Full wwPDB X-ray Structure Validation Report ⓘ

Feb 4, 2024 – 11:48 AM EST

PDB ID	:	1RIT
Title	:	Crystal structure of Peanut lectin in complex with meso-tetrasulphonatophenylporphyrin and lactose
Authors	:	Goel, M.; Kaur, K.J.; Maiya, B.G.; Swamy, M.J.; Salunke, D.M.
Deposited on	:	2003-11-17
Resolution	:	2.85 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:

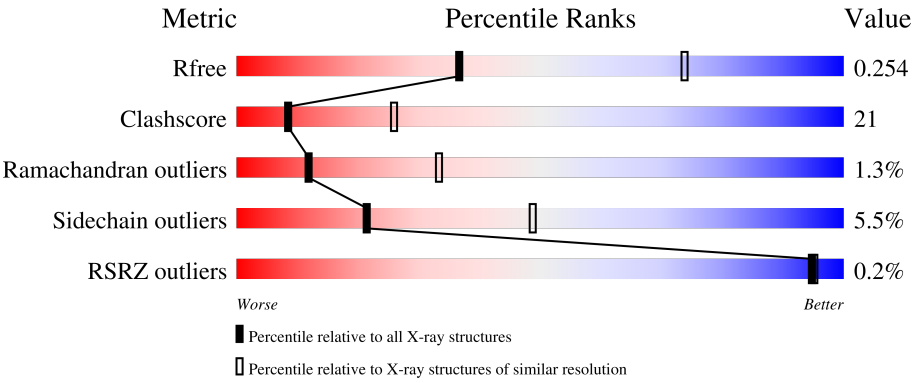
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	236	55% 39%
1	B	236	56% 38%
1	C	236	64% 32%
1	D	236	65% 30%
2	E	2	50% 50%

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Mol	Chain	Length	Quality of chain
2	F	2	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7772 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.

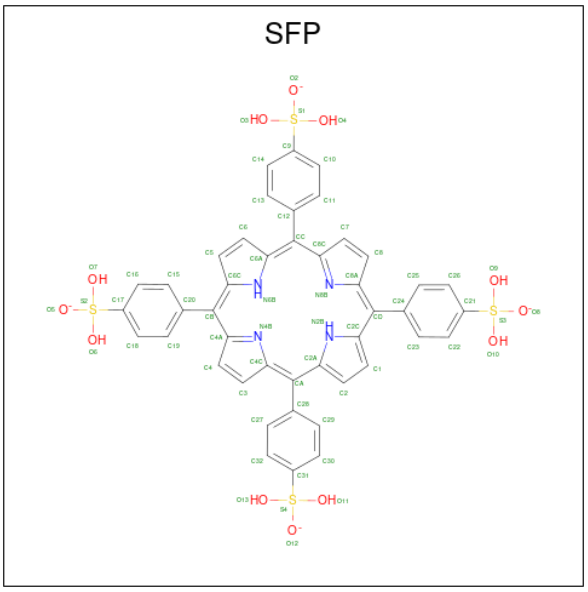
- Molecule 1 is a protein called Galactose-binding lectin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	232	Total	C	N	O	S	0	0	0
			1743	1102	287	352	2			
1	B	232	Total	C	N	O	S	0	0	0
			1743	1102	287	352	2			
1	C	232	Total	C	N	O	S	0	0	0
			1743	1102	287	352	2			
1	D	232	Total	C	N	O	S	0	0	0
			1743	1102	287	352	2			

- Molecule 2 is an oligosaccharide called beta-D-galactopyranose-(1-4)-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	O		0	0	0
			23	12	11				
2	F	2	Total	C	O		0	0	0
			23	12	11				

- Molecule 3 is 5,10,15,20-TETRAKIS(4-SULPFONATOPHENYL)-21H,23H-PORPHINE (three-letter code: SFP) (formula: $C_{44}H_{34}N_4O_{12}S_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			64	44	4	12	4		
3	A	1	Total	C	N	O	S	0	0
			64	44	4	12	4		
3	A	1	Total	C	N	O	S	0	0
			64	44	4	12	4		
3	A	1	Total	C	N	O	S	0	0
			64	44	4	12	4		
3	B	1	Total	C	N	O	S	0	0
			64	44	4	12	4		
3	B	1	Total	C	N	O	S	0	0
			64	44	4	12	4		
3	B	1	Total	C	N	O	S	0	0
			64	44	4	12	4		
3	C	1	Total	C	N	O	S	0	0
			64	44	4	12	4		
3	C	1	Total	C	N	O	S	0	0
			64	44	4	12	4		
3	D	1	Total	C	N	O	S	0	0
			64	44	4	12	4		
3	D	1	Total	C	N	O	S	0	0
			64	44	4	12	4		

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

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

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

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 6 is water.

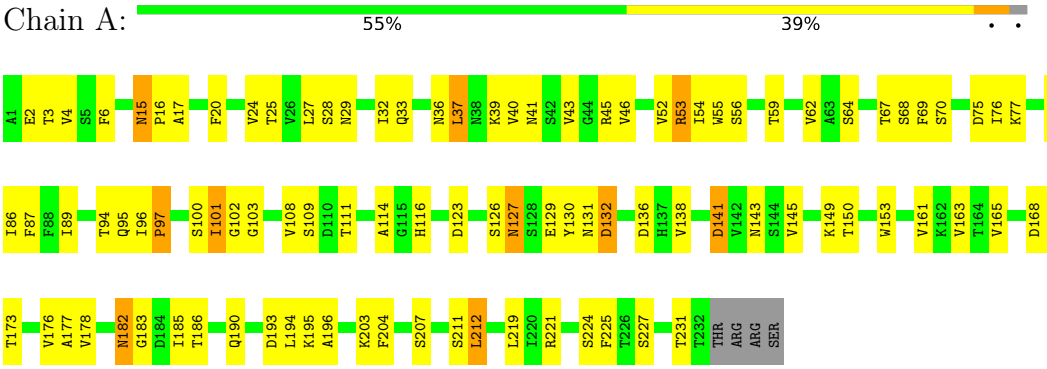
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	16	Total O 16 16	0	0
6	B	7	Total O 7 7	0	0
6	C	9	Total O 9 9	0	0
6	D	10	Total O 10 10	0	0

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.

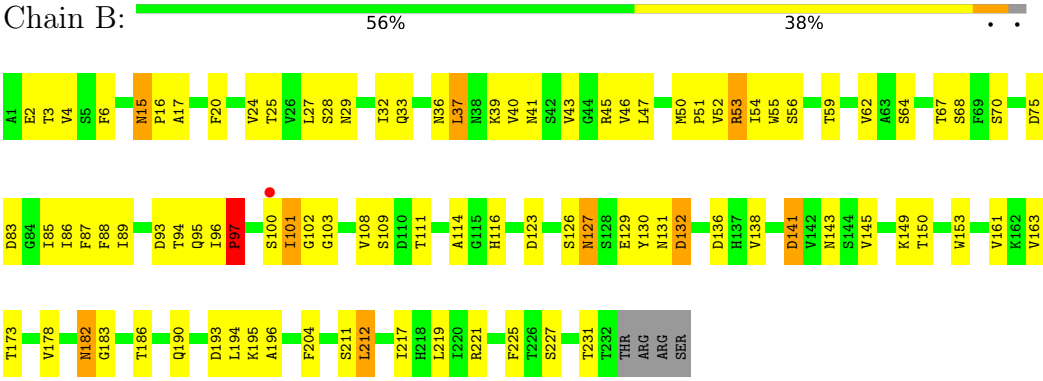
• Molecule 1: Galactose-binding lectin

Chain A:



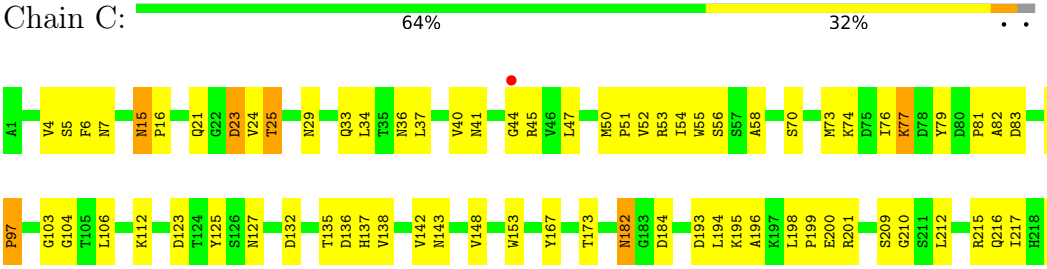
• Molecule 1: Galactose-binding lectin

Chain B:



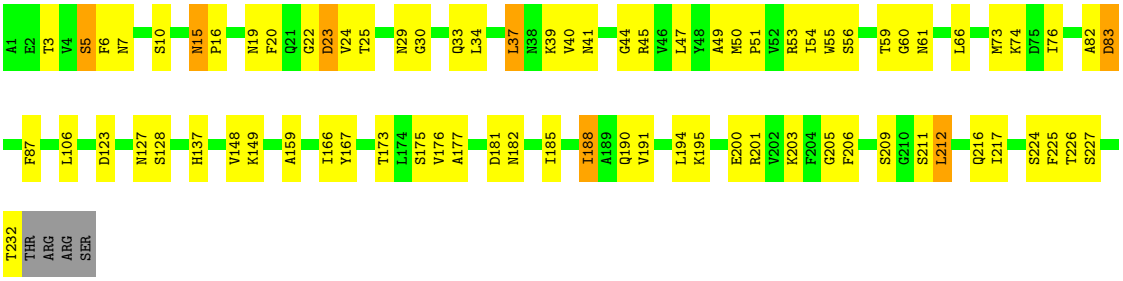
• Molecule 1: Galactose-binding lectin

Chain C:



• Molecule 1: Galactose-binding lectin

Chain D:



• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain E:

• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	94.90Å 94.90Å 144.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	100.00 – 2.85 54.18 – 2.85	Depositor EDS
% Data completeness (in resolution range)	(Not available) (100.00-2.85) 76.9 (54.18-2.85)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.37 (at 2.86Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.235 , 0.260 0.229 , 0.254	Depositor DCC
R_{free} test set	2579 reflections (8.66%)	wwPDB-VP
Wilson B-factor (Å^2)	55.7	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 60.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l 0.397 for h,-h-k,-l 0.028 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	7772	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.32% 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: BGC, GAL, MN, SFP, CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.43	0/1779	0.72	0/2426
1	B	0.44	0/1779	0.72	0/2426
1	C	0.45	0/1779	0.69	0/2426
1	D	0.42	0/1779	0.70	0/2426
All	All	0.44	0/7116	0.71	0/9704

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

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	1743	0	1699	96	0
1	B	1743	0	1699	86	0
1	C	1743	0	1699	58	0
1	D	1743	0	1699	65	0
2	E	23	0	21	1	0
2	F	23	0	21	3	0
3	A	256	0	120	16	0
3	B	192	0	90	7	0
3	C	128	0	60	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	128	0	60	5	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	16	0	0	5	0
6	B	7	0	0	1	0
6	C	9	0	0	1	0
6	D	10	0	0	0	0
All	All	7772	0	7168	310	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 21.

