Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 06:47 PM EDT

PDB ID	:	2WP6
Title	:	Trypanosoma brucei trypanothione reductase in complex with 3,4- dihydro-quinazoline inhibitor (DDD00071494)
Authors	:	Alphey, M.S.; Patterson, S.; Fairlamb, A.H.
Deposited on	:	2009-08-03
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 ⓘ 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:

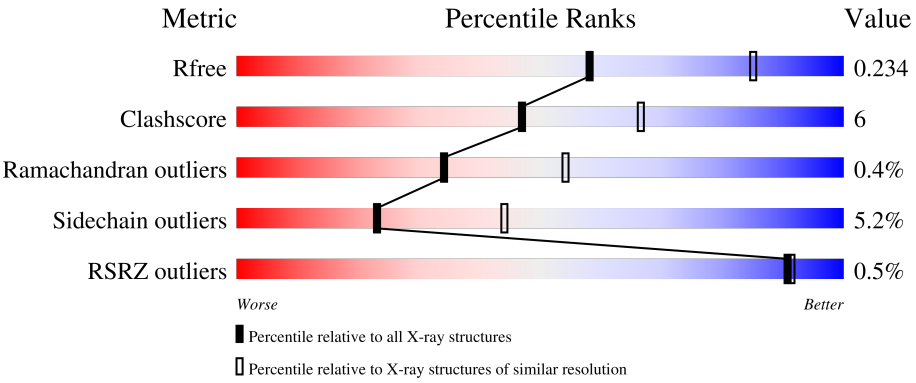
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	495	86% 13%
1	B	495	83% 14%
1	C	495	80% 16%
1	D	495	84% 14%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	WP6	A	1000	-	-	X	-
3	WP6	B	1000	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 16217 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.

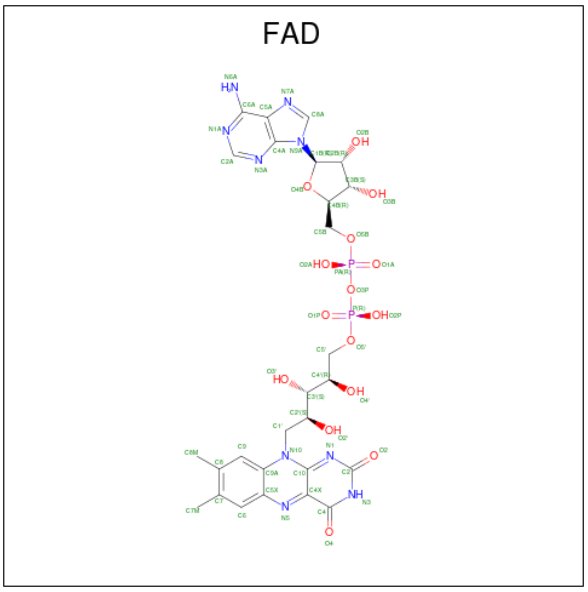
- Molecule 1 is a protein called TRYPANOTHIONE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	490	Total 3745	C 2384	N 636	O 705	S 20	0	3	0
1	B	488	Total 3744	C 2383	N 636	O 706	S 19	0	6	0
1	C	488	Total 3744	C 2383	N 635	O 707	S 19	0	6	0
1	D	489	Total 3752	C 2387	N 637	O 708	S 20	0	7	0

There are 12 discrepancies between the modelled and reference sequences:

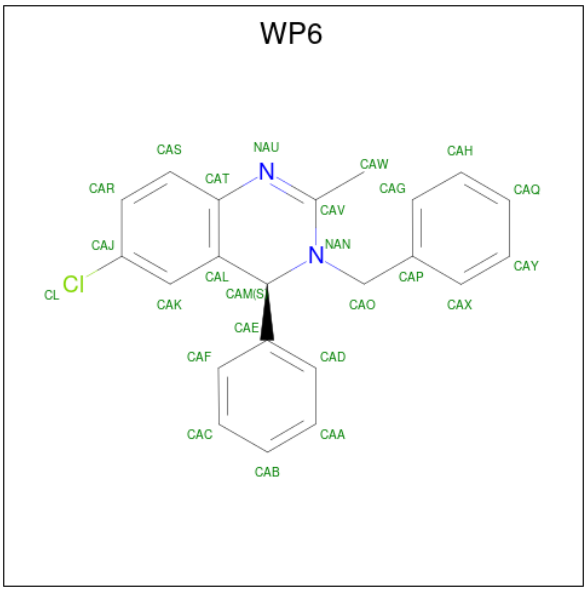
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q389T8
A	-1	SER	-	expression tag	UNP Q389T8
A	0	HIS	-	expression tag	UNP Q389T8
B	-2	GLY	-	expression tag	UNP Q389T8
B	-1	SER	-	expression tag	UNP Q389T8
B	0	HIS	-	expression tag	UNP Q389T8
C	-2	GLY	-	expression tag	UNP Q389T8
C	-1	SER	-	expression tag	UNP Q389T8
C	0	HIS	-	expression tag	UNP Q389T8
D	-2	GLY	-	expression tag	UNP Q389T8
D	-1	SER	-	expression tag	UNP Q389T8
D	0	HIS	-	expression tag	UNP Q389T8

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is (4S)-3-BENZYL-6-CHLORO-2-METHYL-4-PHENYL-3,4-DIHYDROQUINAZOLINE (three-letter code: WP6) (formula: $C_{22}H_{19}ClN_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	0	0
			25	22	1	2		
3	B	1	Total	C	Cl	N	0	0
			25	22	1	2		
3	C	1	Total	C	Cl	N	0	0
			25	22	1	2		
3	D	1	Total	C	Cl	N	0	0
			25	22	1	2		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	B	1	Total	Cl	0	0
			1	1		
4	C	2	Total	Cl	0	0
			2	2		
4	D	1	Total	Cl	0	0
			1	1		

- Molecule 5 is water.

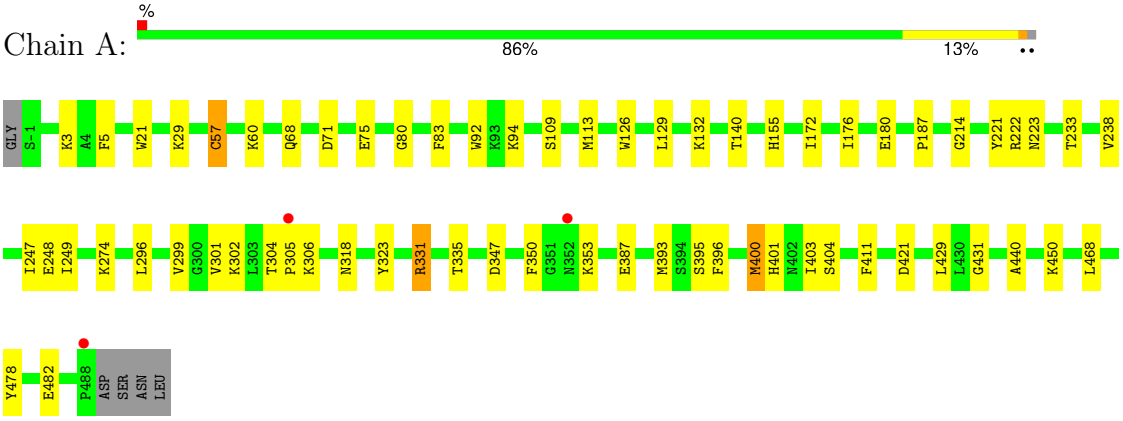
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	272	Total	O	0	0
			272	272		
5	B	211	Total	O	0	0
			211	211		
5	C	197	Total	O	0	0
			197	197		
5	D	235	Total	O	0	0
			235	235		

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.

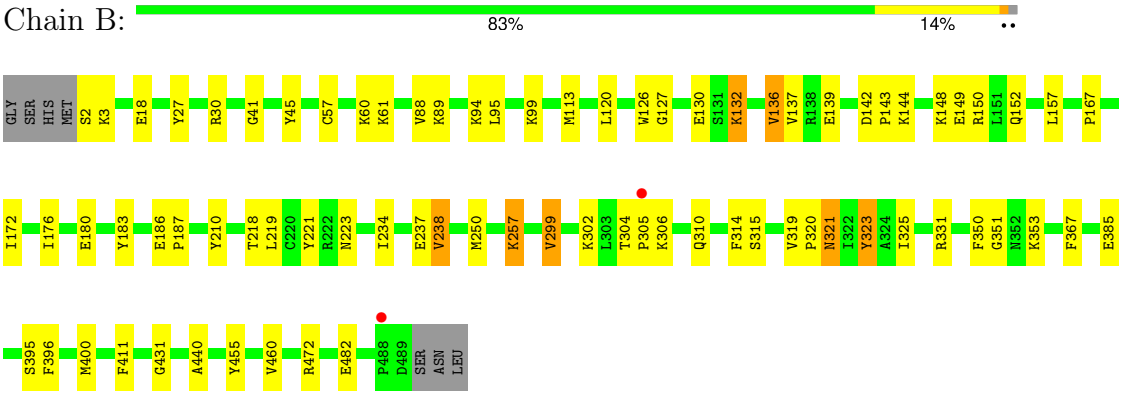
• Molecule 1: TRYPANOTHIONE REDUCTASE

Chain A:



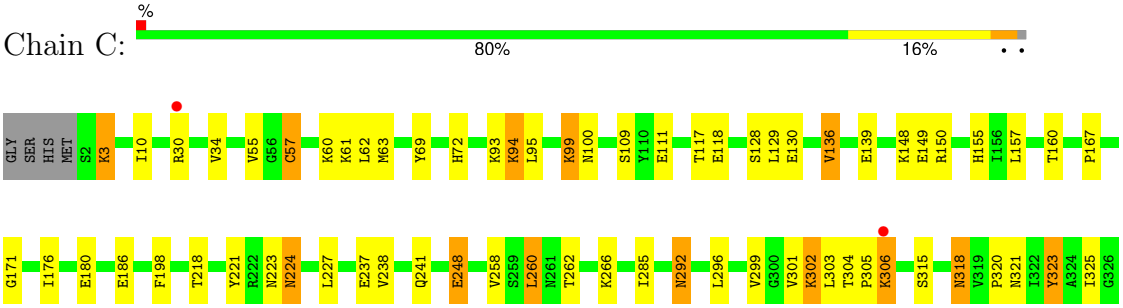
• Molecule 1: TRYPANOTHIONE REDUCTASE

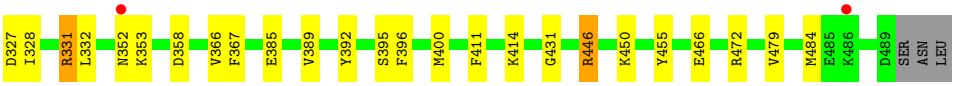
Chain B:



• Molecule 1: TRYPANOTHIONE REDUCTASE

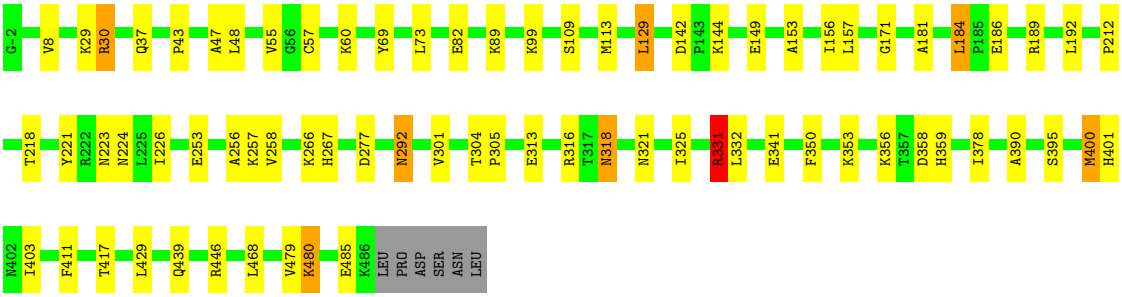
Chain C:





• Molecule 1: TRYPANOTHIONE REDUCTASE

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	101.65Å 63.21Å 170.50Å 90.00° 97.82° 90.00°	Depositor
Resolution (Å)	46.77 – 2.50 46.77 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.77-2.50) 99.9 (46.77-2.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.04 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.163 , 0.236 0.162 , 0.234	Depositor DCC
R_{free} test set	3741 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	24.8	Xtriage
Anisotropy	0.445	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 38.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16217	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.60% 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: WP6, FAD, CL

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	0.87	0/3834	0.81	1/5200 (0.0%)
1	B	0.80	0/3841	0.79	1/5211 (0.0%)
1	C	0.79	0/3841	0.79	2/5212 (0.0%)
1	D	0.83	0/3852	0.81	4/5223 (0.1%)
All	All	0.83	0/15368	0.80	8/20846 (0.0%)

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	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	347	ASP	CB-CG-OD1	6.32	123.99	118.30
1	C	260	LEU	CA-CB-CG	5.58	128.13	115.30
1	D	316	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	D	358	ASP	CB-CG-OD1	5.14	122.93	118.30
1	C	327	ASP	CB-CG-OD1	5.07	122.86	118.30
1	D	331[A]	ARG	NE-CZ-NH1	-5.04	117.78	120.30
1	D	331[B]	ARG	NE-CZ-NH1	-5.04	117.78	120.30
1	B	460	VAL	CB-CA-C	-5.00	101.90	111.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	214	GLY	Peptide
1	B	350	PHE	Peptide

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	3745	0	3760	48	0
1	B	3744	0	3756	45	0
1	C	3744	0	3758	52	0
1	D	3752	0	3765	48	0
2	A	53	0	31	1	0
2	B	53	0	31	0	0
2	C	53	0	31	2	0
2	D	53	0	31	0	0
3	A	25	0	19	9	0
3	B	25	0	19	9	0
3	C	25	0	19	0	0
3	D	25	0	19	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
4	D	1	0	0	0	0
5	A	272	0	0	3	0
5	B	211	0	0	3	0
5	C	197	0	0	2	0
5	D	235	0	0	5	0
All	All	16217	0	15239	188	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 6.

All (188) 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:113:MET:CE	3:A:1000:WP6:HAO1	1.77	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:PRO:O	1:B:321:ASN:ND2	2.01	0.94
1:A:113:MET:HE3	3:A:1000:WP6:HAO1	1.50	0.89
1:B:302:LYS:HD3	1:B:310:GLN:HE22	1.38	0.87
1:A:331[A]:ARG:NH2	5:A:2203:HOH:O	2.13	0.80
1:A:233:THR:HG21	1:A:393:MET:CE	2.14	0.77
1:A:83:PHE:HB3	1:B:88:VAL:HG22	1.66	0.77
1:D:318:ASN:H	1:D:318:ASN:HD22	1.31	0.77
1:A:113:MET:CE	3:A:1000:WP6:CAO	2.61	0.77
1:A:233:THR:HG21	1:A:393:MET:HE3	1.65	0.76
1:B:302:LYS:HD3	1:B:310:GLN:NE2	2.00	0.75
1:D:331[B]:ARG:HH21	1:D:331[B]:ARG:CG	2.01	0.73
1:B:113:MET:HE3	3:B:1000:WP6:CAP	2.17	0.73
1:A:113:MET:HE3	3:A:1000:WP6:CAO	2.17	0.73
1:B:113:MET:CE	3:B:1000:WP6:HAO1	2.20	0.71
1:D:304:THR:HB	1:D:305:PRO:CD	2.22	0.70
1:B:234:ILE:O	1:B:238:VAL:HG12	1.92	0.70
1:A:29:LYS:HD2	1:A:350:PHE:CD1	2.29	0.68
1:D:181:ALA:HA	1:D:184:LEU:HD22	1.75	0.68
1:A:113:MET:HE1	3:A:1000:WP6:HAO1	1.76	0.67
1:D:142:ASP:OD1	1:D:144[B]:LYS:HG2	1.95	0.66
1:A:129:LEU:HD23	1:A:299:VAL:HG21	1.77	0.64
1:B:130:GLU:HB2	1:B:136:VAL:CG2	2.28	0.64
1:D:341:GLU:OE2	1:D:359:HIS:HE1	1.80	0.64
1:D:301:VAL:HA	1:D:318:ASN:HD21	1.64	0.63
1:D:157:LEU:HD11	1:D:325:ILE:HG12	1.80	0.63
1:B:455[A]:TYR:CZ	1:B:472:ARG:HG3	2.34	0.62
1:B:237:GLU:OE1	5:B:2093:HOH:O	2.15	0.62
1:D:390:ALA:HB3	1:D:417:THR:OG1	2.00	0.62
1:D:400:MET:HG3	1:D:401:HIS:N	2.15	0.61
1:A:94:LYS:HG3	5:B:2028:HOH:O	1.99	0.61
1:A:302:LYS:H	1:A:318:ASN:ND2	1.98	0.61
1:C:301:VAL:HA	1:C:318:ASN:HD21	1.65	0.60
1:C:117:THR:O	5:C:2035:HOH:O	2.16	0.60
1:B:27:TYR:CE1	1:B:351:GLY:O	2.55	0.60
1:C:93:LYS:NZ	1:C:186[B]:GLU:CD	2.55	0.59
1:D:429:LEU:HD21	1:D:468:LEU:HD21	1.85	0.59
1:B:120:LEU:O	5:B:2038:HOH:O	2.17	0.58
1:D:253:GLU:HA	5:D:2137:HOH:O	2.03	0.58
1:C:93:LYS:HZ1	1:C:186[B]:GLU:CD	2.06	0.58
1:D:331[B]:ARG:CG	1:D:331[B]:ARG:NH2	2.66	0.58
1:A:113:MET:HE3	3:A:1000:WP6:CAP	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:ASP:O	1:A:75:GLU:HG3	2.04	0.57
1:B:113:MET:CE	3:B:1000:WP6:CAP	2.83	0.57
1:C:34:VAL:HG12	2:C:998:FAD:H2A	1.87	0.56
1:C:296:LEU:HD12	1:C:303:LEU:HD21	1.86	0.56
1:B:218:THR:HG21	1:B:250:MET:CE	2.35	0.56
1:A:318:ASN:HD22	1:A:318:ASN:H	1.54	0.56
1:A:301:VAL:HA	1:A:318:ASN:HD21	1.71	0.56
1:D:304:THR:HB	1:D:305:PRO:HD3	1.87	0.55
1:B:126:TRP:O	1:B:137:VAL:HA	2.06	0.55
1:B:113:MET:HE3	3:B:1000:WP6:HAO1	1.89	0.54
1:A:429:LEU:HD21	1:A:468:LEU:HD21	1.88	0.54
1:A:221:TYR:CE2	1:A:223:ASN:HB2	2.43	0.54
1:A:302:LYS:H	1:A:318:ASN:HD21	1.55	0.54
1:D:331[B]:ARG:NH2	1:D:331[B]:ARG:HG3	2.23	0.54
1:C:160:THR:OG1	1:C:328:ILE:HD12	2.08	0.54
1:D:318:ASN:HD22	1:D:318:ASN:N	2.03	0.53
1:B:299:VAL:HG23	1:B:319:VAL:HG21	1.90	0.53
1:A:304:THR:HB	1:A:305:PRO:HD2	1.90	0.53
1:D:331[B]:ARG:HH21	1:D:331[B]:ARG:HG2	1.74	0.52
1:B:315:SER:O	1:B:323:TYR:HB3	2.09	0.52
1:A:440:ALA:HB3	1:B:440:ALA:HB3	1.90	0.52
1:C:198:PHE:HB2	1:C:366:VAL:HG13	1.91	0.52
1:C:304:THR:HB	1:C:305:PRO:HD2	1.91	0.52
1:C:292:ASN:ND2	1:C:292:ASN:H	2.07	0.52
1:D:331[B]:ARG:HH21	1:D:331[B]:ARG:HG3	1.73	0.52
1:A:129:LEU:HD22	1:A:296:LEU:HD23	1.92	0.52
1:B:113:MET:CE	3:B:1000:WP6:CAO	2.88	0.52
1:B:113:MET:HE3	3:B:1000:WP6:CAO	2.41	0.51
1:B:148:LYS:C	1:B:149:GLU:HG2	2.31	0.51
1:C:218:THR:HG23	1:C:248:GLU:HG2	1.91	0.51
1:B:148:LYS:O	1:B:149:GLU:HG2	2.10	0.51
1:C:63:MET:HG2	1:C:95:LEU:HD21	1.92	0.51
1:A:21:TRP:CD1	3:A:1000:WP6:HAW2	2.45	0.51
1:D:257:LYS:HE3	5:D:2141:HOH:O	2.10	0.50
1:A:172:ILE:O	1:A:172:ILE:HG13	2.11	0.50
1:C:304:THR:C	1:C:306:LYS:H	2.15	0.50
1:B:142:ASP:C	1:B:144:LYS:H	2.15	0.50
1:B:127:GLY:HA2	1:B:136:VAL:O	2.12	0.50
1:C:171:GLY:HA3	1:C:258:VAL:O	2.12	0.49
1:D:189:ARG:HA	1:D:212:PRO:HD2	1.93	0.49
1:C:411:PHE:CD1	1:C:431:GLY:HA3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:TYR:HA	1:A:482:GLU:O	2.12	0.49
1:C:302:LYS:H	1:C:318:ASN:ND2	2.11	0.49
1:B:314:PHE:O	1:B:315:SER:HB2	2.12	0.49
1:C:99:LYS:HD2	1:C:100:ASN:N	2.27	0.49
1:B:455[A]:TYR:CE1	1:B:472:ARG:HG3	2.48	0.49
1:B:411:PHE:CD1	1:B:431:GLY:HA3	2.48	0.48
1:A:113:MET:CE	3:A:1000:WP6:CAP	2.91	0.48
1:A:176:ILE:HB	1:A:180:GLU:HB2	1.96	0.48
1:A:129:LEU:HD23	1:A:299:VAL:CG2	2.41	0.48
1:C:62:LEU:HD13	1:D:403:ILE:CD1	2.44	0.48
1:D:129:LEU:HD11	1:D:156:ILE:HG21	1.95	0.48
1:C:221:TYR:CE2	1:C:223:ASN:HB2	2.49	0.48
1:A:401:HIS:HA	1:A:404:SER:OG	2.14	0.48
1:C:3:LYS:HA	1:C:3:LYS:HD3	1.55	0.48
1:A:68:GLN:NE2	5:A:2038:HOH:O	2.45	0.48
1:B:221:TYR:CE2	1:B:223:ASN:HB2	2.48	0.47
1:B:186:GLU:HB2	1:B:187:PRO:HD2	1.97	0.47
1:C:479:VAL:HB	1:C:484:MET:CE	2.44	0.47
1:D:30:ARG:HG3	1:D:30:ARG:HH11	1.79	0.47
1:B:257:LYS:HB3	1:B:257:LYS:HE3	1.55	0.47
1:D:192:LEU:HA	1:D:218:THR:O	2.15	0.47
1:B:176:ILE:HB	1:B:180:GLU:HB2	1.97	0.47
1:C:227:LEU:HD12	1:C:238:VAL:HG11	1.97	0.47
1:C:320:PRO:O	1:C:321[B]:ASN:OD1	2.33	0.47
1:C:358:ASP:OD2	1:C:446:ARG:NH2	2.48	0.46
1:B:130:GLU:HB2	1:B:136:VAL:HG22	1.96	0.46
1:B:157:LEU:HD11	1:B:325:ILE:HG12	1.97	0.46
1:C:57:CYS:HB3	2:C:998:FAD:C4	2.46	0.46
1:C:62:LEU:HD13	1:D:403:ILE:HD11	1.96	0.46
1:D:29:LYS:HE3	1:D:350:PHE:CD1	2.50	0.46
1:D:47:ALA:O	1:D:48:LEU:C	2.53	0.46
1:A:233:THR:HG21	1:A:393:MET:HE1	1.93	0.46
1:B:18:GLU:OE1	3:B:1000:WP6:NAU	2.49	0.46
1:C:148:LYS:O	1:C:149:GLU:HG2	2.15	0.46
1:D:331[B]:ARG:HB3	1:D:332:LEU:H	1.54	0.46
1:A:400:MET:HG3	1:A:401:HIS:N	2.31	0.46
1:C:331:ARG:HB3	1:C:332:LEU:H	1.64	0.46
1:A:318:ASN:ND2	1:A:318:ASN:H	2.14	0.45
1:C:396:PHE:CD1	1:C:396:PHE:N	2.85	0.45
1:A:421:ASP:O	1:A:450:LYS:HD3	2.17	0.45
1:C:61:LYS:NZ	5:C:2015:HOH:O	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:221:TYR:CE2	1:D:223:ASN:HB2	2.51	0.45
1:B:395:SER:O	1:B:396:PHE:HB3	2.17	0.45
1:A:155:HIS:HB3	1:A:323:TYR:HE2	1.82	0.45
1:D:313:GLU:HB3	1:D:356:LYS:HD2	1.99	0.45
1:A:80:GLY:HA2	1:B:94:LYS:HG2	1.98	0.44
1:A:126:TRP:CD1	1:A:140:THR:HA	2.53	0.44
1:C:157:LEU:HD11	1:C:325:ILE:HG12	1.99	0.44
1:A:3:LYS:HB2	1:A:5:PHE:CE2	2.52	0.44
1:A:132:LYS:HB2	5:A:2071:HOH:O	2.17	0.44
1:C:99:LYS:HD2	1:C:99:LYS:C	2.38	0.44
1:D:256:ALA:O	1:D:257:LYS:HB3	2.17	0.44
1:D:479:VAL:O	1:D:480:LYS:C	2.55	0.44
1:A:113:MET:HE1	3:A:1000:WP6:CAO	2.43	0.44
1:C:455[A]:TYR:CZ	1:C:472:ARG:HD3	2.53	0.44
1:A:274:LYS:HE3	1:A:274:LYS:HB2	1.53	0.44
1:C:130:GLU:HB2	1:C:136:VAL:CG2	2.47	0.44
1:D:341:GLU:OE2	1:D:359:HIS:CE1	2.68	0.44
1:B:218:THR:HG21	1:B:250:MET:HE2	1.99	0.43
1:D:8:VAL:CG2	1:D:153:ALA:HB2	2.47	0.43
1:D:446:ARG:NH1	5:D:2207:HOH:O	2.45	0.43
1:B:2:SER:C	1:B:3:LYS:HG2	2.39	0.43
3:B:1000:WP6:HAM	3:B:1000:WP6:HAX	1.99	0.43
1:D:292:ASN:HB2	5:D:2155:HOH:O	2.18	0.43
1:D:267:HIS:ND1	1:D:277:ASP:OD2	2.46	0.43
1:D:378:ILE:HG12	5:D:2188:HOH:O	2.19	0.43
1:A:57:CYS:HB3	2:A:998:FAD:C4	2.49	0.43
1:D:304:THR:CB	1:D:305:PRO:CD	2.93	0.43
1:C:93:LYS:NZ	1:C:186[B]:GLU:OE1	2.52	0.43
1:D:331[A]:ARG:HB3	1:D:332:LEU:H	1.59	0.42
1:A:395:SER:HA	1:A:411:PHE:O	2.18	0.42
1:C:237:GLU:O	1:C:241:GLN:HG3	2.19	0.42
1:C:395:SER:HA	1:C:411:PHE:O	2.19	0.42
1:C:148:LYS:C	1:C:149:GLU:HG2	2.40	0.42
1:A:247:ILE:HG22	1:A:249:ILE:HD12	2.01	0.42
1:D:69:TYR:O	1:D:73:LEU:HG	2.19	0.42
1:C:61:LYS:HE3	1:C:367:PHE:CE1	2.55	0.42
1:C:94:LYS:NZ	1:D:82:GLU:OE2	2.51	0.42
1:D:109:SER:O	1:D:113:MET:HG3	2.20	0.42
1:A:411:PHE:CD1	1:A:431:GLY:HA3	2.55	0.42
1:C:69:TYR:HA	1:C:72:HIS:HB2	2.02	0.42
1:C:315:SER:O	1:C:323:TYR:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:LYS:HE3	1:B:367:PHE:CE1	2.55	0.41
1:C:176:ILE:HB	1:C:180:GLU:HB2	2.02	0.41
1:A:92:TRP:HB3	1:A:187:PRO:HD3	2.03	0.41
1:B:304:THR:O	1:B:305:PRO:C	2.57	0.41
1:C:299:VAL:HG23	1:C:301:VAL:HG23	2.02	0.41
1:B:219:LEU:C	1:B:219:LEU:HD23	2.41	0.41
1:C:167:PRO:HD3	1:C:285:ILE:CD1	2.50	0.41
1:D:171:GLY:HA3	1:D:258:VAL:O	2.21	0.41
1:C:292:ASN:H	1:C:292:ASN:HD22	1.68	0.41
1:C:392:TYR:O	1:C:414:LYS:HA	2.21	0.41
1:B:167:PRO:HD2	1:B:172:ILE:HD11	2.03	0.41
1:C:155:HIS:HB3	1:C:323:TYR:HE2	1.86	0.41
1:D:318:ASN:N	1:D:318:ASN:ND2	2.66	0.41
1:B:95:LEU:HD22	1:B:210:TYR:CZ	2.56	0.40
1:D:37:GLN:OE1	1:D:43:PRO:HD2	2.20	0.40
1:A:396:PHE:CD1	1:A:396:PHE:N	2.89	0.40
1:B:41:GLY:HA2	1:B:183:TYR:CZ	2.57	0.40
1:C:237:GLU:HG3	1:C:241:GLN:HE21	1.87	0.40
1:C:466:GLU:HA	1:D:439:GLN:OE1	2.21	0.40
1:C:479:VAL:HB	1:C:484:MET:HE3	2.02	0.40
1:D:395:SER:HA	1:D:411:PHE:O	2.22	0.40
3:B:1000:WP6:HAW1	3:B:1000:WP6:HAO2	1.90	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	491/495 (99%)	473 (96%)	18 (4%)	0	100	100
1	B	492/495 (99%)	471 (96%)	18 (4%)	3 (1%)	25	43
1	C	492/495 (99%)	471 (96%)	19 (4%)	2 (0%)	34	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	494/495 (100%)	472 (96%)	19 (4%)	3 (1%)	25 43
All	All	1969/1980 (99%)	1887 (96%)	74 (4%)	8 (0%)	34 54

