Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 11:43 pm BST

PDB ID	:	2WPC
Title	:	Trypanosoma brucei trypanothione reductase in complex with 3,4- dihydro-quinazoline inhibitor (DDD00073357)
Authors	:	Alphey, M.S.; Patterson, S.; Fairlamb, A.H.
Deposited on	:	2009-08-05
Resolution	:	2.10 Å(reported)

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

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

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

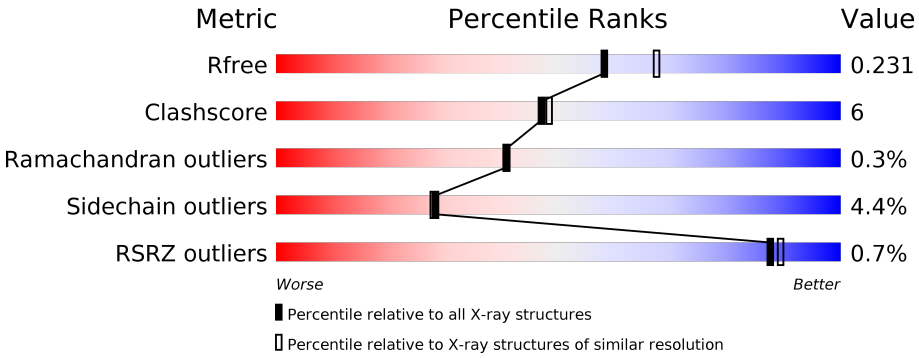
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	495	% 85% 13% ··
1	B	495	% 82% 15% · ·
1	C	495	% 82% 16% ··
1	D	495	% 84% 14% ··

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16689 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.

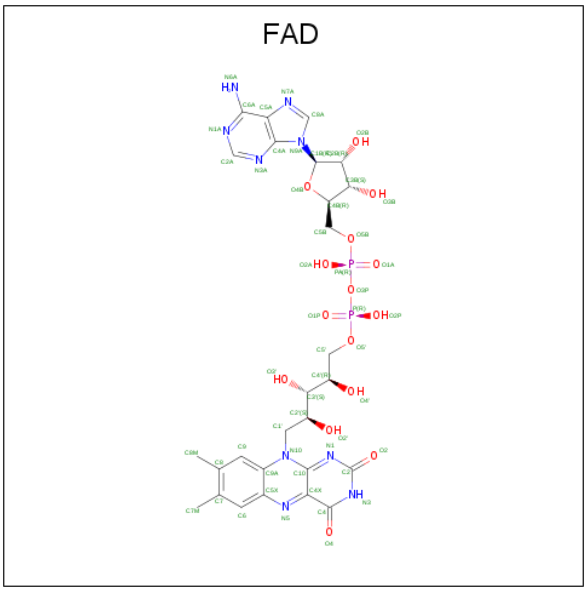
- Molecule 1 is a protein called TRYPANOTHIONE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	489	Total	C	N	O	S	0	0	0
			3715	2362	632	701	20			
1	B	487	Total	C	N	O	S	0	3	0
			3716	2365	634	698	19			
1	C	492	Total	C	N	O	S	0	1	0
			3740	2378	636	706	20			
1	D	490	Total	C	N	O	S	0	1	0
			3728	2371	633	704	20			

There are 12 discrepancies between the modelled and reference sequences:

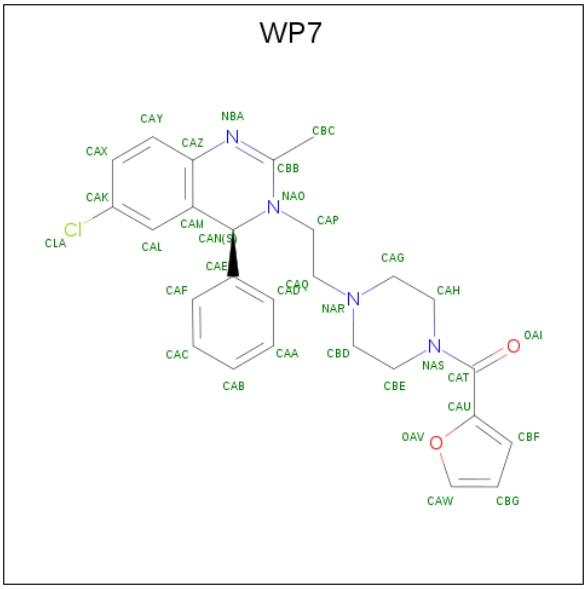
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q389T8
A	-1	SER	-	expression tag	UNP Q389T8
A	0	HIS	-	expression tag	UNP Q389T8
B	-2	GLY	-	expression tag	UNP Q389T8
B	-1	SER	-	expression tag	UNP Q389T8
B	0	HIS	-	expression tag	UNP Q389T8
C	-2	GLY	-	expression tag	UNP Q389T8
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)-6-CHLORO-3-{2-[4-(FURAN-2-YLCARBONYL)PIPERAZIN-1-YL]ETHYL}-2-METHYL-4-PHENYL-3,4-DIHYDROQUINAZOLINE (three-letter code: WP7) (formula: $C_{26}H_{27}ClN_4O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			33	26	1	4	2		
3	B	1	Total	C	Cl	N	O	0	0
			33	26	1	4	2		
3	C	1	Total	C	Cl	N	O	0	0
			33	26	1	4	2		
3	D	1	Total	C	Cl	N	O	0	0
			33	26	1	4	2		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	3	Total	Cl	0	0
			3	3		
4	A	3	Total	Cl	0	0
			3	3		
4	D	3	Total	Cl	0	0
			3	3		
4	C	2	Total	Cl	0	0
			2	2		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Na	0	0
			2	2		
5	A	2	Total	Na	0	0
			2	2		
5	D	2	Total	Na	0	0
			2	2		
5	C	2	Total	Na	0	0
			2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	364	Total	O	0	0
			364	364		
6	B	343	Total	O	0	0
			343	343		
6	C	350	Total	O	0	0
			350	350		

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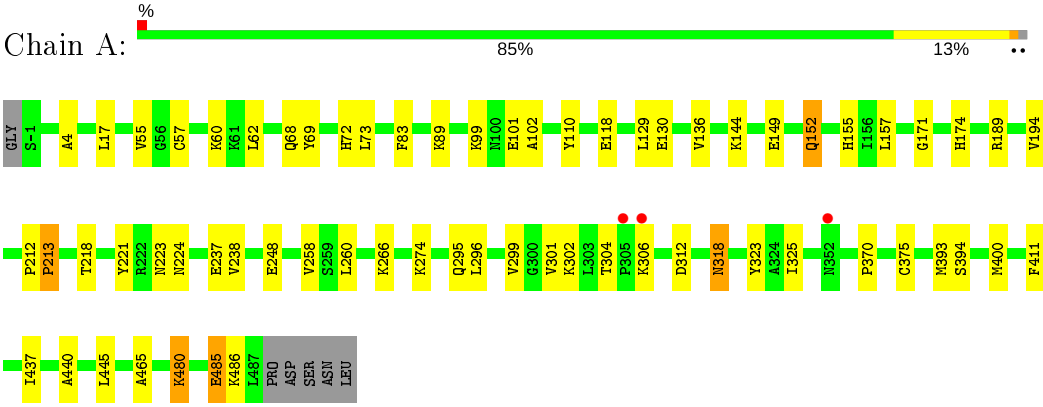
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	370	Total	O	0	0
			370	370		

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.

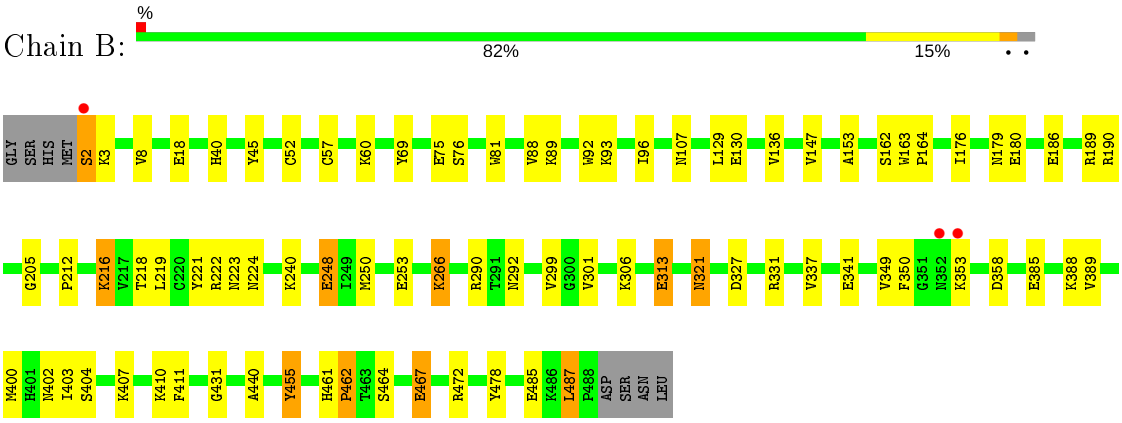
- Molecule 1: TRYPANOTHIONE REDUCTASE

Chain A:



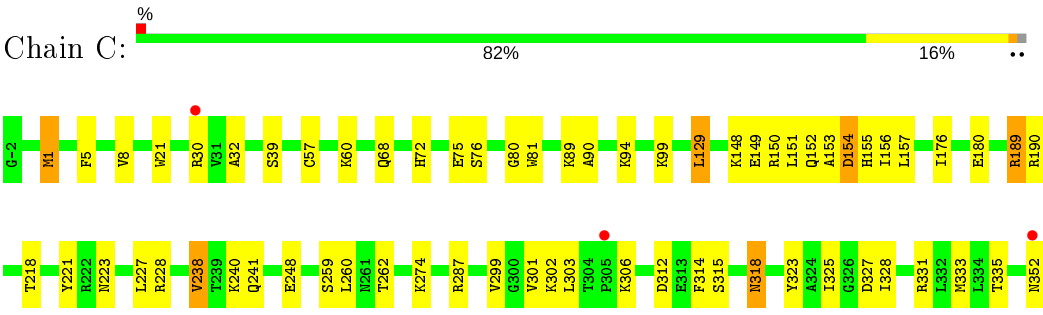
- Molecule 1: TRYPANOTHIONE REDUCTASE

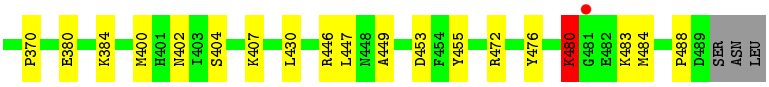
Chain B:



- Molecule 1: TRYPANOTHIONE REDUCTASE

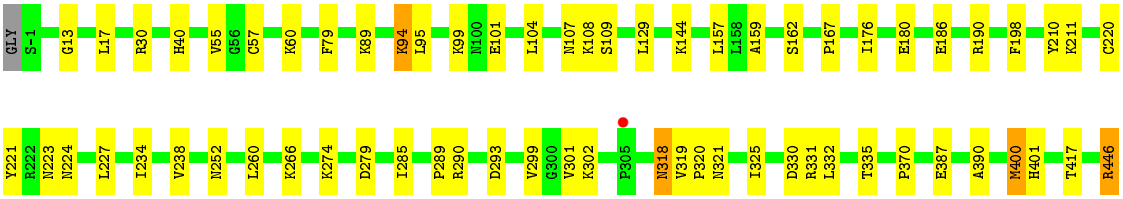
Chain C:

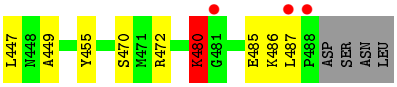




- Molecule 1: TRYPANOTHIONE REDUCTASE

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	101.25Å 63.43Å 169.37Å 90.00° 98.58° 90.00°	Depositor
Resolution (Å)	46.88 – 2.10 46.86 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.88-2.10) 94.2 (46.86-2.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.27 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.165 , 0.232 0.165 , 0.231	Depositor DCC
R_{free} test set	5868 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	18.9	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 55.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16689	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 8.74% 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: NA, WP7, 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	1.16	7/3793 (0.2%)	0.94	1/5144 (0.0%)
1	B	1.08	4/3803 (0.1%)	0.91	4/5158 (0.1%)
1	C	1.08	0/3822	0.90	4/5183 (0.1%)
1	D	1.14	6/3810 (0.2%)	0.92	2/5168 (0.0%)
All	All	1.12	17/15228 (0.1%)	0.92	11/20653 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	118	GLU	CG-CD	5.97	1.60	1.51
1	D	220	CYS	CB-SG	-5.80	1.72	1.81
1	A	110	TYR	CE1-CZ	5.78	1.46	1.38
1	A	102	ALA	CA-CB	5.76	1.64	1.52
1	D	198	PHE	CE1-CZ	5.75	1.48	1.37
1	B	205	GLY	N-CA	5.71	1.54	1.46
1	A	194	VAL	CB-CG2	5.47	1.64	1.52
1	B	69	TYR	CE2-CZ	5.32	1.45	1.38
1	D	109	SER	CB-OG	-5.30	1.35	1.42
1	D	162	SER	CB-OG	5.29	1.49	1.42
1	B	248	GLU	CD-OE1	5.27	1.31	1.25
1	B	455	TYR	CD1-CE1	5.27	1.47	1.39
1	D	159	ALA	CA-CB	5.15	1.63	1.52
1	A	202	GLU	CB-CG	5.10	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	PHE	CD1-CE1	5.04	1.49	1.39
1	A	149	GLU	CG-CD	5.03	1.59	1.51
1	D	79	PHE	CE2-CZ	5.02	1.46	1.37

