



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2020 – 03:15 PM BST

PDB ID : 4CKU
Title : Three dimensional structure of plasmepsin II in complex with hydroxyethylamine-based inhibitor
Authors : Tars, K.; Leitans, J.; Jaudzems, K.
Deposited on : 2014-01-08
Resolution : 1.85 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 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 : 2.13
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) : 2.13

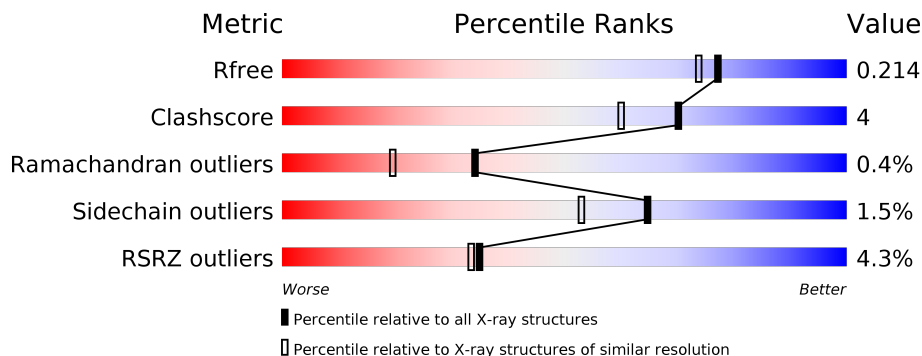
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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

Mol	Chain	Length	Quality of chain
1	A	329	
1	B	329	
1	C	329	
1	D	329	
1	E	329	
1	F	329	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 16812 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.

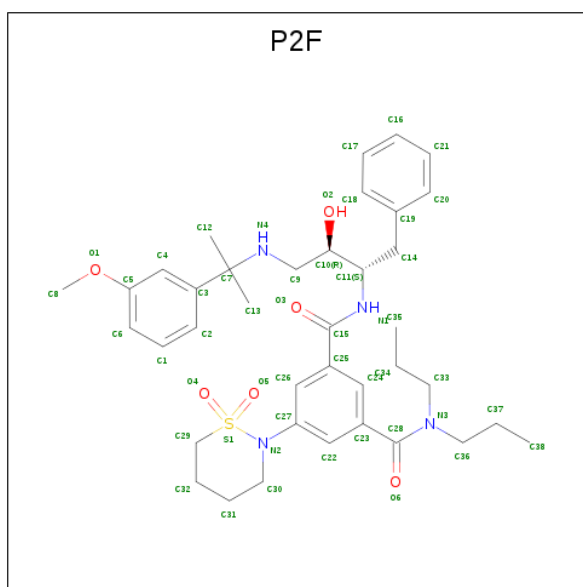
- Molecule 1 is a protein called PLASMEPSIN-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	323	2550	1656	395	489	10	0	0	0
1	B	327	2583	1678	401	494	10	0	1	0
1	C	322	2525	1635	392	488	10	0	0	0
1	D	323	2539	1641	396	492	10	0	0	0
1	E	322	2542	1646	394	492	10	0	1	0
1	F	329	2590	1680	401	499	10	0	3	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	205	SER	MET	conflict	UNP P46925
B	205	SER	MET	conflict	UNP P46925
C	205	SER	MET	conflict	UNP P46925
D	205	SER	MET	conflict	UNP P46925
E	205	SER	MET	conflict	UNP P46925
F	205	SER	MET	conflict	UNP P46925

- Molecule 2 is 5-[1,1-bis(oxidanylidene)-1,2-thiazinan-2-yl]-N3-[(2S,3R)-4-[2-(3-methoxyphenyl)propan-2-ylamino]-3-oxidanyl-1-phenyl-butan-2-yl]-N1,N1-dipropyl-benzene-1,3-dicarboxamide (three-letter code: P2F) (formula: C₃₈H₅₂N₄O₆S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			49	38	4	6	1		
2	B	1	Total	C	N	O	S	0	0
			49	38	4	6	1		
2	C	1	Total	C	N	O	S	0	0
			49	38	4	6	1		
2	D	1	Total	C	N	O	S	0	0
			49	38	4	6	1		
2	E	1	Total	C	N	O	S	0	0
			49	38	4	6	1		
2	F	1	Total	C	N	O	S	0	0
			49	38	4	6	1		

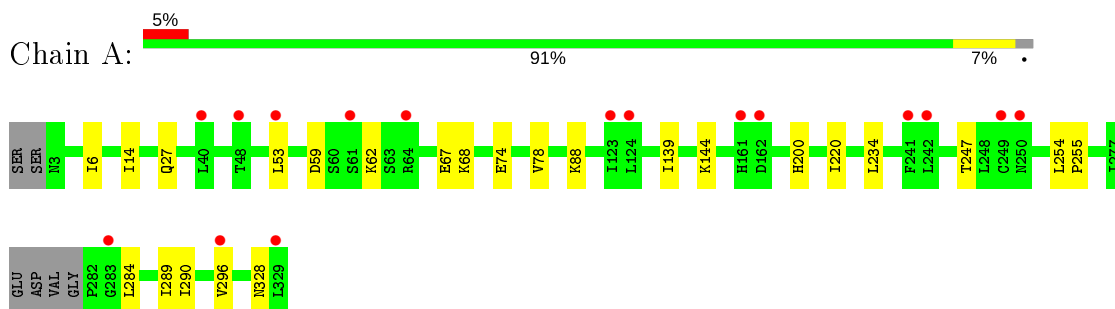
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	183	Total	O	0	0
			183	183		
3	B	217	Total	O	0	0
			217	217		
3	C	197	Total	O	0	0
			197	197		
3	D	216	Total	O	0	0
			216	216		
3	E	181	Total	O	0	0
			181	181		
3	F	195	Total	O	0	0
			195	195		

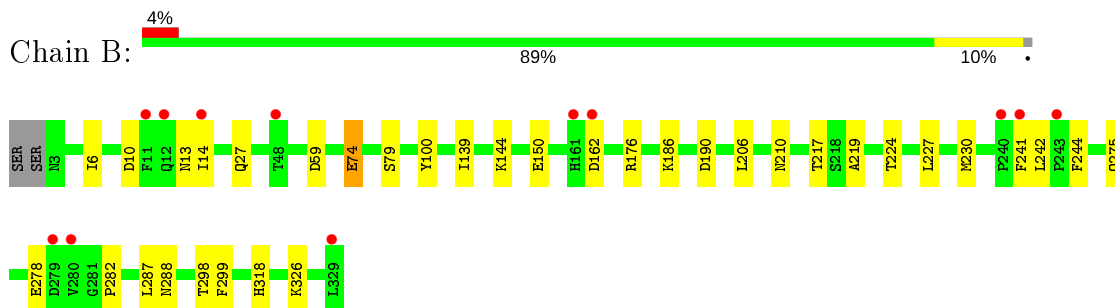
3 Residue-property plots [i](#)

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.

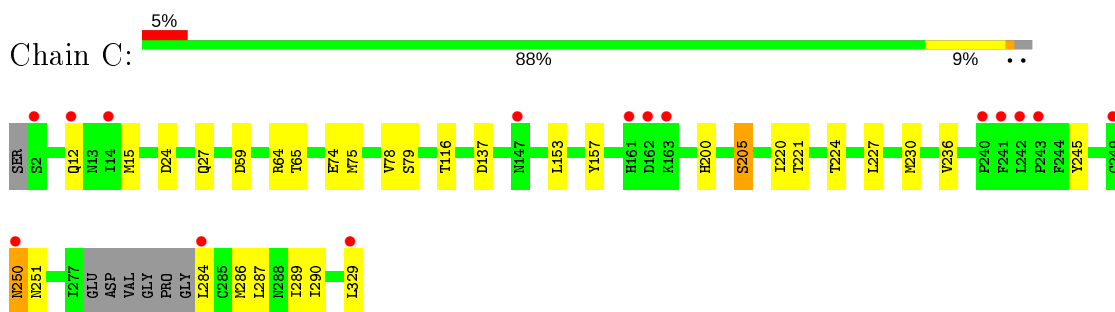
- Molecule 1: PLASMEPSIN-2



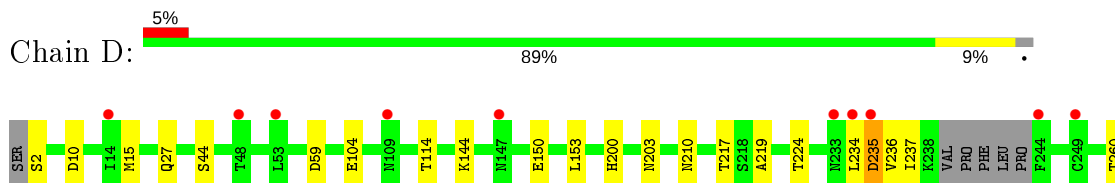
- Molecule 1: PLASMEPSIN-2

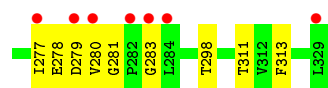


- Molecule 1: PLASMEPSIN-2

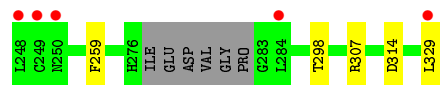
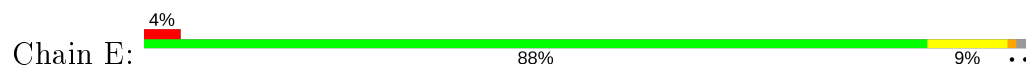


- Molecule 1: PLASMEPSIN-2

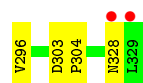
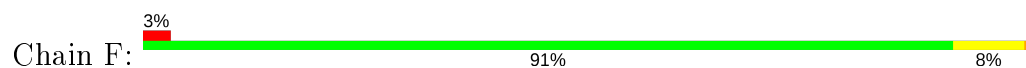