All (310) 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:A:41:ASN:HB2	1:A:100:SER:O	1.63	0.97
1:B:41:ASN:HB2	1:B:100:SER:O	1.63	0.96
1:C:15:ASN:HD22	1:C:16:PRO:HD2	1.31	0.96
1:C:29:ASN:HA	1:D:217:ILE:HD13	1.49	0.94
1:B:15:ASN:ND2	1:B:17:ALA:H	1.68	0.91
1:A:15:ASN:ND2	1:A:17:ALA:H	1.70	0.89
1:B:59:THR:HG21	1:B:231:THR:HG22	1.56	0.86
1:A:59:THR:HG21	1:A:231:THR:HG22	1.58	0.85
1:A:219:LEU:HD11	3:A:243:SFP:H22	1.59	0.83
1:B:4:VAL:HG21	1:B:52:VAL:HG13	1.61	0.82
1:C:217:ILE:HD13	1:D:29:ASN:HA	1.61	0.82
1:A:4:VAL:HG21	1:A:52:VAL:HG13	1.60	0.81
1:B:43:VAL:HG12	1:B:96:ILE:HD11	1.61	0.81
1:B:15:ASN:C	1:B:15:ASN:HD22	1.87	0.78
1:A:127:ASN:H	1:A:132:ASP:HB2	1.48	0.77
1:B:127:ASN:H	1:B:132:ASP:HB2	1.49	0.77
1:A:15:ASN:C	1:A:15:ASN:HD22	1.88	0.77
1:A:101:ILE:HG13	1:A:102:GLY:N	2.00	0.77
1:A:41:ASN:CB	1:A:100:SER:O	2.33	0.77
1:A:43:VAL:HG12	1:A:96:ILE:HD11	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:ASN:CB	1:B:100:SER:O	2.33	0.76
1:B:101:ILE:HG13	1:B:102:GLY:N	1.99	0.76
1:C:77:LYS:H	1:C:77:LYS:HD2	1.52	0.73
1:A:101:ILE:CG1	1:A:102:GLY:N	2.51	0.73
1:B:101:ILE:CG1	1:B:102:GLY:N	2.50	0.73
1:A:101:ILE:HG22	3:A:251:SFP:O6	1.88	0.73
1:C:77:LYS:H	1:C:77:LYS:CD	2.02	0.73
1:A:52:VAL:HA	6:A:255:HOH:O	1.89	0.72
3:C:240:SFP:O10	6:C:254:HOH:O	2.07	0.71
1:B:15:ASN:HD22	1:B:16:PRO:N	1.88	0.71
1:A:82:ALA:HB1	1:A:83:ASP:HA	1.74	0.70
1:C:15:ASN:HD22	1:C:16:PRO:CD	2.04	0.69
1:A:15:ASN:HD22	1:A:16:PRO:N	1.90	0.69
1:D:34:LEU:O	1:D:44:GLY:HA3	1.92	0.68
1:B:219:LEU:HD11	3:B:245:SFP:H22	1.75	0.67
1:D:55:TRP:O	1:D:200:GLU:HG3	1.95	0.67
1:D:19:ASN:ND2	1:D:49:ALA:HA	2.10	0.66
1:B:82:ALA:HB1	1:B:83:ASP:HA	1.78	0.66
1:D:24:VAL:HG21	1:D:45:ARG:O	1.96	0.66
1:B:24:VAL:HG21	1:B:45:ARG:O	1.96	0.65
1:A:138:VAL:HG23	1:A:153:TRP:HB2	1.79	0.65
1:D:55:TRP:CZ3	1:D:195:LYS:HE3	2.33	0.64
1:B:15:ASN:HD22	1:B:17:ALA:H	1.45	0.63
1:B:138:VAL:HG23	1:B:153:TRP:HB2	1.80	0.63
1:D:127:ASN:HD21	2:F:2:GAL:H3	1.62	0.63
1:A:203:LYS:HB3	6:A:267:HOH:O	1.98	0.63
1:B:217:ILE:HD13	3:B:245:SFP:H23	1.80	0.62
1:D:40:VAL:HG12	1:D:41:ASN:ND2	2.14	0.62
1:C:21:GLN:O	1:C:24:VAL:HG23	1.99	0.62
3:A:243:SFP:C26	3:A:244:SFP:H25	2.30	0.62
1:D:59:THR:C	1:D:61:ASN:H	2.03	0.62
1:A:24:VAL:HG21	1:A:45:ARG:O	2.00	0.61
1:B:40:VAL:O	1:B:41:ASN:CG	2.38	0.61
1:A:101:ILE:CG1	1:A:102:GLY:H	2.13	0.61
1:B:101:ILE:CG1	1:B:102:GLY:H	2.13	0.61
1:D:49:ALA:O	1:D:203:LYS:HE2	2.01	0.61
1:B:25:THR:HG23	1:B:33:GLN:HB3	1.81	0.61
1:C:182:ASN:HD21	1:C:184:ASP:HB2	1.64	0.61
3:C:239:SFP:H15	3:C:240:SFP:H14	1.81	0.61
1:A:15:ASN:HD22	1:A:17:ALA:H	1.46	0.61
1:D:7:ASN:OD1	1:D:224:SER:HB3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ILE:HG22	1:A:86:ILE:N	2.17	0.60
1:C:34:LEU:O	1:C:44:GLY:HA3	2.00	0.60
1:A:62:VAL:O	1:A:169:SER:HB2	2.02	0.60
1:D:23:ASP:OD1	1:D:39:LYS:HD3	2.01	0.60
3:A:244:SFP:H27	3:A:244:SFP:H3	1.84	0.60
1:A:25:THR:HG23	1:A:33:GLN:HB3	1.84	0.60
3:A:244:SFP:H27	3:A:244:SFP:C3	2.32	0.59
1:D:82:ALA:HB1	1:D:83:ASP:HA	1.84	0.59
3:A:244:SFP:H3	3:A:244:SFP:C27	2.32	0.59
1:A:40:VAL:O	1:A:41:ASN:CG	2.41	0.59
1:A:56:SER:HB3	1:A:59:THR:OG1	2.03	0.59
1:D:127:ASN:HD21	2:F:2:GAL:C3	2.16	0.58
1:C:142:VAL:HG12	1:C:142:VAL:O	2.04	0.58
1:D:59:THR:O	1:D:61:ASN:N	2.35	0.58
1:D:159:ALA:HB1	1:D:181:ASP:HB2	1.85	0.58
1:C:40:VAL:HG13	1:C:212:LEU:HB2	1.86	0.58
1:D:53:ARG:NH2	3:D:241:SFP:O12	2.35	0.58
1:B:56:SER:HB3	1:B:59:THR:OG1	2.04	0.57
1:D:25:THR:HG23	1:D:33:GLN:HB3	1.87	0.57
1:D:44:GLY:O	1:D:45:ARG:HG2	2.04	0.57
1:B:101:ILE:HG22	3:B:238:SFP:O6	2.04	0.57
1:C:6:PHE:CZ	1:C:225:PHE:HB3	2.39	0.57
1:D:123:ASP:HB3	1:D:137:HIS:CE1	2.40	0.57
1:B:85:ILE:HG22	1:B:86:ILE:N	2.20	0.56
1:D:73:MET:HA	1:D:217:ILE:O	2.06	0.56
1:A:94:THR:HG23	1:A:94:THR:O	2.06	0.56
1:B:94:THR:O	1:B:94:THR:HG23	2.05	0.56
1:D:15:ASN:HD22	1:D:16:PRO:HD2	1.68	0.56
1:C:193:ASP:HB3	1:C:196:ALA:HB3	1.87	0.55
1:A:15:ASN:ND2	1:A:15:ASN:C	2.58	0.55
1:C:15:ASN:ND2	1:C:16:PRO:HD2	2.12	0.55
1:D:87:PHE:HD1	1:D:206:PHE:CE1	2.25	0.55
3:D:241:SFP:H15	3:D:242:SFP:H14	1.87	0.55
1:C:95:GLN:O	1:C:97:PRO:HD3	2.07	0.55
1:A:172:LYS:HE2	1:A:193:ASP:OD2	2.07	0.55
1:D:106:LEU:HA	1:D:209:SER:OG	2.07	0.55
1:B:182:ASN:HD22	1:B:183:GLY:N	2.04	0.55
1:B:54:ILE:HG13	1:B:55:TRP:HD1	1.71	0.55
1:B:62:VAL:O	1:B:169:SER:HB2	2.06	0.55
1:C:104:GLY:HA3	1:C:127:ASN:ND2	2.22	0.55
1:C:76:ILE:HD11	1:C:215:ARG:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:TYR:CZ	1:D:194:LEU:HG	2.42	0.55
1:C:55:TRP:CE3	1:C:195:LYS:HG3	2.42	0.54
1:B:15:ASN:ND2	1:B:15:ASN:C	2.57	0.54
1:A:32:ILE:HD13	1:A:46:VAL:HG21	1.90	0.54
1:A:127:ASN:H	1:A:132:ASP:CB	2.18	0.54
1:B:182:ASN:HD22	1:B:183:GLY:H	1.55	0.54
1:D:53:ARG:HH22	3:D:242:SFP:H32	1.73	0.54
1:A:85:ILE:HG22	1:A:86:ILE:H	1.73	0.54
1:A:101:ILE:CG2	3:A:251:SFP:S2	2.95	0.54
1:C:4:VAL:O	1:C:226:THR:HA	2.07	0.54
1:C:24:VAL:HG21	1:C:45:ARG:O	2.08	0.54
1:C:73:MET:HA	1:C:217:ILE:O	2.08	0.54
1:D:74:LYS:O	1:D:216:GLN:HB2	2.09	0.53
1:C:123:ASP:HB3	1:C:137:HIS:CE1	2.43	0.53
1:B:127:ASN:H	1:B:132:ASP:CB	2.19	0.53
1:C:225:PHE:CZ	1:C:227:SER:HB3	2.44	0.53
1:B:101:ILE:HG12	1:B:102:GLY:H	1.73	0.53
1:B:130:TYR:O	1:B:131:ASN:HB2	2.08	0.53
1:A:193:ASP:HB3	1:A:196:ALA:HB3	1.91	0.53
1:B:32:ILE:HD13	1:B:46:VAL:HG21	1.90	0.52
1:C:7:ASN:OD1	1:C:224:SER:HB3	2.09	0.52
1:A:54:ILE:HG13	1:A:55:TRP:HD1	1.75	0.52
1:A:101:ILE:HG12	1:A:102:GLY:H	1.74	0.52
1:B:182:ASN:HD22	1:B:182:ASN:N	2.07	0.52
1:C:53:ARG:NH1	3:C:239:SFP:O12	2.41	0.52
3:A:250:SFP:C5	3:A:251:SFP:H9	2.40	0.52
1:A:20:PHE:CE1	1:A:46:VAL:HG23	2.45	0.51
1:B:172:LYS:HE2	1:B:193:ASP:OD2	2.10	0.51
1:B:212:LEU:O	1:B:212:LEU:HD23	2.09	0.51
1:D:55:TRP:CE3	1:D:195:LYS:HE3	2.46	0.51
1:A:70:SER:HA	1:A:161:VAL:O	2.11	0.51
1:A:212:LEU:HD23	1:A:212:LEU:O	2.11	0.51
1:B:70:SER:HA	1:B:161:VAL:O	2.10	0.51
1:B:95:GLN:HA	1:B:95:GLN:NE2	2.26	0.51
1:A:4:VAL:HG21	1:A:52:VAL:CG1	2.37	0.51
1:B:20:PHE:CE1	1:B:46:VAL:HG23	2.46	0.51
1:A:182:ASN:HD22	1:A:183:GLY:N	2.09	0.51
1:B:193:ASP:HB3	1:B:196:ALA:HB3	1.93	0.51
1:B:123:ASP:OD2	1:B:132:ASP:OD2	2.30	0.50
1:D:212:LEU:HB3	2:F:1:BGC:O2	2.11	0.50
1:A:6:PHE:CZ	1:A:225:PHE:HB3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:TYR:O	1:A:131:ASN:HB2	2.10	0.50
1:C:74:LYS:HE2	1:D:10:SER:HB3	1.92	0.50
1:A:68:SER:HA	1:A:163:VAL:O	2.11	0.50
1:D:6:PHE:CZ	1:D:225:PHE:HB3	2.46	0.50
1:B:6:PHE:CZ	1:B:225:PHE:HB3	2.46	0.50
1:A:182:ASN:HD22	1:A:183:GLY:H	1.60	0.50
3:A:243:SFP:H26	3:A:244:SFP:H25	1.93	0.49
1:A:116:HIS:HA	1:A:143:ASN:OD1	2.13	0.49
1:A:221:ARG:NH1	6:A:263:HOH:O	2.32	0.49
1:A:182:ASN:HD22	1:A:182:ASN:N	2.09	0.49
1:B:54:ILE:HG13	1:B:55:TRP:CD1	2.47	0.49
1:B:182:ASN:ND2	1:B:183:GLY:N	2.60	0.49
1:C:76:ILE:HG13	1:C:79:TYR:HB2	1.94	0.49
1:C:182:ASN:N	1:C:182:ASN:HD22	2.11	0.49
1:D:37:LEU:HG	1:D:76:ILE:HD13	1.95	0.49
1:D:201:ARG:HG3	1:D:201:ARG:HH11	1.77	0.49
1:A:2:GLU:OE1	1:A:53:ARG:NH1	2.46	0.48
1:A:25:THR:CG2	1:A:33:GLN:HB3	2.43	0.48
1:A:64:SER:OG	1:A:169:SER:HB3	2.13	0.48
1:A:95:GLN:NE2	1:A:95:GLN:HA	2.28	0.48
1:B:97:PRO:HG2	1:B:108:VAL:HA	1.95	0.48
1:C:54:ILE:HG13	1:C:55:TRP:HD1	1.78	0.48
1:B:25:THR:CG2	1:B:33:GLN:HB3	2.42	0.48
1:C:198:LEU:HB3	1:C:199:PRO:HD2	1.95	0.48
1:D:5:SER:HA	1:D:225:PHE:O	2.13	0.48
1:A:141:ASP:OD2	1:A:145:VAL:HA	2.13	0.48
1:A:149:LYS:HG2	1:A:150:THR:N	2.28	0.48
1:A:178:VAL:HB	1:A:186:THR:HB	1.95	0.48
1:A:221:ARG:HG2	1:A:221:ARG:HH11	1.79	0.48
1:B:85:ILE:HG22	1:B:86:ILE:H	1.79	0.48
1:D:22:GLY:C	1:D:24:VAL:H	2.17	0.48
1:C:29:ASN:HA	1:D:217:ILE:CD1	2.32	0.48
1:B:37:LEU:HG	1:B:76:ILE:HD13	1.96	0.47
1:C:125:TYR:CZ	2:E:2:GAL:H5	2.49	0.47
1:A:101:ILE:O	1:A:211:SER:CB	2.63	0.47
1:A:123:ASP:OD2	1:A:132:ASP:OD2	2.33	0.47
1:B:212:LEU:HD21	3:B:238:SFP:C30	2.44	0.47
1:B:221:ARG:HG2	1:B:221:ARG:HH11	1.79	0.47
3:B:237:SFP:C5	3:B:238:SFP:H9	2.44	0.47
1:D:10:SER:HB2	1:D:30:GLY:HA3	1.96	0.47
1:A:101:ILE:CG2	3:A:251:SFP:O6	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:SER:HA	1:B:163:VAL:O	2.14	0.47
1:A:37:LEU:HG	1:A:76:ILE:HD13	1.96	0.47
1:A:54:ILE:HG13	1:A:55:TRP:CD1	2.49	0.47
1:A:97:PRO:HG2	1:A:108:VAL:HA	1.96	0.47
1:B:3:THR:HG23	1:B:227:SER:O	2.14	0.47
1:D:20:PHE:HD1	1:D:24:VAL:HG11	1.79	0.47
1:D:22:GLY:O	1:D:24:VAL:N	2.47	0.47
1:B:173:THR:HG21	1:C:173:THR:HG21	1.96	0.47
1:C:217:ILE:CD1	1:D:29:ASN:HA	2.38	0.47
3:D:241:SFP:C6A	3:D:242:SFP:H9	2.45	0.47
1:A:20:PHE:CD1	1:A:46:VAL:HG23	2.50	0.46
1:B:36:ASN:HB3	1:B:39:LYS:HG3	1.96	0.46
1:A:126:SER:HA	1:A:132:ASP:HB3	1.97	0.46
1:B:221:ARG:HG2	1:B:221:ARG:NH1	2.31	0.46
1:B:75:ASP:O	3:B:245:SFP:H29	2.14	0.46
1:B:101:ILE:CG2	3:B:238:SFP:S2	3.03	0.46
1:B:178:VAL:HB	1:B:186:THR:HB	1.98	0.46
1:B:172:LYS:HD3	1:B:193:ASP:HA	1.98	0.46
1:C:41:ASN:HA	1:C:210:GLY:O	2.15	0.46
1:B:43:VAL:CG1	1:B:96:ILE:HD11	2.39	0.46
1:B:109:SER:HB2	1:B:114:ALA:O	2.15	0.46
1:A:75:ASP:O	3:A:243:SFP:H29	2.15	0.46
1:B:149:LYS:HG2	1:B:150:THR:N	2.29	0.46
1:B:64:SER:OG	1:B:169:SER:HB3	2.15	0.46
1:C:23:ASP:HB3	1:C:36:ASN:HB2	1.97	0.46
1:C:167:TYR:CZ	1:C:194:LEU:HG	2.51	0.46
1:D:185:ILE:HG13	1:D:185:ILE:O	2.15	0.46
1:B:27:LEU:C	1:B:29:ASN:H	2.19	0.45
1:C:33:GLN:HA	1:C:219:LEU:HD23	1.99	0.45
1:A:172:LYS:HD3	1:A:193:ASP:HA	1.97	0.45
1:D:53:ARG:NH2	3:D:242:SFP:H32	2.29	0.45
1:B:126:SER:HA	1:B:132:ASP:HB3	1.97	0.45
1:B:141:ASP:OD2	1:B:145:VAL:HA	2.17	0.45
1:B:101:ILE:O	1:B:211:SER:CB	2.64	0.45
1:A:127:ASN:HB3	1:A:129:GLU:CD	2.37	0.45
1:A:221:ARG:NH1	1:A:221:ARG:HG2	2.32	0.45
1:D:56:SER:O	1:D:59:THR:O	2.35	0.45
1:C:4:VAL:HG21	1:C:52:VAL:HG13	1.99	0.45
1:B:127:ASN:HB3	1:B:129:GLU:CD	2.37	0.45
1:B:116:HIS:HA	1:B:143:ASN:OD1	2.17	0.45
1:D:47:LEU:HD23	1:D:205:GLY:HA3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:THR:HG21	1:B:87:PHE:CZ	2.51	0.44
1:B:149:LYS:HE3	1:B:190:GLN:OE1	2.17	0.44
1:C:5:SER:HB2	1:C:226:THR:OG1	2.17	0.44
1:C:106:LEU:HA	1:C:209:SER:OG	2.17	0.44
1:D:190:GLN:HE21	1:D:191:VAL:H	1.65	0.44
1:A:15:ASN:HD22	1:A:16:PRO:CD	2.30	0.44
1:A:46:VAL:O	1:A:46:VAL:CG1	2.65	0.44
1:A:182:ASN:ND2	1:A:183:GLY:N	2.65	0.44
1:D:59:THR:C	1:D:61:ASN:N	2.69	0.44
1:D:188:ILE:HG23	1:D:188:ILE:O	2.17	0.44
1:A:101:ILE:O	1:A:211:SER:HA	2.18	0.44
1:B:20:PHE:CD1	1:B:46:VAL:HG23	2.53	0.44
1:B:32:ILE:CD1	1:B:46:VAL:HG21	2.47	0.44
1:C:138:VAL:HG23	1:C:153:TRP:CB	2.48	0.44
1:D:39:LYS:HB3	1:D:39:LYS:HE2	1.76	0.44
1:A:67:THR:HG21	1:A:87:PHE:CZ	2.53	0.44
1:A:27:LEU:C	1:A:29:ASN:H	2.21	0.44
1:D:176:VAL:HG12	1:D:177:ALA:N	2.33	0.44
1:D:6:PHE:CE2	1:D:225:PHE:HB3	2.53	0.43
1:A:37:LEU:HB3	3:A:243:SFP:H17	2.00	0.43
1:A:67:THR:HG22	1:A:165:VAL:HB	2.00	0.43
1:D:82:ALA:CB	1:D:83:ASP:HA	2.44	0.43
1:D:148:VAL:O	1:D:148:VAL:CG1	2.67	0.43
1:B:101:ILE:O	1:B:211:SER:HA	2.19	0.43
1:D:54:ILE:HG13	1:D:55:TRP:CD1	2.54	0.43
1:A:46:VAL:O	1:A:46:VAL:HG13	2.18	0.43
1:A:173:THR:HG21	1:D:173:THR:HG21	2.01	0.43
1:A:149:LYS:HE3	1:A:190:GLN:OE1	2.19	0.42
1:C:24:VAL:HG12	1:C:25:THR:N	2.33	0.42
1:C:56:SER:OG	1:C:58:ALA:HB3	2.19	0.42
1:A:3:THR:HG23	1:A:227:SER:O	2.19	0.42
1:A:109:SER:HB2	1:A:114:ALA:O	2.18	0.42
1:A:171:THR:CG2	1:D:149:LYS:NZ	2.82	0.42
1:A:45:ARG:HG3	1:A:96:ILE:HD12	2.01	0.42
1:B:2:GLU:OE1	1:B:53:ARG:NH1	2.53	0.42
1:C:70:SER:OG	1:C:221:ARG:HB2	2.19	0.42
1:C:142:VAL:O	1:C:143:ASN:HB2	2.19	0.42
1:D:40:VAL:O	1:D:211:SER:O	2.37	0.42
1:A:69:PHE:CE1	1:A:163:VAL:HB	2.54	0.42
1:A:193:ASP:OD1	1:A:195:LYS:HB3	2.19	0.42
3:A:250:SFP:C6	3:A:251:SFP:H9	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:LEU:HD21	1:B:88:PHE:CZ	2.55	0.42
1:A:86:ILE:HG22	1:A:207:SER:O	2.19	0.42
1:A:171:THR:HG22	1:D:149:LYS:NZ	2.33	0.42
1:B:138:VAL:HG23	1:B:153:TRP:CB	2.47	0.42
1:D:3:THR:HG23	1:D:227:SER:O	2.19	0.42
1:A:89:ILE:HG12	1:A:204:PHE:CE1	2.54	0.42
3:A:250:SFP:C1	3:A:251:SFP:H25	2.49	0.42
1:B:194:LEU:HD23	1:B:194:LEU:HA	1.84	0.42
1:C:138:VAL:HG23	1:C:153:TRP:HB2	2.02	0.42
1:D:50:MET:HA	1:D:51:PRO:HD3	1.77	0.42
1:C:82:ALA:HB1	1:C:83:ASP:HA	2.02	0.42
1:A:221:ARG:NH2	6:A:263:HOH:O	2.43	0.42
3:A:244:SFP:C23	3:A:244:SFP:H8	2.50	0.42
1:C:50:MET:HA	1:C:51:PRO:HD3	1.71	0.42
1:C:95:GLN:HA	1:C:95:GLN:NE2	2.35	0.42
1:C:225:PHE:CE1	1:C:227:SER:HB3	2.55	0.42
1:A:36:ASN:HB3	1:A:39:LYS:HG3	2.02	0.42
1:B:15:ASN:HD22	1:B:16:PRO:CD	2.33	0.42
1:B:89:ILE:HG12	1:B:204:PHE:CE1	2.55	0.42
1:C:83:ASP:OD2	1:C:210:GLY:HA2	2.20	0.41
1:C:127:ASN:H	1:C:132:ASP:HB2	1.85	0.41
3:A:244:SFP:C3	3:A:244:SFP:C27	2.89	0.41
1:A:194:LEU:HD23	1:A:194:LEU:HA	1.84	0.41
1:C:55:TRP:CD2	1:C:195:LYS:HG3	2.55	0.41
1:D:44:GLY:C	1:D:45:ARG:HG2	2.41	0.41
1:A:168:ASP:HB3	1:A:171:THR:OG1	2.20	0.41
1:B:76:ILE:HG13	1:B:76:ILE:O	2.20	0.41
1:A:138:VAL:HG23	1:A:153:TRP:CB	2.49	0.41
1:B:50:MET:HA	1:B:51:PRO:HD3	1.96	0.41
1:B:93:ASP:CG	6:B:258:HOH:O	2.59	0.41
1:A:224:SER:HB3	6:A:254:HOH:O	2.19	0.41
1:D:190:GLN:NE2	1:D:191:VAL:H	2.18	0.41
1:A:176:VAL:HG12	1:A:177:ALA:N	2.36	0.41
1:B:4:VAL:HG21	1:B:52:VAL:CG1	2.40	0.41
1:B:55:TRP:CD2	1:B:195:LYS:HG3	2.56	0.41
1:C:135:THR:O	1:C:136:ASP:C	2.58	0.41
1:A:185:ILE:HG23	1:D:226:THR:HG21	2.03	0.41
1:A:32:ILE:CD1	1:A:46:VAL:HG21	2.50	0.41
1:D:148:VAL:O	1:D:148:VAL:HG12	2.21	0.41
1:B:47:LEU:HD21	1:B:88:PHE:HZ	1.85	0.40
1:D:66:LEU:CD1	1:D:166:ILE:HG12	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:LEU:HD21	1:C:88:PHE:CZ	2.57	0.40
1:C:81:PRO:HB3	1:C:216:GLN:NE2	2.37	0.40
1:C:55:TRP:CD1	1:C:200:GLU:HA	2.56	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	230/236 (98%)	204 (89%)	23 (10%)	3 (1%)	12 33
1	B	230/236 (98%)	204 (89%)	22 (10%)	4 (2%)	9 27
1	C	230/236 (98%)	202 (88%)	26 (11%)	2 (1%)	17 43
1	D	230/236 (98%)	208 (90%)	19 (8%)	3 (1%)	12 33
All	All	920/944 (98%)	818 (89%)	90 (10%)	12 (1%)	12 33

