Full wwPDB X-ray Structure Validation Report (i)

May 21, 2020 – 11:36 pm BST

PDB ID	:	2FDP
Title	:	Crystal structure of beta-secretase complexed with an amino-ethylene inhibitor
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Deposited on	:	2005-12-14
Resolution	:	2.50 Å(reported)

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

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

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

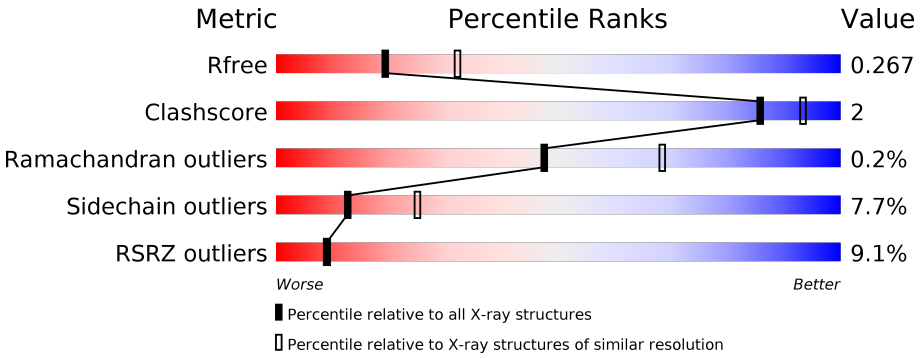
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 <=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	388	9% 80% 15%
1	B	388	9% 84% 11% 5%
1	C	388	8% 81% 14%

2 Entry composition

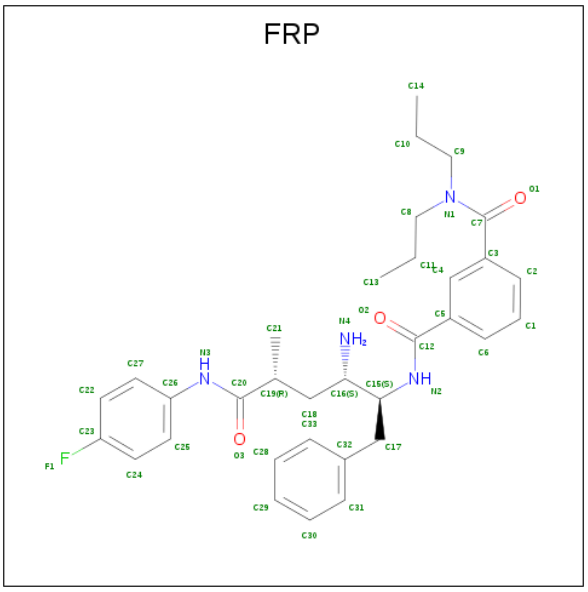
There are 3 unique types of molecules in this entry. The entry contains 9008 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Beta-secretase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	S	0	0	0
			2940	1882	489	555	14			
1	B	369	Total	C	N	O	S	0	0	0
			2908	1865	484	545	14			
1	C	374	Total	C	N	O	S	0	0	0
			2937	1881	489	553	14			

- Molecule 2 is N1-((2S,3S,5R)-3-AMINO-6-(4-FLUOROPHENYLAMINO)-5-METHYL-6-OXO-1-PHENYLHEXAN-2-YL)-N3,N3-DIPROPYLISOPHTHALAMIDE (three-letter code: FRP) (formula: $C_{33}H_{41}FN_4O_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			41	33	1	4	3		
2	B	1	Total	C	F	N	O	0	0
			41	33	1	4	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	F	N	O	0	0
			41	33	1	4	3		

- Molecule 3 is water.

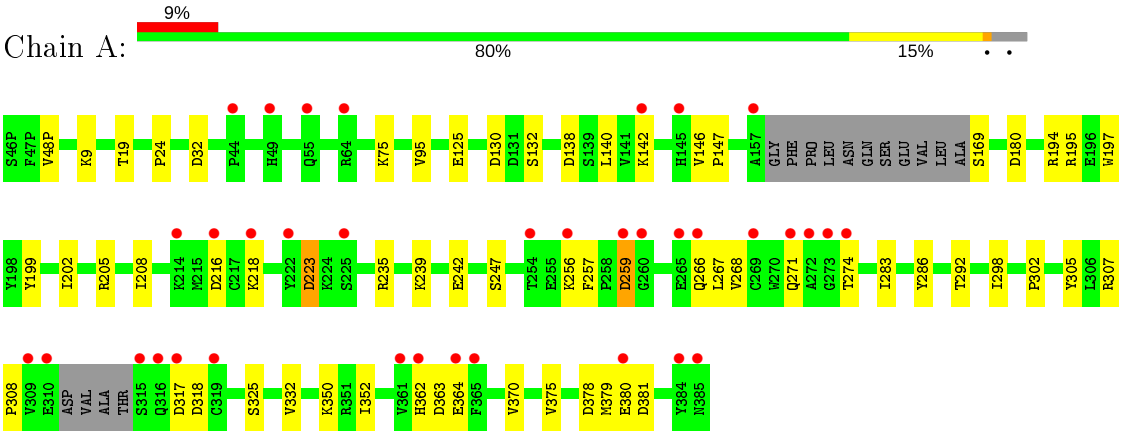
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	36	Total	O	0	0
			36	36		
3	B	35	Total	O	0	0
			35	35		
3	C	29	Total	O	0	0
			29	29		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

