



# Full wwPDB X-ray Structure Validation Report ⓘ

May 19, 2020 – 03:48 pm BST

PDB ID : 2WPF  
Title : Trypanosoma brucei trypanothione reductase in complex with 3,4- dihydro-quinazoline inhibitor (DDD00085762)  
Authors : Alphey, M.S.; Patterson, S.; Fairlamb, A.H.  
Deposited on : 2009-08-06  
Resolution : 1.90 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](mailto: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.

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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

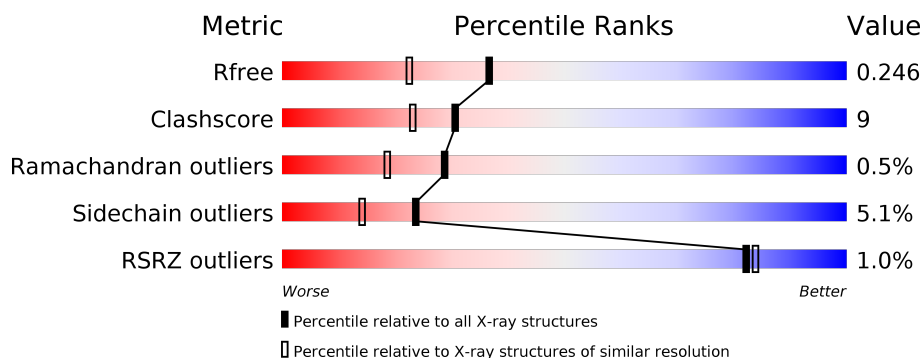
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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

Mol	Chain	Length	Quality of chain
1	A	495	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 19%, green 77%, grey 3%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>77%</span> <span>19%</span> <span>..</span> </div> </div>
1	B	495	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 20%, green 76%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>76%</span> <span>20%</span> <span>..</span> </div> </div>
1	C	495	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 21%, green 76%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>76%</span> <span>21%</span> <span>..</span> </div> </div>
1	D	495	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 17%, green 80%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>80%</span> <span>17%</span> <span>..</span> </div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16503 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.

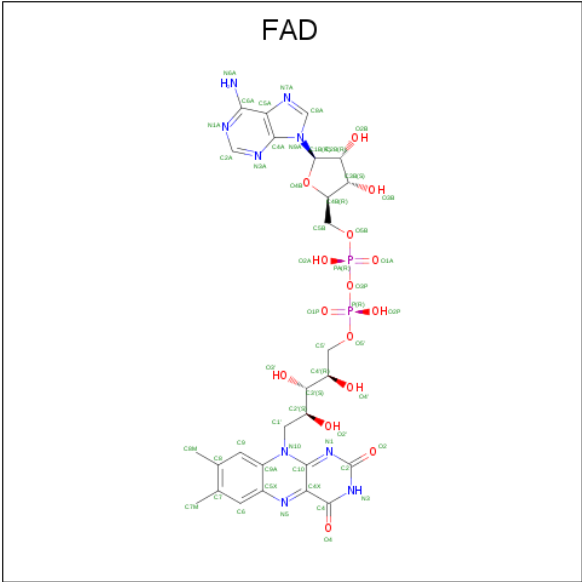
- Molecule 1 is a protein called TRYPANOTHIONE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	490	Total	C	N	O	S	0	2	0
			3733	2374	636	702	21			
1	B	487	Total	C	N	O	S	0	2	0
			3702	2353	631	699	19			
1	C	487	Total	C	N	O	S	0	3	0
			3716	2364	630	703	19			
1	D	491	Total	C	N	O	S	0	2	0
			3737	2376	635	706	20			

There are 12 discrepancies between the modelled and reference sequences:

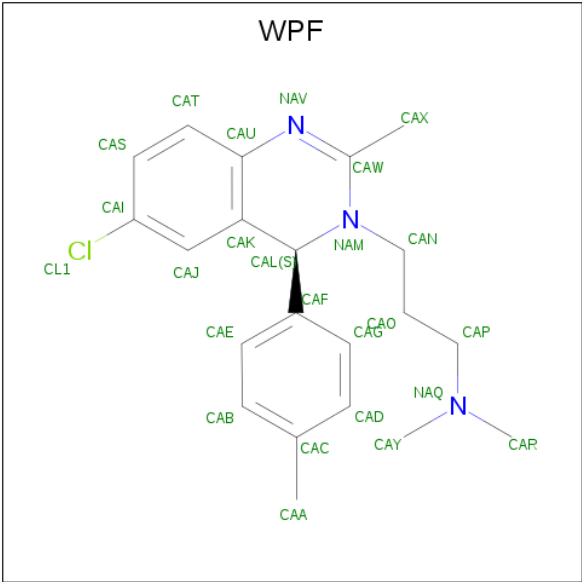
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P39051
A	-1	SER	-	expression tag	UNP P39051
A	0	HIS	-	expression tag	UNP P39051
B	-2	GLY	-	expression tag	UNP P39051
B	-1	SER	-	expression tag	UNP P39051
B	0	HIS	-	expression tag	UNP P39051
C	-2	GLY	-	expression tag	UNP P39051
C	-1	SER	-	expression tag	UNP P39051
C	0	HIS	-	expression tag	UNP P39051
D	-2	GLY	-	expression tag	UNP P39051
D	-1	SER	-	expression tag	UNP P39051
D	0	HIS	-	expression tag	UNP P39051

- 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 3-[(4S)-6-CHLORO-2-METHYL-4-(4-METHYLPHENYL)QUINAZOLI N-3(4H)-YL]-N,N-DIMETHYLPROPAN-1-AMINE (three-letter code: WPF) (formula: C<sub>21</sub>H<sub>26</sub>ClN<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	0	0
			25	21	1	3		
3	B	1	Total	C	Cl	N	0	0
			25	21	1	3		
3	C	1	Total	C	Cl	N	0	0
			25	21	1	3		
3	D	1	Total	C	Cl	N	0	0
			25	21	1	3		

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

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

- Molecule 5 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Br	0	0
			1	1		
5	D	2	Total	Br	0	0
			2	2		

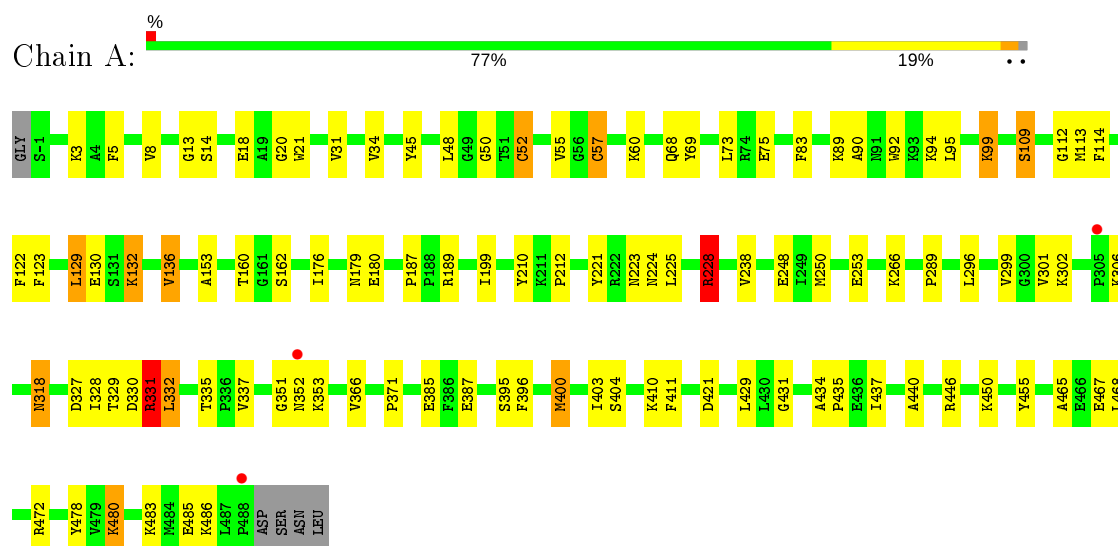
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	374	Total	O	0	0
			374	374		
6	B	290	Total	O	0	0
			290	290		
6	C	282	Total	O	0	0
			282	282		
6	D	347	Total	O	0	0
			347	347		

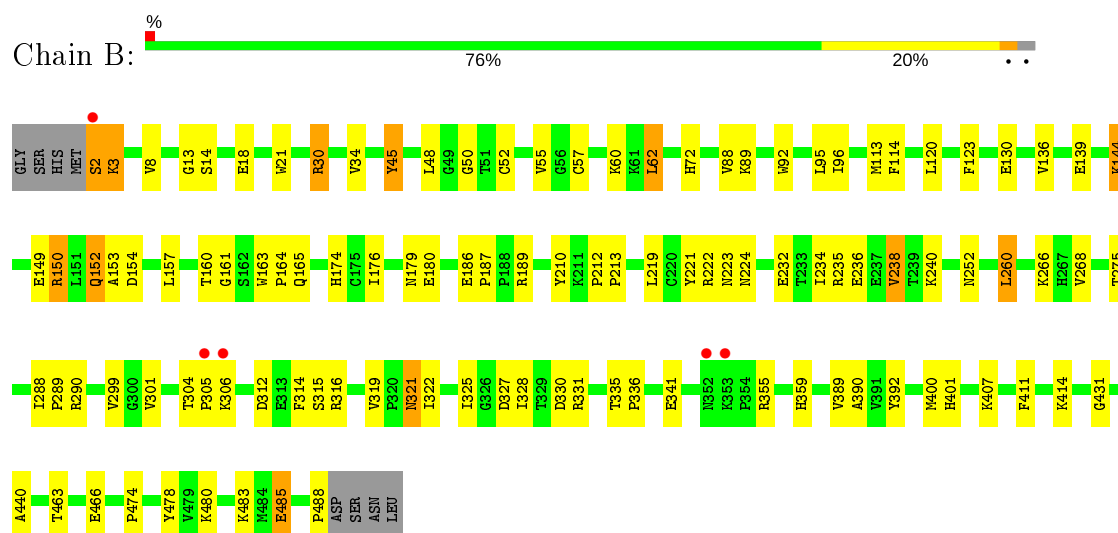
### 3 Residue-property plots [i](#)

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.

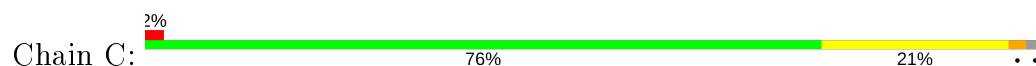
#### • Molecule 1: TRYPANOTHIONE REDUCTASE

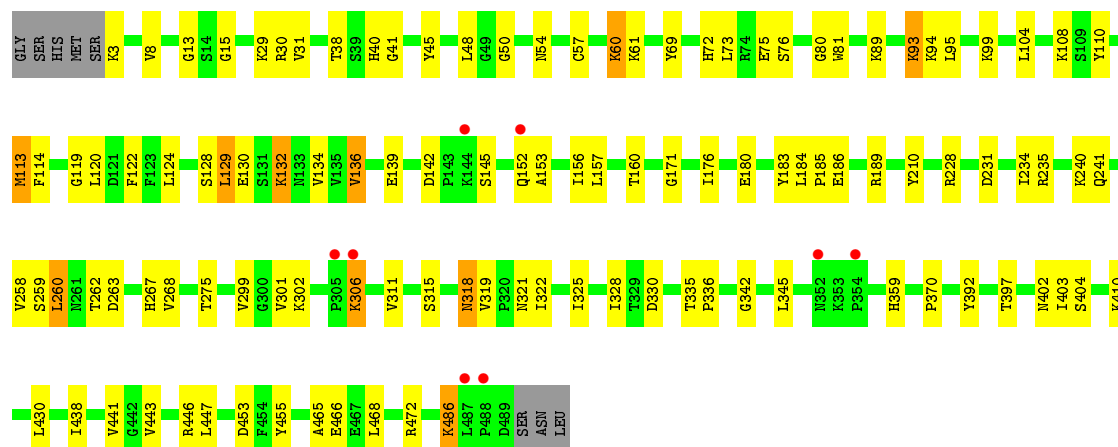


#### • Molecule 1: TRYPANOTHIONE REDUCTASE

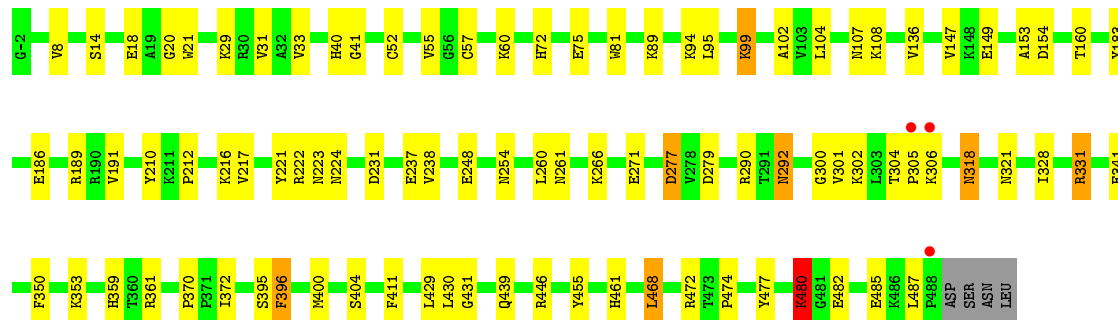
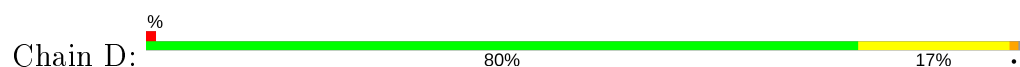