- Molecule 1: PLASMEPSIN-2



- Molecule 1: PLASMEPSIN-2



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	201.95Å 115.25Å 93.17Å 90.00° 110.75° 90.00°	Depositor
Resolution (Å)	29.98 – 1.85 29.98 – 1.85	Depositor EDS
% Data completeness (in resolution range)	97.9 (29.98-1.85) 97.9 (29.98-1.85)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 1.85Å)	Xtrriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.158 , 0.209 0.168 , 0.214	Depositor DCC
R_{free} test set	8325 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	18.7	Xtrriage
Anisotropy	0.049	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 54.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16812	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: P2F

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	0.89	0/2616	0.90	0/3561
1	B	0.93	0/2653	0.91	1/3613 (0.0%)
1	C	0.91	0/2588	0.92	1/3526 (0.0%)
1	D	0.89	0/2601	0.91	0/3538
1	E	0.96	0/2609	0.97	6/3553 (0.2%)
1	F	0.95	1/2665 (0.0%)	0.95	3/3632 (0.1%)
All	All	0.92	1/15732 (0.0%)	0.93	11/21423 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	104	GLU	CD-OE2	-5.66	1.19	1.25

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	19	ASP	CB-CG-OD1	7.02	124.62	118.30
1	E	307	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	E	314	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	B	190	ASP	CB-CG-OD2	-5.74	113.14	118.30
1	E	198	ASP	CB-CG-OD1	5.63	123.37	118.30
1	F	153	LEU	CA-CB-CG	5.48	127.90	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	190	ASP	CB-CG-OD1	5.39	123.15	118.30
1	E	190	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	E	64	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	C	75	MET	CG-SD-CE	5.16	108.45	100.20
1	F	64	ARG	NE-CZ-NH1	5.09	122.84	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	201	VAL	Peptide
1	F	31	PHE	Peptide

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	2550	0	2467	16	0
1	B	2583	0	2509	24	0
1	C	2525	0	2430	21	0
1	D	2539	0	2452	21	0
1	E	2542	0	2452	17	0
1	F	2590	0	2511	16	0
2	A	49	0	52	3	0
2	B	49	0	52	1	0
2	C	49	0	52	3	0
2	D	49	0	52	3	0
2	E	49	0	52	0	0
2	F	49	0	52	3	0
3	A	183	0	0	9	0
3	B	217	0	0	4	0
3	C	197	0	0	1	0
3	D	216	0	0	3	0
3	E	181	0	0	0	0
3	F	195	0	0	2	0
All	All	16812	0	15133	111	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 4.

All (111) 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:F:27:GLN:HE22	1:F:59:ASP:H	1.09	0.98
1:C:27:GLN:HE22	1:C:59:ASP:H	1.17	0.91
1:E:27:GLN:HE22	1:E:59:ASP:H	1.20	0.88
1:B:144:LYS:HE3	3:B:2212:HOH:O	1.76	0.85
1:A:200:HIS:HD2	3:A:2128:HOH:O	1.60	0.84
1:D:224:THR:HG21	1:E:74:GLU:HG2	1.60	0.83
1:B:27:GLN:HE22	1:B:59:ASP:H	1.27	0.81
1:D:27:GLN:HE22	1:D:59:ASP:H	1.24	0.81
1:F:218:SER:O	1:F:288:ASN:ND2	2.21	0.72
1:B:74:GLU:HG2	1:C:224:THR:HG21	1.70	0.72
1:A:27:GLN:HE22	1:A:59:ASP:H	1.37	0.71
1:F:292:LEU:HD21	2:F:400:P2F:H83C	1.73	0.69
1:E:6:ILE:HD11	1:E:93[A]:VAL:HG12	1.74	0.69
1:C:64:ARG:HD2	3:C:2021:HOH:O	1.94	0.67
1:E:6:ILE:CD1	1:E:93[A]:VAL:HG12	2.25	0.66
2:A:400:P2F:C32	3:A:2183:HOH:O	2.46	0.64
1:D:15:MET:HG2	2:D:400:P2F:H351	1.79	0.63
1:D:144:LYS:HE3	1:D:150:GLU:O	1.99	0.63
1:F:11:PHE:O	1:F:14:ILE:HG22	1.99	0.63
1:D:236:VAL:C	1:D:237:ILE:HD13	2.19	0.62
1:A:14:ILE:HG22	2:A:400:P2F:H351	1.81	0.61
1:C:15:MET:HG2	2:C:400:P2F:H351	1.83	0.60
1:A:6:ILE:N	1:A:6:ILE:HD12	2.16	0.59
1:C:236:VAL:CG1	1:C:245:TYR:HB3	2.33	0.58
2:A:400:P2F:H321	3:A:2183:HOH:O	2.02	0.58
1:C:78:VAL:HG21	2:C:400:P2F:H82C	1.86	0.57
1:A:200:HIS:CD2	3:A:2128:HOH:O	2.46	0.55
1:F:1:SER:HB3	3:F:2003:HOH:O	2.06	0.55
3:B:2165:HOH:O	1:C:74:GLU:HG3	2.07	0.54
1:D:200:HIS:CD2	3:D:2155:HOH:O	2.59	0.54
1:B:144:LYS:CE	3:B:2212:HOH:O	2.44	0.54
1:E:226:PHE:O	1:E:230:MET:HG2	2.09	0.52
3:B:2165:HOH:O	1:C:74:GLU:CG	2.58	0.52
1:E:44:SER:HB2	1:E:104:GLU:HG2	1.90	0.52
1:D:44:SER:HB2	1:D:104:GLU:HG2	1.92	0.51
1:B:6:ILE:N	1:B:6:ILE:HD12	2.26	0.50
1:B:74:GLU:HG3	1:B:74:GLU:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:239:VAL:HG12	1:E:242:LEU:HD12	1.94	0.50
1:F:222:VAL:CG2	1:F:227:LEU:HB2	2.42	0.49
1:B:176:ARG:O	1:B:326:LYS:HD2	2.12	0.49
1:C:227:LEU:HA	1:C:230:MET:HG2	1.95	0.49
1:A:67:GLU:HB2	1:A:88:LYS:HB3	1.95	0.48
1:C:78:VAL:CG2	2:C:400:P2F:H82C	2.42	0.48
1:D:278:GLU:OE2	1:D:283:GLY:N	2.45	0.48
1:E:106:ILE:O	1:E:106:ILE:HG22	2.12	0.47
1:B:227:LEU:HA	1:B:230:MET:HG2	1.96	0.47
1:F:44:SER:HB2	1:F:104:GLU:HG3	1.96	0.47
1:B:278:GLU:OE1	1:B:282:PRO:HA	2.14	0.47
1:D:277:ILE:O	1:D:280:VAL:HG22	2.15	0.47
1:F:1:SER:CB	3:F:2003:HOH:O	2.61	0.47
1:A:74:GLU:HG2	1:F:224:THR:HG21	1.97	0.46
1:E:100:TYR:CZ	1:E:139:ILE:HG13	2.50	0.46
1:C:200:HIS:CD2	1:C:205:SER:HB2	2.51	0.46
1:F:11:PHE:O	1:F:14:ILE:CG2	2.64	0.46
1:A:234:LEU:CD1	1:A:255:PRO:HD3	2.46	0.45
1:B:74:GLU:HG2	1:C:224:THR:CG2	2.44	0.45
1:D:210:ASN:O	1:D:298:THR:HA	2.17	0.45
1:E:236:VAL:CG1	1:E:245:TYR:HB3	2.46	0.45
1:C:287:LEU:N	1:C:287:LEU:HD12	2.31	0.45
1:C:24:ASP:HB3	1:C:65:THR:OG1	2.16	0.45
1:D:234:LEU:O	1:D:235:ASP:HB2	2.16	0.45
1:F:64:ARG:NE	1:F:64:ARG:HA	2.32	0.45
1:F:240:PRO:O	1:F:242:LEU:HD12	2.16	0.45
1:B:186:LYS:HD3	1:B:318:HIS:O	2.17	0.45
1:A:6:ILE:N	1:A:6:ILE:CD1	2.80	0.45
1:B:144:LYS:NZ	1:B:150:GLU:O	2.45	0.45
1:B:206:LEU:HD23	1:B:299:PHE:HE1	1.82	0.45
1:D:278:GLU:HA	1:D:281:GLY:O	2.17	0.44
1:A:296:VAL:HG22	3:A:2170:HOH:O	2.17	0.44
1:B:100:TYR:CZ	1:B:139:ILE:HG22	2.52	0.44
1:E:210:ASN:O	1:E:298:THR:HA	2.17	0.44
1:A:220:ILE:O	1:A:289:ILE:HA	2.18	0.44
1:B:287:LEU:HD12	1:B:287:LEU:N	2.33	0.44
1:B:217:THR:HG22	1:B:219:ALA:H	1.82	0.44
1:D:217:THR:HG22	1:D:219:ALA:H	1.83	0.44
1:B:224:THR:HG21	1:C:74:GLU:HG3	2.00	0.43
1:E:329:LEU:HD12	1:E:329:LEU:HA	1.87	0.43
1:C:250:ASN:C	1:C:250:ASN:ND2	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:THR:HG21	1:A:254:LEU:HD11	2.01	0.43
1:C:221:THR:HA	1:C:290:ILE:O	2.19	0.42
1:D:114:THR:HG23	2:D:400:P2F:H381	2.00	0.42
1:F:290:ILE:HG13	2:F:400:P2F:H322	2.01	0.42
1:A:53:LEU:HB2	3:A:2041:HOH:O	2.17	0.42
1:D:153:LEU:C	1:D:153:LEU:HD12	2.40	0.42
1:E:240:PRO:O	1:E:241:PHE:CB	2.67	0.42
1:F:303:ASP:N	1:F:304:PRO:CD	2.82	0.42
1:D:203:ASN:HB2	3:D:2159:HOH:O	2.20	0.42
1:B:14:ILE:HG22	2:B:400:P2F:H351	2.01	0.42
1:B:210:ASN:O	1:B:298:THR:HA	2.20	0.42
1:C:153:LEU:C	1:C:153:LEU:HD12	2.40	0.42
1:B:241:PHE:C	1:B:242:LEU:HD12	2.41	0.41
1:C:157:TYR:CZ	1:C:329:LEU:HD13	2.55	0.41
1:D:236:VAL:O	1:D:237:ILE:HD13	2.20	0.41
1:D:311:THR:HG1	1:D:313:PHE:HE1	1.66	0.41
1:A:78:VAL:HG23	3:A:2059:HOH:O	2.21	0.41
1:D:144:LYS:CE	1:D:150:GLU:O	2.66	0.41
1:B:242:LEU:HD23	1:B:244:PHE:CD2	2.55	0.41
1:F:214:ASP:OD2	2:F:400:P2F:N4	2.54	0.41
1:D:260:THR:HG23	3:D:2155:HOH:O	2.20	0.41
1:B:10:ASP:OD1	1:B:13:ASN:HA	2.21	0.41
1:E:75:MET:O	1:E:81:THR:HA	2.21	0.41
1:B:288:ASN:HD22	1:B:288:ASN:HA	1.65	0.41
1:A:68:LYS:HD2	3:A:2050:HOH:O	2.20	0.40
1:C:220:ILE:O	1:C:289:ILE:HA	2.21	0.40
1:D:15:MET:HE2	2:D:400:P2F:H353	2.03	0.40
1:A:62:LYS:HE2	3:A:2045:HOH:O	2.21	0.40
1:B:100:TYR:CZ	1:B:139:ILE:CG2	3.04	0.40
1:E:198:ASP:O	1:E:259:PHE:HA	2.21	0.40
1:E:44:SER:HB2	1:E:104:GLU:CG	2.50	0.40
1:F:44:SER:HB2	1:F:104:GLU:CG	2.51	0.40
1:C:116:THR:HB	1:E:116:THR:HG23	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	319/329 (97%)	308 (97%)	11 (3%)	0	100	100
1	B	326/329 (99%)	315 (97%)	10 (3%)	1 (0%)	41	26
1	C	318/329 (97%)	307 (96%)	9 (3%)	2 (1%)	25	12
1	D	319/329 (97%)	309 (97%)	8 (2%)	2 (1%)	25	12
1	E	319/329 (97%)	313 (98%)	6 (2%)	0	100	100
1	F	330/329 (100%)	318 (96%)	10 (3%)	2 (1%)	25	12
All	All	1931/1974 (98%)	1870 (97%)	54 (3%)	7 (0%)	34	19

