Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2024 – 07:02 pm GMT

PDB ID	:	8QRT
Title	:	Acyl-ACP thioesterase from Lemna paucicostata in complex with a spirolactam
Authors	:	Freigang, J.
Deposited on	:	2023-10-09
Resolution	:	2.00 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

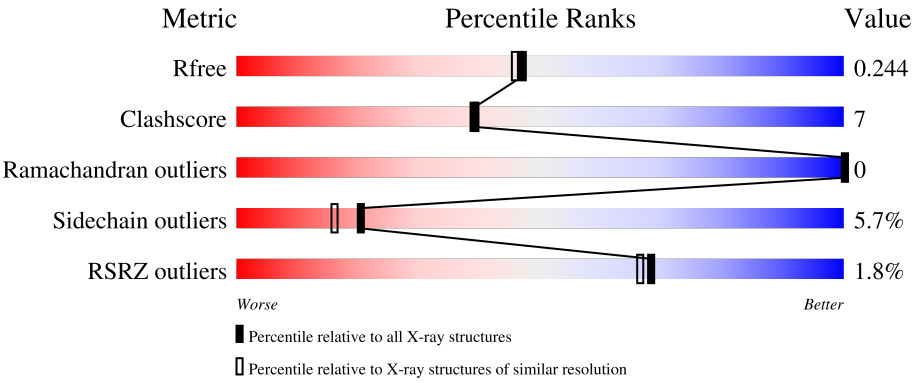
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	AAA	320	% 71% 12% • 16%
1	BBB	320	% 69% 12% • 17%
1	CCC	320	3% 71% 12% • 16%
1	DDD	320	% 71% 10% • 17%

2 Entry composition

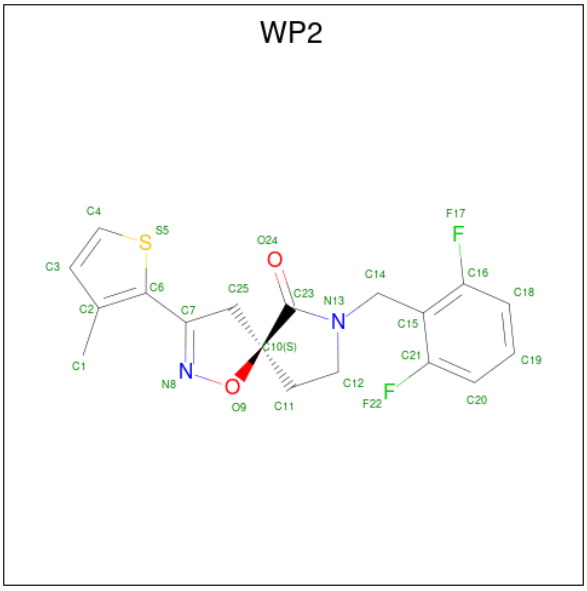
There are 3 unique types of molecules in this entry. The entry contains 9388 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Acyl-acp thioesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	270	Total	C	N	O	S	0	0	0
			2186	1370	388	418	10			
1	BBB	266	Total	C	N	O	S	0	0	0
			2158	1354	383	411	10			
1	CCC	270	Total	C	N	O	S	0	0	0
			2186	1370	388	418	10			
1	DDD	266	Total	C	N	O	S	0	0	0
			2158	1354	383	411	10			

- Molecule 2 is (5 {S})-7-[[2,6-bis(fluoranyl)phenyl]methyl]-3-(3-methylthiophen-2-yl)-1-oxa-2,7-diazaspiro[4.4]non-2-en-6-one (three-letter code: WP2) (formula: $C_{18}H_{16}F_2N_2O_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	AAA	1	Total	C	F	N	O	S	0	0
			25	18	2	2	2	1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	BBB	1	Total	C	F	N	O	S	0	0
			25	18	2	2	2	1		
2	CCC	1	Total	C	F	N	O	S	0	0
			25	18	2	2	2	1		
2	DDD	1	Total	C	F	N	O	S	0	0
			25	18	2	2	2	1		

- Molecule 3 is water.

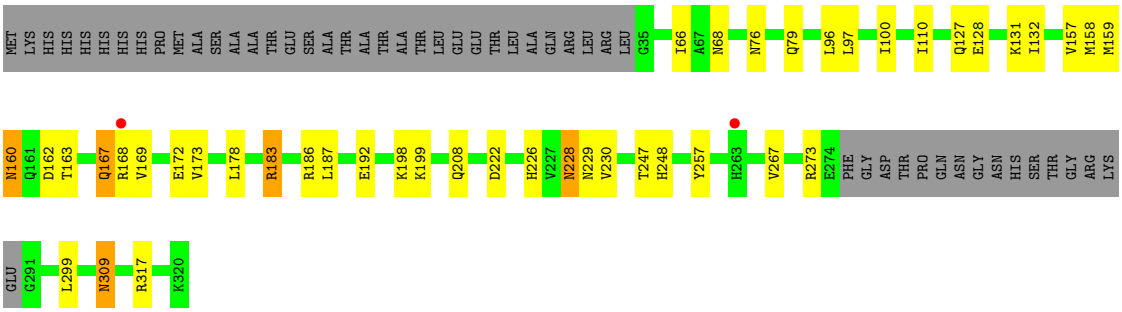
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	155	Total	O	0	0
			155	155		
3	BBB	162	Total	O	0	0
			162	162		
3	CCC	145	Total	O	0	0
			145	145		
3	DDD	138	Total	O	0	0
			138	138		

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.