#### • Molecule 1: TRYPANOTHIONE REDUCTASE





### • Molecule 1: TRYPANOTHIONE REDUCTASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.82Å 62.76Å 167.44Å 90.00° 98.13° 90.00°	Depositor
Resolution (Å)	19.89 – 1.90 19.89 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.89-1.90) 99.4 (19.89-1.90)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.78 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, $R_{free}$	0.185 , 0.247 0.185 , 0.246	Depositor DCC
$R_{free}$ test set	8048 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.0	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 50.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	16503	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.34% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: WPF, BR, 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	1.10	3/3818 (0.1%)	1.00	3/5178 (0.1%)
1	B	0.98	1/3785 (0.0%)	0.93	7/5135 (0.1%)
1	C	0.97	2/3803 (0.1%)	0.92	4/5161 (0.1%)
1	D	1.04	1/3822 (0.0%)	0.95	6/5184 (0.1%)
All	All	1.02	7/15228 (0.0%)	0.95	20/20658 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	228	ARG	CG-CD	6.56	1.68	1.51
1	C	240	LYS	CD-CE	5.77	1.65	1.51
1	A	366	VAL	CB-CG1	5.28	1.64	1.52
1	C	240	LYS	CE-NZ	5.23	1.62	1.49
1	A	136	VAL	CB-CG2	-5.11	1.42	1.52
1	D	33	VAL	CB-CG2	-5.10	1.42	1.52
1	B	238	VAL	CB-CG1	-5.09	1.42	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	331[A]	ARG	NE-CZ-NH2	-9.95	115.33	120.30
1	A	331[B]	ARG	NE-CZ-NH2	-9.95	115.33	120.30
1	A	228	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	B	290	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	B	312	ASP	CB-CG-OD1	5.85	123.57	118.30
1	B	260	LEU	CA-CB-CG	5.71	128.44	115.30
1	D	361	ARG	NE-CZ-NH1	-5.67	117.46	120.30
1	D	154	ASP	CB-CG-OD1	5.48	123.23	118.30
1	D	279	ASP	CB-CG-OD1	-5.48	113.36	118.30
1	C	453	ASP	CB-CG-OD1	-5.34	113.49	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	62	LEU	CB-CG-CD1	-5.33	101.95	111.00
1	C	260	LEU	CB-CG-CD2	5.26	119.94	111.00
1	B	266	LYS	CD-CE-NZ	-5.21	99.72	111.70
1	D	260	LEU	CA-CB-CG	5.20	127.26	115.30
1	B	488	PRO	N-CA-CB	5.13	109.45	103.30
1	D	468	LEU	CB-CG-CD2	5.12	119.70	111.00
1	C	235	ARG	NE-CZ-NH1	-5.09	117.76	120.30
1	D	279	ASP	CB-CG-OD2	5.05	122.84	118.30
1	B	312	ASP	CB-CG-OD2	-5.03	113.77	118.30
1	C	263	ASP	CB-CG-OD1	5.03	122.82	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3733	0	3750	74	0
1	B	3702	0	3701	75	0
1	C	3716	0	3725	76	0
1	D	3737	0	3747	61	0
2	A	53	0	31	0	0
2	B	53	0	31	1	0
2	C	53	0	31	0	0
2	D	53	0	31	0	0
3	A	25	0	26	4	0
3	B	25	0	26	3	0
3	C	25	0	26	8	0
3	D	25	0	26	3	0
4	A	3	0	0	1	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
5	B	1	0	0	0	0
5	D	2	0	0	0	0
6	A	374	0	0	14	0
6	B	290	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	282	0	0	5	0
6	D	347	0	0	8	0
All	All	16503	0	15151	278	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 9.

