Full wwPDB X-ray Structure Validation Report ⓘ

Nov 1, 2021 – 04:36 PM EDT

PDB ID	:	1WRL
Title	:	Crystal structure of the N-terminal domain of human cardiac troponin C in complex with trifluoperazine (monoclinic crystal form)
Authors	:	Takeda, S.; Igarashi, T.; Oishi, Y.; Mori, H.
Deposited on	:	2004-10-20
Resolution	:	2.60 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

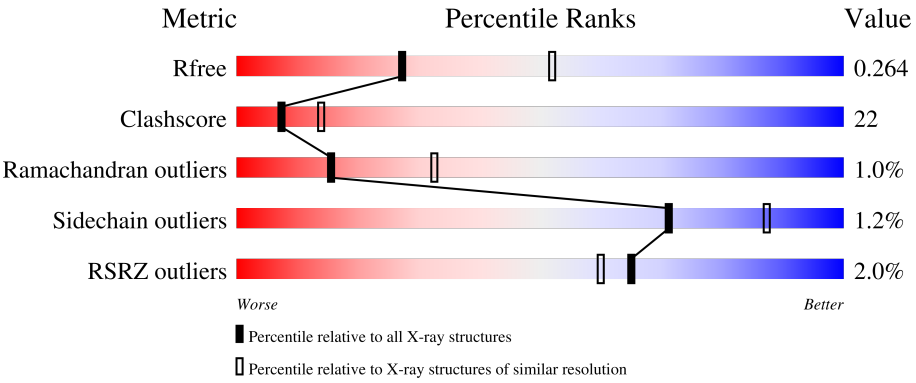
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	88	60% 33% 7%
1	B	88	2% 74% 19% 6%
1	C	88	57% 38% 6%
1	D	88	3% 51% 41% 7%
1	E	88	53% 40% 6%

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Mol	Chain	Length	Quality of chain
1	F	88	3% 51% 41% 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
3	TFP	A	204	-	-	X	-
3	TFP	B	203	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4301 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 Troponin C, slow skeletal and cardiac muscles.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	82	Total	C	N	O	S	0	0	0
			642	402	99	135	6			
1	B	83	Total	C	N	O	S	0	0	0
			650	406	100	138	6			
1	C	83	Total	C	N	O	S	0	0	0
			650	406	100	138	6			
1	D	82	Total	C	N	O	S	0	0	0
			642	401	99	137	5			
1	E	83	Total	C	N	O	S	0	0	0
			650	406	100	138	6			
1	F	82	Total	C	N	O	S	0	0	0
			642	401	99	137	5			

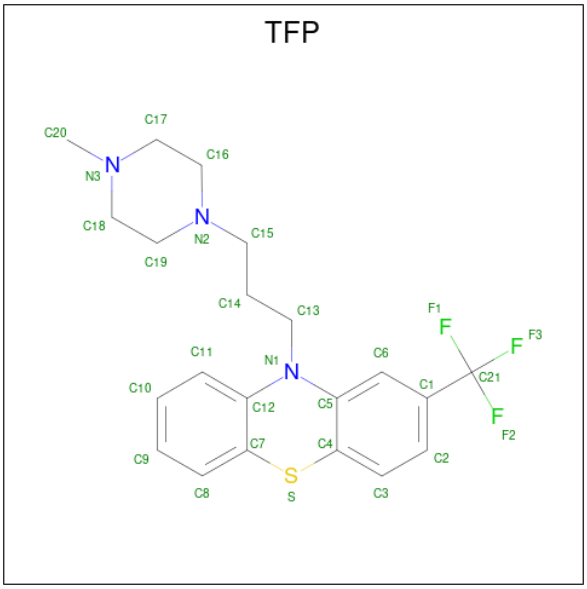
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	35	SER	CYS	engineered mutation	UNP P63316
A	84	SER	CYS	engineered mutation	UNP P63316
B	35	SER	CYS	engineered mutation	UNP P63316
B	84	SER	CYS	engineered mutation	UNP P63316
C	35	SER	CYS	engineered mutation	UNP P63316
C	84	SER	CYS	engineered mutation	UNP P63316
D	35	SER	CYS	engineered mutation	UNP P63316
D	84	SER	CYS	engineered mutation	UNP P63316
E	35	SER	CYS	engineered mutation	UNP P63316
E	84	SER	CYS	engineered mutation	UNP P63316
F	35	SER	CYS	engineered mutation	UNP P63316
F	84	SER	CYS	engineered mutation	UNP P63316

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is 10-[3-(4-METHYL-PIPERAZIN-1-YL)-PROPYL]-2-TRIFLUOROMETHYL-10H-PHENOTHIAZINE (three-letter code: TFP) (formula: $C_{21}H_{24}F_3N_3S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C F N S 28 21 3 3 1	0	0
3	A	1	Total C F N S 28 21 3 3 1	0	0
3	B	1	Total C F N S 28 21 3 3 1	0	0
3	B	1	Total C F N S 28 21 3 3 1	0	0
3	C	1	Total C F N S 28 21 3 3 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	F	N	S	0	0
			28	21	3	3	1		
3	D	1	Total	C	F	N	S	0	0
			28	21	3	3	1		
3	D	1	Total	C	F	N	S	0	0
			28	21	3	3	1		
3	E	1	Total	C	F	N	S	0	0
			28	21	3	3	1		
3	E	1	Total	C	F	N	S	0	0
			28	21	3	3	1		
3	F	1	Total	C	F	N	S	0	0
			28	21	3	3	1		
3	F	1	Total	C	F	N	S	0	0
			28	21	3	3	1		

- Molecule 4 is water.

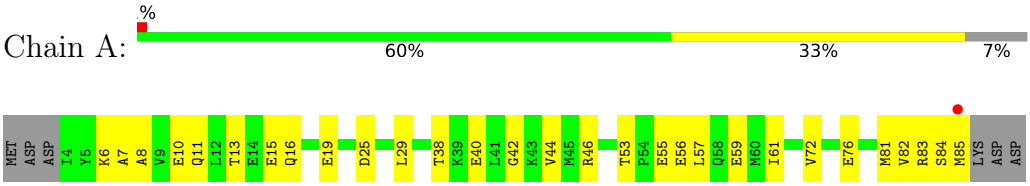
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	20	Total	O	0	0
			20	20		
4	B	27	Total	O	0	0
			27	27		
4	C	10	Total	O	0	0
			10	10		
4	D	10	Total	O	0	0
			10	10		
4	E	12	Total	O	0	0
			12	12		
4	F	4	Total	O	0	0
			4	4		

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.

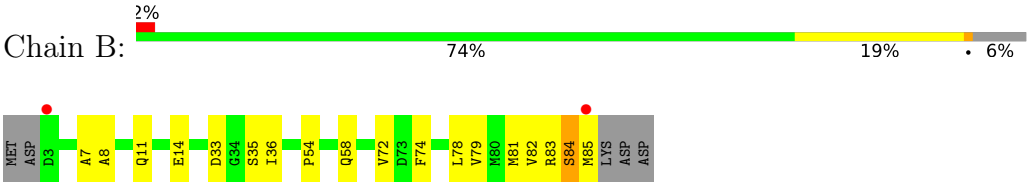
• Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain A:



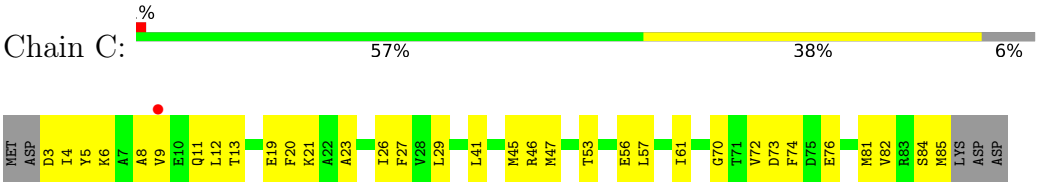
• Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain B:



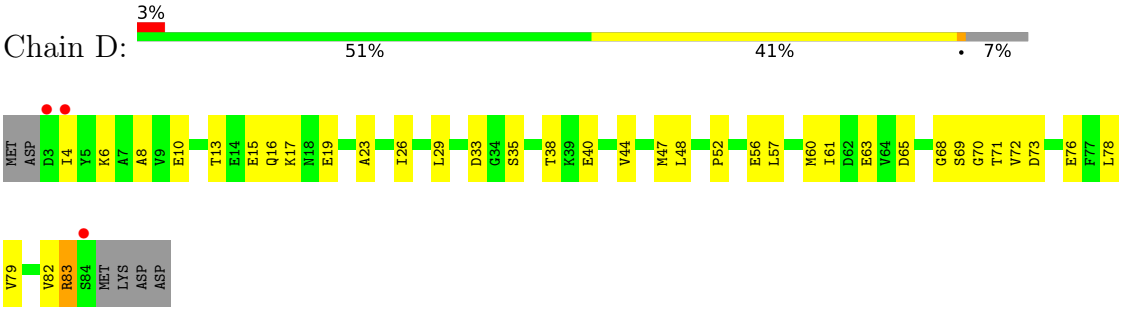
• Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain C:



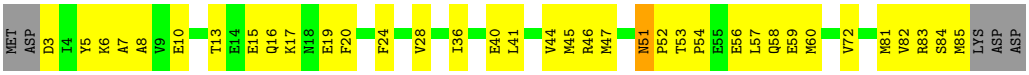
• Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain D:



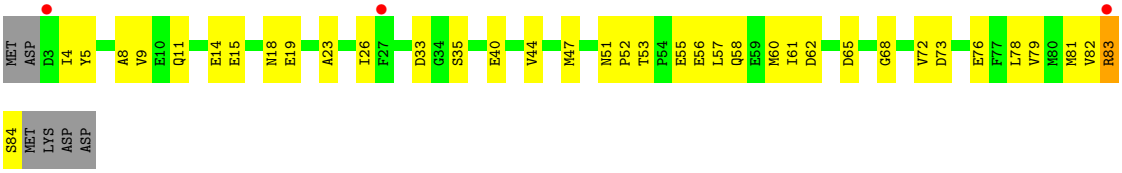
• Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain E:



• Molecule 1: Troponin C, slow skeletal and cardiac muscles

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	48.93Å 67.46Å 90.28Å 90.00° 96.75° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 48.59 – 2.61	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.60) 99.6 (48.59-2.61)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.07 (at 2.61Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.240 , 0.273 0.229 , 0.264	Depositor DCC
R_{free} test set	862 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å^2)	44.0	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 52.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4301	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.68 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.2462e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: TFP, 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	0.34	0/649	0.52	0/870
1	B	0.35	0/657	0.55	0/881
1	C	0.31	0/657	0.52	0/881
1	D	0.31	0/649	0.48	0/871
1	E	0.32	0/657	0.52	0/881
1	F	0.29	0/649	0.47	0/871
All	All	0.32	0/3918	0.51	0/5255

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	642	0	619	37	0
1	B	650	0	623	21	0
1	C	650	0	623	32	0
1	D	642	0	614	28	0
1	E	650	0	623	34	0
1	F	642	0	615	30	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	56	0	48	11	0
3	B	56	0	48	9	0
3	C	56	0	48	5	0
3	D	56	0	48	3	0
3	E	56	0	48	6	0
3	F	56	0	48	4	0
4	A	20	0	0	1	0
4	B	27	0	0	0	0
4	C	10	0	0	0	0
4	D	10	0	0	0	0
4	E	12	0	0	2	0
4	F	4	0	0	0	0
All	All	4301	0	4005	183	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 22.