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	13	ASN
1	B	162	ASP
1	C	12	GLN
1	D	279	ASP
1	F	202	GLY
1	D	235	ASP
1	C	251	ASN

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	285/294 (97%)	280 (98%)	5 (2%)	59	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	289/294 (98%)	286 (99%)	3 (1%)	76	69
1	C	281/294 (96%)	275 (98%)	6 (2%)	53	38
1	D	283/294 (96%)	281 (99%)	2 (1%)	84	79
1	E	285/294 (97%)	281 (99%)	4 (1%)	67	55
1	F	290/294 (99%)	285 (98%)	5 (2%)	60	47
All	All	1713/1764 (97%)	1688 (98%)	25 (2%)	65	53

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	139	ILE
1	A	144	LYS
1	A	284	LEU
1	A	290	ILE
1	A	328	ASN
1	B	74	GLU
1	B	79	SER
1	B	275	GLN
1	C	79	SER
1	C	137	ASP
1	C	205	SER
1	C	250	ASN
1	C	284	LEU
1	C	286	MET
1	D	2	SER
1	D	10	ASP
1	E	15	MET
1	E	64	ARG
1	E	74	GLU
1	E	79	SER
1	F	15	MET
1	F	218	SER
1	F	233	ASN
1	F	296	VAL
1	F	328	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	27	GLN
1	A	76	ASN
1	A	146	GLN
1	A	200	HIS
1	A	233	ASN
1	B	27	GLN
1	B	146	GLN
1	B	275	GLN
1	B	288	ASN
1	C	27	GLN
1	C	146	GLN
1	C	200	HIS
1	C	232	GLN
1	C	250	ASN
1	D	3	ASN
1	D	27	GLN
1	D	146	GLN
1	D	200	HIS
1	E	27	GLN
1	E	146	GLN
1	E	228	ASN
1	E	288	ASN
1	F	3	ASN
1	F	27	GLN
1	F	146	GLN
1	F	147	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

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	P2F	E	400	-	50,52,52	1.54	6 (12%)	66,73,73	1.65	16 (24%)
2	P2F	C	400	-	50,52,52	1.75	7 (14%)	66,73,73	1.74	14 (21%)
2	P2F	B	400	-	50,52,52	1.38	4 (8%)	66,73,73	1.94	14 (21%)
2	P2F	F	400	-	50,52,52	1.57	4 (8%)	66,73,73	1.77	20 (30%)
2	P2F	D	400	-	50,52,52	1.39	3 (6%)	66,73,73	1.54	9 (13%)
2	P2F	A	400	-	50,52,52	1.62	5 (10%)	66,73,73	1.81	16 (24%)

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	P2F	E	400	-	-	6/48/62/62	0/4/4/4
2	P2F	C	400	-	-	9/48/62/62	0/4/4/4
2	P2F	B	400	-	-	10/48/62/62	0/4/4/4
2	P2F	F	400	-	-	7/48/62/62	0/4/4/4
2	P2F	D	400	-	-	7/48/62/62	0/4/4/4
2	P2F	A	400	-	-	8/48/62/62	0/4/4/4

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	400	P2F	C29-S1	-8.34	1.66	1.76
2	C	400	P2F	C29-S1	-8.31	1.66	1.76
2	A	400	P2F	C29-S1	-7.70	1.66	1.76
2	E	400	P2F	C29-S1	-7.03	1.67	1.76
2	B	400	P2F	C29-S1	-7.01	1.67	1.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	400	P2F	C29-S1	-6.30	1.68	1.76
2	A	400	P2F	C30-N2	-4.68	1.44	1.48
2	C	400	P2F	C27-N2	-4.11	1.39	1.44
2	C	400	P2F	C30-N2	-3.89	1.45	1.48
2	A	400	P2F	C27-N2	-3.86	1.39	1.44
2	E	400	P2F	C27-N2	-3.06	1.40	1.44
2	E	400	P2F	C30-N2	-2.85	1.46	1.48
2	E	400	P2F	C22-C23	-2.78	1.35	1.39
2	F	400	P2F	C30-N2	-2.57	1.46	1.48
2	C	400	P2F	C28-N3	2.55	1.40	1.34
2	B	400	P2F	C28-N3	2.45	1.40	1.34
2	C	400	P2F	C22-C23	-2.43	1.35	1.39
2	C	400	P2F	C26-C25	-2.30	1.36	1.39
2	D	400	P2F	C30-N2	-2.30	1.46	1.48
2	D	400	P2F	C11-N1	2.28	1.50	1.46
2	E	400	P2F	C15-N1	2.26	1.39	1.34
2	F	400	P2F	C27-N2	-2.25	1.41	1.44
2	E	400	P2F	C24-C25	-2.22	1.36	1.39
2	B	400	P2F	C15-N1	2.18	1.38	1.34
2	F	400	P2F	C22-C23	-2.18	1.36	1.39
2	C	400	P2F	O5-S1	2.17	1.45	1.43
2	B	400	P2F	C26-C27	2.12	1.43	1.39
2	A	400	P2F	C28-N3	2.11	1.39	1.34
2	A	400	P2F	C1-C2	2.00	1.43	1.38