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	266	LYS	CD-CE-NZ	-7.18	95.18	111.70
1	C	287	ARG	NE-CZ-NH2	-6.75	116.93	120.30
1	C	312	ASP	CB-CG-OD1	6.44	124.10	118.30
1	D	290	ARG	NE-CZ-NH2	-6.41	117.10	120.30
1	A	312	ASP	CB-CG-OD1	5.96	123.67	118.30
1	C	190	ARG	NE-CZ-NH2	-5.85	117.37	120.30
1	B	487	LEU	CB-CG-CD2	-5.81	101.12	111.00
1	C	190	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	D	446	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	B	290	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	B	358	ASP	CB-CG-OD1	5.12	122.91	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	2	SER	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	3715	0	3725	38	0
1	B	3716	0	3736	57	0
1	C	3740	0	3752	55	0
1	D	3728	0	3738	43	0
2	A	53	0	31	0	0
2	B	53	0	31	0	0
2	C	53	0	31	0	0
2	D	53	0	31	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	33	0	27	0	0
3	B	33	0	27	2	0
3	C	33	0	27	2	0
3	D	33	0	27	2	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	C	2	0	0	0	0
4	D	3	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
6	A	364	0	0	6	0
6	B	343	0	0	12	0
6	C	350	0	0	11	0
6	D	370	0	0	7	0
All	All	16689	0	15183	189	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 (189) 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:D:480:LYS:HA	1:D:480:LYS:HE2	1.32	1.12
1:A:129:LEU:HD23	1:A:299:VAL:HG21	1.45	0.98
1:A:393:MET:HE2	1:A:414:LYS:HE3	1.48	0.95
1:A:485:GLU:HG2	1:A:486:LYS:HD2	1.55	0.86
1:C:94:LYS:HE2	6:C:3074:HOH:O	1.79	0.81
1:A:274:LYS:HD2	6:A:3205:HOH:O	1.79	0.81
1:D:101:GLU:HG3	6:D:3081:HOH:O	1.84	0.77
1:D:480:LYS:HA	1:D:480:LYS:CE	2.10	0.75
1:A:393:MET:CE	1:A:414:LYS:HE3	2.17	0.75
1:B:130:GLU:HB2	1:B:136:VAL:CG2	2.16	0.74
1:A:129:LEU:HD23	1:A:299:VAL:CG2	2.18	0.73
1:C:299:VAL:HG23	1:C:301:VAL:HG23	1.71	0.73
1:A:370:PRO:HD2	6:A:3298:HOH:O	1.88	0.73
1:C:318:ASN:H	1:C:318:ASN:HD22	1.36	0.73
1:D:486:LYS:HB2	6:D:3361:HOH:O	1.86	0.73
1:C:241:GLN:OE1	1:C:370:PRO:HG3	1.88	0.73
1:C:80:GLY:HA2	1:D:94:LYS:HG2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:TRP:HZ2	3:C:1000:WP7:HBF	1.57	0.69
1:C:301:VAL:HA	1:C:318:ASN:HD21	1.58	0.69
1:D:224:ASN:HD22	1:D:252:ASN:HD21	1.38	0.69
1:D:289:PRO:HG3	1:D:330:ASP:HB2	1.74	0.69
1:C:455:TYR:CZ	1:C:472:ARG:HD3	2.27	0.69
1:A:72:HIS:HD2	6:B:3036:HOH:O	1.75	0.68
1:C:380:GLU:O	1:C:384[B]:LYS:HD2	1.94	0.67
1:D:387:GLU:HA	1:D:480:LYS:HE3	1.78	0.65
1:B:218:THR:HG23	1:B:248:GLU:HG2	1.79	0.64
1:A:302:LYS:H	1:A:318:ASN:HD21	1.46	0.64
1:C:189:ARG:HA	1:C:212:PRO:HD2	1.80	0.64
1:A:318:ASN:H	1:A:318:ASN:HD22	1.47	0.63
1:A:4:ALA:HA	1:A:152:GLN:HG3	1.80	0.63
3:D:1000:WP7:HBE1	3:D:1000:WP7:CBF	2.28	0.63
1:A:295:GLN:HG3	6:A:3245:HOH:O	1.99	0.62
1:C:318:ASN:HD22	1:C:318:ASN:N	1.97	0.62
1:D:390:ALA:HB3	1:D:417:THR:OG1	1.99	0.62
1:B:464:SER:O	1:B:467:GLU:HB2	2.00	0.62
1:D:221:TYR:CE2	1:D:223:ASN:HB2	2.35	0.62
1:C:94:LYS:NZ	6:C:3076:HOH:O	2.32	0.62
1:D:13:GLY:HA3	2:D:998:FAD:H52A	1.81	0.62
1:B:130:GLU:HB2	1:B:136:VAL:HG23	1.82	0.61
1:A:302:LYS:H	1:A:318:ASN:ND2	1.99	0.61
1:C:331:ARG:HB3	6:C:3249:HOH:O	2.00	0.61
1:C:299:VAL:CG2	1:C:301:VAL:HG23	2.30	0.61
1:B:2:SER:C	1:B:3:LYS:HG3	2.21	0.60
1:D:387:GLU:HG3	1:D:480:LYS:HD2	1.83	0.60
1:B:189:ARG:HA	1:B:212:PRO:HD2	1.84	0.59
1:D:129:LEU:HD23	1:D:299:VAL:HG21	1.82	0.59
1:B:129:LEU:HD23	1:B:299:VAL:HG21	1.84	0.59
1:B:266:LYS:N	1:B:266:LYS:HD2	2.17	0.59
1:D:302:LYS:H	1:D:318:ASN:HD21	1.50	0.59
1:D:318:ASN:H	1:D:318:ASN:HD22	1.50	0.59
1:B:313:GLU:HG3	6:B:3224:HOH:O	2.03	0.59
1:B:147:VAL:HG23	6:B:3104:HOH:O	2.02	0.58
1:D:302:LYS:H	1:D:318:ASN:ND2	2.02	0.58
1:C:274:LYS:HE2	6:C:3209:HOH:O	2.04	0.57
1:D:144:LYS:HE2	6:D:3125:HOH:O	2.05	0.57
1:B:162:SER:HB3	1:B:327:ASP:HB3	1.86	0.57
1:A:62:LEU:HD22	1:B:403:ILE:HD12	1.85	0.57
1:A:129:LEU:HD22	1:A:296:LEU:HD23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:CYS:HB3	6:B:3004:HOH:O	2.05	0.56
1:D:104:LEU:HG	1:D:108:LYS:HE3	1.88	0.56
1:A:152:GLN:OE1	6:A:3128:HOH:O	2.18	0.56
1:D:227:LEU:HD12	1:D:238:VAL:HG11	1.86	0.56
1:C:240:LYS:HE2	6:C:3170:HOH:O	2.05	0.55
1:C:155:HIS:HB3	1:C:323:TYR:HE2	1.71	0.55
1:A:221:TYR:CE2	1:A:223:ASN:HB2	2.42	0.55
1:B:219:LEU:HD23	1:B:219:LEU:C	2.28	0.55
1:B:337:VAL:O	1:B:341:GLU:HG3	2.07	0.54
1:B:331:ARG:HB3	6:B:3240:HOH:O	2.07	0.54
1:D:211:LYS:NZ	6:D:3174:HOH:O	2.40	0.54
1:B:240:LYS:HD3	6:B:3057:HOH:O	2.06	0.54
1:A:130:GLU:HB2	1:A:136:VAL:HG23	1.90	0.53
1:B:411:PHE:CD1	1:B:431:GLY:HA3	2.44	0.53
1:D:400:MET:HG3	1:D:401:HIS:N	2.24	0.53
1:B:455:TYR:CZ	1:B:472:ARG:HD3	2.44	0.52
1:B:130:GLU:HB2	1:B:136:VAL:HG22	1.91	0.52
1:C:154:ASP:HB3	1:C:155:HIS:CD2	2.45	0.52
1:D:95:LEU:HD22	1:D:210:TYR:CZ	2.45	0.52
1:B:190[B]:ARG:HD3	1:B:216:LYS:HB3	1.91	0.51
1:B:410:LYS:HE2	6:B:3162:HOH:O	2.10	0.51
1:A:83:PHE:HB3	1:B:88:VAL:HG22	1.92	0.51
1:C:402:ASN:HA	1:C:407:LYS:HD3	1.92	0.51
1:C:449:ALA:HB2	1:D:447:LEU:HD11	1.93	0.51
1:A:301:VAL:HA	1:A:318:ASN:HD21	1.74	0.51
1:C:480:LYS:HE3	6:C:3334:HOH:O	2.10	0.51
1:D:446:ARG:HD3	6:D:3335:HOH:O	2.09	0.51
1:C:302:LYS:H	1:C:318:ASN:ND2	2.09	0.50
3:D:1000:WP7:HBE1	3:D:1000:WP7:HBF	1.93	0.50
1:A:411:PHE:CD1	1:A:431:GLY:HA3	2.46	0.50
1:C:75:GLU:HG2	1:C:404:SER:HB2	1.93	0.50
1:C:407:LYS:HB2	6:C:3292:HOH:O	2.10	0.50
1:B:349:VAL:HG12	1:B:350:PHE:CD1	2.46	0.50
1:A:130:GLU:HB2	1:A:136:VAL:CG2	2.42	0.50
1:A:189:ARG:HA	1:A:212:PRO:HD2	1.93	0.50
1:B:402:ASN:HA	1:B:407:LYS:HD3	1.92	0.50
1:B:40:HIS:H	1:B:107:ASN:ND2	2.09	0.49
1:D:234:ILE:O	1:D:238:VAL:HG12	2.13	0.49
1:C:129:LEU:HD11	1:C:156:ILE:HG21	1.95	0.49
1:A:218:THR:HG23	1:A:248:GLU:HG2	1.95	0.49
1:B:353:LYS:CB	6:B:3247:HOH:O	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:PHE:HB2	1:C:366:VAL:HG13	1.94	0.49
1:C:68:GLN:HG2	6:C:3049:HOH:O	2.13	0.49
1:D:293:ASP:HB2	6:D:3234:HOH:O	2.12	0.48
1:B:353:LYS:HB3	6:B:3247:HOH:O	2.11	0.48
1:A:157:LEU:HD11	1:A:325:ILE:HG12	1.96	0.48
1:D:387:GLU:HG3	1:D:480:LYS:CD	2.44	0.48
1:A:69:TYR:O	1:A:73:LEU:HG	2.14	0.47
1:B:75:GLU:HB3	1:B:404:SER:HB2	1.96	0.47
1:C:476:TYR:CE2	1:C:483:LYS:HE3	2.50	0.47
1:D:40:HIS:H	1:D:107:ASN:ND2	2.12	0.47
1:C:89:LYS:HG2	1:C:90:ALA:N	2.30	0.47
1:B:176:ILE:HB	1:B:180:GLU:HB2	1.97	0.47
1:B:455:TYR:CD2	1:B:472:ARG:HB3	2.50	0.47
1:C:480:LYS:CE	6:C:3334:HOH:O	2.63	0.47
1:C:148:LYS:C	1:C:149:GLU:HG2	2.34	0.47
1:C:325:ILE:O	1:C:328:ILE:HG22	2.14	0.47
3:C:1000:WP7:HAQ2	6:C:3348:HOH:O	2.14	0.47
1:C:318:ASN:ND2	1:C:318:ASN:N	2.64	0.46
1:C:94:LYS:HB3	1:C:94:LYS:HE3	1.60	0.46
1:D:301:VAL:HA	1:D:318:ASN:HD21	1.81	0.46
1:C:218:THR:HG23	1:C:248:GLU:HG2	1.97	0.46
1:C:314:PHE:O	1:C:315:SER:HB2	2.15	0.46
1:A:440:ALA:HB3	1:B:440:ALA:HB3	1.98	0.46
1:C:227:LEU:HD12	1:C:238:VAL:HG11	1.98	0.46
1:B:129:LEU:HD23	1:B:299:VAL:CG2	2.46	0.46
1:B:250:MET:HE2	1:B:253:GLU:HG3	1.98	0.46
1:B:321:ASN:HD22	1:B:321:ASN:N	2.13	0.46
1:C:352:ASN:O	1:C:354:PRO:HD3	2.16	0.46
1:C:176:ILE:HB	1:C:180:GLU:HB2	1.96	0.46
1:C:72:HIS:HD2	6:C:3056:HOH:O	1.98	0.46
1:B:163:TRP:CG	1:B:164:PRO:HD2	2.51	0.45
1:D:455:TYR:CD2	1:D:472:ARG:HB3	2.50	0.45
1:A:4:ALA:CA	1:A:152:GLN:HG3	2.46	0.45
1:C:447:LEU:HD11	1:D:449:ALA:HB2	1.98	0.45
1:C:5:PHE:HE2	1:C:151:LEU:HD22	1.82	0.45
1:A:198:PHE:O	1:A:202:GLU:HG3	2.16	0.45
1:A:304:THR:HG21	6:A:3250:HOH:O	2.16	0.45
1:D:190:ARG:NH2	1:D:279:ASP:OD1	2.48	0.45
1:C:80:GLY:CA	1:D:94:LYS:HG2	2.45	0.45
1:B:18:GLU:OE1	3:B:1000:WP7:NBA	2.50	0.45
1:B:8:VAL:HG23	1:B:153:ALA:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:HIS:H	1:D:107:ASN:HD21	1.65	0.45
1:C:8:VAL:HG22	1:C:32:ALA:HB3	1.99	0.44
3:B:1000:WP7:HAP2	3:B:1000:WP7:HBC1	1.81	0.44
1:D:176:ILE:HB	1:D:180:GLU:HB2	2.00	0.44
1:A:437:ILE:HG12	1:A:465:ALA:HB2	2.00	0.44
1:B:190[A]:ARG:NH1	6:B:3132:HOH:O	2.30	0.43
1:D:157:LEU:HD11	1:D:325:ILE:HG12	2.01	0.43
1:C:370:PRO:HG2	1:C:430:LEU:HD11	2.01	0.43
1:C:484:MET:SD	1:C:488:PRO:HD3	2.58	0.43
1:A:155:HIS:HB3	1:A:323:TYR:HE2	1.82	0.43
1:B:45:TYR:CD1	1:B:179:ASN:HB3	2.54	0.43
1:D:319:VAL:HA	1:D:320:PRO:HD3	1.97	0.43
1:B:190[B]:ARG:CD	1:B:216:LYS:HB3	2.49	0.43
1:B:222:ARG:NH1	6:B:3180:HOH:O	2.51	0.43
1:B:299:VAL:HG23	1:B:301:VAL:HG23	2.01	0.43
1:B:40:HIS:H	1:B:107:ASN:HD21	1.67	0.43
1:B:388:LYS:HE2	1:B:388:LYS:HB3	1.86	0.43
1:B:349:VAL:HG12	1:B:350:PHE:CE1	2.54	0.42
1:B:76:SER:HB2	1:B:81:TRP:HB2	2.00	0.42
1:C:8:VAL:HG23	1:C:153:ALA:HB2	2.02	0.42
1:B:250:MET:CE	1:B:253:GLU:HG3	2.50	0.42
1:B:92:TRP:O	1:B:96:ILE:HG12	2.19	0.42
1:A:171:GLY:HA3	1:A:258:VAL:O	2.20	0.42
1:D:370:PRO:HD2	6:D:3301:HOH:O	2.20	0.42
1:B:2:SER:C	1:B:3:LYS:CG	2.88	0.42
1:A:375:CYS:SG	1:A:445:LEU:HD22	2.59	0.42
1:D:331:ARG:HG2	1:D:332:LEU:H	1.84	0.42
1:C:453:ASP:CG	1:D:447:LEU:HD21	2.39	0.42
1:B:389:VAL:HB	1:B:478:TYR:HB2	2.02	0.42
1:A:144:LYS:HB2	1:A:144:LYS:HE3	1.77	0.41
1:C:76:SER:HB2	1:C:81:TRP:HB2	2.02	0.41
1:C:1:MET:HA	1:C:1:MET:HE2	2.01	0.41
1:B:45:TYR:CG	1:B:179:ASN:HB3	2.55	0.41
1:B:353:LYS:CA	6:B:3247:HOH:O	2.68	0.41
1:C:221:TYR:CE2	1:C:223:ASN:HB2	2.56	0.41
1:C:157:LEU:HD11	1:C:325:ILE:HG12	2.01	0.41
1:C:302:LYS:HD3	1:C:303:LEU:O	2.21	0.41
1:D:17:LEU:HA	1:D:17:LEU:HD23	1.98	0.41
1:C:327:ASP:OD1	1:C:333:MET:HA	2.20	0.41
1:D:485:GLU:O	1:D:486:LYS:HG2	2.20	0.41
1:A:17:LEU:HD23	1:A:17:LEU:HA	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:HIS:CE1	1:A:260:LEU:HG	2.56	0.41
1:A:68:GLN:NE2	6:A:3049:HOH:O	2.53	0.41
1:B:461:HIS:HA	1:B:462:PRO:HA	1.92	0.40
1:B:190[A]:ARG:HB2	1:B:190[A]:ARG:HE	1.72	0.40
1:B:221:TYR:CE2	1:B:223:ASN:HB2	2.55	0.40
1:C:5:PHE:CE2	1:C:151:LEU:HD22	2.55	0.40
1:B:93:LYS:NZ	1:B:186:GLU:OE2	2.55	0.40
1:D:167:PRO:HD3	1:D:285:ILE:CD1	2.51	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	487/495 (98%)	472 (97%)	12 (2%)	3 (1%)	25	21
1	B	488/495 (99%)	473 (97%)	15 (3%)	0	100	100
1	C	491/495 (99%)	475 (97%)	15 (3%)	1 (0%)	47	49
1	D	489/495 (99%)	473 (97%)	14 (3%)	2 (0%)	34	32
All	All	1955/1980 (99%)	1893 (97%)	56 (3%)	6 (0%)	41	41