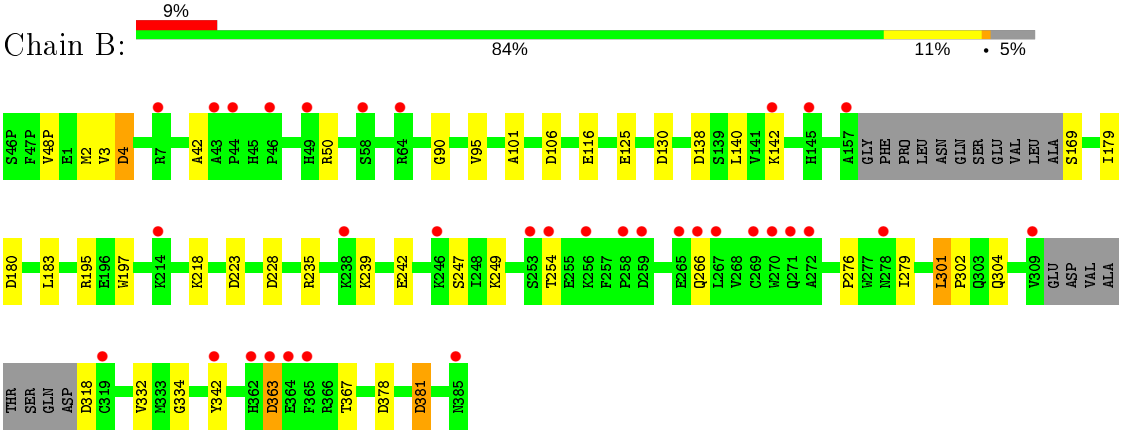
- Molecule 1: Beta-secretase 1

Chain A:



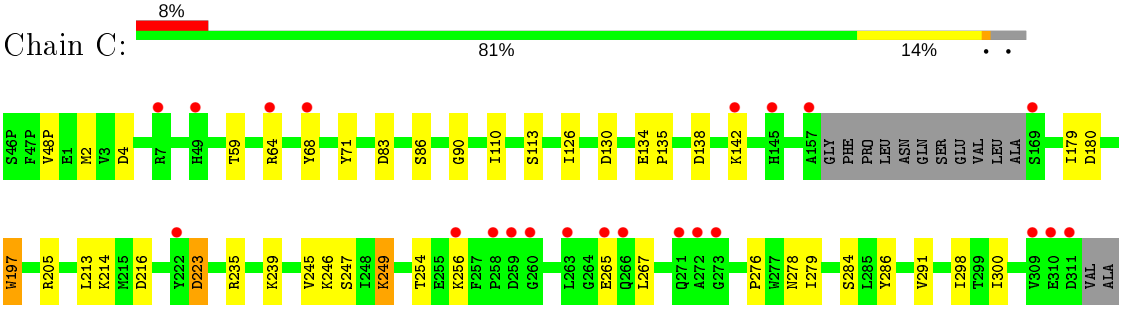
- Molecule 1: Beta-secretase 1

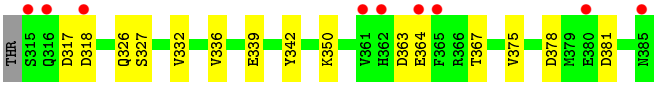
Chain B:



- Molecule 1: Beta-secretase 1

Chain C:




THR
S315
Q316
D317
D318
Q326
S327
V332
V336
E339
Y342
K350
V361
H362
D363
E364
F365
R366
T367
V375
D378
M379
E380
D381
N385

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	81.19Å 102.19Å 99.53Å 90.00° 103.21° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 19.79 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.9 (20.00-2.50) 98.9 (19.79-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.55 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.225 , 0.254 0.244 , 0.267	Depositor DCC
R_{free} test set	2794 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	42.7	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 25.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9008	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.30	0/3014	0.64	12/4092 (0.3%)
1	B	0.30	0/2982	0.64	10/4049 (0.2%)
1	C	0.30	0/3011	0.64	11/4089 (0.3%)
All	All	0.30	0/9007	0.64	33/12230 (0.3%)