All (183) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:SER:OG	3:B:203:TFP:H11	1.56	1.03
1:E:81:MET:HE1	3:E:212:TFP:H6	1.47	0.94
3:A:204:TFP:H171	1:B:85:MET:SD	2.14	0.87
1:A:81:MET:HE1	3:A:204:TFP:H6	1.67	0.76
1:E:84:SER:HB2	3:E:212:TFP:H10	1.67	0.76
1:C:3:ASP:O	1:C:6:LYS:HB3	1.88	0.74
1:D:8:ALA:HB3	1:D:82:VAL:HG11	1.69	0.74
1:C:23:ALA:O	1:C:26:ILE:HG22	1.87	0.73
1:C:3:ASP:OD2	1:C:4:ILE:HG12	1.88	0.73
1:A:13:THR:H	1:A:16:GLN:HE21	1.35	0.73
1:A:53:THR:OG1	1:A:56:GLU:HG3	1.88	0.73
1:F:72:VAL:HG13	1:F:76:GLU:HB2	1.71	0.72
1:A:84:SER:HB2	3:A:204:TFP:H10	1.70	0.72
1:C:81:MET:HE1	3:C:208:TFP:H6	1.72	0.71
1:B:8:ALA:HB3	1:B:82:VAL:HG11	1.72	0.71
1:A:42:GLY:O	1:A:46:ARG:HG2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61:ILE:HG23	1:D:72:VAL:HG23	1.73	0.69
1:E:8:ALA:HB3	1:E:82:VAL:HG11	1.74	0.69
1:D:13:THR:O	1:D:17:LYS:HG3	1.93	0.68
1:A:46:ARG:HH21	1:A:46:ARG:HG3	1.58	0.67
3:B:203:TFP:H11	3:B:203:TFP:H141	1.77	0.67
1:A:55:GLU:HG2	1:F:11:GLN:HG2	1.77	0.66
1:F:72:VAL:HA	1:F:76:GLU:OE1	1.98	0.63
1:A:85:MET:HG3	1:B:85:MET:HE2	1.81	0.63
1:D:15:GLU:O	1:D:19:GLU:HG3	1.98	0.63
1:A:6:LYS:O	1:A:10:GLU:HG2	1.99	0.63
1:C:23:ALA:HB2	3:D:205:TFP:H9	1.80	0.63
1:E:6:LYS:HB3	1:E:6:LYS:HZ3	1.64	0.62
1:A:13:THR:OG1	1:A:16:GLN:HG3	2.00	0.62
1:A:15:GLU:O	1:A:19:GLU:HG3	2.00	0.61
1:F:9:VAL:HG22	1:F:82:VAL:HG21	1.80	0.61
1:A:7:ALA:O	1:A:11:GLN:HG2	2.01	0.61
1:E:8:ALA:HB3	1:E:82:VAL:CG1	2.29	0.61
1:A:13:THR:H	1:A:16:GLN:NE2	1.97	0.61
1:C:26:ILE:HD12	1:C:29:LEU:HD12	1.83	0.61
1:C:9:VAL:O	1:C:12:LEU:HB2	2.01	0.60
1:D:65:ASP:OD1	1:D:70:GLY:N	2.34	0.60
1:F:58:GLN:HG3	1:F:62:ASP:OD2	2.02	0.60
3:A:204:TFP:H141	3:A:204:TFP:H11	1.82	0.60
1:C:61:ILE:HG21	1:C:70:GLY:O	2.02	0.59
1:E:45:MET:HG2	3:E:210:TFP:S	2.43	0.59
3:B:203:TFP:H141	3:B:203:TFP:C11	2.33	0.59
1:E:51:ASN:H	1:E:51:ASN:HD22	1.51	0.59
1:E:53:THR:OG1	1:E:56:GLU:HG3	2.04	0.58
3:A:204:TFP:H132	3:B:203:TFP:H132	1.86	0.58
1:A:13:THR:HG23	1:A:16:GLN:HE21	1.69	0.57
1:C:82:VAL:C	1:C:84:SER:H	2.07	0.57
1:F:65:ASP:HA	1:F:76:GLU:OE2	2.04	0.57
1:A:8:ALA:HB3	1:A:82:VAL:HG11	1.84	0.57
1:C:81:MET:O	1:C:84:SER:HB2	2.05	0.57
1:B:84:SER:OG	3:B:203:TFP:C11	2.43	0.56
1:F:33:ASP:OD2	1:F:35:SER:HB2	2.06	0.56
1:D:56:GLU:O	1:D:60:MET:HG3	2.06	0.56
1:E:13:THR:HG23	1:E:16:GLN:HE21	1.70	0.55
1:F:40:GLU:O	1:F:44:VAL:HG23	2.06	0.55
1:F:78:LEU:O	1:F:82:VAL:HG23	2.07	0.55
1:F:73:ASP:OD2	1:F:76:GLU:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:TYR:O	1:C:9:VAL:HG23	2.07	0.54
1:D:23:ALA:O	1:D:26:ILE:HG22	2.08	0.54
1:A:40:GLU:O	1:A:44:VAL:HG23	2.07	0.54
1:D:33:ASP:OD1	1:D:35:SER:HB2	2.08	0.54
1:E:40:GLU:O	1:E:44:VAL:HG23	2.08	0.53
1:A:11:GLN:HE21	1:A:11:GLN:HA	1.74	0.53
1:A:61:ILE:HD12	1:A:72:VAL:HG23	1.90	0.53
1:D:4:ILE:HG13	1:D:4:ILE:O	2.08	0.53
1:C:47:MET:HE3	1:D:47:MET:SD	2.49	0.52
1:E:6:LYS:HB3	1:E:6:LYS:NZ	2.25	0.52
1:E:19:GLU:OE1	3:F:209:TFP:H152	2.08	0.52
1:F:61:ILE:HG23	1:F:72:VAL:HG23	1.92	0.52
1:A:11:GLN:HA	1:A:11:GLN:NE2	2.25	0.52
1:E:24:PHE:O	1:E:28:VAL:HG22	2.09	0.52
1:C:41:LEU:HG	1:C:45:MET:HE3	1.91	0.52
3:C:208:TFP:H11	3:C:208:TFP:H141	1.92	0.51
1:A:46:ARG:HG3	1:A:46:ARG:NH2	2.26	0.50
1:D:40:GLU:O	1:D:44:VAL:HG23	2.11	0.50
1:E:3:ASP:OD1	1:E:6:LYS:NZ	2.43	0.50
1:E:13:THR:O	1:E:17:LYS:HG3	2.12	0.50
1:E:3:ASP:HA	1:E:6:LYS:NZ	2.26	0.50
1:E:20:PHE:CE1	1:E:81:MET:HE3	2.46	0.50
1:C:8:ALA:O	1:C:11:GLN:HB2	2.12	0.50
1:C:82:VAL:C	1:C:84:SER:N	2.65	0.50
1:A:83:ARG:HG3	1:A:83:ARG:HH11	1.76	0.49
1:B:79:VAL:O	1:B:83:ARG:HG3	2.12	0.49
3:E:210:TFP:H9	1:F:23:ALA:HB2	1.93	0.49
1:C:53:THR:OG1	1:C:56:GLU:HG3	2.13	0.49
1:B:8:ALA:HB3	1:B:82:VAL:CG1	2.42	0.49
3:E:212:TFP:H131	3:F:211:TFP:S	2.53	0.49
3:E:212:TFP:H141	3:E:212:TFP:H11	1.95	0.49
1:A:38:THR:HG23	4:A:215:HOH:O	2.13	0.48
1:A:55:GLU:O	1:A:59:GLU:HG3	2.14	0.48
3:A:204:TFP:C17	1:B:85:MET:SD	2.96	0.48
1:B:74:PHE:CZ	1:B:78:LEU:HD21	2.49	0.48
1:D:73:ASP:OD2	1:D:76:GLU:HG3	2.13	0.48
1:E:82:VAL:O	1:E:85:MET:HB3	2.13	0.48
1:D:60:MET:O	1:D:63:GLU:HB3	2.13	0.48
1:A:13:THR:HG23	1:A:16:GLN:NE2	2.29	0.47
1:D:52:PRO:HA	1:D:56:GLU:OE2	2.14	0.47
1:A:85:MET:CG	1:B:85:MET:HE2	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:VAL:HG13	1:D:76:GLU:HB2	1.95	0.47
1:D:17:LYS:NZ	1:D:78:LEU:HD13	2.30	0.47
1:B:33:ASP:OD1	1:B:35:SER:HB2	2.14	0.47
1:C:19:GLU:OE1	3:D:205:TFP:H152	2.15	0.47
1:F:9:VAL:CG2	1:F:82:VAL:HG21	2.45	0.47
1:F:81:MET:O	3:F:211:TFP:H151	2.15	0.47
1:F:84:SER:O	3:F:211:TFP:H11	2.14	0.47
1:F:53:THR:OG1	1:F:56:GLU:HG3	2.15	0.46
1:F:15:GLU:O	1:F:19:GLU:HG3	2.14	0.46
1:D:4:ILE:O	1:D:4:ILE:CG1	2.62	0.46
1:F:5:TYR:O	1:F:9:VAL:HG23	2.16	0.46
1:B:36:ILE:HB	1:B:72:VAL:HB	1.97	0.46
1:E:46:ARG:NH2	4:E:213:HOH:O	2.49	0.46
1:F:56:GLU:O	1:F:60:MET:HG3	2.15	0.46
1:C:21:LYS:HA	1:C:74:PHE:CE1	2.51	0.46
1:E:3:ASP:O	1:E:6:LYS:HB3	2.15	0.45
1:C:81:MET:CE	3:C:208:TFP:H6	2.45	0.45
1:D:26:ILE:HD12	1:D:29:LEU:HD11	1.98	0.45
1:E:15:GLU:HG2	1:E:19:GLU:OE2	2.17	0.45
1:F:52:PRO:HG2	1:F:57:LEU:HD21	1.98	0.45
1:C:20:PHE:CE1	1:C:81:MET:CE	3.00	0.45
1:B:83:ARG:O	1:B:84:SER:C	2.54	0.45
1:C:61:ILE:HG23	1:C:72:VAL:HG23	1.98	0.45
1:A:85:MET:SD	1:B:85:MET:CE	3.04	0.45
1:C:84:SER:HA	3:C:208:TFP:H10	1.98	0.45
1:E:45:MET:HE1	1:E:57:LEU:HD23	1.98	0.45
1:C:45:MET:HE1	1:C:57:LEU:HD23	1.98	0.45
3:A:204:TFP:H131	3:B:203:TFP:S	2.57	0.44
1:A:85:MET:SD	1:B:85:MET:HE2	2.56	0.44
1:C:8:ALA:HB3	1:C:82:VAL:HG11	1.99	0.44
1:D:79:VAL:O	1:D:83:ARG:HG3	2.16	0.44
1:E:5:TYR:CD1	1:E:83:ARG:HA	2.53	0.44
1:E:36:ILE:HB	1:E:72:VAL:HB	1.98	0.44
1:B:54:PRO:O	1:B:58:GLN:HG3	2.18	0.44
1:F:4:ILE:HG12	1:F:4:ILE:O	2.15	0.44
1:F:55:GLU:H	1:F:55:GLU:CD	2.20	0.44
1:E:7:ALA:HA	1:E:10:GLU:OE1	2.17	0.44
1:E:6:LYS:O	1:E:10:GLU:HG3	2.18	0.43
1:E:41:LEU:HD11	1:E:45:MET:HE2	2.00	0.43
1:E:52:PRO:HG2	4:E:213:HOH:O	2.18	0.43
1:D:63:GLU:HG2	1:D:83:ARG:NH1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:PHE:CE1	1:C:81:MET:HE3	2.53	0.43
1:A:85:MET:O	1:A:85:MET:HG2	2.19	0.43
1:A:72:VAL:HA	1:A:76:GLU:OE1	2.19	0.43
1:F:5:TYR:CD1	1:F:83:ARG:HG2	2.54	0.43
1:B:14:GLU:HG2	1:E:59:GLU:OE1	2.19	0.43
1:C:41:LEU:HG	1:C:45:MET:CE	2.49	0.43
1:D:13:THR:OG1	1:D:16:GLN:HG3	2.19	0.42
1:C:45:MET:CE	1:C:57:LEU:HD23	2.49	0.42
1:D:69:SER:C	1:D:71:THR:H	2.22	0.42
1:B:7:ALA:O	1:B:11:GLN:HG2	2.19	0.42
1:B:81:MET:O	3:B:203:TFP:H191	2.19	0.42
1:E:45:MET:HE1	1:E:60:MET:SD	2.60	0.42
3:C:208:TFP:H132	3:D:207:TFP:H142	2.01	0.42
1:E:47:MET:HE2	1:F:47:MET:SD	2.60	0.42
1:D:6:LYS:O	1:D:10:GLU:HG3	2.19	0.42
1:B:84:SER:OG	3:B:203:TFP:H141	2.19	0.42
1:C:23:ALA:HA	1:D:48:LEU:O	2.20	0.41
1:D:44:VAL:O	1:D:47:MET:HG2	2.19	0.41
1:F:5:TYR:CG	1:F:83:ARG:HG2	2.55	0.41
1:F:23:ALA:O	1:F:26:ILE:HG22	2.20	0.41
1:A:57:LEU:O	1:A:61:ILE:HG12	2.20	0.41
1:D:72:VAL:HA	1:D:76:GLU:OE1	2.20	0.41
1:C:26:ILE:HG23	1:C:27:PHE:CD1	2.54	0.41
1:C:82:VAL:O	1:C:84:SER:N	2.53	0.41
1:A:25:ASP:O	1:A:29:LEU:HG	2.20	0.41
1:A:83:ARG:HG3	1:A:83:ARG:NH1	2.35	0.41
1:F:79:VAL:HG12	1:F:83:ARG:HG3	2.01	0.41
1:D:38:THR:O	1:D:57:LEU:HD13	2.21	0.41
1:C:3:ASP:N	1:C:6:LYS:HB2	2.36	0.41
1:A:46:ARG:NH2	1:A:46:ARG:CG	2.84	0.41
1:A:81:MET:HE1	3:A:204:TFP:H142	2.02	0.41
1:B:84:SER:CB	3:B:203:TFP:H11	2.47	0.41
1:D:8:ALA:CB	1:D:82:VAL:HG11	2.44	0.41
1:C:73:ASP:OD2	1:C:76:GLU:HG3	2.22	0.40
1:F:14:GLU:O	1:F:18:ASN:ND2	2.54	0.40
1:F:61:ILE:HG23	1:F:72:VAL:CG2	2.52	0.40
1:A:82:VAL:HA	3:A:204:TFP:H182	2.03	0.40
1:E:54:PRO:O	1:E:58:GLN:HG3	2.21	0.40
1:A:72:VAL:HG13	1:A:76:GLU:HB2	2.04	0.40
1:A:84:SER:HB2	3:A:204:TFP:C10	2.46	0.40
3:A:204:TFP:H141	3:A:204:TFP:C11	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:20:PHE:CE1	1:E:81:MET:CE	3.03	0.40
1:E:41:LEU:HG	1:E:45:MET:CE	2.51	0.40
1:F:8:ALA:HB3	1:F:82:VAL:HG11	2.02	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	80/88 (91%)	77 (96%)	3 (4%)	0	100 100
1	B	81/88 (92%)	79 (98%)	1 (1%)	1 (1%)	13 27
1	C	81/88 (92%)	74 (91%)	7 (9%)	0	100 100
1	D	80/88 (91%)	75 (94%)	3 (4%)	2 (2%)	5 9
1	E	81/88 (92%)	75 (93%)	6 (7%)	0	100 100
1	F	80/88 (91%)	70 (88%)	8 (10%)	2 (2%)	5 9
All	All	483/528 (92%)	450 (93%)	28 (6%)	5 (1%)	15 32

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	83	ARG
1	D	68	GLY
1	F	68	GLY
1	B	84	SER
1	D	83	ARG