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	23	ASP
1	A	103	GLY
1	B	103	GLY
1	C	23	ASP
1	A	28	SER
1	B	28	SER
1	A	77	LYS
1	B	77	LYS
1	C	103	GLY
1	B	97	PRO
1	D	60	GLY
1	D	188	ILE

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	197/201 (98%)	185 (94%)	12 (6%)	18	43
1	B	197/201 (98%)	185 (94%)	12 (6%)	18	43
1	C	197/201 (98%)	187 (95%)	10 (5%)	24	52
1	D	197/201 (98%)	188 (95%)	9 (5%)	27	56
All	All	788/804 (98%)	745 (94%)	43 (6%)	21	49

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	37	LEU
1	A	53	ARG
1	A	97	PRO
1	A	101	ILE
1	A	111	THR
1	A	127	ASN
1	A	132	ASP
1	A	136	ASP
1	A	141	ASP
1	A	182	ASN
1	A	212	LEU
1	B	15	ASN
1	B	37	LEU
1	B	53	ARG
1	B	97	PRO
1	B	101	ILE
1	B	111	THR
1	B	127	ASN
1	B	132	ASP
1	B	136	ASP
1	B	141	ASP
1	B	182	ASN
1	B	212	LEU

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Mol	Chain	Res	Type
1	C	15	ASN
1	C	25	THR
1	C	37	LEU
1	C	77	LYS
1	C	97	PRO
1	C	112	LYS
1	C	148	VAL
1	C	182	ASN
1	C	201	ARG
1	C	232	THR
1	D	5	SER
1	D	15	ASN
1	D	37	LEU
1	D	83	ASP
1	D	128	SER
1	D	175	SER
1	D	182	ASN
1	D	212	LEU
1	D	232	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	19	ASN
1	A	33	GLN
1	A	61	ASN
1	A	95	GLN
1	A	182	ASN
1	A	216	GLN
1	B	15	ASN
1	B	19	ASN
1	B	31	ASN
1	B	33	GLN
1	B	61	ASN
1	B	95	GLN
1	B	182	ASN
1	B	216	GLN
1	C	15	ASN
1	C	31	ASN
1	C	33	GLN
1	C	41	ASN

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Mol	Chain	Res	Type
1	C	61	ASN
1	C	95	GLN
1	C	182	ASN
1	C	216	GLN
1	D	15	ASN
1	D	19	ASN
1	D	33	GLN
1	D	41	ASN
1	D	61	ASN
1	D	95	GLN
1	D	127	ASN
1	D	182	ASN
1	D	190	GLN
1	D	216	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

4 monosaccharides 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	$\#\|Z\| > 2$
2	BGC	E	1	2	12,12,12	1.12	1 (8%)	17,17,17	0.54	0
2	GAL	E	2	2	11,11,12	0.88	0	15,15,17	1.08	1 (6%)
2	BGC	F	1	2	12,12,12	1.18	1 (8%)	17,17,17	0.51	0
2	GAL	F	2	2	11,11,12	1.00	0	15,15,17	1.02	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	E	1	2	-	0/2/22/22	0/1/1/1
2	GAL	E	2	2	-	0/2/19/22	0/1/1/1
2	BGC	F	1	2	-	2/2/22/22	0/1/1/1
2	GAL	F	2	2	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1	BGC	C4-C5	2.22	1.57	1.53
2	E	1	BGC	C4-C5	2.19	1.57	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	2	GAL	C3-C4-C5	-2.68	105.45	110.24
2	F	2	GAL	C3-C4-C5	-2.45	105.87	110.24

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	1	BGC	C4-C5-C6-O6
2	F	1	BGC	O5-C5-C6-O6

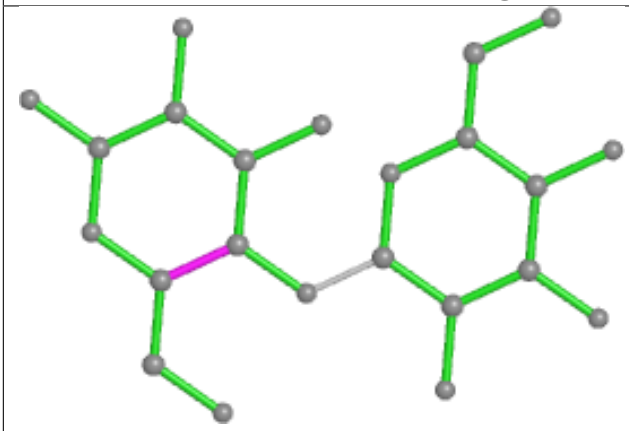
There are no ring outliers.

3 monomers are involved in 4 short contacts:

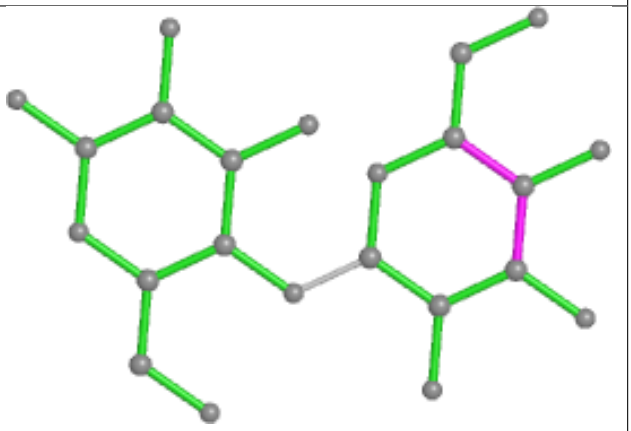
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	GAL	1	0
2	F	2	GAL	2	0
2	F	1	BGC	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

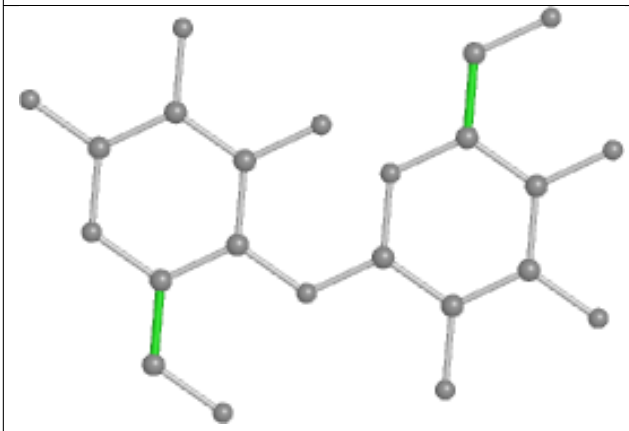
Oligosaccharide Chain E



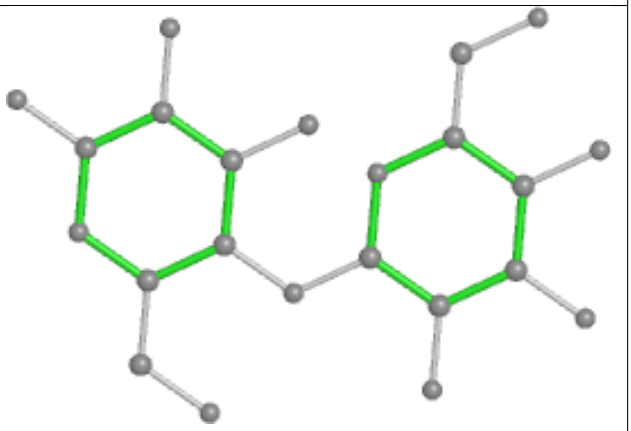
Bond lengths



Bond angles

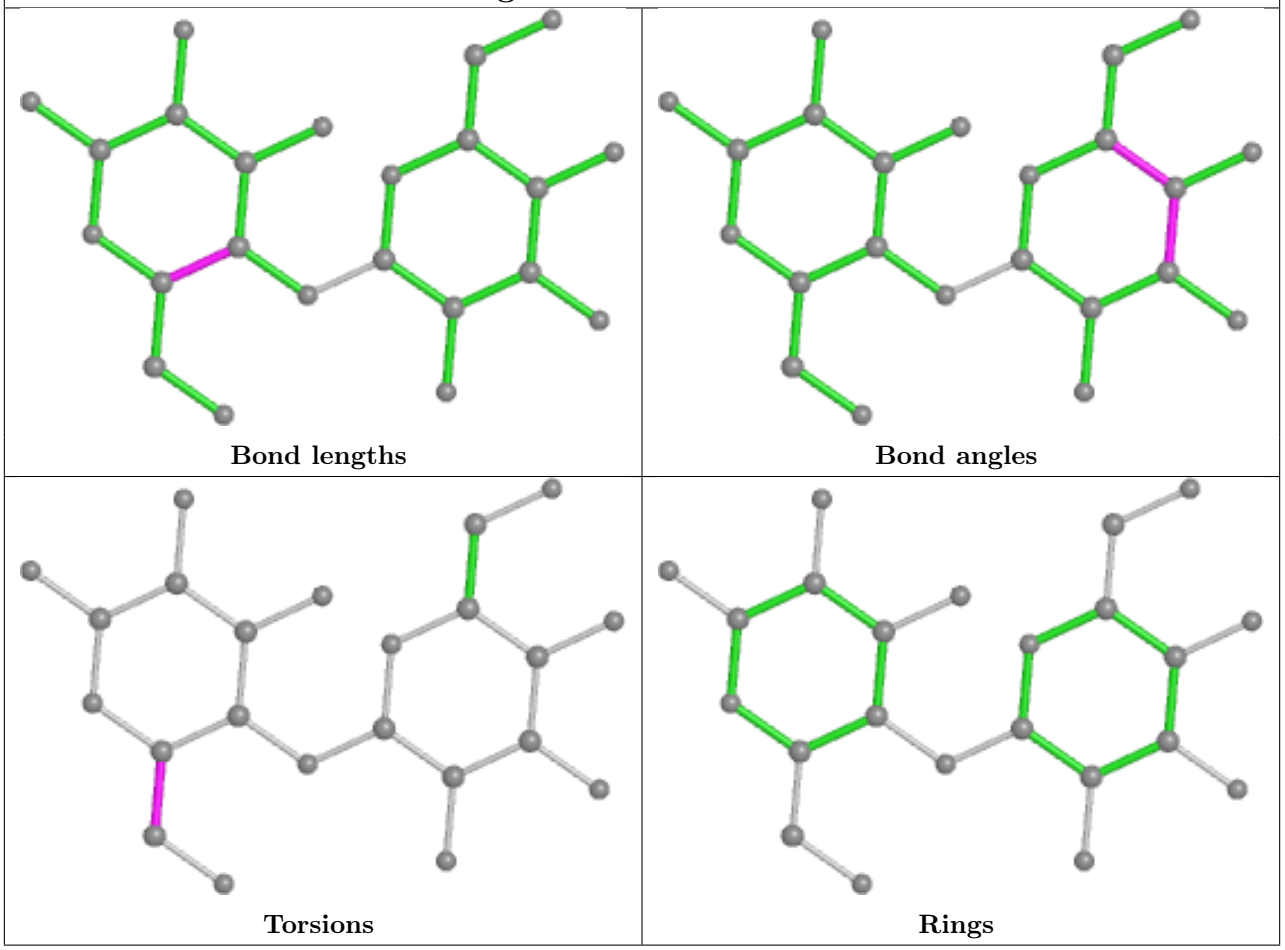


Torsions



Rings

Oligosaccharide Chain F



5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 8 are monoatomic - leaving 11 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	$\#\|Z\| > 2$
3	SFP	C	239	-	44,72,72	1.57	11 (25%)	38,112,112	0.78	0
3	SFP	A	250	-	44,72,72	1.46	8 (18%)	38,112,112	0.68	0
3	SFP	C	240	-	44,72,72	1.61	11 (25%)	38,112,112	0.77	1 (2%)
3	SFP	D	242	-	44,72,72	1.58	7 (15%)	38,112,112	0.79	0
3	SFP	B	245	-	44,72,72	1.40	7 (15%)	38,112,112	0.84	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	SFP	A	251	-	44,72,72	1.51	10 (22%)	38,112,112	0.72	0
3	SFP	A	243	-	44,72,72	1.45	8 (18%)	38,112,112	0.76	0
3	SFP	A	244	-	44,72,72	1.66	9 (20%)	38,112,112	0.87	2 (5%)
3	SFP	B	237	-	44,72,72	1.47	7 (15%)	38,112,112	0.67	0
3	SFP	B	238	-	44,72,72	1.46	8 (18%)	38,112,112	0.77	1 (2%)
3	SFP	D	241	-	44,72,72	1.54	9 (20%)	38,112,112	0.72	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	SFP	C	239	-	-	0/0/90/90	0/8/9/9
3	SFP	A	250	-	-	0/0/90/90	0/8/9/9
3	SFP	C	240	-	-	0/0/90/90	0/8/9/9
3	SFP	D	242	-	-	0/0/90/90	0/8/9/9
3	SFP	B	245	-	-	0/0/90/90	0/8/9/9
3	SFP	A	251	-	-	0/0/90/90	0/8/9/9
3	SFP	A	243	-	-	0/0/90/90	0/8/9/9
3	SFP	A	244	-	-	0/0/90/90	0/8/9/9
3	SFP	B	237	-	-	0/0/90/90	0/8/9/9
3	SFP	B	238	-	-	0/0/90/90	0/8/9/9
3	SFP	D	241	-	-	0/0/90/90	0/8/9/9