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	216	ASP	CB-CG-OD2	6.37	124.03	118.30
1	C	4	ASP	CB-CG-OD2	5.94	123.64	118.30
1	A	130	ASP	CB-CG-OD2	5.92	123.63	118.30
1	B	381	ASP	CB-CG-OD2	5.86	123.58	118.30
1	A	317	ASP	CB-CG-OD2	5.86	123.58	118.30
1	B	4	ASP	CB-CG-OD2	5.84	123.55	118.30
1	B	130	ASP	CB-CG-OD2	5.74	123.47	118.30
1	C	130	ASP	CB-CG-OD2	5.66	123.40	118.30
1	A	381	ASP	CB-CG-OD2	5.66	123.39	118.30
1	C	318	ASP	CB-CG-OD2	5.61	123.35	118.30
1	C	381	ASP	CB-CG-OD2	5.55	123.29	118.30
1	A	138	ASP	CB-CG-OD2	5.45	123.20	118.30
1	B	318	ASP	CB-CG-OD2	5.45	123.20	118.30
1	A	180	ASP	CB-CG-OD2	5.41	123.17	118.30
1	A	363	ASP	CB-CG-OD2	5.36	123.12	118.30
1	C	138	ASP	CB-CG-OD2	5.33	123.10	118.30
1	B	106	ASP	CB-CG-OD2	5.28	123.05	118.30
1	B	180	ASP	CB-CG-OD2	5.25	123.03	118.30
1	B	138	ASP	CB-CG-OD2	5.23	123.01	118.30
1	B	363	ASP	CB-CG-OD2	5.23	123.01	118.30
1	C	378	ASP	CB-CG-OD2	5.19	122.97	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	83	ASP	CB-CG-OD2	5.18	122.97	118.30
1	B	223	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	259	ASP	CB-CG-OD2	5.15	122.94	118.30
1	A	32	ASP	CB-CG-OD2	5.13	122.92	118.30
1	B	378	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	318	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	216	ASP	CB-CG-OD2	5.05	122.85	118.30
1	A	378	ASP	CB-CG-OD2	5.05	122.84	118.30
1	A	223	ASP	CB-CG-OD2	5.03	122.83	118.30
1	C	223	ASP	CB-CG-OD2	5.03	122.82	118.30
1	C	180	ASP	CB-CG-OD2	5.03	122.82	118.30
1	C	363	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2940	0	2849	12	0
1	B	2908	0	2826	10	0
1	C	2937	0	2841	13	0
2	A	41	0	41	1	0
2	B	41	0	41	1	0
2	C	41	0	41	2	0
3	A	36	0	0	0	0
3	B	35	0	0	0	0
3	C	29	0	0	0	0
All	All	9008	0	8639	38	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 2.

All (38) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:PHE:HD2	1:A:268:VAL:HG21	1.71	0.56
1:C:110:ILE:HB	1:C:113:SER:HB3	1.89	0.55
1:B:235:ARG:HB2	1:B:332:VAL:HB	1.88	0.55
2:C:386:FRP:H27	2:C:386:FRP:O3	2.08	0.54
1:A:235:ARG:HB2	1:A:332:VAL:HB	1.91	0.53
1:C:235:ARG:HB2	1:C:332:VAL:HB	1.91	0.52
1:C:2:MET:HG2	1:C:90:GLY:HA2	1.92	0.52
1:B:301:LEU:HB3	1:B:302:PRO:HD2	1.93	0.51
1:A:194:ARG:HD2	1:A:202:ILE:HD11	1.95	0.49
1:C:276:PRO:HB2	1:C:279:ILE:HG12	1.95	0.48
1:B:2:MET:HG2	1:B:90:GLY:HA2	1.96	0.48
1:A:208:ILE:HG12	1:A:283:ILE:HG12	1.95	0.48
1:C:245:VAL:O	1:C:249:LYS:HB2	2.14	0.48
1:B:95:VAL:HG11	1:B:140:LEU:HA	1.97	0.47
1:A:95:VAL:HG11	1:A:140:LEU:HA	1.97	0.47
2:B:386:FRP:H27	2:B:386:FRP:O3	2.15	0.47
1:A:19:THR:HB	1:A:24:PRO:HB3	1.97	0.46
1:A:298:ILE:HG22	1:A:370:VAL:HG22	1.97	0.45
1:B:276:PRO:HB2	1:B:279:ILE:HG12	1.99	0.45
1:C:235:ARG:HB3	1:C:327:SER:HB2	1.96	0.45
1:B:50:ARG:O	1:B:116:GLU:HG2	2.16	0.45
2:A:386:FRP:O3	2:A:386:FRP:H27	2.17	0.44
1:A:302:PRO:HA	1:A:305:TYR:CE2	2.54	0.43
1:C:126:ILE:HG23	1:C:197:TRP:HB2	2.00	0.43
1:B:179:ILE:HG23	1:B:342:TYR:HE2	1.83	0.42
1:B:228:ASP:O	1:B:334:GLY:HA2	2.19	0.42
1:B:3:VAL:HG13	1:B:183:LEU:HD21	2.02	0.42
1:C:134:GLU:HA	1:C:135:PRO:HD3	1.94	0.42
1:A:307:ARG:HA	1:A:308:PRO:HD3	1.86	0.42
1:A:199:TYR:HB3	1:A:352:ILE:HD11	2.02	0.42
1:A:205:ARG:HB3	1:A:286:TYR:HB2	2.02	0.42
1:C:278:ASN:H	1:C:278:ASN:HD22	1.69	0.41
1:B:42:ALA:HB2	1:B:101:ALA:HB1	2.03	0.41
1:C:205:ARG:HB3	1:C:286:TYR:HB2	2.03	0.41
1:C:298:ILE:HD12	1:C:300:ILE:HD11	2.03	0.41
1:A:146:VAL:HA	1:A:147:PRO:HD3	1.96	0.40
1:C:71:TYR:HB3	2:C:386:FRP:H15	2.04	0.40
1:C:179:ILE:HG23	1:C:342:TYR:HE2	1.86	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	367/388 (95%)	356 (97%)	10 (3%)	1 (0%)	41 61
1	B	363/388 (94%)	353 (97%)	10 (3%)	0	100 100
1	C	368/388 (95%)	358 (97%)	9 (2%)	1 (0%)	41 61
All	All	1098/1164 (94%)	1067 (97%)	29 (3%)	2 (0%)	47 68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	223	ASP
1	A	223	ASP

