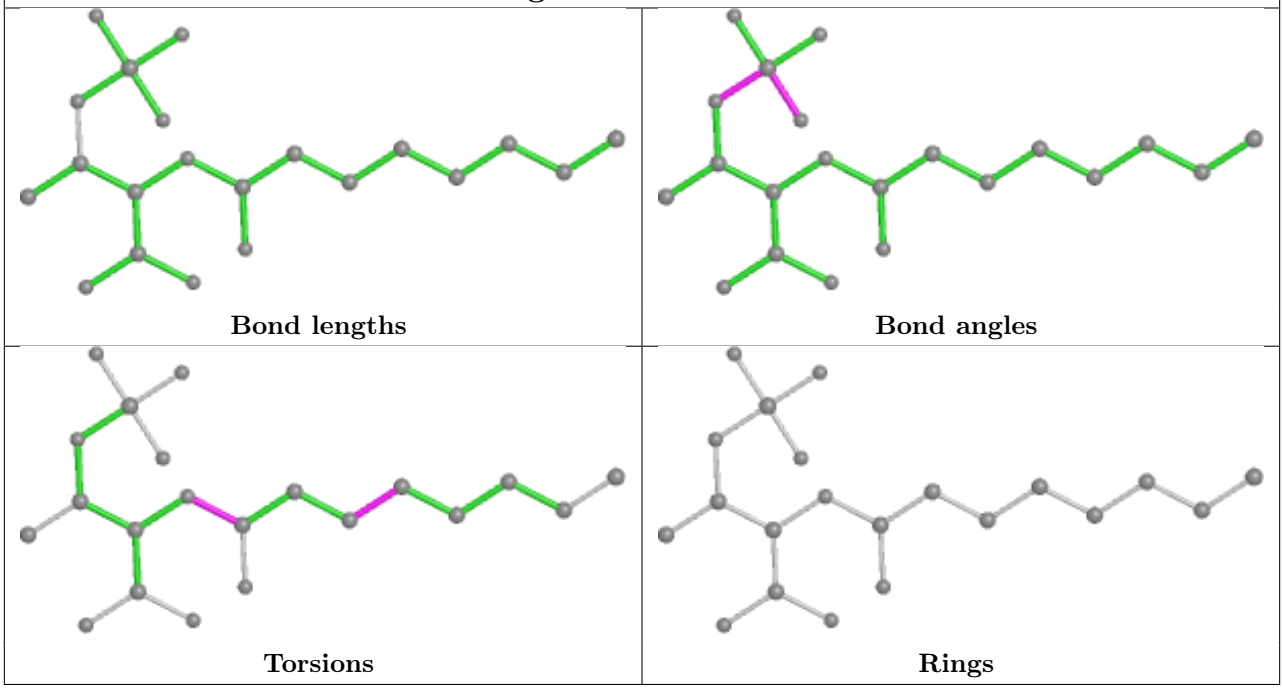


Rings

Ligand TP7 A 602



Ligand TP7 G 602



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	542/553 (98%)	-0.63	0 100 100	9, 19, 40, 64	0
1	D	542/553 (98%)	-0.26	2 (0%) 92 94	9, 19, 40, 65	0
1	G	542/553 (98%)	-0.63	1 (0%) 95 96	12, 23, 45, 78	0
1	J	542/553 (98%)	-0.45	0 100 100	9, 19, 42, 73	0
2	B	442/443 (99%)	-0.28	4 (0%) 84 88	12, 26, 48, 82	0
2	E	442/443 (99%)	-0.46	2 (0%) 91 93	11, 24, 48, 70	0
2	H	442/443 (99%)	-0.31	2 (0%) 91 93	11, 27, 47, 76	0
2	K	442/443 (99%)	-0.58	0 100 100	11, 22, 43, 66	0
3	C	262/265 (98%)	-0.37	3 (1%) 80 85	17, 30, 59, 92	0
3	F	261/265 (98%)	-0.35	1 (0%) 92 94	14, 27, 54, 75	0
3	I	262/265 (98%)	-0.30	3 (1%) 80 85	22, 38, 62, 79	0
3	L	263/265 (99%)	-0.38	3 (1%) 80 85	11, 26, 54, 83	0
All	All	4984/5044 (98%)	-0.43	21 (0%) 92 94	9, 24, 49, 92	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	63	ASP	3.8
3	L	2	SER	3.6
3	C	63	ASP	3.4
2	H	443	LEU	3.4
3	L	49	GLY	3.4
2	B	442	GLN	3.0
1	D	511	ILE	2.9
3	C	37	GLU	2.9
2	E	442	GLN	2.7
2	E	443	LEU	2.7
3	C	49	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	98	ASP	2.4
2	B	441	ASP	2.4
3	F	63	ASP	2.3
2	H	442	GLN	2.2
3	L	60	ASP	2.2
3	I	2	SER	2.2
3	I	182	GLU	2.1
1	D	475	PRO	2.1