All (95) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	244	SFP	C29-C30	4.91	1.47	1.36
3	C	240	SFP	C13-C14	4.20	1.45	1.36
3	D	242	SFP	C13-C14	4.17	1.45	1.36
3	C	239	SFP	C29-C30	3.50	1.44	1.36
3	A	250	SFP	C13-C14	3.46	1.43	1.36
3	B	237	SFP	C13-C14	3.44	1.43	1.36
3	C	239	SFP	C13-C14	3.42	1.43	1.36
3	C	240	SFP	C27-C32	3.38	1.43	1.36
3	A	251	SFP	C29-C30	3.34	1.43	1.36
3	B	238	SFP	C29-C30	3.31	1.43	1.36
3	D	241	SFP	C29-C30	3.31	1.43	1.36
3	D	242	SFP	C29-C30	3.22	1.43	1.36
3	B	245	SFP	C29-C30	3.21	1.43	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	243	SFP	C29-C30	3.18	1.43	1.36
3	D	241	SFP	C13-C14	3.12	1.43	1.36
3	A	243	SFP	C11-C10	2.97	1.42	1.36
3	B	245	SFP	C11-C10	2.94	1.42	1.36
3	A	244	SFP	C13-C14	2.89	1.42	1.36
3	D	242	SFP	C23-C22	2.88	1.42	1.36
3	A	251	SFP	C19-C18	2.88	1.42	1.36
3	D	242	SFP	C27-C32	2.84	1.42	1.36
3	A	251	SFP	C13-C14	2.83	1.42	1.36
3	A	251	SFP	C11-C10	2.79	1.42	1.36
3	B	238	SFP	C13-C14	2.76	1.42	1.36
3	C	239	SFP	C27-C32	2.76	1.42	1.36
3	A	251	SFP	C11-C12	2.72	1.48	1.41
3	A	243	SFP	C11-C12	2.69	1.48	1.41
3	B	238	SFP	C11-C12	2.64	1.48	1.41
3	B	237	SFP	C27-C32	2.64	1.42	1.36
3	D	242	SFP	C11-C12	2.64	1.48	1.41
3	A	250	SFP	C11-C12	2.61	1.48	1.41
3	A	244	SFP	C11-C12	2.61	1.48	1.41
3	A	243	SFP	C27-C32	2.58	1.42	1.36
3	D	241	SFP	C11-C12	2.54	1.48	1.41
3	C	240	SFP	C11-C12	2.54	1.48	1.41
3	A	244	SFP	C27-C28	2.53	1.48	1.41
3	D	241	SFP	C27-C32	2.53	1.41	1.36
3	C	240	SFP	C23-C22	2.52	1.41	1.36
3	B	237	SFP	C11-C12	2.51	1.48	1.41
3	C	240	SFP	C29-C30	2.50	1.41	1.36
3	B	245	SFP	C11-C12	2.50	1.48	1.41
3	B	238	SFP	C19-C18	2.50	1.41	1.36
3	A	243	SFP	C23-C24	2.49	1.48	1.41
3	A	244	SFP	C29-C28	2.48	1.48	1.41
3	B	245	SFP	C27-C32	2.48	1.41	1.36
3	A	244	SFP	C15-C16	2.47	1.41	1.36
3	D	242	SFP	C25-C24	2.46	1.47	1.41
3	B	238	SFP	C15-C20	2.43	1.47	1.41
3	C	240	SFP	C19-C18	2.42	1.41	1.36
3	B	238	SFP	C11-C10	2.42	1.41	1.36
3	A	250	SFP	C29-C30	2.40	1.41	1.36
3	B	237	SFP	C29-C30	2.38	1.41	1.36
3	C	239	SFP	C15-C16	2.37	1.41	1.36
3	C	239	SFP	C11-C12	2.37	1.47	1.41
3	C	240	SFP	C23-C24	2.36	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	250	SFP	C27-C32	2.35	1.41	1.36
3	D	241	SFP	C11-C10	2.33	1.41	1.36
3	C	240	SFP	C15-C20	2.32	1.47	1.41
3	B	245	SFP	C23-C24	2.31	1.47	1.41
3	D	241	SFP	C25-C24	2.30	1.47	1.41
3	A	244	SFP	C11-C10	2.30	1.41	1.36
3	A	251	SFP	C23-C24	2.28	1.47	1.41
3	B	238	SFP	C19-C20	2.28	1.47	1.41
3	A	250	SFP	C19-C18	2.28	1.41	1.36
3	A	244	SFP	C23-C22	2.28	1.41	1.36
3	B	237	SFP	C19-C20	2.25	1.47	1.41
3	A	251	SFP	C23-C22	2.24	1.41	1.36
3	B	245	SFP	C27-C28	2.23	1.47	1.41
3	A	250	SFP	C23-C24	2.21	1.47	1.41
3	C	239	SFP	C23-C24	2.21	1.47	1.41
3	C	239	SFP	C23-C22	2.21	1.41	1.36
3	C	239	SFP	C25-C24	2.21	1.47	1.41
3	B	245	SFP	C19-C18	2.20	1.41	1.36
3	A	244	SFP	C23-C24	2.20	1.47	1.41
3	D	241	SFP	C19-C18	2.19	1.41	1.36
3	C	239	SFP	C11-C10	2.18	1.41	1.36
3	B	237	SFP	C15-C20	2.18	1.47	1.41
3	A	251	SFP	C19-C20	2.17	1.47	1.41
3	B	238	SFP	C23-C24	2.17	1.47	1.41
3	A	243	SFP	C13-C14	2.17	1.41	1.36
3	D	242	SFP	C15-C20	2.16	1.47	1.41
3	C	240	SFP	C25-C24	2.16	1.47	1.41
3	A	243	SFP	C19-C20	2.13	1.47	1.41
3	C	239	SFP	C27-C28	2.12	1.47	1.41
3	A	251	SFP	C15-C20	2.08	1.47	1.41
3	A	243	SFP	C19-C18	2.08	1.41	1.36
3	D	241	SFP	C23-C24	2.07	1.46	1.41
3	A	250	SFP	C23-C22	2.07	1.41	1.36
3	B	237	SFP	C23-C24	2.06	1.46	1.41
3	C	240	SFP	C27-C28	2.03	1.46	1.41
3	A	251	SFP	C27-C28	2.03	1.46	1.41
3	A	250	SFP	C19-C20	2.03	1.46	1.41
3	C	239	SFP	C19-C20	2.02	1.46	1.41
3	D	241	SFP	C27-C28	2.01	1.46	1.41
3	C	240	SFP	C14-C9	2.00	1.46	1.39

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	244	SFP	C29-C28-C27	-2.26	116.64	118.65
3	C	240	SFP	C14-C13-C12	-2.19	117.44	120.82
3	B	238	SFP	C29-C28-C27	2.18	120.58	118.65
3	A	244	SFP	C25-C24-C23	-2.17	116.72	118.65
3	B	245	SFP	C19-C20-C15	2.08	120.50	118.65

There are no chirality outliers.

There are no torsion outliers.

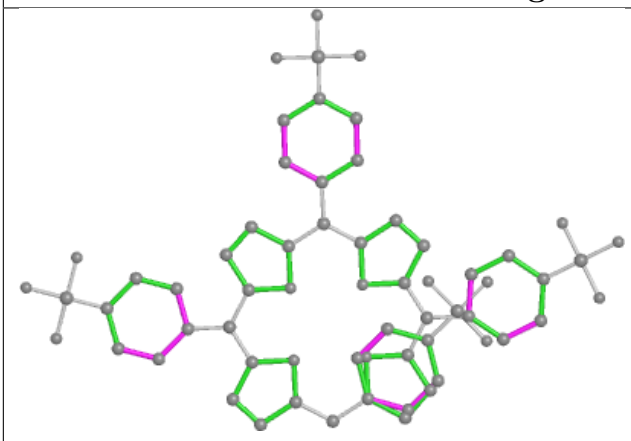
There are no ring outliers.

11 monomers are involved in 31 short contacts:

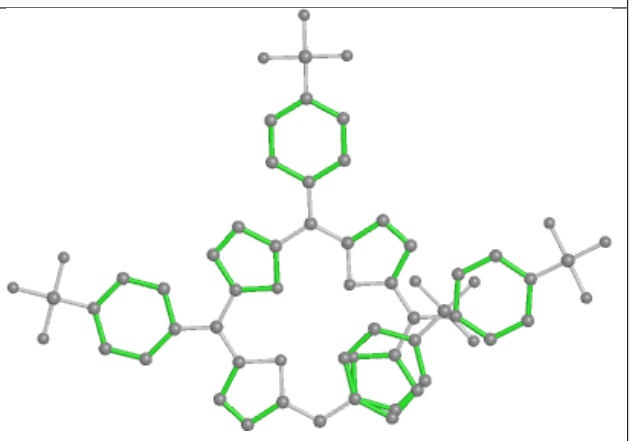
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	239	SFP	2	0
3	A	250	SFP	3	0
3	C	240	SFP	2	0
3	D	242	SFP	4	0
3	B	245	SFP	3	0
3	A	251	SFP	6	0
3	A	243	SFP	5	0
3	A	244	SFP	7	0
3	B	237	SFP	1	0
3	B	238	SFP	4	0
3	D	241	SFP	3	0

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.