All (278) 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:B:2:SER:O	1:B:3:LYS:HG2	1.61	0.99
1:B:8:VAL:HG23	1:B:153:ALA:HB2	1.51	0.91
1:B:130:GLU:HB2	1:B:136:VAL:HG23	1.53	0.91
1:C:130:GLU:HB2	1:C:136:VAL:CG2	2.01	0.89
1:C:301:VAL:HA	1:C:318:ASN:HD21	1.46	0.80
1:A:485:GLU:HG2	1:A:486:LYS:HD3	1.65	0.79
1:C:241:GLN:OE1	1:C:370:PRO:HG3	1.84	0.78
1:D:331:ARG:HG3	1:D:331:ARG:HH11	1.49	0.78
3:A:1000:WPF:HAX1	6:A:2023:HOH:O	1.83	0.77
1:A:331[A]:ARG:NH2	6:A:2278:HOH:O	2.18	0.76
1:C:299:VAL:HG23	1:C:301:VAL:HG23	1.67	0.75
1:D:318:ASN:H	1:D:318:ASN:HD22	1.35	0.75
1:D:331:ARG:CG	1:D:331:ARG:HH11	1.99	0.74
1:B:30:ARG:HH21	1:B:30:ARG:HG3	1.53	0.73
1:B:174:HIS:HD2	6:B:2054:HOH:O	1.69	0.72
1:A:52[A]:CYS:HB3	6:A:2017:HOH:O	1.90	0.72
1:B:139:GLU:HG3	6:B:2085:HOH:O	1.90	0.72
1:C:302:LYS:H	1:C:318:ASN:ND2	1.88	0.71
1:D:429:LEU:HD21	1:D:468:LEU:HD21	1.71	0.71
1:C:130:GLU:HB2	1:C:136:VAL:HG22	1.72	0.71
1:D:221:TYR:CE2	1:D:223:ASN:HB2	2.27	0.69
1:C:142:ASP:O	1:C:145:SER:OG	2.11	0.69
1:B:224[A]:ASN:HD22	1:B:252:ASN:HD21	1.41	0.69
1:C:157:LEU:HD11	1:C:325:ILE:HG12	1.75	0.69
1:A:21:TRP:CD1	3:A:1000:WPF:HAX3	2.28	0.68
1:D:136:VAL:HG23	1:D:147:VAL:HG13	1.76	0.68
1:D:72:HIS:HE1	6:D:2047:HOH:O	1.75	0.68
1:B:130:GLU:HB2	1:B:136:VAL:CG2	2.24	0.67
6:A:2060:HOH:O	1:B:72:HIS:HD2	1.78	0.66
1:B:485:GLU:HG3	1:B:485:GLU:O	1.96	0.65
1:B:8:VAL:HG23	1:B:153:ALA:CB	2.24	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:PHE:O	1:B:315:SER:HB2	1.97	0.64
1:A:485:GLU:HG2	1:A:486:LYS:CD	2.28	0.64
1:B:186:GLU:HB2	1:B:187:PRO:HD2	1.79	0.64
1:A:318:ASN:H	1:A:318:ASN:HD22	1.46	0.63
1:C:319:VAL:HG11	1:C:322:ILE:HD12	1.81	0.63
1:C:110:TYR:OH	3:C:1000:WPF:HAJ	1.99	0.63
1:D:21:TRP:CD1	3:D:1000:WPF:HAX3	2.33	0.63
1:D:301:VAL:HA	1:D:318:ASN:HD21	1.62	0.63
1:D:237:GLU:HB3	1:D:430:LEU:CD2	2.29	0.62
1:B:319:VAL:HG11	1:B:322:ILE:HD12	1.80	0.62
1:A:446:ARG:NE	6:A:2338:HOH:O	2.30	0.62
1:B:299:VAL:CG2	1:B:301:VAL:HG23	2.30	0.62
1:C:319:VAL:CG1	1:C:322:ILE:HD12	2.30	0.61
1:D:304:THR:HB	1:D:305:PRO:HD2	1.82	0.61
1:D:370:PRO:HG2	6:D:2300:HOH:O	2.01	0.61
1:B:8:VAL:CG2	1:B:153:ALA:HB2	2.29	0.61
1:D:238:VAL:HG21	1:D:372:ILE:HD11	1.82	0.60
1:C:113:MET:HB2	3:C:1000:WPF:HAA1	1.83	0.60
1:A:440:ALA:HB3	1:B:440:ALA:HB3	1.82	0.59
1:D:189:ARG:HA	1:D:212:PRO:HD2	1.84	0.59
1:A:434:ALA:HB3	1:A:435:PRO:HD3	1.84	0.59
1:A:48:LEU:HD11	1:A:114:PHE:HE2	1.67	0.59
6:C:2026:HOH:O	1:D:72:HIS:HD2	1.85	0.59
1:A:69:TYR:O	1:A:73:LEU:HG	2.03	0.58
1:D:480:LYS:HA	1:D:480:LYS:HE2	1.84	0.58
1:C:397:THR:OG1	1:C:410:LYS:HD3	2.04	0.58
1:A:302:LYS:H	1:A:318:ASN:ND2	2.01	0.58
1:B:2:SER:C	1:B:3:LYS:HG2	2.24	0.58
1:C:189:ARG:NH1	6:C:2102:HOH:O	2.35	0.58
1:A:8:VAL:CG2	1:A:153:ALA:HB2	2.34	0.57
1:C:72:HIS:HD2	6:C:2037:HOH:O	1.87	0.57
1:A:411:PHE:CD1	1:A:431:GLY:HA3	2.40	0.57
1:C:403:ILE:HD11	1:D:102:ALA:HB2	1.86	0.57
1:B:341:GLU:OE2	1:B:359:HIS:HE1	1.87	0.57
1:D:29:LYS:HE3	1:D:350:PHE:CD1	2.40	0.57
1:B:316:ARG:HB3	6:B:2203:HOH:O	2.04	0.57
1:D:216:LYS:HE3	1:D:248[A]:GLU:HB2	1.87	0.56
1:D:136:VAL:CG2	1:D:147:VAL:HG13	2.35	0.56
1:A:302:LYS:H	1:A:318:ASN:HD21	1.54	0.56
1:C:31:VAL:N	1:C:119:GLY:O	2.37	0.55
1:B:221:TYR:CE2	1:B:223:ASN:HB2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:52:CYS:HB3	6:D:2041:HOH:O	2.05	0.55
1:A:266:LYS:N	1:A:266:LYS:HD2	2.21	0.55
1:B:234:ILE:O	1:B:238:VAL:HG12	2.06	0.55
1:A:478:TYR:CE1	1:A:483:LYS:HB2	2.42	0.55
1:D:331:ARG:NH1	1:D:331:ARG:HG3	2.14	0.55
1:C:318:ASN:H	1:C:318:ASN:HD22	1.54	0.55
1:D:237:GLU:HB3	1:D:430:LEU:HD23	1.89	0.54
1:B:2:SER:O	1:B:3:LYS:CG	2.46	0.54
1:A:199:ILE:HD12	4:A:1491:CL:CL	2.45	0.54
1:C:157:LEU:HD13	1:C:345:LEU:CD2	2.38	0.53
1:D:14:SER:HA	3:D:1000:WPF:HAS	1.89	0.53
1:A:299:VAL:HG23	1:A:301:VAL:HG23	1.90	0.53
1:B:335:THR:HB	1:B:336:PRO:HD3	1.90	0.53
1:B:21:TRP:CD1	3:B:1000:WPF:HAX3	2.43	0.53
1:A:400:MET:HB3	6:B:2024:HOH:O	2.08	0.53
1:A:289:PRO:HG3	1:A:330:ASP:HB2	1.90	0.53
1:A:446:ARG:HG2	1:A:446:ARG:HH11	1.73	0.53
1:A:68:GLN:NE2	6:A:2057:HOH:O	2.42	0.52
1:C:176:ILE:HB	1:C:180:GLU:HB2	1.90	0.52
1:B:95:LEU:HD22	1:B:210:TYR:CZ	2.44	0.52
1:D:300:GLY:HA2	6:D:2079:HOH:O	2.10	0.52
1:B:400:MET:HG3	1:B:401:HIS:N	2.25	0.52
1:B:411:PHE:CD1	1:B:431:GLY:HA3	2.45	0.52
1:B:2:SER:C	1:B:3:LYS:CG	2.78	0.52
1:A:403:ILE:CD1	1:B:62:LEU:HD13	2.40	0.52
1:C:60:LYS:HD2	1:C:60:LYS:C	2.29	0.52
1:B:222:ARG:O	1:B:252:ASN:HA	2.10	0.51
1:B:186:GLU:HB2	1:B:187:PRO:CD	2.41	0.51
1:D:18:GLU:OE1	3:D:1000:WPF:NAV	2.44	0.51
1:A:92:TRP:CB	1:A:187:PRO:HG3	2.41	0.51
1:B:174:HIS:HE1	6:B:2101:HOH:O	1.93	0.51
1:C:76:SER:HB2	1:C:81:TRP:HB2	1.92	0.51
1:A:8:VAL:HG23	1:A:153:ALA:HB2	1.92	0.51
1:B:219:LEU:HD23	1:B:219:LEU:C	2.31	0.51
1:C:113:MET:HG3	3:C:1000:WPF:HAB	1.93	0.51
1:C:93:LYS:NZ	1:C:186[B]:GLU:OE1	2.36	0.50
1:A:48:LEU:HD11	1:A:114:PHE:CE2	2.46	0.50
1:C:110:TYR:CZ	3:C:1000:WPF:HAJ	2.47	0.50
1:C:171:GLY:HA3	1:C:258:VAL:O	2.11	0.50
1:C:302:LYS:H	1:C:318:ASN:HD21	1.58	0.50
1:A:75:GLU:HG2	1:A:404:SER:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:TYR:CE1	3:C:1000:WPF:HAJ	2.46	0.50
1:D:318:ASN:N	1:D:318:ASN:HD22	2.04	0.50
1:C:160:THR:OG1	1:C:328:ILE:HD12	2.11	0.50
1:A:221:TYR:CE2	1:A:223:ASN:HB2	2.47	0.50
1:B:92:TRP:CZ2	1:B:96:ILE:HD11	2.47	0.50
1:D:341:GLU:OE2	1:D:359:HIS:HE1	1.95	0.50
1:D:95:LEU:HD22	1:D:210:TYR:CZ	2.46	0.50
1:D:261:ASN:ND2	1:D:277:ASP:OD1	2.44	0.49
1:A:14:SER:HA	3:A:1000:WPF:HAS	1.94	0.49
1:D:395:SER:O	1:D:396:PHE:HB3	2.12	0.49
1:B:189:ARG:HA	1:B:212:PRO:HD2	1.95	0.49
1:A:446:ARG:CG	6:A:2339:HOH:O	2.59	0.49
1:A:485:GLU:OE2	1:A:486:LYS:HE2	2.13	0.49
1:B:114:PHE:CE1	1:B:120:LEU:HG	2.47	0.49
1:C:48:LEU:HD11	1:C:114:PHE:HE2	1.78	0.49
1:B:14:SER:HA	3:B:1000:WPF:HAS	1.94	0.49
1:D:29:LYS:HE3	1:D:350:PHE:HD1	1.77	0.48
1:B:232:GLU:O	1:B:236:GLU:HG3	2.12	0.48
1:A:421:ASP:O	1:A:450:LYS:HE3	2.12	0.48
1:C:268:VAL:O	1:C:275:THR:HA	2.14	0.48
1:A:446:ARG:HG3	6:A:2339:HOH:O	2.14	0.48
1:C:438:ILE:O	1:C:441:VAL:HB	2.14	0.48
1:A:329:THR:O	1:A:331[A]:ARG:HD2	2.13	0.48
1:D:52:CYS:CB	6:D:2041:HOH:O	2.59	0.47
1:A:189:ARG:HA	1:A:212:PRO:HD2	1.95	0.47
1:B:18:GLU:OE1	3:B:1000:WPF:NAV	2.48	0.47
1:A:225:LEU:H	1:A:228:ARG:HH21	1.63	0.47
1:D:104:LEU:HG	1:D:108:LYS:HE3	1.96	0.47
1:D:160:THR:OG1	1:D:328:ILE:HD12	2.13	0.47
1:C:38:THR:HG23	1:C:124:LEU:HD13	1.96	0.47
1:A:129:LEU:HD22	1:A:296:LEU:HD23	1.95	0.47
1:A:301:VAL:HA	1:A:318:ASN:HD21	1.78	0.47
1:B:331:ARG:HG3	6:B:2207:HOH:O	2.14	0.47
1:D:254:ASN:ND2	1:D:271:GLU:OE2	2.47	0.47
1:B:3:LYS:HE3	1:B:149:GLU:OE1	2.15	0.46
1:D:455:TYR:CE2	1:D:472:ARG:HB2	2.50	0.46
1:B:389:VAL:HB	1:B:478:TYR:HB2	1.97	0.46
1:D:20:GLY:HA2	1:D:31:VAL:HG11	1.98	0.46
1:A:332:LEU:HD13	1:A:337:VAL:HG21	1.98	0.46
1:A:112:GLY:HA3	6:A:2097:HOH:O	2.16	0.46
1:C:299:VAL:CG2	1:C:301:VAL:HG23	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:ARG:NH1	6:B:2140:HOH:O	2.48	0.46
1:C:95:LEU:HD22	1:C:210:TYR:CZ	2.50	0.46
1:D:75:GLU:HB3	1:D:404:SER:HB2	1.96	0.46
1:C:114:PHE:CE1	1:C:120:LEU:HG	2.51	0.46
1:D:411:PHE:CD1	1:D:431:GLY:HA3	2.51	0.46
1:A:403:ILE:HD12	1:B:62:LEU:HD13	1.98	0.46
1:B:176:ILE:HB	1:B:180:GLU:HB2	1.98	0.46
1:A:176:ILE:HB	1:A:180:GLU:HB2	1.98	0.45
1:A:52[A]:CYS:HB2	1:A:57:CYS:SG	2.56	0.45
1:C:335:THR:HB	1:C:336:PRO:HD3	1.98	0.45
1:A:130:GLU:HB2	1:A:136:VAL:CG2	2.47	0.45
1:C:29:LYS:HA	1:C:29:LYS:HD3	1.71	0.45
1:B:299:VAL:HG23	1:B:301:VAL:HG23	1.99	0.45
1:A:34:VAL:HA	1:A:123:PHE:O	2.17	0.45
1:A:302:LYS:NZ	6:A:2252:HOH:O	2.38	0.45
1:C:113:MET:CB	3:C:1000:WPF:HAB	2.47	0.45
1:C:89:LYS:HE2	6:D:2058:HOH:O	2.16	0.45
1:A:160:THR:OG1	1:A:328:ILE:HD12	2.16	0.45
1:B:154:ASP:O	1:B:321:ASN:HB2	2.17	0.45
1:D:222:ARG:HH12	1:D:254:ASN:ND2	2.15	0.45
1:A:45:TYR:CG	1:A:179:ASN:HB3	2.52	0.45
1:D:474:PRO:HG2	1:D:477:TYR:CE1	2.52	0.45
1:A:109:SER:O	1:A:113:MET:HG3	2.17	0.44
1:A:351:GLY:O	1:A:353:LYS:HG3	2.17	0.44
1:D:222:ARG:NH1	1:D:254:ASN:ND2	2.65	0.44
1:B:130:GLU:OE2	1:B:150:ARG:NH1	2.45	0.44
1:D:446:ARG:NH1	6:D:2314:HOH:O	2.50	0.44
1:B:165:GLN:HB2	1:B:288:ILE:HG23	2.00	0.44
1:B:52:CYS:HB3	6:B:2016:HOH:O	2.17	0.44
1:D:41:GLY:HA2	1:D:183:TYR:CZ	2.53	0.44
1:B:161:GLY:HA2	1:B:327:ASP:HB2	2.00	0.44
1:C:104:LEU:HG	1:C:108:LYS:HE3	1.99	0.44
1:D:191:VAL:CG1	1:D:217:VAL:HG22	2.47	0.44
1:A:114:PHE:CG	1:A:122:PHE:HB2	2.52	0.44
1:B:48:LEU:HD11	1:B:114:PHE:HE2	1.82	0.44
1:B:152:GLN:HG2	1:B:152:GLN:H	1.59	0.44
1:C:447:LEU:HD23	1:C:447:LEU:HA	1.78	0.44
1:A:83:PHE:HB3	1:B:88:VAL:HG22	2.00	0.44
1:D:221:TYR:CZ	1:D:223:ASN:HB2	2.52	0.44
1:A:250:MET:CE	1:A:253:GLU:HG3	2.48	0.44
2:B:998:FAD:H9	2:B:998:FAD:H1'1	1.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:GLY:HA2	1:A:50:GLY:HA3	1.99	0.44
1:B:48:LEU:HD11	1:B:114:PHE:CE2	2.53	0.44
1:A:132:LYS:HB2	6:A:2110:HOH:O	2.18	0.43
1:A:396:PHE:CD1	1:A:396:PHE:N	2.86	0.43
1:B:304:THR:HB	1:B:305:PRO:HD2	2.00	0.43
1:B:392:TYR:O	1:B:414:LYS:HA	2.19	0.43
1:C:15:GLY:HA3	1:C:325:ILE:HD12	2.01	0.43
1:C:486:LYS:HD2	1:C:486:LYS:HA	1.82	0.43
1:D:331:ARG:CG	1:D:331:ARG:NH1	2.69	0.43
1:A:351:GLY:O	1:A:352:ASN:C	2.57	0.43
1:A:429:LEU:HD21	1:A:468:LEU:HD21	2.00	0.43
1:B:478:TYR:CE1	1:B:483:LYS:HB2	2.54	0.43
1:C:392:TYR:CD2	1:C:392:TYR:N	2.86	0.43
1:C:75:GLU:HB3	1:C:404:SER:HB2	2.00	0.43
1:C:80:GLY:HA2	1:D:94:LYS:HG2	2.00	0.43
1:B:144:LYS:O	1:B:144:LYS:HG2	2.18	0.43
1:C:231:ASP:HB3	1:C:234:ILE:HB	2.01	0.43
1:D:302:LYS:H	1:D:318:ASN:ND2	2.16	0.43
1:A:3:LYS:HB2	1:A:5:PHE:CE2	2.54	0.43
1:A:92:TRP:HB3	1:A:187:PRO:HG3	2.00	0.43
1:C:359:HIS:HB2	6:C:2210:HOH:O	2.19	0.43
1:D:292:ASN:HD22	1:D:292:ASN:HA	1.65	0.43
1:B:114:PHE:CD1	1:B:120:LEU:HG	2.54	0.42
1:B:160:THR:OG1	1:B:328:ILE:HD12	2.19	0.42
1:D:474:PRO:HG2	1:D:477:TYR:CZ	2.54	0.42
1:A:18:GLU:OE1	3:A:1000:WPF:NAV	2.52	0.42
1:A:162:SER:HB3	1:A:327:ASP:HB3	2.00	0.42
1:A:455:TYR:CZ	1:A:472:ARG:HD2	2.54	0.42
1:C:48:LEU:HD11	1:C:114:PHE:CE2	2.54	0.42
1:D:8:VAL:CG2	1:D:153:ALA:HB2	2.49	0.42
1:C:465:ALA:HB1	1:D:439:GLN:HB3	2.02	0.42
1:D:40:HIS:H	1:D:107:ASN:ND2	2.18	0.42
1:B:268:VAL:O	1:B:275:THR:HA	2.20	0.42
1:C:129:LEU:HD11	1:C:156:ILE:HG21	2.00	0.42
1:C:311:VAL:HB	1:C:315:SER:HA	2.02	0.42
1:A:89:LYS:HG2	1:A:90:ALA:N	2.34	0.42
1:A:248:GLU:HG2	6:A:2178:HOH:O	2.20	0.42
1:C:455:TYR:CD2	1:C:472:ARG:HB3	2.55	0.42
1:D:99:LYS:C	1:D:99:LYS:HD2	2.39	0.42
1:B:34:VAL:HA	1:B:123:PHE:O	2.20	0.42
1:C:370:PRO:HG2	1:C:430:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:468:LEU:HA	1:C:468:LEU:HD23	1.85	0.42
1:A:395:SER:HA	1:A:411:PHE:O	2.18	0.42
1:A:446:ARG:HD2	6:A:2339:HOH:O	2.19	0.42
1:B:45:TYR:CG	1:B:179:ASN:HB3	2.55	0.42
1:C:38:THR:HG22	1:C:122:PHE:CE2	2.54	0.42
1:A:95:LEU:HD22	1:A:210:TYR:CZ	2.54	0.41
1:B:13:GLY:HA2	1:B:50:GLY:HA3	2.01	0.41
1:C:466:GLU:HA	1:D:439:GLN:OE1	2.19	0.41
1:C:336:PRO:HG3	1:D:461:HIS:HB2	2.02	0.41
1:B:463:THR:O	1:B:466:GLU:HG2	2.20	0.41
1:C:184:LEU:HA	1:C:185:PRO:HD3	1.99	0.41
1:C:41:GLY:HA2	1:C:183:TYR:CZ	2.55	0.41
1:A:99:LYS:C	1:A:99:LYS:HD2	2.41	0.41
1:C:402:ASN:O	6:C:2233:HOH:O	2.22	0.41
1:A:92:TRP:HB2	1:A:187:PRO:HG3	2.02	0.41
1:A:20:GLY:HA2	1:A:31:VAL:HG11	2.03	0.41
1:B:152:GLN:HB3	6:B:2092:HOH:O	2.21	0.41
1:C:113:MET:CG	3:C:1000:WPF:HAB	2.49	0.41
1:C:306:LYS:HB3	1:C:330:ASP:OD2	2.20	0.41
1:C:40:HIS:HB3	1:C:54:ASN:OD1	2.19	0.41
1:C:69:TYR:O	1:C:73:LEU:HG	2.21	0.41
1:A:371:PRO:HD3	6:A:2057:HOH:O	2.21	0.41
1:B:130:GLU:CD	1:B:150:ARG:HH22	2.24	0.41
1:C:130:GLU:OE1	1:C:134:VAL:HG11	2.21	0.41
1:B:240:LYS:HD2	6:B:2045:HOH:O	2.20	0.41
1:C:69:TYR:HB2	1:D:81:TRP:NE1	2.35	0.41
1:C:113:MET:HB2	3:C:1000:WPF:HAB	2.03	0.41
1:C:8:VAL:CG2	1:C:153:ALA:HB2	2.50	0.41
1:C:60:LYS:HD2	1:C:61:LYS:N	2.36	0.41
1:D:223:ASN:ND2	6:D:2167:HOH:O	2.35	0.41
1:B:163:TRP:CG	1:B:164:PRO:HD2	2.56	0.40
1:B:232:GLU:HA	1:B:235:ARG:HD3	2.03	0.40
1:B:289:PRO:HG3	1:B:330:ASP:HB2	2.03	0.40
1:C:443:VAL:O	1:C:446:ARG:HB3	2.22	0.40
1:C:325:ILE:HD13	1:C:342:GLY:HA2	2.03	0.40
1:C:13:GLY:HA2	1:C:50:GLY:CA	2.52	0.40
1:B:390:ALA:HB1	1:B:474:PRO:HB3	2.03	0.40
1:A:437:ILE:HG12	1:A:465:ALA:HB2	2.03	0.40
1:D:304:THR:HB	1:D:305:PRO:CD	2.50	0.40
1:B:157:LEU:HD21	1:B:325:ILE:CD1	2.52	0.40
1:C:267:HIS:CE1	1:C:275:THR:HB	2.57	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	490/495 (99%)	472 (96%)	16 (3%)	2 (0%)	34	24
1	B	487/495 (98%)	468 (96%)	16 (3%)	3 (1%)	25	15
1	C	488/495 (99%)	471 (96%)	15 (3%)	2 (0%)	34	24
1	D	491/495 (99%)	475 (97%)	13 (3%)	3 (1%)	25	15
All	All	1956/1980 (99%)	1886 (96%)	60 (3%)	10 (0%)	29	18