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	P2F	O5-S1-O4	-6.92	109.09	118.36
2	C	400	P2F	O5-S1-O4	-6.22	110.02	118.36
2	B	400	P2F	C31-C30-N2	-6.08	102.43	111.76
2	B	400	P2F	C23-C28-N3	5.73	126.00	118.72
2	D	400	P2F	O5-S1-O4	-5.38	111.16	118.36
2	C	400	P2F	C31-C30-N2	-5.37	103.53	111.76
2	A	400	P2F	C31-C30-N2	-5.29	103.64	111.76
2	F	400	P2F	C8-O1-C5	4.90	128.15	117.51
2	F	400	P2F	O5-S1-O4	-4.81	111.92	118.36
2	E	400	P2F	C31-C30-N2	-4.72	104.53	111.76
2	C	400	P2F	C8-O1-C5	4.23	126.69	117.51
2	A	400	P2F	C23-C28-N3	4.17	124.01	118.72
2	D	400	P2F	C31-C30-N2	-4.11	105.45	111.76
2	A	400	P2F	C36-N3-C33	-3.69	108.23	116.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	400	P2F	O6-C28-C23	-3.65	113.13	120.23
2	B	400	P2F	C11-N1-C15	-3.56	116.54	123.01
2	A	400	P2F	O5-S1-O4	-3.55	113.61	118.36
2	A	400	P2F	C14-C11-N1	-3.54	104.91	110.07
2	D	400	P2F	C11-N1-C15	-3.53	116.58	123.01
2	B	400	P2F	C36-N3-C33	-3.46	108.75	116.69
2	A	400	P2F	C1-C2-C3	3.45	124.38	120.76
2	F	400	P2F	C9-N4-C7	-3.45	112.78	116.57
2	E	400	P2F	C13-C7-C12	3.34	113.55	109.55
2	F	400	P2F	C14-C11-N1	-3.32	105.23	110.07
2	A	400	P2F	C9-N4-C7	-3.29	112.95	116.57
2	D	400	P2F	C8-O1-C5	3.25	124.57	117.51
2	E	400	P2F	C8-O1-C5	3.19	124.44	117.51
2	B	400	P2F	O4-S1-C29	3.17	113.84	109.56
2	A	400	P2F	C33-N3-C28	-3.13	110.28	121.25
2	C	400	P2F	O4-S1-C29	3.03	113.65	109.56
2	F	400	P2F	C25-C26-C27	-3.00	116.17	119.59
2	E	400	P2F	O4-S1-C29	2.99	113.61	109.56
2	E	400	P2F	O5-S1-O4	-2.99	114.35	118.36
2	D	400	P2F	C33-N3-C28	-2.99	110.76	121.25
2	B	400	P2F	C33-N3-C28	-2.97	110.83	121.25
2	F	400	P2F	C36-N3-C28	-2.96	110.86	121.25
2	C	400	P2F	C23-C28-N3	2.91	122.42	118.72
2	F	400	P2F	C11-N1-C15	-2.90	117.74	123.01
2	A	400	P2F	C30-N2-C27	2.84	122.43	116.87
2	E	400	P2F	C36-N3-C28	-2.80	111.42	121.25
2	A	400	P2F	O5-S1-N2	-2.78	103.61	108.71
2	A	400	P2F	C11-N1-C15	-2.75	118.00	123.01
2	E	400	P2F	O5-S1-C29	-2.74	105.85	109.56
2	F	400	P2F	C26-C27-N2	2.68	124.53	119.31
2	D	400	P2F	C26-C27-N2	2.60	124.39	119.31
2	C	400	P2F	O4-S1-N2	2.60	113.48	108.71
2	A	400	P2F	C36-N3-C28	-2.56	112.27	121.25
2	E	400	P2F	C18-C19-C20	2.54	122.16	118.17
2	C	400	P2F	C14-C11-N1	-2.52	106.39	110.07
2	A	400	P2F	C19-C14-C11	-2.52	108.96	113.33
2	E	400	P2F	C11-N1-C15	-2.49	118.48	123.01
2	B	400	P2F	O6-C28-C23	-2.47	115.43	120.23
2	E	400	P2F	C33-N3-C28	-2.46	112.63	121.25
2	A	400	P2F	O6-C28-C23	-2.44	115.48	120.23
2	E	400	P2F	C26-C27-N2	2.43	124.05	119.31
2	E	400	P2F	C23-C28-N3	2.43	121.80	118.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	400	P2F	C32-C31-C30	2.42	115.87	111.19
2	E	400	P2F	C9-N4-C7	-2.41	113.92	116.57
2	C	400	P2F	C31-C32-C29	2.40	115.87	112.35
2	F	400	P2F	C31-C30-N2	-2.40	108.08	111.76
2	A	400	P2F	O4-S1-N2	2.40	113.11	108.71
2	C	400	P2F	C33-N3-C28	-2.38	112.88	121.25
2	D	400	P2F	C36-N3-C33	-2.36	111.28	116.69
2	D	400	P2F	C19-C14-C11	-2.33	109.30	113.33
2	F	400	P2F	C23-C22-C27	2.32	122.24	119.59
2	F	400	P2F	C33-N3-C28	-2.32	113.11	121.25
2	B	400	P2F	O5-S1-C29	-2.30	106.45	109.56
2	F	400	P2F	C22-C27-N2	-2.30	114.82	119.31
2	C	400	P2F	C1-C2-C3	2.28	123.16	120.76
2	B	400	P2F	O6-C28-N3	-2.28	118.56	122.34
2	B	400	P2F	C26-C27-N2	2.28	123.75	119.31
2	F	400	P2F	C14-C19-C18	-2.25	116.43	120.91
2	F	400	P2F	O5-S1-N2	-2.25	104.59	108.71
2	B	400	P2F	O5-S1-N2	2.23	112.81	108.71
2	E	400	P2F	O2-C10-C9	-2.21	105.23	109.69
2	C	400	P2F	C36-N3-C33	-2.21	111.62	116.69
2	B	400	P2F	C10-C9-N4	-2.20	107.72	110.74
2	E	400	P2F	C22-C27-N2	-2.20	115.02	119.31
2	B	400	P2F	C19-C14-C11	-2.18	109.54	113.33
2	F	400	P2F	C23-C28-N3	2.16	121.46	118.72
2	C	400	P2F	O2-C10-C9	-2.14	105.37	109.69
2	A	400	P2F	C6-C1-C2	-2.13	117.23	120.25
2	E	400	P2F	C17-C18-C19	-2.12	117.39	120.63
2	D	400	P2F	C5-C4-C3	2.12	122.92	120.14
2	F	400	P2F	C13-C7-C12	2.06	112.02	109.55
2	F	400	P2F	C17-C18-C19	-2.02	117.53	120.63
2	F	400	P2F	O2-C10-C9	-2.01	105.64	109.69
2	F	400	P2F	C26-C25-C24	2.00	122.04	119.63
2	F	400	P2F	O6-C28-C23	-2.00	116.33	120.23

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	400	P2F	C23-C28-N3-C36
2	E	400	P2F	O6-C28-N3-C36
2	B	400	P2F	C26-C27-N2-S1
2	B	400	P2F	C22-C27-N2-S1

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Mol	Chain	Res	Type	Atoms
2	B	400	P2F	C23-C28-N3-C33
2	B	400	P2F	O6-C28-N3-C33
2	F	400	P2F	C23-C28-N3-C36
2	F	400	P2F	O6-C28-N3-C36
2	D	400	P2F	O6-C28-N3-C36
2	D	400	P2F	C37-C36-N3-C28
2	A	400	P2F	C23-C28-N3-C33
2	A	400	P2F	O6-C28-N3-C33
2	D	400	P2F	C23-C28-N3-C36
2	A	400	P2F	C4-C5-O1-C8
2	D	400	P2F	N3-C36-C37-C38
2	A	400	P2F	C6-C5-O1-C8
2	F	400	P2F	C34-C33-N3-C36
2	B	400	P2F	C6-C5-O1-C8
2	F	400	P2F	N3-C33-C34-C35
2	C	400	P2F	C37-C36-N3-C28
2	B	400	P2F	C4-C5-O1-C8
2	C	400	P2F	O6-C28-N3-C33
2	C	400	P2F	N3-C36-C37-C38
2	E	400	P2F	N3-C36-C37-C38
2	A	400	P2F	C34-C33-N3-C36
2	C	400	P2F	C34-C33-N3-C36
2	E	400	P2F	C34-C33-N3-C36
2	B	400	P2F	C34-C33-N3-C36
2	C	400	P2F	C4-C5-O1-C8
2	C	400	P2F	C6-C5-O1-C8
2	C	400	P2F	C23-C28-N3-C36
2	C	400	P2F	C26-C27-N2-C30
2	A	400	P2F	C26-C27-N2-C30
2	A	400	P2F	C22-C27-N2-C30
2	D	400	P2F	C26-C27-N2-S1
2	D	400	P2F	C22-C27-N2-S1
2	F	400	P2F	C34-C33-N3-C28
2	B	400	P2F	N3-C36-C37-C38
2	F	400	P2F	C37-C36-N3-C33
2	E	400	P2F	C6-C5-O1-C8
2	B	400	P2F	C37-C36-N3-C28
2	E	400	P2F	C37-C36-N3-C33
2	A	400	P2F	C37-C36-N3-C33
2	C	400	P2F	C22-C27-N2-C30
2	F	400	P2F	C26-C27-N2-C30
2	B	400	P2F	C13-C7-N4-C9

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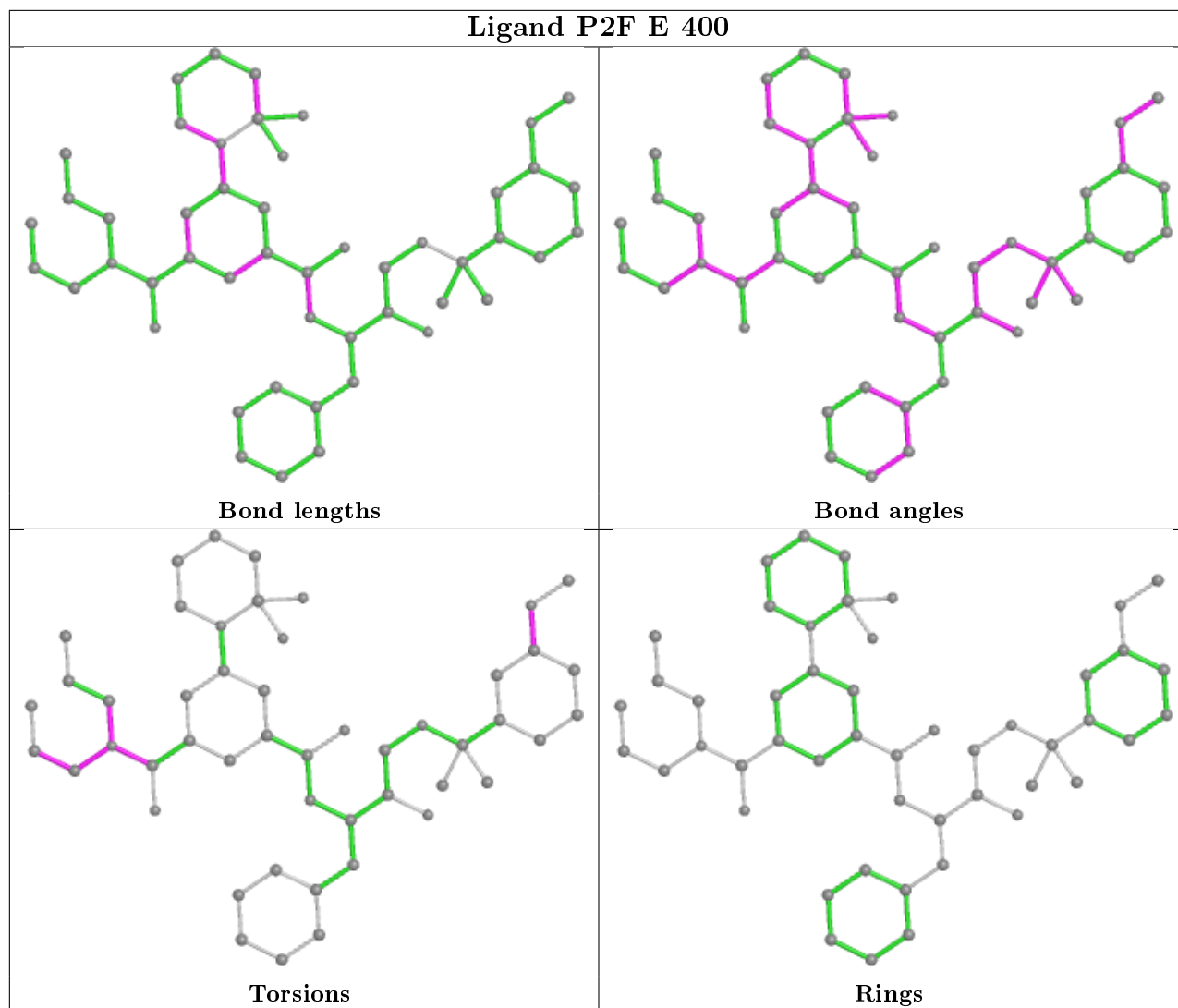
Mol	Chain	Res	Type	Atoms
2	D	400	P2F	C34-C33-N3-C36