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	319/331 (96%)	292 (92%)	27 (8%)	10 21
1	B	315/331 (95%)	296 (94%)	19 (6%)	19 37
1	C	317/331 (96%)	290 (92%)	27 (8%)	10 21
All	All	951/993 (96%)	878 (92%)	73 (8%)	13 25

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48(P)	VAL

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Mol	Chain	Res	Type
1	A	9	LYS
1	A	75	LYS
1	A	125	GLU
1	A	132	SER
1	A	142	LYS
1	A	169	SER
1	A	195	ARG
1	A	197	TRP
1	A	218	LYS
1	A	239	LYS
1	A	242	GLU
1	A	247	SER
1	A	256	LYS
1	A	259	ASP
1	A	266	GLN
1	A	267	LEU
1	A	271	GLN
1	A	274	THR
1	A	292	THR
1	A	325	SER
1	A	350	LYS
1	A	362	HIS
1	A	364	GLU
1	A	375	VAL
1	A	379	MET
1	A	380	GLU
1	B	48(P)	VAL
1	B	4	ASP
1	B	125	GLU
1	B	142	LYS
1	B	169	SER
1	B	195	ARG
1	B	197	TRP
1	B	218	LYS
1	B	239	LYS
1	B	242	GLU
1	B	247	SER
1	B	249	LYS
1	B	254	THR
1	B	266	GLN
1	B	301	LEU
1	B	304	GLN

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Mol	Chain	Res	Type
1	B	363	ASP
1	B	367	THR
1	B	381	ASP
1	C	48(P)	VAL
1	C	59	THR
1	C	64	ARG
1	C	68	TYR
1	C	86	SER
1	C	142	LYS
1	C	197	TRP
1	C	213	LEU
1	C	214	LYS
1	C	239	LYS
1	C	246	LYS
1	C	247	SER
1	C	249	LYS
1	C	254	THR
1	C	256	LYS
1	C	265	GLU
1	C	267	LEU
1	C	284	SER
1	C	291	VAL
1	C	317	ASP
1	C	326	GLN
1	C	336	VAL
1	C	339	GLU
1	C	350	LYS
1	C	364	GLU
1	C	367	THR
1	C	375	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	HIS
1	B	304	GLN
1	C	278	ASN
1	C	304	GLN
1	C	326	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

3 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	FRP	A	386	-	43,43,43	0.61	1 (2%)	52,57,57	0.95	3 (5%)
2	FRP	C	386	-	43,43,43	0.63	1 (2%)	52,57,57	0.91	2 (3%)
2	FRP	B	386	-	43,43,43	0.64	1 (2%)	52,57,57	0.95	3 (5%)

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	FRP	A	386	-	-	4/42/42/42	0/3/3/3
2	FRP	C	386	-	-	4/42/42/42	0/3/3/3
2	FRP	B	386	-	-	2/42/42/42	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	386	FRP	C26-N3	-2.50	1.36	1.41
2	B	386	FRP	C26-N3	-2.48	1.36	1.41
2	A	386	FRP	C26-N3	-2.30	1.37	1.41

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	386	FRP	C17-C15-N2	-2.87	105.89	110.07
2	C	386	FRP	C17-C15-N2	-2.72	106.10	110.07
2	B	386	FRP	C17-C15-N2	-2.72	106.11	110.07
2	A	386	FRP	C3-C7-N1	2.48	121.86	118.72
2	C	386	FRP	C3-C7-N1	2.28	121.61	118.72
2	B	386	FRP	C22-C23-C24	-2.24	119.84	122.83
2	A	386	FRP	C22-C23-C24	-2.22	119.88	122.83
2	B	386	FRP	C3-C7-N1	2.03	121.29	118.72

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	386	FRP	N4-C16-C18-C19
2	C	386	FRP	C16-C18-C19-C21
2	B	386	FRP	N4-C16-C18-C19
2	A	386	FRP	C14-C10-C9-N1
2	C	386	FRP	C13-C11-C8-N1
2	A	386	FRP	C15-C17-C32-C33
2	A	386	FRP	C15-C17-C32-C31
2	A	386	FRP	C13-C11-C8-N1
2	B	386	FRP	C14-C10-C9-N1
2	C	386	FRP	C15-C16-C18-C19

There are no ring outliers.