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	132	LYS
1	B	3	LYS
1	B	45	TYR
1	D	480	LYS
1	A	480	LYS
1	D	396	PHE
1	C	45	TYR
1	D	55	VAL
1	A	55	VAL
1	B	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	405/407 (100%)	381 (94%)	24 (6%)	19	10
1	B	399/407 (98%)	382 (96%)	17 (4%)	29	19
1	C	403/407 (99%)	382 (95%)	21 (5%)	23	14
1	D	405/407 (100%)	382 (94%)	23 (6%)	20	11
All	All	1612/1628 (99%)	1527 (95%)	85 (5%)	24	13

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52[A]	CYS
1	A	52[B]	CYS
1	A	57	CYS
1	A	60	LYS
1	A	94	LYS
1	A	99	LYS
1	A	109	SER
1	A	129	LEU
1	A	132	LYS
1	A	224	ASN
1	A	228	ARG
1	A	238	VAL
1	A	306	LYS
1	A	318	ASN
1	A	331[A]	ARG
1	A	331[B]	ARG
1	A	332	LEU
1	A	335	THR
1	A	385	GLU
1	A	387	GLU
1	A	400	MET
1	A	410	LYS
1	A	467	GLU
1	A	480	LYS
1	B	2	SER
1	B	30	ARG
1	B	57	CYS
1	B	60	LYS
1	B	89	LYS
1	B	113	MET
1	B	144	LYS
1	B	150	ARG
1	B	152	GLN

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Mol	Chain	Res	Type
1	B	213	PRO
1	B	260	LEU
1	B	306	LYS
1	B	321	ASN
1	B	355	ARG
1	B	407	LYS
1	B	480	LYS
1	B	485	GLU
1	C	3	LYS
1	C	30	ARG
1	C	57	CYS
1	C	60	LYS
1	C	93	LYS
1	C	94	LYS
1	C	99	LYS
1	C	113	MET
1	C	128	SER
1	C	129	LEU
1	C	132	LYS
1	C	136	VAL
1	C	139	GLU
1	C	152	GLN
1	C	228	ARG
1	C	259	SER
1	C	260	LEU
1	C	262	THR
1	C	306	LYS
1	C	318	ASN
1	C	486	LYS
1	D	57	CYS
1	D	60	LYS
1	D	89	LYS
1	D	99	LYS
1	D	149	GLU
1	D	186	GLU
1	D	224[A]	ASN
1	D	224[B]	ASN
1	D	231	ASP
1	D	266	LYS
1	D	277	ASP
1	D	290	ARG
1	D	292	ASN

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Mol	Chain	Res	Type
1	D	306	LYS
1	D	318	ASN
1	D	321	ASN
1	D	331	ARG
1	D	353	LYS
1	D	400	MET
1	D	480	LYS
1	D	482	GLU
1	D	485	GLU
1	D	487	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	152	GLN
1	A	318	ASN
1	B	72	HIS
1	B	107	ASN
1	B	174	HIS
1	B	310	GLN
1	B	359	HIS
1	C	72	HIS
1	C	107	ASN
1	C	152	GLN
1	C	310	GLN
1	C	318	ASN
1	D	72	HIS
1	D	107	ASN
1	D	152	GLN
1	D	223	ASN
1	D	292	ASN
1	D	295	GLN
1	D	318	ASN
1	D	321	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 [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 18 ligands modelled in this entry, 10 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	A	998	-	51,58,58	1.26	5 (9%)	60,89,89	1.96	14 (23%)
2	FAD	C	998	-	51,58,58	1.28	5 (9%)	60,89,89	2.27	18 (30%)
3	WPF	C	1000	-	27,27,27	2.53	9 (33%)	34,38,38	1.91	8 (23%)
2	FAD	B	998	-	51,58,58	1.32	4 (7%)	60,89,89	2.29	13 (21%)
3	WPF	D	1000	-	27,27,27	2.26	6 (22%)	34,38,38	1.71	4 (11%)
2	FAD	D	998	-	51,58,58	1.16	3 (5%)	60,89,89	2.00	12 (20%)
3	WPF	A	1000	-	27,27,27	2.19	6 (22%)	34,38,38	1.77	7 (20%)
3	WPF	B	1000	-	27,27,27	2.32	7 (25%)	34,38,38	1.95	7 (20%)

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	A	998	-	-	5/30/50/50	0/6/6/6
2	FAD	C	998	-	-	5/30/50/50	0/6/6/6
3	WPF	C	1000	-	-	4/10/26/26	0/3/3/3
2	FAD	B	998	-	-	4/30/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	WPF	D	1000	-	-	2/10/26/26	0/3/3/3
2	FAD	D	998	-	-	4/30/50/50	0/6/6/6
3	WPF	A	1000	-	-	3/10/26/26	0/3/3/3
3	WPF	B	1000	-	-	1/10/26/26	0/3/3/3

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1000	WPF	CAW-NAV	8.83	1.41	1.29
3	C	1000	WPF	CAW-NAV	8.75	1.41	1.29
3	D	1000	WPF	CAW-NAV	8.66	1.41	1.29
3	A	1000	WPF	CAW-NAV	8.39	1.40	1.29
3	C	1000	WPF	CAK-CAL	5.65	1.57	1.51
2	B	998	FAD	C2A-N3A	4.87	1.39	1.32
3	A	1000	WPF	CAX-CAW	4.53	1.56	1.49
2	C	998	FAD	C2A-N3A	4.34	1.39	1.32
3	D	1000	WPF	CAK-CAL	4.16	1.56	1.51
3	B	1000	WPF	CAK-CAL	3.59	1.55	1.51
2	A	998	FAD	C5X-N5	3.55	1.41	1.35
3	B	1000	WPF	CAL-NAM	3.29	1.50	1.48
3	B	1000	WPF	CAX-CAW	3.28	1.54	1.49
2	B	998	FAD	C2A-N1A	3.24	1.39	1.33
3	D	1000	WPF	CAX-CAW	3.23	1.54	1.49
3	C	1000	WPF	CAX-CAW	3.17	1.54	1.49
2	D	998	FAD	C4X-N5	3.11	1.37	1.33
2	B	998	FAD	C4-N3	2.93	1.38	1.33
3	B	1000	WPF	CAW-NAM	2.92	1.43	1.35
3	D	1000	WPF	CAN-NAM	2.84	1.51	1.46
3	C	1000	WPF	CAL-NAM	2.83	1.49	1.48
3	A	1000	WPF	CAK-CAL	2.80	1.54	1.51
2	D	998	FAD	C4-N3	2.77	1.37	1.33
3	C	1000	WPF	CAF-CAL	2.71	1.56	1.52
2	C	998	FAD	C10-N1	2.70	1.36	1.33
3	C	1000	WPF	CAJ-CAI	2.70	1.42	1.38
2	A	998	FAD	C1'-N10	2.66	1.51	1.48
3	A	1000	WPF	CAJ-CAI	2.65	1.42	1.38
3	C	1000	WPF	CAN-NAM	2.54	1.51	1.46
2	D	998	FAD	C2A-N3A	2.54	1.36	1.32
2	B	998	FAD	C9A-C5X	-2.41	1.37	1.42
2	C	998	FAD	C2A-N1A	2.38	1.38	1.33
3	D	1000	WPF	CAW-NAM	2.34	1.41	1.35
2	A	998	FAD	C2A-N3A	2.34	1.35	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1000	WPF	CAN-NAM	2.33	1.50	1.46
3	C	1000	WPF	CAW-NAM	2.32	1.41	1.35
3	B	1000	WPF	CAS-CAI	2.25	1.42	1.38
2	A	998	FAD	C4A-N3A	2.24	1.38	1.35
2	C	998	FAD	C4-C4X	-2.24	1.37	1.41
2	C	998	FAD	C5X-N5	2.23	1.39	1.35
2	A	998	FAD	O3B-C3B	2.22	1.48	1.43
3	D	1000	WPF	CAE-CAF	2.19	1.42	1.39
3	C	1000	WPF	CAI-CL1	2.07	1.79	1.74
3	B	1000	WPF	CAJ-CAI	2.03	1.41	1.38
3	A	1000	WPF	CAD-CAG	2.03	1.42	1.38