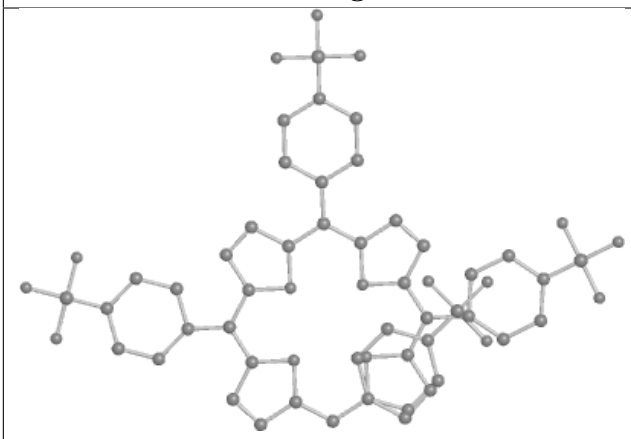
Ligand SFP C 239



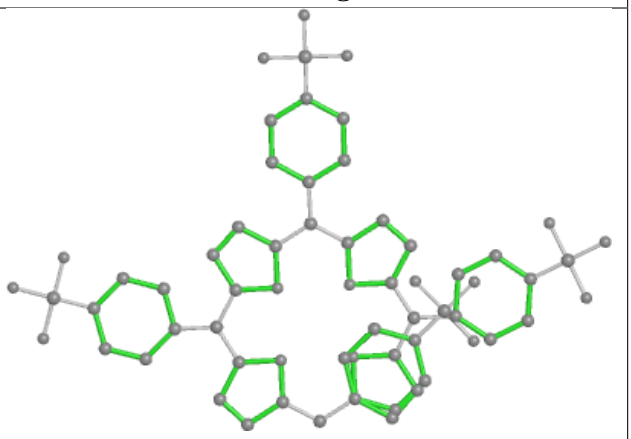
Bond lengths



Bond angles

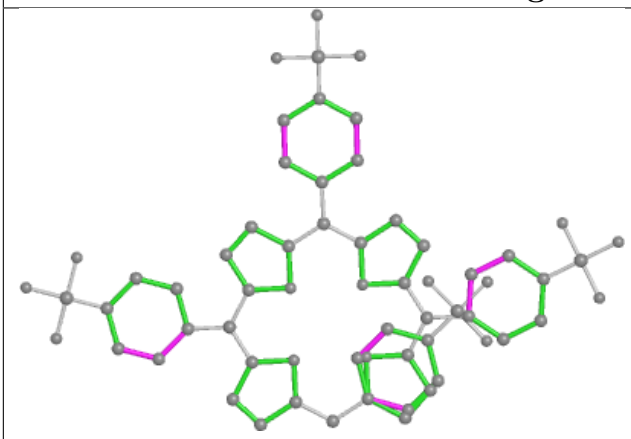


Torsions

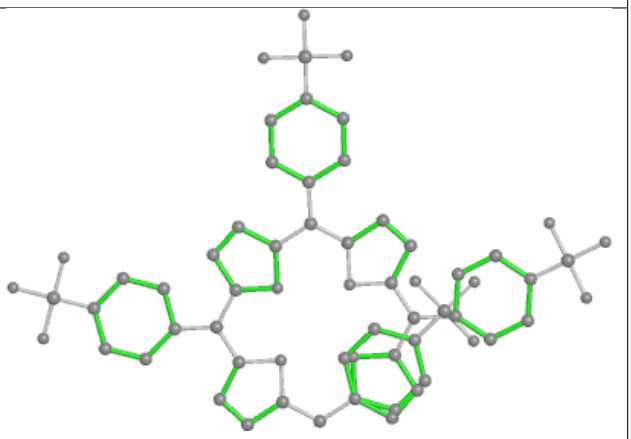


Rings

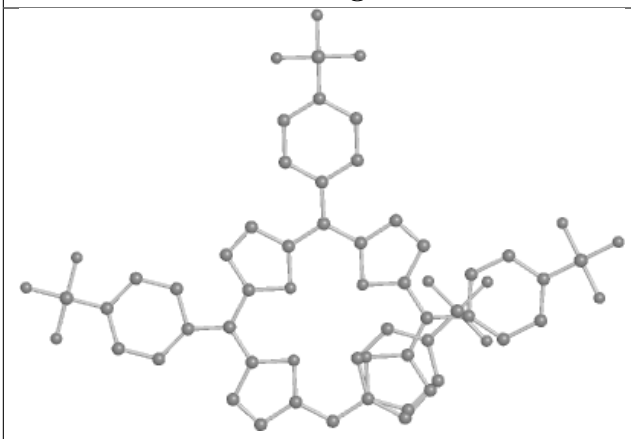
Ligand SFP A 250



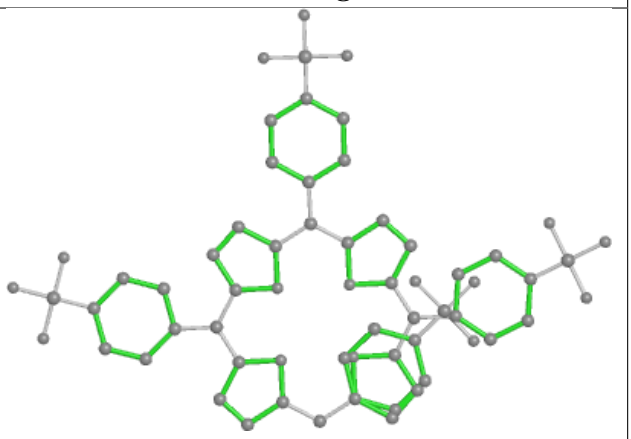
Bond lengths



Bond angles

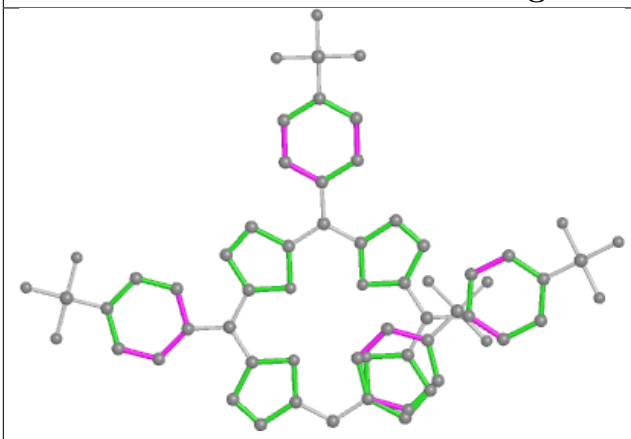


Torsions

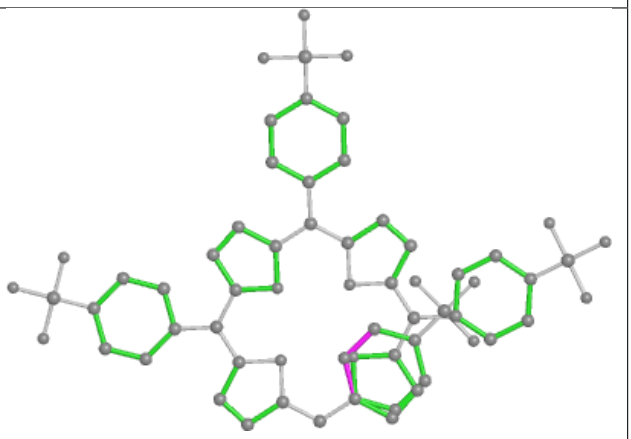


Rings

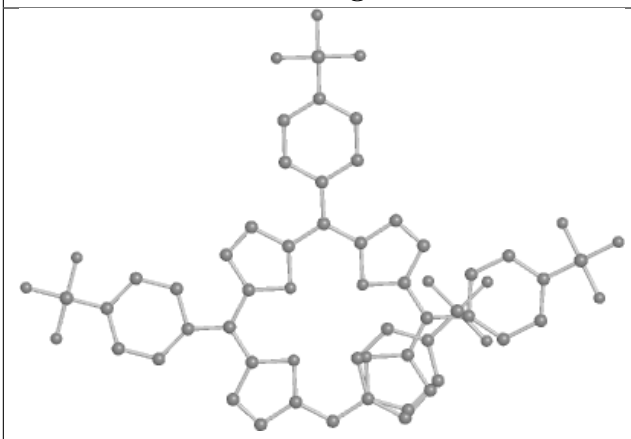
Ligand SFP C 240



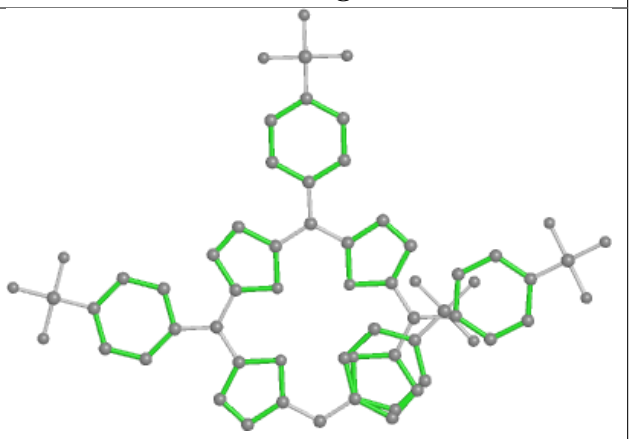
Bond lengths



Bond angles

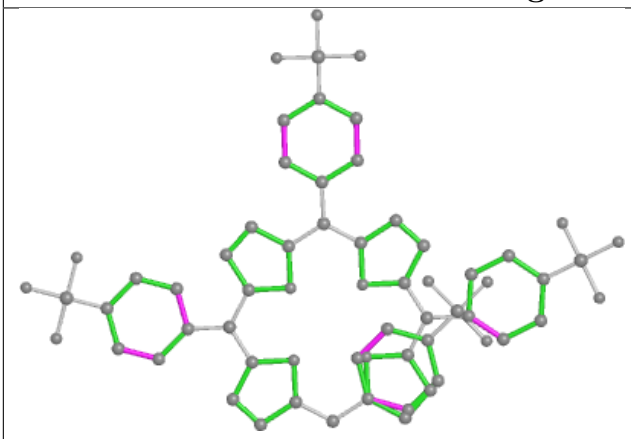


Torsions

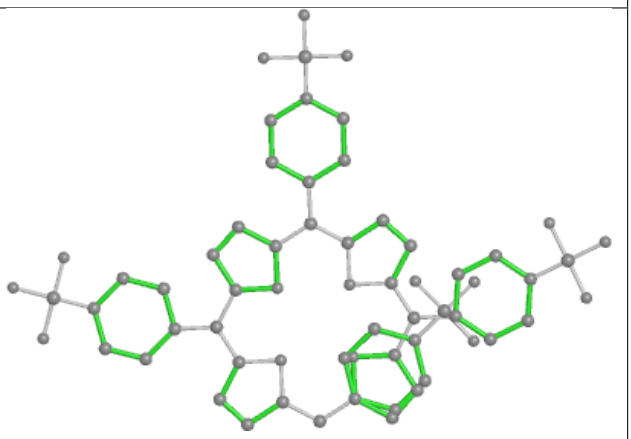


Rings

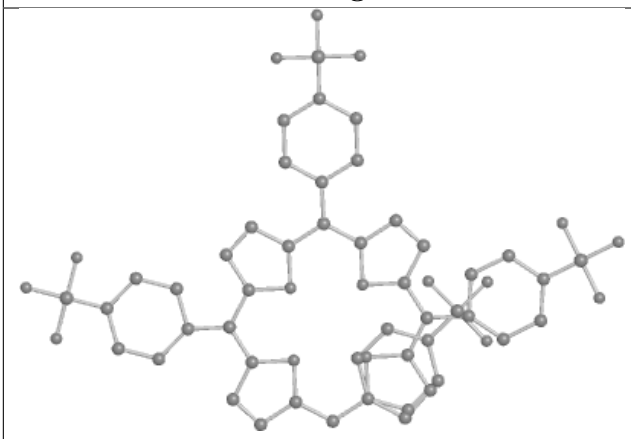
Ligand SFP D 242



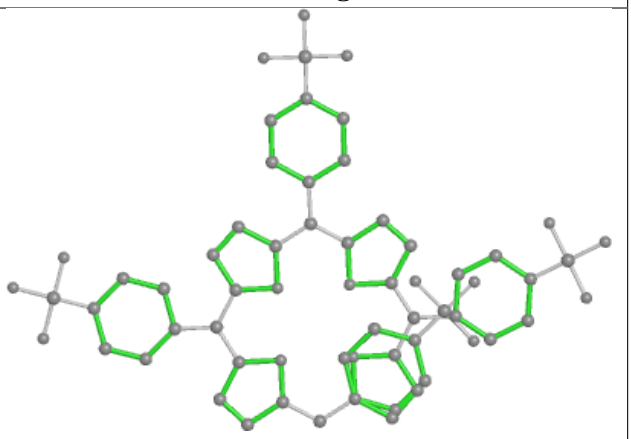
Bond lengths



Bond angles

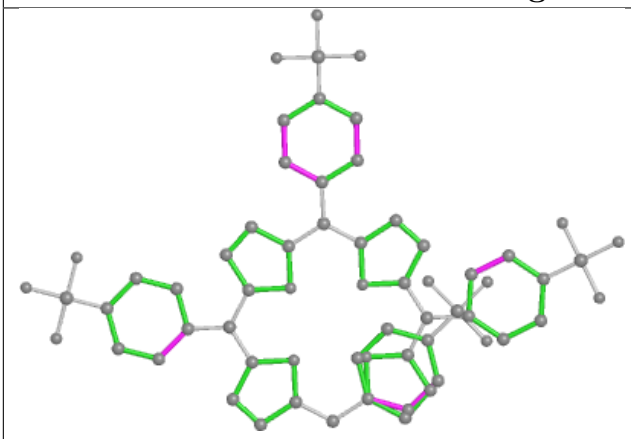


Torsions

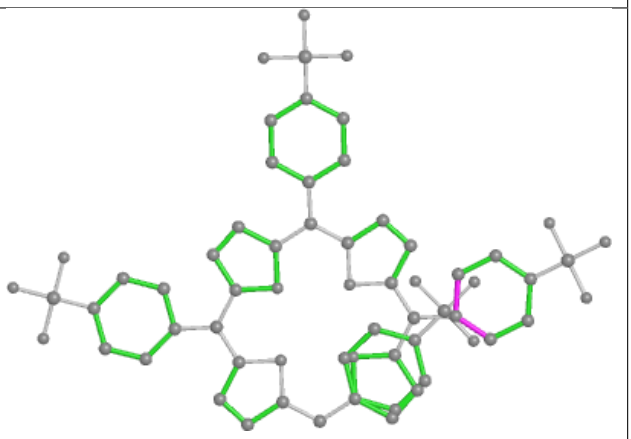


Rings

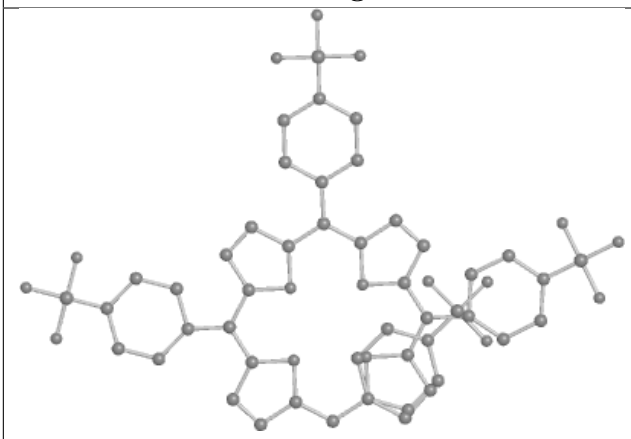
Ligand SFP B 245



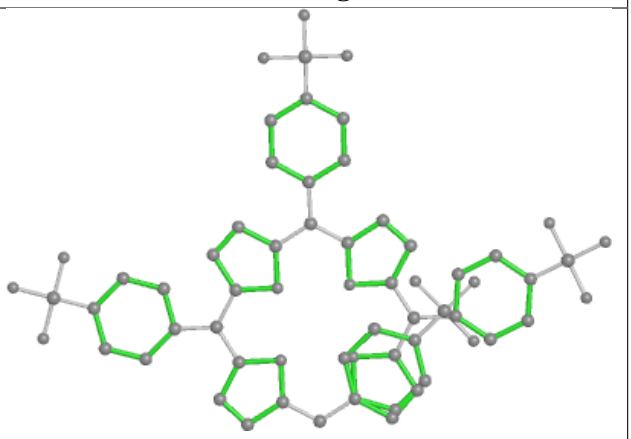
Bond lengths



Bond angles

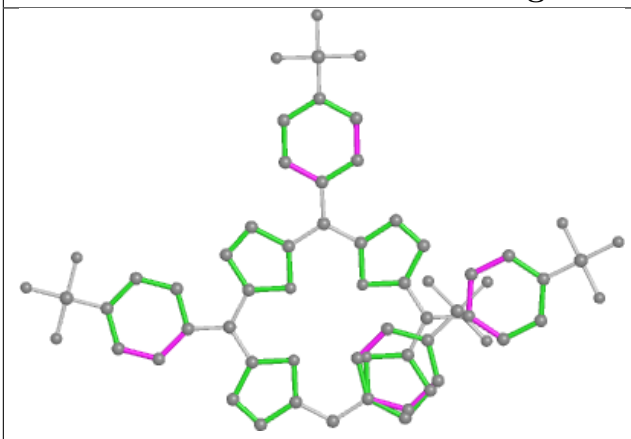


Torsions

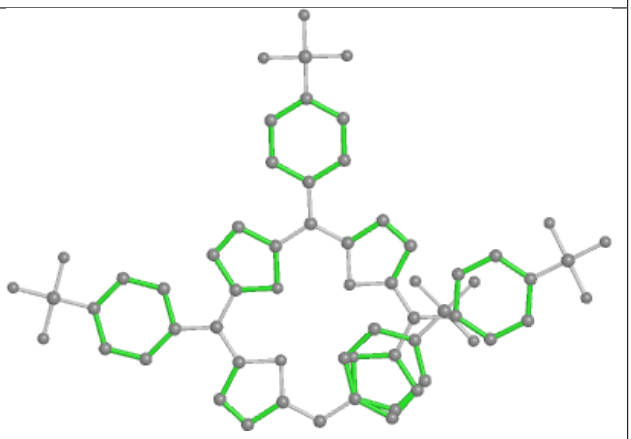


Rings

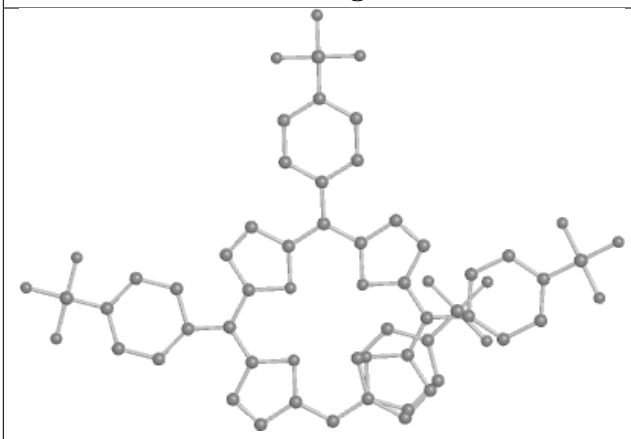
Ligand SFP A 251



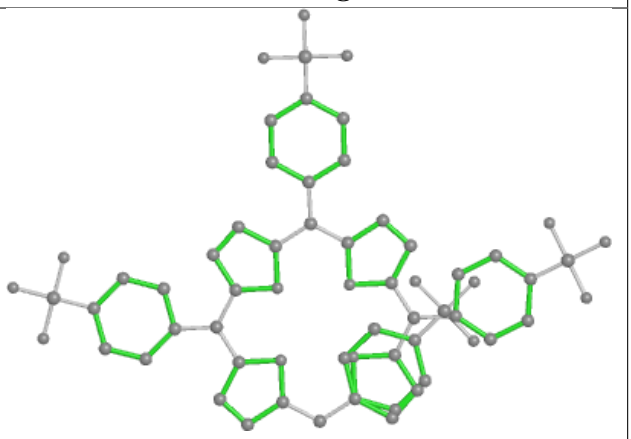
Bond lengths



Bond angles

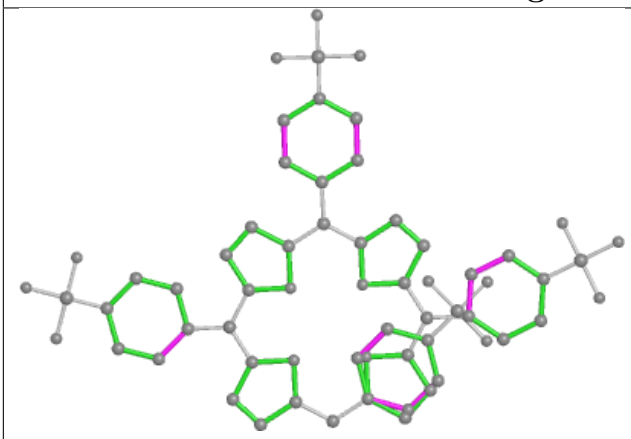


Torsions

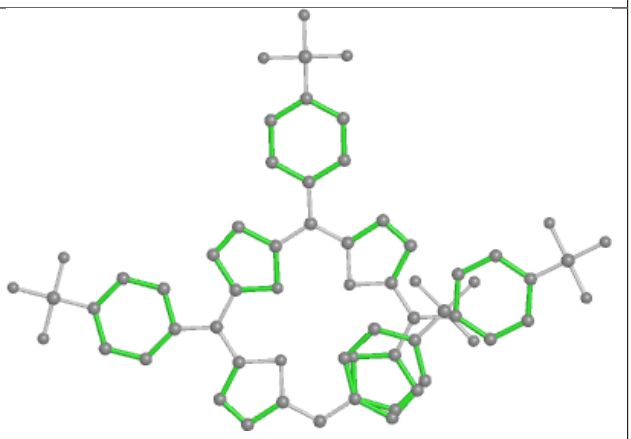


Rings

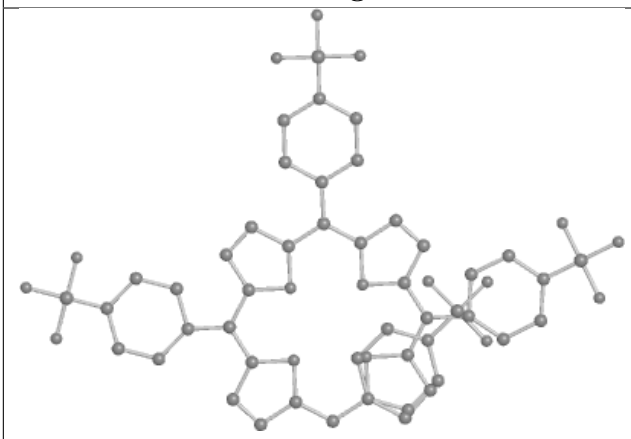
Ligand SFP A 243



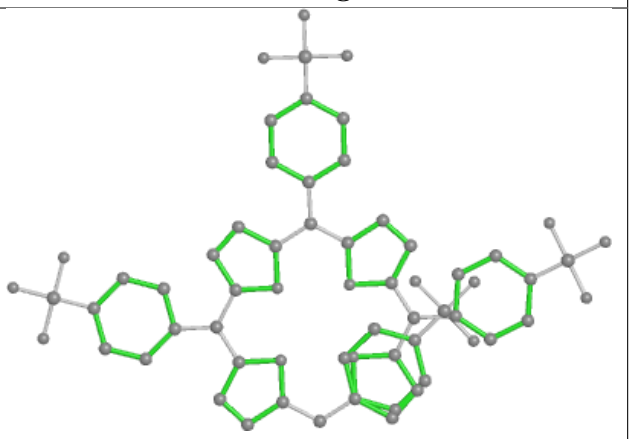
Bond lengths



Bond angles

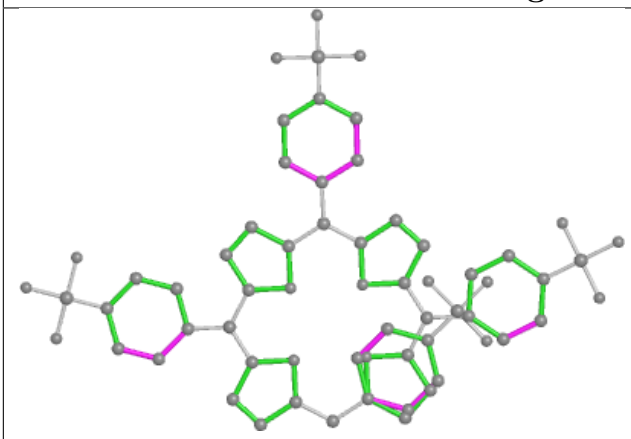


Torsions

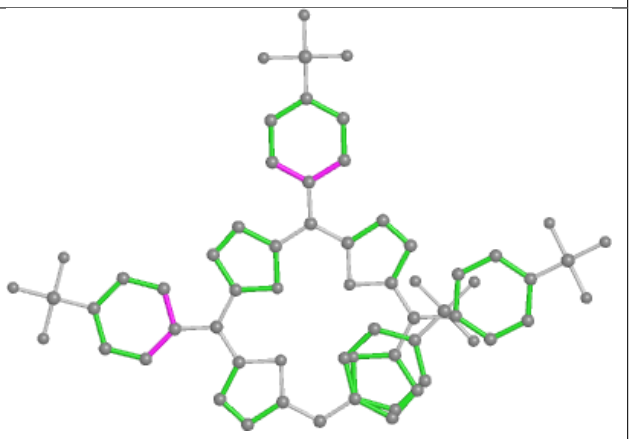


Rings

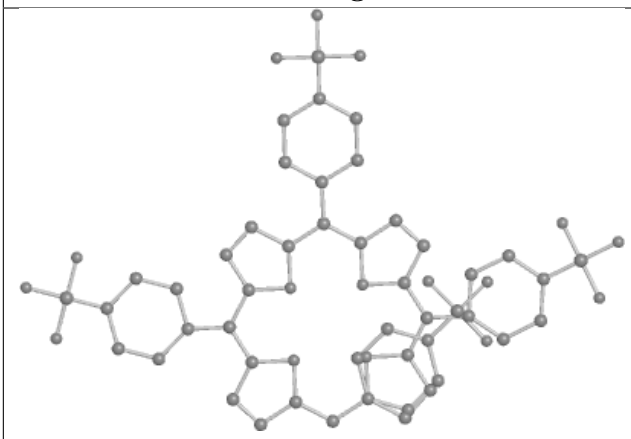
Ligand SFP A 244



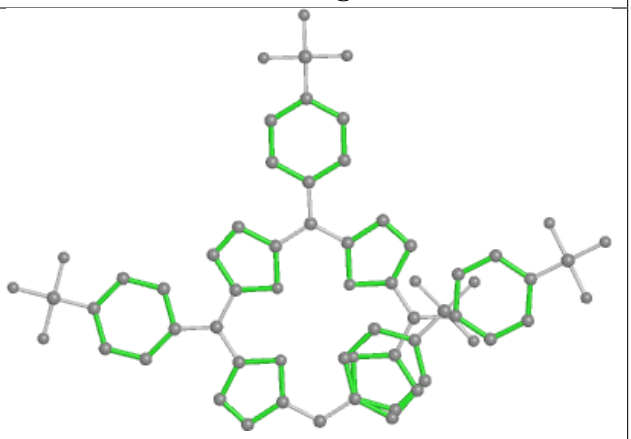