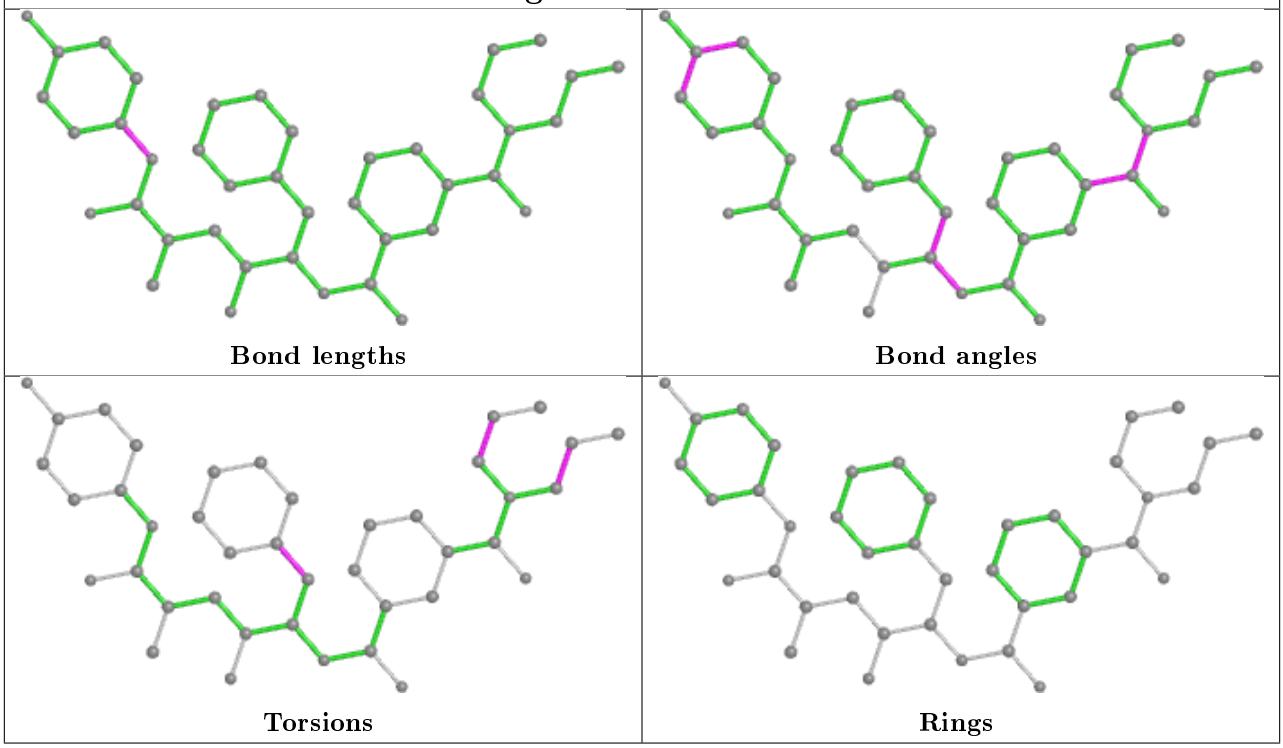
3 monomers are involved in 4 short contacts:

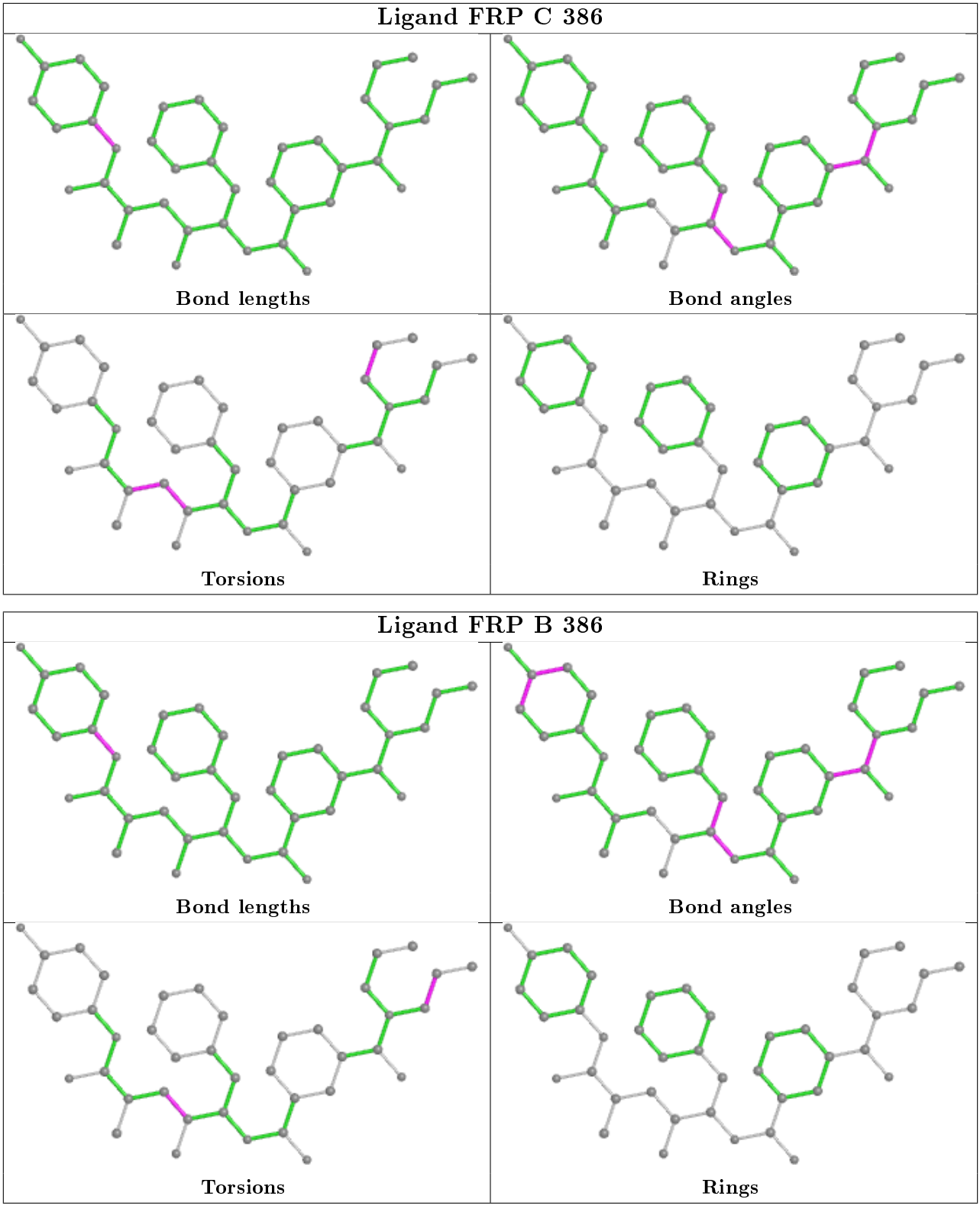
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	386	FRP	1	0
2	C	386	FRP	2	0
2	B	386	FRP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for 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 FRP A 386