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	998	FAD	C4-N3-C2	9.71	123.34	115.14
2	D	998	FAD	C4-N3-C2	7.42	121.41	115.14
2	C	998	FAD	C1'-N10-C9A	6.46	123.37	118.29
3	A	1000	WPF	CAF-CAL-NAM	-6.40	102.48	111.55
2	C	998	FAD	N3A-C2A-N1A	-6.27	118.87	128.68
2	B	998	FAD	C4X-N5-C5X	6.21	122.98	116.77
2	C	998	FAD	C4-N3-C2	6.10	120.30	115.14
3	B	1000	WPF	CAF-CAL-NAM	-5.90	103.19	111.55
2	B	998	FAD	C4X-C4-N3	-5.85	115.43	123.43
2	A	998	FAD	C4-N3-C2	5.85	120.08	115.14
3	C	1000	WPF	CAU-NAV-CAW	5.70	123.54	118.19
2	C	998	FAD	C4X-N5-C5X	5.70	122.46	116.77
3	B	1000	WPF	CAU-NAV-CAW	5.63	123.48	118.19
2	D	998	FAD	C4X-N5-C5X	5.47	122.24	116.77
3	D	1000	WPF	CAU-NAV-CAW	5.37	123.23	118.19
2	B	998	FAD	N3A-C2A-N1A	-5.19	120.56	128.68
2	A	998	FAD	C2A-N1A-C6A	4.99	127.29	118.75
2	A	998	FAD	N3A-C2A-N1A	-4.85	121.11	128.68
2	D	998	FAD	C4X-C4-N3	-4.82	116.84	123.43
2	C	998	FAD	C5X-C9A-N10	4.31	120.84	117.72
2	A	998	FAD	C4X-N5-C5X	4.26	121.03	116.77
3	D	1000	WPF	CAF-CAL-NAM	-4.25	105.53	111.55
2	D	998	FAD	N3A-C2A-N1A	-4.07	122.32	128.68
3	C	1000	WPF	CAS-CAI-CAJ	-4.06	116.14	121.53
2	D	998	FAD	C10-C4X-N5	-4.02	118.47	121.26
2	B	998	FAD	C10-C4X-N5	-4.02	118.48	121.26
3	D	1000	WPF	CAK-CAU-NAV	-3.84	118.83	122.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	998	FAD	C10-C4X-N5	-3.79	118.64	121.26
2	B	998	FAD	C4-C4X-C10	3.72	122.41	119.95
2	C	998	FAD	C4X-C4-N3	-3.66	118.43	123.43
2	B	998	FAD	C1'-N10-C10	3.65	121.68	118.41
2	D	998	FAD	C4'-C3'-C2'	-3.59	105.90	113.36
3	B	1000	WPF	CAT-CAU-CAK	3.40	122.43	119.49
3	A	1000	WPF	CAU-NAV-CAW	3.40	121.38	118.19
3	B	1000	WPF	CAK-CAU-NAV	-3.35	119.27	122.17
3	C	1000	WPF	CAI-CAJ-CAK	3.29	123.88	119.77
2	A	998	FAD	C5A-C6A-N1A	-3.28	112.92	120.35
2	C	998	FAD	C4-C4X-C10	3.26	122.11	119.95
2	A	998	FAD	C4X-C4-N3	-3.20	119.06	123.43
2	D	998	FAD	C5X-C9A-N10	3.19	120.03	117.72
2	C	998	FAD	C9A-C5X-N5	-3.18	117.39	122.36
3	C	1000	WPF	CAK-CAU-NAV	-3.15	119.43	122.17
3	C	1000	WPF	CAF-CAL-NAM	-3.04	107.23	111.55
2	C	998	FAD	O3'-C3'-C2'	-2.95	101.69	108.81
2	B	998	FAD	O4B-C1B-C2B	-2.94	102.63	106.93
2	D	998	FAD	C1'-N10-C9A	2.93	120.60	118.29
2	B	998	FAD	C5X-C9A-N10	2.92	119.83	117.72
2	A	998	FAD	O2'-C2'-C3'	2.78	115.86	109.10
2	D	998	FAD	C4A-C5A-N7A	-2.77	106.51	109.40
2	C	998	FAD	C9A-N10-C10	-2.76	118.29	121.91
3	B	1000	WPF	CAX-CAW-NAV	-2.62	115.96	119.34
3	C	1000	WPF	CAO-CAN-NAM	-2.62	109.27	113.31
2	C	998	FAD	C7-C6-C5X	-2.61	117.53	121.22
3	C	1000	WPF	CAK-CAL-NAM	2.56	114.11	110.39
3	A	1000	WPF	CAO-CAP-NAQ	-2.51	106.98	113.79
2	A	998	FAD	O4B-C1B-C2B	-2.47	103.32	106.93
3	A	1000	WPF	CAT-CAU-CAK	2.46	121.61	119.49
2	C	998	FAD	C5B-C4B-C3B	-2.42	106.11	115.18
2	A	998	FAD	C1'-C2'-C3'	-2.38	103.14	109.79
2	B	998	FAD	C9A-C5X-N5	-2.38	118.64	122.36
3	A	1000	WPF	CAK-CAU-NAV	-2.34	120.14	122.17
3	A	1000	WPF	CAB-CAE-CAF	-2.33	118.85	121.20
3	C	1000	WPF	CAJ-CAI-CL1	2.30	122.03	119.15
3	B	1000	WPF	CAF-CAL-CAK	-2.30	108.82	112.78
2	C	998	FAD	O5'-P-O1P	-2.30	100.08	109.07
3	D	1000	WPF	CAT-CAU-CAK	2.30	121.47	119.49
2	D	998	FAD	C9A-C5X-N5	-2.29	118.78	122.36
3	B	1000	WPF	CAK-CAL-NAM	2.24	113.65	110.39
2	C	998	FAD	N6A-C6A-N1A	2.20	123.15	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	998	FAD	O4'-C4'-C5'	-2.20	104.97	109.92
2	D	998	FAD	O5B-C5B-C4B	-2.19	101.46	108.99
2	C	998	FAD	C5A-C6A-N6A	-2.18	117.04	120.35
2	D	998	FAD	C6-C5X-C9A	2.15	121.87	119.05
2	A	998	FAD	C5'-C4'-C3'	-2.13	108.10	112.20
2	C	998	FAD	C4'-C3'-C2'	-2.11	108.97	113.36
2	B	998	FAD	C4A-C5A-N7A	-2.11	107.20	109.40
3	A	1000	WPF	CAG-CAD-CAC	-2.09	118.58	121.38
2	B	998	FAD	C6-C5X-N5	2.09	121.35	119.05
2	A	998	FAD	O3'-C3'-C2'	2.06	113.79	108.81
2	C	998	FAD	C1B-N9A-C4A	-2.06	123.02	126.64
2	C	998	FAD	C7M-C7-C8	-2.05	116.53	120.74
2	B	998	FAD	C8M-C8-C7	2.03	124.89	120.74
2	A	998	FAD	O5B-C5B-C4B	-2.01	102.09	108.99

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	998	FAD	PA-O3P-P-O5'
2	D	998	FAD	PA-O3P-P-O5'
2	A	998	FAD	O4B-C4B-C5B-O5B
2	C	998	FAD	O4B-C4B-C5B-O5B
2	C	998	FAD	C3B-C4B-C5B-O5B
3	C	1000	WPF	CAN-CAO-CAP-NAQ
3	A	1000	WPF	CAN-CAO-CAP-NAQ
3	C	1000	WPF	NAM-CAN-CAO-CAP
3	C	1000	WPF	CAO-CAP-NAQ-CAR
3	D	1000	WPF	CAN-CAO-CAP-NAQ
2	A	998	FAD	C3B-C4B-C5B-O5B
2	C	998	FAD	PA-O3P-P-O5'
2	B	998	FAD	PA-O3P-P-O5'
2	A	998	FAD	P-O3P-PA-O1A
2	C	998	FAD	P-O3P-PA-O2A
2	B	998	FAD	P-O3P-PA-O2A
3	C	1000	WPF	CAO-CAP-NAQ-CAY
3	D	1000	WPF	CAO-CAP-NAQ-CAR
3	A	1000	WPF	CAO-CAP-NAQ-CAY
2	A	998	FAD	P-O3P-PA-O2A
2	D	998	FAD	P-O3P-PA-O2A
2	C	998	FAD	P-O3P-PA-O1A
2	D	998	FAD	O4B-C4B-C5B-O5B

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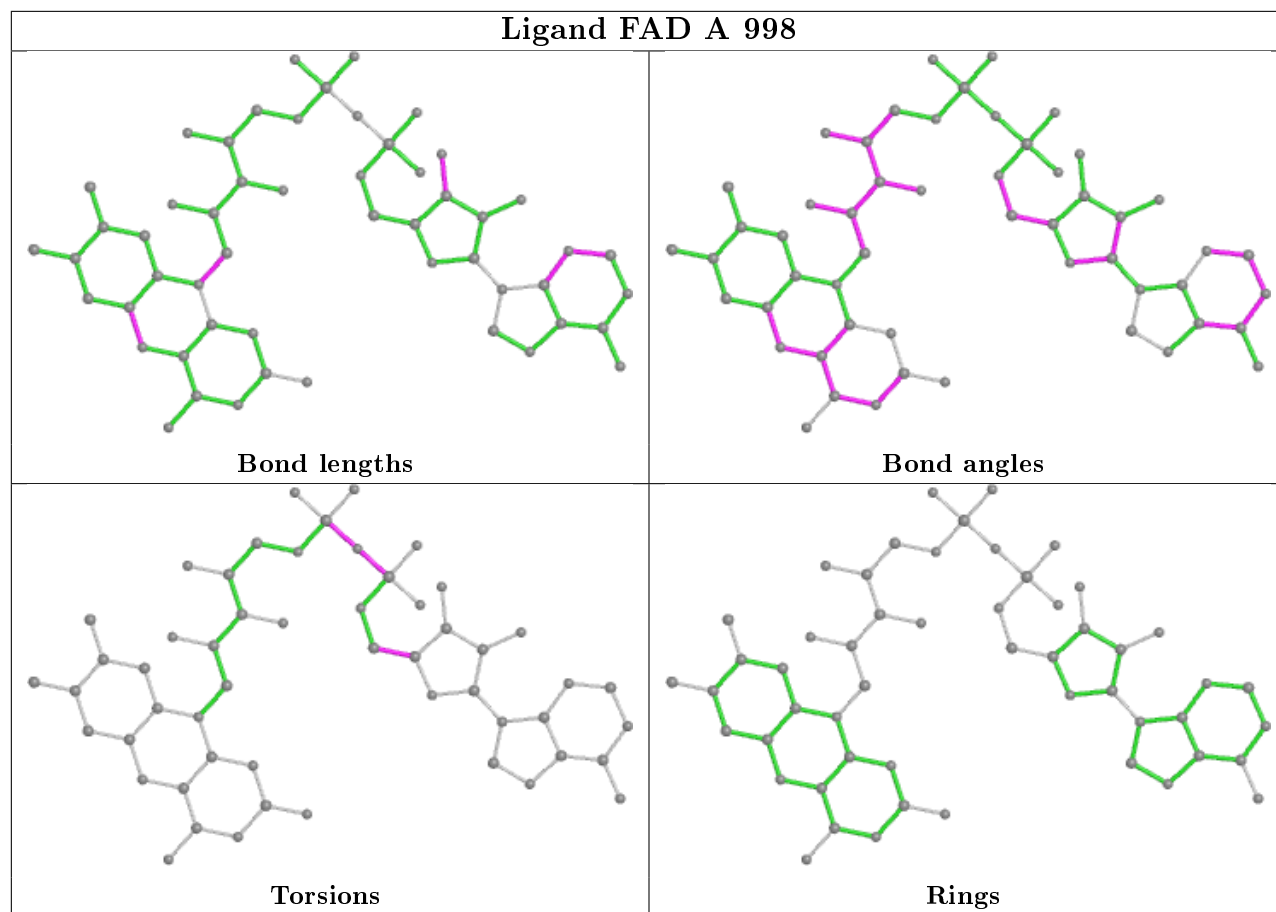
Mol	Chain	Res	Type	Atoms
3	A	1000	WPF	CAO-CAP-NAQ-CAR
2	B	998	FAD	O4B-C4B-C5B-O5B
2	B	998	FAD	P-O3P-PA-O1A
2	D	998	FAD	P-O3P-PA-O1A
3	B	1000	WPF	CAN-CAO-CAP-NAQ

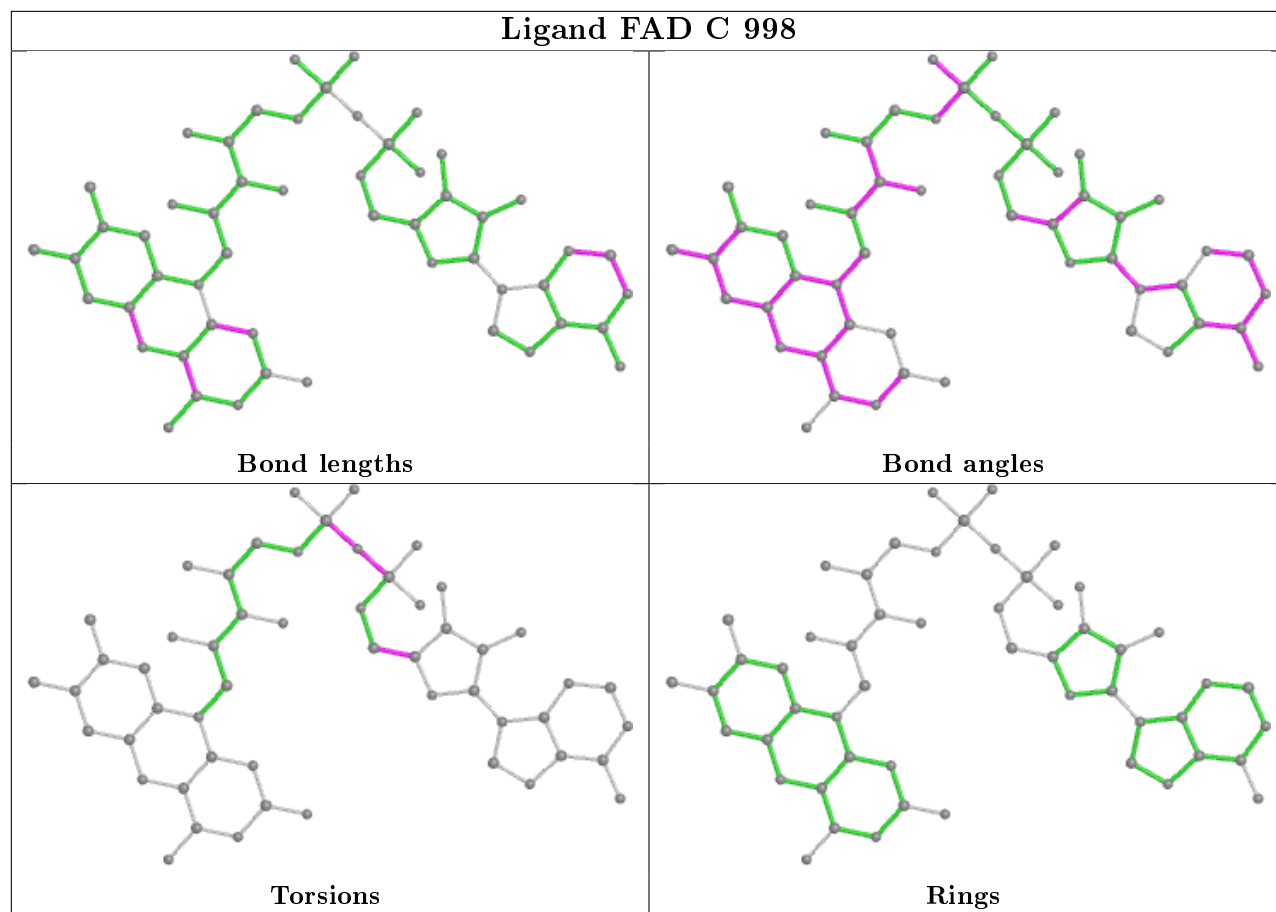
There are no ring outliers.

