



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:40 PM UTC

PDB ID : 2WPE / pdb_00002wpe
Title : Trypanosoma brucei trypanothione reductase in complex with 3,4- dihydro-quinazoline inhibitor (DDD00073359)
Authors : Alpey, M.S.; Patterson, S.; Fairlamb, A.H.
Deposited on : 2009-08-06
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

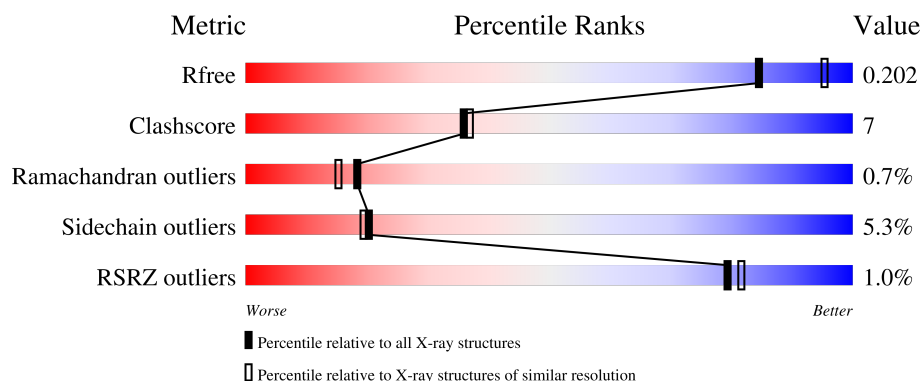
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	 83% 14% ..
1	B	495	 2% 78% 18% ..
1	C	495	 2% 74% 21% ..
1	D	495	 81% 14% ..

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 16447 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
			3735	2375	637	703	20			
1	B	486	Total	C	N	O	S	0	2	0
			3704	2358	631	696	19			
1	C	484	Total	C	N	O	S	0	4	0
			3698	2352	628	699	19			
1	D	489	Total	C	N	O	S	0	4	0
			3732	2371	635	706	20			

There are 12 discrepancies between the modelled and reference sequences:

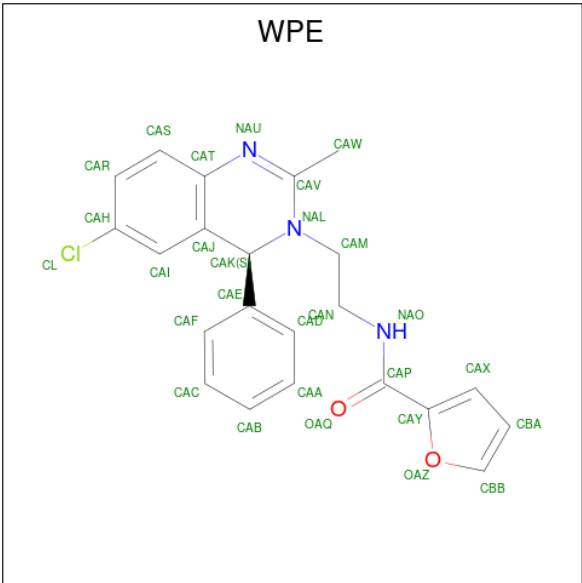
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q389T8
A	-1	SER	-	expression tag	UNP Q389T8
A	0	HIS	-	expression tag	UNP Q389T8
B	-2	GLY	-	expression tag	UNP Q389T8
B	-1	SER	-	expression tag	UNP Q389T8
B	0	HIS	-	expression tag	UNP Q389T8
C	-2	GLY	-	expression tag	UNP Q389T8
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 (CCD ID: 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 N-{2-[(4S)-6-CHLORO-2-METHYL-4-PHENYLQUINAZOLIN-3(4H)-YL]ETHYL}FURAN-2-CARBOXAMIDE (CCD ID: WPE) (formula: C₂₂H₂₀ClN₃O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			28	22	1	3	2		
3	B	1	Total	C	Cl	N	O	0	0
			28	22	1	3	2		
3	C	1	Total	C	Cl	N	O	0	0
			28	22	1	3	2		
3	D	1	Total	C	Cl	N	O	0	0
			28	22	1	3	2		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

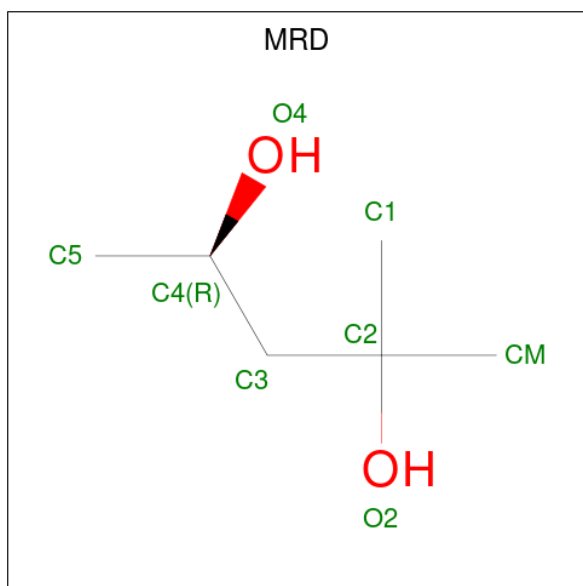
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total	Cl	0	0
			4	4		
5	B	5	Total	Cl	0	0
			5	5		
5	C	5	Total	Cl	0	0
			5	5		
5	D	4	Total	Cl	0	0
			4	4		

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			8	6	2		

- Molecule 7 is (4R)-2-METHYLPENTANE-2,4-DIOL (CCD ID: MRD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	C	O	0	0
			8	6	2		

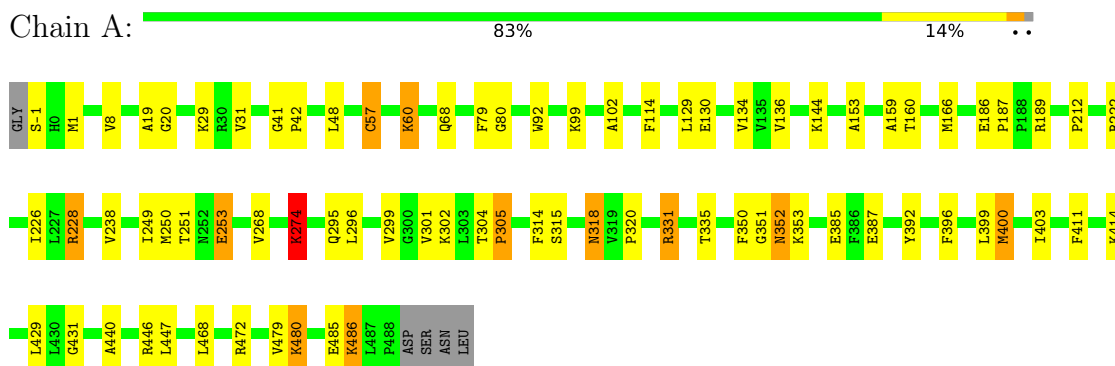
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	365	Total 365	O 365	0	0
8	B	265	Total 265	O 265	0	0
8	C	265	Total 265	O 265	0	0
8	D	321	Total 321	O 321	0	0

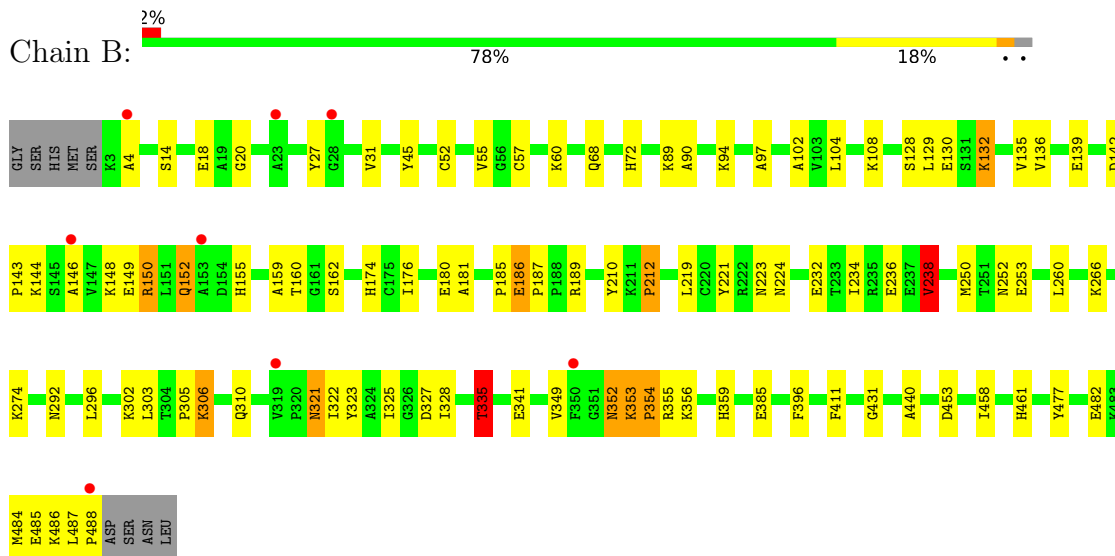
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