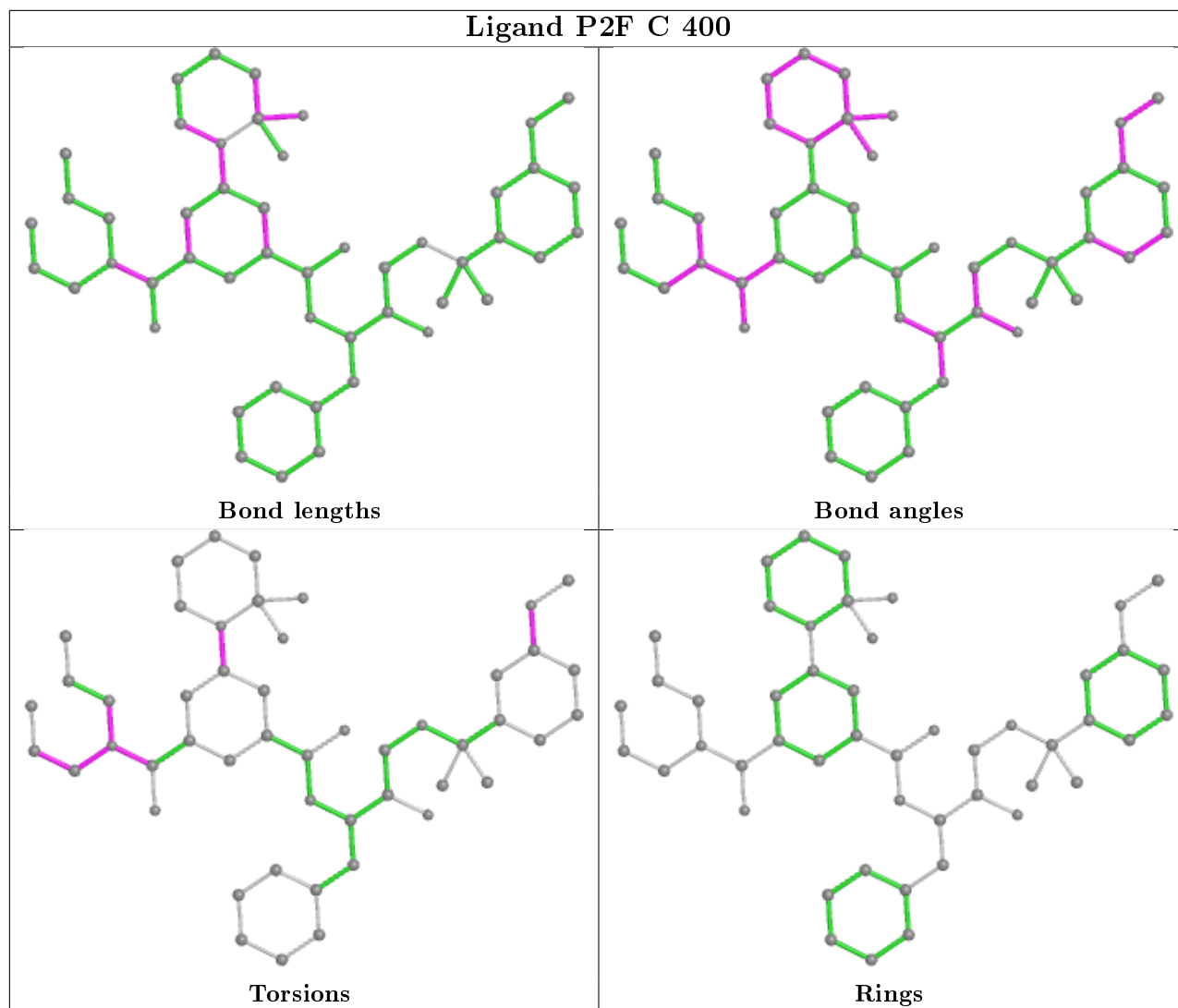
There are no ring outliers.

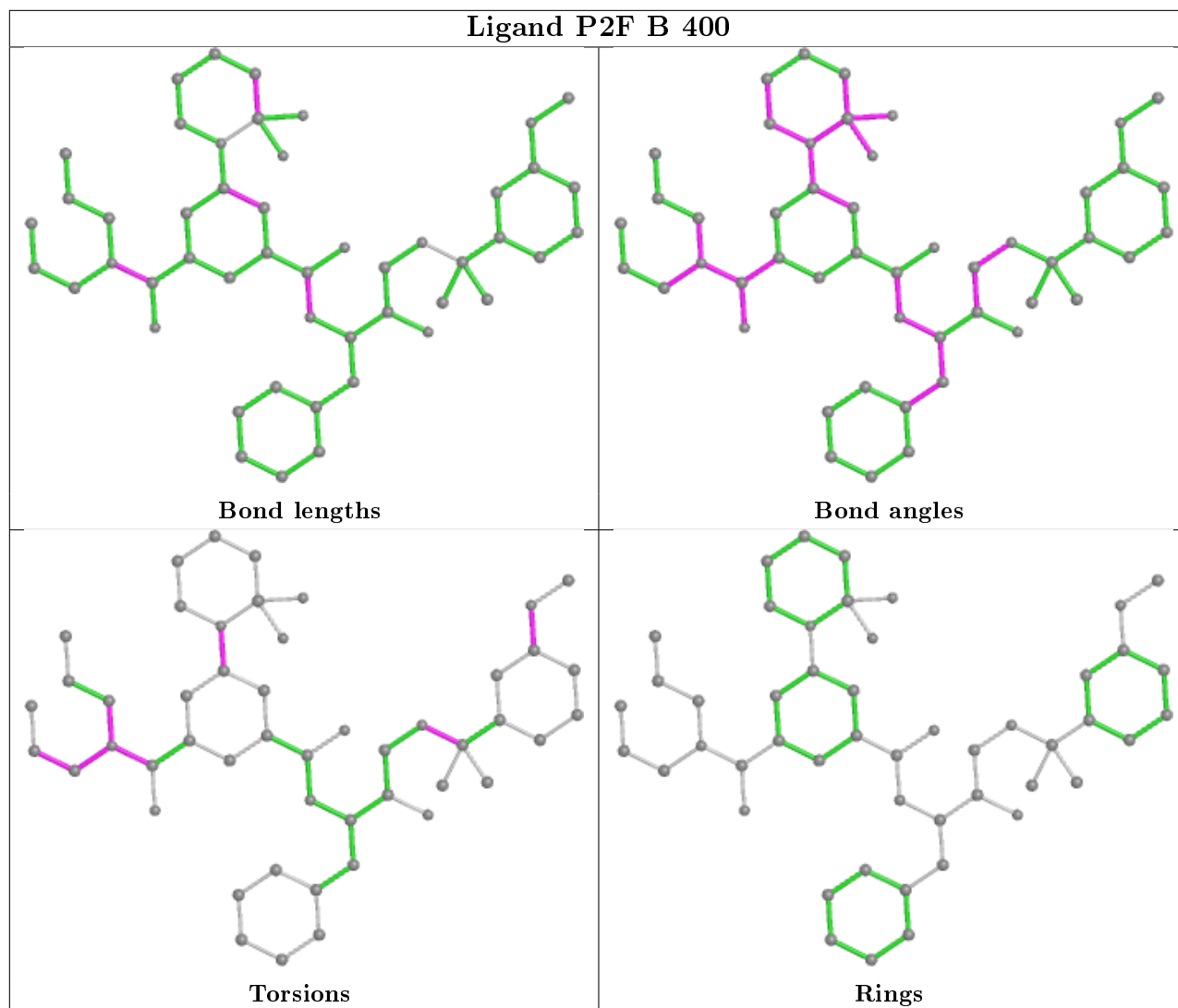
5 monomers are involved in 13 short contacts:

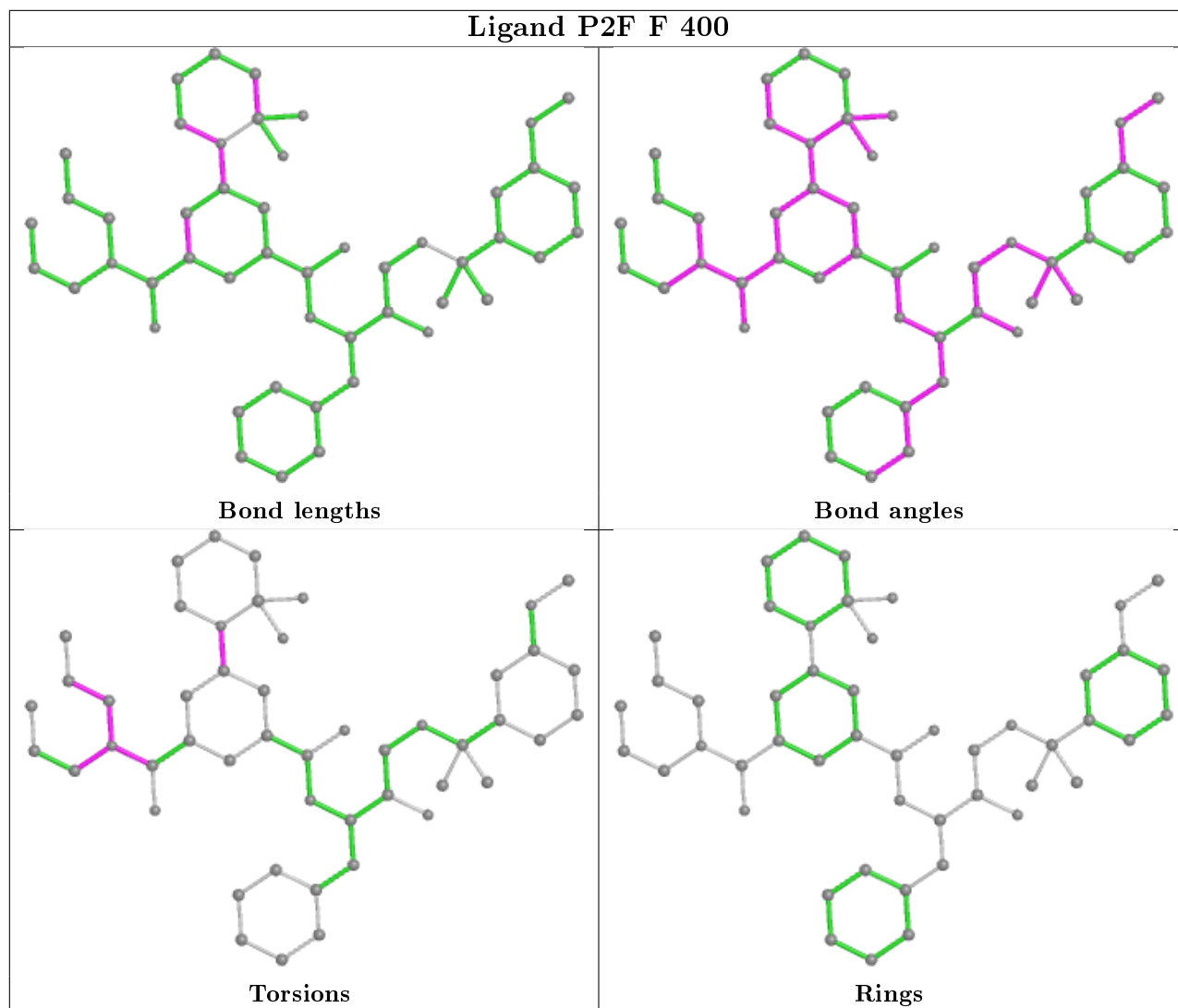
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	400	P2F	3	0
2	B	400	P2F	1	0
2	F	400	P2F	3	0
2	D	400	P2F	3	0
2	A	400	P2F	3	0

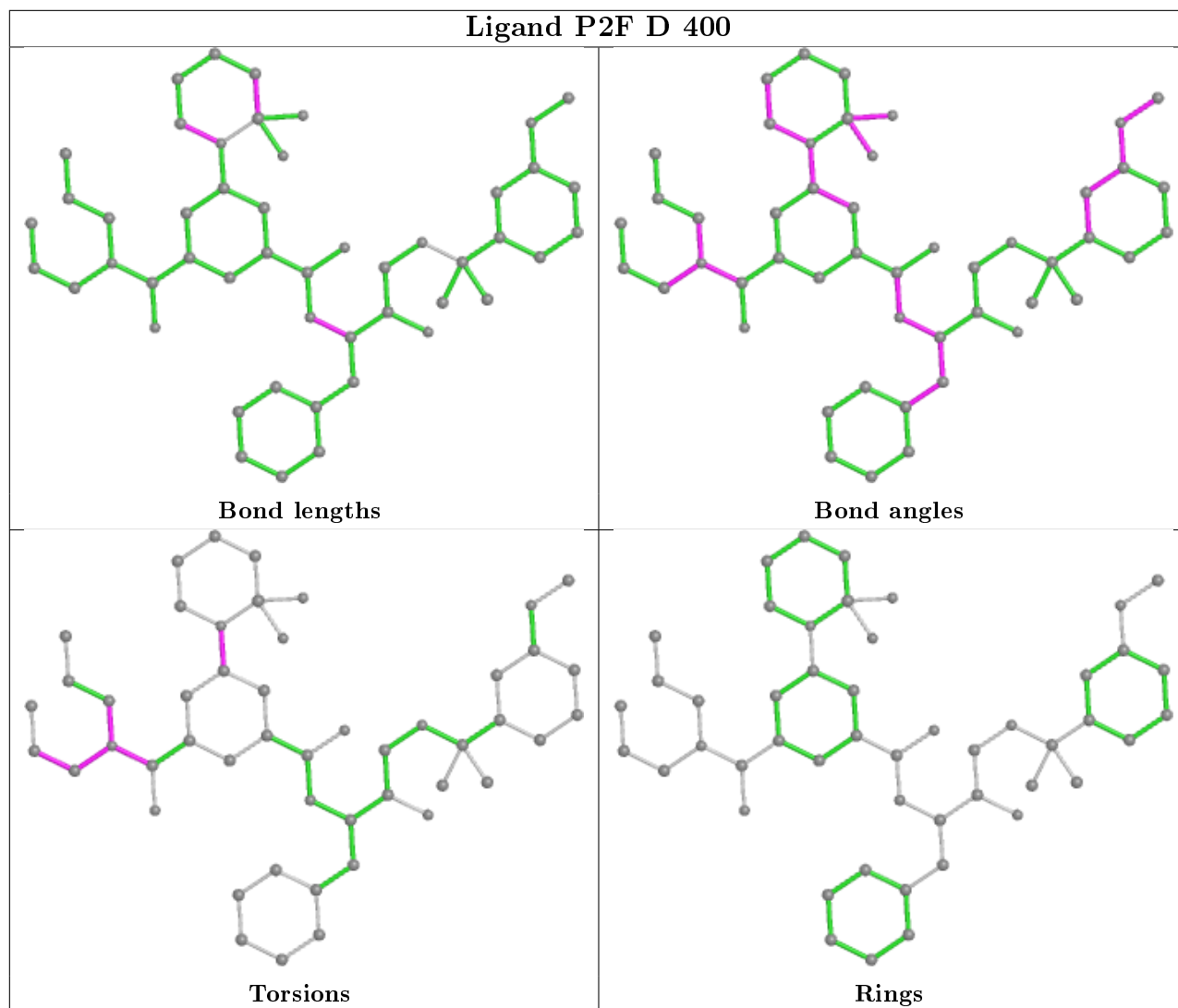
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