5 monomers are involved in 19 short contacts:

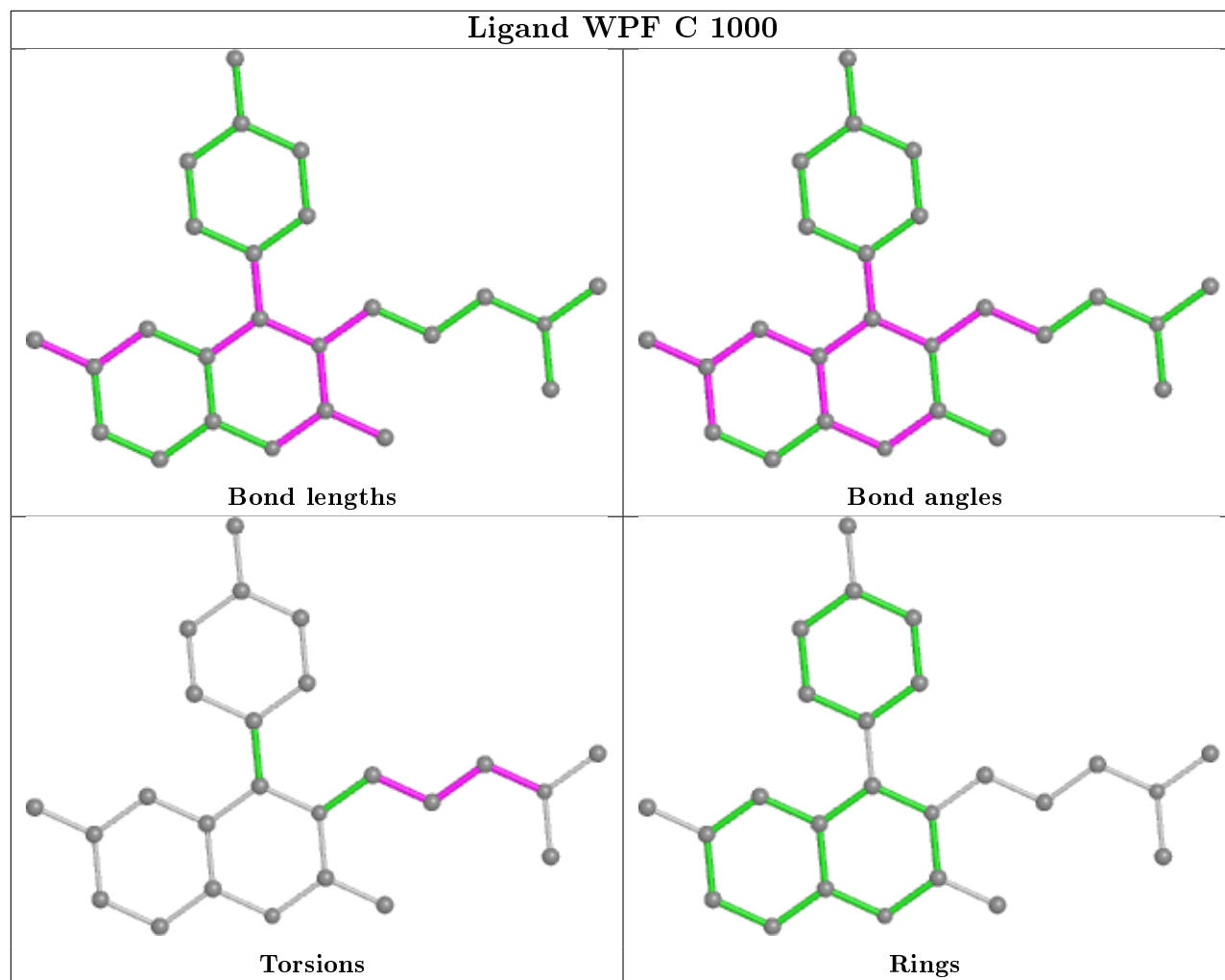
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1000	WPF	8	0
2	B	998	FAD	1	0
3	D	1000	WPF	3	0
3	A	1000	WPF	4	0
3	B	1000	WPF	3	0

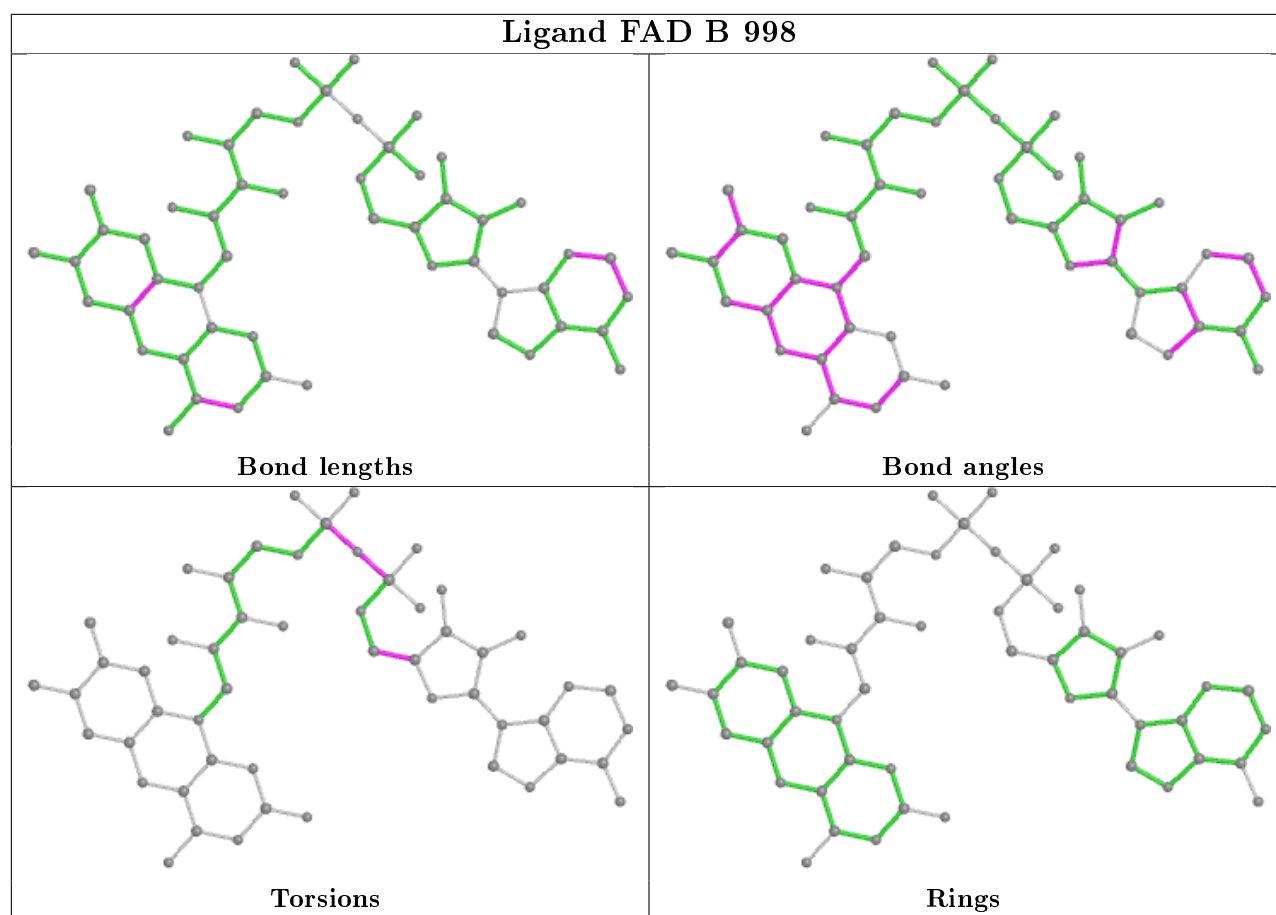
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