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	480	LYS
1	C	480	LYS
1	D	480	LYS
1	A	213	PRO
1	D	55	VAL
1	A	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	402/407 (99%)	385 (96%)	17 (4%)	30	30
1	B	402/407 (99%)	387 (96%)	15 (4%)	34	35
1	C	405/407 (100%)	383 (95%)	22 (5%)	22	20
1	D	404/407 (99%)	387 (96%)	17 (4%)	30	30
All	All	1613/1628 (99%)	1542 (96%)	71 (4%)	28	28

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	CYS
1	A	60	LYS
1	A	89	LYS
1	A	99	LYS
1	A	101	GLU
1	A	152	GLN
1	A	213	PRO
1	A	224	ASN
1	A	237	GLU
1	A	238	VAL
1	A	266	LYS
1	A	306	LYS
1	A	318	ASN
1	A	394	SER
1	A	400	MET
1	A	480	LYS
1	A	485	GLU
1	B	57	CYS
1	B	60	LYS
1	B	89	LYS
1	B	216	LYS
1	B	224	ASN
1	B	292	ASN
1	B	306	LYS

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Mol	Chain	Res	Type
1	B	313	GLU
1	B	321	ASN
1	B	385	GLU
1	B	400	MET
1	B	462	PRO
1	B	467	GLU
1	B	485	GLU
1	B	487	LEU
1	C	1	MET
1	C	30	ARG
1	C	39	SER
1	C	57	CYS
1	C	60	LYS
1	C	99	LYS
1	C	129	LEU
1	C	150	ARG
1	C	152	GLN
1	C	154	ASP
1	C	189	ARG
1	C	228	ARG
1	C	238	VAL
1	C	259	SER
1	C	260	LEU
1	C	262	THR
1	C	306	LYS
1	C	318	ASN
1	C	335	THR
1	C	400	MET
1	C	446	ARG
1	C	480	LYS
1	D	30	ARG
1	D	57	CYS
1	D	60	LYS
1	D	89	LYS
1	D	94	LYS
1	D	99	LYS
1	D	186	GLU
1	D	260	LEU
1	D	266	LYS
1	D	274	LYS
1	D	318	ASN
1	D	321	ASN

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Mol	Chain	Res	Type
1	D	335	THR
1	D	400	MET
1	D	470	SER
1	D	480	LYS
1	D	487	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	72	HIS
1	A	152	GLN
1	A	318	ASN
1	B	107	ASN
1	B	224	ASN
1	B	310	GLN
1	B	321	ASN
1	C	72	HIS
1	C	107	ASN
1	C	152	GLN
1	C	318	ASN
1	D	107	ASN
1	D	152	GLN
1	D	224	ASN
1	D	295	GLN
1	D	318	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 27 ligands modelled in this entry, 19 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	$\#\|Z\| > 2$
2	FAD	B	998	-	51,58,58	1.32	7 (13%)	60,89,89	2.17	13 (21%)
2	FAD	A	998	-	51,58,58	1.45	7 (13%)	60,89,89	1.97	15 (25%)
2	FAD	C	998	-	51,58,58	1.26	7 (13%)	60,89,89	1.69	8 (13%)
3	WP7	C	1000	-	33,37,37	1.93	6 (18%)	42,52,52	1.80	9 (21%)
3	WP7	A	1000	-	33,37,37	1.94	7 (21%)	42,52,52	1.78	8 (19%)
3	WP7	D	1000	-	33,37,37	2.58	10 (30%)	42,52,52	1.90	11 (26%)
2	FAD	D	998	-	51,58,58	1.96	10 (19%)	60,89,89	2.11	18 (30%)
3	WP7	B	1000	-	33,37,37	2.54	9 (27%)	42,52,52	1.78	10 (23%)

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	FAD	B	998	-	-	5/30/50/50	0/6/6/6
2	FAD	A	998	-	-	4/30/50/50	0/6/6/6
2	FAD	C	998	-	-	5/30/50/50	0/6/6/6
3	WP7	C	1000	-	-	2/13/43/43	0/5/5/5
3	WP7	A	1000	-	-	2/13/43/43	0/5/5/5
3	WP7	D	1000	-	-	0/13/43/43	0/5/5/5
2	FAD	D	998	-	-	5/30/50/50	0/6/6/6
3	WP7	B	1000	-	-	1/13/43/43	0/5/5/5

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1000	WP7	CBB-NBA	9.01	1.41	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1000	WP7	CBB-NBA	8.43	1.41	1.29
2	D	998	FAD	C10-N1	6.66	1.41	1.33
3	B	1000	WP7	CAU-CAT	5.91	1.58	1.49
3	C	1000	WP7	CBB-NBA	5.58	1.37	1.29
3	B	1000	WP7	CAN-NAO	5.49	1.51	1.48
3	D	1000	WP7	CAU-CAT	5.40	1.58	1.49
3	D	1000	WP7	CBC-CBB	5.25	1.57	1.49
3	C	1000	WP7	CBC-CBB	4.94	1.57	1.49
2	D	998	FAD	C2A-N3A	4.84	1.39	1.32
2	D	998	FAD	C4-N3	4.65	1.41	1.33
2	A	998	FAD	C4X-N5	4.54	1.39	1.33
3	A	1000	WP7	CAU-CAT	4.50	1.56	1.49
3	C	1000	WP7	CAU-CAT	4.49	1.56	1.49
3	A	1000	WP7	CBC-CBB	4.17	1.55	1.49
3	B	1000	WP7	CBC-CBB	4.17	1.55	1.49
2	D	998	FAD	C4X-N5	4.10	1.39	1.33
3	D	1000	WP7	CAN-NAO	3.97	1.50	1.48
3	D	1000	WP7	CBB-NAO	3.68	1.45	1.35
2	D	998	FAD	C2A-N1A	3.66	1.40	1.33
3	A	1000	WP7	CAH-NAS	3.64	1.53	1.47
2	A	998	FAD	C10-N1	3.64	1.37	1.33
3	A	1000	WP7	CBB-NBA	3.53	1.34	1.29
2	B	998	FAD	C2A-N3A	3.45	1.37	1.32
3	A	1000	WP7	CBE-NAS	3.43	1.53	1.47
3	B	1000	WP7	CBE-NAS	3.31	1.52	1.47
2	B	998	FAD	C5X-N5	3.29	1.40	1.35
2	C	998	FAD	C2A-N3A	3.19	1.37	1.32
3	B	1000	WP7	CAL-CAK	3.10	1.43	1.38
3	B	1000	WP7	CAH-NAS	3.04	1.52	1.47
2	D	998	FAD	C5X-N5	2.99	1.40	1.35
2	A	998	FAD	C4-N3	2.96	1.38	1.33
2	C	998	FAD	C4-N3	2.94	1.38	1.33
2	C	998	FAD	C2A-N1A	2.93	1.39	1.33
2	A	998	FAD	C2A-N1A	2.91	1.39	1.33
3	C	1000	WP7	CAM-CAN	2.77	1.54	1.51
2	D	998	FAD	C2B-C1B	-2.73	1.49	1.53
3	C	1000	WP7	CAL-CAK	2.65	1.42	1.38
3	C	1000	WP7	CBB-NAO	2.63	1.42	1.35
3	D	1000	WP7	CAM-CAN	2.63	1.54	1.51
3	B	1000	WP7	CBB-NAO	2.59	1.42	1.35
2	B	998	FAD	C5'-C4'	2.54	1.55	1.51
3	B	1000	WP7	CAE-CAN	2.52	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	998	FAD	O4B-C1B	2.42	1.44	1.41
2	A	998	FAD	C1'-N10	2.40	1.50	1.48
2	D	998	FAD	O5B-C5B	-2.39	1.35	1.44
3	A	1000	WP7	CBB-NAO	2.38	1.41	1.35
2	B	998	FAD	C8-C7	-2.33	1.35	1.40
3	D	1000	WP7	CAH-NAS	2.32	1.51	1.47
2	B	998	FAD	C6-C7	2.31	1.43	1.37
2	C	998	FAD	C4X-N5	2.29	1.36	1.33
2	B	998	FAD	C2A-N1A	2.26	1.38	1.33
3	D	1000	WP7	CAK-CLA	-2.25	1.69	1.74
2	A	998	FAD	C9A-N10	2.21	1.41	1.38
2	B	998	FAD	C1'-N10	2.20	1.50	1.48
2	D	998	FAD	O4'-C4'	-2.09	1.38	1.43
2	C	998	FAD	C6-C5X	-2.08	1.38	1.41
2	A	998	FAD	C2A-N3A	2.07	1.35	1.32
2	C	998	FAD	C10-N1	2.06	1.35	1.33
3	D	1000	WP7	CAE-CAN	2.05	1.55	1.52
3	A	1000	WP7	CAZ-NBA	2.03	1.43	1.39
3	D	1000	WP7	CAP-NAO	2.03	1.50	1.46
2	C	998	FAD	C5X-N5	2.01	1.38	1.35