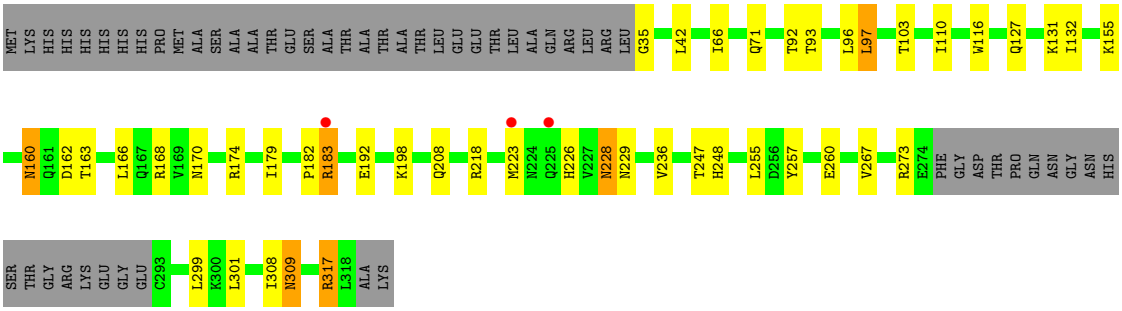
- Molecule 1: Acyl-acp thioesterase

Chain AAA:



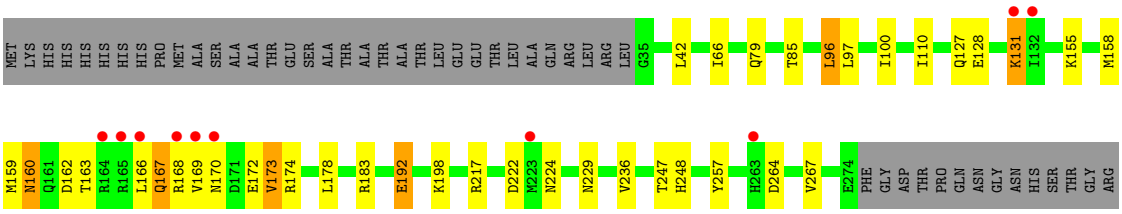
- Molecule 1: Acyl-acp thioesterase

Chain BBB:



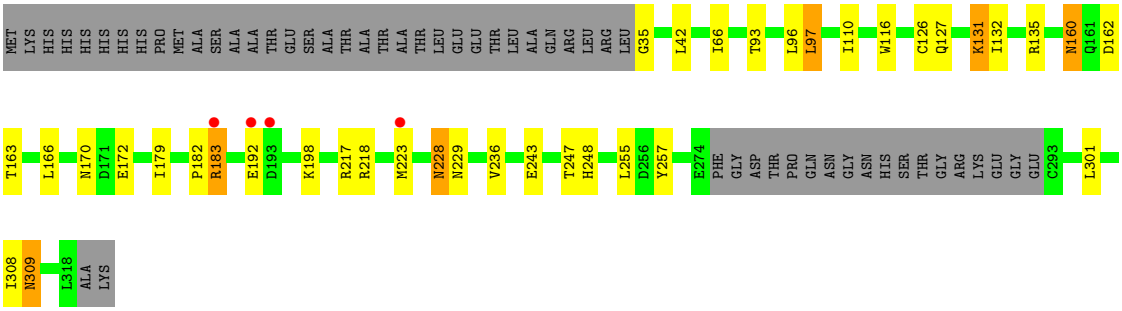
- Molecule 1: Acyl-acp thioesterase

Chain CCC:



• Molecule 1: Acyl-acp thioesterase

Chain DDD:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	80.89Å 52.99Å 148.50Å 90.00° 91.67° 90.00°	Depositor
Resolution (Å)	19.94 – 2.00 19.93 – 2.00	Depositor EDS
% Data completeness (in resolution range)	90.3 (19.94-2.00) 90.4 (19.93-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.45 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.206 , 0.241 0.213 , 0.244	Depositor DCC
R_{free} test set	3734 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å^2)	21.1	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 27.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.189 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9388	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.89% 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: WP2

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	AAA	0.73	0/2228	0.82	0/3014
1	BBB	0.71	0/2200	0.81	1/2979 (0.0%)
1	CCC	0.71	0/2228	0.82	1/3014 (0.0%)
1	DDD	0.70	0/2200	0.82	1/2979 (0.0%)
All	All	0.71	0/8856	0.82	3/11986 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	BBB	218	ARG	NE-CZ-NH1	-5.99	117.31	120.30
1	CCC	312	ARG	NE-CZ-NH1	-5.35	117.62	120.30
1	DDD	218	ARG	NE-CZ-NH1	-5.16	117.72	120.30

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	AAA	2186	0	2156	35	0
1	BBB	2158	0	2129	30	0
1	CCC	2186	0	2156	38	0
1	DDD	2158	0	2129	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	AAA	25	0	0	0	0
2	BBB	25	0	0	0	0
2	CCC	25	0	0	0	0
2	DDD	25	0	0	0	0
3	AAA	155	0	0	9	0
3	BBB	162	0	0	11	0
3	CCC	145	0	0	14	0
3	DDD	138	0	0	9	0
All	All	9388	0	8570	129	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 7.