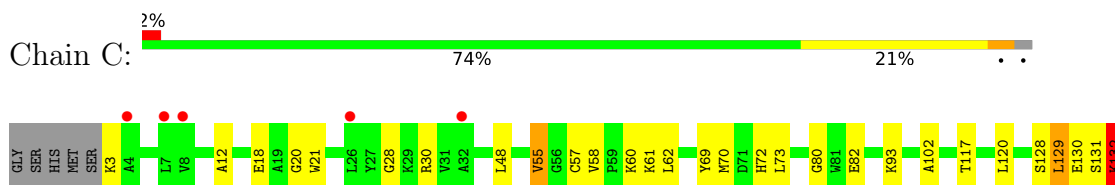
• Molecule 1: TRYPANOTHIONE REDUCTASE

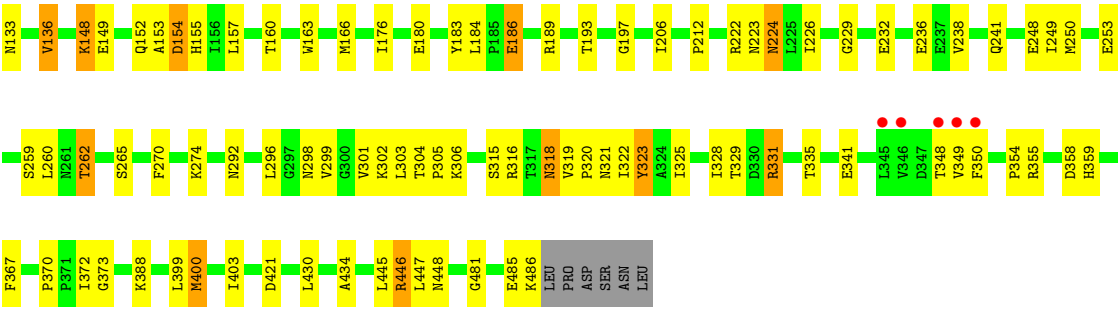


• Molecule 1: TRYPANOTHIONE REDUCTASE

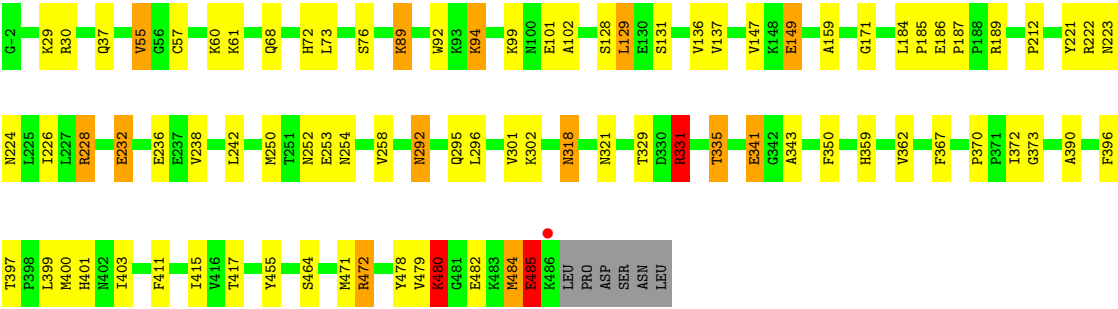
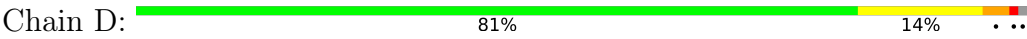


• Molecule 1: TRYPANOTHIONE REDUCTASE





● Molecule 1: TRYPANOTHIONE REDUCTASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	100.64Å 63.29Å 169.16Å 90.00° 98.20° 90.00°	Depositor
Resolution (Å)	45.98 – 2.10 45.98 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.98-2.10) 99.8 (45.98-2.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.168 , 0.230 (Not available) , 0.202	Depositor DCC
R_{free} test set	6169 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	24.1	Xtriage
Anisotropy	0.416	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16447	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: WPE, MPD, MRD, NA, CL, FAD

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	1.47	10/3820 (0.3%)	1.23	9/5181 (0.2%)
1	B	1.34	6/3787 (0.2%)	1.20	14/5135 (0.3%)
1	C	1.31	14/3787 (0.4%)	1.21	15/5138 (0.3%)
1	D	1.37	6/3822 (0.2%)	1.20	15/5183 (0.3%)
All	All	1.38	36/15216 (0.2%)	1.21	53/20637 (0.3%)

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	42	PRO	CA-C	11.90	1.58	1.51
1	D	226	ILE	CA-CB	8.13	1.62	1.54
1	A	102	ALA	CA-CB	7.30	1.64	1.53
1	D	362	VAL	CA-CB	7.29	1.62	1.54
1	A	42	PRO	C-O	-7.26	1.18	1.25
1	B	159	ALA	CA-CB	7.12	1.60	1.53
1	C	434	ALA	CA-CB	6.96	1.62	1.53
1	A	226	ILE	CA-CB	6.83	1.60	1.54
1	C	206	ILE	CA-CB	-6.36	1.46	1.54
1	B	181	ALA	CA-CB	6.24	1.63	1.53
1	A	134	VAL	CA-CB	6.11	1.62	1.54
1	B	97	ALA	CA-CB	5.93	1.62	1.53
1	C	193	THR	CA-CB	5.75	1.61	1.53
1	C	265	SER	CA-C	5.72	1.61	1.53
1	C	58	VAL	CA-CB	5.71	1.61	1.54
1	B	186	GLU	CA-CB	-5.60	1.46	1.53
1	C	62	LEU	C-O	-5.58	1.17	1.24
1	C	270	PHE	N-CA	5.50	1.52	1.45
1	C	259	SER	N-CA	5.41	1.52	1.46
1	D	159	ALA	CA-CB	5.36	1.58	1.53
1	C	226	ILE	CA-CB	5.31	1.61	1.54
1	D	128	SER	N-CA	5.30	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	160	THR	N-CA	5.26	1.53	1.46
1	A	268	VAL	CA-CB	5.25	1.60	1.54
1	B	461	HIS	CA-C	5.21	1.57	1.52
1	A	19	ALA	CA-CB	5.21	1.61	1.53
1	B	238	VAL	CA-CB	5.20	1.60	1.54
1	C	249	ILE	C-O	-5.20	1.18	1.24
1	A	159	ALA	CA-CB	5.18	1.58	1.53
1	D	55	VAL	CA-CB	5.16	1.61	1.54
1	C	262	THR	CA-CB	5.15	1.61	1.53
1	C	55	VAL	CA-CB	5.12	1.61	1.54
1	C	274	LYS	CA-C	5.07	1.59	1.53
1	A	253	GLU	C-O	5.05	1.30	1.23
1	C	197	GLY	N-CA	5.04	1.50	1.45
1	D	343	ALA	C-O	5.04	1.30	1.24

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	186	GLU	N-CA-C	10.41	120.11	108.14
1	C	186[A]	GLU	CA-C-N	-8.24	111.89	120.38
1	C	186[A]	GLU	C-N-CA	-8.24	111.89	120.38
1	C	186[B]	GLU	CA-C-N	-8.24	111.89	120.38
1	C	186[B]	GLU	C-N-CA	-8.24	111.89	120.38
1	D	335	THR	CA-C-N	-7.99	111.57	119.64
1	D	335	THR	C-N-CA	-7.99	111.57	119.64
1	C	292	ASN	N-CA-C	7.11	119.03	111.28
1	B	488	PRO	N-CA-CB	7.08	110.79	103.00
1	D	485	GLU	N-CA-C	6.98	120.98	107.71
1	B	186	GLU	CA-C-N	-6.97	113.20	120.38
1	B	186	GLU	C-N-CA	-6.97	113.20	120.38
1	D	397	THR	CA-C-N	-6.77	112.67	119.92
1	D	397	THR	C-N-CA	-6.77	112.67	119.92
1	D	30	ARG	CA-CB-CG	-6.66	100.78	114.10
1	D	186	GLU	CA-C-N	-6.52	113.66	120.38
1	D	186	GLU	C-N-CA	-6.52	113.66	120.38
1	C	166	MET	CA-C-N	-6.46	113.10	119.76
1	C	166	MET	C-N-CA	-6.46	113.10	119.76
1	C	163	TRP	CA-C-N	-6.02	113.56	119.76
1	C	163	TRP	C-N-CA	-6.02	113.56	119.76
1	B	185	PRO	CA-C-N	-5.99	113.45	122.07
1	B	185	PRO	C-N-CA	-5.99	113.45	122.07
1	C	229	GLY	N-CA-C	-5.95	106.88	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	292	ASN	N-CA-C	5.80	117.40	111.14
1	D	232	GLU	N-CA-C	5.72	117.60	111.36
1	D	373	GLY	N-CA-C	-5.57	101.72	111.46
1	C	148	LYS	N-CA-C	-5.54	107.06	113.88
1	D	149	GLU	CB-CG-CD	-5.49	103.26	112.60
1	D	484	MET	N-CA-C	5.44	115.02	107.73
1	D	292	ASN	N-CA-C	5.40	118.08	111.82
1	A	396	PHE	N-CA-C	-5.39	99.82	108.55
1	A	41	GLY	CA-C-N	-5.33	115.77	119.66
1	A	41	GLY	C-N-CA	-5.33	115.77	119.66
1	B	186	GLU	CB-CG-CD	-5.33	103.55	112.60
1	A	226	ILE	N-CA-C	5.30	118.04	110.09
1	B	212	PRO	CA-C-N	5.29	126.45	119.84
1	B	212	PRO	C-N-CA	5.29	126.45	119.84
1	B	458	ILE	CB-CA-C	5.23	117.94	111.15
1	A	79	PHE	N-CA-C	-5.22	106.15	112.88
1	B	335	THR	CA-C-N	-5.21	114.30	119.56
1	B	335	THR	C-N-CA	-5.21	114.30	119.56
1	C	481	GLY	CA-C-N	-5.20	115.86	122.77
1	C	481	GLY	C-N-CA	-5.20	115.86	122.77
1	A	305	PRO	N-CA-C	-5.18	106.03	113.75
1	C	21	TRP	N-CA-C	-5.17	107.04	113.55
1	A	274	LYS	N-CA-C	-5.08	103.82	110.53
1	D	341	GLU	CA-C-N	5.08	125.58	119.94
1	D	341	GLU	C-N-CA	5.08	125.58	119.94
1	B	325	ILE	CB-CA-C	-5.04	102.61	110.52
1	C	445	LEU	N-CA-C	-5.02	106.67	112.89
1	A	186	GLU	CA-C-N	-5.01	115.22	120.38
1	A	186	GLU	C-N-CA	-5.01	115.22	120.38