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	998	FAD	C1'-N10-C9A	7.00	123.80	118.29
2	B	998	FAD	C4-N3-C2	6.85	120.92	115.14
2	B	998	FAD	N3A-C2A-N1A	-6.65	118.28	128.68
2	A	998	FAD	N3A-C2A-N1A	-6.22	118.96	128.68
3	C	1000	WP7	CAZ-NBA-CBB	6.14	123.96	118.19
2	C	998	FAD	C4-N3-C2	6.01	120.22	115.14
2	D	998	FAD	O3B-C3B-C4B	-5.95	93.84	111.05
2	D	998	FAD	C4X-N5-C5X	5.56	122.33	116.77
3	D	1000	WP7	CAZ-NBA-CBB	5.53	123.39	118.19
2	D	998	FAD	O2A-PA-O5B	5.51	133.35	107.75
2	A	998	FAD	C5X-C9A-N10	5.38	121.61	117.72
2	C	998	FAD	N3A-C2A-N1A	-5.26	120.46	128.68
3	B	1000	WP7	CAZ-NBA-CBB	5.25	123.12	118.19
2	C	998	FAD	C1'-N10-C9A	5.02	122.24	118.29
2	D	998	FAD	N3A-C2A-N1A	-4.94	120.95	128.68
2	D	998	FAD	C4-N3-C2	4.92	119.29	115.14
3	D	1000	WP7	CAL-CAK-CLA	-4.89	113.04	119.15
3	A	1000	WP7	CBE-NAS-CAH	4.85	121.96	112.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	998	FAD	C4X-N5-C5X	4.73	121.50	116.77
2	A	998	FAD	C4X-N5-C5X	4.62	121.39	116.77
2	A	998	FAD	C2A-N1A-C6A	4.33	126.17	118.75
3	B	1000	WP7	OAI-CAT-NAS	-4.09	115.57	122.34
2	B	998	FAD	C10-C4X-N5	-3.90	118.56	121.26
3	B	1000	WP7	CBE-NAS-CAH	3.89	120.10	112.62
2	D	998	FAD	C4A-C5A-N7A	-3.79	105.45	109.40
2	B	998	FAD	C4X-C4-N3	-3.76	118.30	123.43
3	C	1000	WP7	CBD-CBE-NAS	-3.74	102.42	110.44
3	D	1000	WP7	CAM-CAZ-NBA	-3.74	118.93	122.17
2	A	998	FAD	C5A-C6A-N6A	3.69	125.95	120.35
3	C	1000	WP7	CAE-CAN-NAO	-3.68	106.33	111.55
3	A	1000	WP7	CAE-CAN-NAO	-3.64	106.39	111.55
2	A	998	FAD	C1'-N10-C10	3.59	121.62	118.41
3	A	1000	WP7	CAQ-CAP-NAO	-3.58	106.39	112.10
2	B	998	FAD	C4'-C3'-C2'	-3.53	106.02	113.36
3	C	1000	WP7	CAQ-NAR-CBD	3.51	120.20	111.23
2	D	998	FAD	O4B-C4B-C5B	3.47	120.80	109.37
3	D	1000	WP7	OAI-CAT-NAS	-3.47	116.60	122.34
2	D	998	FAD	C4X-C4-N3	-3.47	118.69	123.43
3	D	1000	WP7	CAY-CAX-CAK	-3.44	115.61	119.24
2	C	998	FAD	C4X-C4-N3	-3.34	118.86	123.43
3	A	1000	WP7	CAP-CAQ-NAR	-3.32	104.98	113.02
2	B	998	FAD	C4A-C5A-N7A	-3.20	106.07	109.40
3	C	1000	WP7	CAQ-CAP-NAO	-3.16	107.04	112.10
3	B	1000	WP7	CAQ-CAP-NAO	-3.14	107.08	112.10
2	B	998	FAD	C1'-N10-C10	-3.13	115.61	118.41
3	C	1000	WP7	CBD-NAR-CAG	3.07	115.73	108.83
2	A	998	FAD	C4-N3-C2	2.97	117.65	115.14
3	C	1000	WP7	CAY-CAZ-CAM	2.88	121.97	119.49
3	B	1000	WP7	CAE-CAN-NAO	-2.87	107.48	111.55
2	A	998	FAD	C5A-C6A-N1A	-2.86	113.88	120.35
3	B	1000	WP7	CAP-CAQ-NAR	-2.79	106.27	113.02
2	B	998	FAD	O3'-C3'-C2'	2.78	115.53	108.81
2	D	998	FAD	C6-C5X-N5	2.78	122.11	119.05
3	C	1000	WP7	CAE-CAN-CAM	-2.73	108.09	112.78
2	A	998	FAD	C9A-N10-C10	-2.68	118.40	121.91
3	B	1000	WP7	CAE-CAN-CAM	-2.65	108.21	112.78
2	A	998	FAD	C9A-C5X-N5	-2.63	118.24	122.36
2	A	998	FAD	C4X-C4-N3	-2.59	119.89	123.43
2	C	998	FAD	C4A-C5A-N7A	-2.58	106.71	109.40
2	A	998	FAD	C10-C4X-N5	-2.57	119.48	121.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1000	WP7	CAU-CAT-NAS	2.56	126.35	119.81
3	C	1000	WP7	CAM-CAZ-NBA	-2.55	119.96	122.17
3	A	1000	WP7	CAQ-NAR-CAG	2.52	117.68	111.23
2	D	998	FAD	C9A-C5X-N5	-2.51	118.43	122.36
2	C	998	FAD	C9A-N10-C10	-2.47	118.68	121.91
2	C	998	FAD	C10-C4X-N5	-2.43	119.58	121.26
3	D	1000	WP7	CAE-CAN-NAO	-2.42	108.12	111.55
3	D	1000	WP7	CAQ-NAR-CAG	2.42	117.41	111.23
3	D	1000	WP7	CBE-NAS-CAH	2.40	117.24	112.62
3	A	1000	WP7	CAZ-NBA-CBB	2.37	120.41	118.19
2	C	998	FAD	C5B-C4B-C3B	-2.36	106.32	115.18
2	D	998	FAD	O5B-PA-O1A	-2.36	99.84	109.07
2	D	998	FAD	C1B-N9A-C4A	-2.28	122.63	126.64
2	D	998	FAD	C10-C4X-N5	-2.25	119.70	121.26
2	B	998	FAD	C3B-C2B-C1B	2.24	104.36	100.98
3	D	1000	WP7	CAQ-CAP-NAO	-2.22	108.55	112.10
2	A	998	FAD	C4-C4X-C10	2.22	121.42	119.95
2	D	998	FAD	C4X-C10-N10	-2.19	118.05	120.30
3	D	1000	WP7	CAX-CAK-CLA	2.17	122.74	119.35
3	B	1000	WP7	CAM-CAN-NAO	2.14	113.51	110.39
2	A	998	FAD	C1'-N10-C9A	2.13	119.97	118.29
3	B	1000	WP7	CAL-CAK-CLA	2.13	121.81	119.15
3	D	1000	WP7	CBD-NAR-CAG	2.13	113.63	108.83
2	A	998	FAD	O4B-C1B-C2B	-2.13	103.81	106.93
2	D	998	FAD	O4'-C4'-C5'	-2.13	105.14	109.92
3	A	1000	WP7	CAB-CAC-CAF	2.12	123.42	120.19
2	D	998	FAD	P-O3P-PA	2.12	140.09	132.83
2	B	998	FAD	C4-C4X-C10	2.07	121.32	119.95
3	A	1000	WP7	CAX-CAK-CLA	-2.06	116.14	119.35
2	D	998	FAD	C4'-C3'-C2'	-2.04	109.11	113.36
2	B	998	FAD	C2A-N1A-C6A	2.01	122.19	118.75
2	D	998	FAD	C5X-C9A-N10	2.01	119.17	117.72

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1000	WP7	CAP-CAQ-NAR-CBD
2	D	998	FAD	C5B-O5B-PA-O2A
3	A	1000	WP7	CAP-CAQ-NAR-CBD
3	B	1000	WP7	NAO-CAP-CAQ-NAR
2	C	998	FAD	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
3	A	1000	WP7	CAP-CAQ-NAR-CAG
2	C	998	FAD	C3B-C4B-C5B-O5B
2	A	998	FAD	PA-O3P-P-O5'
2	D	998	FAD	PA-O3P-P-O5'
2	B	998	FAD	PA-O3P-P-O5'
2	C	998	FAD	PA-O3P-P-O5'
2	A	998	FAD	P-O3P-PA-O2A
2	D	998	FAD	P-O3P-PA-O2A
2	B	998	FAD	P-O3P-PA-O2A
2	C	998	FAD	P-O3P-PA-O2A
2	D	998	FAD	C5B-O5B-PA-O1A
3	C	1000	WP7	CAP-CAQ-NAR-CAG
2	A	998	FAD	O4B-C4B-C5B-O5B
2	A	998	FAD	C3B-C4B-C5B-O5B
2	D	998	FAD	C5B-O5B-PA-O3P
2	B	998	FAD	O4B-C4B-C5B-O5B
2	B	998	FAD	P-O3P-PA-O1A
2	C	998	FAD	P-O3P-PA-O1A
2	B	998	FAD	C5'-O5'-P-O1P

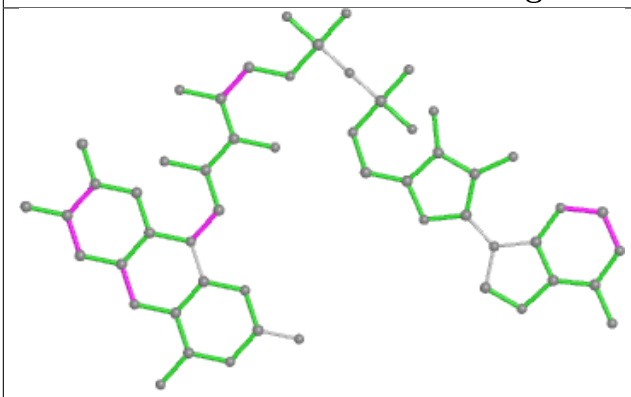
There are no ring outliers.