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	373/388 (96%)	0.48	36 (9%) 7 7	6, 19, 39, 53	0
1	B	369/388 (95%)	0.58	34 (9%) 9 9	5, 20, 34, 51	0
1	C	374/388 (96%)	0.48	31 (8%) 11 11	5, 20, 40, 58	0
All	All	1116/1164 (95%)	0.51	101 (9%) 9 9	5, 19, 38, 58	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	365	PHE	7.4
1	C	259	ASP	7.1
1	A	316	GLN	6.1
1	C	157	ALA	6.0
1	A	157	ALA	5.8
1	B	256	LYS	5.8
1	A	259	ASP	5.0
1	B	254	THR	5.0
1	C	311	ASP	4.8
1	B	364	GLU	4.8
1	B	272	ALA	4.8
1	A	272	ALA	4.6
1	B	309	VAL	4.6
1	A	256	LYS	4.5
1	A	365	PHE	4.5
1	C	385	ASN	4.5
1	A	273	GLY	4.3
1	C	364	GLU	4.2
1	C	49	HIS	4.1
1	C	265	GLU	4.1
1	C	273	GLY	4.1
1	B	265	GLU	4.0
1	B	271	GLN	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	316	GLN	4.0
1	C	361	VAL	3.9
1	B	259	ASP	3.9
1	B	319	CYS	3.8
1	C	64	ARG	3.8
1	A	266	GLN	3.7
1	B	43	ALA	3.7
1	A	385	ASN	3.6
1	C	266	GLN	3.6
1	B	253	SER	3.5
1	C	7	ARG	3.5
1	C	315	SER	3.5
1	A	364	GLU	3.5
1	C	310	GLU	3.5
1	B	157	ALA	3.5
1	C	365	PHE	3.4
1	A	310	GLU	3.4
1	B	266	GLN	3.4
1	A	362	HIS	3.4
1	B	49	HIS	3.4
1	B	267	LEU	3.4
1	C	272	ALA	3.4
1	A	265	GLU	3.3
1	A	380	GLU	3.3
1	A	315	SER	3.3
1	A	55	GLN	3.2
1	C	68	TYR	3.2
1	A	319	CYS	3.1
1	A	361	VAL	3.1
1	B	64	ARG	3.1
1	A	44	PRO	3.0
1	A	64	ARG	3.0
1	B	270	TRP	3.0
1	C	362	HIS	2.9
1	A	309	VAL	2.9
1	B	258	PRO	2.7
1	A	145	HIS	2.7
1	C	318	ASP	2.7
1	C	256	LYS	2.7
1	B	142	LYS	2.6
1	A	254	THR	2.6
1	A	222	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	222	TYR	2.6
1	A	49	HIS	2.6
1	A	271	GLN	2.6
1	A	317	ASP	2.6
1	A	142	LYS	2.6
1	B	214	LYS	2.6
1	C	145	HIS	2.5
1	B	278	ASN	2.5
1	C	271	GLN	2.4
1	C	260	GLY	2.4
1	A	274	THR	2.4
1	C	309	VAL	2.4
1	C	142	LYS	2.4
1	C	380	GLU	2.4
1	B	269	CYS	2.4
1	B	363	ASP	2.4
1	B	46	PRO	2.3
1	C	258	PRO	2.3
1	B	362	HIS	2.3
1	A	216	ASP	2.3
1	B	58	SER	2.3
1	A	269	CYS	2.3
1	C	263	LEU	2.3
1	B	44	PRO	2.3
1	B	385	ASN	2.2
1	A	384	TYR	2.2
1	C	169	SER	2.2
1	B	145	HIS	2.2
1	A	218	LYS	2.2
1	A	225	SER	2.1
1	B	246	LYS	2.1
1	B	342	TYR	2.1
1	B	7	ARG	2.1
1	A	214	LYS	2.1
1	A	260	GLY	2.1
1	B	238	LYS	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 carbohydrates in this entry.