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	71/77 (92%)	71 (100%)	0	100	100
1	B	72/77 (94%)	72 (100%)	0	100	100
1	C	72/77 (94%)	69 (96%)	3 (4%)	30	55
1	D	71/77 (92%)	71 (100%)	0	100	100
1	E	72/77 (94%)	71 (99%)	1 (1%)	67	85
1	F	71/77 (92%)	70 (99%)	1 (1%)	67	85
All	All	429/462 (93%)	424 (99%)	5 (1%)	71	87

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	13	THR
1	C	46	ARG
1	C	85	MET
1	E	51	ASN
1	F	51	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	16	GLN
1	A	18	ASN
1	B	58	GLN
1	C	18	ASN
1	D	11	GLN
1	E	16	GLN
1	E	18	ASN
1	E	51	ASN
1	F	11	GLN
1	F	18	ASN
1	F	51	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 6 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	$\#\|Z\| > 2$
3	TFP	F	211	-	31,31,31	1.92	7 (22%)	45,45,45	1.23	3 (6%)
3	TFP	E	210	-	31,31,31	1.69	7 (22%)	45,45,45	1.22	6 (13%)
3	TFP	F	209	-	31,31,31	1.73	7 (22%)	45,45,45	1.22	6 (13%)
3	TFP	B	201	-	31,31,31	1.65	5 (16%)	45,45,45	1.30	6 (13%)
3	TFP	B	203	-	31,31,31	1.77	4 (12%)	45,45,45	1.61	9 (20%)
3	TFP	A	202	-	31,31,31	1.74	7 (22%)	45,45,45	1.36	9 (20%)
3	TFP	C	206	-	31,31,31	1.64	6 (19%)	45,45,45	1.22	4 (8%)
3	TFP	D	207	-	31,31,31	1.96	7 (22%)	45,45,45	1.28	4 (8%)
3	TFP	E	212	-	31,31,31	1.68	6 (19%)	45,45,45	1.38	5 (11%)
3	TFP	C	208	-	31,31,31	1.64	5 (16%)	45,45,45	1.49	8 (17%)
3	TFP	D	205	-	31,31,31	1.71	7 (22%)	45,45,45	1.25	5 (11%)
3	TFP	A	204	-	31,31,31	1.65	7 (22%)	45,45,45	1.37	5 (11%)

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	TFP	F	211	-	-	0/12/34/34	0/4/4/4
3	TFP	E	210	-	-	0/12/34/34	0/4/4/4
3	TFP	F	209	-	-	0/12/34/34	0/4/4/4
3	TFP	B	201	-	-	0/12/34/34	0/4/4/4
3	TFP	B	203	-	-	3/12/34/34	0/4/4/4
3	TFP	A	202	-	-	1/12/34/34	0/4/4/4
3	TFP	C	206	-	-	0/12/34/34	0/4/4/4
3	TFP	D	207	-	-	0/12/34/34	0/4/4/4
3	TFP	E	212	-	-	2/12/34/34	0/4/4/4
3	TFP	C	208	-	-	1/12/34/34	0/4/4/4
3	TFP	D	205	-	-	0/12/34/34	0/4/4/4
3	TFP	A	204	-	-	2/12/34/34	0/4/4/4

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	207	TFP	C12-C7	4.92	1.46	1.40
3	B	203	TFP	C12-C7	4.85	1.46	1.40
3	F	211	TFP	C12-C7	4.61	1.45	1.40
3	D	207	TFP	C4-S	-4.43	1.68	1.76
3	F	209	TFP	C4-S	-4.38	1.68	1.76
3	F	211	TFP	C4-S	-4.30	1.68	1.76
3	A	202	TFP	C4-S	-4.28	1.68	1.76
3	D	205	TFP	C4-S	-4.26	1.68	1.76
3	B	201	TFP	C4-S	-4.23	1.69	1.76
3	B	203	TFP	C12-N1	4.19	1.47	1.40
3	C	206	TFP	C12-C7	4.11	1.45	1.40
3	E	212	TFP	C12-C7	4.10	1.45	1.40
3	B	203	TFP	C4-S	-4.02	1.69	1.76
3	A	202	TFP	C12-C7	4.01	1.45	1.40
3	C	208	TFP	C12-C7	3.95	1.45	1.40
3	A	204	TFP	C12-C7	3.95	1.45	1.40
3	E	210	TFP	C12-C7	3.89	1.45	1.40
3	B	201	TFP	C12-C7	3.87	1.45	1.40
3	E	212	TFP	C4-S	-3.87	1.69	1.76
3	F	209	TFP	C12-C7	3.84	1.45	1.40
3	D	205	TFP	C12-C7	3.82	1.45	1.40
3	E	210	TFP	C4-S	-3.79	1.69	1.76
3	C	206	TFP	C4-S	-3.78	1.69	1.76
3	D	207	TFP	C5-C4	3.73	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	211	TFP	C5-C4	3.71	1.44	1.40
3	F	211	TFP	C12-N1	3.71	1.46	1.40
3	A	204	TFP	C4-S	-3.68	1.69	1.76
3	C	208	TFP	C4-S	-3.65	1.70	1.76
3	D	207	TFP	C12-N1	3.43	1.46	1.40
3	B	203	TFP	C5-C4	3.39	1.44	1.40
3	C	206	TFP	C5-C4	3.35	1.44	1.40
3	D	207	TFP	C11-C12	3.28	1.45	1.39
3	E	212	TFP	C12-N1	3.22	1.45	1.40
3	E	210	TFP	C5-C4	3.18	1.44	1.40
3	F	209	TFP	C5-C4	3.16	1.44	1.40
3	A	204	TFP	C5-C4	3.14	1.44	1.40
3	F	211	TFP	C11-C12	3.12	1.44	1.39
3	A	202	TFP	C12-N1	3.11	1.45	1.40
3	A	204	TFP	C12-N1	3.10	1.45	1.40
3	D	205	TFP	C5-C4	3.07	1.44	1.40
3	E	212	TFP	C5-C4	3.07	1.44	1.40
3	D	207	TFP	C5-N1	3.06	1.45	1.40
3	C	208	TFP	C12-N1	2.99	1.45	1.40
3	F	211	TFP	C5-N1	2.95	1.45	1.40
3	A	202	TFP	C5-C4	2.93	1.43	1.40
3	F	209	TFP	C11-C12	2.91	1.44	1.39
3	C	208	TFP	C11-C12	2.91	1.44	1.39
3	D	205	TFP	C11-C12	2.91	1.44	1.39
3	A	202	TFP	C11-C12	2.89	1.44	1.39
3	E	210	TFP	C11-C12	2.85	1.44	1.39
3	B	201	TFP	C11-C12	2.82	1.44	1.39
3	F	209	TFP	C12-N1	2.76	1.44	1.40
3	C	208	TFP	C5-C4	2.74	1.43	1.40
3	E	212	TFP	C11-C12	2.72	1.44	1.39
3	C	206	TFP	C11-C12	2.71	1.44	1.39
3	B	201	TFP	C12-N1	2.69	1.44	1.40
3	B	201	TFP	C5-C4	2.66	1.43	1.40
3	D	207	TFP	C6-C5	2.65	1.43	1.39
3	E	210	TFP	C5-N1	2.60	1.44	1.40
3	D	205	TFP	C12-N1	2.58	1.44	1.40
3	A	204	TFP	C11-C12	2.57	1.43	1.39
3	F	211	TFP	C6-C5	2.56	1.43	1.39
3	D	205	TFP	C5-N1	2.47	1.44	1.40
3	E	210	TFP	C12-N1	2.37	1.44	1.40
3	D	205	TFP	C6-C5	2.31	1.43	1.39
3	E	210	TFP	C6-C5	2.27	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	209	TFP	C6-C5	2.20	1.43	1.39
3	C	206	TFP	C12-N1	2.20	1.44	1.40
3	F	209	TFP	C5-N1	2.19	1.44	1.40
3	A	204	TFP	C6-C5	2.15	1.43	1.39
3	A	202	TFP	C5-N1	2.12	1.43	1.40
3	A	204	TFP	C21-C1	2.12	1.54	1.49
3	E	212	TFP	C6-C5	2.11	1.43	1.39
3	C	206	TFP	C5-N1	2.08	1.43	1.40
3	A	202	TFP	C6-C5	2.06	1.43	1.39

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	203	TFP	C13-N1-C12	5.54	126.25	119.03
3	A	202	TFP	C18-N3-C17	4.11	115.28	109.52
3	C	208	TFP	C7-C12-N1	-3.83	114.35	119.94
3	C	208	TFP	C11-C12-N1	3.77	126.70	121.77
3	B	201	TFP	C18-N3-C17	3.72	114.73	109.52
3	E	212	TFP	C15-N2-C16	-3.52	102.24	111.23
3	B	203	TFP	C13-N1-C5	-3.29	114.74	119.03
3	A	204	TFP	C11-C12-N1	3.23	125.99	121.77
3	B	203	TFP	C11-C12-N1	3.22	125.98	121.77
3	A	204	TFP	C15-N2-C16	-3.20	103.05	111.23
3	E	212	TFP	C11-C12-N1	3.09	125.81	121.77
3	D	207	TFP	C15-N2-C16	-2.94	103.72	111.23
3	D	205	TFP	C15-N2-C16	-2.93	103.74	111.23
3	A	204	TFP	C7-C12-N1	-2.93	115.66	119.94
3	F	211	TFP	C15-N2-C16	-2.93	103.75	111.23
3	E	212	TFP	C7-C12-N1	-2.91	115.69	119.94
3	B	203	TFP	C15-N2-C16	-2.91	103.80	111.23
3	C	208	TFP	C15-N2-C16	-2.81	104.05	111.23
3	C	206	TFP	C15-N2-C16	-2.81	104.06	111.23
3	E	210	TFP	C15-N2-C16	-2.76	104.18	111.23
3	F	209	TFP	C15-N2-C16	-2.75	104.21	111.23
3	A	202	TFP	C16-C17-N3	2.64	113.78	110.80
3	D	207	TFP	F3-C21-C1	2.62	118.69	112.93
3	B	203	TFP	F3-C21-C1	2.61	118.66	112.93
3	F	211	TFP	F2-C21-C1	2.60	118.62	112.93
3	C	206	TFP	C18-N3-C17	2.54	113.08	109.52
3	D	205	TFP	F3-C21-C1	2.50	118.42	112.93
3	B	201	TFP	F3-C21-C1	2.48	118.38	112.93
3	E	210	TFP	F3-C21-C1	2.48	118.36	112.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	208	TFP	F3-C21-C1	2.47	118.36	112.93
3	A	204	TFP	F3-C21-C1	2.47	118.34	112.93
3	E	210	TFP	F2-C21-C1	2.45	118.31	112.93
3	C	206	TFP	F3-C21-C1	2.44	118.28	112.93
3	B	201	TFP	F2-C21-C1	2.43	118.27	112.93
3	F	209	TFP	F3-C21-C1	2.43	118.26	112.93
3	E	212	TFP	F3-C21-C1	2.42	118.24	112.93
3	C	208	TFP	C13-N1-C12	2.39	122.14	119.03
3	A	204	TFP	F2-C21-C1	2.38	118.16	112.93
3	F	209	TFP	C18-N3-C17	2.38	112.85	109.52
3	F	209	TFP	F2-C21-C1	2.35	118.09	112.93
3	C	208	TFP	F2-C21-C1	2.33	118.04	112.93
3	A	202	TFP	F3-C21-C1	2.33	118.04	112.93
3	D	205	TFP	C14-C13-N1	-2.32	105.75	112.99
3	F	211	TFP	F3-C21-C1	2.32	118.01	112.93
3	B	203	TFP	C7-C12-N1	-2.31	116.56	119.94
3	E	212	TFP	F2-C21-C1	2.31	117.99	112.93
3	C	208	TFP	C18-N3-C17	2.29	112.73	109.52
3	A	202	TFP	F2-C21-C1	2.28	117.94	112.93
3	A	202	TFP	C19-C18-N3	2.25	113.35	110.80
3	D	205	TFP	F2-C21-C1	2.24	117.85	112.93
3	F	209	TFP	C14-C13-N1	-2.21	106.08	112.99
3	B	201	TFP	C15-N2-C16	-2.21	105.59	111.23
3	B	203	TFP	C6-C1-C21	-2.20	116.61	119.58
3	D	207	TFP	C18-N3-C17	2.18	112.58	109.52
3	B	203	TFP	C18-N3-C17	2.18	112.57	109.52
3	A	202	TFP	C15-N2-C16	-2.16	105.72	111.23
3	E	210	TFP	C14-C13-N1	-2.13	106.35	112.99
3	B	201	TFP	C14-C13-N1	-2.11	106.39	112.99
3	D	205	TFP	C18-N3-C17	2.11	112.47	109.52
3	D	207	TFP	F2-C21-C1	2.08	117.48	112.93
3	A	202	TFP	C2-C1-C6	2.08	121.76	117.76
3	B	201	TFP	C20-N3-C17	-2.06	107.57	110.66
3	B	203	TFP	F2-C21-C1	2.06	117.45	112.93
3	A	202	TFP	C20-N3-C18	-2.06	107.58	110.66
3	C	206	TFP	F2-C21-C1	2.06	117.44	112.93
3	E	210	TFP	C18-N3-C17	2.05	112.39	109.52
3	C	208	TFP	C4-C5-N1	-2.03	116.97	119.94
3	A	202	TFP	C20-N3-C17	-2.02	107.64	110.66
3	E	210	TFP	C2-C1-C6	2.02	121.65	117.76
3	F	209	TFP	C2-C1-C6	2.01	121.63	117.76

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	203	TFP	C14-C13-N1-C12
3	E	212	TFP	N1-C13-C14-C15
3	C	208	TFP	N1-C13-C14-C15
3	B	203	TFP	N1-C13-C14-C15
3	A	204	TFP	N1-C13-C14-C15
3	B	203	TFP	C14-C13-N1-C5
3	A	204	TFP	C14-C13-N1-C5
3	E	212	TFP	C14-C13-N1-C5
3	A	202	TFP	C14-C13-N1-C5

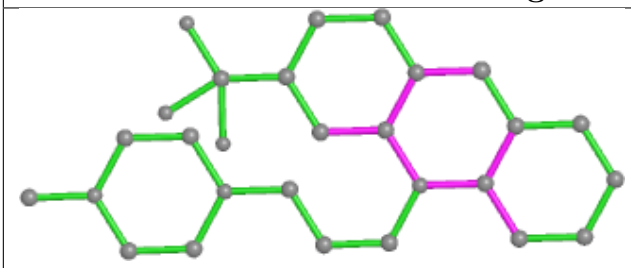
There are no ring outliers.