4 monomers are involved in 7 short contacts:

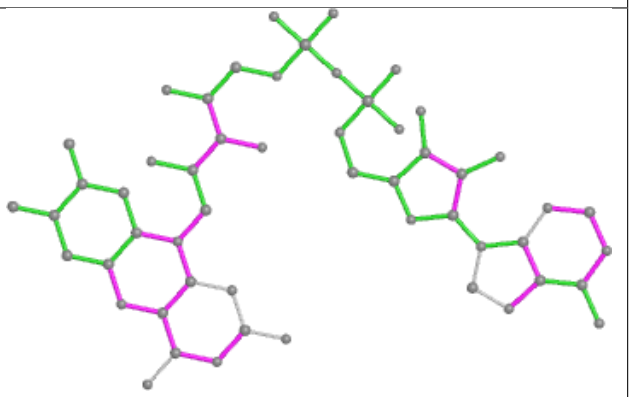
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1000	WP7	2	0
3	D	1000	WP7	2	0
2	D	998	FAD	1	0
3	B	1000	WP7	2	0

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.

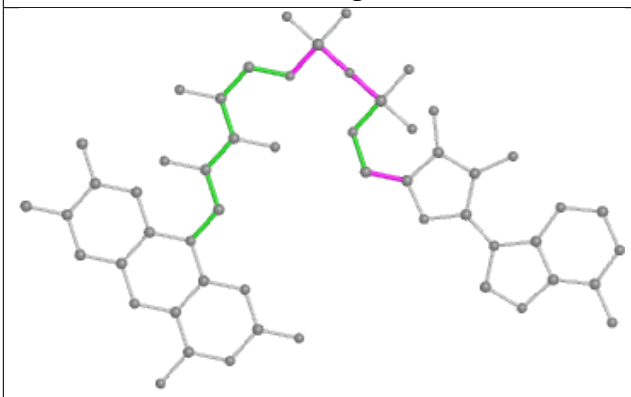
Ligand FAD B 998



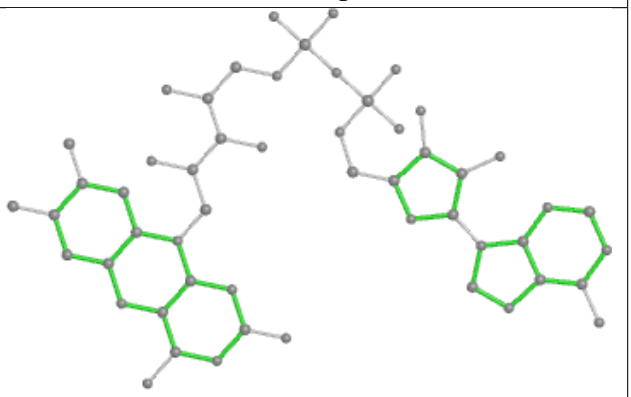
Bond lengths



Bond angles

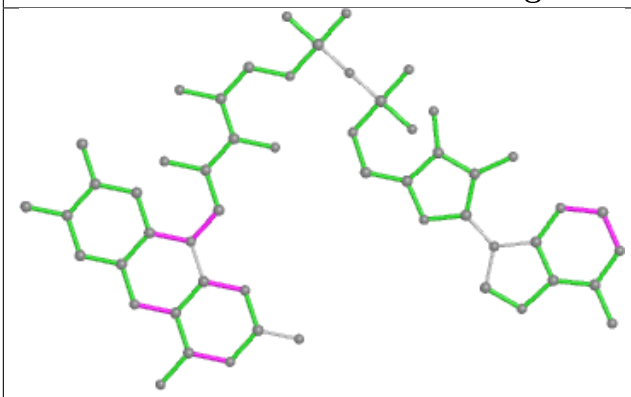


Torsions

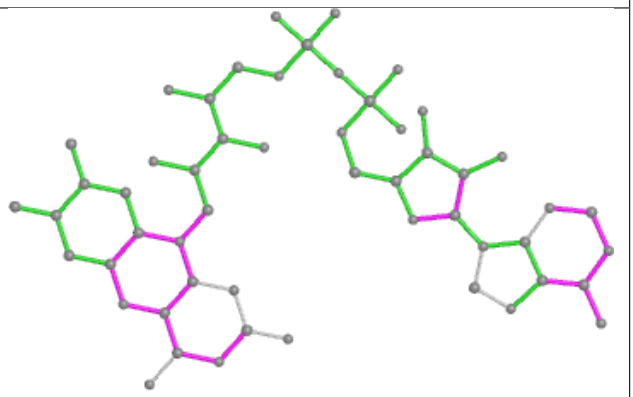


Rings

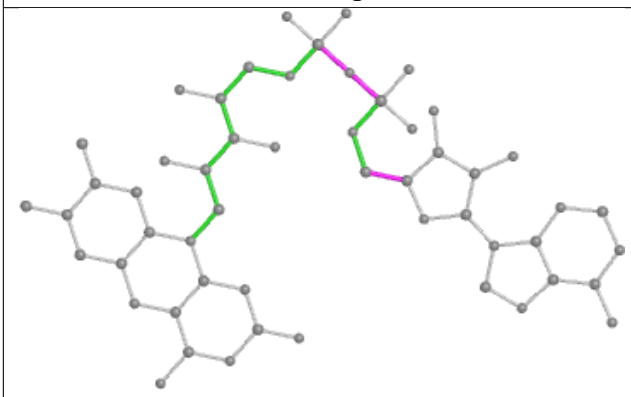
Ligand FAD A 998



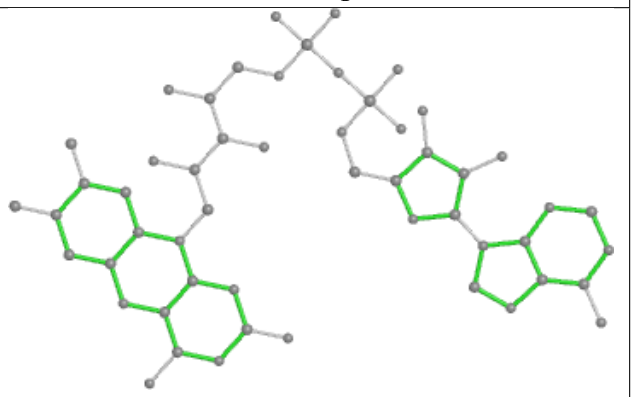
Bond lengths



Bond angles

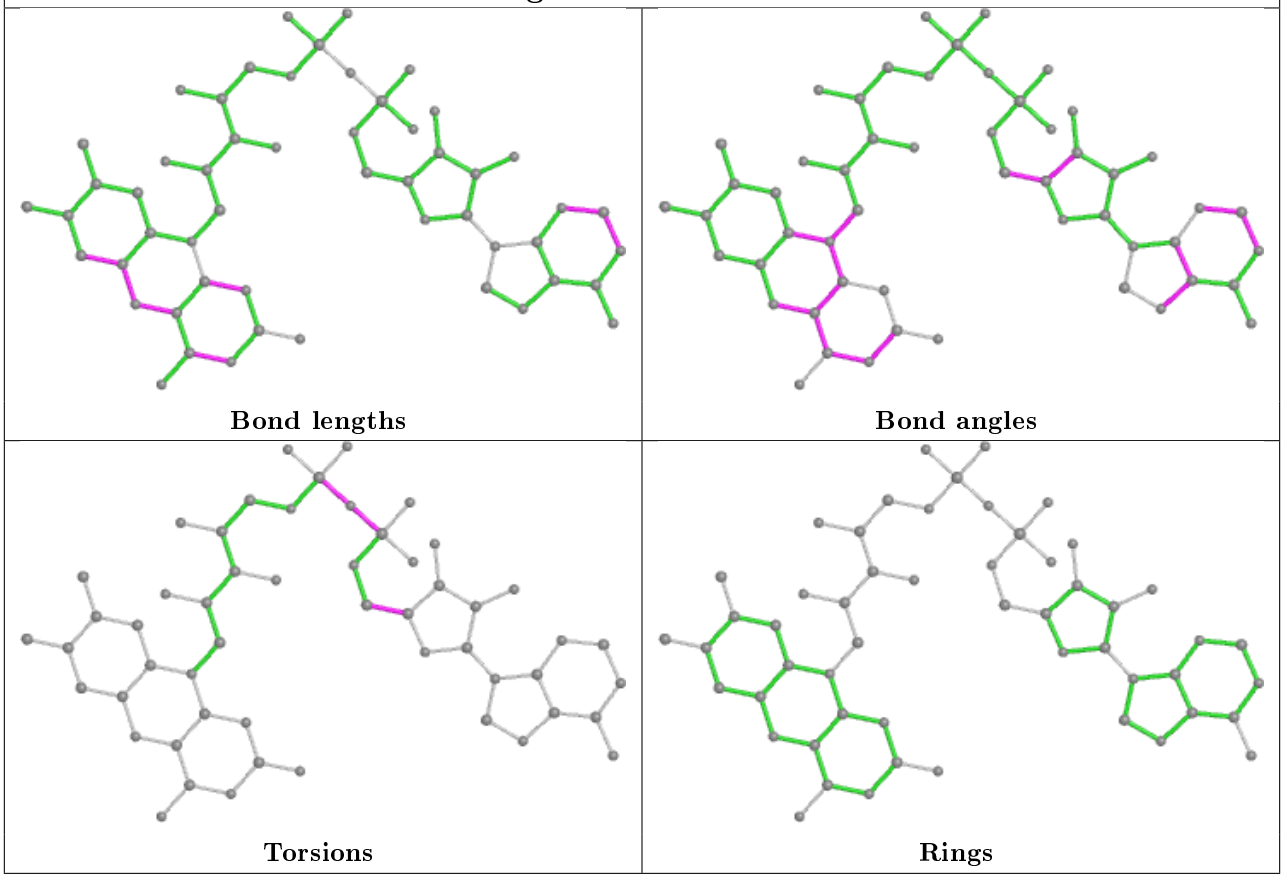


Torsions

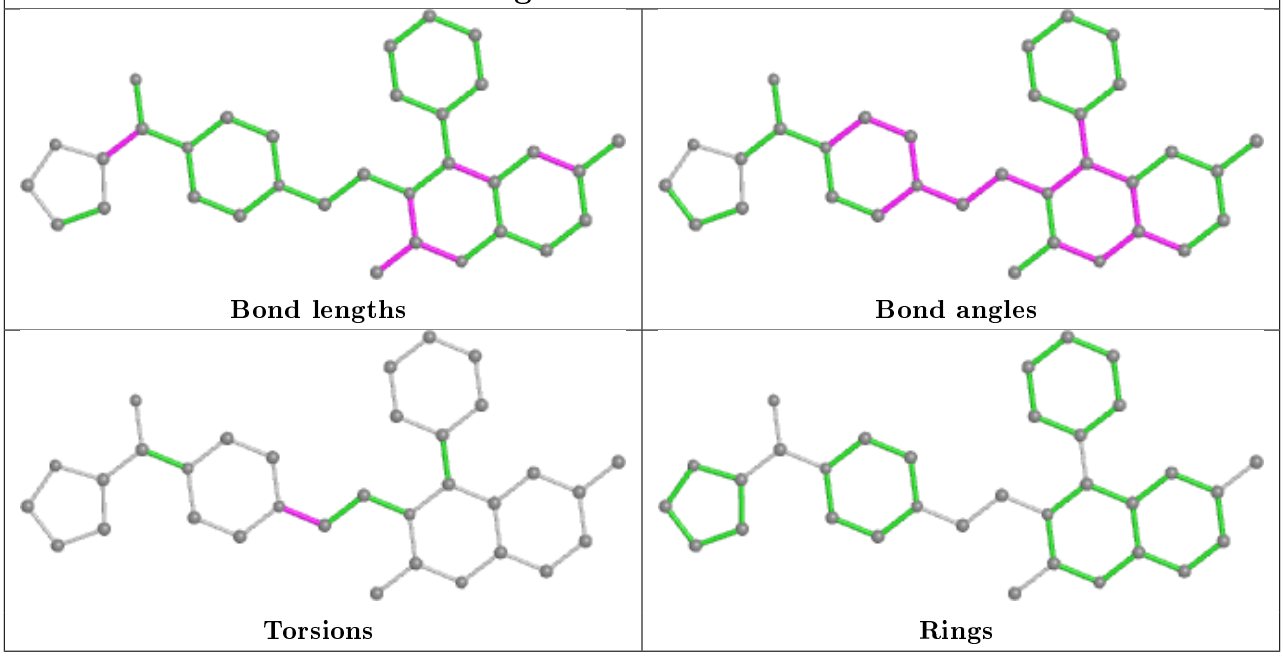


Rings

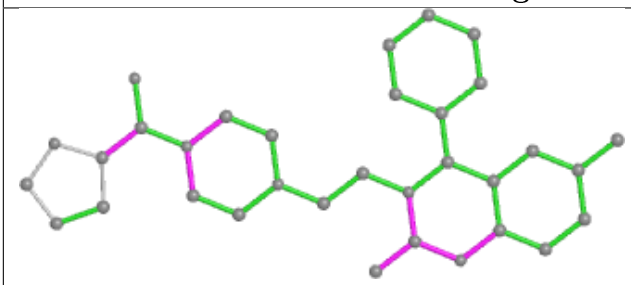
Ligand FAD C 998



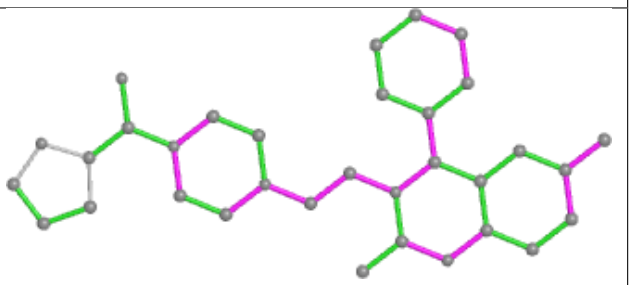
Ligand WP7 C 1000



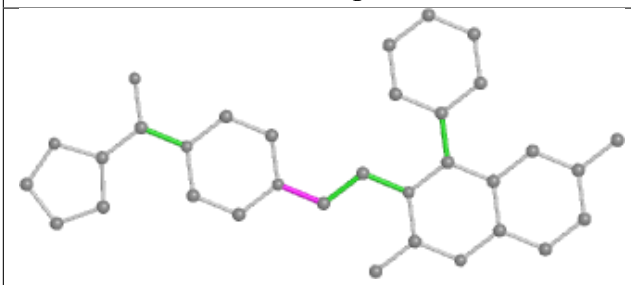
Ligand WP7 A 1000



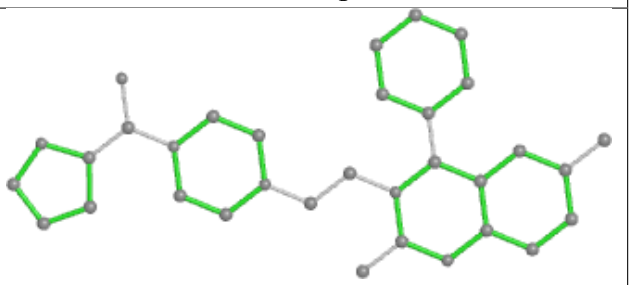
Bond lengths



Bond angles

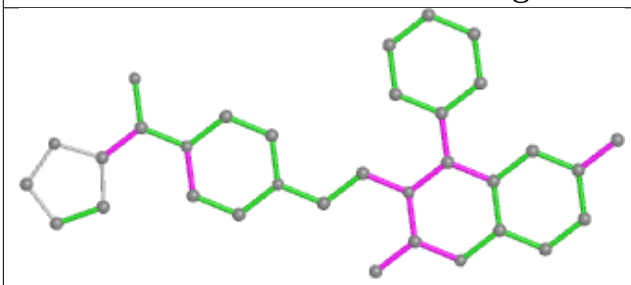


Torsions

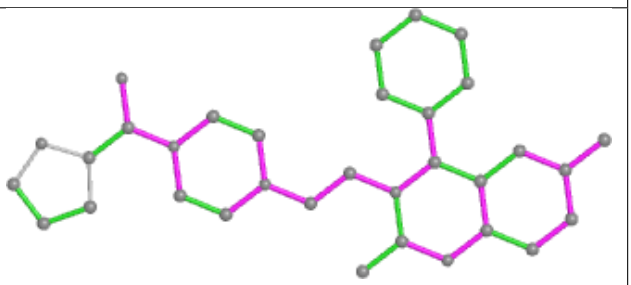


Rings