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	3735	0	3751	47	0
1	B	3704	0	3723	54	0
1	C	3698	0	3709	69	0
1	D	3732	0	3737	58	0
2	A	53	0	31	2	0
2	B	53	0	31	0	0
2	C	53	0	31	0	0
2	D	53	0	31	0	0
3	A	28	0	20	0	0
3	B	28	0	20	3	0
3	C	28	0	20	1	0
3	D	28	0	20	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	4	0	0	2	0
5	B	5	0	0	0	0
5	C	5	0	0	1	0
5	D	4	0	0	0	0
6	A	8	0	14	2	0
7	D	8	0	14	0	0
8	A	365	0	0	11	0
8	B	265	0	0	6	0
8	C	265	0	0	5	0
8	D	321	0	0	12	0
All	All	16447	0	15152	221	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (221) 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:321:ASN:HB2	8:D:2232:HOH:O	1.41	1.17
1:A:485:GLU:HG2	1:A:486:LYS:HD2	1.20	1.08
1:B:352:ASN:C	1:B:352:ASN:HD22	1.74	0.94
1:D:292:ASN:HB2	8:D:2213:HOH:O	1.71	0.91
1:C:130:GLU:HB2	1:C:136:VAL:CG2	2.00	0.90
1:C:241:GLN:OE1	1:C:370:PRO:HG3	1.72	0.88
1:C:155:HIS:HD1	1:C:323:TYR:HH	1.19	0.87
1:D:318:ASN:H	1:D:318:ASN:HD22	1.18	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:MET:HE2	1:C:253:GLU:HG3	1.60	0.82
1:D:341:GLU:OE2	1:D:359:HIS:HE1	1.64	0.81
1:B:305:PRO:O	1:B:306:LYS:HB2	1.80	0.81
1:B:224:ASN:HD22	1:B:252:ASN:HD21	1.30	0.80
1:C:304:THR:HB	1:C:305:PRO:HD2	1.65	0.78
1:A:485:GLU:HG2	1:A:486:LYS:CD	2.08	0.76
1:C:20:GLY:O	1:C:120:LEU:HD13	1.85	0.76
1:D:370:PRO:HD2	8:D:2261:HOH:O	1.86	0.76
1:C:93:LYS:NZ	1:C:186[B]:GLU:OE2	2.20	0.75
1:A:318:ASN:HD22	1:A:318:ASN:H	1.36	0.74
1:C:155:HIS:HB3	1:C:323:TYR:HE2	1.53	0.73
1:C:301:VAL:HA	1:C:318:ASN:HD21	1.54	0.72
1:D:101[B]:GLU:HG2	8:D:2065:HOH:O	1.90	0.72
1:C:132:LYS:HD2	1:C:321[B]:ASN:OD1	1.91	0.70
1:B:352:ASN:C	1:B:352:ASN:ND2	2.49	0.70
1:C:117:THR:O	8:C:2059:HOH:O	2.11	0.69
1:B:274[A]:LYS:HG3	8:B:2156:HOH:O	1.92	0.68
1:D:455:TYR:CE2	1:D:472:ARG:HB2	2.29	0.67
1:A:166:MET:HG3	6:A:1494:MPD:H53	1.79	0.65
1:C:80:GLY:HA2	1:D:94:LYS:HG2	1.79	0.65
1:A:400:MET:HB3	8:A:2051:HOH:O	1.96	0.65
1:B:155:HIS:HB3	1:B:323:TYR:HE2	1.61	0.65
1:B:234:ILE:O	1:B:238:VAL:HG12	1.97	0.64
1:B:132:LYS:HZ2	1:B:132:LYS:HB3	1.62	0.64
8:A:2061:HOH:O	1:B:72:HIS:HD2	1.81	0.63
1:D:189:ARG:HA	1:D:212:PRO:HD2	1.80	0.62
1:A:129:LEU:HD22	1:A:296:LEU:HD23	1.82	0.62
1:B:482:GLU:HG3	1:B:484:MET:CE	2.29	0.62
1:D:318:ASN:H	1:D:318:ASN:ND2	1.94	0.62
1:B:186:GLU:HB2	1:B:187:PRO:CD	2.29	0.62
1:B:224:ASN:ND2	1:B:252:ASN:HD21	1.98	0.62
1:D:318:ASN:HD22	1:D:318:ASN:N	1.94	0.62
1:C:148:LYS:C	1:C:149:GLU:HG2	2.25	0.61
1:D:482:GLU:HG2	1:D:484:MET:CE	2.30	0.61
1:B:250:MET:HE2	1:B:253:GLU:HG3	1.81	0.61
1:C:133:ASN:ND2	1:C:153:ALA:O	2.22	0.61
1:B:186:GLU:HB2	1:B:187:PRO:HD2	1.83	0.60
1:C:318:ASN:H	1:C:318:ASN:HD22	1.47	0.60
1:D:329:THR:OG1	1:D:331[A]:ARG:NH1	2.35	0.60
1:B:353:LYS:O	1:B:354:PRO:C	2.45	0.60
1:C:222:ARG:HD2	5:C:1490:CL:CL	2.39	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:390:ALA:HB3	1:D:417:THR:OG1	2.00	0.60
1:D:232:GLU:O	1:D:236:GLU:HG3	2.02	0.60
1:B:341:GLU:OE2	1:B:359:HIS:HE1	1.84	0.59
1:C:485:GLU:HB3	8:C:2259:HOH:O	2.02	0.58
1:D:331[A]:ARG:HH11	1:D:331[A]:ARG:HB2	1.67	0.58
1:A:429:LEU:HD21	1:A:468:LEU:HD21	1.86	0.58
1:C:315:SER:O	1:C:323:TYR:HB3	2.04	0.58
1:B:4:ALA:HA	1:B:152:GLN:HG2	1.85	0.58
1:A:304:THR:HB	1:A:305:PRO:HD2	1.86	0.58
1:C:348:THR:HG22	1:C:348:THR:O	2.04	0.57
1:C:130:GLU:HB2	1:C:136:VAL:HG22	1.85	0.57
1:C:148:LYS:O	1:C:149:GLU:HG2	2.05	0.57
1:D:331[A]:ARG:NH2	8:D:2236:HOH:O	2.34	0.57
1:C:370:PRO:HG2	1:C:430:LEU:HD11	1.85	0.56
1:C:93:LYS:HZ1	1:C:186[B]:GLU:CD	2.14	0.56
1:A:295:GLN:NE2	8:A:2233:HOH:O	2.38	0.56
1:B:219:LEU:C	1:B:219:LEU:HD23	2.31	0.56
1:A:411:PHE:CD1	1:A:431:GLY:HA3	2.40	0.55
1:C:319:VAL:HG11	1:C:322:ILE:HD12	1.87	0.55
1:B:104:LEU:HG	1:B:108:LYS:HE3	1.87	0.55
1:C:61:LYS:HE3	1:C:367:PHE:CE1	2.41	0.55
1:A:446:ARG:NE	8:A:2330:HOH:O	2.38	0.55
1:A:446:ARG:HB2	8:A:2285:HOH:O	2.07	0.55
1:B:162:SER:HB3	1:B:327:ASP:HB3	1.89	0.55
1:C:93:LYS:NZ	1:C:186[B]:GLU:CD	2.65	0.55
1:C:296:LEU:HD12	1:C:303:LEU:HD21	1.88	0.55
1:D:482:GLU:HG2	1:D:484:MET:HE2	1.88	0.54
1:A:29:LYS:HD2	1:A:350:PHE:CD1	2.42	0.54
1:A:228:ARG:NH2	5:A:1493:CL:CL	2.67	0.54
1:C:132:LYS:HG3	1:C:133:ASN:OD1	2.07	0.54
1:D:480:LYS:HA	1:D:480:LYS:HE3	1.89	0.54
1:C:223:ASN:HB3	1:C:224[A]:ASN:OD1	2.07	0.54
1:A:68:GLN:NE2	8:A:2058:HOH:O	2.39	0.53
1:C:403:ILE:HD11	1:D:102:ALA:HB2	1.90	0.53
1:D:29:LYS:HE3	1:D:350:PHE:CD1	2.44	0.53
1:C:73:LEU:CD2	1:D:73:LEU:HD23	2.39	0.53
1:D:72:HIS:HD2	8:D:2053:HOH:O	1.91	0.53
1:B:18:GLU:OE1	3:B:1000:WPE:NAU	2.42	0.52
1:C:154:ASP:HB3	1:C:155:HIS:CD2	2.44	0.52
1:D:171:GLY:HA3	1:D:258:VAL:O	2.08	0.52
1:D:415:ILE:HD12	1:D:471:MET:HE3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:329:THR:OG1	1:C:331:ARG:HD2	2.09	0.51
1:C:131:SER:O	1:C:133:ASN:N	2.44	0.51
1:C:176:ILE:HB	1:C:180:GLU:HB2	1.91	0.51
1:D:221:TYR:CE2	1:D:223:ASN:HB2	2.46	0.51
1:C:160:THR:OG1	1:C:328:ILE:HD12	2.11	0.51
1:C:299:VAL:HG23	1:C:301:VAL:HG23	1.92	0.51
1:A:301:VAL:HA	1:A:318:ASN:HD21	1.75	0.50
1:C:82:GLU:OE1	1:D:89:LYS:HE3	2.10	0.50
1:C:130:GLU:HB2	1:C:136:VAL:HG21	1.90	0.50
1:D:359:HIS:HD2	8:D:2254:HOH:O	1.95	0.50
1:B:132:LYS:NZ	1:B:321:ASN:OD1	2.44	0.50
1:B:232:GLU:O	1:B:236:GLU:HG3	2.11	0.50
1:B:189:ARG:HA	1:B:212:PRO:HD2	1.93	0.50
1:D:136:VAL:HG13	1:D:147:VAL:HG13	1.94	0.50
1:C:189:ARG:HA	1:C:212:PRO:HD2	1.92	0.50