All (129) 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:BBB:71:GLN:HG2	3:BBB:540:HOH:O	1.50	1.09
1:AAA:158:MET:HE1	1:AAA:173:VAL:HG11	1.66	0.76
1:CCC:158:MET:HE1	1:CCC:169:VAL:HG13	1.68	0.75
1:AAA:158:MET:SD	3:AAA:627:HOH:O	2.45	0.74
1:AAA:158:MET:CE	1:AAA:173:VAL:HG11	2.17	0.74
1:BBB:223:MET:SD	3:BBB:645:HOH:O	2.45	0.74
1:AAA:226:HIS:HD2	3:AAA:513:HOH:O	1.72	0.72
1:BBB:92:THR:HB	3:BBB:529:HOH:O	1.90	0.72
1:CCC:155:LYS:CE	3:CCC:633:HOH:O	2.35	0.72
1:CCC:158:MET:CE	1:CCC:169:VAL:HG13	2.22	0.70
1:DDD:243:GLU:HB3	3:DDD:638:HOH:O	1.91	0.69
1:AAA:158:MET:HE1	1:AAA:169:VAL:HG13	1.76	0.67
1:AAA:158:MET:CE	1:AAA:169:VAL:HG13	2.25	0.67
1:BBB:236:VAL:HG23	3:BBB:524:HOH:O	1.97	0.65
1:CCC:170:ASN:O	1:CCC:173:VAL:HG23	1.98	0.63
1:AAA:172:GLU:HG3	3:AAA:516:HOH:O	1.97	0.62
1:AAA:158:MET:HE1	1:AAA:173:VAL:CG1	2.31	0.60
1:AAA:183:ARG:HD3	1:AAA:183:ARG:H	1.67	0.59
1:DDD:183:ARG:N	1:DDD:183:ARG:HD2	2.17	0.59
1:CCC:183:ARG:HD2	1:CCC:183:ARG:N	2.17	0.59
1:CCC:155:LYS:HD2	3:CCC:633:HOH:O	2.01	0.59
1:BBB:174:ARG:NH2	3:BBB:501:HOH:O	2.36	0.59
1:CCC:264:ASP:HB3	3:CCC:563:HOH:O	2.03	0.58
1:DDD:35:GLY:N	3:DDD:501:HOH:O	2.35	0.58
1:CCC:236:VAL:HG23	3:CCC:505:HOH:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:222:ASP:HB2	3:AAA:504:HOH:O	2.07	0.55
1:CCC:170:ASN:ND2	1:CCC:172:GLU:HG2	2.22	0.54
1:BBB:226:HIS:HE1	3:BBB:555:HOH:O	1.91	0.54
1:CCC:292:GLU:HG2	3:CCC:624:HOH:O	2.05	0.54
1:AAA:160:ASN:HB2	1:AAA:167:GLN:HE22	1.72	0.54
1:CCC:183:ARG:NE	3:CCC:501:HOH:O	2.31	0.54
1:DDD:132:ILE:HG12	1:DDD:166:LEU:HD23	1.90	0.54
1:CCC:170:ASN:HD22	1:CCC:172:GLU:HG2	1.71	0.54
1:DDD:183:ARG:HG3	3:DDD:624:HOH:O	2.07	0.54
1:CCC:229:ASN:ND2	1:CCC:257:TYR:OH	2.41	0.53
1:DDD:217:ARG:HD2	3:DDD:593:HOH:O	2.07	0.53
1:CCC:131:LYS:HE2	3:CCC:625:HOH:O	2.07	0.53
1:DDD:66:ILE:HG21	1:DDD:110:ILE:HD11	1.90	0.52
1:AAA:79:GLN:NE2	3:AAA:502:HOH:O	2.41	0.52
3:AAA:629:HOH:O	1:BBB:223:MET:HG2	2.10	0.52
1:BBB:183:ARG:N	1:BBB:183:ARG:HD2	2.24	0.52
1:CCC:160:ASN:HB2	1:CCC:167:GLN:HE22	1.74	0.51
1:AAA:187:LEU:HD12	1:AAA:187:LEU:N	2.25	0.51
1:AAA:76:ASN:HD21	1:BBB:116:TRP:HE1	1.58	0.51
1:BBB:132:ILE:HG12	1:BBB:166:LEU:HD23	1.92	0.51
1:CCC:155:LYS:HE2	3:CCC:633:HOH:O	2.07	0.51
1:CCC:174:ARG:NH1	1:CCC:178:LEU:HD11	2.26	0.51
1:DDD:35:GLY:HA3	3:DDD:542:HOH:O	2.11	0.51
1:AAA:128:GLU:HB2	1:AAA:178:LEU:HD21	1.93	0.50
1:BBB:71:GLN:CG	3:BBB:540:HOH:O	2.24	0.50
1:DDD:93:THR:HG22	1:DDD:97:LEU:HD22	1.94	0.50
1:BBB:93:THR:HG22	1:BBB:97:LEU:HD22	1.94	0.49
1:AAA:100:ILE:HD11	1:AAA:159:MET:HE2	1.93	0.49
1:CCC:160:ASN:HD22	1:CCC:163:THR:H	1.61	0.49
1:DDD:183:ARG:HD2	1:DDD:183:ARG:H	1.77	0.49
1:BBB:66:ILE:HG21	1:BBB:110:ILE:HD11	1.95	0.49
1:CCC:96:LEU:HD13	3:CCC:540:HOH:O	2.12	0.49
1:DDD:160:ASN:HD22	1:DDD:163:THR:H	1.59	0.49
1:DDD:35:GLY:N	3:DDD:503:HOH:O	2.46	0.48
1:CCC:100:ILE:HD11	1:CCC:159:MET:HE2	1.95	0.48
1:AAA:229:ASN:ND2	1:AAA:257:TYR:OH	2.43	0.47
1:AAA:160:ASN:HD22	1:AAA:163:THR:H	1.63	0.47
1:BBB:160:ASN:HD22	1:BBB:163:THR:H	1.61	0.47
3:CCC:608:HOH:O	1:DDD:223:MET:HE2	2.14	0.47
1:CCC:192:GLU:HG2	3:CCC:575:HOH:O	2.15	0.46
1:BBB:160:ASN:ND2	1:BBB:162:ASP:H	2.12	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:42:LEU:HD13	1:BBB:182:PRO:HA	1.97	0.46
1:DDD:301:LEU:HG	1:DDD:308:ILE:HD11	1.98	0.46
1:AAA:158:MET:HE3	1:AAA:169:VAL:HG13	1.98	0.46
1:BBB:183:ARG:CD	1:BBB:183:ARG:H	2.28	0.46