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	352	ASN
1	B	132	LYS
1	D	480	LYS
1	B	45	TYR
1	B	143	PRO
1	C	55	VAL
1	D	226	ILE
1	D	55	VAL

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	406/407 (100%)	392 (97%)	14 (3%)	37 63
1	B	406/407 (100%)	384 (95%)	22 (5%)	22 42
1	C	407/407 (100%)	373 (92%)	34 (8%)	11 21
1	D	407/407 (100%)	386 (95%)	21 (5%)	23 44
All	All	1626/1628 (100%)	1535 (94%)	91 (6%)	23 40

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	CYS
1	A	60	LYS
1	A	109	SER
1	A	222	ARG
1	A	238	VAL
1	A	248	GLU

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Mol	Chain	Res	Type
1	A	306	LYS
1	A	331[A]	ARG
1	A	331[B]	ARG
1	A	335	THR
1	A	353	LYS
1	A	387	GLU
1	A	400	MET
1	A	403	ILE
1	B	30	ARG
1	B	57	CYS
1	B	60	LYS
1	B	89	LYS
1	B	99	LYS
1	B	132	LYS
1	B	136	VAL
1	B	139[A]	GLU
1	B	139[B]	GLU
1	B	150	ARG
1	B	152	GLN
1	B	238	VAL
1	B	257	LYS
1	B	299	VAL
1	B	306	LYS
1	B	321	ASN
1	B	323	TYR
1	B	331	ARG
1	B	353	LYS
1	B	385	GLU
1	B	400	MET
1	B	482	GLU
1	C	3	LYS
1	C	10	ILE
1	C	30[A]	ARG
1	C	30[B]	ARG
1	C	57	CYS
1	C	60	LYS
1	C	94	LYS
1	C	99	LYS
1	C	109	SER
1	C	111	GLU
1	C	118	GLU
1	C	128	SER

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Mol	Chain	Res	Type
1	C	129	LEU
1	C	136	VAL
1	C	139	GLU
1	C	150	ARG
1	C	224[A]	ASN
1	C	224[B]	ASN
1	C	248	GLU
1	C	260	LEU
1	C	262	THR
1	C	266	LYS
1	C	292	ASN
1	C	302	LYS
1	C	306	LYS
1	C	318	ASN
1	C	323	TYR
1	C	331	ARG
1	C	353	LYS
1	C	385	GLU
1	C	389	VAL
1	C	400	MET
1	C	446	ARG
1	C	450	LYS
1	D	30	ARG
1	D	57	CYS
1	D	60	LYS
1	D	89	LYS
1	D	99	LYS
1	D	129	LEU
1	D	149	GLU
1	D	184	LEU
1	D	186	GLU
1	D	224[A]	ASN
1	D	224[B]	ASN
1	D	266	LYS
1	D	292	ASN
1	D	318	ASN
1	D	321[A]	ASN
1	D	321[B]	ASN
1	D	331[A]	ARG
1	D	331[B]	ARG
1	D	353	LYS
1	D	400	MET

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Mol	Chain	Res	Type
1	D	485	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	223	ASN
1	A	295	GLN
1	A	318	ASN
1	A	359	HIS
1	B	107	ASN
1	B	133	ASN
1	B	245	ASN
1	B	310	GLN
1	B	352	ASN
1	B	456	ASN
1	C	107	ASN
1	C	152	GLN
1	C	245	ASN
1	C	292	ASN
1	C	318	ASN
1	D	68	GLN
1	D	107	ASN
1	D	152	GLN
1	D	208	ASN
1	D	245	ASN
1	D	292	ASN
1	D	318	ASN
1	D	359	HIS

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 (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 5 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	WP6	A	1000	-	28,28,28	2.38	5 (17%)	33,39,39	1.50	3 (9%)
3	WP6	B	1000	-	28,28,28	2.34	6 (21%)	33,39,39	1.35	2 (6%)
3	WP6	D	1000	-	28,28,28	2.52	5 (17%)	33,39,39	1.15	2 (6%)
2	FAD	A	998	-	54,58,58	1.04	3 (5%)	71,89,89	1.53	12 (16%)
2	FAD	D	998	-	54,58,58	1.13	4 (7%)	71,89,89	1.39	6 (8%)
2	FAD	C	998	-	54,58,58	1.21	4 (7%)	71,89,89	1.64	16 (22%)
3	WP6	C	1000	-	28,28,28	2.17	5 (17%)	33,39,39	1.44	7 (21%)
2	FAD	B	998	-	54,58,58	1.16	4 (7%)	71,89,89	1.63	13 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	WP6	A	1000	-	-	0/8/24/24	0/4/4/4
3	WP6	B	1000	-	-	0/8/24/24	0/4/4/4
3	WP6	D	1000	-	-	0/8/24/24	0/4/4/4
2	FAD	A	998	-	-	3/30/50/50	0/6/6/6
2	FAD	D	998	-	-	5/30/50/50	0/6/6/6
2	FAD	C	998	-	-	4/30/50/50	0/6/6/6
3	WP6	C	1000	-	-	0/8/24/24	0/4/4/4
2	FAD	B	998	-	-	3/30/50/50	0/6/6/6