1:A:440:ALA:HB3	1:B:440:ALA:HB3	1.93	0.50
1:B:14:SER:HA	3:B:1000:WPE:HAR	1.94	0.50
1:C:304:THR:HB	1:C:305:PRO:CD	2.38	0.50
1:A:302:LYS:H	1:A:318:ASN:ND2	2.09	0.49
1:A:99:LYS:HD2	1:A:99:LYS:C	2.37	0.49
1:C:232:GLU:O	1:C:236:GLU:HG3	2.12	0.49
1:A:20:GLY:HA2	1:A:31:VAL:HG11	1.94	0.49
1:B:296:LEU:HD12	1:B:303:LEU:HD21	1.94	0.49
1:B:305:PRO:O	1:B:306:LYS:CB	2.53	0.49
1:D:61:LYS:HE3	1:D:367:PHE:CE1	2.47	0.49
1:B:130:GLU:OE1	1:B:150:ARG:NH2	2.45	0.49
1:D:321:ASN:CB	8:D:2232:HOH:O	2.23	0.49
1:D:222:ARG:HH12	1:D:254:ASN:ND2	2.10	0.49
6:A:1494:MPD:H51	8:A:2134:HOH:O	2.13	0.49
1:D:370:PRO:HG2	8:D:2176:HOH:O	2.13	0.49
1:A:250:MET:HE2	1:A:253:GLU:HG3	1.93	0.48
1:B:274[A]:LYS:HG2	8:B:2155:HOH:O	2.14	0.48
1:D:295:GLN:NE2	8:D:2216:HOH:O	2.45	0.48
1:A:222:ARG:NH2	5:A:1490:CL:CL	2.84	0.48
1:C:302:LYS:H	1:C:318:ASN:ND2	2.11	0.48
1:D:222:ARG:NH1	1:D:254:ASN:ND2	2.62	0.48
1:A:479:VAL:O	1:A:480:LYS:C	2.57	0.48
1:A:302:LYS:H	1:A:318:ASN:HD21	1.62	0.48
1:B:176:ILE:HB	1:B:180:GLU:HB2	1.96	0.47
1:C:155:HIS:ND1	1:C:323:TYR:OH	2.27	0.47
1:D:250:MET:HE2	1:D:253:GLU:HG3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:GLU:HB2	1:A:136:VAL:HG23	1.95	0.47
1:C:69:TYR:CD1	1:D:76:SER:HB3	2.50	0.47
1:D:301:VAL:HA	1:D:318:ASN:HD21	1.79	0.47
1:B:310:GLN:HB3	8:B:2172:HOH:O	2.14	0.47
1:C:155:HIS:HB3	1:C:323:TYR:CE2	2.43	0.47
1:A:314:PHE:O	1:A:315:SER:HB2	2.16	0.46
1:B:139:GLU:HG3	1:B:146:ALA:HB3	1.97	0.46
1:C:12:ALA:HB1	1:C:48:LEU:HD12	1.96	0.46
1:C:349:VAL:HG12	1:C:350:PHE:CE1	2.51	0.46
1:D:136:VAL:HG12	1:D:137:VAL:N	2.31	0.46
1:D:68:GLN:NE2	8:D:2045:HOH:O	2.48	0.46
1:C:421:ASP:OD1	1:C:421:ASP:C	2.59	0.46
1:A:331[A]:ARG:NH2	8:A:2260:HOH:O	2.49	0.45
1:D:478:TYR:HA	1:D:482:GLU:O	2.15	0.45
1:B:52:CYS:HB2	1:B:335:THR:OG1	2.16	0.45
1:C:72:HIS:HD2	8:C:2033:HOH:O	1.99	0.45
1:C:18:GLU:OE1	3:C:1000:WPE:NAU	2.49	0.45
1:D:302:LYS:H	1:D:318:ASN:ND2	2.14	0.45
1:A:385:GLU:HB3	8:A:2300:HOH:O	2.17	0.45
1:B:352:ASN:ND2	1:B:352:ASN:O	2.47	0.45
1:B:477:TYR:CD1	1:B:487:LEU:HD13	2.52	0.45
1:C:399:LEU:O	1:C:400:MET:C	2.60	0.45
1:C:320:PRO:O	1:C:321[B]:ASN:OD1	2.34	0.45
1:C:372:ILE:HG22	1:C:373:GLY:N	2.32	0.45
1:C:447:LEU:C	1:C:448[B]:ASN:HD22	2.25	0.45
1:D:99:LYS:HD2	1:D:99:LYS:C	2.41	0.45
1:C:485:GLU:C	1:C:486:LYS:HG2	2.41	0.44
1:A:392:TYR:O	1:A:414:LYS:HA	2.17	0.44
1:B:221:TYR:CE2	1:B:223:ASN:HB2	2.51	0.44
1:B:132:LYS:HB3	1:B:132:LYS:NZ	2.31	0.44
1:A:57:CYS:HB3	2:A:998:FAD:C4	2.47	0.44
1:B:90:ALA:HB1	1:B:210:TYR:CD1	2.53	0.44
1:A:8:VAL:CG2	1:A:153:ALA:HB2	2.48	0.44
1:D:129:LEU:HD22	1:D:296:LEU:HD23	1.99	0.44
1:C:316:ARG:HG2	1:C:323:TYR:CD1	2.53	0.43
1:D:411:PHE:CZ	1:D:464:SER:HB3	2.53	0.43
1:C:183:TYR:O	1:C:184:LEU:C	2.59	0.43
1:A:60:LYS:HD2	1:A:60:LYS:C	2.43	0.43
1:A:304:THR:HB	1:A:305:PRO:CD	2.48	0.43
1:C:102:ALA:HB1	1:D:399:LEU:HD11	2.00	0.43
1:D:479:VAL:O	1:D:480:LYS:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:ASN:H	1:A:318:ASN:ND2	2.11	0.43
1:B:411:PHE:CD1	1:B:431:GLY:HA3	2.53	0.43
1:B:321:ASN:HD22	1:B:321:ASN:C	2.26	0.43
1:D:184:LEU:HA	1:D:185:PRO:HD3	1.94	0.43
1:B:160:THR:OG1	1:B:328:ILE:HD12	2.18	0.43
1:B:266:LYS:HD2	1:B:266:LYS:N	2.33	0.43
1:C:70:MET:HE2	8:C:2028:HOH:O	2.19	0.42
1:C:130:GLU:CB	1:C:136:VAL:CG2	2.86	0.42
1:C:358:ASP:OD2	1:C:446:ARG:NH2	2.51	0.42
1:D:92:TRP:HB3	1:D:187:PRO:HD3	2.01	0.42
1:A:399:LEU:HD11	1:B:102:ALA:HB1	1.99	0.42
1:C:341:GLU:OE2	1:C:359:HIS:HE1	2.02	0.42
1:D:485:GLU:N	1:D:485:GLU:OE1	2.53	0.42
1:A:80:GLY:HA2	1:B:94:LYS:HG2	2.01	0.42
1:A:446:ARG:NH1	1:B:453:ASP:OD1	2.52	0.42
1:A:351:GLY:O	1:A:352:ASN:C	2.61	0.42
1:C:157:LEU:HD11	1:C:325:ILE:HG12	2.01	0.42
1:B:20:GLY:HA2	1:B:31:VAL:HG11	2.02	0.42
3:B:1000:WPE:HAM2	3:B:1000:WPE:HAW3	1.78	0.42
1:D:238:VAL:HG21	1:D:372:ILE:HD11	2.01	0.42
1:B:52:CYS:HB3	8:B:2015:HOH:O	2.20	0.41
1:C:331:ARG:N	8:C:2191:HOH:O	2.53	0.41
1:D:136:VAL:CG1	1:D:137:VAL:N	2.82	0.41
1:A:68:GLN:HB3	8:A:2059:HOH:O	2.19	0.41
1:B:68:GLN:NE2	8:B:2022:HOH:O	2.46	0.41
1:A:274:LYS:HB2	1:A:274:LYS:HE3	1.41	0.41
1:A:447:LEU:HD23	1:A:447:LEU:HA	1.95	0.41
1:B:27:TYR:OH	1:B:353:LYS:HE3	2.20	0.41
1:C:318:ASN:HD22	1:C:318:ASN:N	2.16	0.41
1:A:144:LYS:HB2	1:A:144:LYS:HE2	1.92	0.41
1:C:129:LEU:HD22	1:C:296:LEU:HD23	2.02	0.41
1:A:129:LEU:HD23	1:A:299:VAL:HG21	2.03	0.41
1:D:222:ARG:NH2	8:D:2163:HOH:O	2.53	0.41
1:A:189:ARG:HA	1:A:212:PRO:HD2	2.02	0.41
1:B:174:HIS:HE1	8:B:2081:HOH:O	2.03	0.41
1:D:224[A]:ASN:ND2	1:D:252:ASN:OD1	2.54	0.41
1:B:142:ASP:HA	1:B:143:PRO:HD3	1.94	0.41
1:B:396:PHE:CD2	1:B:396:PHE:C	2.99	0.41
1:C:485:GLU:HG3	1:C:486:LYS:HG2	2.03	0.41
1:D:302:LYS:H	1:D:318:ASN:HD21	1.69	0.41
1:A:331[B]:ARG:HB3	8:A:2264:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:400:MET:HG3	1:D:401:HIS:N	2.36	0.40
1:A:48:LEU:HD11	1:A:114:PHE:HE2	1.86	0.40
1:A:92:TRP:HB3	1:A:187:PRO:HD3	2.03	0.40
2:A:998:FAD:H9	2:A:998:FAD:H1'1	1.89	0.40
1:B:148:LYS:C	1:B:149:GLU:HG2	2.46	0.40
1:D:228:ARG:HE	1:D:228:ARG:HB3	1.21	0.40
1:D:238:VAL:O	1:D:242:LEU:HG	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	490/495 (99%)	477 (97%)	12 (2%)	1 (0%)	43	44
1	B	486/495 (98%)	469 (96%)	12 (2%)	5 (1%)	12	9
1	C	486/495 (98%)	458 (94%)	24 (5%)	4 (1%)	16	12
1	D	491/495 (99%)	473 (96%)	13 (3%)	5 (1%)	12	9
All	All	1953/1980 (99%)	1877 (96%)	61 (3%)	15 (1%)	18	12