1	G	24	TYR	2.1
2	B	443	LEU	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, 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
1	MHS	J	260	11/12	0.95	0.10	18,31,39,39	0
1	MHS	G	260	11/12	0.96	0.13	21,26,32,34	0
1	MHS	D	260	11/12	0.97	0.12	15,26,38,38	0
1	DYA	D	452	8/9	0.97	0.09	12,15,19,20	0
1	MHS	A	260	11/12	0.97	0.07	19,21,28,29	0
1	AGM	G	274	12/13	0.97	0.12	12,18,20,21	0
1	AGM	A	274	12/13	0.97	0.16	10,15,22,22	0
1	AGM	J	274	12/13	0.97	0.15	8,16,18,20	0
1	MGN	A	402	10/11	0.98	0.09	11,12,17,18	0
1	AGM	D	274	12/13	0.98	0.16	7,14,16,20	0
1	MGN	G	402	10/11	0.98	0.08	15,18,24,28	0
1	GL3	G	447	4/5	0.98	0.07	18,18,19,20	0
1	DYA	G	452	8/9	0.98	0.07	17,22,28,29	0
1	SMC	G	454	7/8	0.98	0.07	17,18,23,27	0
1	MGN	D	402	10/11	0.98	0.08	9,14,18,19	0
1	DYA	A	452	8/9	0.98	0.08	12,16,20,23	0
1	MGN	J	402	10/11	0.98	0.11	8,10,18,21	0
1	DYA	J	452	8/9	0.98	0.13	7,12,16,27	0
1	SMC	A	454	7/8	0.99	0.08	11,11,22,23	0
1	SMC	D	454	7/8	0.99	0.09	9,13,16,18	0
1	GL3	A	447	4/5	0.99	0.07	15,16,17,20	0
1	GL3	J	447	4/5	0.99	0.09	12,12,14,14	0
1	GL3	D	447	4/5	0.99	0.07	13,18,19,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	SMC	J	454	7/8	0.99	0.11	6,12,15,19	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