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1000	WP6	CAV-NAU	10.02	1.42	1.29
3	A	1000	WP6	CAV-NAU	8.80	1.40	1.29
3	B	1000	WP6	CAV-NAU	8.66	1.40	1.29
3	C	1000	WP6	CAV-NAU	8.56	1.40	1.29
3	B	1000	WP6	CAW-CAV	5.30	1.57	1.49
3	A	1000	WP6	CAM-NAN	5.02	1.51	1.48
3	D	1000	WP6	CAW-CAV	4.51	1.56	1.49
3	D	1000	WP6	CAL-CAM	4.40	1.56	1.51
2	C	998	FAD	C2A-N3A	4.27	1.38	1.32
2	B	998	FAD	C2A-N3A	4.17	1.38	1.32
3	A	1000	WP6	CAW-CAV	4.03	1.55	1.49
2	D	998	FAD	C2A-N3A	3.89	1.38	1.32
3	C	1000	WP6	CAL-CAM	3.56	1.55	1.51
2	A	998	FAD	C2A-N3A	3.48	1.37	1.32
3	D	1000	WP6	CAM-NAN	3.42	1.50	1.48
2	C	998	FAD	C4X-N5	3.41	1.38	1.30
2	A	998	FAD	C4X-N5	3.17	1.37	1.30
3	B	1000	WP6	CAE-CAM	3.16	1.57	1.52
2	D	998	FAD	C10-N1	3.15	1.39	1.33
2	D	998	FAD	C4X-N5	3.14	1.37	1.30
3	B	1000	WP6	CAM-NAN	3.11	1.50	1.48
3	C	1000	WP6	CAO-CAP	3.04	1.56	1.51
3	B	1000	WP6	CAO-CAP	2.99	1.56	1.51
2	B	998	FAD	C4X-N5	2.99	1.37	1.30
2	C	998	FAD	C2A-N1A	2.97	1.39	1.33
3	D	1000	WP6	CAV-NAN	2.87	1.43	1.35
2	C	998	FAD	C10-N1	2.69	1.38	1.33
3	B	1000	WP6	CAV-NAN	2.68	1.42	1.35
3	A	1000	WP6	CAE-CAM	2.65	1.56	1.52
2	A	998	FAD	C2A-N1A	2.51	1.38	1.33
2	D	998	FAD	C2A-N1A	2.48	1.38	1.33
3	C	1000	WP6	CAW-CAV	2.43	1.53	1.49
2	B	998	FAD	C10-N1	2.41	1.38	1.33
2	B	998	FAD	C2A-N1A	2.37	1.38	1.33
3	C	1000	WP6	CAV-NAN	2.34	1.41	1.35
3	A	1000	WP6	CAV-NAN	2.32	1.41	1.35

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	998	FAD	N3A-C2A-N1A	-6.73	119.54	128.67
2	C	998	FAD	N3A-C2A-N1A	-6.37	120.02	128.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	998	FAD	N3A-C2A-N1A	-5.93	120.63	128.67
2	D	998	FAD	N3A-C2A-N1A	-5.58	121.10	128.67
3	B	1000	WP6	CAT-NAU-CAV	4.70	122.19	118.16
3	A	1000	WP6	CAT-NAU-CAV	4.59	122.11	118.16
3	C	1000	WP6	CAT-NAU-CAV	4.15	121.72	118.16
2	C	998	FAD	O2A-PA-O3P	4.02	118.14	107.27
3	D	1000	WP6	CAT-NAU-CAV	3.82	121.44	118.16
2	A	998	FAD	C4X-C10-N10	3.63	121.67	116.48
2	B	998	FAD	O2A-PA-O3P	3.55	116.86	107.27
3	A	1000	WP6	CAE-CAM-CAL	-3.53	106.46	112.75
2	D	998	FAD	C4X-C10-N10	3.46	121.43	116.48
2	B	998	FAD	C9A-C5X-N5	-3.44	118.81	122.45
2	C	998	FAD	C9A-C5X-N5	-3.39	118.86	122.45
2	B	998	FAD	O4B-C1B-N9A	-3.20	104.50	108.75
2	B	998	FAD	C4-N3-C2	-3.17	120.02	125.64
2	D	998	FAD	C10-C4X-N5	-3.10	118.47	124.81
2	A	998	FAD	C4-C4X-N5	3.09	122.47	118.21
2	A	998	FAD	C10-C4X-N5	-3.05	118.59	124.81
2	B	998	FAD	C4X-C4-N3	2.97	120.81	113.25
3	D	1000	WP6	CAE-CAM-NAN	-2.95	107.65	111.65
2	A	998	FAD	C9A-C5X-N5	-2.90	119.37	122.45
2	D	998	FAD	O2A-PA-O3P	2.89	115.09	107.27
2	A	998	FAD	C4-N3-C2	-2.89	120.51	125.64
3	A	1000	WP6	CAE-CAM-NAN	-2.85	107.78	111.65
2	A	998	FAD	O3B-C3B-C4B	-2.83	102.97	111.08
2	C	998	FAD	O3P-P-O1P	-2.76	102.40	110.70
2	C	998	FAD	C4X-C10-N10	2.75	120.42	116.48
3	C	1000	WP6	CAS-CAR-CAJ	2.72	121.98	119.24
2	A	998	FAD	O2A-PA-O3P	2.72	114.63	107.27
2	B	998	FAD	C4X-C10-N10	2.71	120.36	116.48
2	C	998	FAD	C4-N3-C2	-2.70	120.84	125.64
2	D	998	FAD	C4-C4X-N5	2.66	121.88	118.21
2	C	998	FAD	C4X-C4-N3	2.64	119.97	113.25
2	A	998	FAD	C10-N1-C2	2.59	122.45	116.85
2	C	998	FAD	O3P-PA-O1A	-2.56	103.01	110.70
2	C	998	FAD	O4-C4-C4X	-2.51	119.90	126.53
2	C	998	FAD	C4B-O4B-C1B	-2.50	107.63	109.92
3	C	1000	WP6	CAE-CAM-NAN	-2.50	108.27	111.65
2	B	998	FAD	C4A-C5A-N7A	-2.46	106.74	109.34
2	C	998	FAD	C10-C4X-N5	-2.44	119.82	124.81
2	D	998	FAD	C4-N3-C2	-2.40	121.39	125.64
2	B	998	FAD	C6-C5X-N5	2.40	122.42	118.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	998	FAD	C4-C4X-N5	2.39	121.51	118.21
2	B	998	FAD	C5X-C9A-N10	2.39	120.13	117.97
2	A	998	FAD	C4X-C4-N3	2.36	119.26	113.25
2	B	998	FAD	C10-C4X-N5	-2.35	120.01	124.81
2	C	998	FAD	C10-N1-C2	2.32	121.87	116.85
2	C	998	FAD	O4B-C1B-N9A	-2.30	105.70	108.75
3	C	1000	WP6	CAE-CAM-CAL	-2.27	108.71	112.75
3	C	1000	WP6	CAL-CAM-NAN	2.26	113.67	110.39
2	B	998	FAD	O3B-C3B-C4B	-2.21	104.73	111.08
3	B	1000	WP6	CAE-CAM-CAL	-2.21	108.81	112.75
3	C	1000	WP6	CAW-CAV-NAU	-2.19	116.53	119.32
3	C	1000	WP6	CAL-CAT-NAU	-2.16	120.30	122.16
2	C	998	FAD	C5X-N5-C4X	2.16	121.58	118.09
2	C	998	FAD	C4X-C10-N1	-2.10	119.45	124.59
2	C	998	FAD	C5'-C4'-C3'	-2.08	108.30	112.22
2	A	998	FAD	C4X-C10-N1	-2.04	119.58	124.59
2	A	998	FAD	C5X-N5-C4X	2.03	121.37	118.09

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	998	FAD	O4B-C4B-C5B-O5B
2	D	998	FAD	O4B-C4B-C5B-O5B
2	D	998	FAD	C3B-C4B-C5B-O5B
2	C	998	FAD	C3B-C4B-C5B-O5B
2	A	998	FAD	PA-O3P-P-O5'
2	B	998	FAD	PA-O3P-P-O5'
2	C	998	FAD	PA-O3P-P-O5'
2	D	998	FAD	PA-O3P-P-O5'
2	B	998	FAD	P-O3P-PA-O2A
2	D	998	FAD	P-O3P-PA-O2A
2	A	998	FAD	P-O3P-PA-O1A
2	C	998	FAD	PA-O3P-P-O2P
2	D	998	FAD	P-O3P-PA-O1A
2	A	998	FAD	PA-O3P-P-O2P
2	B	998	FAD	P-O3P-PA-O1A

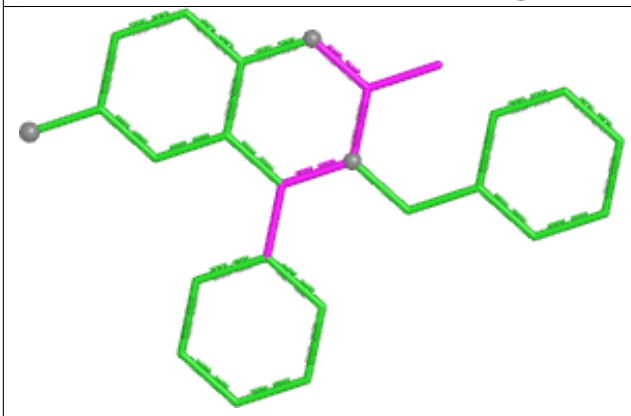
There are no ring outliers.

4 monomers are involved in 21 short contacts:

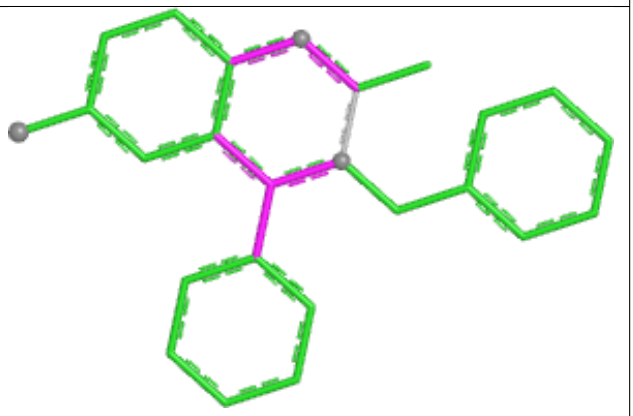
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1000	WP6	9	0
3	B	1000	WP6	9	0
2	A	998	FAD	1	0
2	C	998	FAD	2	0

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.