9 monomers are involved in 34 short contacts:

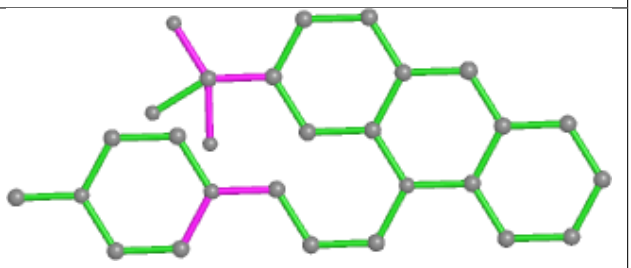
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	211	TFP	3	0
3	E	210	TFP	2	0
3	F	209	TFP	1	0
3	B	203	TFP	9	0
3	D	207	TFP	1	0
3	E	212	TFP	4	0
3	C	208	TFP	5	0
3	D	205	TFP	2	0
3	A	204	TFP	11	0

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.

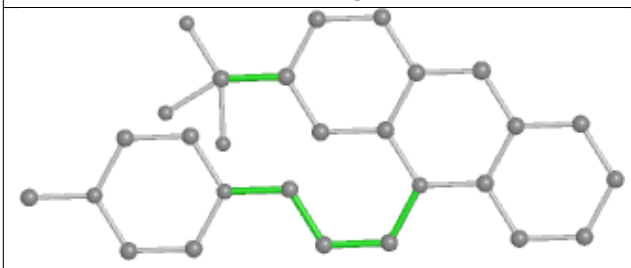
Ligand TFP F 211



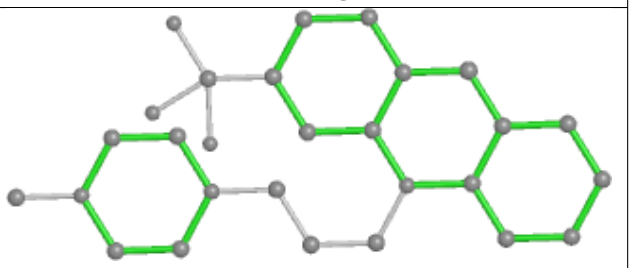
Bond lengths



Bond angles

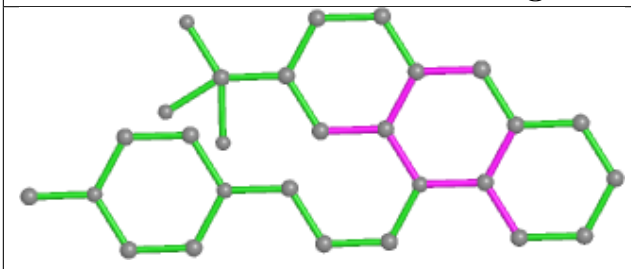


Torsions

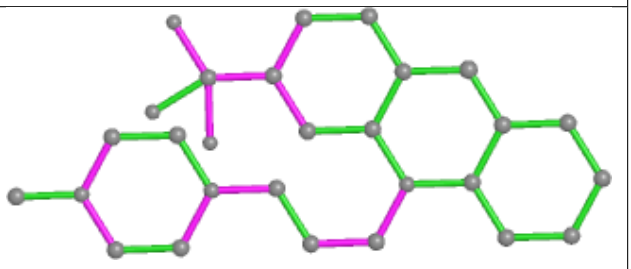


Rings

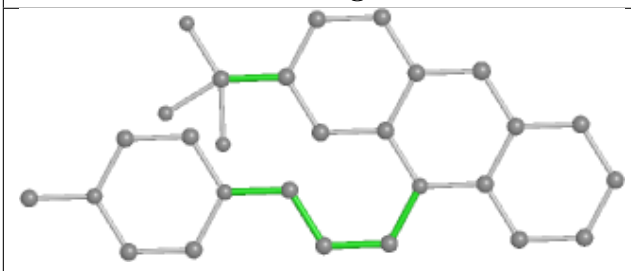
Ligand TFP E 210



Bond lengths



Bond angles



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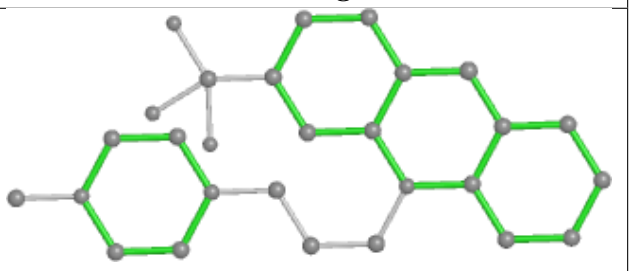
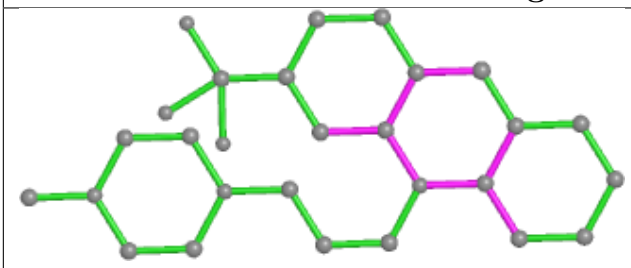
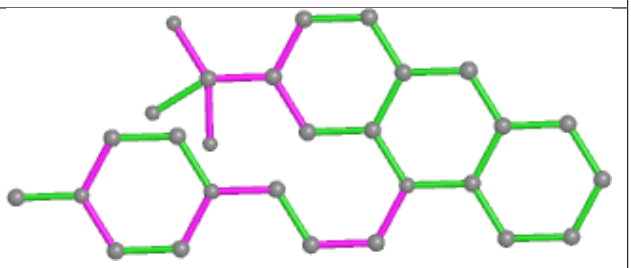


Rings

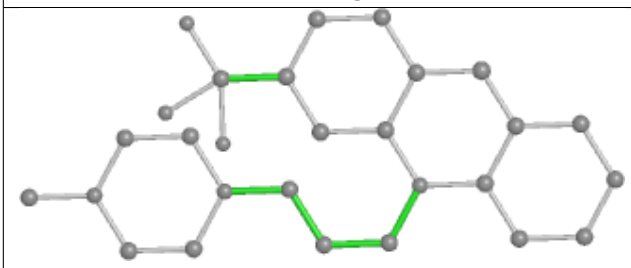
Ligand TFP F 209



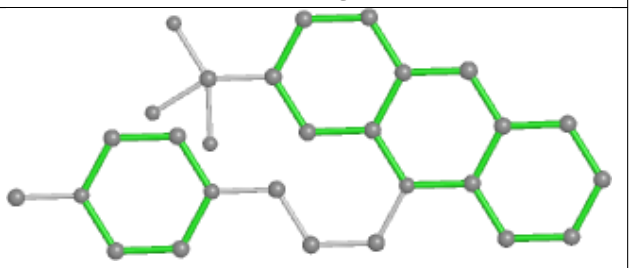
Bond lengths



Bond angles

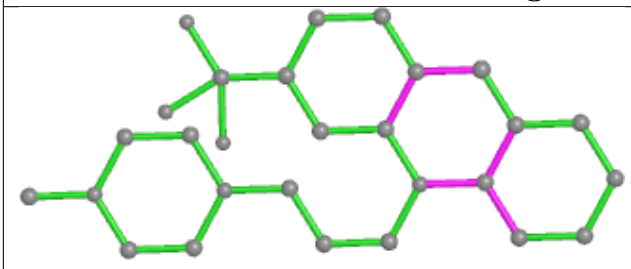


Torsions



Rings

Ligand TFP B 201



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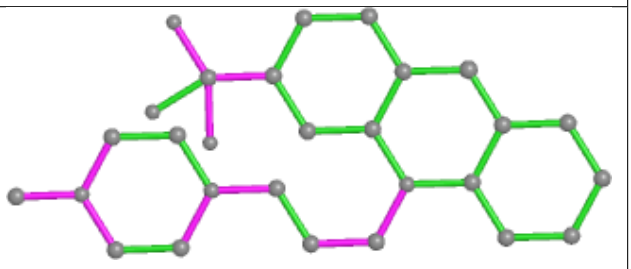
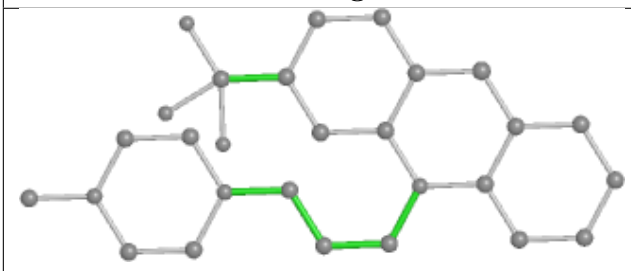


Bond angles



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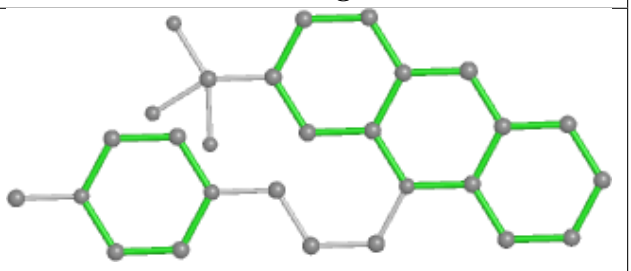

Rings

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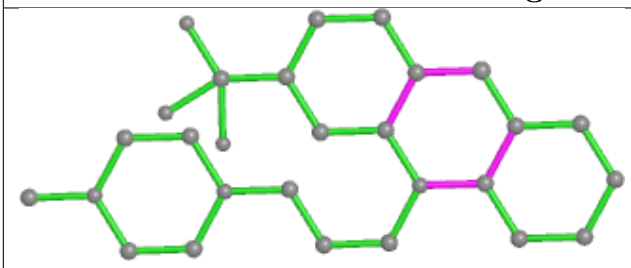
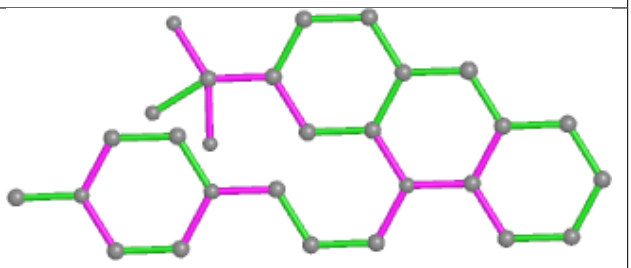
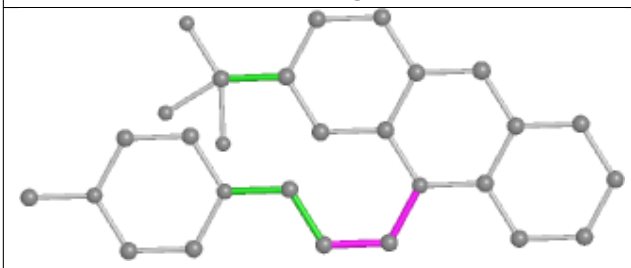


Bond lengths



Bond angles



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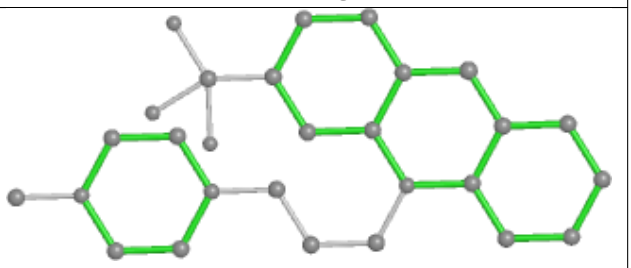
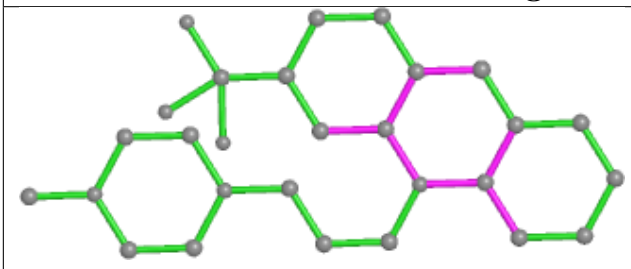


Rings

Ligand TFP A 202



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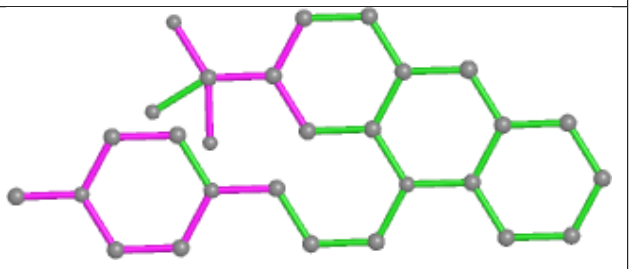
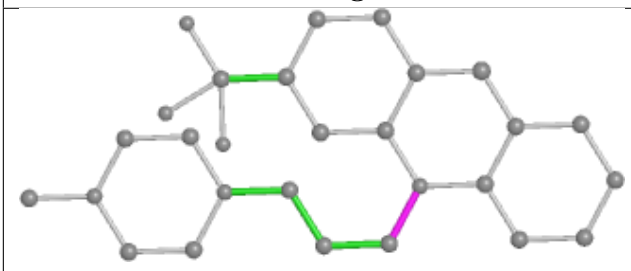