1:CCC:160:ASN:ND2	1:CCC:162:ASP:H	2.14	0.46
1:AAA:160:ASN:ND2	1:AAA:162:ASP:H	2.14	0.46
1:DDD:160:ASN:ND2	1:DDD:162:ASP:H	2.13	0.46
1:CCC:170:ASN:HB3	1:CCC:173:VAL:HG22	1.97	0.45
1:CCC:299:LEU:HD22	3:CCC:505:HOH:O	2.16	0.45
1:CCC:309:ASN:HD22	1:CCC:309:ASN:C	2.20	0.45
1:CCC:217:ARG:HB3	3:DDD:523:HOH:O	2.17	0.45
1:BBB:183:ARG:N	1:BBB:183:ARG:CD	2.80	0.44
1:AAA:247:THR:OG1	1:AAA:248:HIS:HD2	2.00	0.44
1:BBB:301:LEU:HG	1:BBB:308:ILE:HD11	1.99	0.44
1:AAA:186:ARG:C	1:AAA:187:LEU:HD12	2.38	0.44
1:CCC:128:GLU:HB2	1:CCC:178:LEU:HD21	1.99	0.44
1:AAA:228:ASN:C	1:AAA:228:ASN:HD22	2.21	0.44
1:AAA:66:ILE:HG21	1:AAA:110:ILE:HD11	1.99	0.44
1:AAA:183:ARG:N	1:AAA:183:ARG:CD	2.81	0.44
1:DDD:183:ARG:HA	3:DDD:624:HOH:O	2.18	0.44
1:AAA:309:ASN:C	1:AAA:309:ASN:HD22	2.22	0.43
1:CCC:183:ARG:HD2	1:CCC:183:ARG:H	1.81	0.43
1:BBB:35:GLY:HA3	3:BBB:533:HOH:O	2.19	0.43
1:DDD:183:ARG:H	1:DDD:183:ARG:CD	2.30	0.43
1:BBB:229:ASN:ND2	1:BBB:257:TYR:OH	2.50	0.43
1:DDD:229:ASN:ND2	1:DDD:257:TYR:OH	2.50	0.43
1:DDD:183:ARG:N	1:DDD:183:ARG:CD	2.82	0.43
1:DDD:131:LYS:HD2	3:DDD:587:HOH:O	2.19	0.42
1:DDD:228:ASN:HD22	1:DDD:228:ASN:C	2.22	0.42
1:BBB:309:ASN:C	1:BBB:309:ASN:HD22	2.22	0.42
1:CCC:155:LYS:CD	3:CCC:633:HOH:O	2.58	0.42
1:AAA:183:ARG:H	1:AAA:183:ARG:CD	2.32	0.42
1:AAA:199:LYS:HD3	3:AAA:635:HOH:O	2.19	0.42
1:AAA:229:ASN:N	3:AAA:501:HOH:O	2.40	0.42
1:CCC:267:VAL:CG1	1:CCC:299:LEU:HG	2.50	0.42
1:DDD:309:ASN:HD22	1:DDD:309:ASN:C	2.22	0.42
1:AAA:68:ASN:OD1	1:AAA:230:VAL:HG21	2.19	0.42
1:CCC:42:LEU:HD11	1:CCC:183:ARG:CZ	2.50	0.42
1:CCC:131:LYS:CE	3:CCC:625:HOH:O	2.65	0.41
1:AAA:226:HIS:CD2	3:AAA:513:HOH:O	2.57	0.41
1:CCC:85:THR:HB	1:DDD:116:TRP:CZ3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:228:ASN:C	1:BBB:228:ASN:HD22	2.23	0.41
1:BBB:267:VAL:CG1	1:BBB:299:LEU:HG	2.51	0.41
1:CCC:247:THR:OG1	1:CCC:248:HIS:HD2	2.03	0.41
1:CCC:158:MET:HE3	1:CCC:169:VAL:HG13	2.02	0.41
1:AAA:267:VAL:CG1	1:AAA:299:LEU:HG	2.51	0.41
1:AAA:158:MET:HE2	1:AAA:173:VAL:HG11	2.02	0.41
1:BBB:317:ARG:HD2	3:BBB:562:HOH:O	2.20	0.41
1:DDD:42:LEU:HD13	1:DDD:182:PRO:HA	2.03	0.41
1:DDD:126:CYS:HA	1:DDD:135:ARG:O	2.21	0.41
1:DDD:247:THR:OG1	1:DDD:248:HIS:HD2	2.04	0.41
1:BBB:155:LYS:HB3	3:BBB:625:HOH:O	2.20	0.41
1:BBB:236:VAL:HG21	1:BBB:255:LEU:HD21	2.02	0.41
1:BBB:247:THR:OG1	1:BBB:248:HIS:HD2	2.04	0.41
1:CCC:222:ASP:C	1:CCC:224:ASN:H	2.24	0.41
1:DDD:236:VAL:HG21	1:DDD:255:LEU:HD21	2.02	0.41
1:BBB:208:GLN:NE2	1:BBB:273:ARG:H	2.18	0.40
1:AAA:208:GLN:NE2	1:AAA:273:ARG:H	2.20	0.40
1:CCC:66:ILE:HG21	1:CCC:110:ILE:HD11	2.02	0.40
1:CCC:183:ARG:N	1:CCC:183:ARG:CD	2.83	0.40
1:DDD:42:LEU:HD11	1:DDD:183:ARG:CZ	2.50	0.40
1:AAA:132:ILE:HG13	1:AAA:157:VAL:HG12	2.02	0.40
1:BBB:260:GLU:HG2	3:BBB:502:HOH:O	2.21	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	AAA	266/320 (83%)	262 (98%)	4 (2%)	0	100	100
1	BBB	262/320 (82%)	259 (99%)	3 (1%)	0	100	100
1	CCC	266/320 (83%)	262 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	DDD	262/320 (82%)	259 (99%)	3 (1%)	0	100	100
All	All	1056/1280 (82%)	1042 (99%)	14 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	AAA	242/282 (86%)	229 (95%)	13 (5%)	22	18
1	BBB	240/282 (85%)	225 (94%)	15 (6%)	18	13
1	CCC	242/282 (86%)	228 (94%)	14 (6%)	20	15
1	DDD	240/282 (85%)	227 (95%)	13 (5%)	22	18
All	All	964/1128 (86%)	909 (94%)	55 (6%)	20	16