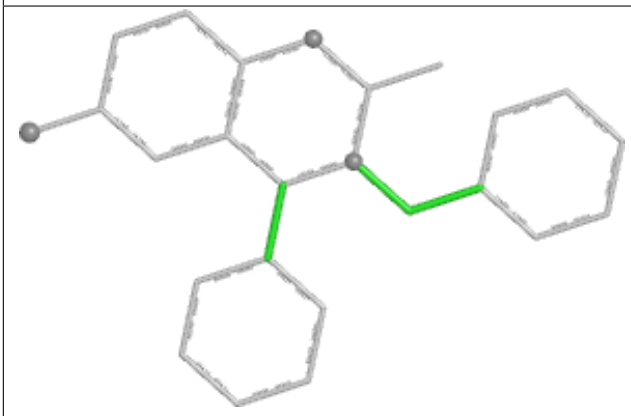
Ligand WP6 A 1000



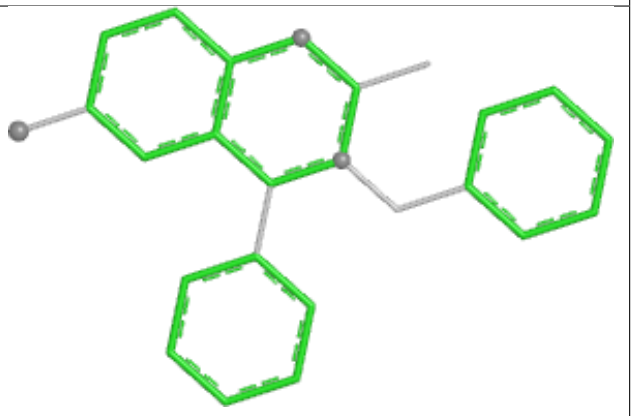
Bond lengths



Bond angles

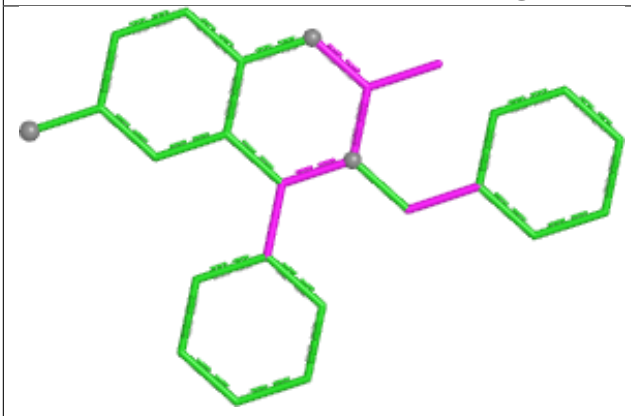


Torsions

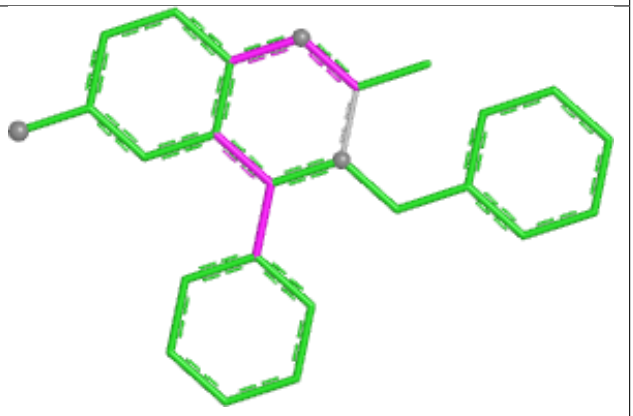


Rings

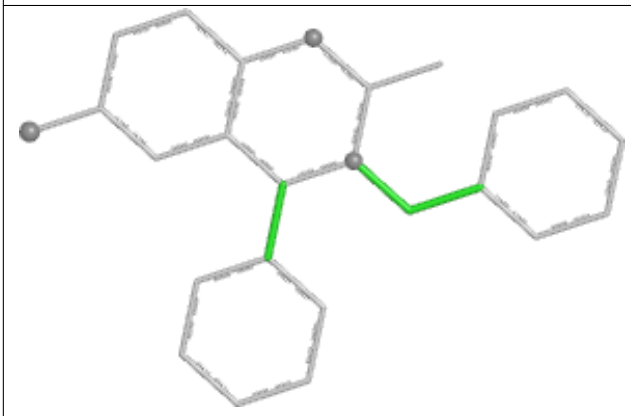
Ligand WP6 B 1000



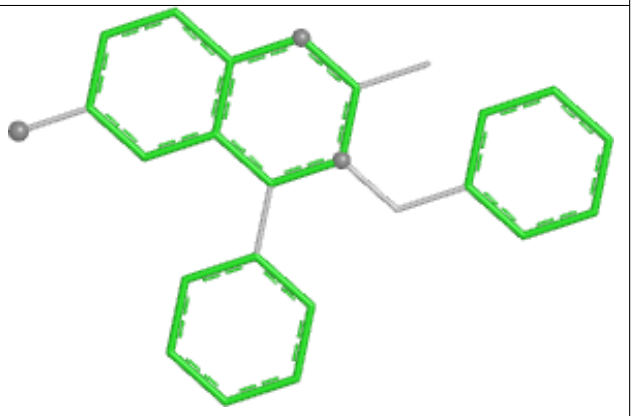
Bond lengths



Bond angles

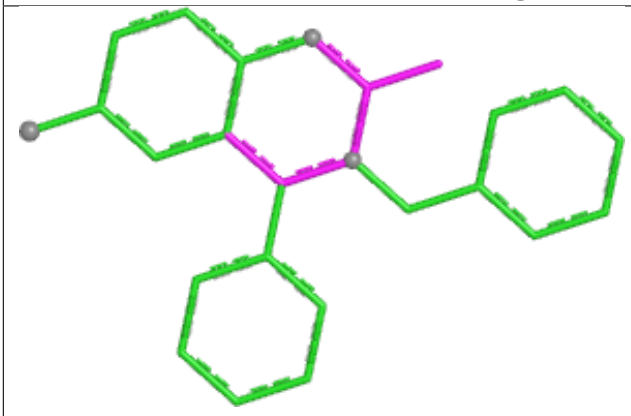


Torsions

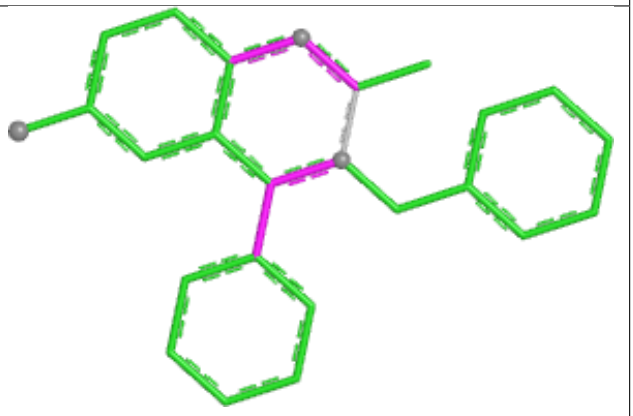


Rings

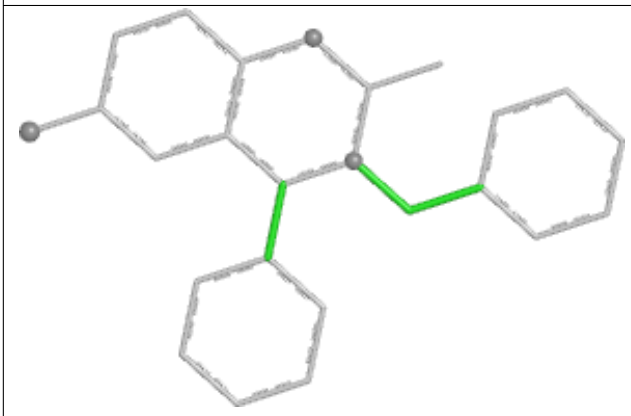
Ligand WP6 D 1000



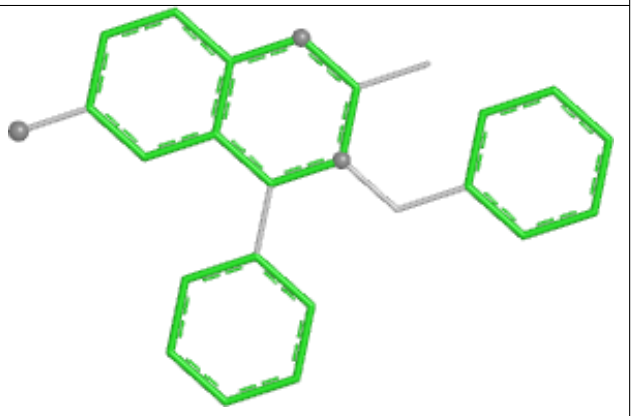
Bond lengths



Bond angles

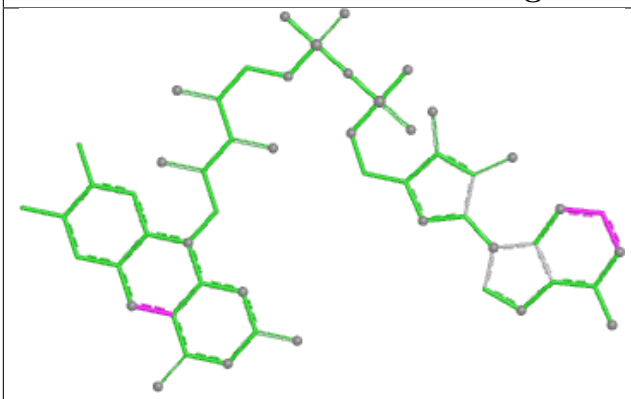


Torsions

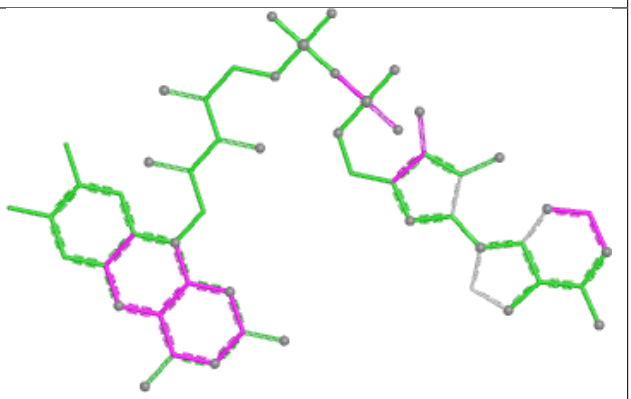


Rings

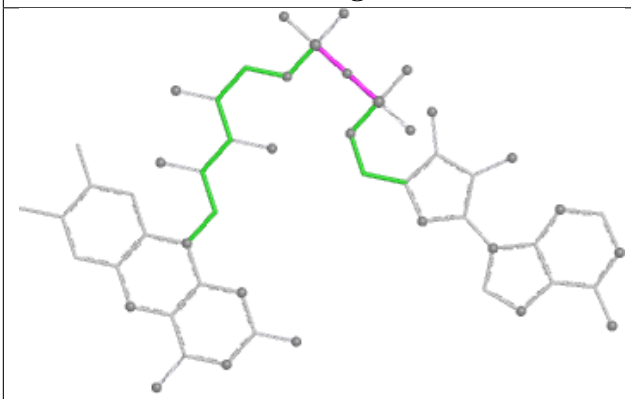
Ligand FAD A 998



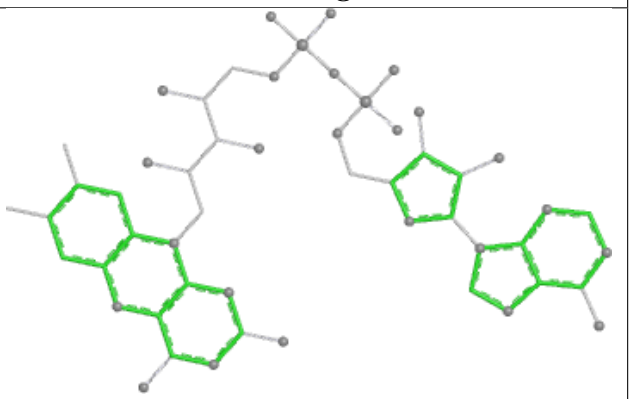
Bond lengths