6.4 Ligands (i)

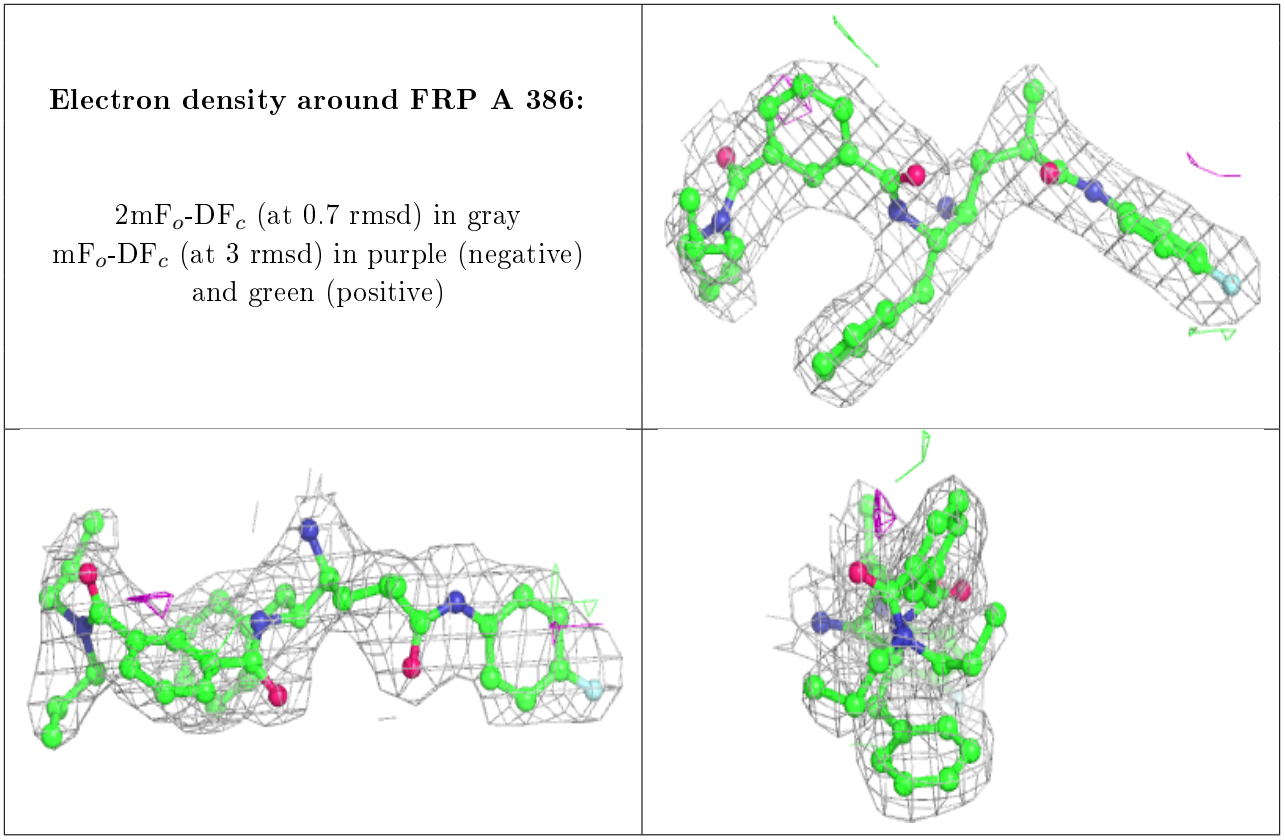
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FRP	A	386	41/41	0.95	0.15	10,13,19,21	0
2	FRP	C	386	41/41	0.95	0.15	11,15,19,21	0
2	FRP	B	386	41/41	0.95	0.15	12,14,20,20	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.

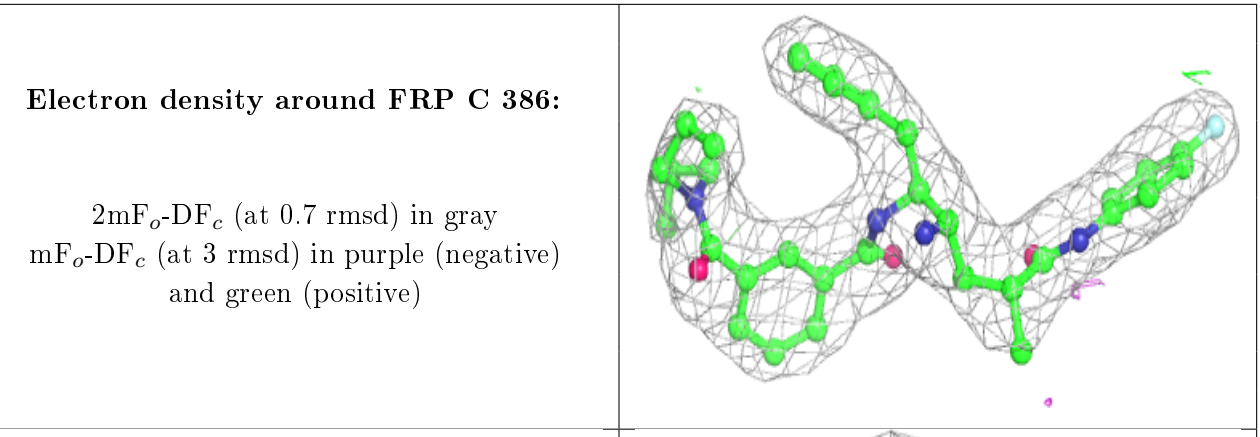
Electron density around FRP A 386:

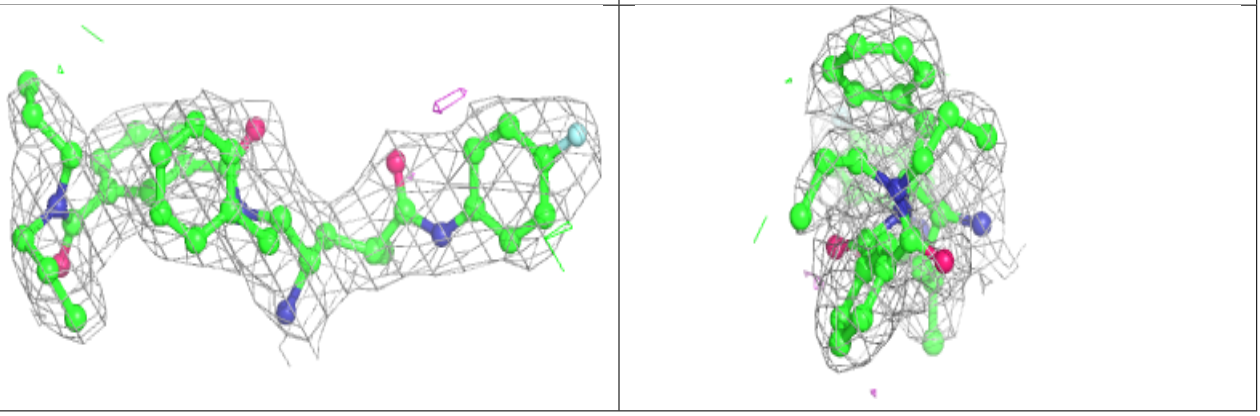
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around FRP C 386:

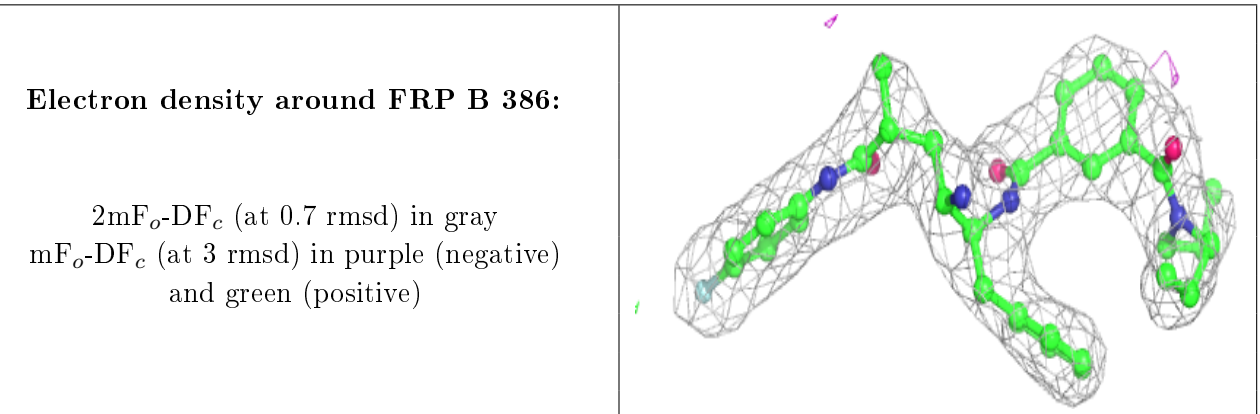
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

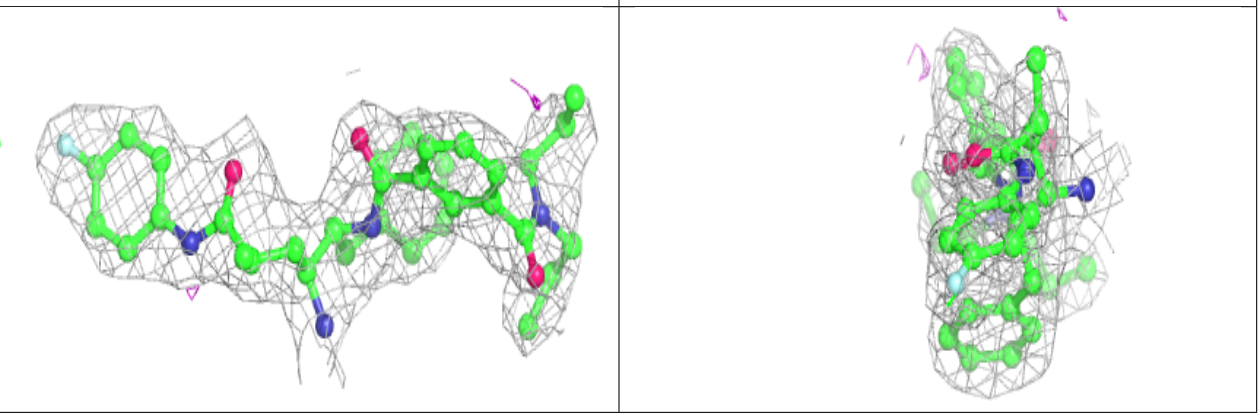




Electron density around FRP B 386:

$2mF_o$-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.