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	96	LEU
1	AAA	97	LEU
1	AAA	127	GLN
1	AAA	131	LYS
1	AAA	160	ASN
1	AAA	167	GLN
1	AAA	168	ARG
1	AAA	183	ARG
1	AAA	192	GLU
1	AAA	198	LYS
1	AAA	228	ASN
1	AAA	309	ASN
1	AAA	317	ARG
1	BBB	96	LEU
1	BBB	97	LEU
1	BBB	103	THR

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Mol	Chain	Res	Type
1	BBB	127	GLN
1	BBB	131	LYS
1	BBB	160	ASN
1	BBB	168	ARG
1	BBB	170	ASN
1	BBB	179	ILE
1	BBB	183	ARG
1	BBB	192	GLU
1	BBB	198	LYS
1	BBB	228	ASN
1	BBB	309	ASN
1	BBB	317	ARG
1	CCC	79	GLN
1	CCC	96	LEU
1	CCC	97	LEU
1	CCC	127	GLN
1	CCC	131	LYS
1	CCC	160	ASN
1	CCC	166	LEU
1	CCC	167	GLN
1	CCC	168	ARG
1	CCC	173	VAL
1	CCC	192	GLU
1	CCC	198	LYS
1	CCC	309	ASN
1	CCC	317	ARG
1	DDD	96	LEU
1	DDD	97	LEU
1	DDD	127	GLN
1	DDD	131	LYS
1	DDD	160	ASN
1	DDD	170	ASN
1	DDD	172	GLU
1	DDD	179	ILE
1	DDD	183	ARG
1	DDD	192	GLU
1	DDD	198	LYS
1	DDD	228	ASN
1	DDD	309	ASN

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

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 monosaccharides in this entry.