Bond lengths



Bond angles

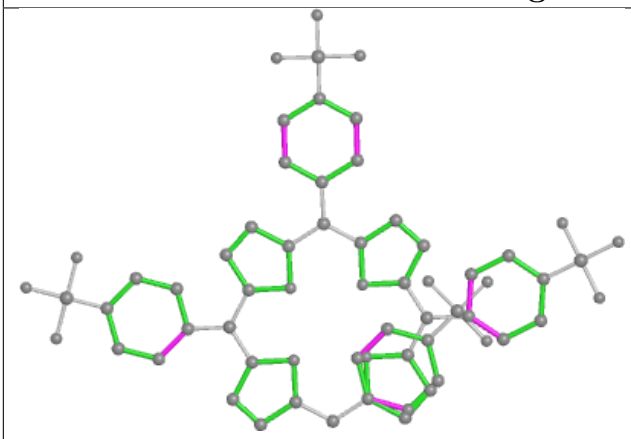


Torsions

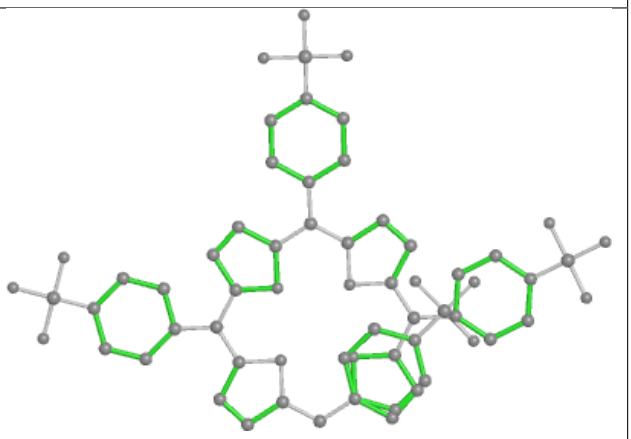


Rings

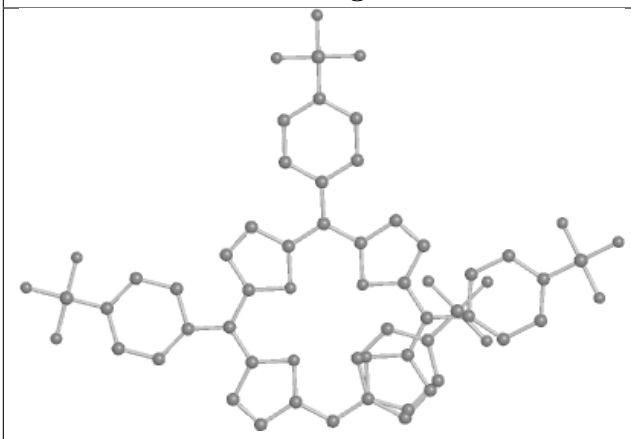
Ligand SFP B 237



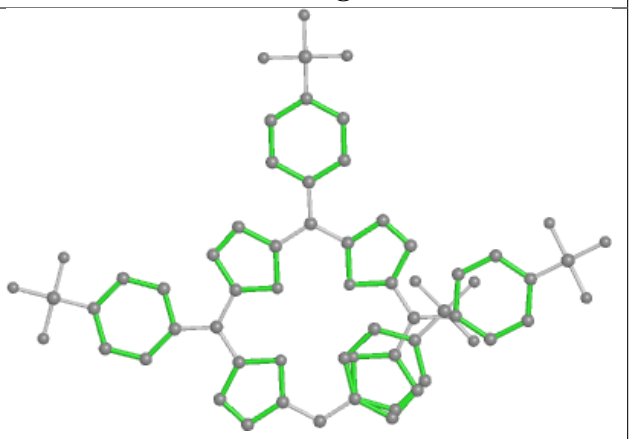
Bond lengths



Bond angles

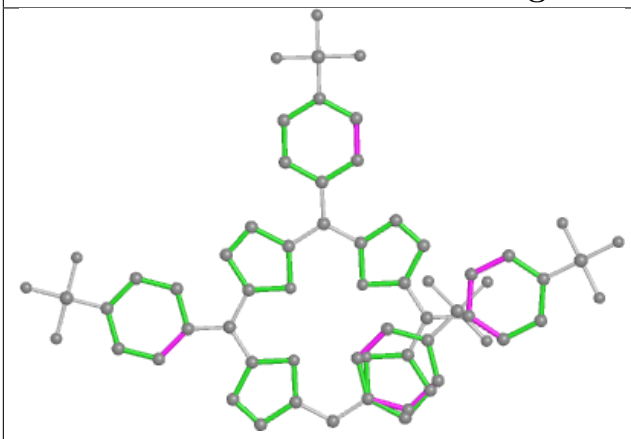


Torsions

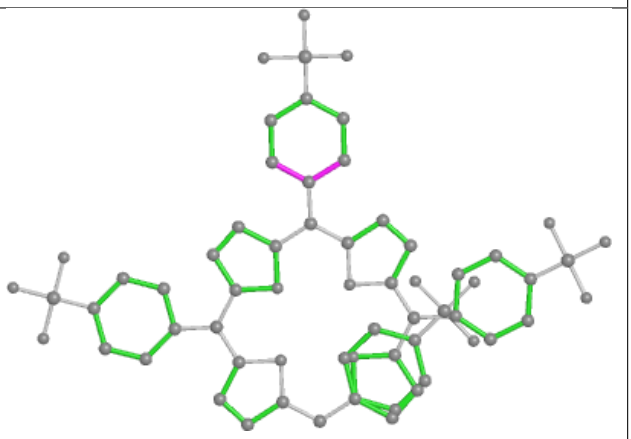


Rings

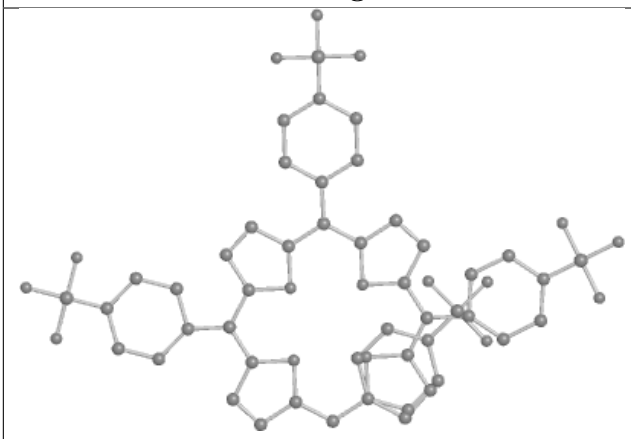
Ligand SFP B 238



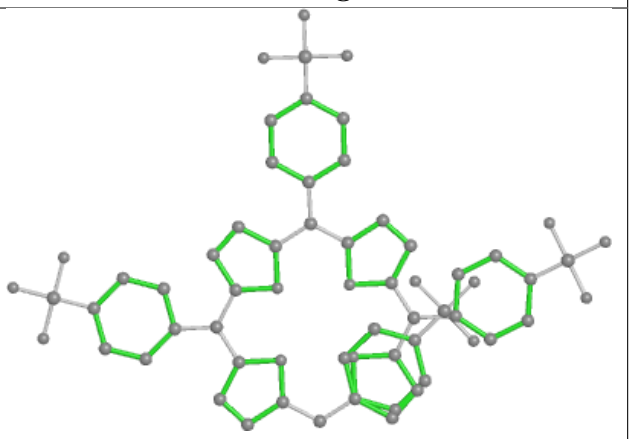
Bond lengths



Bond angles

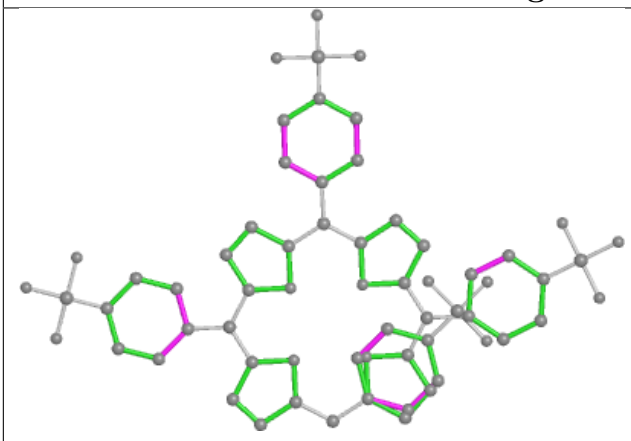


Torsions

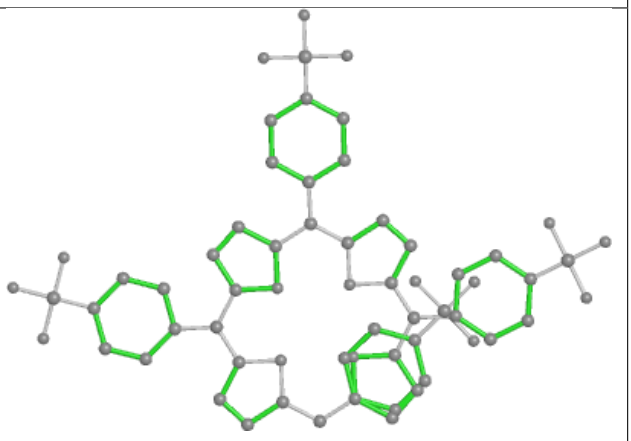


Rings

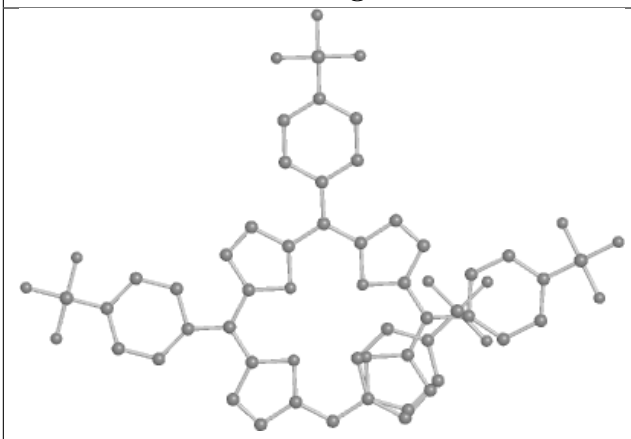
Ligand SFP D 241



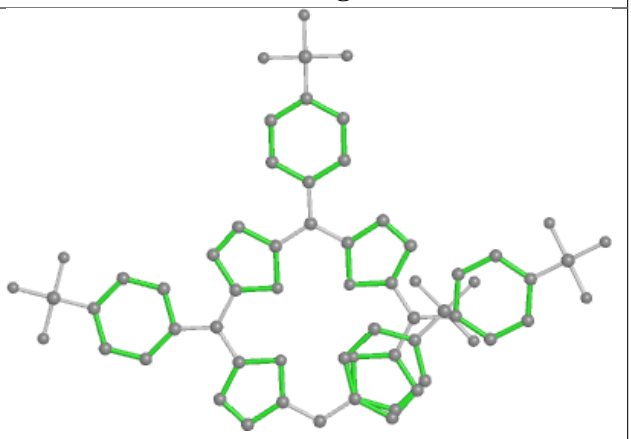
Bond lengths



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	232/236 (98%)	-0.42	0 100 100	25, 53, 96, 169	0
1	B	232/236 (98%)	-0.40	1 (0%) 92 92	24, 52, 95, 169	0
1	C	232/236 (98%)	-0.32	1 (0%) 92 92	32, 67, 113, 152	0
1	D	232/236 (98%)	-0.32	0 100 100	28, 67, 115, 147	0
All	All	928/944 (98%)	-0.36	2 (0%) 95 95	24, 59, 110, 169	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	100	SER	3.0
1	C	44	GLY	2.9

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

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

6.3 Carbohydrates

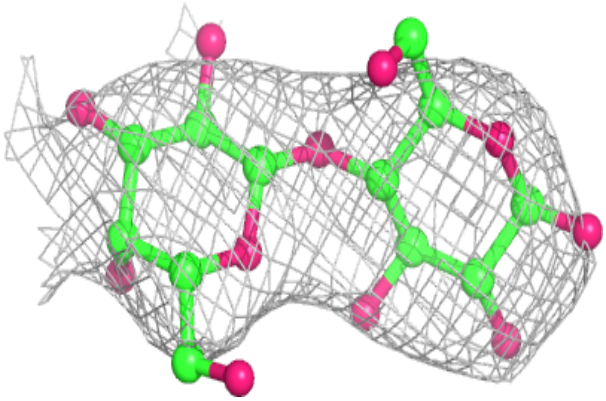
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

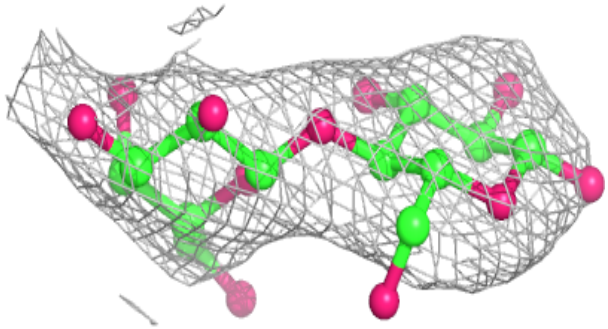
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BGC	E	1	12/12	0.92	0.21	134,137,142,144	0
2	BGC	F	1	12/12	0.93	0.20	129,139,143,145	0
2	GAL	F	2	11/12	0.95	0.25	115,118,124,126	0
2	GAL	E	2	11/12	0.98	0.28	124,129,130,133	0

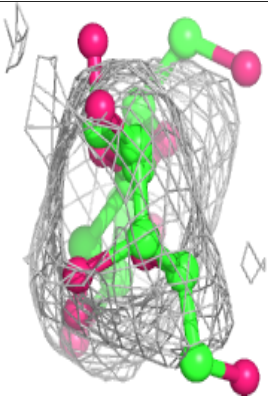
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