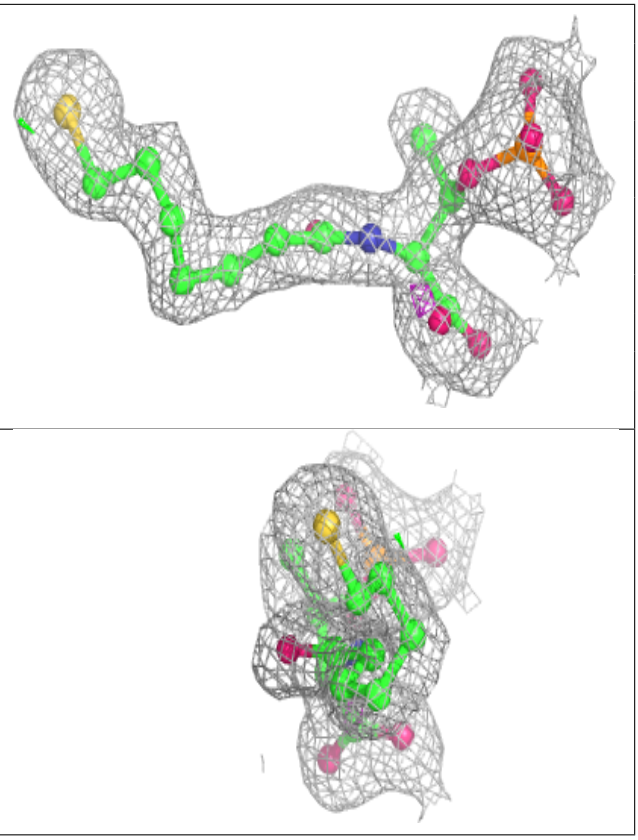
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	COM	A	601	7/7	0.96	0.10	19,25,28,29	0
4	COM	D	601	7/7	0.97	0.09	20,25,26,28	0
5	TP7	D	602	21/21	0.97	0.08	10,24,30,33	0
5	TP7	G	602	21/21	0.97	0.09	19,31,39,44	0
5	TP7	J	602	21/21	0.97	0.10	17,29,38,43	0
4	COM	G	601	7/7	0.98	0.10	25,31,34,34	0
4	COM	J	601	7/7	0.98	0.08	17,25,34,37	0
5	TP7	A	602	21/21	0.98	0.09	10,25,36,39	0
6	F43	A	603	62/62	0.98	0.08	5,13,20,25	0
6	F43	D	603	62/62	0.98	0.08	1,15,25,29	0
6	F43	G	603	62/62	0.98	0.08	9,22,31,35	0
6	F43	J	603	62/62	0.98	0.11	3,14,23,30	0
7	K	J	606	1/1	0.98	0.05	25,25,25,25	0
7	K	G	604	1/1	0.99	0.03	30,30,30,30	0
7	K	J	604	1/1	0.99	0.07	19,19,19,19	0
7	K	J	605	1/1	0.99	0.07	26,26,26,26	0
7	K	A	604	1/1	0.99	0.04	24,24,24,24	0
7	K	D	604	1/1	1.00	0.03	22,22,22,22	0
7	K	D	605	1/1	1.00	0.08	15,15,15,15	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.

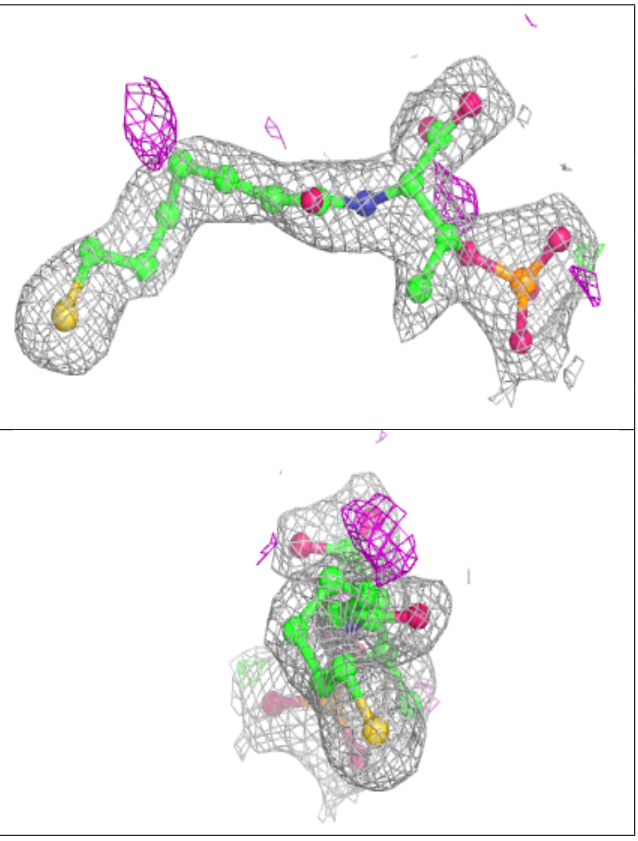
Electron density around TP7 D 602:

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



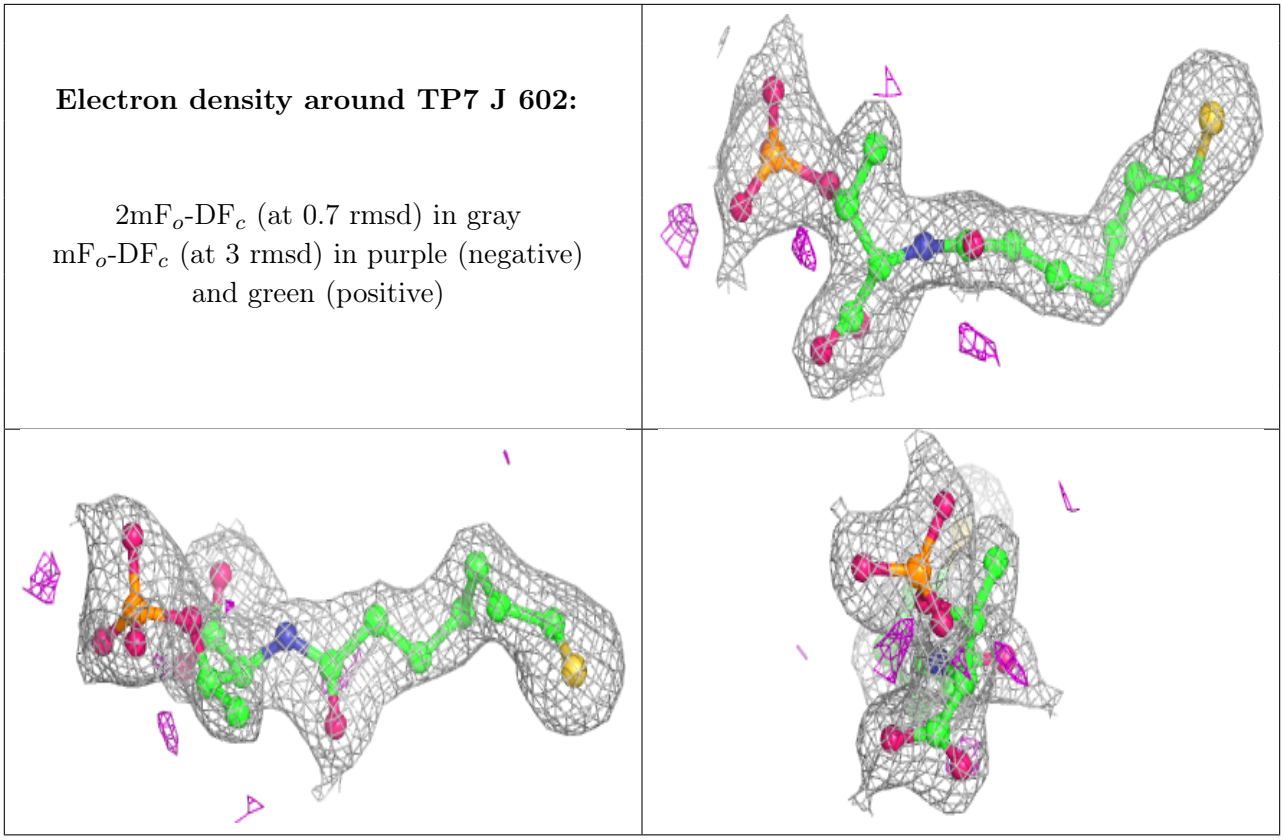
Electron density around TP7 G 602:

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



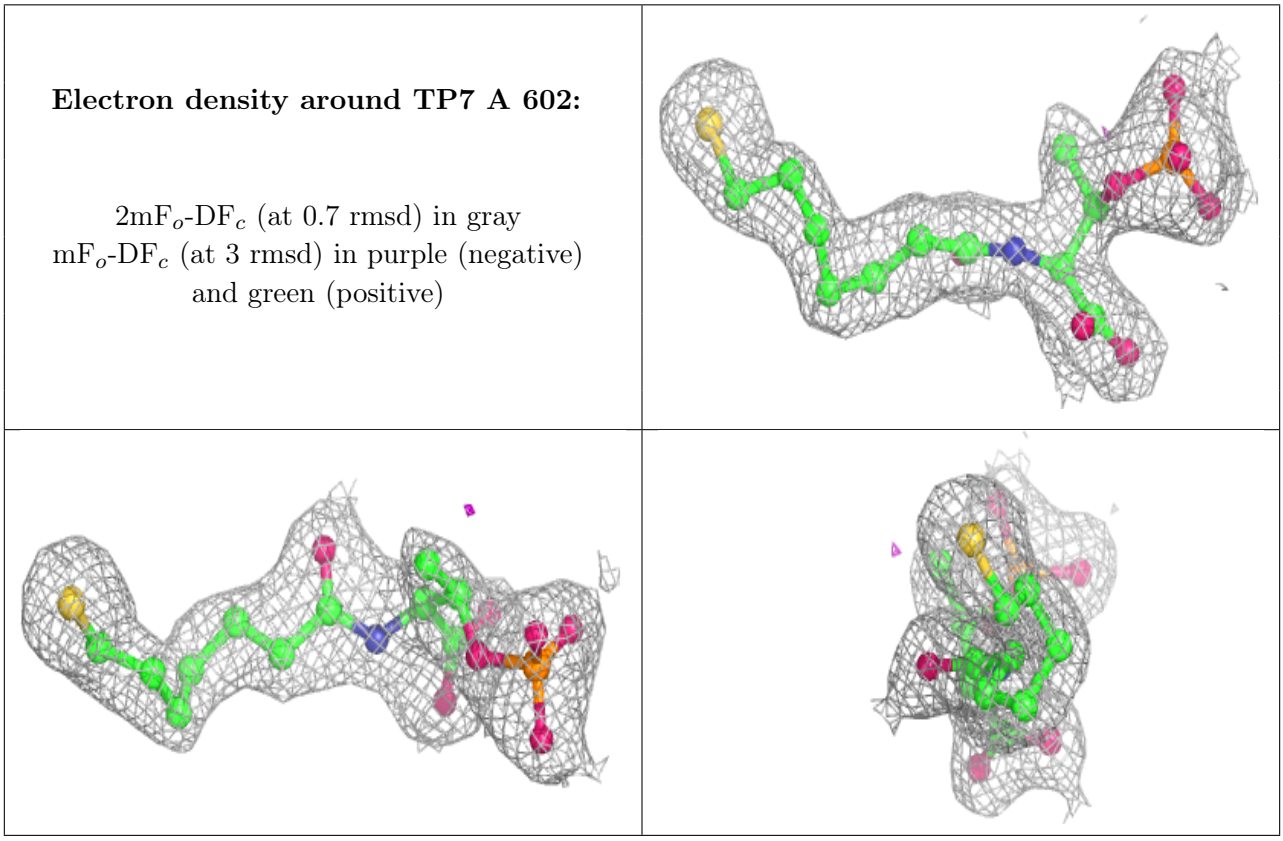
Electron density around TP7 J 602:

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



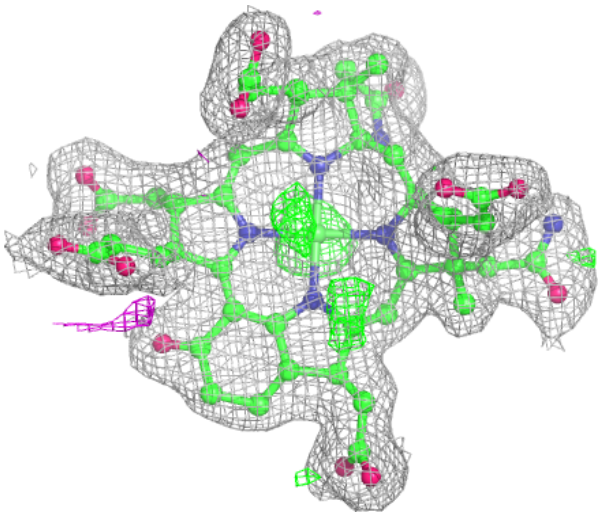
Electron density around TP7 A 602:

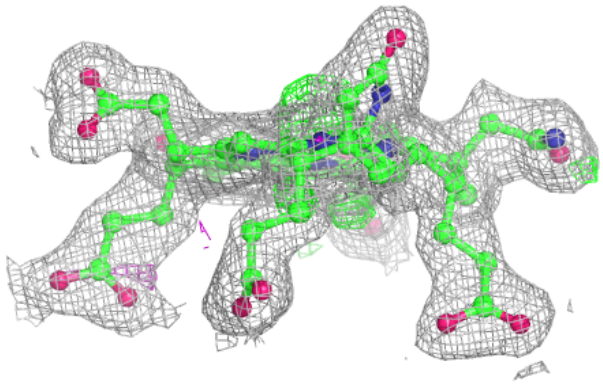
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

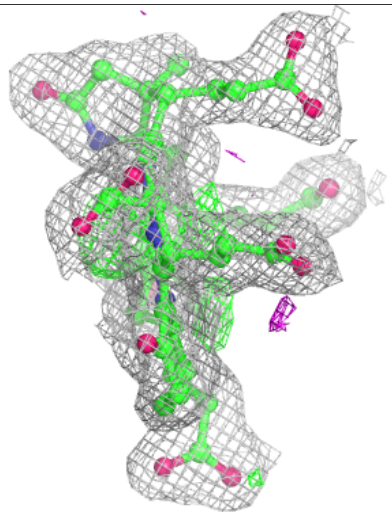


Electron density around F43 A 603:

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

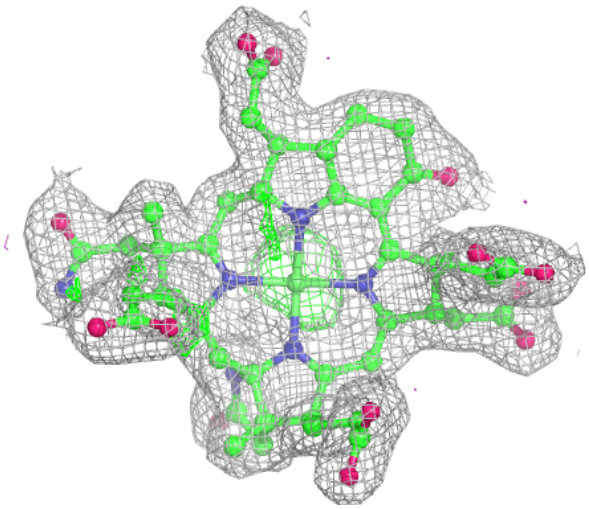


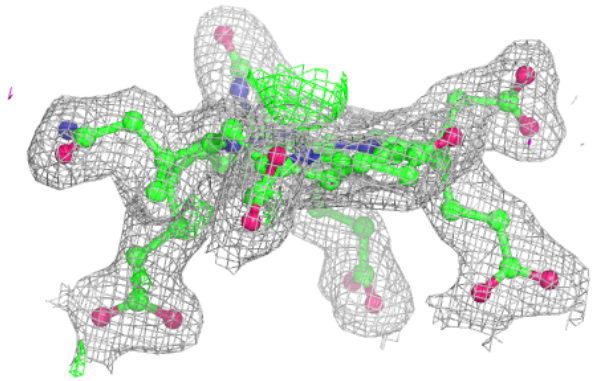




Electron density around F43 D 603:

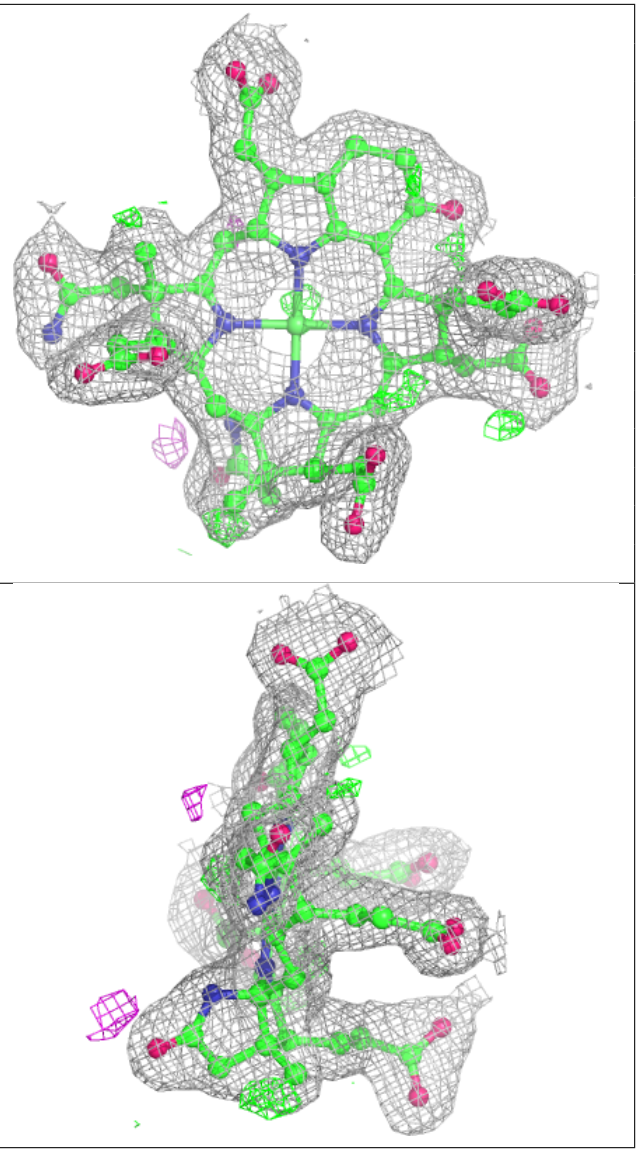
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





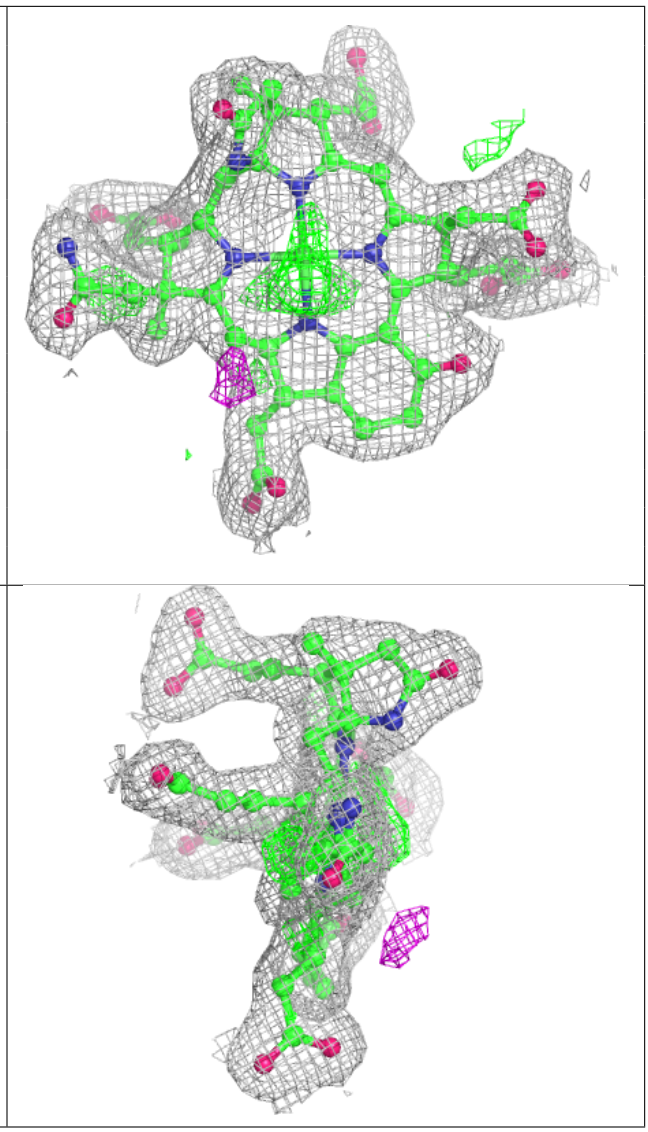
Electron density around F43 G 603:

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



Electron density around F43 J 603:

$2mF_o$-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.