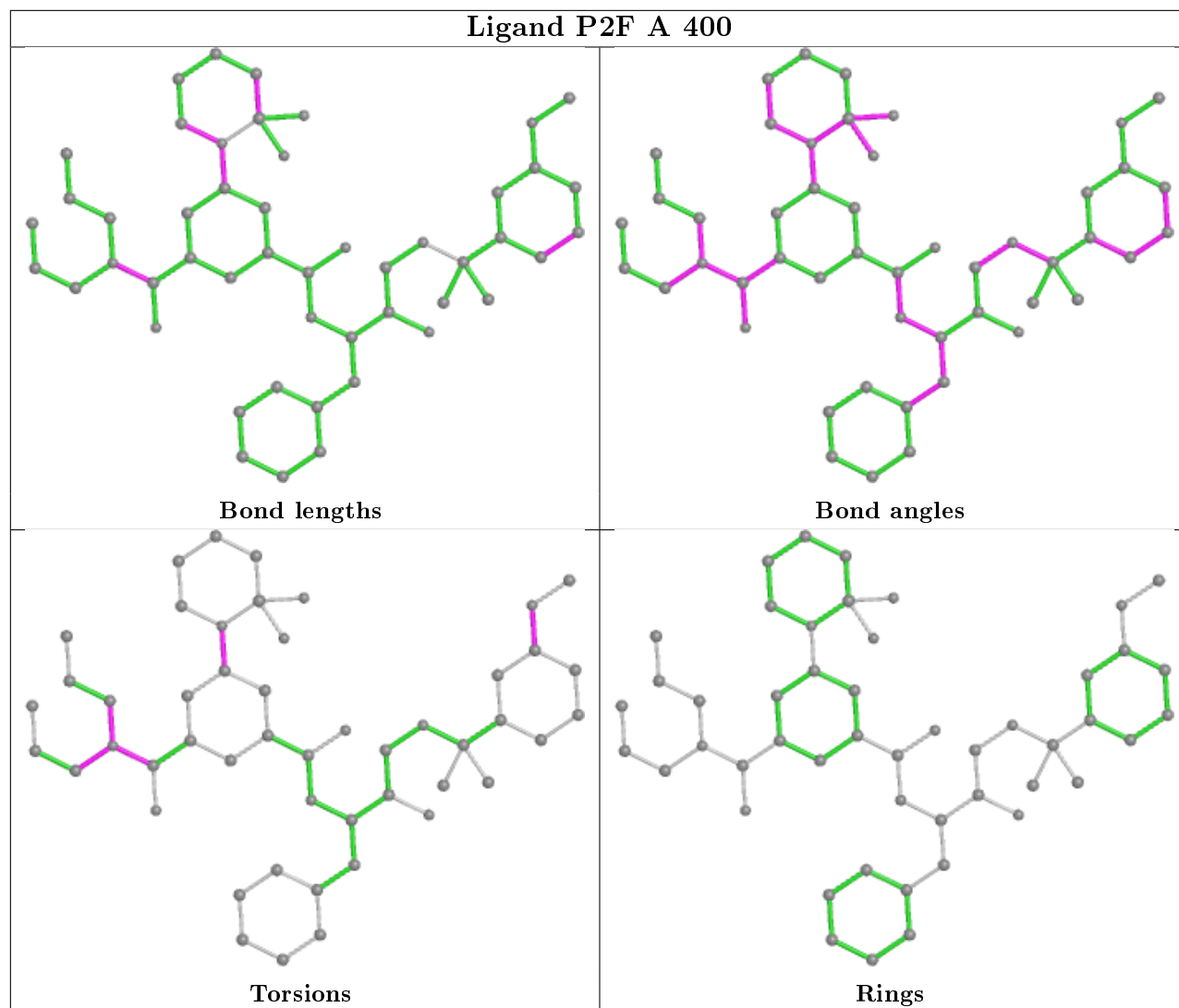












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	323/329 (98%)	0.06	16 (4%) 28 27	11, 24, 48, 63	0
1	B	327/329 (99%)	-0.14	12 (3%) 41 39	9, 20, 50, 75	0
1	C	322/329 (97%)	-0.01	15 (4%) 31 30	11, 21, 49, 74	0
1	D	323/329 (98%)	-0.03	17 (5%) 26 25	10, 21, 48, 70	0
1	E	322/329 (97%)	-0.05	13 (4%) 38 36	8, 20, 48, 71	0
1	F	329/329 (100%)	-0.11	11 (3%) 46 44	8, 19, 47, 78	0
All	All	1946/1974 (98%)	-0.05	84 (4%) 35 33	8, 21, 49, 78	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	241	PHE	7.5
1	E	241	PHE	6.4
1	C	329	LEU	6.4
1	F	329	LEU	5.6
1	C	14	ILE	4.9
1	A	53	LEU	4.9
1	A	48	THR	4.7
1	D	280	VAL	4.7
1	C	241	PHE	4.4
1	A	241	PHE	4.3
1	B	329	LEU	4.1
1	E	284	LEU	4.1
1	F	241	PHE	3.8
1	D	279	ASP	3.8
1	E	329	LEU	3.8
1	D	14	ILE	3.7
1	F	242	LEU	3.7
1	B	280	VAL	3.6
1	D	282	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	248	LEU	3.5
1	E	242	LEU	3.5
1	A	283	GLY	3.4
1	C	240	PRO	3.2
1	E	244	PHE	3.2
1	F	11	PHE	3.2
1	C	243	PRO	3.1
1	B	14	ILE	3.1
1	E	243	PRO	3.0
1	A	329	LEU	3.0
1	D	283	GLY	3.0
1	E	249	CYS	3.0
1	B	162	ASP	2.9
1	B	12	GLN	2.9
1	F	328	ASN	2.8
1	C	2	SER	2.8
1	F	282	PRO	2.7
1	A	40	LEU	2.7
1	D	284	LEU	2.7
1	A	162	ASP	2.6
1	C	161	HIS	2.6
1	A	123	ILE	2.6
1	C	12	GLN	2.6
1	C	284	LEU	2.5
1	F	124	LEU	2.5
1	D	233	ASN	2.5
1	B	48	THR	2.5
1	D	147	ASN	2.5
1	B	240	PRO	2.5
1	B	243	PRO	2.5
1	C	162	ASP	2.5
1	F	244	PHE	2.4
1	E	162	ASP	2.4
1	D	244	PHE	2.4
1	D	48	THR	2.4
1	E	250	ASN	2.4
1	B	161	HIS	2.4
1	F	283	GLY	2.4
1	E	203	ASN	2.3
1	F	280	VAL	2.3
1	A	124	LEU	2.3
1	C	250	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	329	LEU	2.3
1	D	234	LEU	2.2
1	A	161	HIS	2.2
1	E	240	PRO	2.2
1	D	235	ASP	2.2
1	A	242	LEU	2.2
1	B	279	ASP	2.2
1	A	61	SER	2.1
1	A	64	ARG	2.1
1	D	249	CYS	2.1
1	C	163	LYS	2.1
1	A	250	ASN	2.1
1	B	11	PHE	2.1
1	A	296	VAL	2.1
1	C	242	LEU	2.1
1	C	147	ASN	2.1
1	E	32	ILE	2.1
1	F	126	LEU	2.1
1	D	53	LEU	2.0
1	A	249	CYS	2.0
1	C	249	CYS	2.0
1	D	109	ASN	2.0
1	D	277	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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](#)

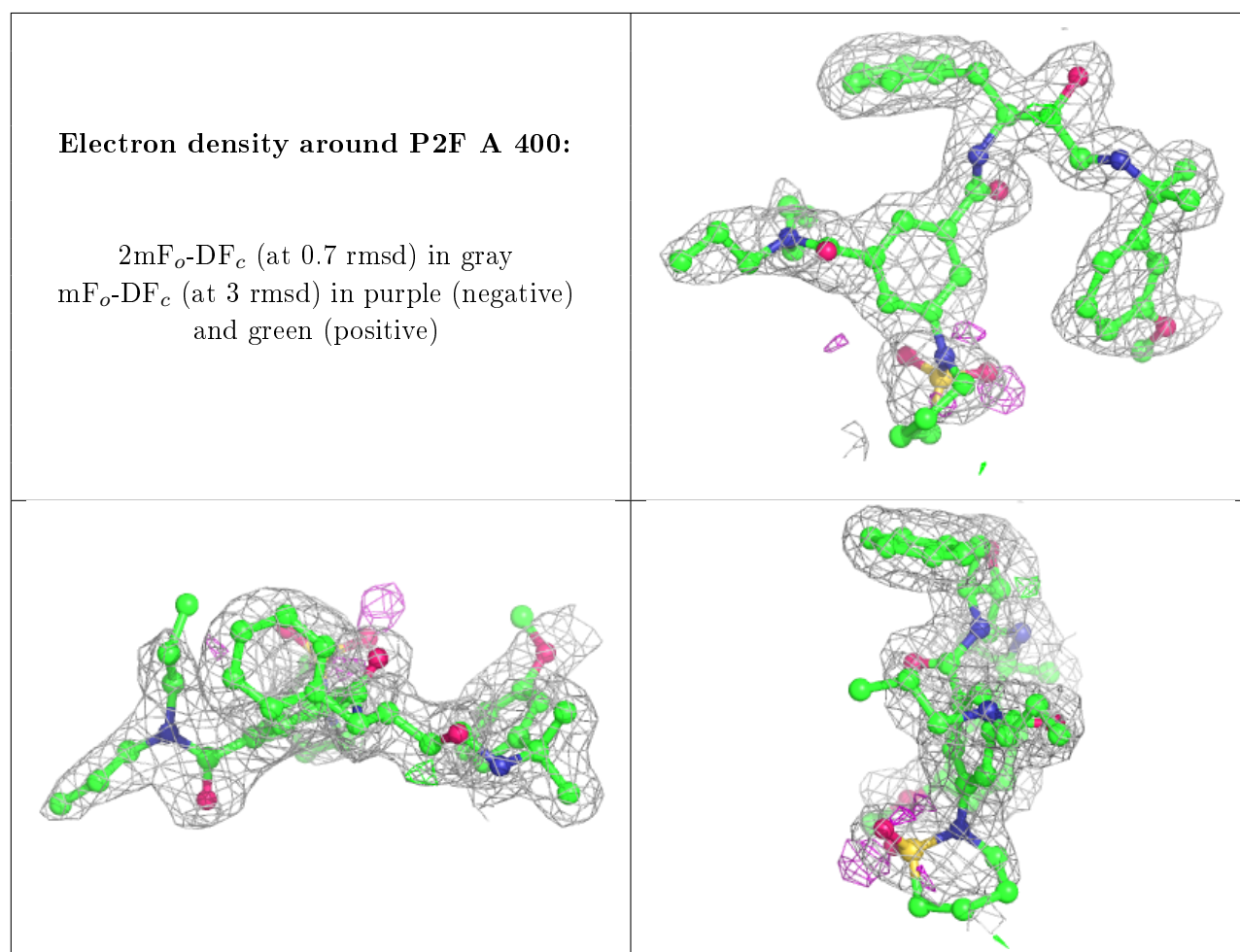
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

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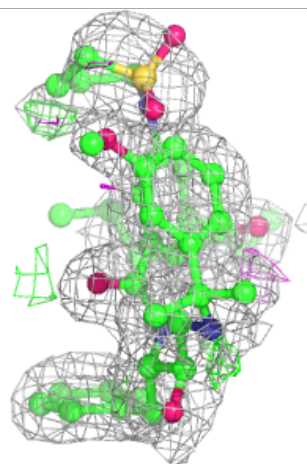
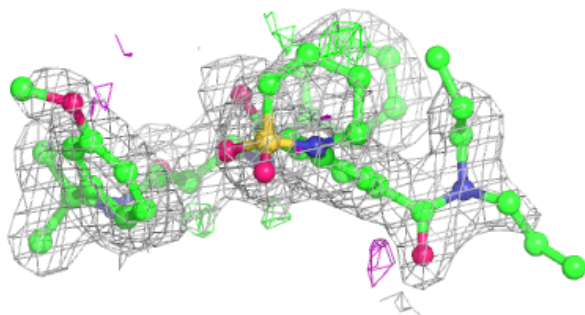
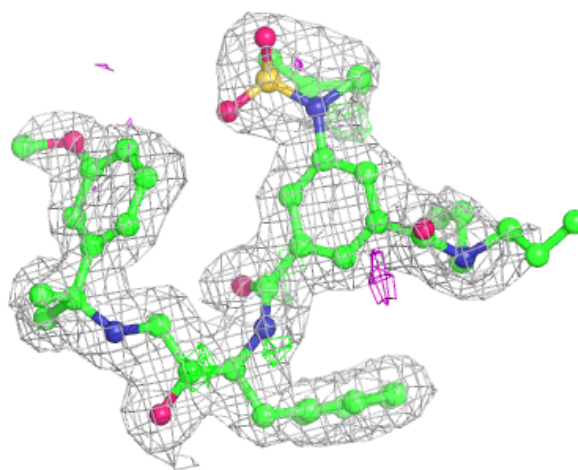
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	P2F	A	400	49/49	0.89	0.13	17,27,64,71	0
2	P2F	B	400	49/49	0.90	0.14	17,28,67,78	0
2	P2F	F	400	49/49	0.90	0.13	16,30,59,64	0
2	P2F	D	400	49/49	0.90	0.14	17,30,75,84	0
2	P2F	C	400	49/49	0.90	0.13	19,32,68,70	0
2	P2F	E	400	49/49	0.92	0.12	17,23,63,72	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.