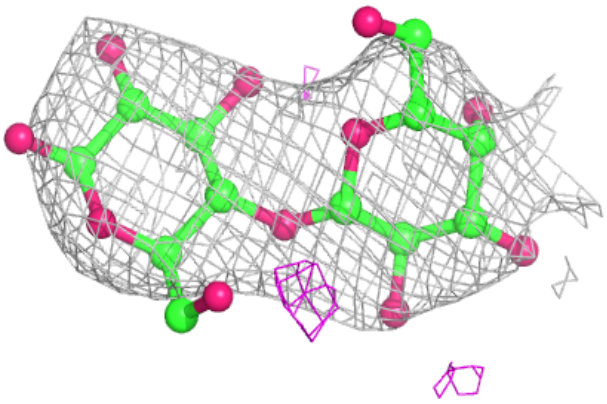


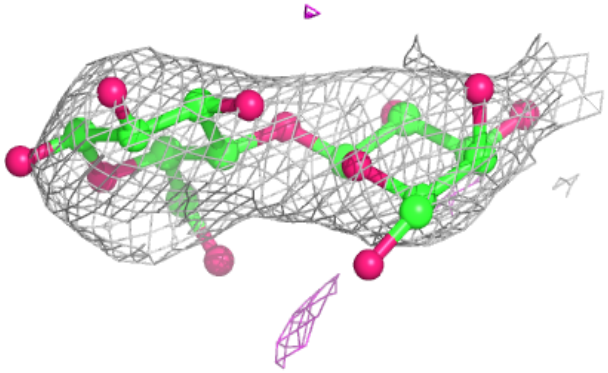


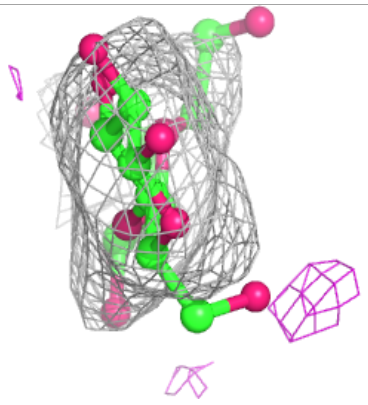


Electron density around Chain F:

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







6.4 Ligands (i)

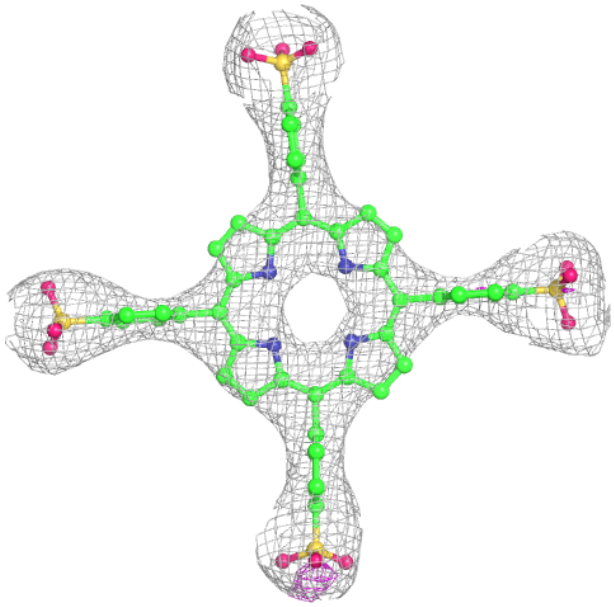
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

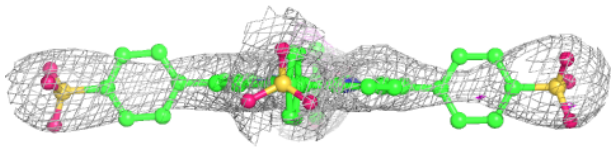
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SFP	C	239	64/64	0.89	0.27	140,148,160,162	0
3	SFP	A	244	64/64	0.90	0.28	137,145,157,158	0
3	SFP	D	241	64/64	0.90	0.26	136,144,156,158	0
3	SFP	C	240	64/64	0.95	0.20	94,103,115,116	0
3	SFP	B	245	64/64	0.96	0.17	88,96,108,109	0
3	SFP	A	243	64/64	0.96	0.18	83,92,103,105	0
3	SFP	A	250	64/64	0.96	0.17	80,88,100,101	0
3	SFP	B	237	64/64	0.96	0.16	72,80,92,94	0
3	SFP	D	242	64/64	0.96	0.19	90,99,111,112	0
3	SFP	B	238	64/64	0.97	0.16	77,86,97,99	0
3	SFP	A	251	64/64	0.97	0.17	83,91,103,104	0
4	CA	D	254	1/1	0.98	0.12	57,57,57,57	0
4	CA	C	252	1/1	0.99	0.10	50,50,50,50	0
4	CA	A	248	1/1	0.99	0.10	42,42,42,42	0
5	MN	A	249	1/1	0.99	0.07	62,62,62,62	0
5	MN	B	251	1/1	0.99	0.09	57,57,57,57	0
5	MN	C	253	1/1	0.99	0.10	69,69,69,69	0
5	MN	D	255	1/1	0.99	0.09	75,75,75,75	0
4	CA	B	250	1/1	1.00	0.11	39,39,39,39	0

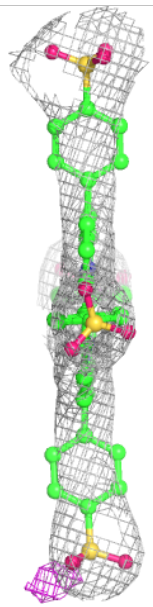
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SFP C 239:

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

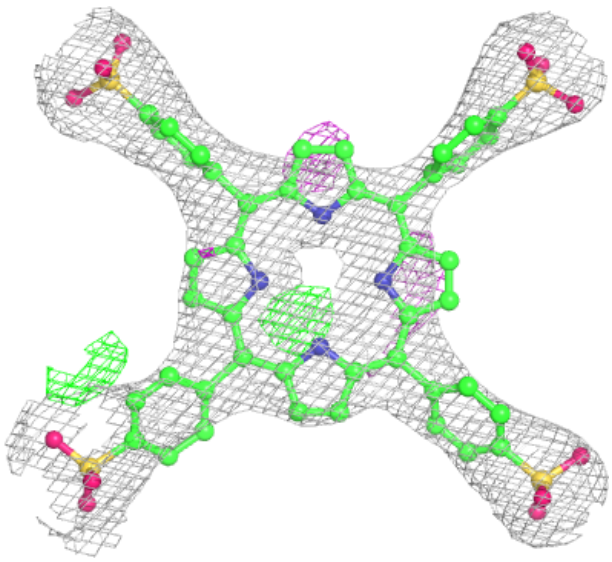


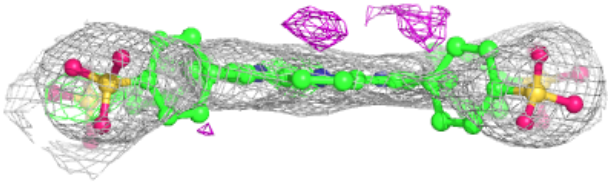


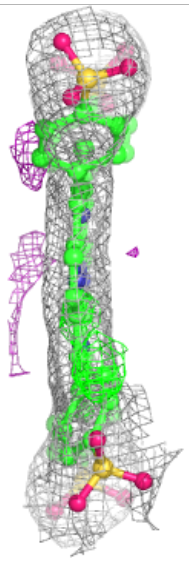


Electron density around SFP A 244:

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

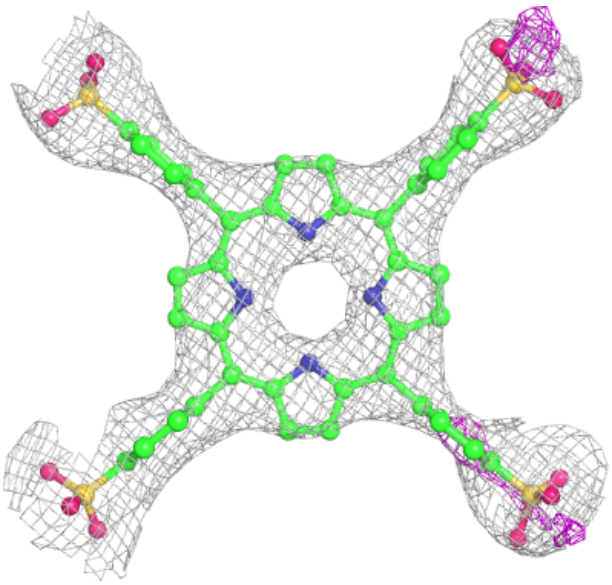


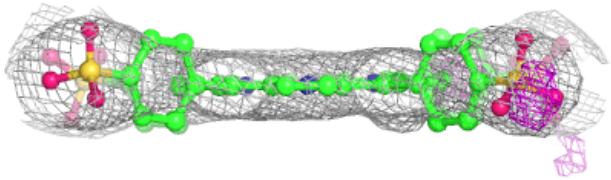


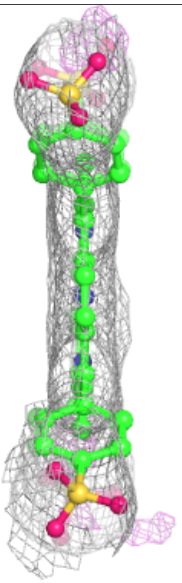


Electron density around SFP D 241:

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

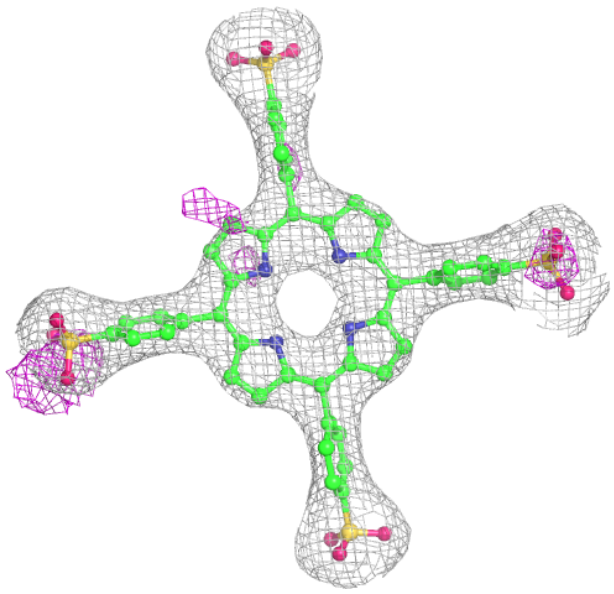


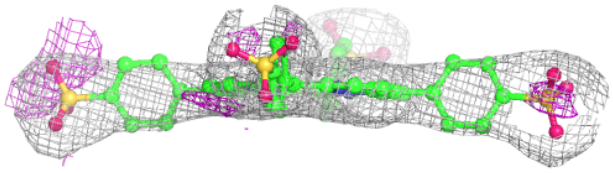


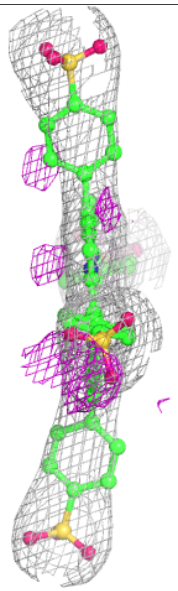


Electron density around SFP C 240:

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

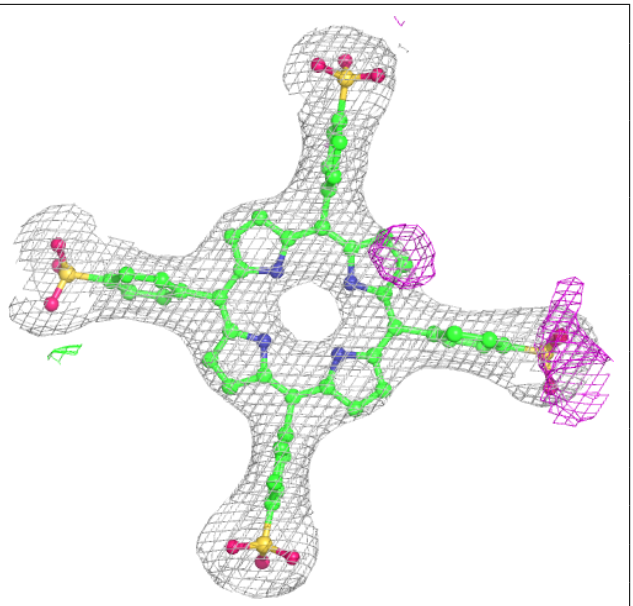


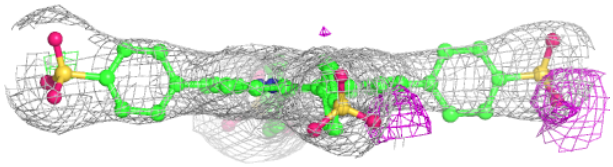


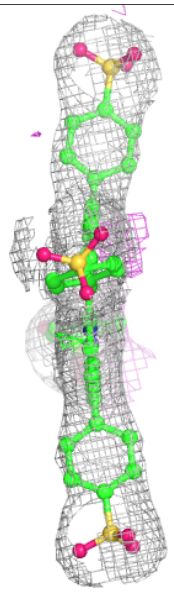


Electron density around SFP B 245:

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

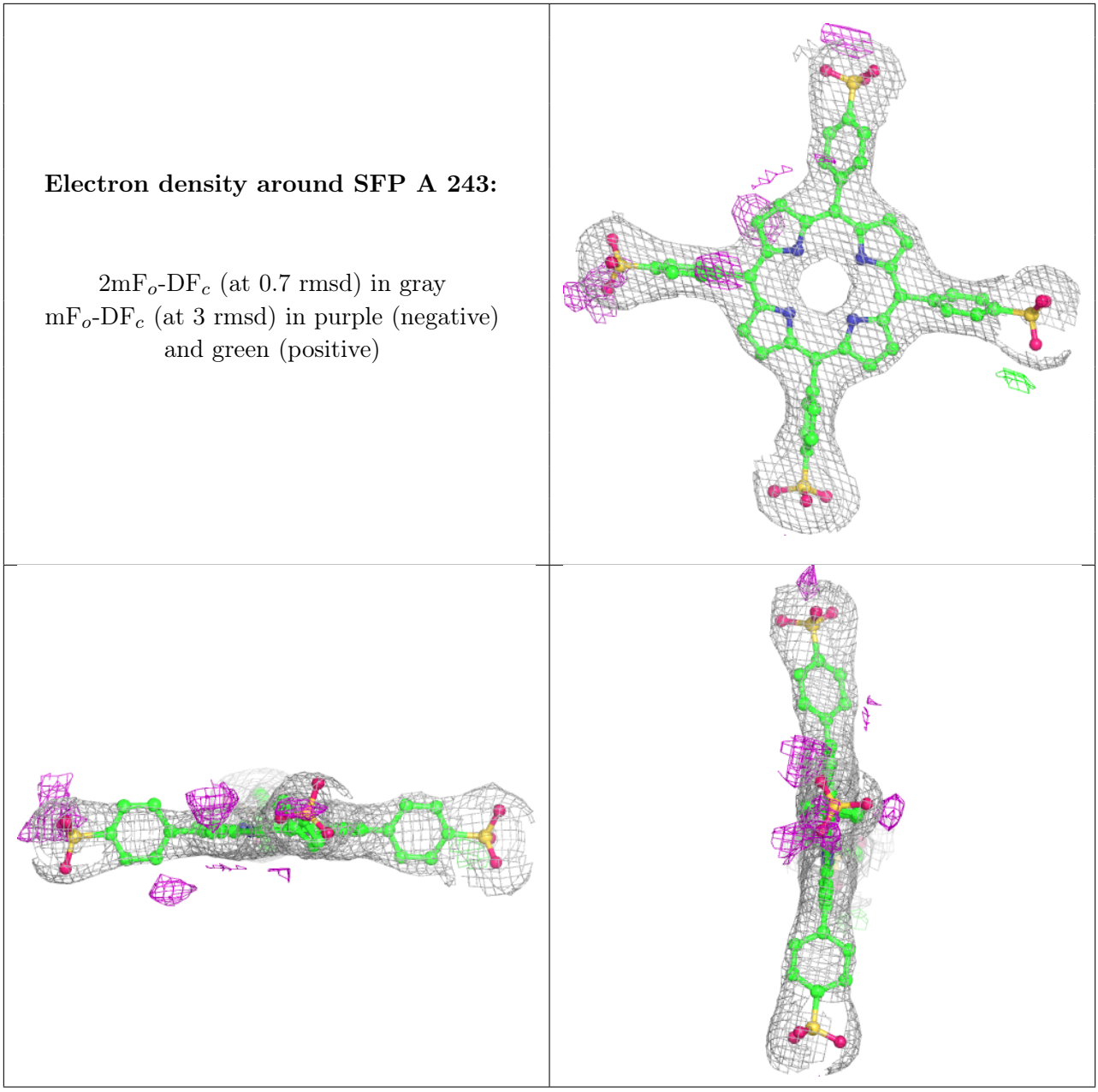






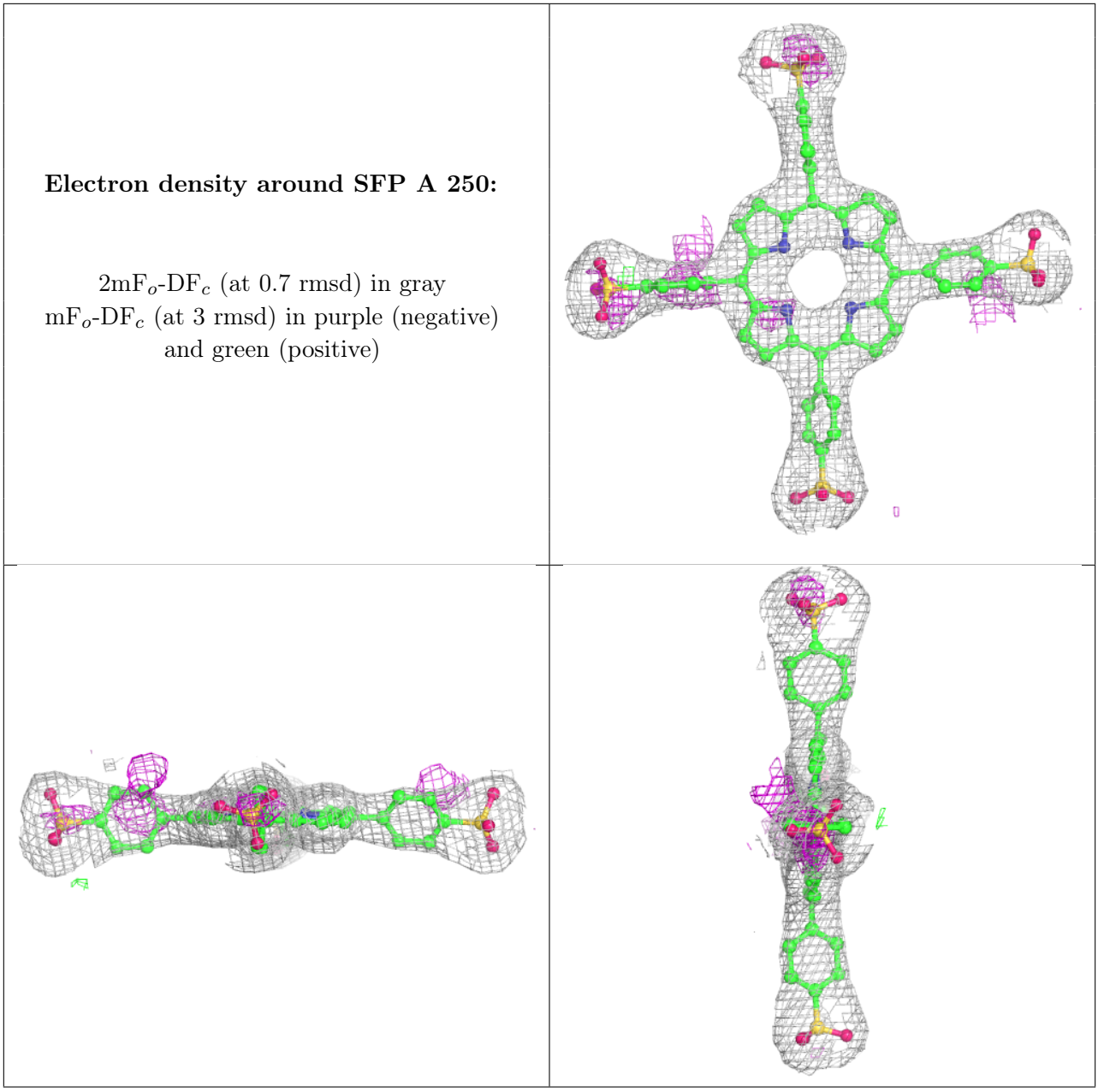
Electron density around SFP A 243:

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



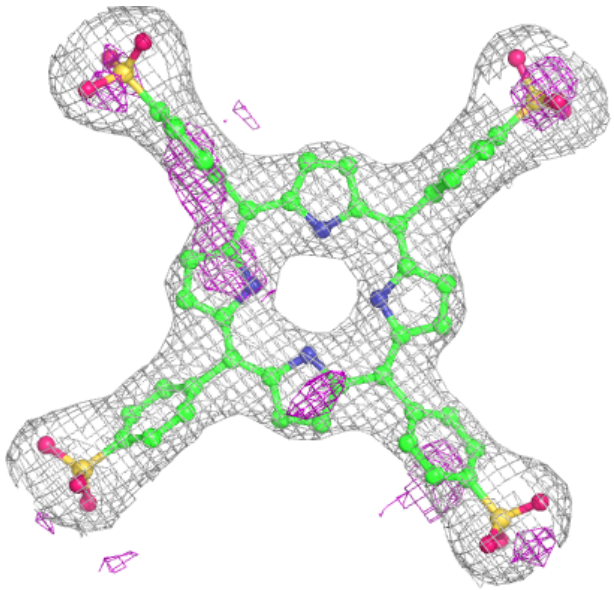
Electron density around SFP A 250:

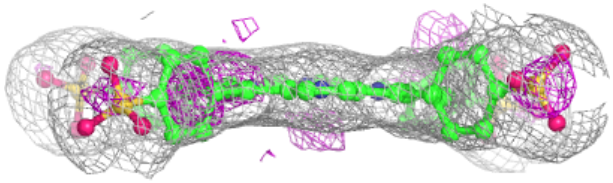
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

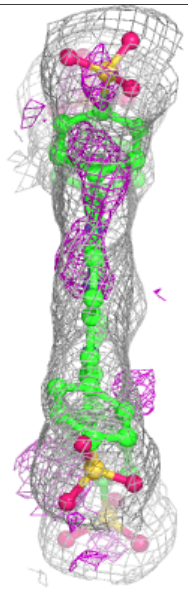


Electron density around SFP B 237:

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

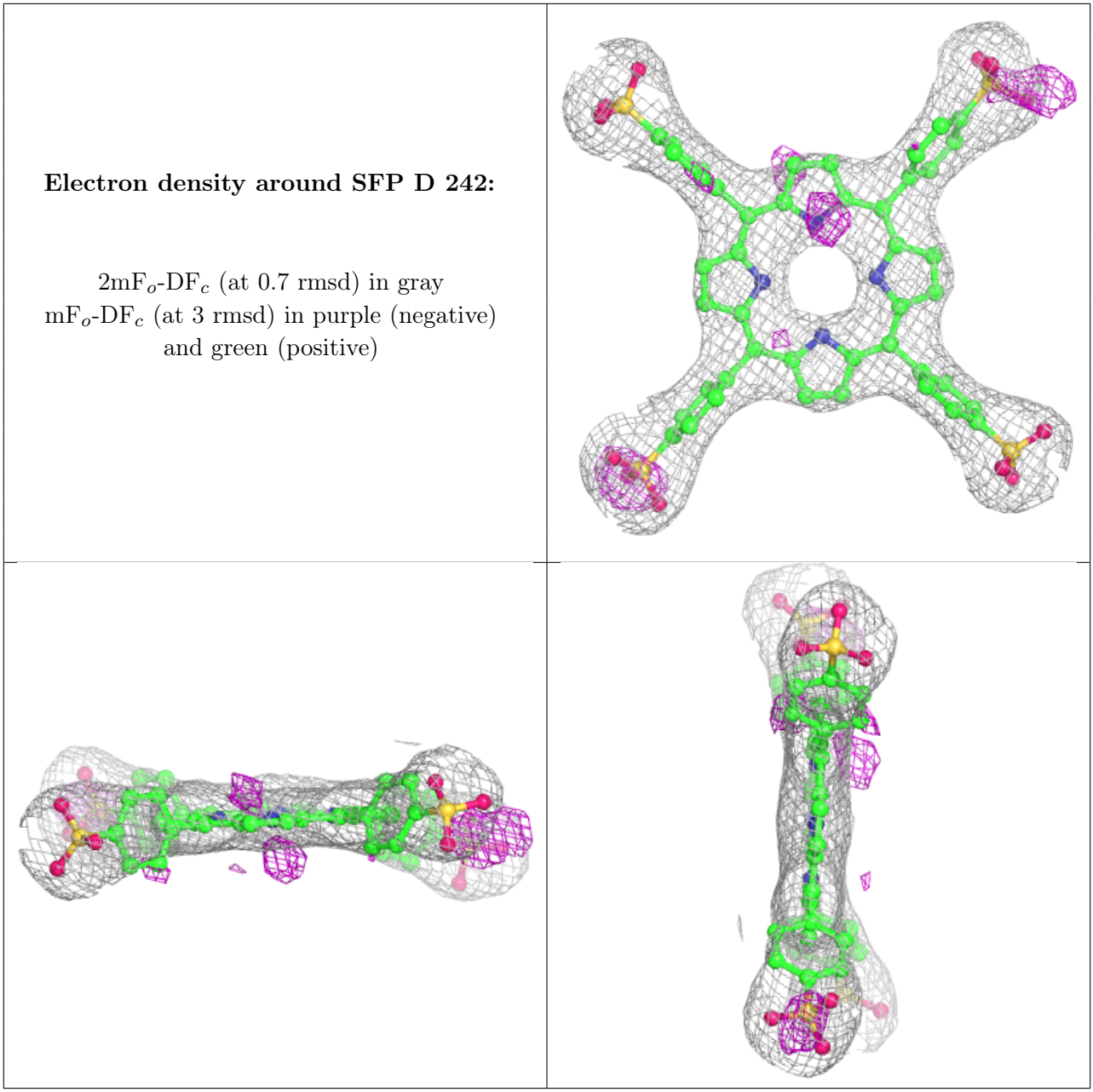






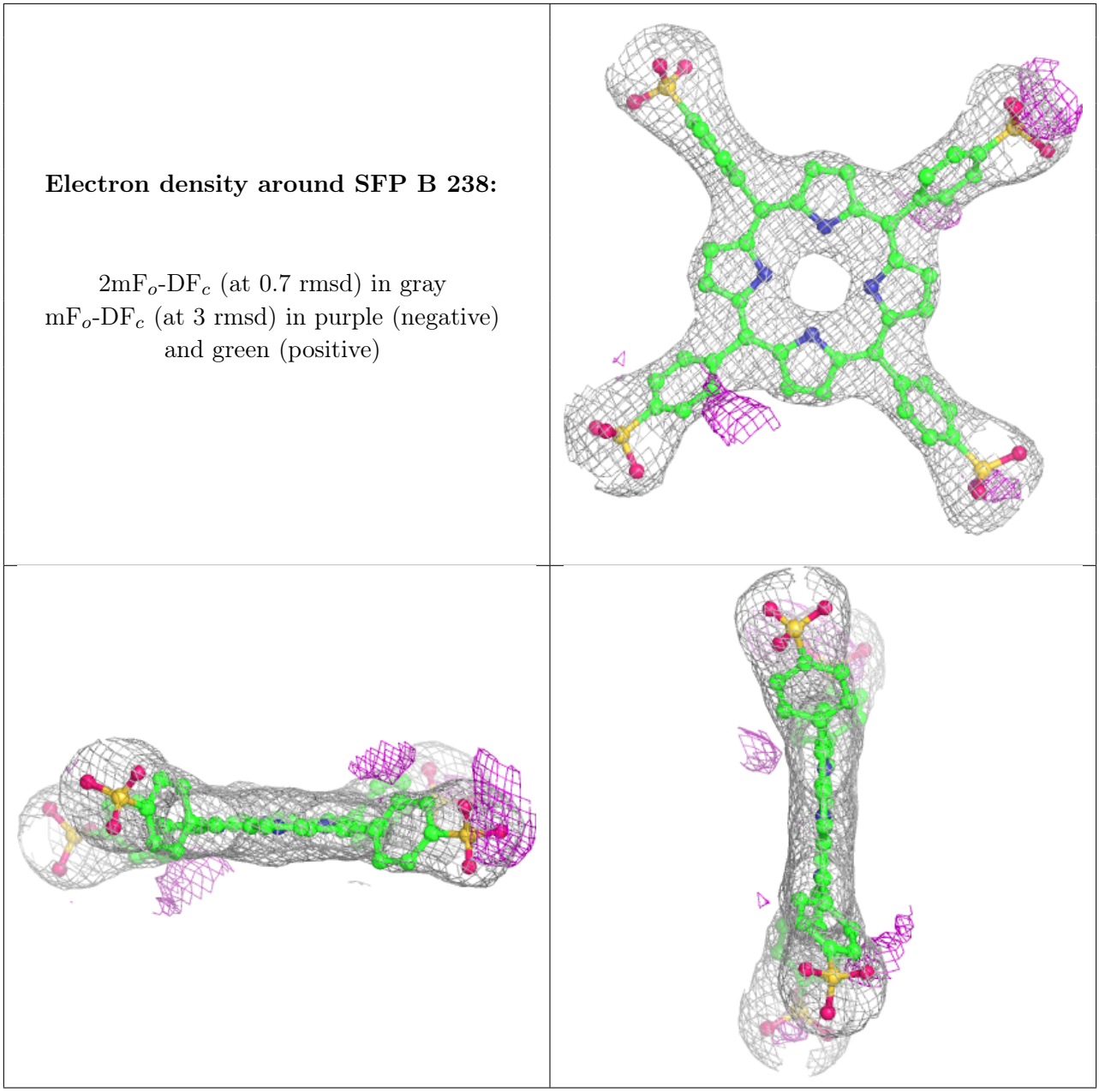
Electron density around SFP D 242:

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



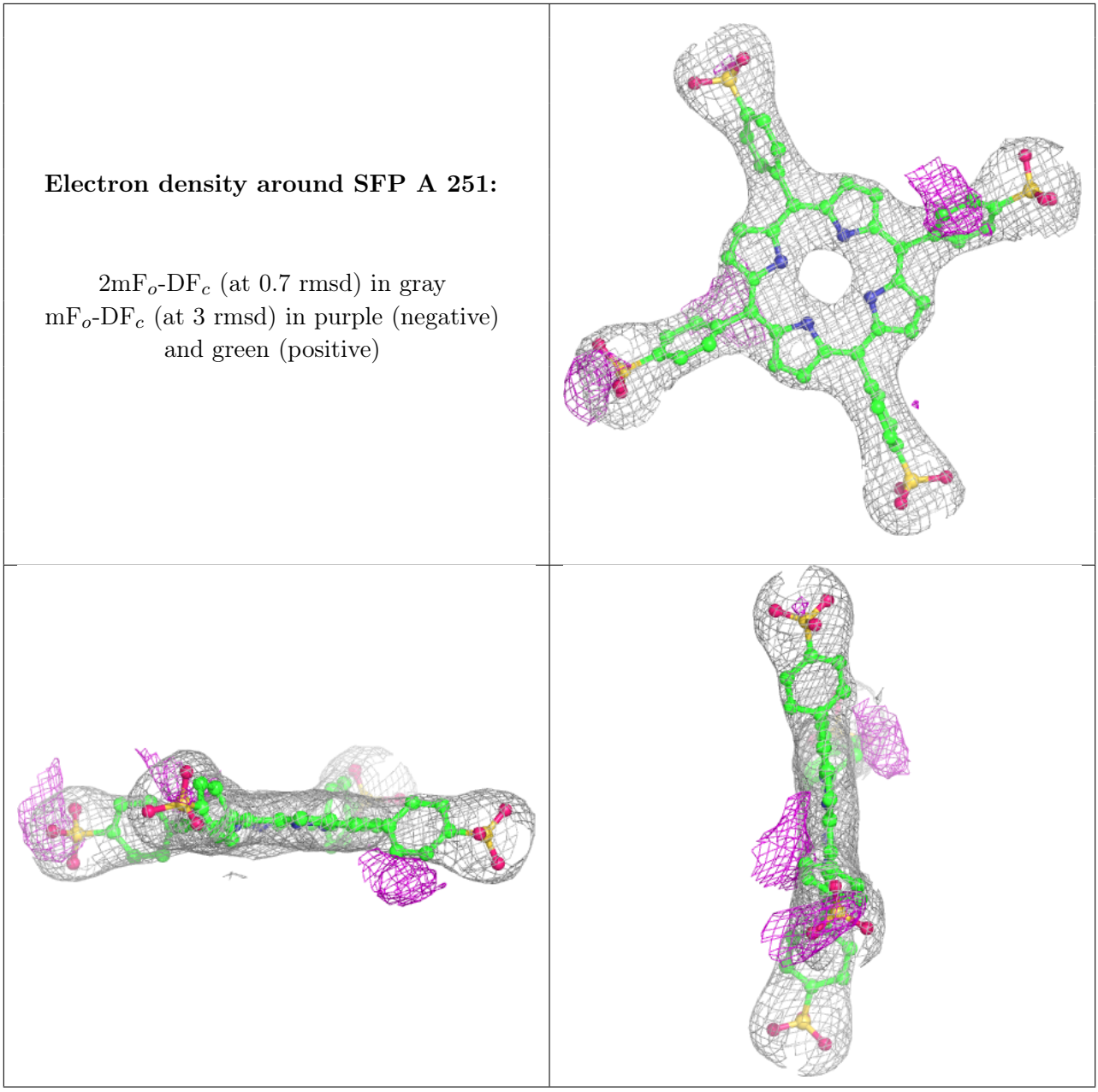
Electron density around SFP B 238:

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



Electron density around SFP A 251:

$2mF_o$-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.