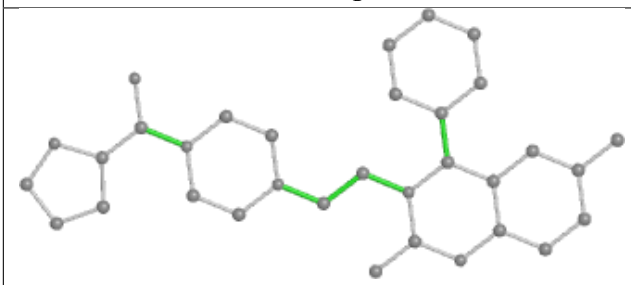
Ligand WP7 D 1000



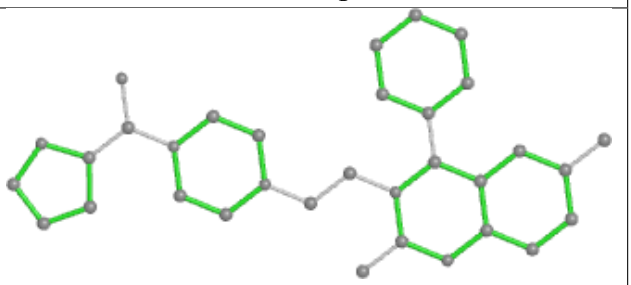
Bond lengths



Bond angles

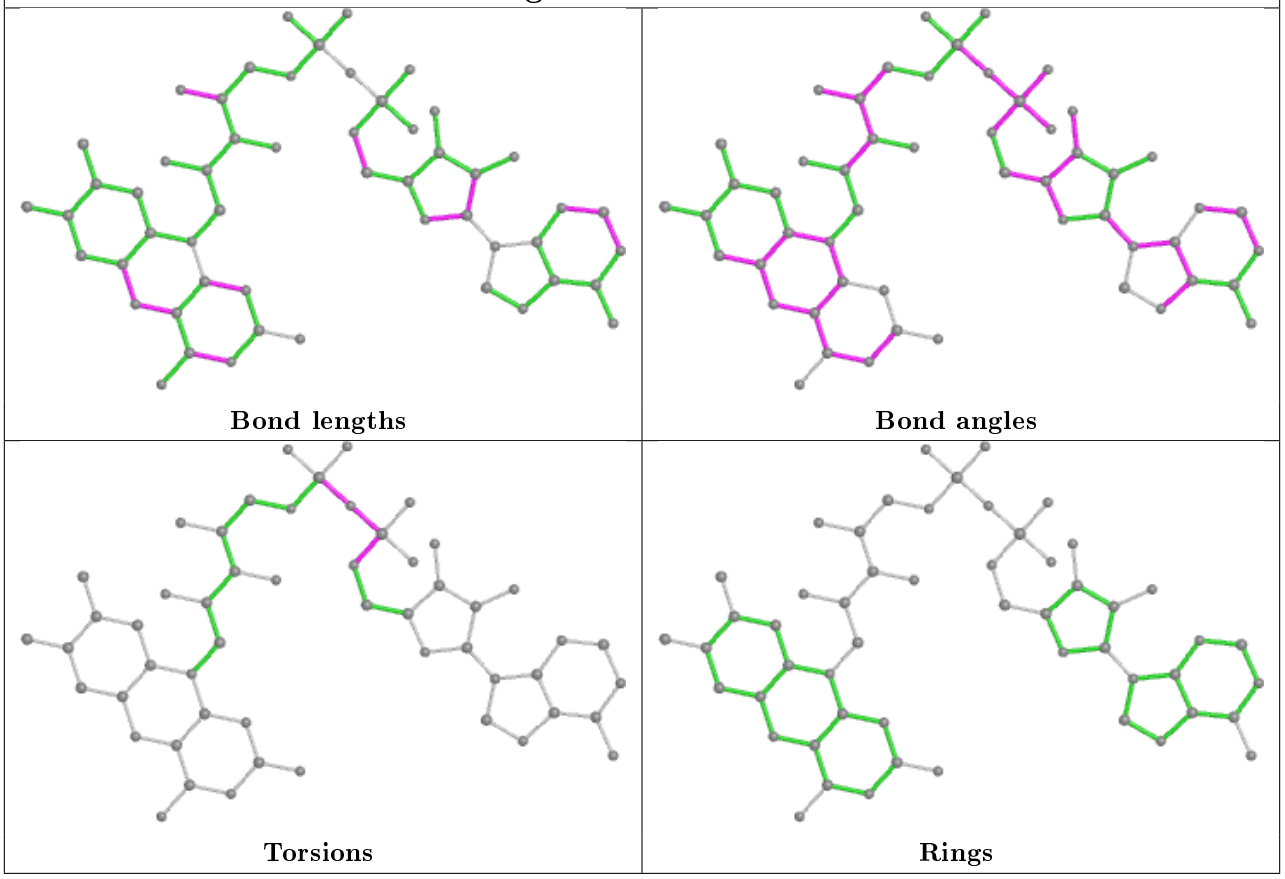


Torsions



Rings

Ligand FAD D 998



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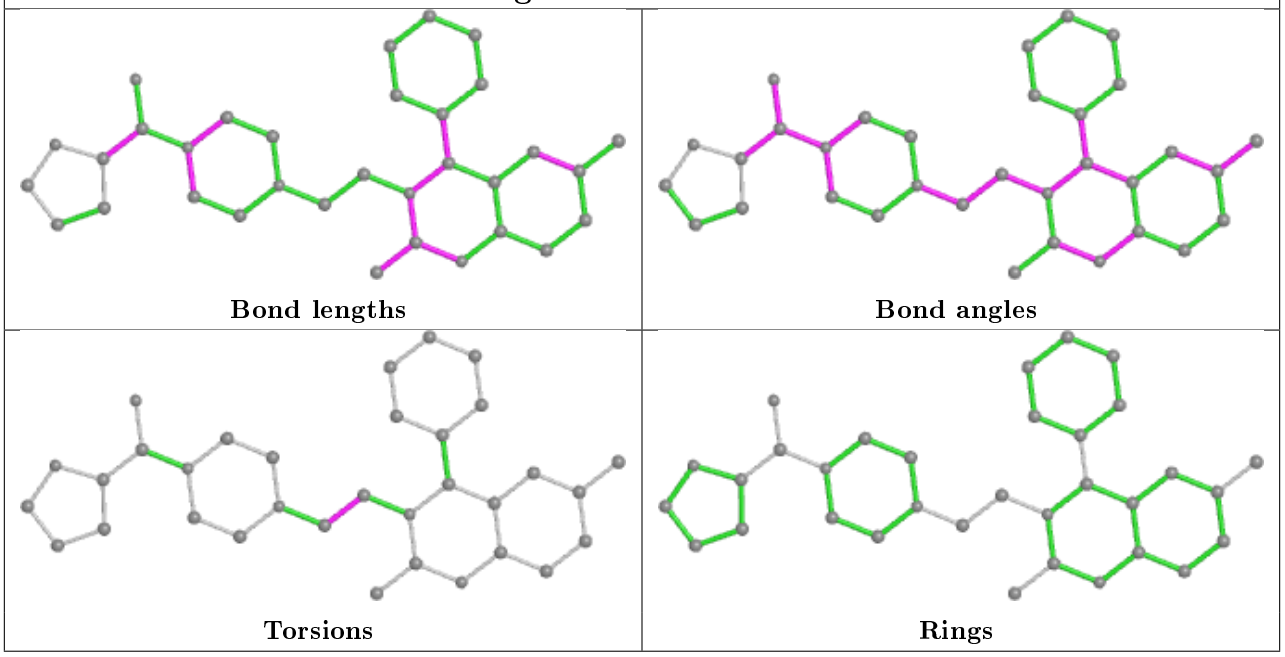


5.7 Other polymers (i)

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	489/495 (98%)	-0.48	3 (0%)	89	91	7, 16, 29, 40	0
1	B	487/495 (98%)	-0.27	3 (0%)	89	91	9, 20, 37, 48	0
1	C	492/495 (99%)	-0.26	4 (0%)	86	88	8, 20, 41, 53	0
1	D	490/495 (98%)	-0.45	4 (0%)	86	88	8, 17, 29, 56	0
All	All	1958/1980 (98%)	-0.37	14 (0%)	87	89	7, 18, 37, 56	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	488	PRO	5.3
1	B	352	ASN	4.0
1	D	487	LEU	3.8
1	C	352	ASN	3.5
1	D	305	PRO	2.7
1	A	305	PRO	2.6
1	A	352	ASN	2.5
1	B	353	LYS	2.5
1	C	30	ARG	2.4
1	B	2	SER	2.2
1	C	481	GLY	2.2
1	A	306	LYS	2.1
1	C	305	PRO	2.1
1	D	481	GLY	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 (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

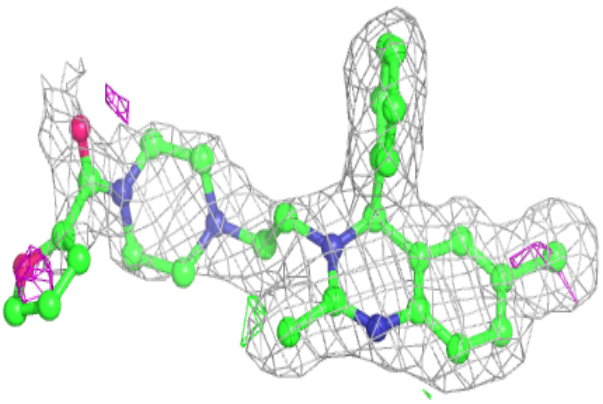
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