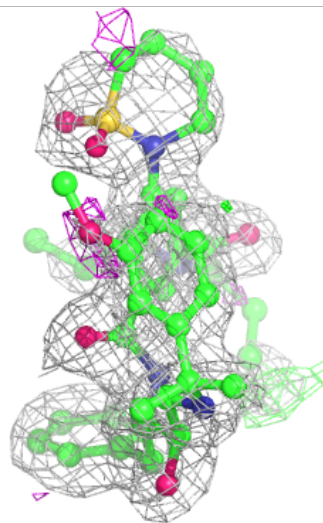
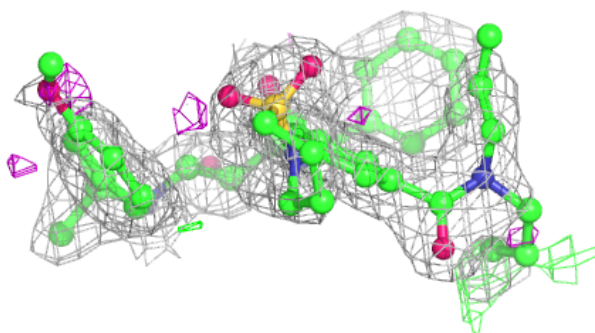
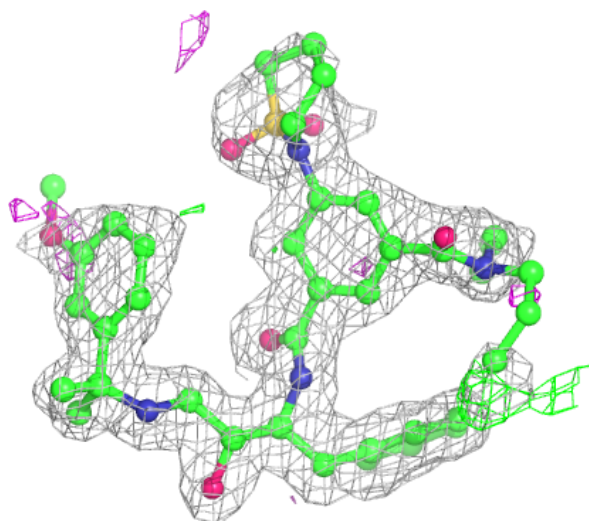
Electron density around P2F B 400:

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



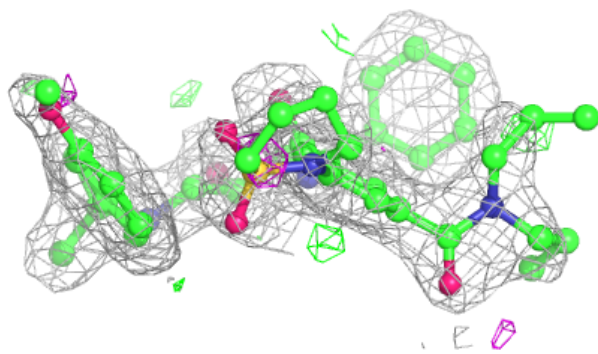
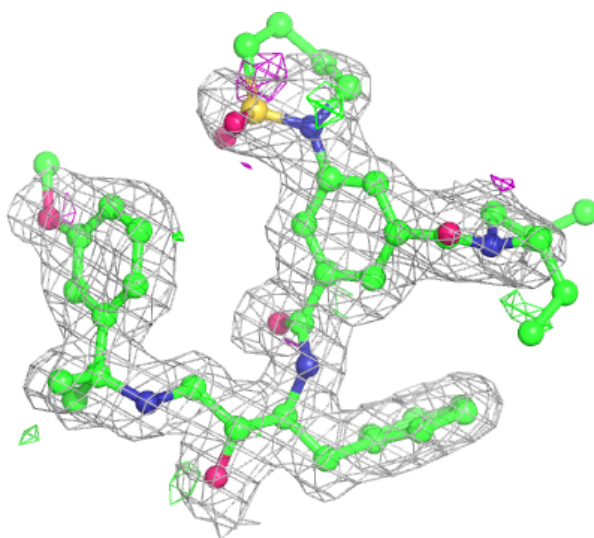
Electron density around P2F F 400:

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



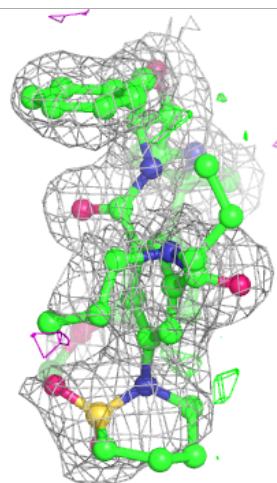
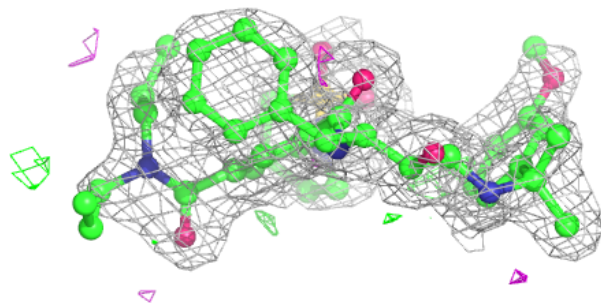
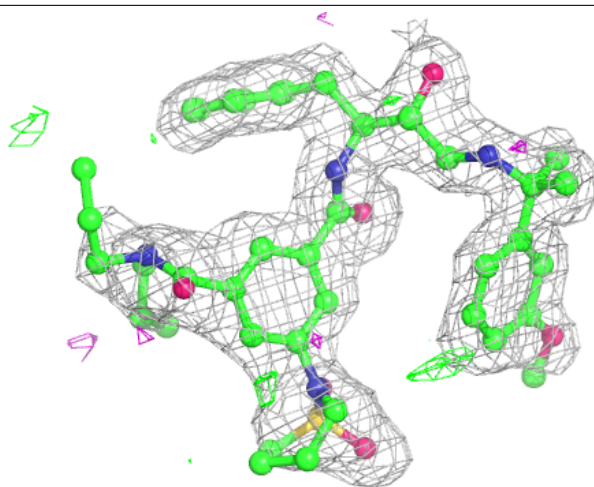
Electron density around P2F D 400:

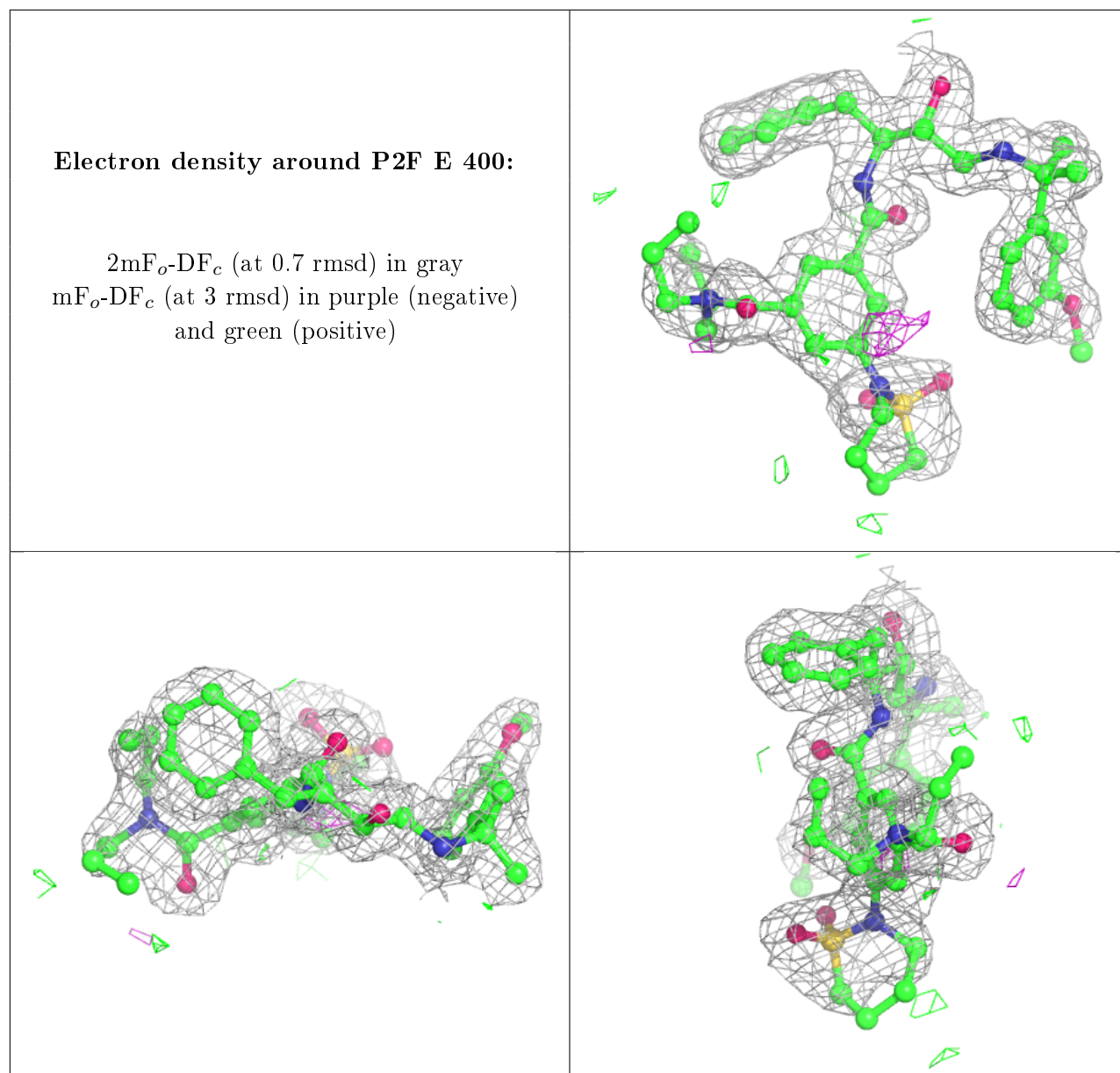
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around P2F C 400:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.