Bond angles

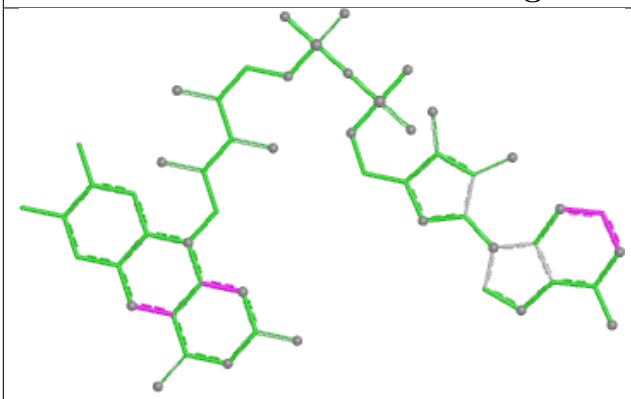


Torsions

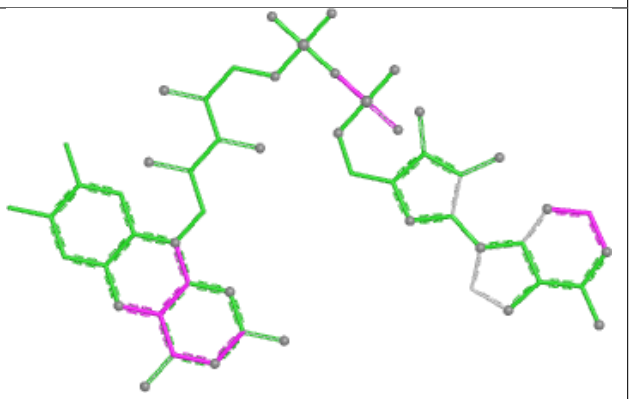


Rings

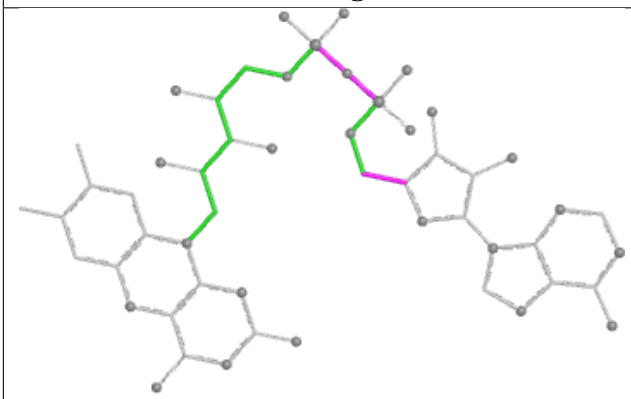
Ligand FAD D 998



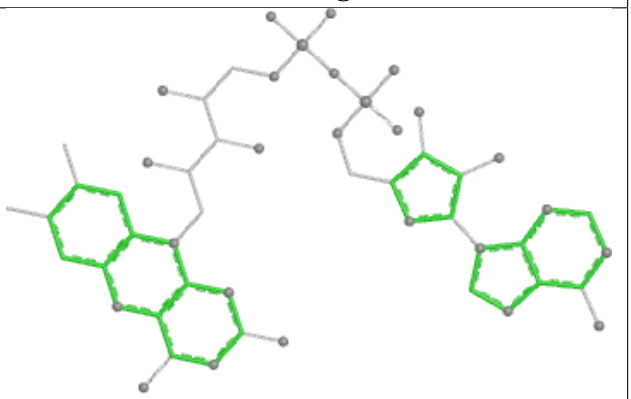
Bond lengths



Bond angles

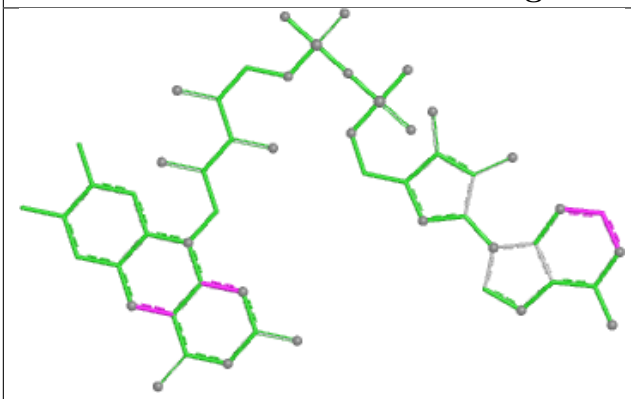


Torsions

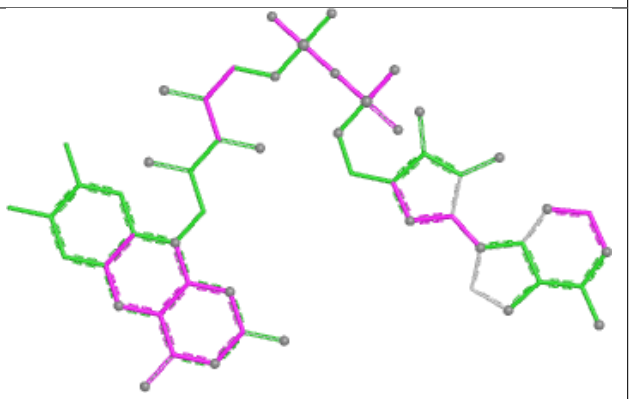


Rings

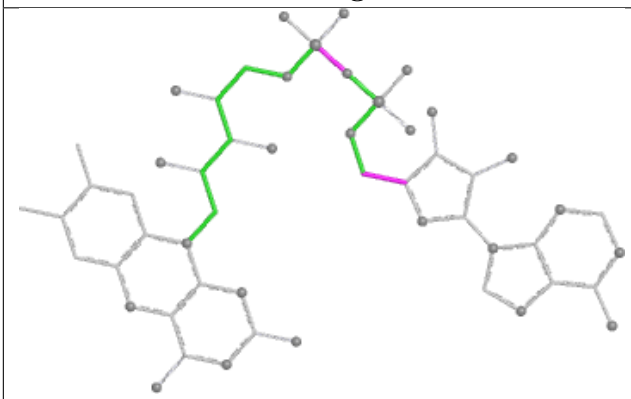
Ligand FAD C 998



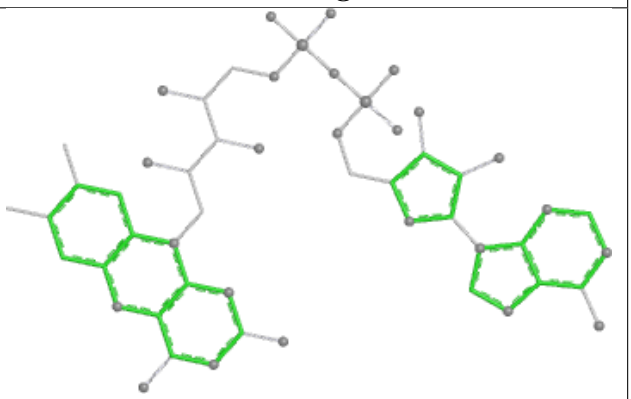
Bond lengths



Bond angles

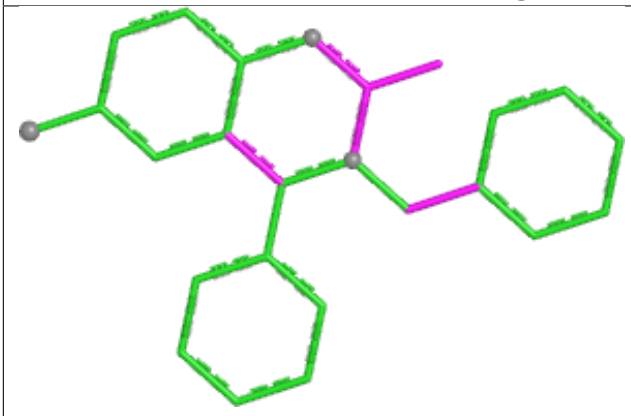


Torsions

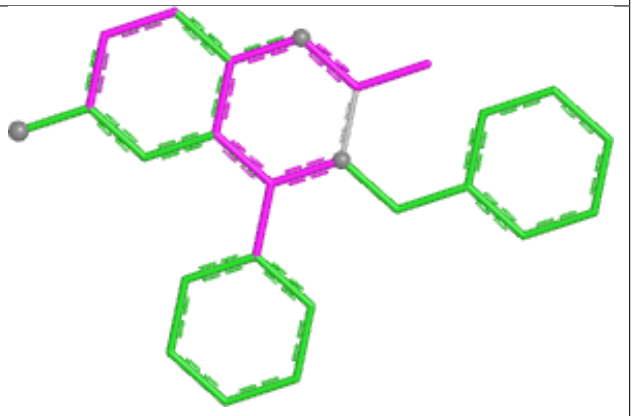


Rings

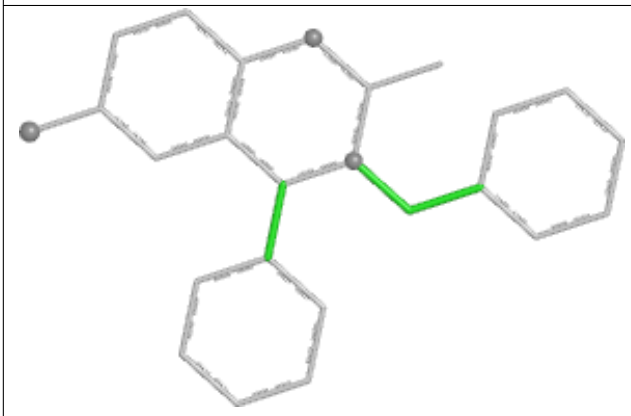
Ligand WP6 C 1000



Bond lengths



Bond angles



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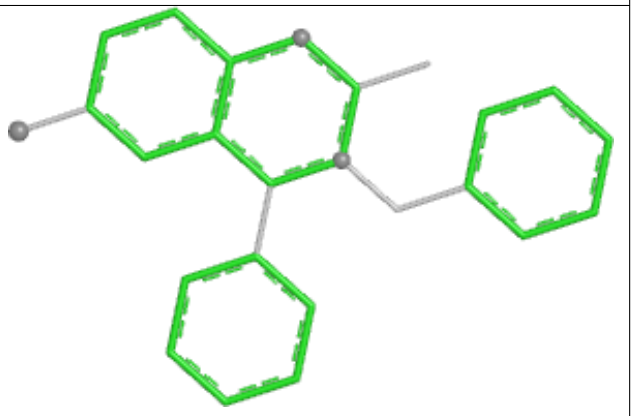
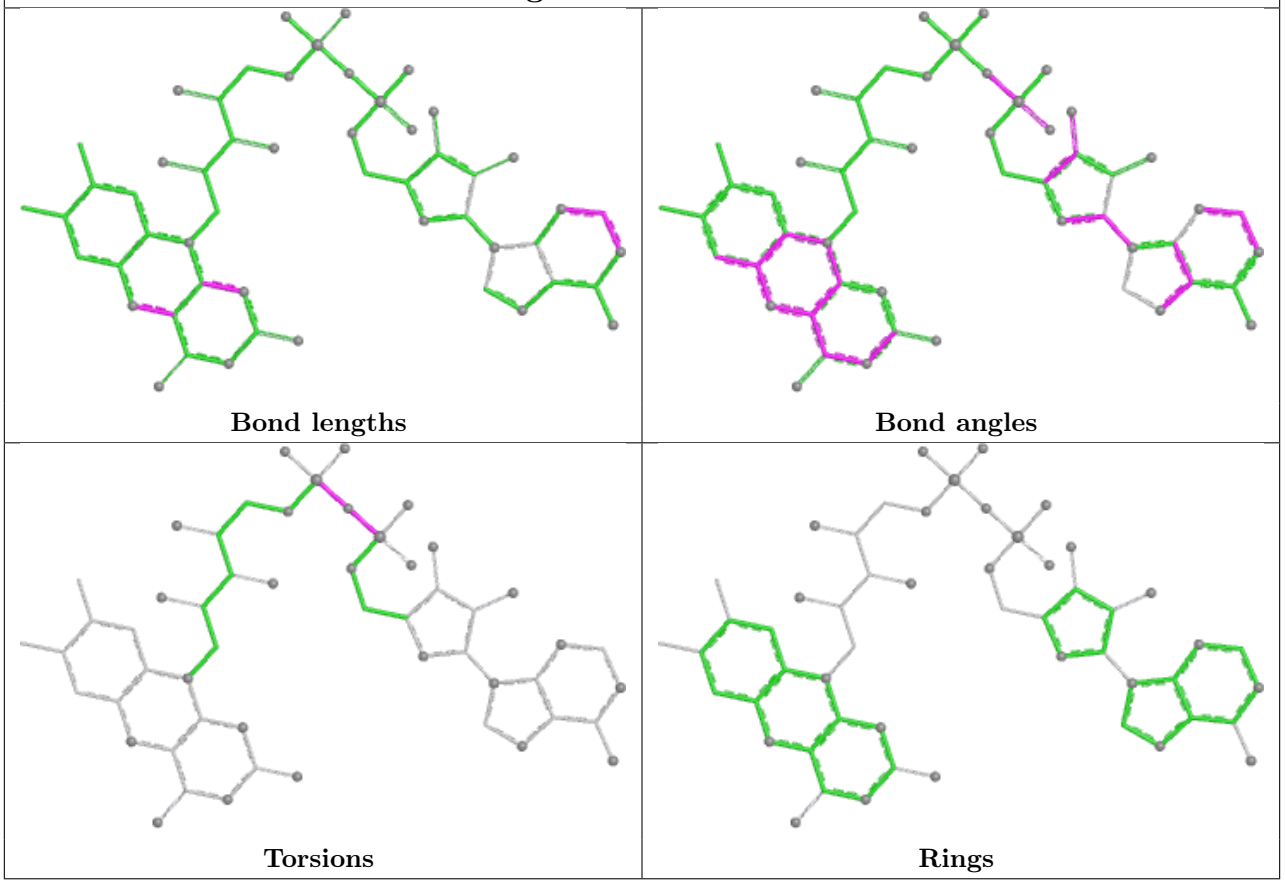