Bond angles



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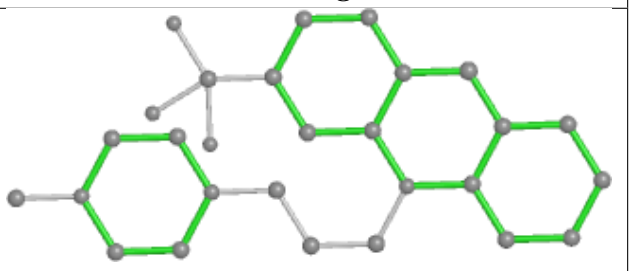
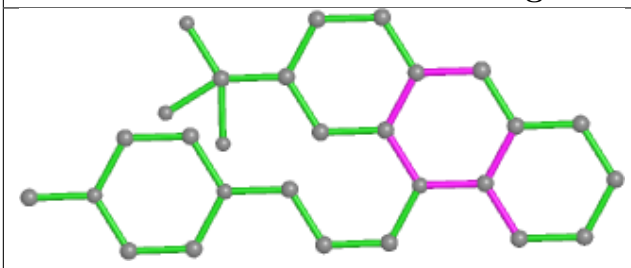


Rings

Ligand TFP C 206



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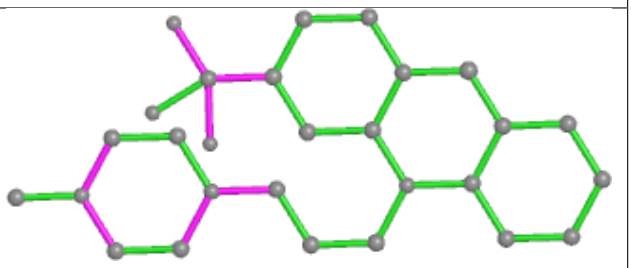
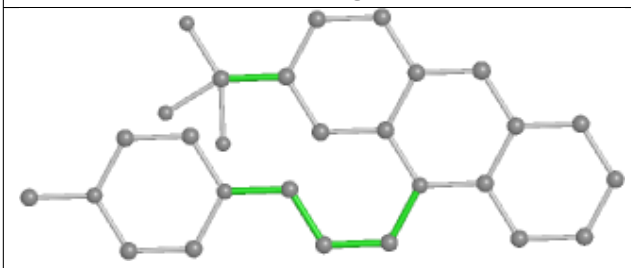


Bond angles



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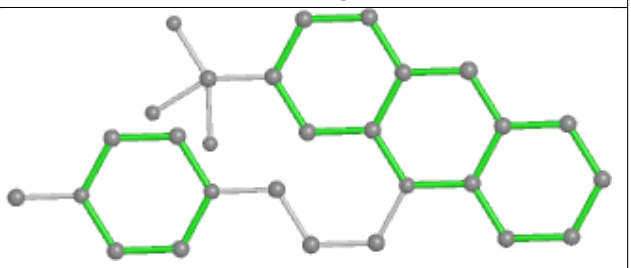
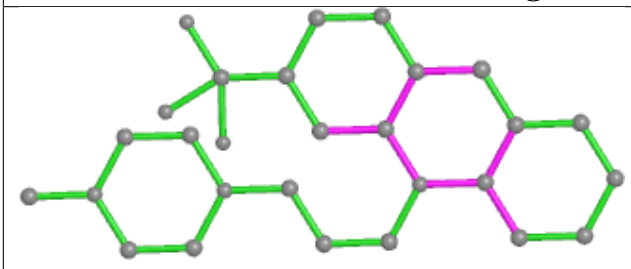


Rings

Ligand TFP D 207



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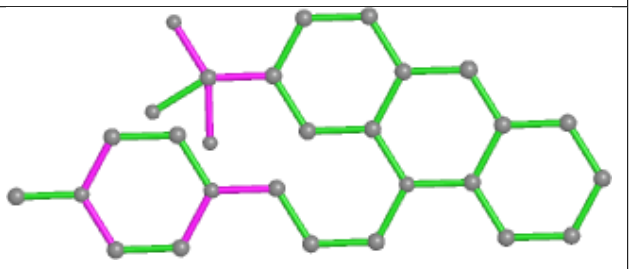
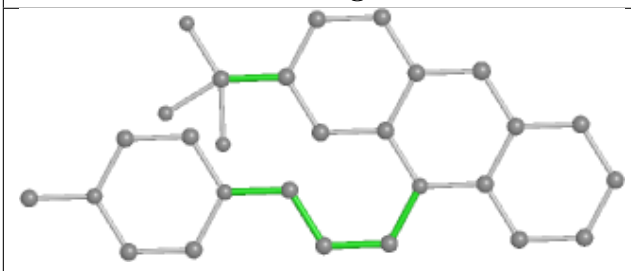


Bond angles



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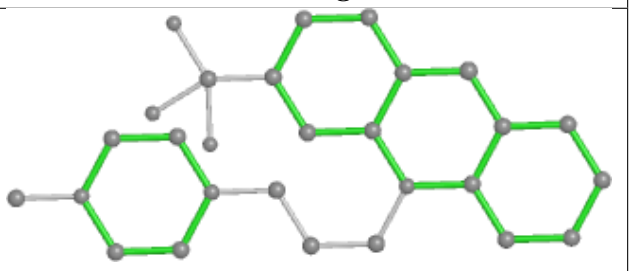
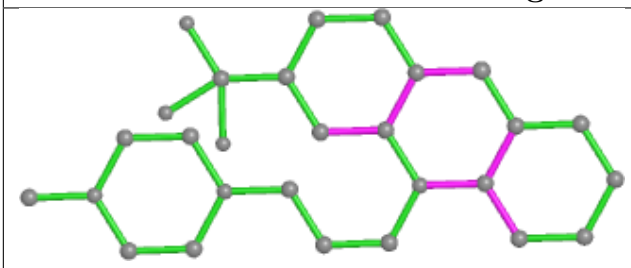
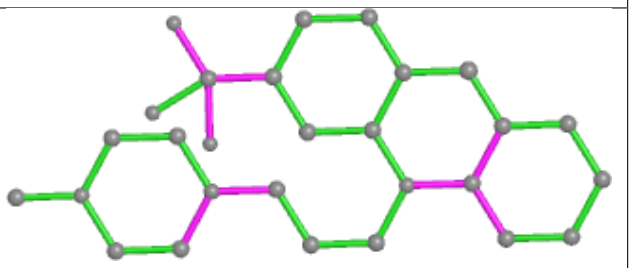


Rings

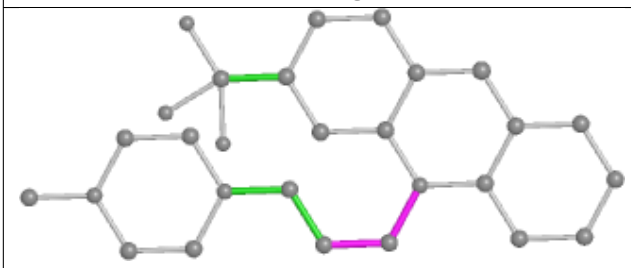
Ligand TFP E 212



Bond lengths



Bond angles



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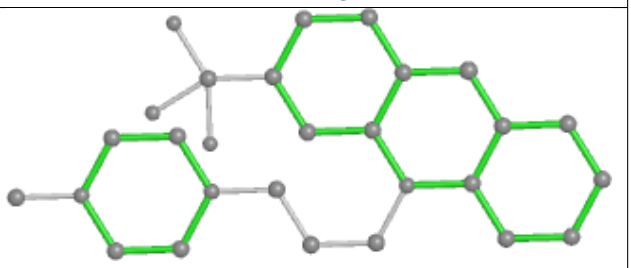
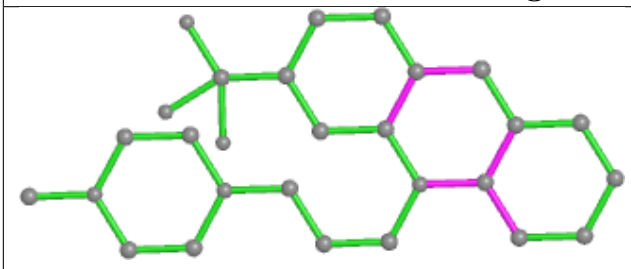


Rings

Ligand TFP C 208



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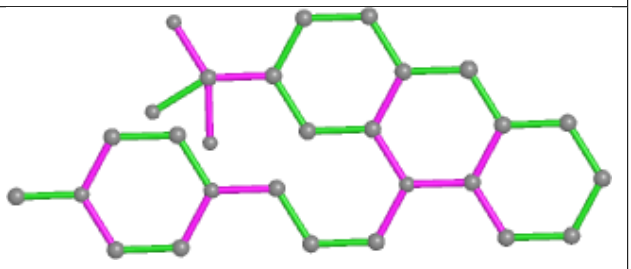
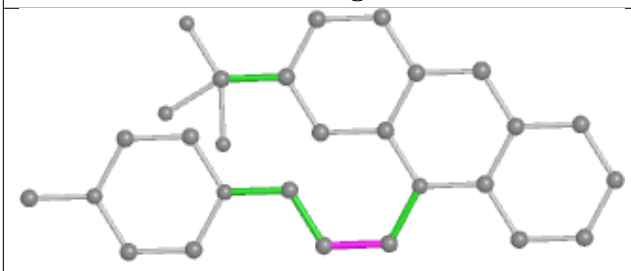


Bond angles



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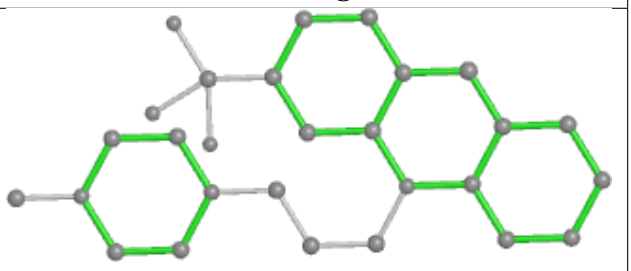
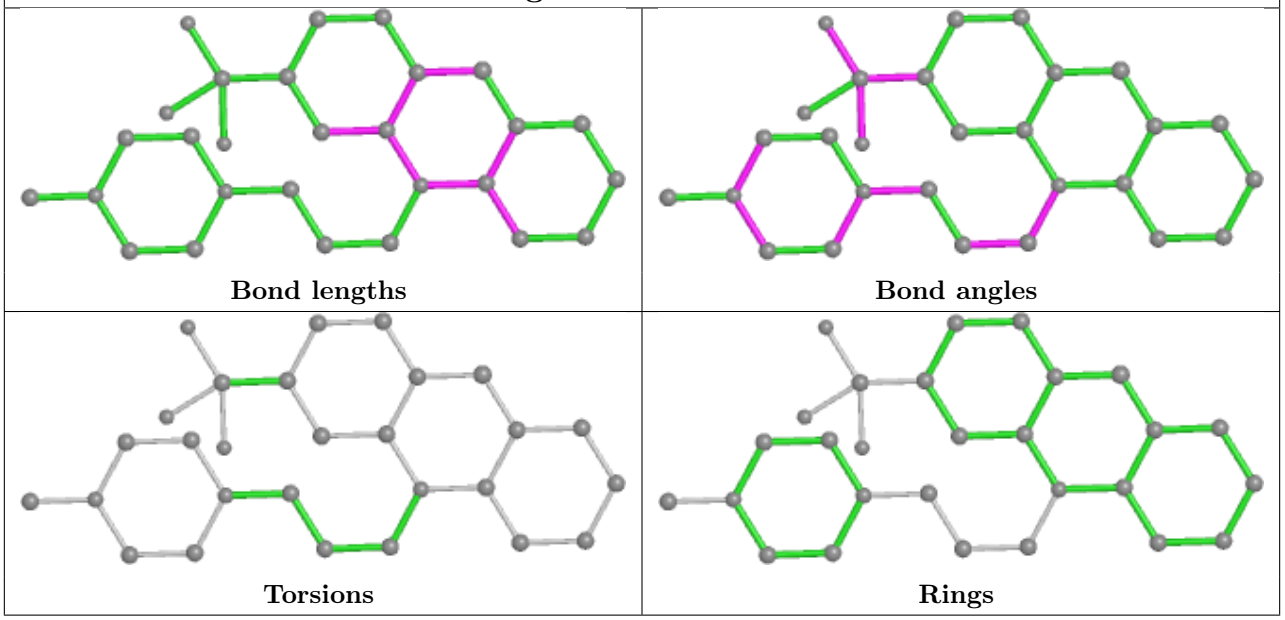
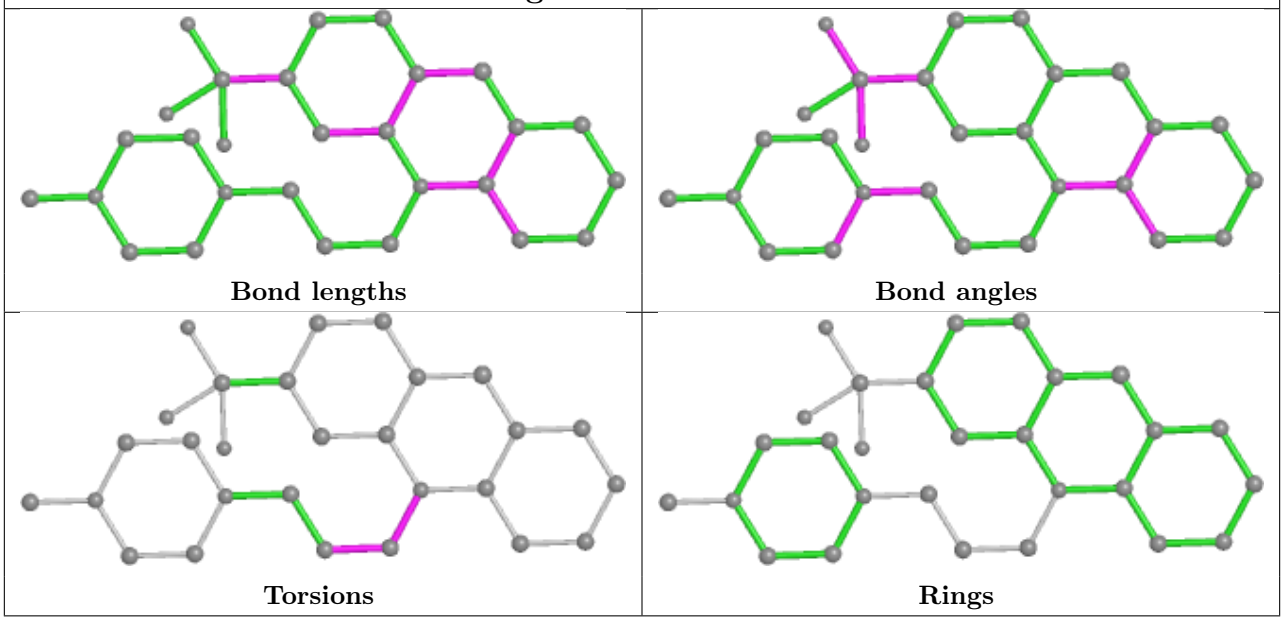