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	132	LYS
1	A	352	ASN
1	C	28	GLY
1	B	306	LYS
1	B	354	PRO
1	D	331[A]	ARG
1	D	331[B]	ARG
1	D	396	PHE

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Mol	Chain	Res	Type
1	D	480	LYS
1	B	45	TYR
1	C	55	VAL
1	C	298	ASN
1	D	55	VAL
1	B	55	VAL
1	B	349	VAL

5.3.2 Protein sidechains ⓘ

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%)	384 (95%)	21 (5%)	21	20
1	B	400/407 (98%)	376 (94%)	24 (6%)	17	15
1	C	401/407 (98%)	375 (94%)	26 (6%)	15	13
1	D	404/407 (99%)	387 (96%)	17 (4%)	26	28
All	All	1610/1628 (99%)	1522 (94%)	88 (6%)	20	18

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	SER
1	A	1	MET
1	A	57	CYS
1	A	60	LYS
1	A	228	ARG
1	A	238	VAL
1	A	249	ILE
1	A	251	THR
1	A	274	LYS
1	A	318	ASN
1	A	320	PRO
1	A	331[A]	ARG
1	A	331[B]	ARG
1	A	335	THR

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Mol	Chain	Res	Type
1	A	353	LYS
1	A	387	GLU
1	A	400	MET
1	A	403	ILE
1	A	472	ARG
1	A	480	LYS
1	A	486	LYS
1	B	57	CYS
1	B	60	LYS
1	B	89	LYS
1	B	128	SER
1	B	129	LEU
1	B	132	LYS
1	B	135	VAL
1	B	136	VAL
1	B	144	LYS
1	B	150	ARG
1	B	152	GLN
1	B	238	VAL
1	B	260	LEU
1	B	302	LYS
1	B	321	ASN
1	B	322	ILE
1	B	335	THR
1	B	352	ASN
1	B	353	LYS
1	B	355	ARG
1	B	356	LYS
1	B	385	GLU
1	B	485	GLU
1	B	486	LYS
1	C	3	LYS
1	C	30	ARG
1	C	57	CYS
1	C	60	LYS
1	C	128	SER
1	C	129	LEU
1	C	132	LYS
1	C	136	VAL
1	C	152	GLN
1	C	154	ASP
1	C	224[A]	ASN

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Mol	Chain	Res	Type
1	C	224[B]	ASN
1	C	238	VAL
1	C	248	GLU
1	C	260	LEU
1	C	262	THR
1	C	306	LYS
1	C	318	ASN
1	C	323	TYR
1	C	331	ARG
1	C	335	THR
1	C	354	PRO
1	C	355	ARG
1	C	388	LYS
1	C	400	MET
1	C	446	ARG
1	D	37	GLN
1	D	57	CYS
1	D	60	LYS
1	D	89	LYS
1	D	94	LYS
1	D	129	LEU
1	D	131	SER
1	D	149	GLU
1	D	228	ARG
1	D	318	ASN
1	D	331[A]	ARG
1	D	331[B]	ARG
1	D	335	THR
1	D	403	ILE
1	D	472	ARG
1	D	480	LYS
1	D	485	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	223	ASN
1	A	252	ASN
1	A	318	ASN
1	A	340	ASN
1	A	352	ASN

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Mol	Chain	Res	Type
1	B	72	HIS
1	B	107	ASN
1	B	174	HIS
1	B	223	ASN
1	B	252	ASN
1	B	310	GLN
1	B	352	ASN
1	B	359	HIS
1	C	72	HIS
1	C	107	ASN
1	C	208	ASN
1	C	252	ASN
1	C	310	GLN
1	C	318	ASN
1	C	340	ASN
1	C	359	HIS
1	D	68	GLN
1	D	72	HIS
1	D	107	ASN
1	D	223	ASN
1	D	252	ASN
1	D	254	ASN
1	D	292	ASN
1	D	318	ASN
1	D	321	ASN
1	D	340	ASN
1	D	352	ASN
1	D	359	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 32 ligands modelled in this entry, 22 are monoatomic - leaving 10 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	-	58,58,58	1.18	5 (8%)	85,89,89	1.70	18 (21%)
6	MPD	A	1494	-	7,7,7	0.81	0	9,10,10	0.73	0
3	WPE	D	1000	-	31,31,31	2.17	7 (22%)	37,43,43	2.15	10 (27%)
7	MRD	D	1492	-	7,7,7	0.65	0	9,10,10	0.84	0
3	WPE	A	1000	-	31,31,31	2.28	9 (29%)	37,43,43	1.89	8 (21%)
3	WPE	C	1000	-	31,31,31	2.47	9 (29%)	37,43,43	1.92	9 (24%)
2	FAD	B	998	-	58,58,58	1.35	7 (12%)	85,89,89	1.75	17 (20%)
2	FAD	D	998	-	58,58,58	1.28	8 (13%)	85,89,89	1.89	19 (22%)
3	WPE	B	1000	-	31,31,31	2.24	7 (22%)	37,43,43	1.77	8 (21%)
2	FAD	C	998	-	58,58,58	1.29	7 (12%)	85,89,89	1.83	19 (22%)