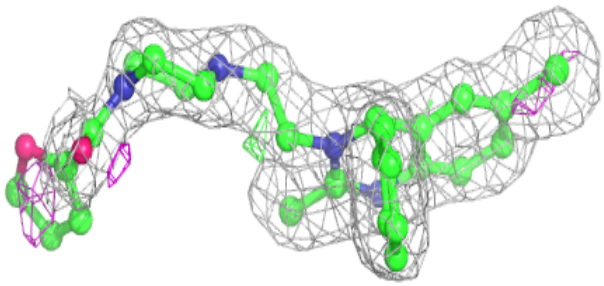
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NA	C	1492	1/1	0.81	0.08	44,44,44,44	0
3	WP7	C	1000	33/33	0.90	0.16	25,32,68,68	0
3	WP7	B	1000	33/33	0.91	0.17	21,27,72,72	0
4	CL	B	2003	1/1	0.93	0.07	34,34,34,34	0
4	CL	D	1491	1/1	0.93	0.08	33,33,33,33	0
3	WP7	A	1000	33/33	0.94	0.14	12,20,61,62	0
5	NA	D	1492	1/1	0.95	0.15	29,29,29,29	0
3	WP7	D	1000	33/33	0.95	0.13	10,18,61,62	0
5	NA	A	1491	1/1	0.95	0.09	19,19,19,19	0
4	CL	C	1491	1/1	0.96	0.04	34,34,34,34	0
5	NA	B	2004	1/1	0.97	0.05	30,30,30,30	0
2	FAD	B	998	53/53	0.97	0.10	7,16,30,31	0
5	NA	A	1492	1/1	0.97	0.08	28,28,28,28	0
2	FAD	C	998	53/53	0.97	0.09	7,17,23,25	0
5	NA	B	2005	1/1	0.97	0.16	32,32,32,32	0
2	FAD	A	998	53/53	0.98	0.09	3,9,12,14	0
5	NA	D	1493	1/1	0.98	0.03	19,19,19,19	0
2	FAD	D	998	53/53	0.98	0.09	2,10,15,23	0
4	CL	A	1490	1/1	0.98	0.10	32,32,32,32	0
5	NA	C	1493	1/1	0.98	0.06	19,19,19,19	0
4	CL	B	2001	1/1	0.99	0.05	20,20,20,20	0
4	CL	C	1490	1/1	0.99	0.07	16,16,16,16	0
4	CL	A	1488	1/1	0.99	0.07	15,15,15,15	0
4	CL	B	2002	1/1	0.99	0.08	15,15,15,15	0
4	CL	A	1489	1/1	0.99	0.06	22,22,22,22	0
4	CL	D	1489	1/1	0.99	0.05	28,28,28,28	0
4	CL	D	1490	1/1	1.00	0.08	16,16,16,16	0

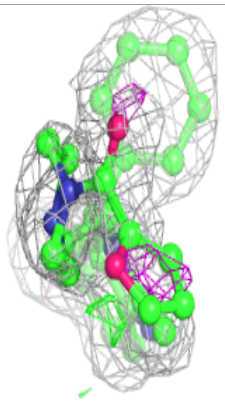
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around WP7 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)

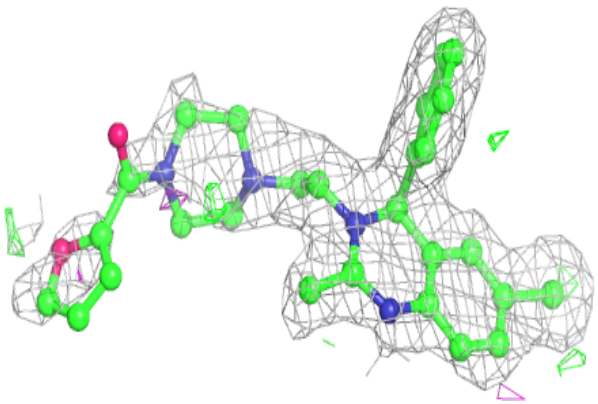


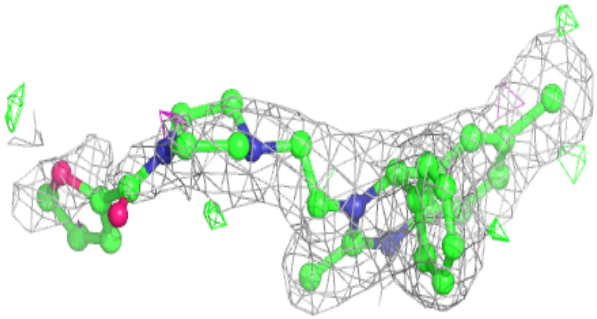


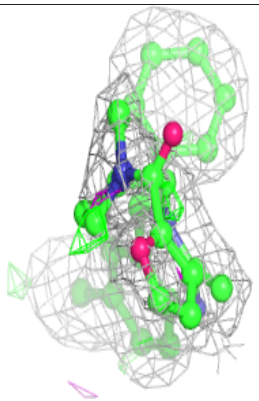


Electron density around WP7 B 1000:

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

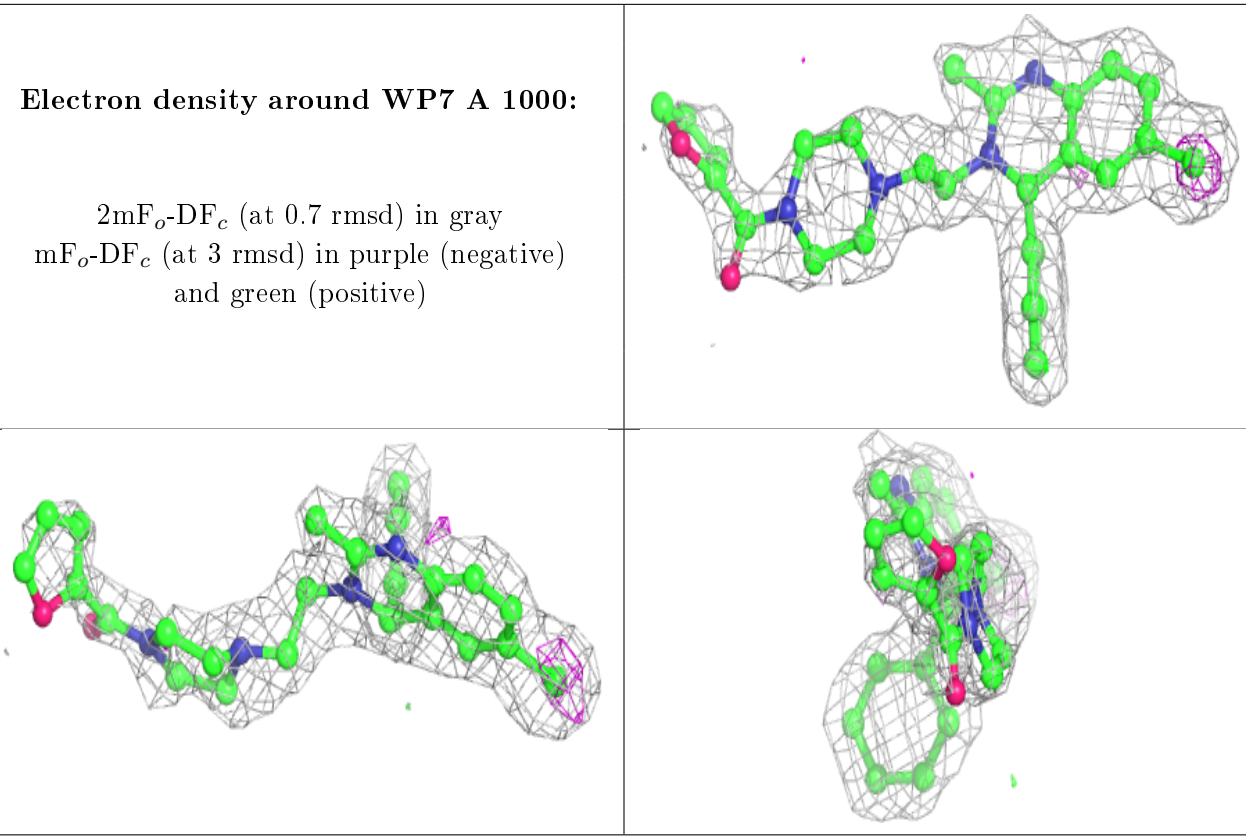






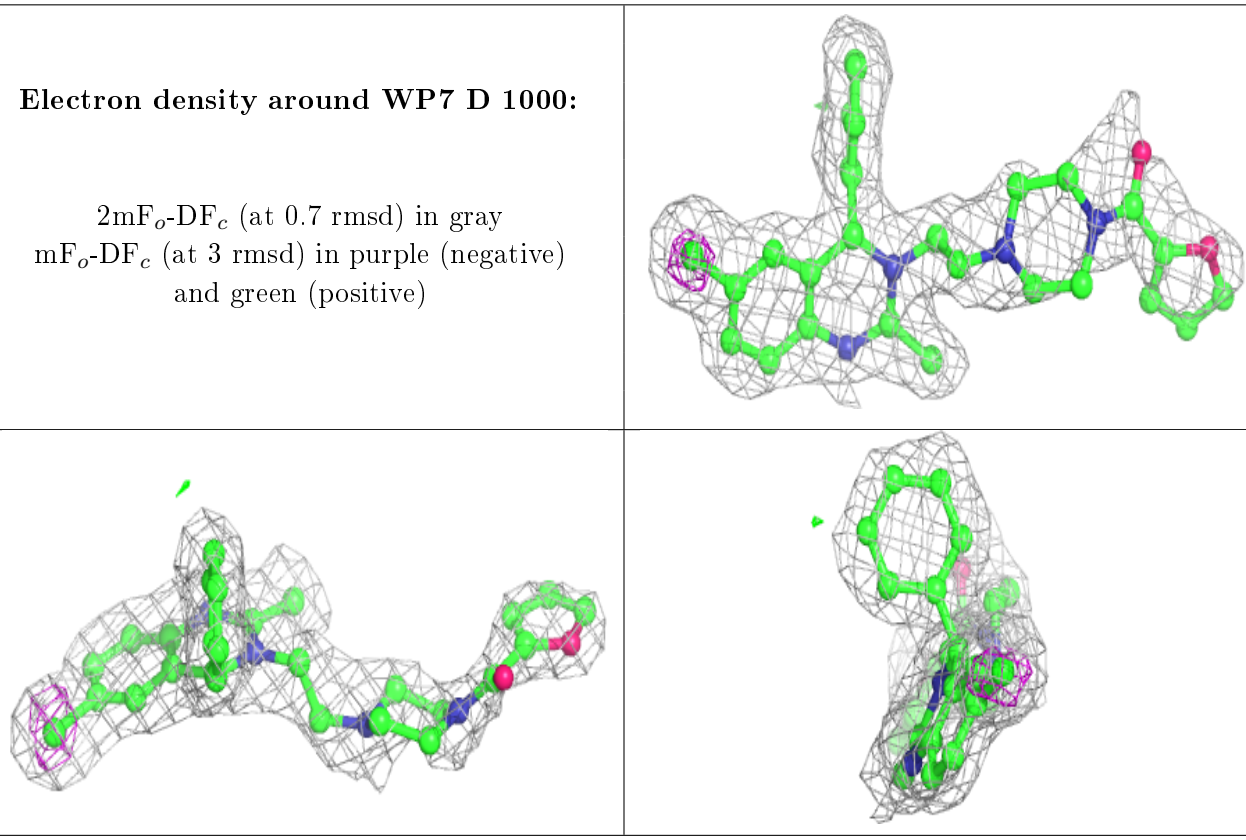
Electron density around WP7 A 1000:

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



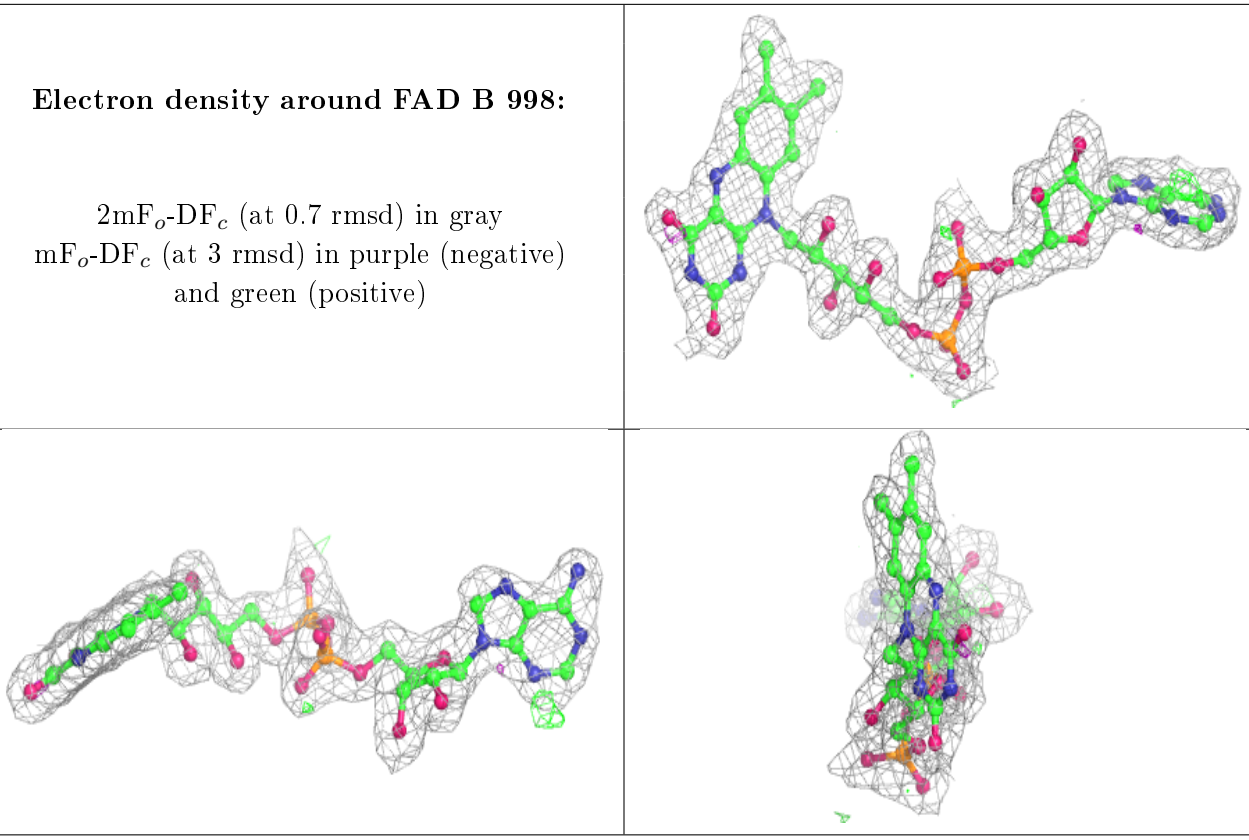
Electron density around WP7 D 1000:

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



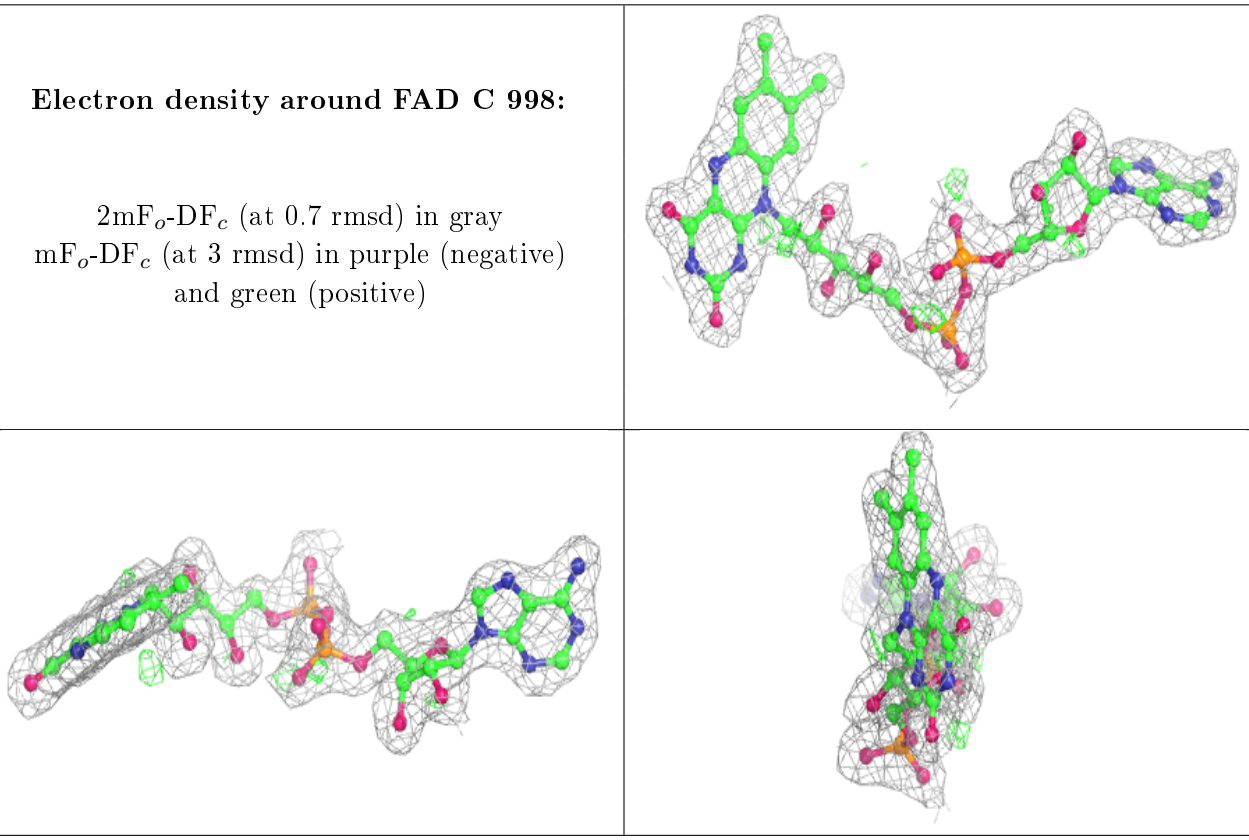
Electron density around FAD B 998:

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



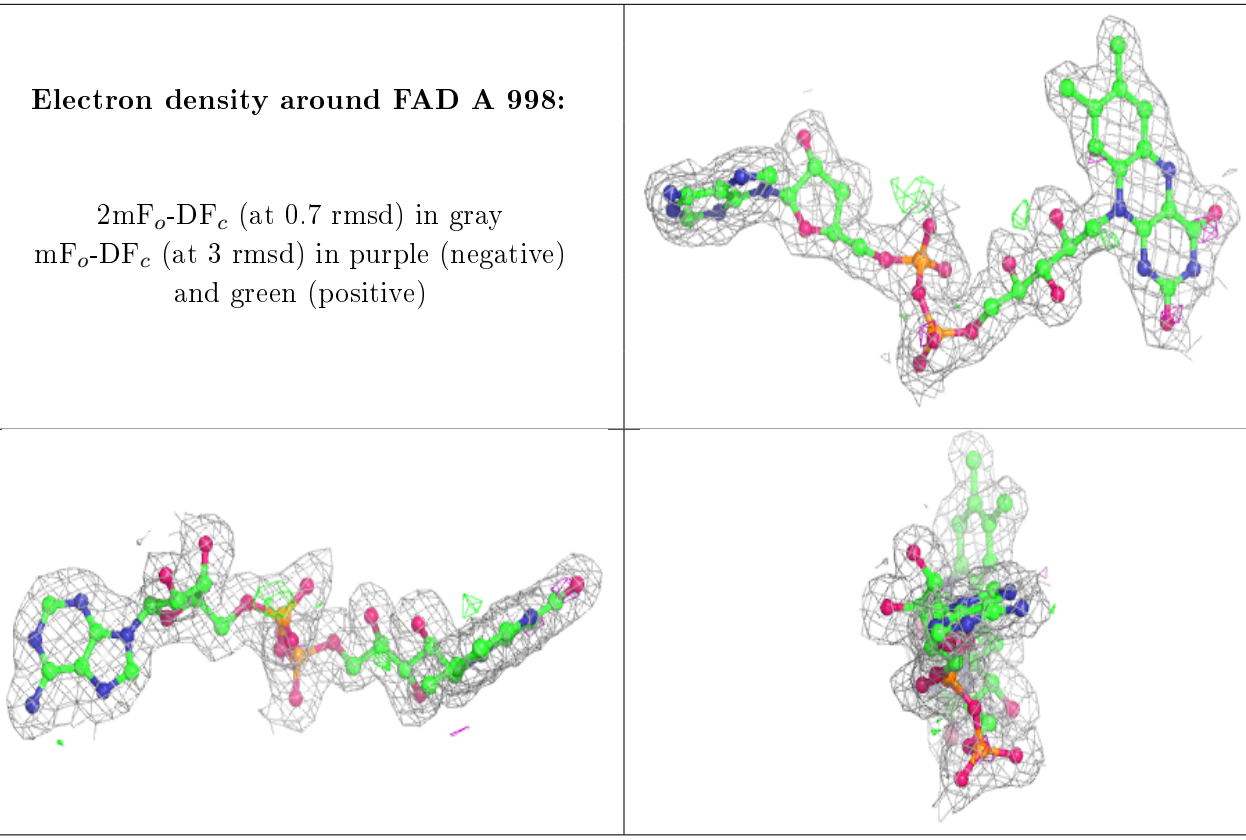
Electron density around FAD C 998:

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



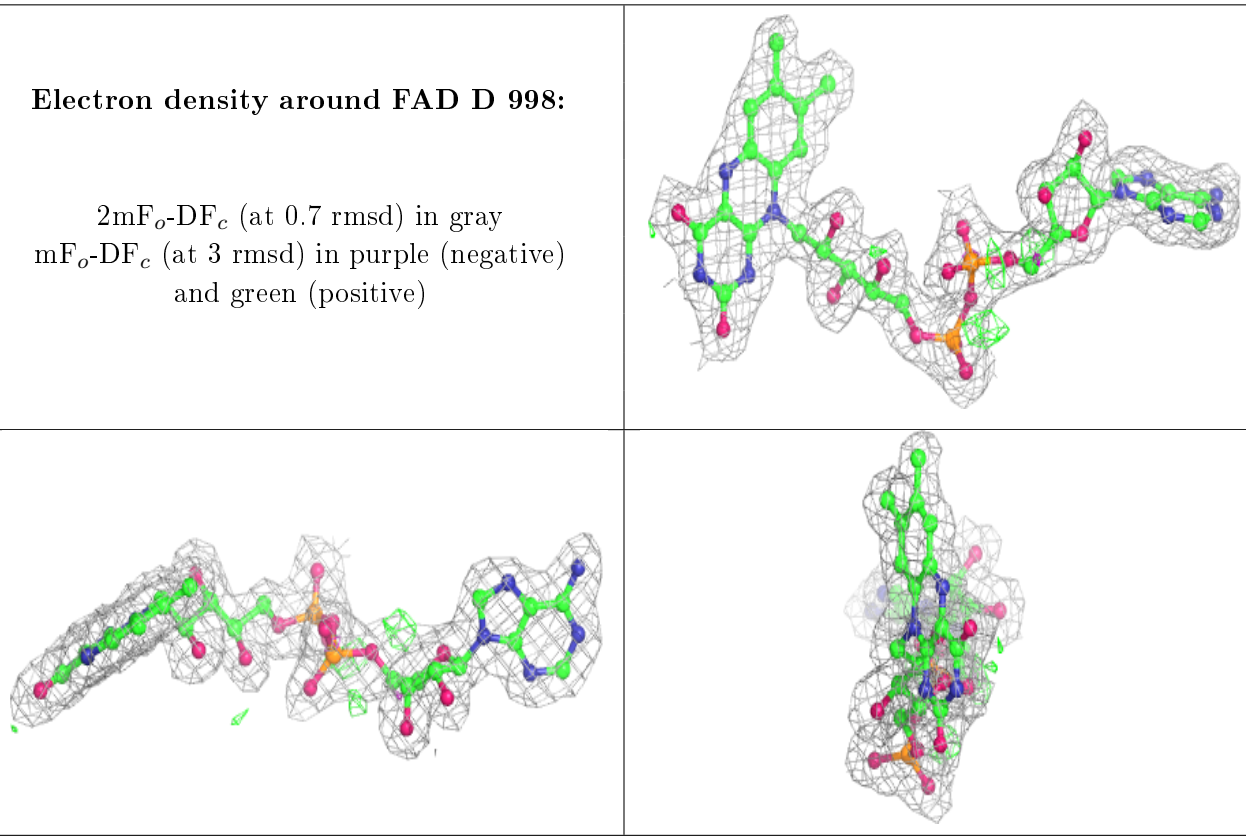
Electron density around FAD A 998:

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



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)



6.5 Other polymers (i)

There are no such residues in this entry.