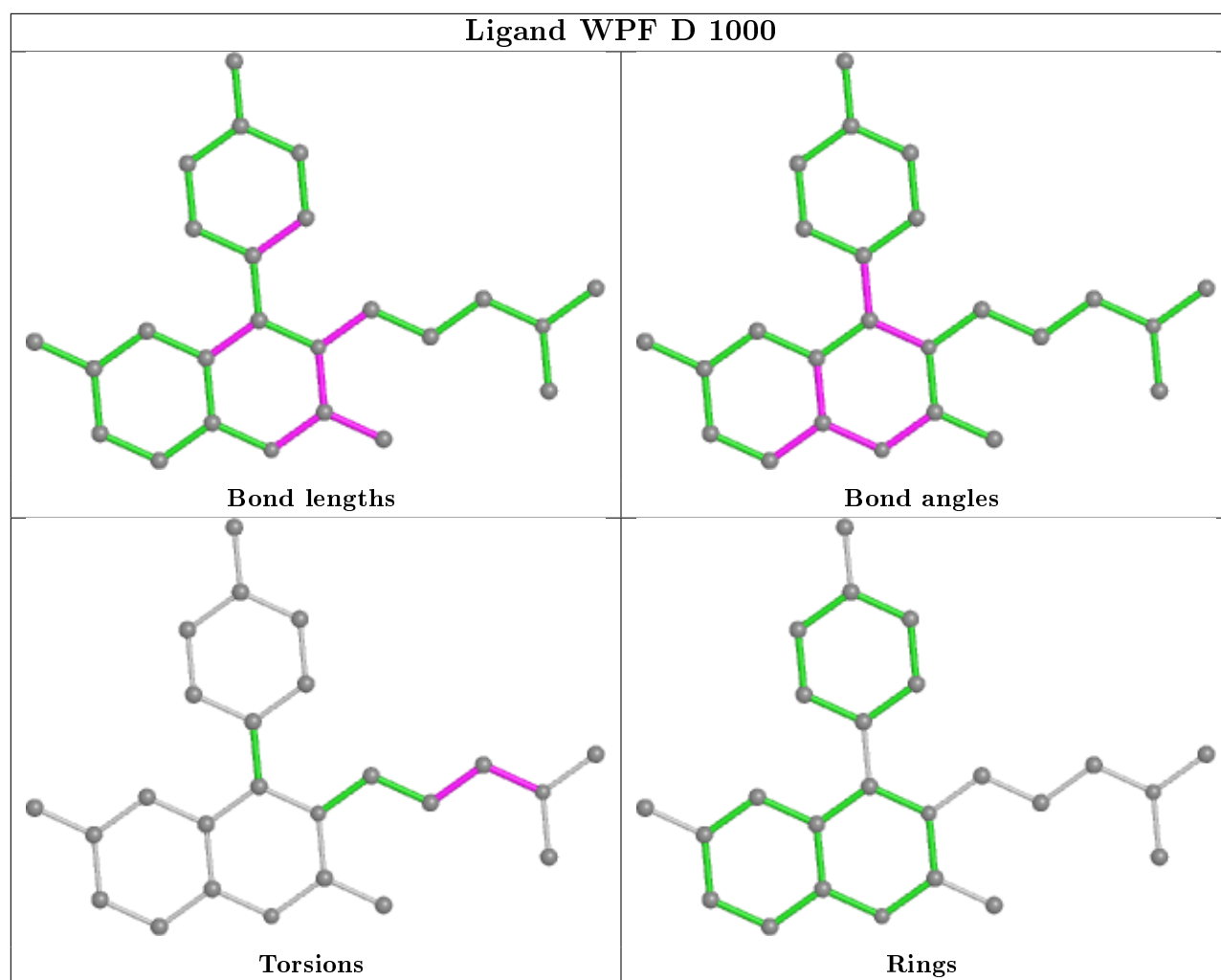




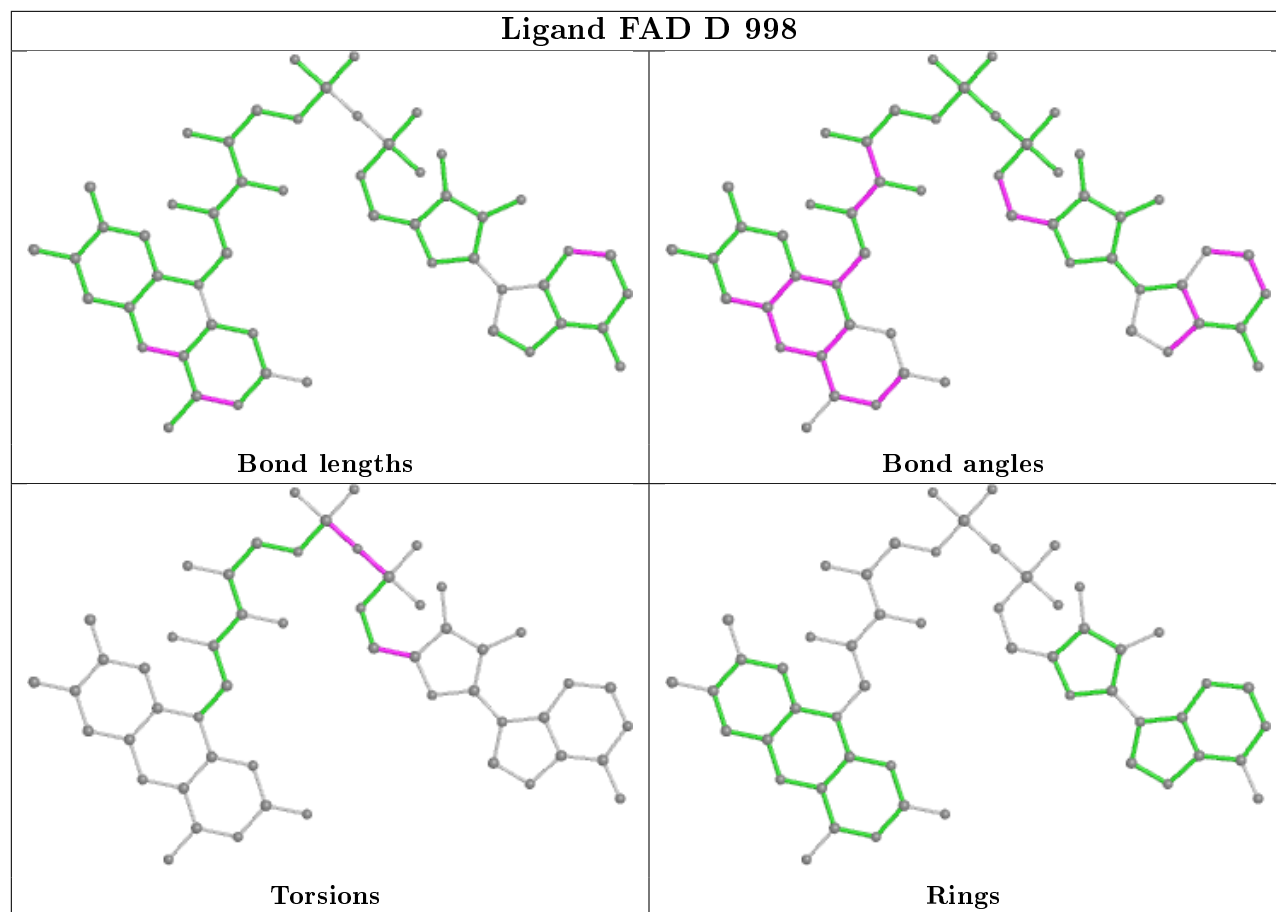
## Ligand WPF C 1000



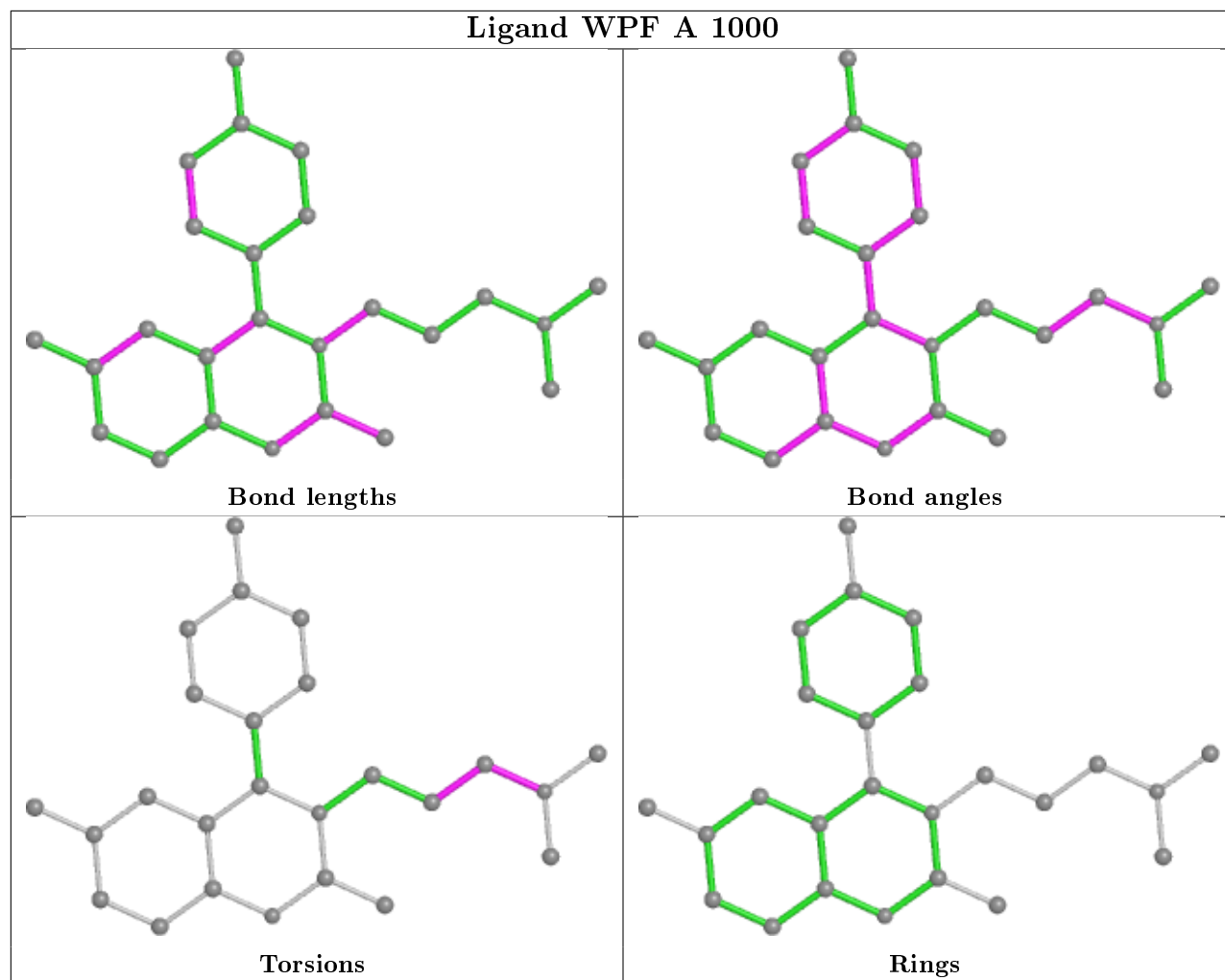


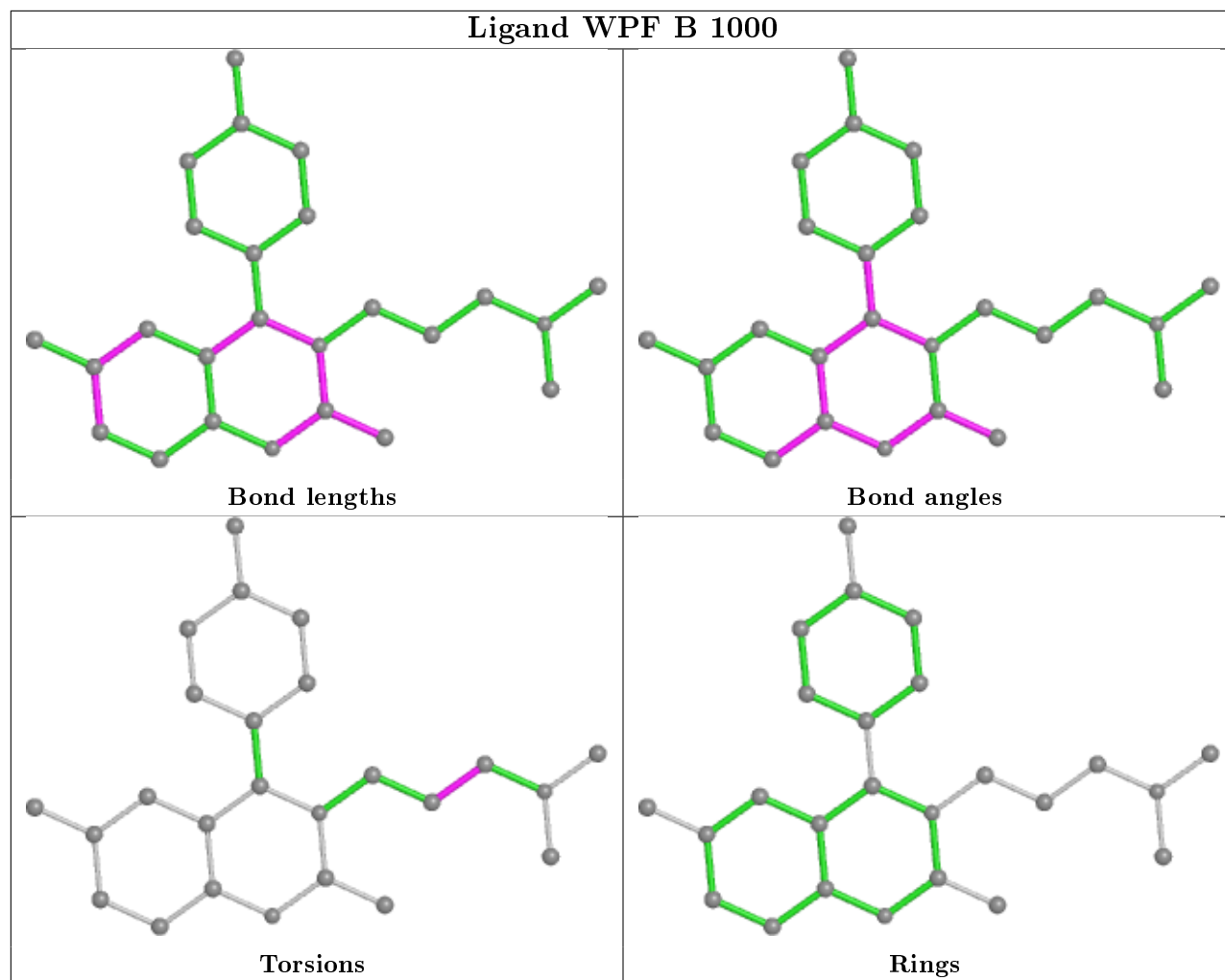






## Ligand WPF A 1000





## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	490/495 (98%)	-0.43	3 (0%) 89 90	9, 19, 33, 46	0
1	B	487/495 (98%)	-0.28	5 (1%) 82 84	13, 24, 41, 53	0
1	C	487/495 (98%)	-0.18	8 (1%) 72 74	12, 24, 45, 57	0
1	D	491/495 (99%)	-0.41	3 (0%) 89 90	10, 20, 33, 47	0
All	All	1955/1980 (98%)	-0.32	19 (0%) 82 84	9, 21, 41, 57	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	352	ASN	4.2
1	B	352	ASN	4.0
1	C	306	LYS	3.5
1	C	305	PRO	3.5
1	D	305	PRO	3.1
1	B	305	PRO	2.9
1	A	352	ASN	2.8
1	B	353	LYS	2.8
1	C	144	LYS	2.6
1	B	306	LYS	2.4
1	B	2	SER	2.3
1	C	487	LEU	2.3
1	A	305	PRO	2.3
1	C	354	PRO	2.2
1	D	488	PRO	2.2
1	A	488	PRO	2.2
1	D	306	LYS	2.2
1	C	152	GLN	2.2
1	C	488	PRO	2.2

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

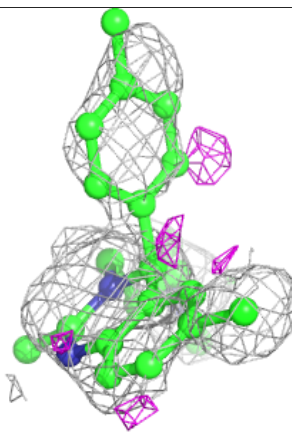
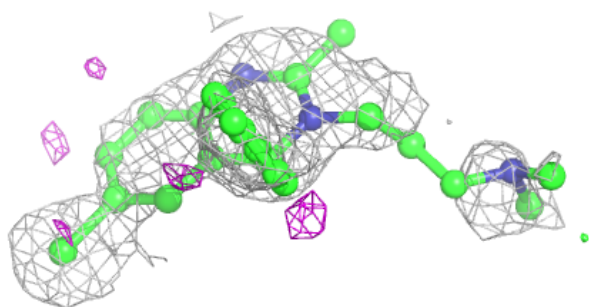
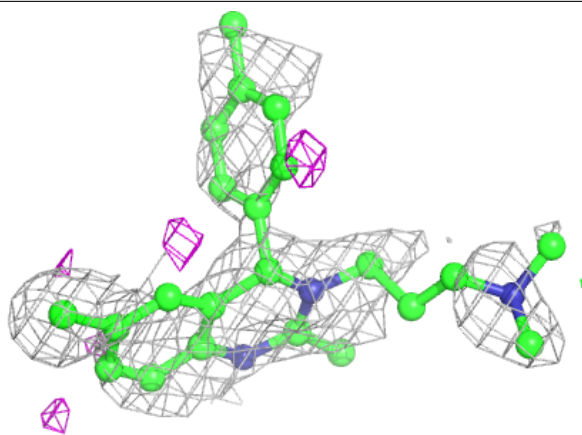
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	WPF	C	1000	25/25	0.81	0.27	48,62,66,67	0
3	WPF	B	1000	25/25	0.90	0.19	36,41,54,55	0
3	WPF	A	1000	25/25	0.91	0.16	22,30,47,48	0
3	WPF	D	1000	25/25	0.92	0.15	25,32,43,46	0
5	BR	D	1489	1/1	0.94	0.09	66,66,66,66	0
5	BR	B	1491	1/1	0.95	0.15	69,69,69,69	0
2	FAD	B	998	53/53	0.97	0.08	15,21,27,28	0
2	FAD	A	998	53/53	0.98	0.07	2,12,16,17	0
4	CL	A	1491	1/1	0.98	0.04	27,27,27,27	0
2	FAD	D	998	53/53	0.98	0.07	11,14,18,19	0
4	CL	C	1491	1/1	0.98	0.04	22,22,22,22	0
2	FAD	C	998	53/53	0.98	0.07	13,21,27,28	0
4	CL	A	1489	1/1	0.99	0.10	17,17,17,17	0
4	CL	C	1490	1/1	0.99	0.08	15,15,15,15	0
4	CL	B	1489	1/1	0.99	0.10	17,17,17,17	0
4	CL	A	1490	1/1	0.99	0.09	19,19,19,19	0
4	CL	B	1490	1/1	1.00	0.08	18,18,18,18	0
5	BR	D	1490	1/1	1.00	0.02	36,36,36,36	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.