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	-	-	4/34/50/50	0/6/6/6
6	MPD	A	1494	-	-	1/5/5/5	-
3	WPE	D	1000	-	-	0/14/30/30	0/4/4/4
7	MRD	D	1492	-	-	3/5/5/5	-
3	WPE	A	1000	-	-	0/14/30/30	0/4/4/4
3	WPE	C	1000	-	-	1/14/30/30	0/4/4/4
2	FAD	B	998	-	-	3/34/50/50	0/6/6/6
2	FAD	D	998	-	-	4/34/50/50	0/6/6/6
3	WPE	B	1000	-	-	0/14/30/30	0/4/4/4
2	FAD	C	998	-	-	4/34/50/50	0/6/6/6

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1000	WPE	CAV-NAU	9.02	1.40	1.29
3	B	1000	WPE	CAV-NAU	9.00	1.40	1.29
3	D	1000	WPE	CAV-NAU	6.28	1.37	1.29
3	A	1000	WPE	CAV-NAU	5.85	1.37	1.29
3	D	1000	WPE	CAJ-CAK	5.08	1.57	1.51
3	A	1000	WPE	CAE-CAK	4.72	1.59	1.52
3	A	1000	WPE	CAY-CAP	4.64	1.56	1.47
3	D	1000	WPE	CAY-CAP	4.56	1.56	1.47
3	D	1000	WPE	CAW-CAV	4.21	1.55	1.49
3	C	1000	WPE	CAY-CAP	4.19	1.55	1.47
2	B	998	FAD	C4X-N5	3.89	1.39	1.30
3	C	1000	WPE	CAW-CAV	3.86	1.55	1.49
3	A	1000	WPE	CAC-CAF	3.84	1.45	1.38
3	A	1000	WPE	CAA-CAD	3.82	1.45	1.38
3	B	1000	WPE	CAY-CAP	3.81	1.55	1.47
3	C	1000	WPE	CAJ-CAK	3.80	1.55	1.51
3	B	1000	WPE	CAE-CAK	3.70	1.58	1.52
2	A	998	FAD	C2A-N1A	3.69	1.40	1.33
3	C	1000	WPE	CAK-NAL	3.54	1.50	1.48
3	A	1000	WPE	CAW-CAV	3.53	1.54	1.49
2	C	998	FAD	C2A-N1A	3.35	1.39	1.33
2	C	998	FAD	O4-C4	3.22	1.29	1.23
2	B	998	FAD	P-O3P	-3.20	1.56	1.59
2	B	998	FAD	C2A-N1A	3.15	1.39	1.33
2	D	998	FAD	C8A-N7A	3.10	1.37	1.31
3	D	1000	WPE	CAE-CAK	3.09	1.57	1.52
2	C	998	FAD	C2A-N3A	3.09	1.39	1.33
3	B	1000	WPE	CAW-CAV	3.07	1.54	1.49
2	C	998	FAD	C10-N1	3.05	1.39	1.33
2	D	998	FAD	C4X-N5	2.97	1.37	1.30
2	D	998	FAD	C5'-C4'	2.89	1.55	1.51
3	D	1000	WPE	CAV-NAL	2.88	1.43	1.35
2	D	998	FAD	O4-C4	2.82	1.28	1.23
3	C	1000	WPE	CAM-NAL	2.78	1.51	1.46
2	C	998	FAD	C5A-N7A	-2.77	1.34	1.39
2	B	998	FAD	C2A-N3A	2.75	1.38	1.33
2	A	998	FAD	C4X-N5	2.75	1.36	1.30
3	A	1000	WPE	CAM-NAL	2.70	1.51	1.46
2	C	998	FAD	C4X-N5	2.63	1.36	1.30
3	C	1000	WPE	CAV-NAL	2.61	1.42	1.35
2	D	998	FAD	C2A-N3A	2.55	1.38	1.33
2	D	998	FAD	C2A-N1A	2.52	1.38	1.33
3	A	1000	WPE	CAC-CAB	2.51	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1000	WPE	CAI-CAH	2.47	1.42	1.38
2	B	998	FAD	C10-N1	2.45	1.38	1.33
3	A	1000	WPE	CAJ-CAK	-2.42	1.49	1.51
2	C	998	FAD	C8A-N7A	2.39	1.36	1.31
2	A	998	FAD	C10-N1	2.39	1.38	1.33
2	B	998	FAD	PA-O3P	-2.38	1.56	1.59
2	D	998	FAD	C10-N1	2.37	1.38	1.33
2	B	998	FAD	C4X-C10	-2.35	1.37	1.44
2	D	998	FAD	PA-O3P	2.31	1.62	1.59
3	B	1000	WPE	CAV-NAL	2.29	1.41	1.35
3	D	1000	WPE	CAI-CAH	2.23	1.41	1.38
3	B	1000	WPE	CAJ-CAK	2.22	1.54	1.51
2	A	998	FAD	C7M-C7	2.16	1.55	1.51
3	B	1000	WPE	CAD-CAE	2.13	1.42	1.39
2	A	998	FAD	C5X-N5	2.10	1.43	1.39
3	C	1000	WPE	CAN-NAO	2.09	1.50	1.46