5.6 Ligand geometry

4 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	WP2	BBB	401	-	23,28,28	1.03	2 (8%)	26,42,42	3.35	12 (46%)
2	WP2	AAA	401	-	23,28,28	0.84	1 (4%)	26,42,42	2.74	9 (34%)
2	WP2	CCC	401	-	23,28,28	0.73	0	26,42,42	2.63	9 (34%)
2	WP2	DDD	401	-	23,28,28	1.05	3 (13%)	26,42,42	3.42	14 (53%)

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	WP2	BBB	401	-	-	0/4/35/35	0/4/4/4
2	WP2	AAA	401	-	-	1/4/35/35	0/4/4/4
2	WP2	CCC	401	-	-	0/4/35/35	0/4/4/4
2	WP2	DDD	401	-	-	0/4/35/35	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	DDD	401	WP2	C23-N13	-2.57	1.32	1.34
2	AAA	401	WP2	C25-C7	2.40	1.52	1.50
2	DDD	401	WP2	C11-C12	2.34	1.57	1.52
2	DDD	401	WP2	O9-N8	2.34	1.46	1.42
2	BBB	401	WP2	C6-C7	-2.18	1.44	1.47
2	BBB	401	WP2	O9-N8	2.00	1.45	1.42

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	DDD	401	WP2	C25-C7-N8	-11.33	106.11	113.96
2	BBB	401	WP2	C25-C7-N8	-11.08	106.28	113.96
2	AAA	401	WP2	C25-C7-N8	-9.46	107.41	113.96
2	DDD	401	WP2	C6-C7-N8	7.94	132.55	120.46
2	BBB	401	WP2	C6-C7-N8	6.48	130.32	120.46
2	BBB	401	WP2	O9-N8-C7	5.87	112.80	109.29
2	CCC	401	WP2	C25-C7-N8	-5.62	110.06	113.96
2	DDD	401	WP2	O9-N8-C7	5.45	112.55	109.29
2	CCC	401	WP2	C6-C7-N8	5.11	128.24	120.46
2	CCC	401	WP2	C14-N13-C23	4.88	127.85	123.38
2	CCC	401	WP2	C11-C12-N13	4.88	108.05	103.62
2	CCC	401	WP2	C11-C10-C25	-4.60	109.93	117.89
2	AAA	401	WP2	C6-C7-N8	4.46	127.25	120.46
2	CCC	401	WP2	C12-N13-C23	-4.13	111.23	114.33
2	BBB	401	WP2	C11-C10-C25	-4.05	110.87	117.89
2	BBB	401	WP2	C11-C12-N13	3.90	107.16	103.62
2	DDD	401	WP2	C21-C15-C16	3.80	119.81	114.51
2	AAA	401	WP2	C12-N13-C23	-3.74	111.53	114.33
2	AAA	401	WP2	C11-C12-N13	3.44	106.74	103.62
2	DDD	401	WP2	C11-C10-C25	-3.36	112.06	117.89
2	AAA	401	WP2	C21-C15-C16	3.29	119.10	114.51
2	BBB	401	WP2	C12-N13-C23	-3.26	111.88	114.33
2	CCC	401	WP2	C21-C15-C16	3.17	118.93	114.51
2	BBB	401	WP2	C21-C15-C16	2.90	118.55	114.51
2	AAA	401	WP2	O9-N8-C7	2.83	110.98	109.29
2	BBB	401	WP2	C18-C16-C15	-2.69	119.14	124.02
2	AAA	401	WP2	C1-C2-C3	-2.68	121.42	125.59
2	DDD	401	WP2	C11-C12-N13	2.62	106.00	103.62
2	AAA	401	WP2	C11-C10-C25	-2.58	113.43	117.89
2	DDD	401	WP2	C1-C2-C3	-2.41	121.83	125.59
2	CCC	401	WP2	C18-C16-C15	-2.36	119.74	124.02
2	DDD	401	WP2	F22-C21-C15	2.36	120.44	117.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	BBB	401	WP2	C10-C25-C7	2.35	103.60	101.21
2	AAA	401	WP2	C18-C16-C15	-2.28	119.89	124.02
2	DDD	401	WP2	C12-N13-C23	-2.28	112.62	114.33
2	DDD	401	WP2	C18-C16-C15	-2.27	119.90	124.02
2	DDD	401	WP2	O24-C23-N13	-2.27	123.92	125.87
2	BBB	401	WP2	F22-C21-C15	2.26	120.32	117.63
2	BBB	401	WP2	C14-C15-C16	-2.17	117.44	122.50
2	DDD	401	WP2	C20-C21-C15	-2.12	120.18	124.02
2	DDD	401	WP2	C25-C7-C6	-2.12	121.23	125.07
2	DDD	401	WP2	C10-C25-C7	2.06	103.30	101.21
2	BBB	401	WP2	F17-C16-C18	2.04	123.14	118.59
2	CCC	401	WP2	F17-C16-C15	2.04	120.06	117.63

There are no chirality outliers.

All (1) torsion outliers are listed below:

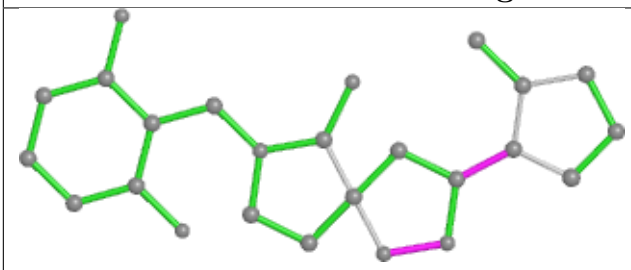
Mol	Chain	Res	Type	Atoms
2	AAA	401	WP2	C15-C14-N13-C12

There are no ring outliers.

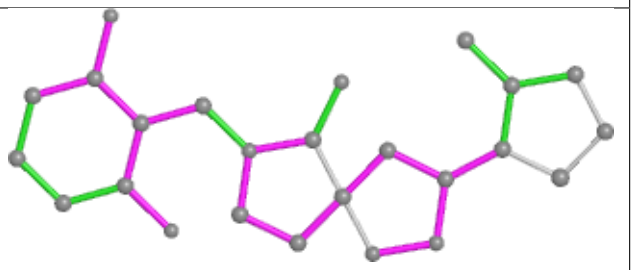
No monomer is involved in short contacts.