Rings

Ligand FAD B 998



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	490/495 (98%)	-0.58	3 (0%)	89	90	6, 17, 33, 47	0
1	B	488/495 (98%)	-0.40	2 (0%)	92	93	9, 22, 44, 59	0
1	C	488/495 (98%)	-0.42	4 (0%)	86	87	10, 22, 47, 60	0
1	D	489/495 (98%)	-0.54	0	100	100	10, 20, 34, 54	0
All	All	1955/1980 (98%)	-0.48	9 (0%)	91	91	6, 20, 42, 60	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	352	ASN	2.5
1	B	488	PRO	2.4
1	A	352	ASN	2.3
1	C	486	LYS	2.3
1	A	488	PRO	2.1
1	C	306	LYS	2.1
1	C	30[A]	ARG	2.1
1	A	305	PRO	2.0
1	B	305	PRO	2.0

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

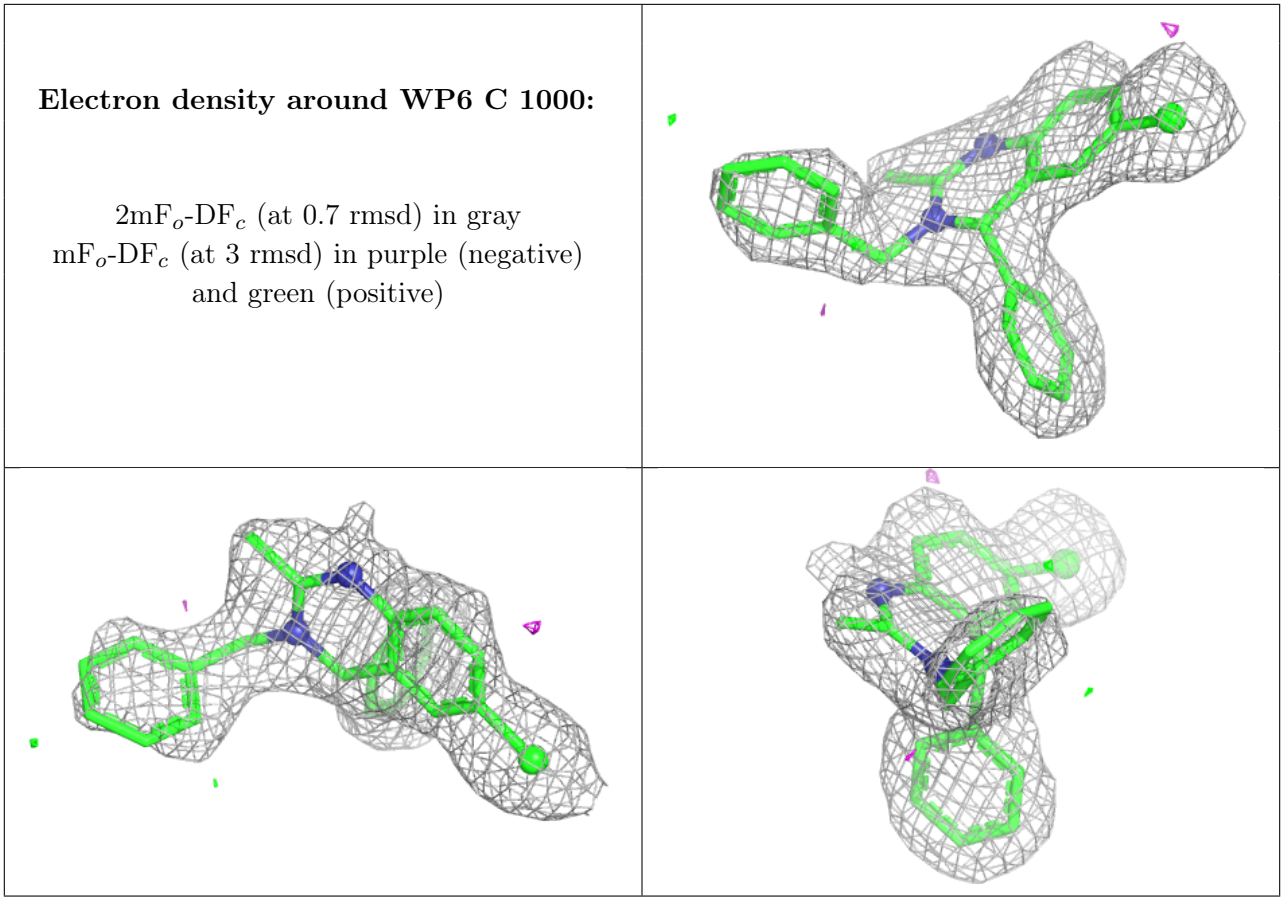
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	WP6	C	1000	25/25	0.95	0.13	25,30,51,52	0
4	CL	D	1487	1/1	0.95	0.08	35,35,35,35	0
3	WP6	A	1000	25/25	0.97	0.12	10,18,30,33	0
3	WP6	B	1000	25/25	0.97	0.12	19,25,31,32	0
2	FAD	B	998	53/53	0.97	0.12	9,19,30,31	0
4	CL	C	1491	1/1	0.97	0.24	35,35,35,35	0
2	FAD	C	998	53/53	0.97	0.11	14,18,25,27	0
3	WP6	D	1000	25/25	0.98	0.09	13,16,30,31	0
4	CL	A	1489	1/1	0.98	0.06	27,27,27,27	0
4	CL	C	1490	1/1	0.98	0.06	37,37,37,37	0
2	FAD	D	998	53/53	0.98	0.10	7,12,17,17	0
2	FAD	A	998	53/53	0.98	0.11	4,10,14,18	0
4	CL	B	1490	1/1	0.99	0.04	27,27,27,27	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.

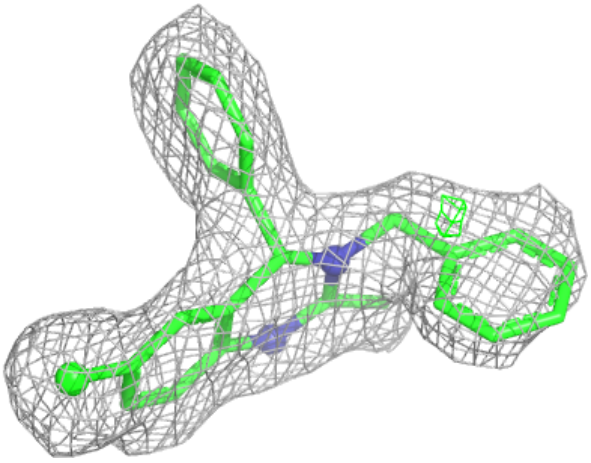
Electron density around WP6 C 1000:

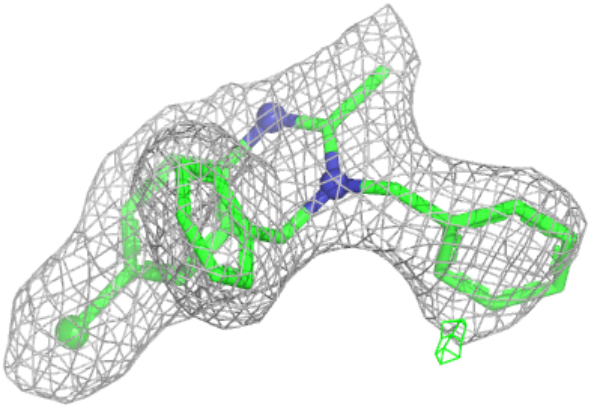
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

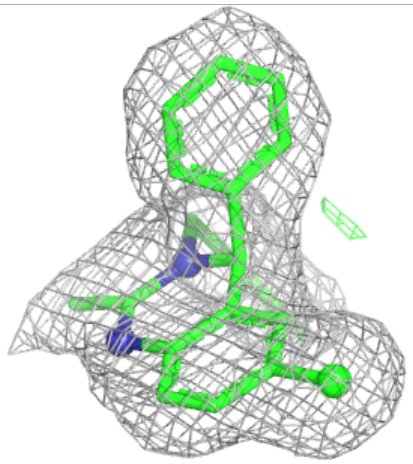


Electron density around WP6 A 1000:

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

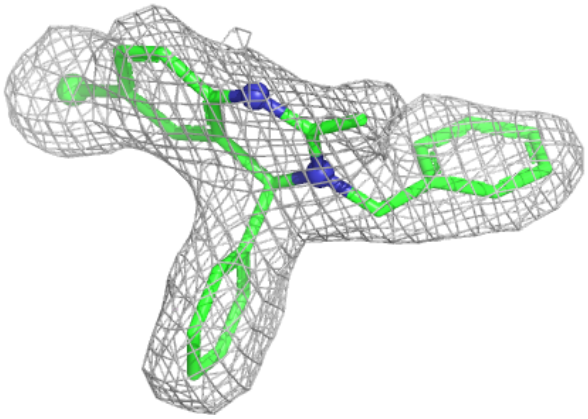


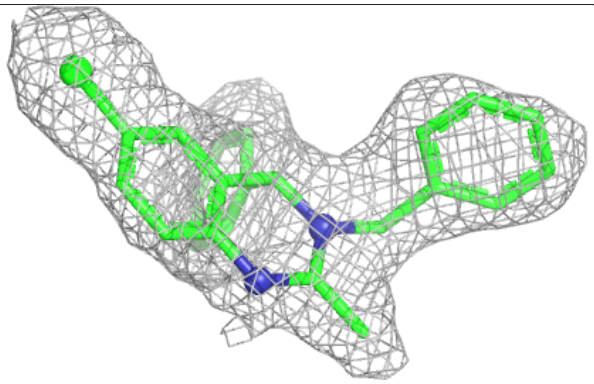


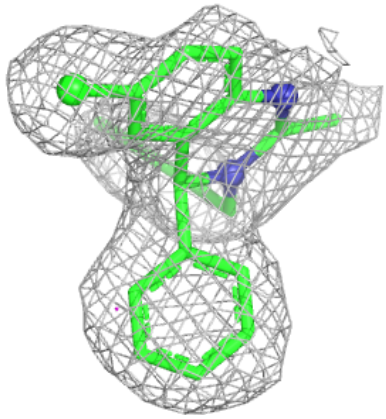


Electron density around WP6 B 1000:

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

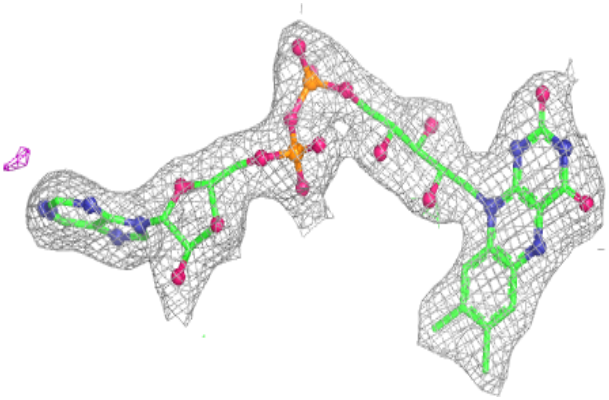


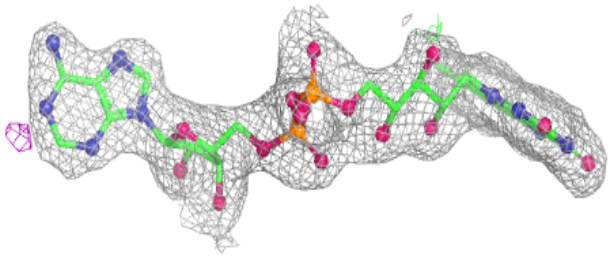


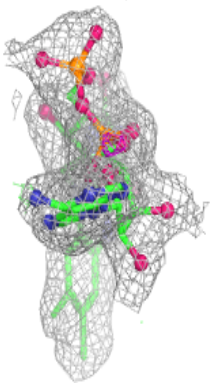


Electron density around FAD B 998:

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

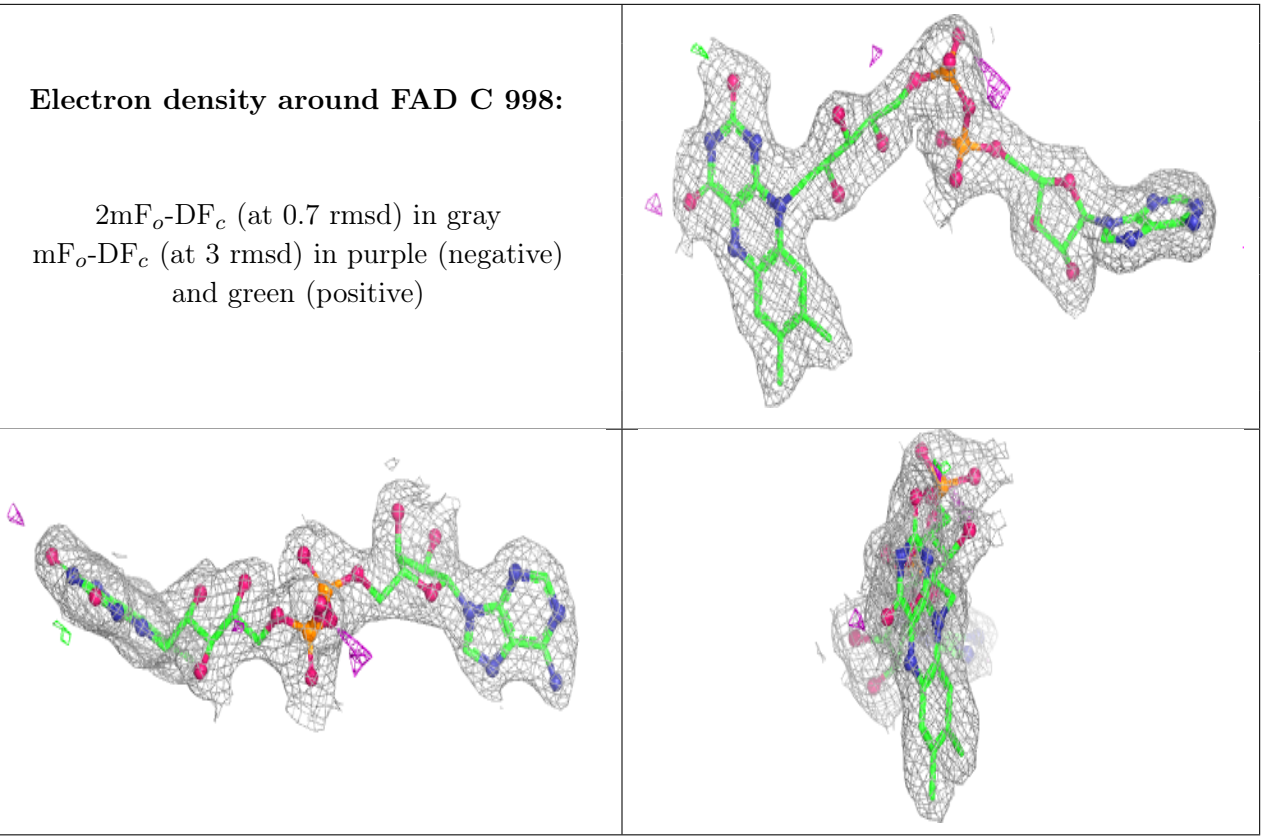






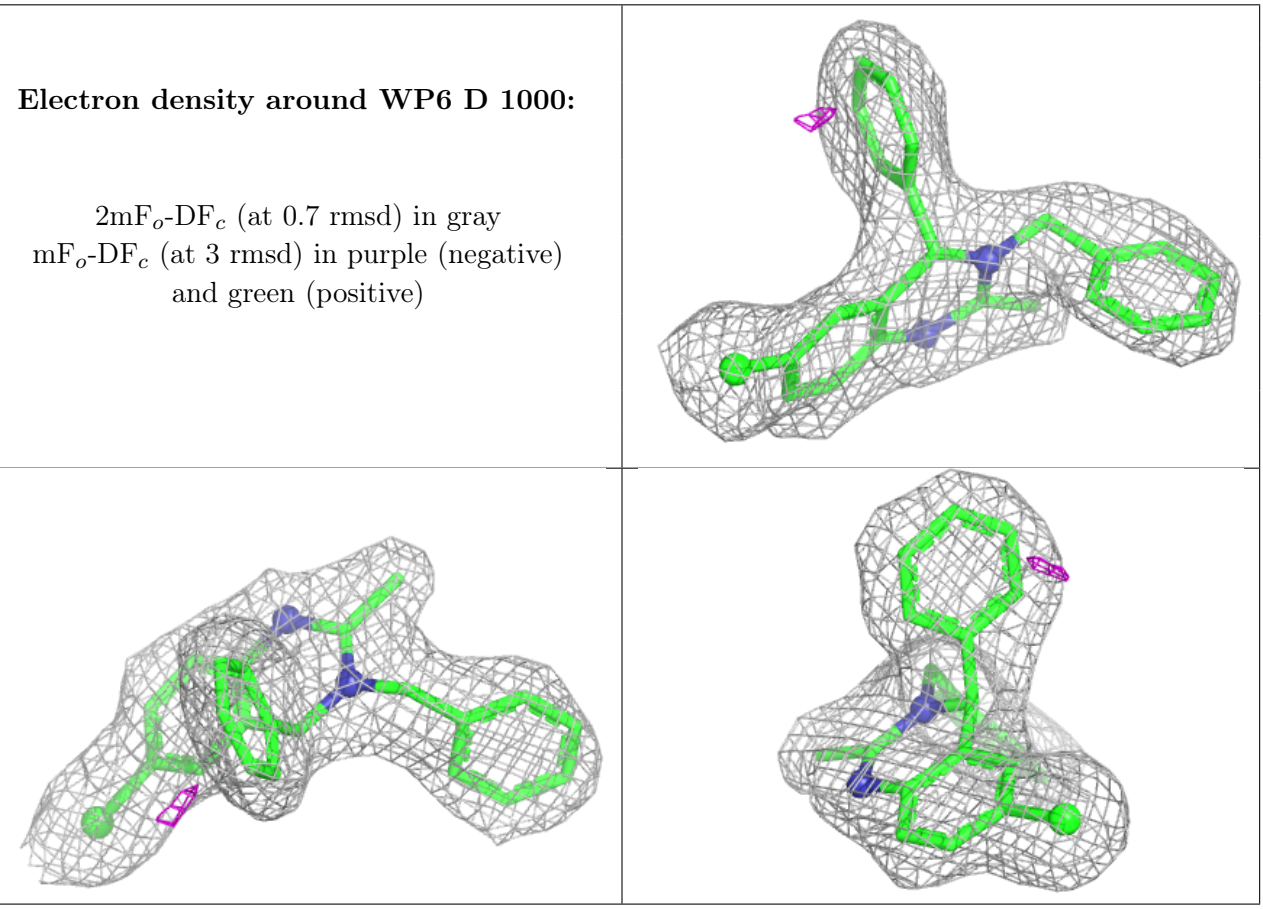
Electron density around FAD C 998:

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



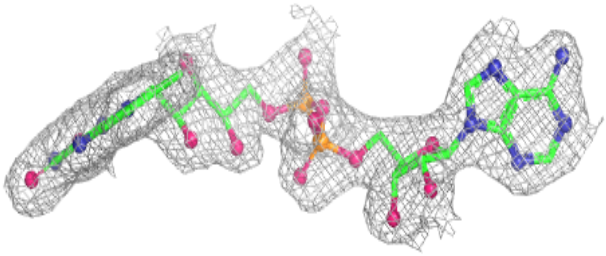
Electron density around WP6 D 1000:

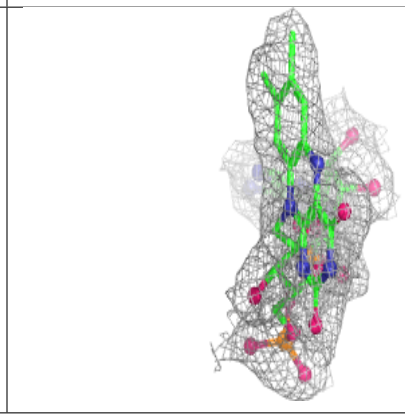
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around FAD D 998:

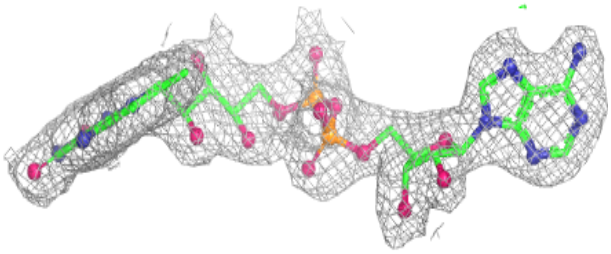
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

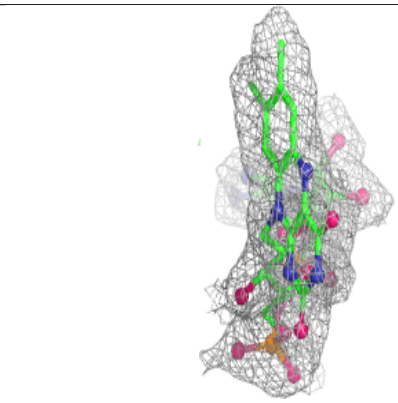




Electron density around FAD A 998:

$2mF_o$-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.