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	998	FAD	N3A-C2A-N1A	-6.81	118.28	128.58
2	A	998	FAD	N3A-C2A-N1A	-6.34	118.98	128.58
2	B	998	FAD	N3A-C2A-N1A	-6.30	119.04	128.58
3	D	1000	WPE	CAN-CAM-NAL	-6.22	106.35	113.74
2	C	998	FAD	N3A-C2A-N1A	-5.56	120.17	128.58
3	D	1000	WPE	CAT-NAU-CAV	5.26	122.68	118.16
2	C	998	FAD	N9A-C8A-N7A	-5.14	106.64	113.94
3	B	1000	WPE	CAN-CAM-NAL	-5.02	107.79	113.74
2	C	998	FAD	C5A-N7A-C8A	4.96	111.24	103.45
3	A	1000	WPE	CAN-CAM-NAL	-4.89	107.94	113.74
2	D	998	FAD	N9A-C8A-N7A	-4.82	107.10	113.94
3	D	1000	WPE	CAS-CAT-CAJ	4.78	123.84	119.54
2	D	998	FAD	C10-C4X-N5	-4.76	115.10	124.81
2	C	998	FAD	C5A-C4A-N3A	-4.72	120.22	126.72
3	C	1000	WPE	CAE-CAK-NAL	-4.71	105.25	111.65
2	B	998	FAD	N9A-C8A-N7A	-4.55	107.48	113.94
3	C	1000	WPE	CAT-NAU-CAV	4.54	122.06	118.16
2	B	998	FAD	C5A-N7A-C8A	4.48	110.48	103.45
2	D	998	FAD	C5A-N7A-C8A	4.46	110.45	103.45
2	D	998	FAD	C5X-N5-C4X	4.33	125.10	118.09
3	A	1000	WPE	CAE-CAK-NAL	-4.31	105.80	111.65
3	C	1000	WPE	CAX-CAY-CAP	-4.19	122.38	132.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	998	FAD	C5A-C4A-N3A	-4.14	121.02	126.72
3	C	1000	WPE	OAZ-CAY-CAP	4.09	128.02	117.98
2	B	998	FAD	O2A-PA-O3P	4.02	118.13	107.27
3	B	1000	WPE	CAM-CAN-NAO	-4.02	103.81	111.56
2	B	998	FAD	C5A-C4A-N3A	-3.89	121.36	126.72
2	A	998	FAD	C4X-C10-N10	3.89	122.04	116.48
2	A	998	FAD	O3P-PA-O1A	-3.74	99.45	110.70
2	A	998	FAD	C2A-N1A-C6A	3.74	124.87	118.73
3	B	1000	WPE	CAE-CAK-NAL	-3.58	106.80	111.65
3	D	1000	WPE	CAE-CAK-NAL	-3.52	106.88	111.65
2	C	998	FAD	O3P-PA-O1A	-3.47	100.26	110.70
3	A	1000	WPE	CAM-CAN-NAO	-3.44	104.91	111.56
2	D	998	FAD	C2A-N3A-C4A	3.39	120.11	111.83
3	D	1000	WPE	OAZ-CAY-CAP	3.35	126.22	117.98
3	C	1000	WPE	OAQ-CAP-CAY	-3.34	115.86	121.10
2	C	998	FAD	C5X-N5-C4X	3.33	123.48	118.09
3	B	1000	WPE	CAX-CAY-CAP	-3.31	124.42	132.04
2	C	998	FAD	N3A-C4A-N9A	3.30	132.78	127.17
2	A	998	FAD	C10-C4X-N5	-3.30	118.06	124.81
2	D	998	FAD	C4-N3-C2	-3.29	119.80	125.64
2	D	998	FAD	C2A-N1A-C6A	3.28	124.12	118.73
2	B	998	FAD	C2A-N3A-C4A	3.27	119.81	111.83
3	A	1000	WPE	OAZ-CAY-CAP	3.27	126.01	117.98
2	A	998	FAD	C4-N3-C2	-3.26	119.85	125.64
2	D	998	FAD	C4X-C10-N10	3.26	121.15	116.48
2	D	998	FAD	C4-C4X-C10	3.23	122.47	116.93
3	D	1000	WPE	CAX-CAY-CAP	-3.21	124.64	132.04
3	A	1000	WPE	CAX-CAY-CAP	-3.21	124.64	132.04
2	C	998	FAD	C10-C4X-N5	-3.18	118.32	124.81
3	B	1000	WPE	OAZ-CAY-CAP	3.17	125.77	117.98
3	A	1000	WPE	CAH-CAI-CAJ	-3.13	115.85	119.74
2	C	998	FAD	C9A-C5X-N5	-3.13	119.13	122.45
2	B	998	FAD	C4A-C5A-N7A	-3.12	107.02	110.58
2	C	998	FAD	C4A-C5A-N7A	-3.08	107.06	110.58
2	D	998	FAD	C4-C4X-N5	3.06	122.43	118.21
2	C	998	FAD	C2A-N3A-C4A	3.05	119.28	111.83
3	A	1000	WPE	CAS-CAT-CAJ	3.01	122.25	119.54
2	B	998	FAD	O4B-C1B-N9A	-2.98	102.36	108.09
2	A	998	FAD	C2B-C1B-N9A	2.97	120.69	113.30
2	A	998	FAD	N9A-C8A-N7A	-2.96	109.73	113.94
2	D	998	FAD	C4A-C5A-N7A	-2.91	107.25	110.58
2	C	998	FAD	C4-C4X-C10	2.86	121.84	116.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1000	WPE	CAE-CAK-CAJ	-2.82	107.73	112.75
2	A	998	FAD	C4-C4X-C10	2.81	121.75	116.93
3	D	1000	WPE	CAM-CAN-NAO	-2.77	106.22	111.56
2	D	998	FAD	N3A-C4A-N9A	2.74	131.83	127.17
2	B	998	FAD	N3A-C4A-N9A	2.73	131.81	127.17
2	C	998	FAD	C6A-C5A-C4A	2.73	120.90	117.18
2	A	998	FAD	O2'-C2'-C3'	2.70	115.57	109.25
2	D	998	FAD	C4X-C10-N1	-2.69	117.98	124.59
2	A	998	FAD	C9A-C5X-N5	-2.67	119.62	122.45
2	B	998	FAD	C4X-C10-N10	2.64	120.27	116.48
2	B	998	FAD	C9A-C5X-N5	-2.59	119.71	122.45
2	C	998	FAD	C4X-C10-N10	2.53	120.10	116.48
2	A	998	FAD	C4A-N9A-C8A	2.51	108.37	105.74
2	D	998	FAD	C9A-C5X-N5	-2.50	119.80	122.45
3	A	1000	WPE	CAS-CAT-NAU	-2.49	115.44	118.61
3	D	1000	WPE	CAJ-CAT-NAU	-2.41	120.08	122.16
2	A	998	FAD	C4X-C10-N1	-2.41	118.69	124.59
3	C	1000	WPE	CAJ-CAK-NAL	2.40	113.89	110.39
3	C	1000	WPE	CAR-CAH-CAI	-2.40	118.39	121.53
3	B	1000	WPE	CAT-NAU-CAV	2.34	120.17	118.16
2	A	998	FAD	C5A-C4A-N3A	-2.33	123.50	126.72
2	C	998	FAD	O2A-PA-O3P	2.33	113.57	107.27
2	A	998	FAD	O4B-C1B-N9A	-2.33	103.62	108.09
2	B	998	FAD	C10-C4X-N5	-2.30	120.12	124.81
2	B	998	FAD	C4A-N9A-C8A	2.30	108.15	105.74
2	C	998	FAD	O4B-C1B-N9A	-2.29	103.69	108.09
2	A	998	FAD	C2A-N3A-C4A	2.29	117.43	111.83
2	C	998	FAD	C2B-C1B-N9A	2.23	118.85	113.30
2	A	998	FAD	C5X-N5-C4X	2.22	121.69	118.09
2	D	998	FAD	O2B-C2B-C1B	-2.22	102.46	110.10
3	D	1000	WPE	CAR-CAH-CAI	2.22	124.43	121.53
2	B	998	FAD	C1'-N10-C9A	2.21	124.92	120.63
3	B	1000	WPE	CAE-CAK-CAJ	-2.19	108.85	112.75
2	B	998	FAD	C2B-C1B-N9A	2.18	118.72	113.30
2	C	998	FAD	C4A-N9A-C8A	2.16	108.00	105.74
2	A	998	FAD	N3A-C4A-N9A	2.13	130.79	127.17
2	D	998	FAD	C4A-N9A-C8A	2.08	107.92	105.74
2	C	998	FAD	C8M-C8-C9	-2.07	115.92	119.57
2	D	998	FAD	O4-C4-N3	-2.06	116.24	120.11
2	B	998	FAD	O3'-C3'-C2'	2.05	113.59	108.93
2	B	998	FAD	C2A-N1A-C6A	2.04	122.07	118.73
3	D	1000	WPE	CAS-CAT-NAU	-2.03	116.02	118.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1000	WPE	CAS-CAR-CAH	2.03	121.29	119.24
3	C	1000	WPE	CAI-CAH-CL	2.00	121.68	119.17

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	998	FAD	PA-O3P-P-O5'
7	D	1492	MRD	C2-C3-C4-C5
3	C	1000	WPE	NAL-CAM-CAN-NAO
2	A	998	FAD	P-O3P-PA-O1A
2	C	998	FAD	PA-O3P-P-O5'
2	D	998	FAD	PA-O3P-P-O5'
2	C	998	FAD	P-O3P-PA-O2A
2	D	998	FAD	P-O3P-PA-O2A
6	A	1494	MPD	C2-C3-C4-C5
2	A	998	FAD	O4B-C4B-C5B-O5B
2	C	998	FAD	O4B-C4B-C5B-O5B
2	B	998	FAD	P-O3P-PA-O2A
2	B	998	FAD	PA-O3P-P-O5'
2	D	998	FAD	O4B-C4B-C5B-O5B
2	A	998	FAD	P-O3P-PA-O2A
2	C	998	FAD	P-O3P-PA-O1A
2	D	998	FAD	P-O3P-PA-O1A
7	D	1492	MRD	C2-C3-C4-O4
7	D	1492	MRD	CM-C2-C3-C4
2	B	998	FAD	O4B-C4B-C5B-O5B

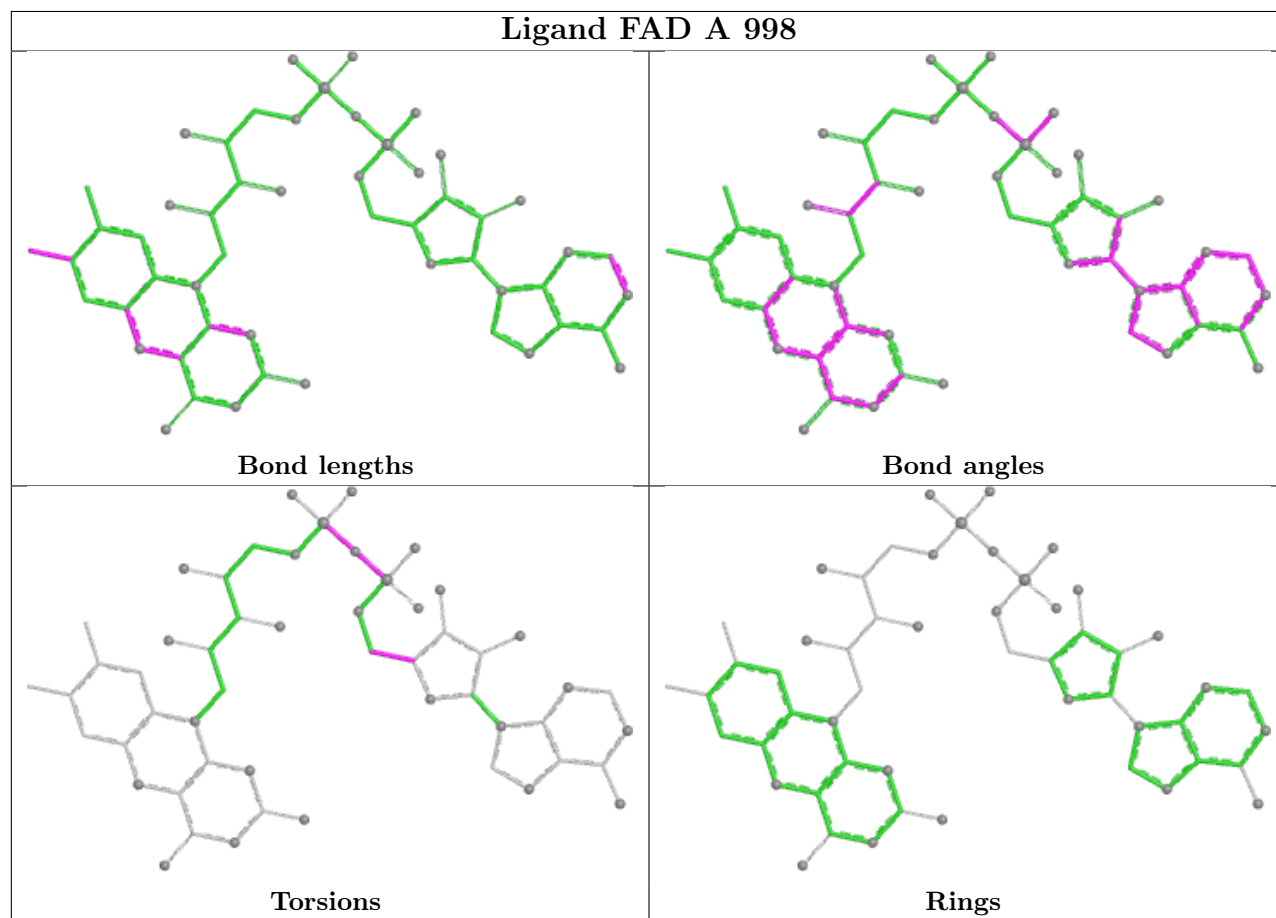
There are no ring outliers.