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.

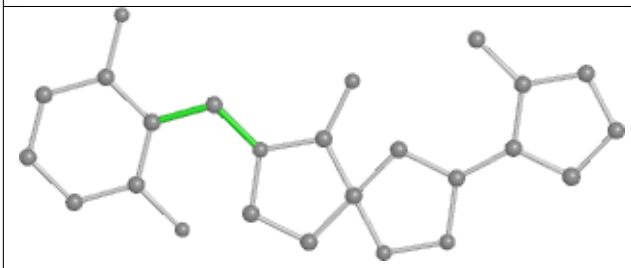
Ligand WP2 BBB 401



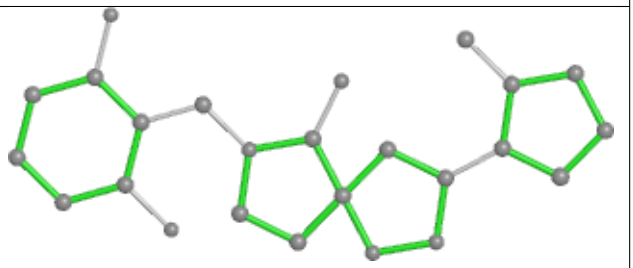
Bond lengths



Bond angles

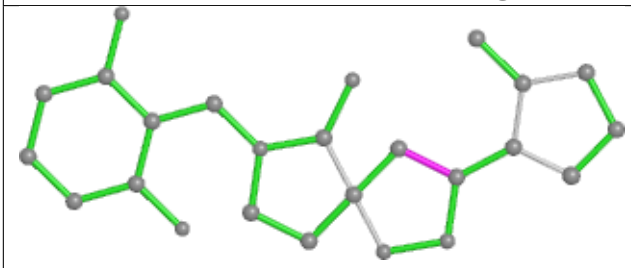


Torsions

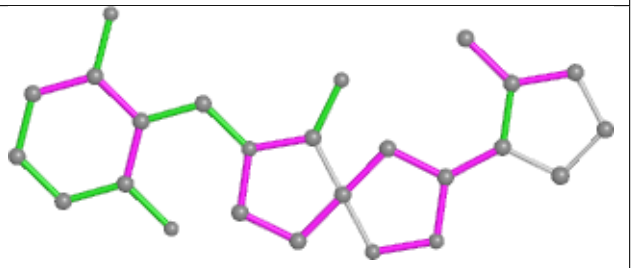


Rings

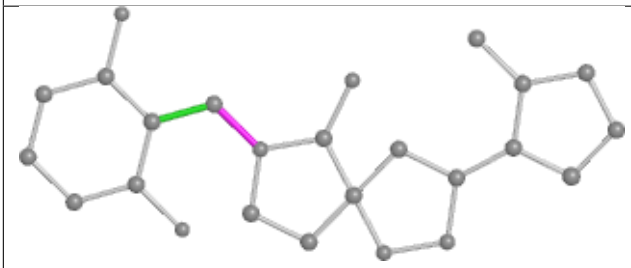
Ligand WP2 AAA 401



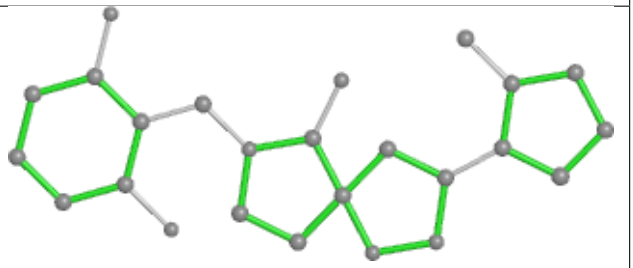
Bond lengths



Bond angles

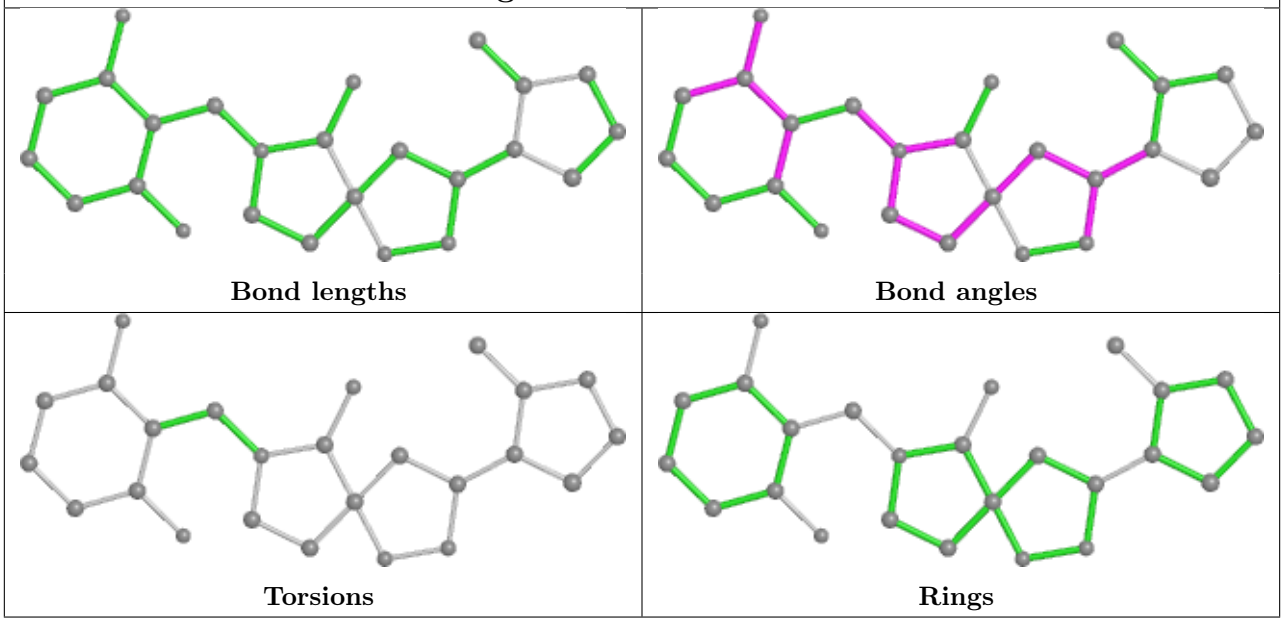


Torsions

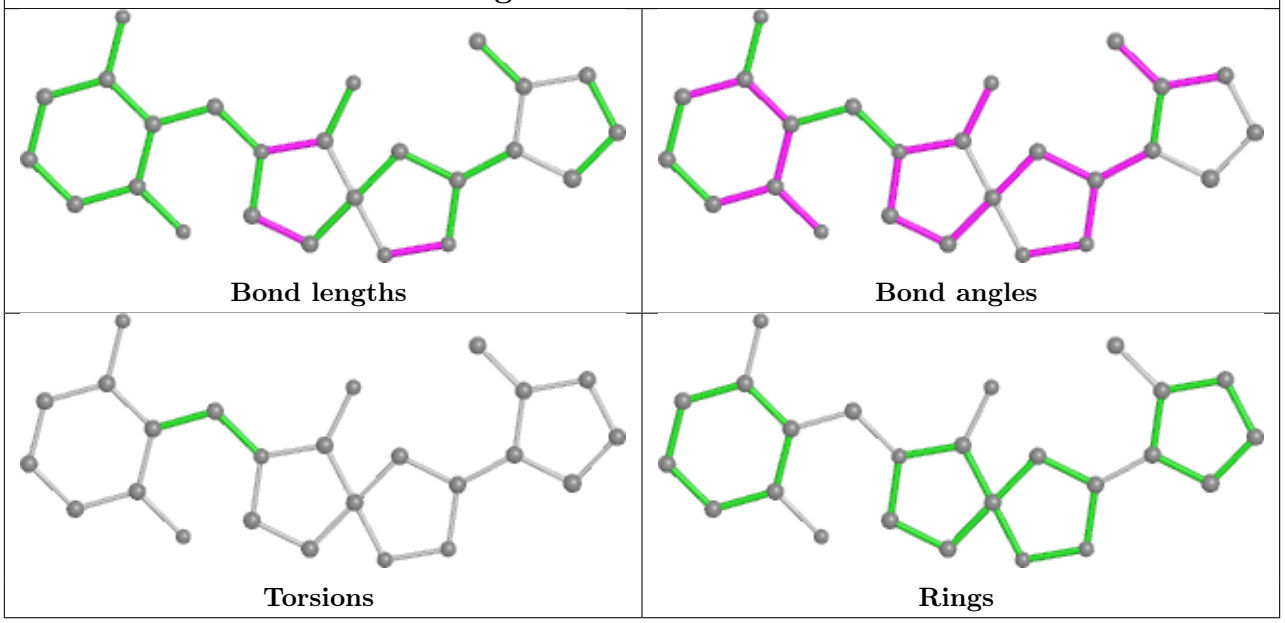


Rings

Ligand WP2 CCC 401



Ligand WP2 DDD 401



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	AAA	270/320 (84%)	-0.33	2 (0%)	87	87	12, 23, 56, 76	0
1	BBB	266/320 (83%)	-0.44	3 (1%)	80	79	13, 21, 42, 60	0
1	CCC	270/320 (84%)	-0.27	10 (3%)	41	41	13, 25, 60, 81	0
1	DDD	266/320 (83%)	-0.41	4 (1%)	73	72	13, 23, 43, 66	0
All	All	1072/1280 (83%)	-0.36	19 (1%)	68	66	12, 23, 51, 81	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DDD	183	ARG	3.8
1	CCC	223	MET	3.5
1	CCC	168	ARG	3.2
1	AAA	168	ARG	3.0
1	CCC	263	HIS	2.8
1	DDD	192	GLU	2.6
1	CCC	131	LYS	2.5
1	BBB	223	MET	2.5
1	AAA	263	HIS	2.4
1	BBB	183	ARG	2.4
1	CCC	132	ILE	2.4
1	DDD	193	ASP	2.3
1	CCC	164	ARG	2.3
1	CCC	166	LEU	2.2
1	CCC	170	ASN	2.1
1	CCC	165	ARG	2.1
1	DDD	223	MET	2.1
1	CCC	169	VAL	2.1
1	BBB	225	GLN	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)

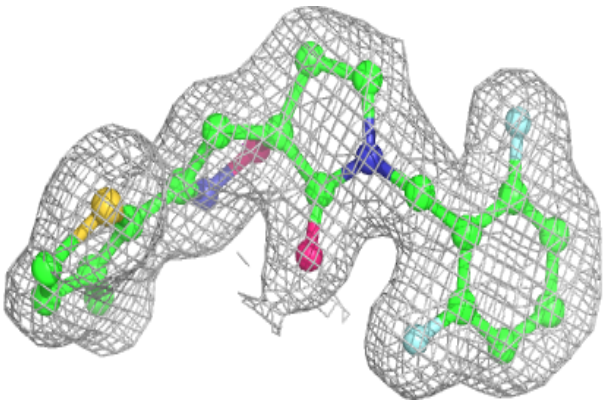
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

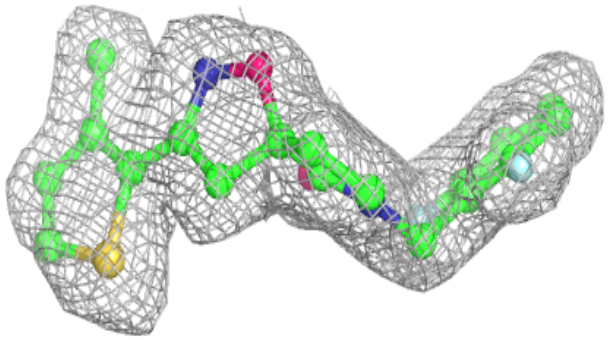
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	WP2	CCC	401	25/25	0.94	0.10	21,26,30,32	0
2	WP2	BBB	401	25/25	0.96	0.10	18,21,25,26	0
2	WP2	AAA	401	25/25	0.97	0.08	19,20,28,30	0
2	WP2	DDD	401	25/25	0.97	0.09	17,22,30,31	0