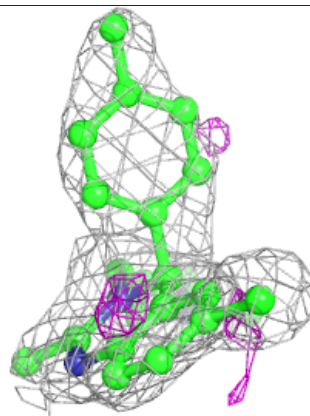
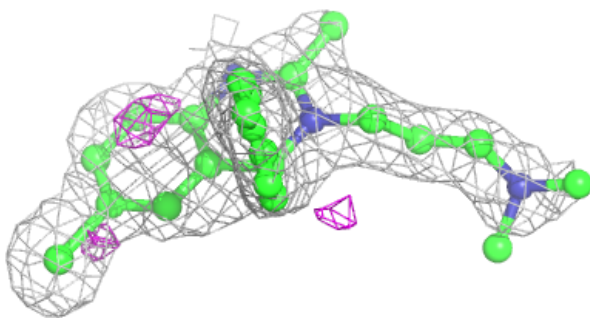
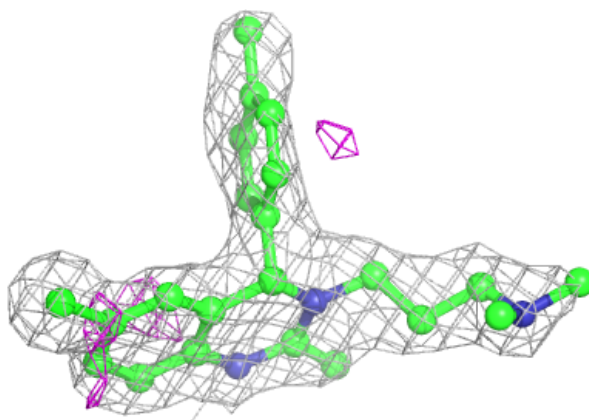
**Electron density around WPF C 1000:**

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



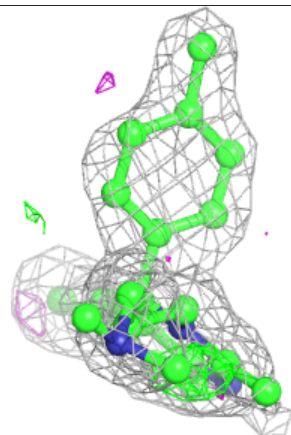
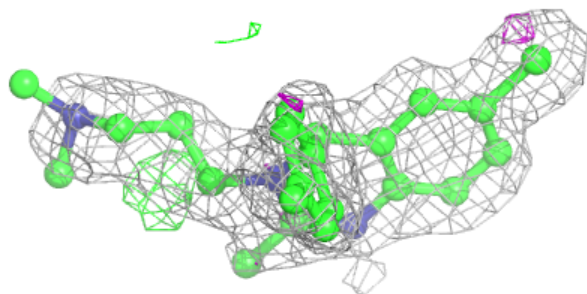
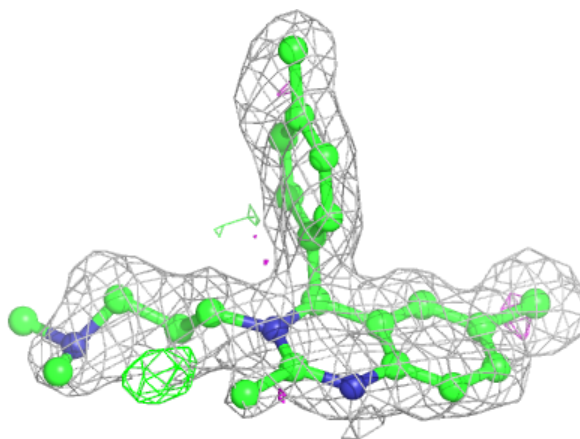
**Electron density around WPF B 1000:**

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



**Electron density around WPF A 1000:**

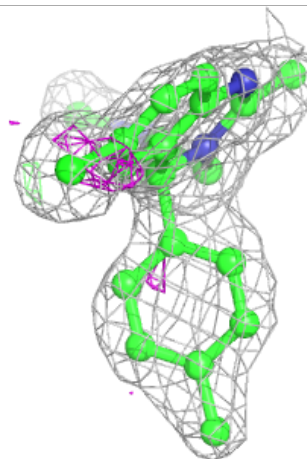
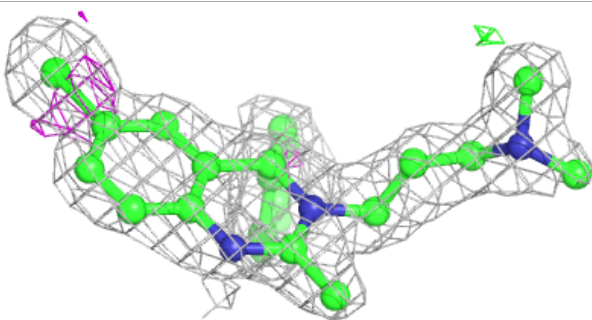
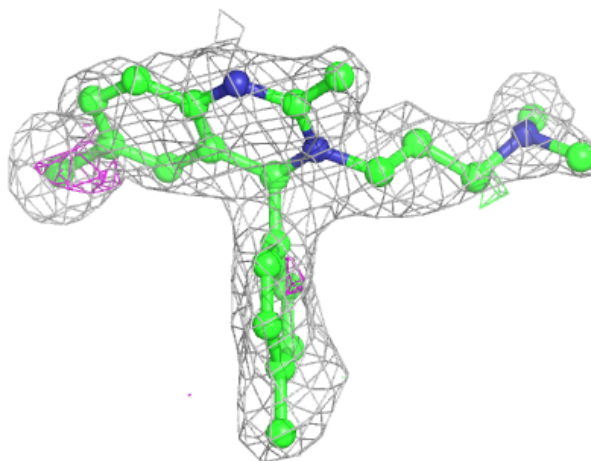
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





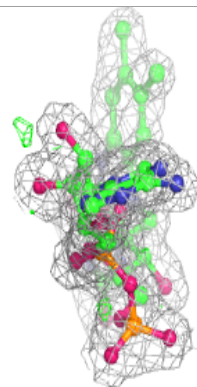
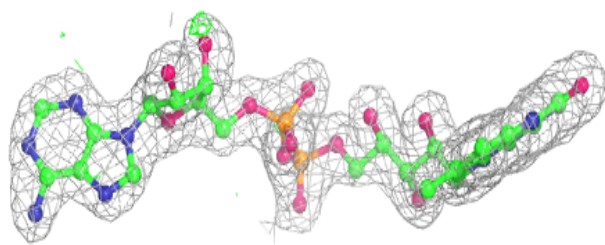
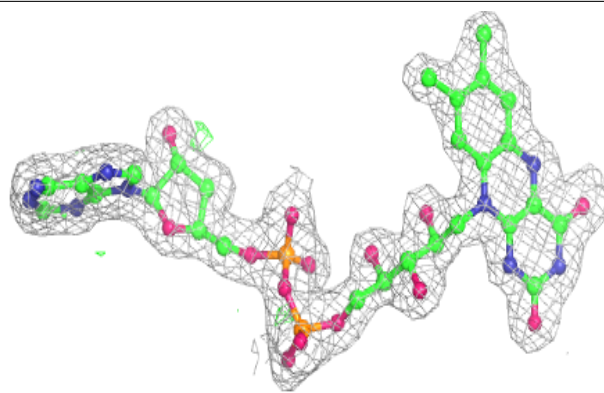
**Electron density around WPF D 1000:**

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

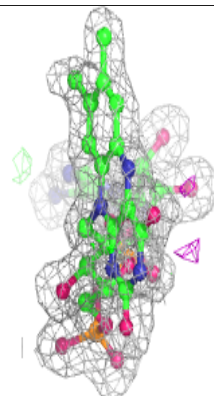
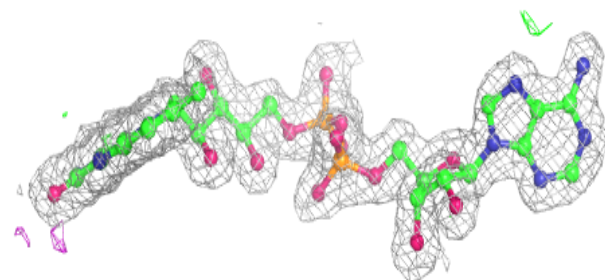
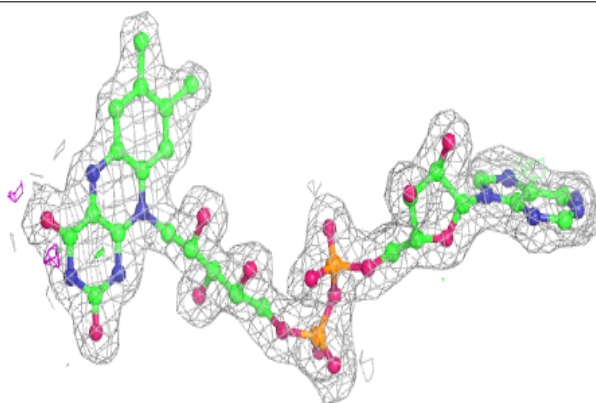


**Electron density around FAD B 998:**

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

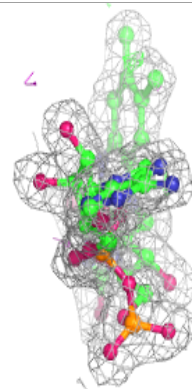
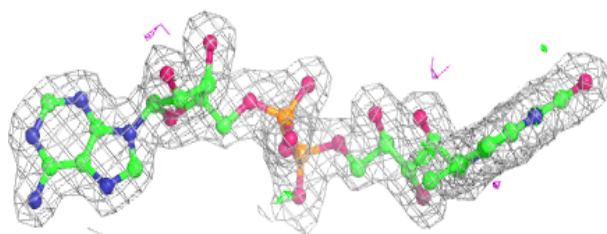
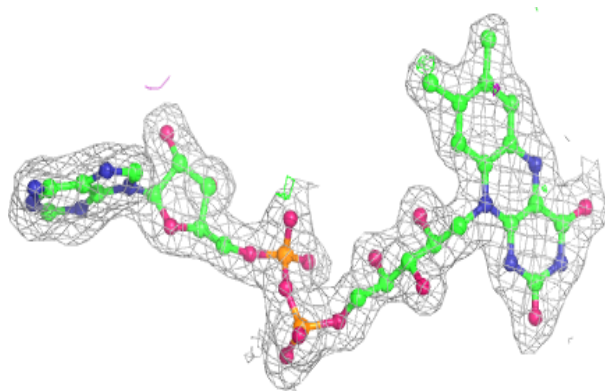
**Electron density around FAD A 998:**

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

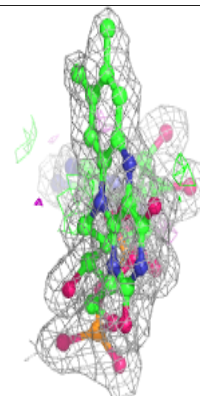
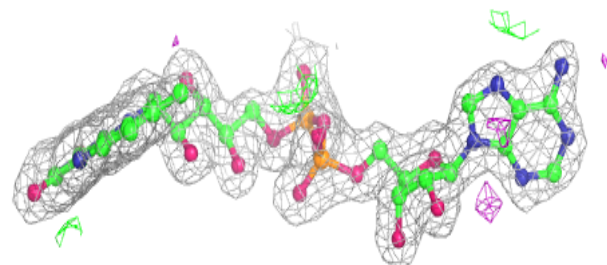
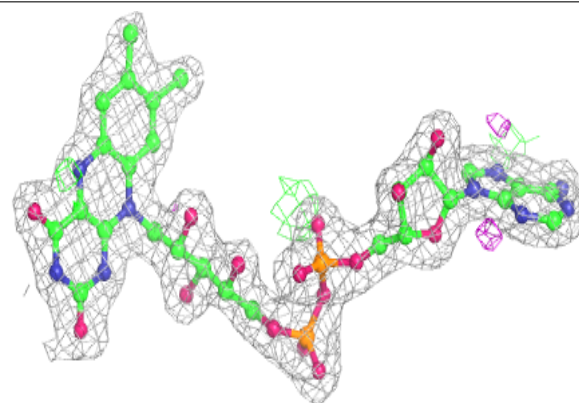


**Electron density around FAD D 998:**

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

**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)



## 6.5 Other polymers

There are no such residues in this entry.