Rings

Ligand TFP D 205



Ligand TFP A 204



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	82/88 (93%)	-0.07	1 (1%) 79 76	23, 39, 67, 86	0
1	B	83/88 (94%)	-0.13	2 (2%) 59 53	22, 34, 67, 92	0
1	C	83/88 (94%)	0.02	1 (1%) 79 76	24, 49, 93, 99	0
1	D	82/88 (93%)	0.15	3 (3%) 41 34	29, 52, 76, 97	0
1	E	83/88 (94%)	-0.05	0 100 100	21, 38, 73, 93	0
1	F	82/88 (93%)	0.35	3 (3%) 41 34	32, 68, 89, 105	0
All	All	495/528 (93%)	0.04	10 (2%) 65 60	21, 45, 85, 105	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	85	MET	4.4
1	D	3	ASP	3.5
1	F	83	ARG	3.2
1	B	3	ASP	3.0
1	D	84	SER	2.8
1	D	4	ILE	2.5
1	C	9	VAL	2.4
1	F	3	ASP	2.3
1	F	27	PHE	2.1
1	A	85	MET	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

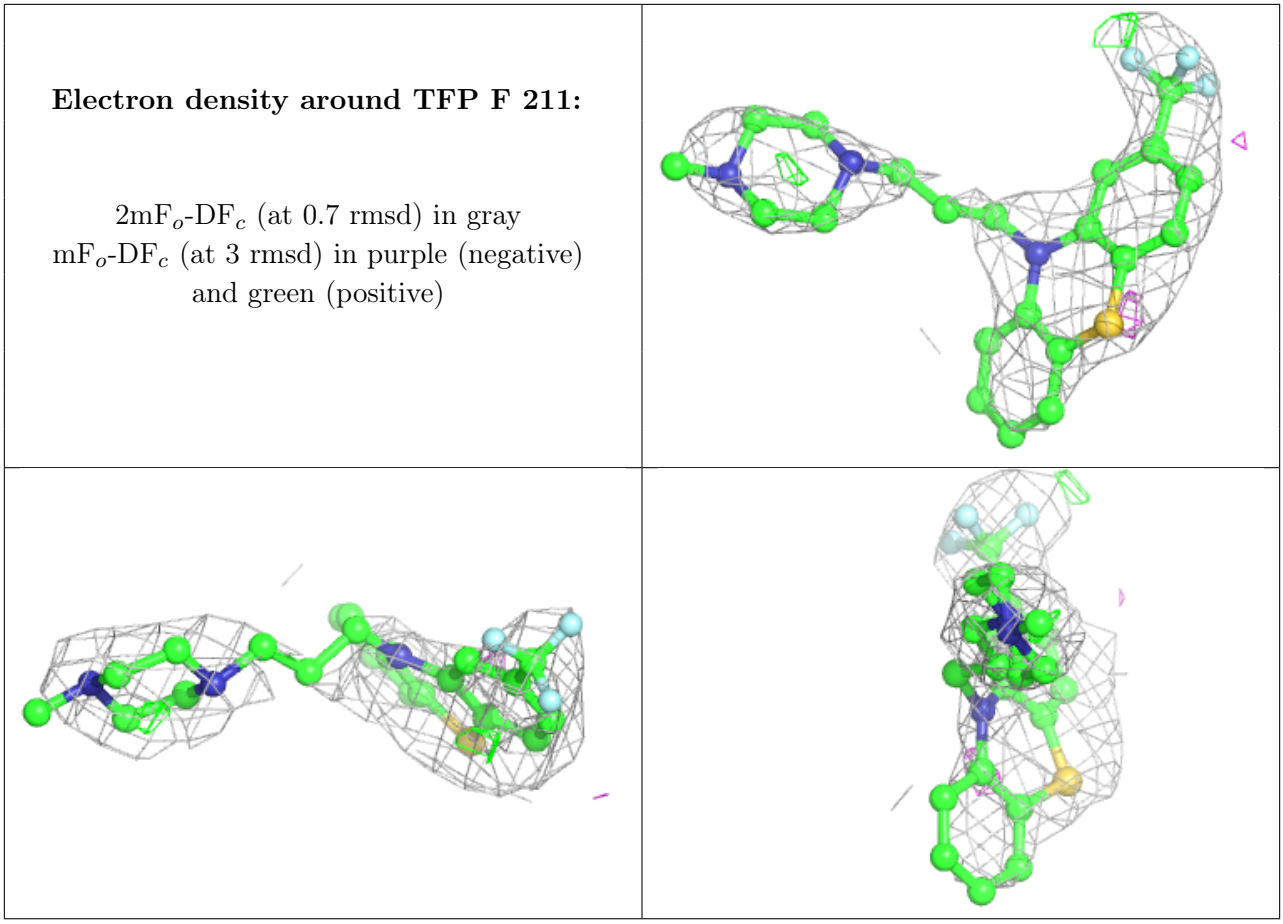
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	TFP	F	211	28/28	0.78	0.39	92,93,96,96	0
3	TFP	C	206	28/28	0.80	0.28	56,63,71,74	0
3	TFP	D	207	28/28	0.81	0.38	82,86,88,89	0
3	TFP	C	208	28/28	0.84	0.35	75,85,101,102	0
3	TFP	F	209	28/28	0.84	0.33	54,69,89,90	0
3	TFP	E	210	28/28	0.85	0.27	53,59,73,74	0
3	TFP	E	212	28/28	0.86	0.33	71,83,92,94	0
3	TFP	A	204	28/28	0.86	0.28	53,59,73,74	0
3	TFP	B	201	28/28	0.86	0.26	50,59,73,74	0
3	TFP	B	203	28/28	0.87	0.28	58,62,70,74	0
3	TFP	D	205	28/28	0.87	0.38	73,81,96,96	0
3	TFP	A	202	28/28	0.88	0.21	41,51,64,64	0
2	CA	D	104	1/1	0.94	0.10	52,52,52,52	0
2	CA	F	106	1/1	0.94	0.10	57,57,57,57	0
2	CA	E	105	1/1	0.97	0.10	31,31,31,31	0
2	CA	C	103	1/1	0.97	0.08	48,48,48,48	0
2	CA	A	101	1/1	0.99	0.13	30,30,30,30	0
2	CA	B	102	1/1	0.99	0.14	24,24,24,24	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.

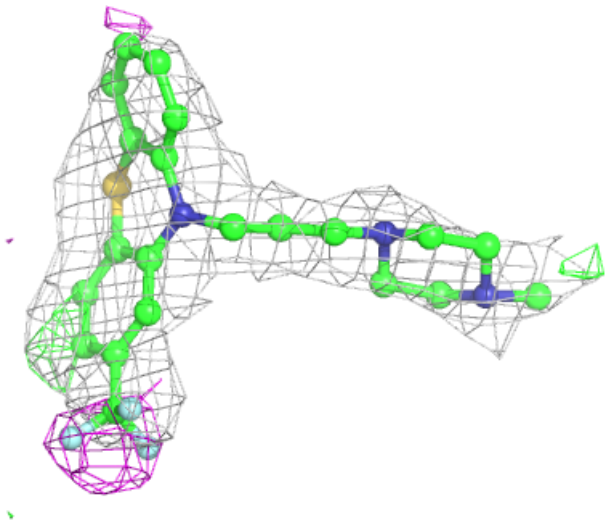
Electron density around TFP F 211:

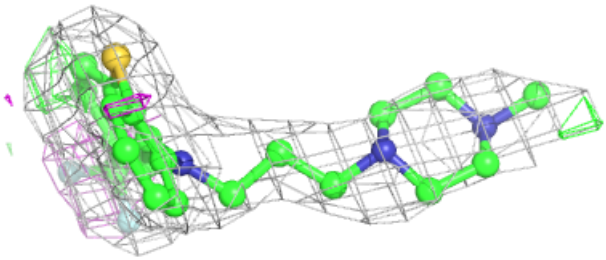
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

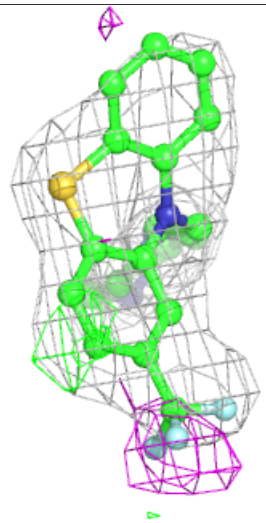


Electron density around TFP C 206:

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

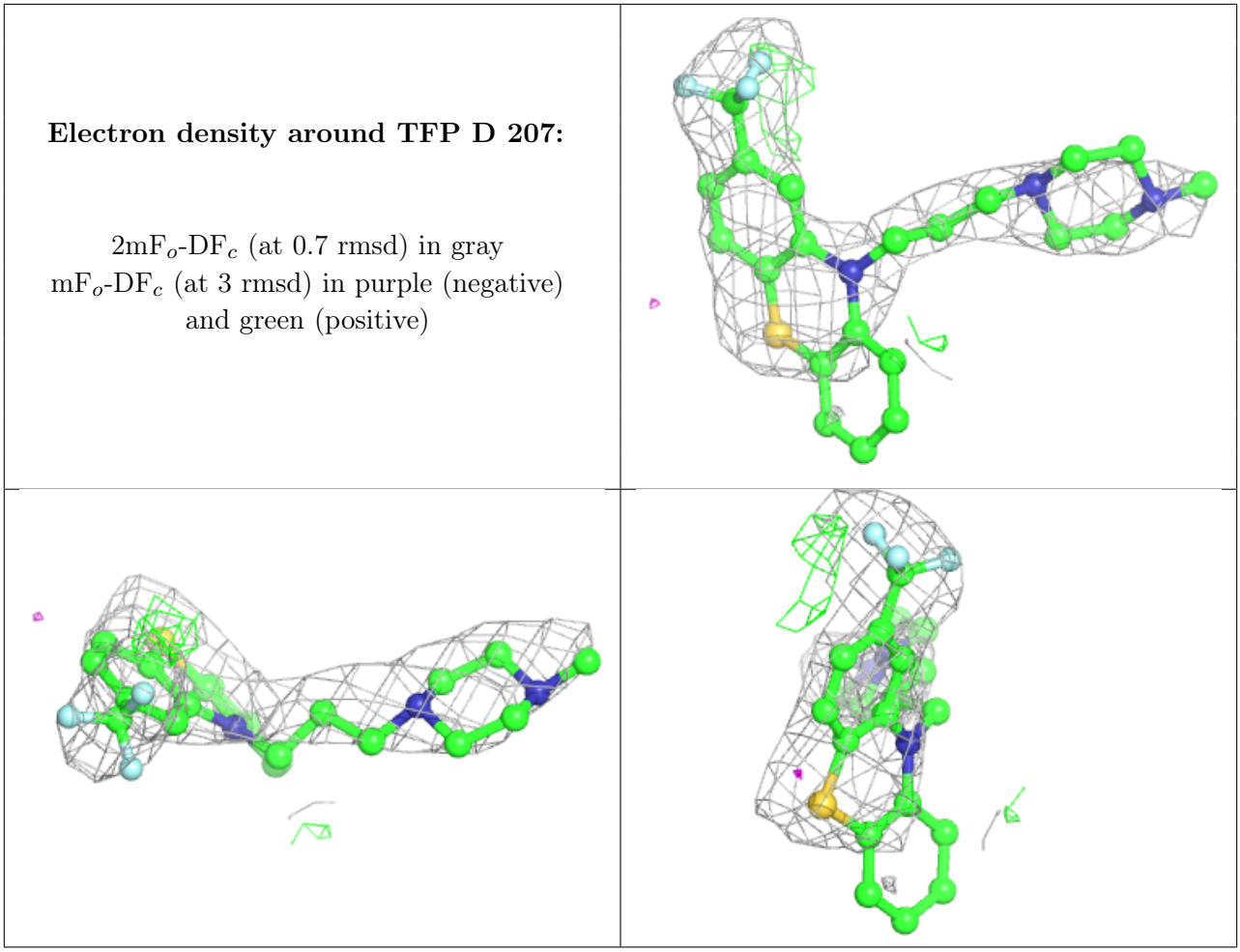






Electron density around TFP D 207:

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



Electron density around TFP C 208:

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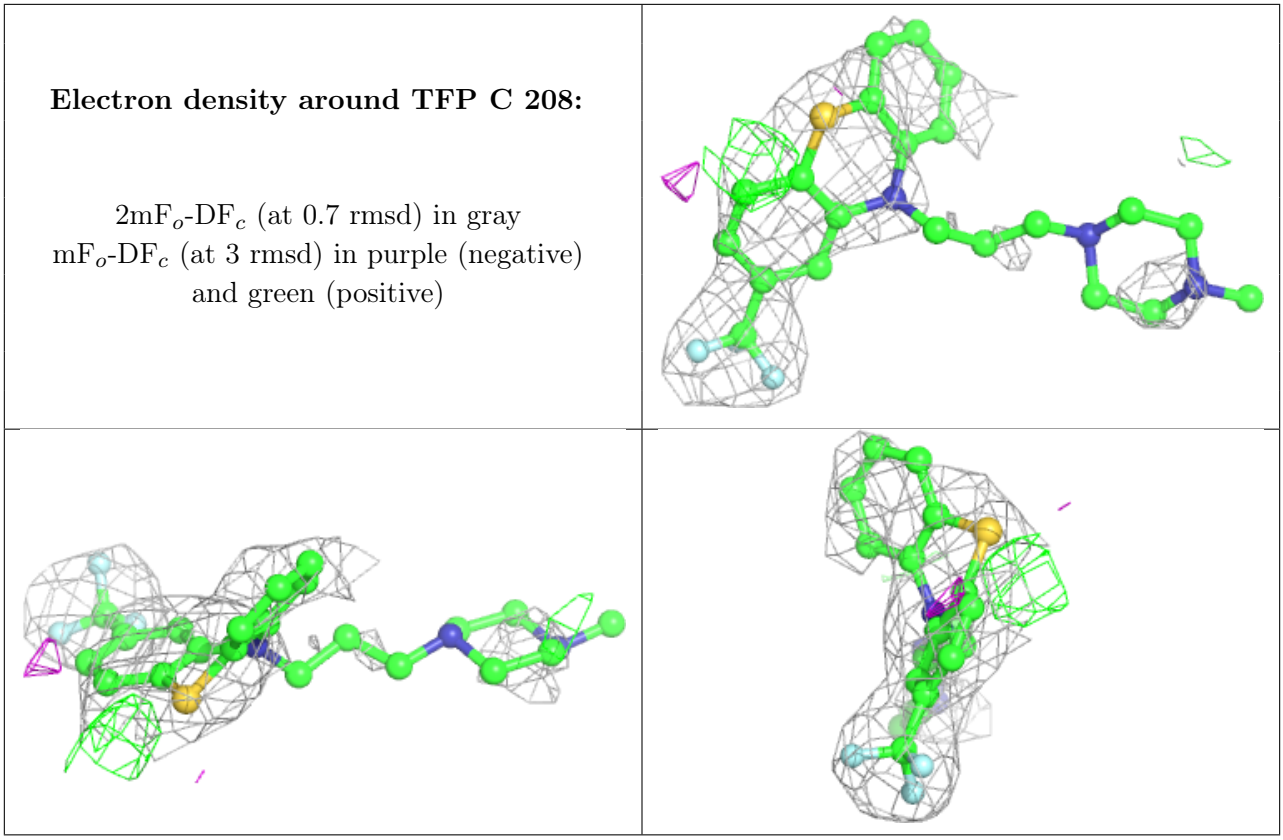
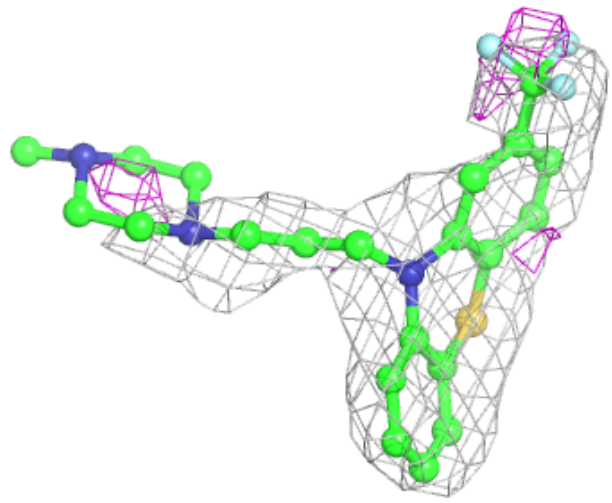
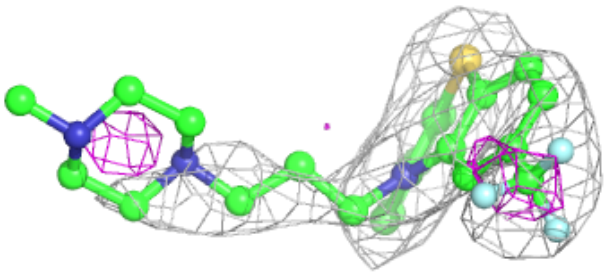
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

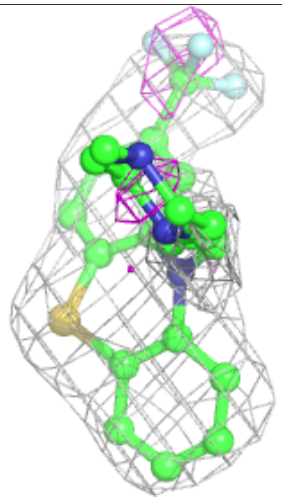


Electron density around TFP F 209:

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

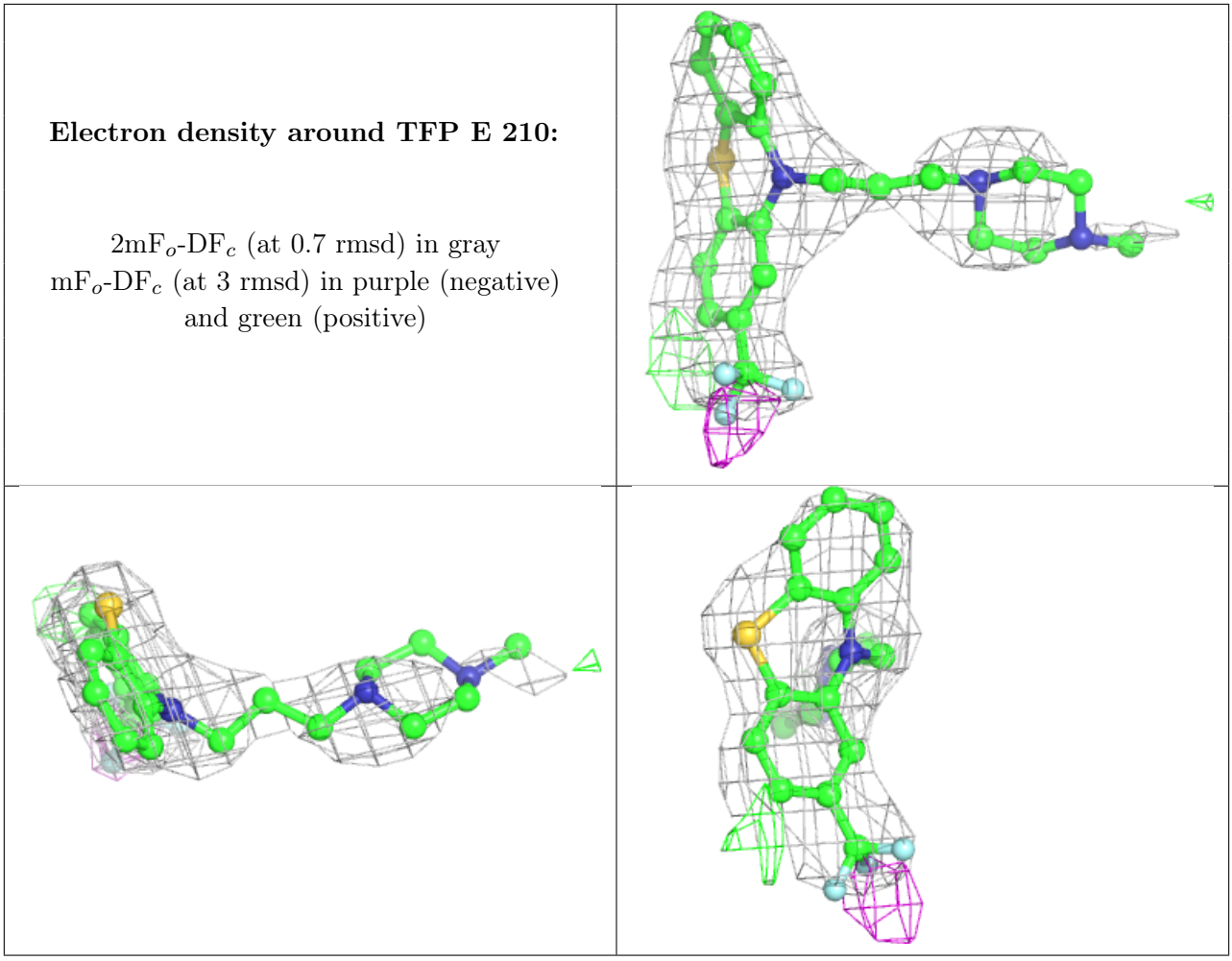






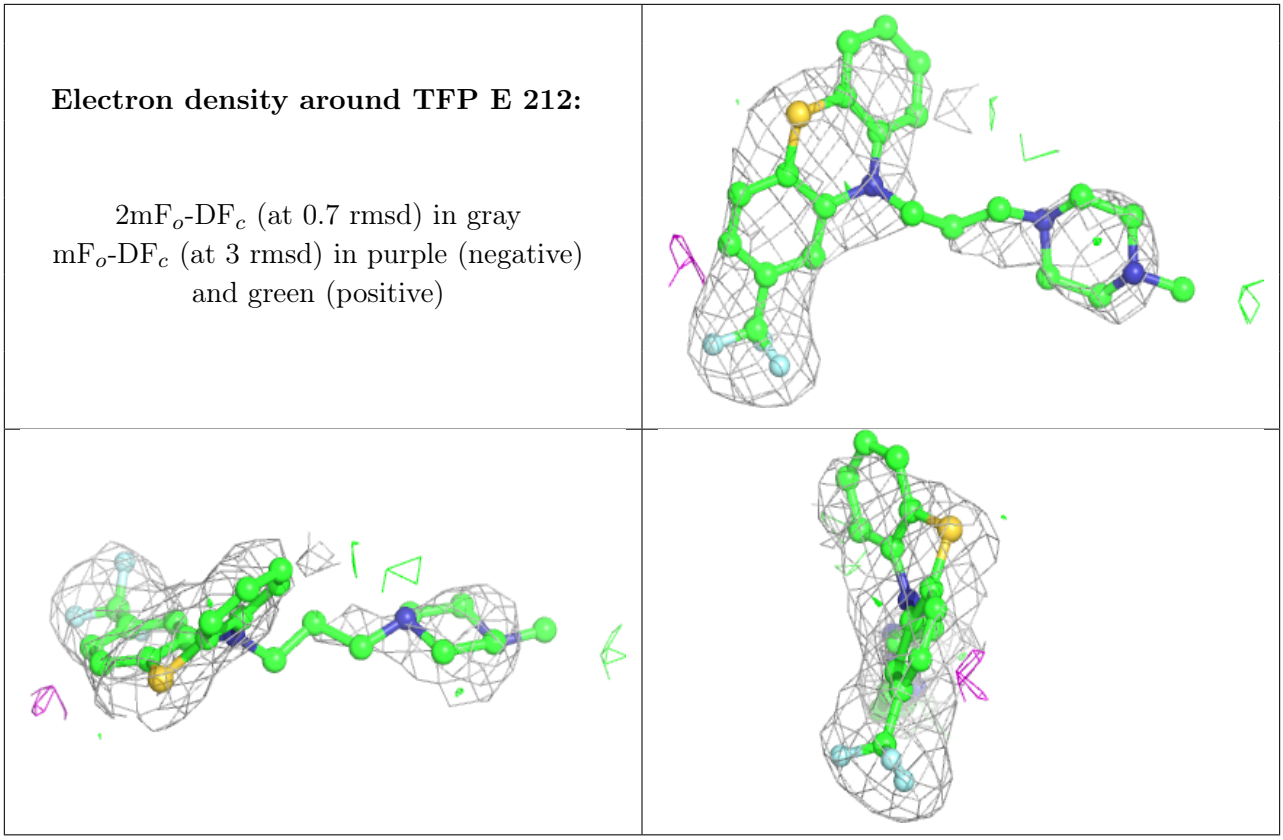
Electron density around TFP E 210:

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



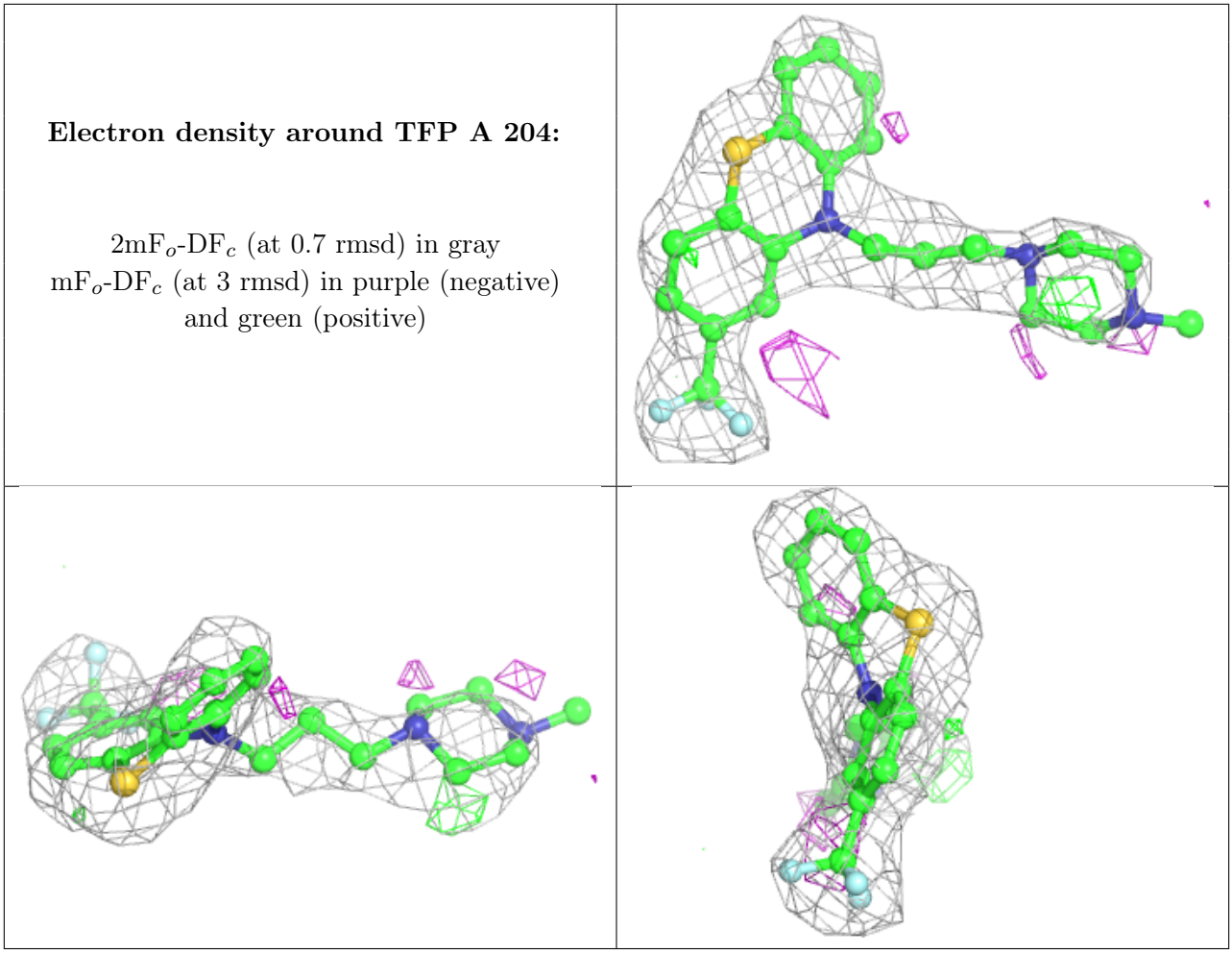
Electron density around TFP E 212:

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



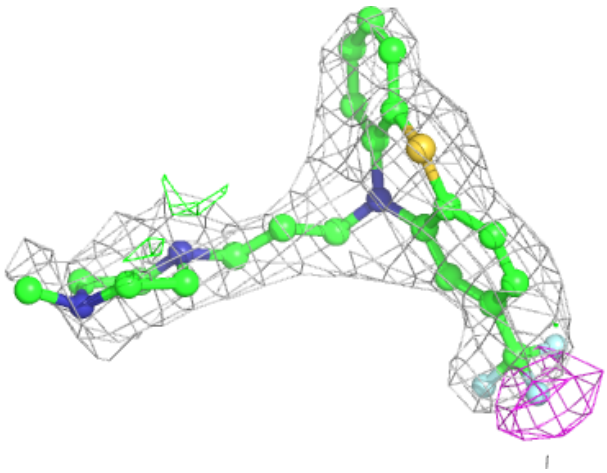
Electron density around TFP A 204:

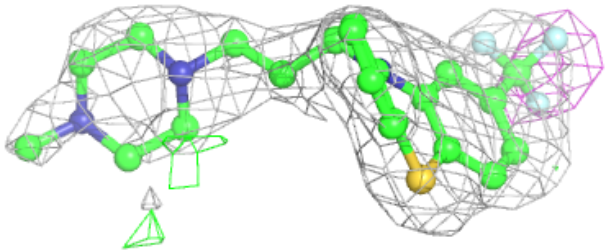
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

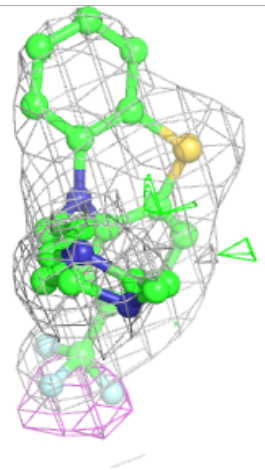


Electron density around TFP B 201:

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

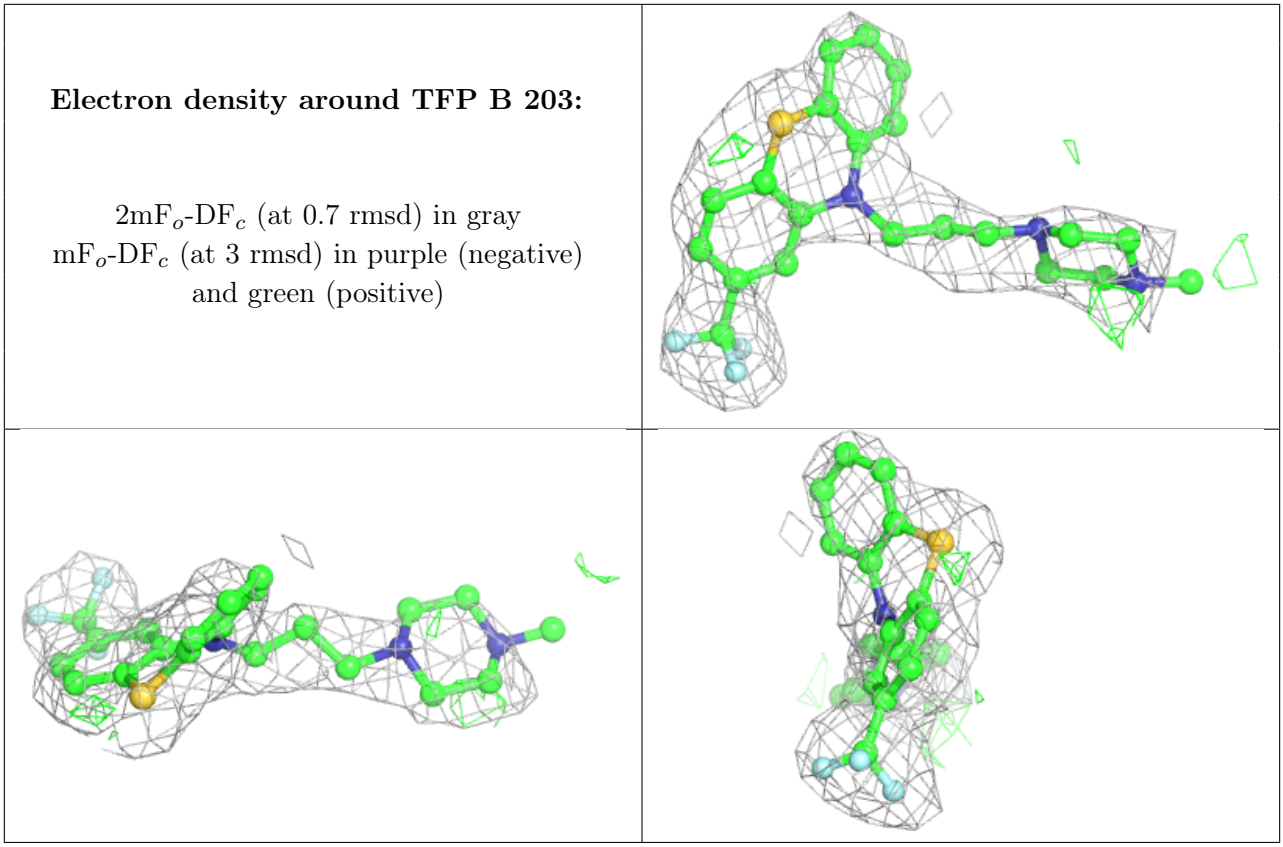






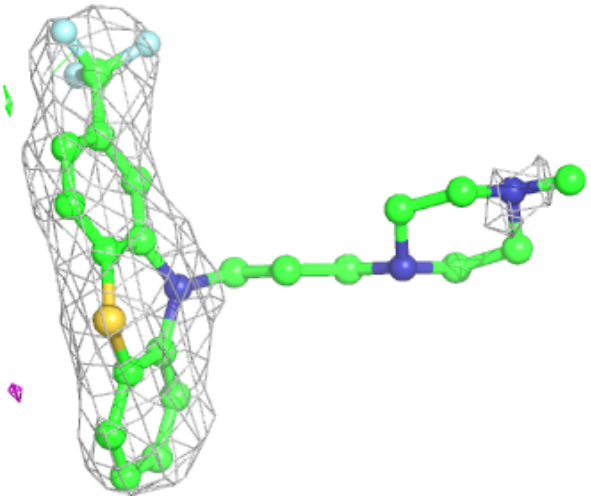
Electron density around TFP B 203:

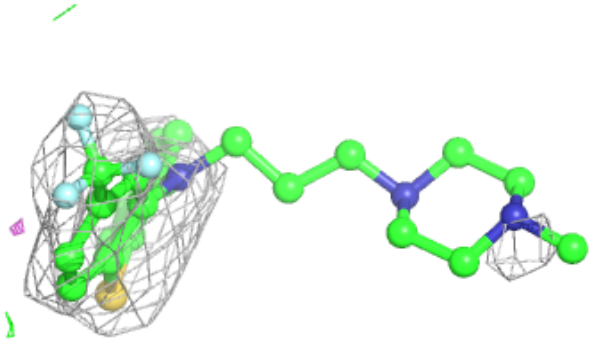
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

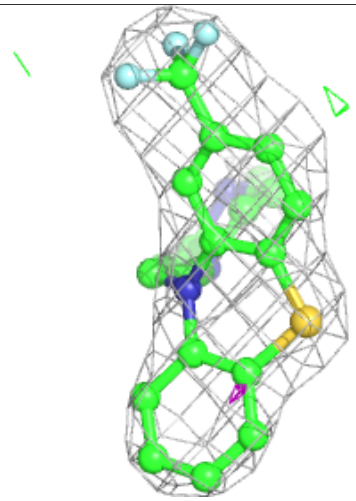


Electron density around TFP D 205:

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







Electron density around TFP A 202:

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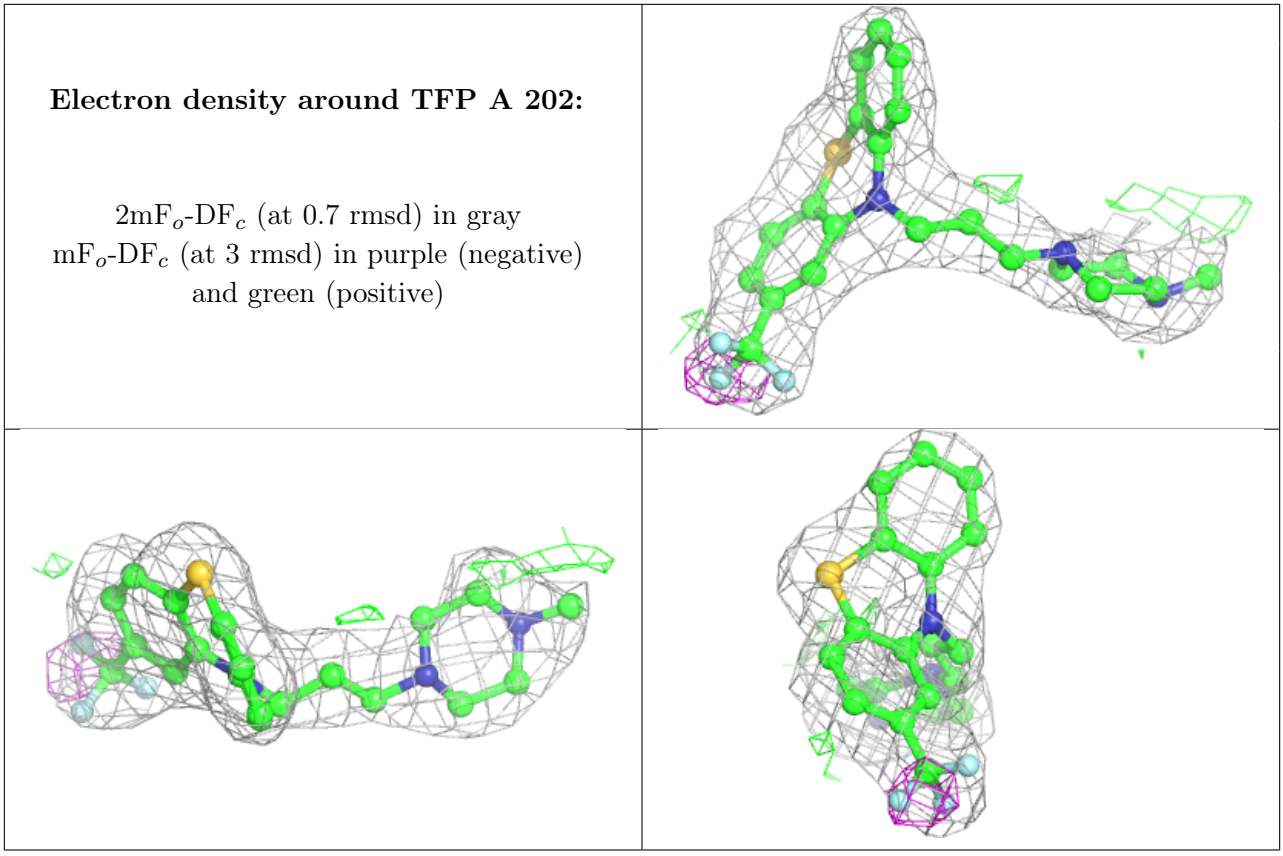
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.