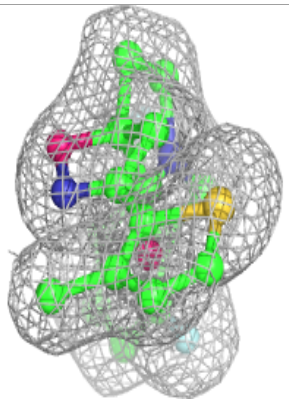
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around WP2 CCC 401:

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

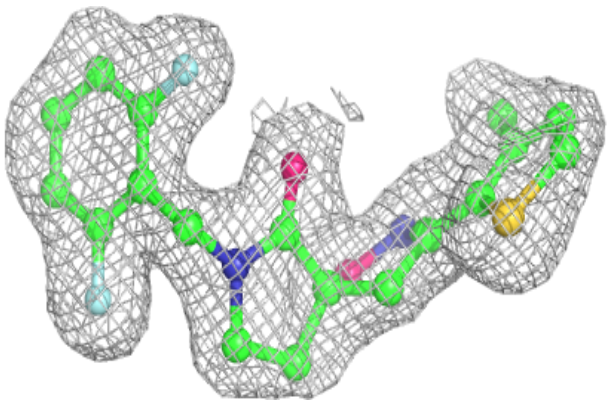


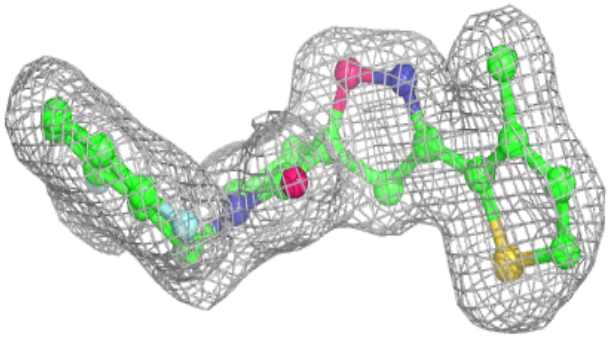


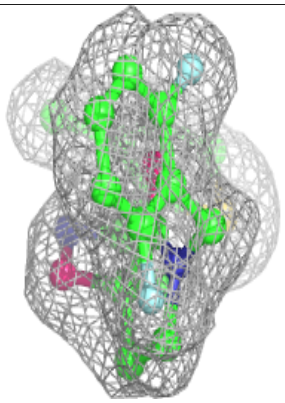


Electron density around WP2 BBB 401:

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

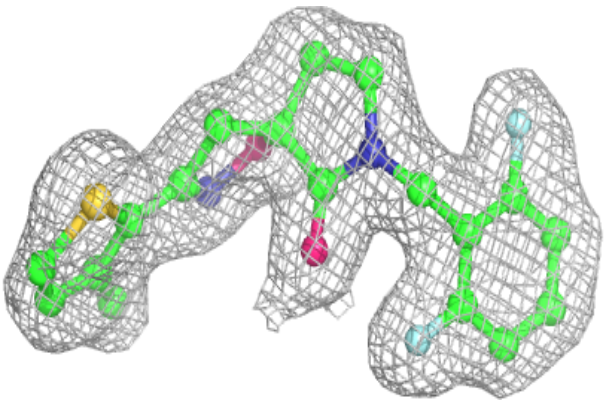


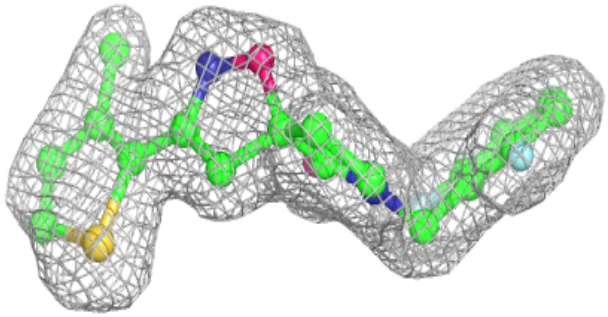


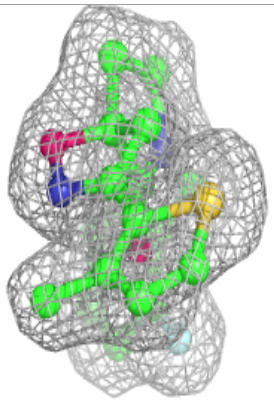


Electron density around WP2 AAA 401:

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

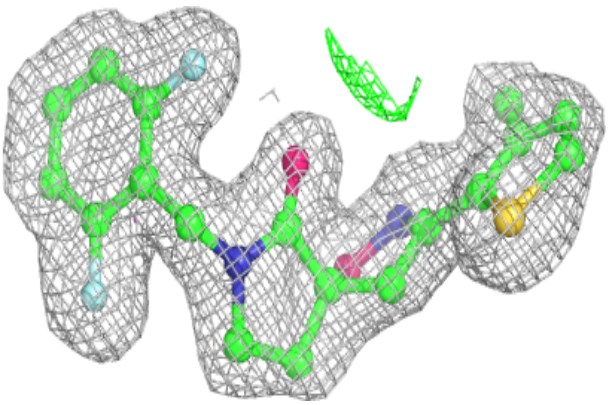


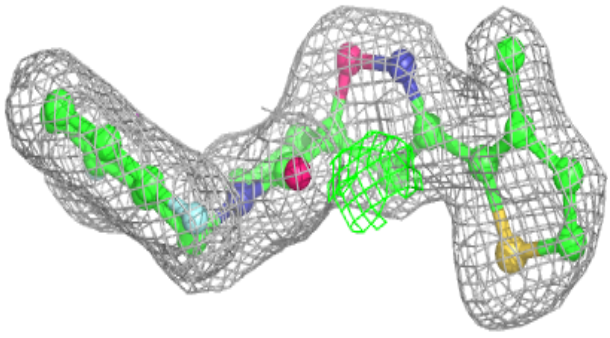


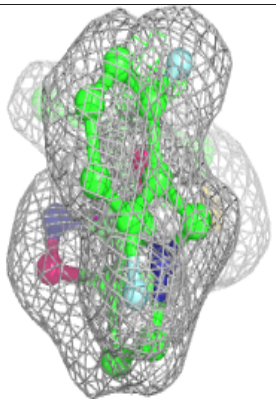


Electron density around WP2 DDD 401:

$2mF_o$-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.