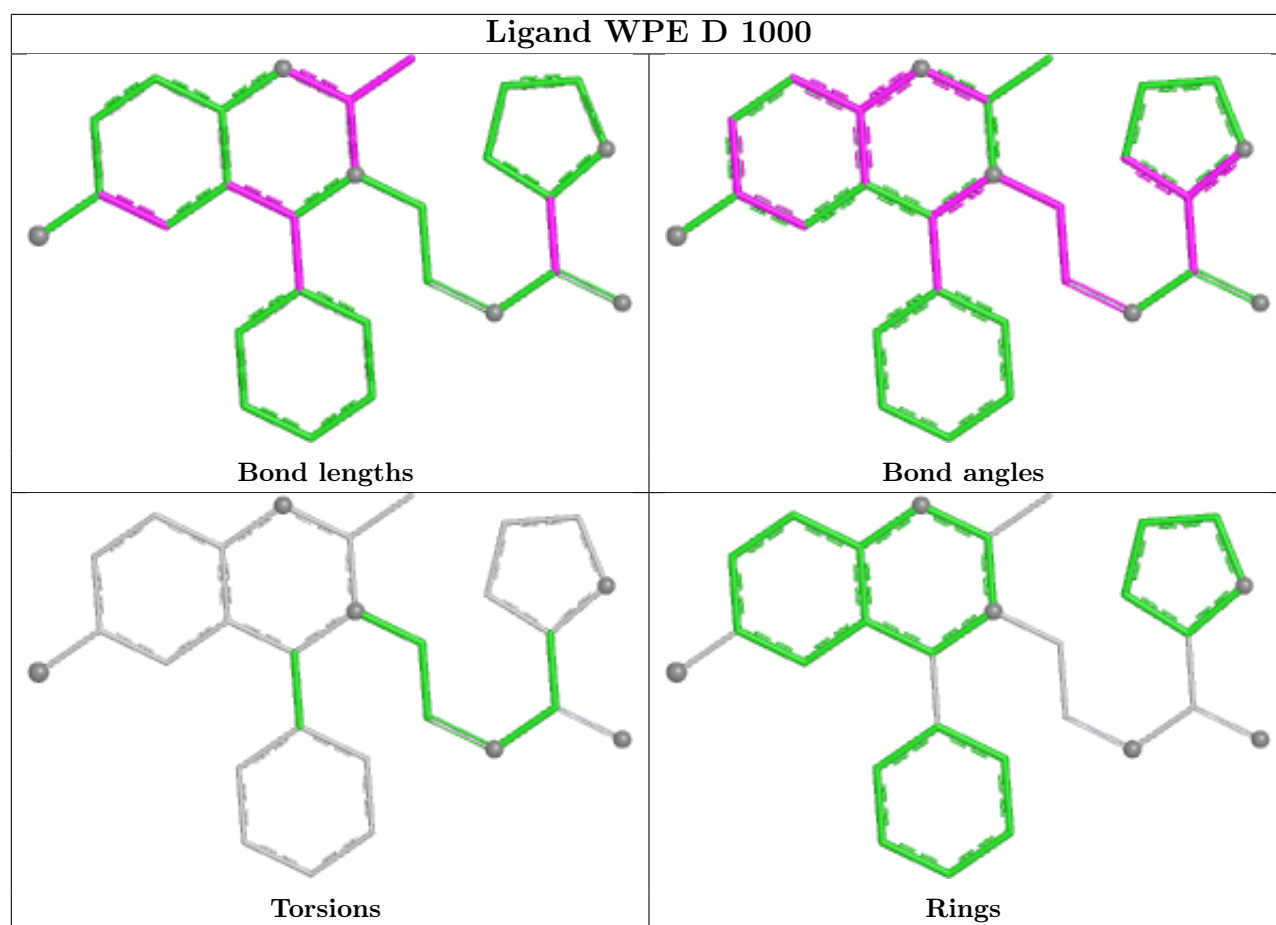
4 monomers are involved in 8 short contacts:

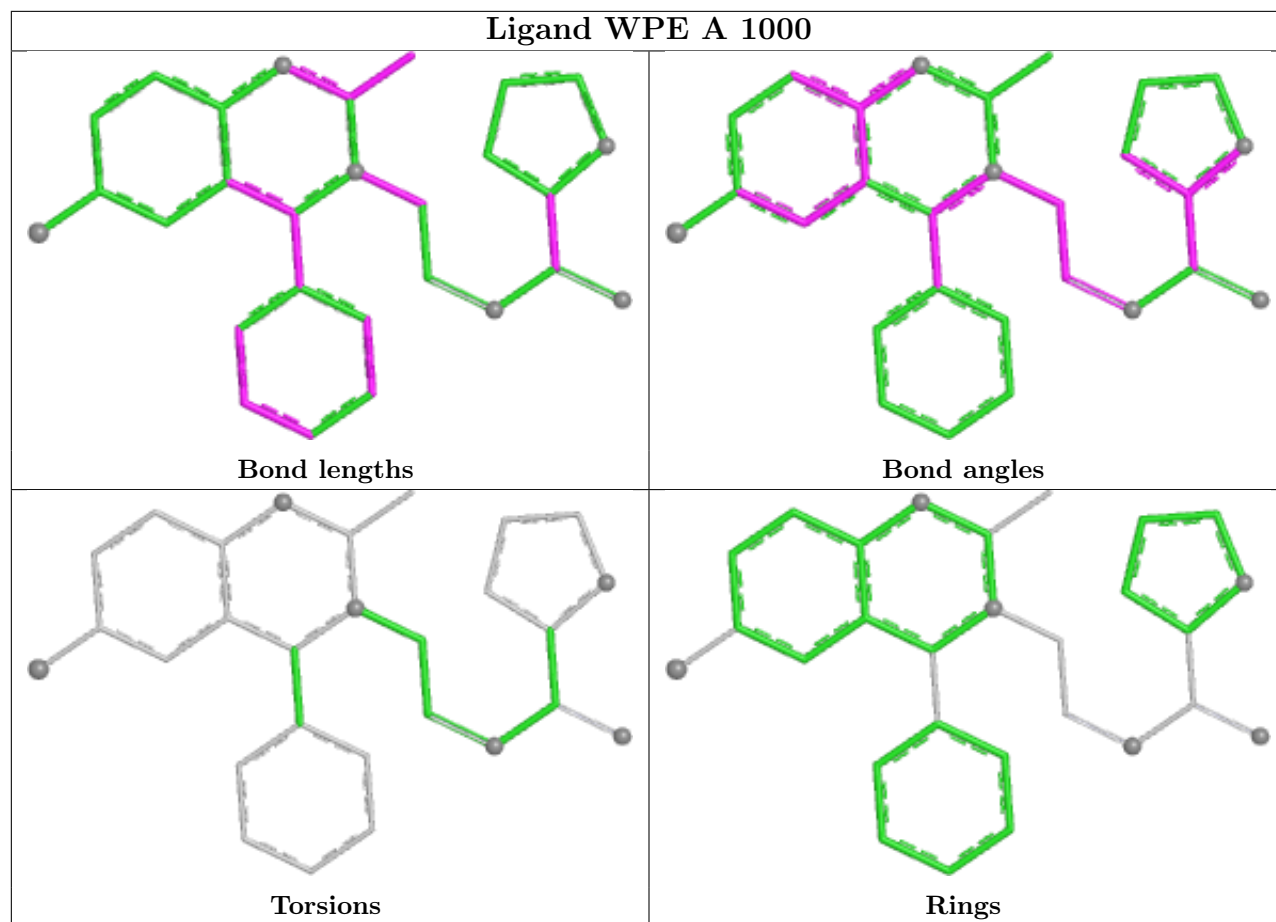
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	998	FAD	2	0
6	A	1494	MPD	2	0
3	C	1000	WPE	1	0
3	B	1000	WPE	3	0

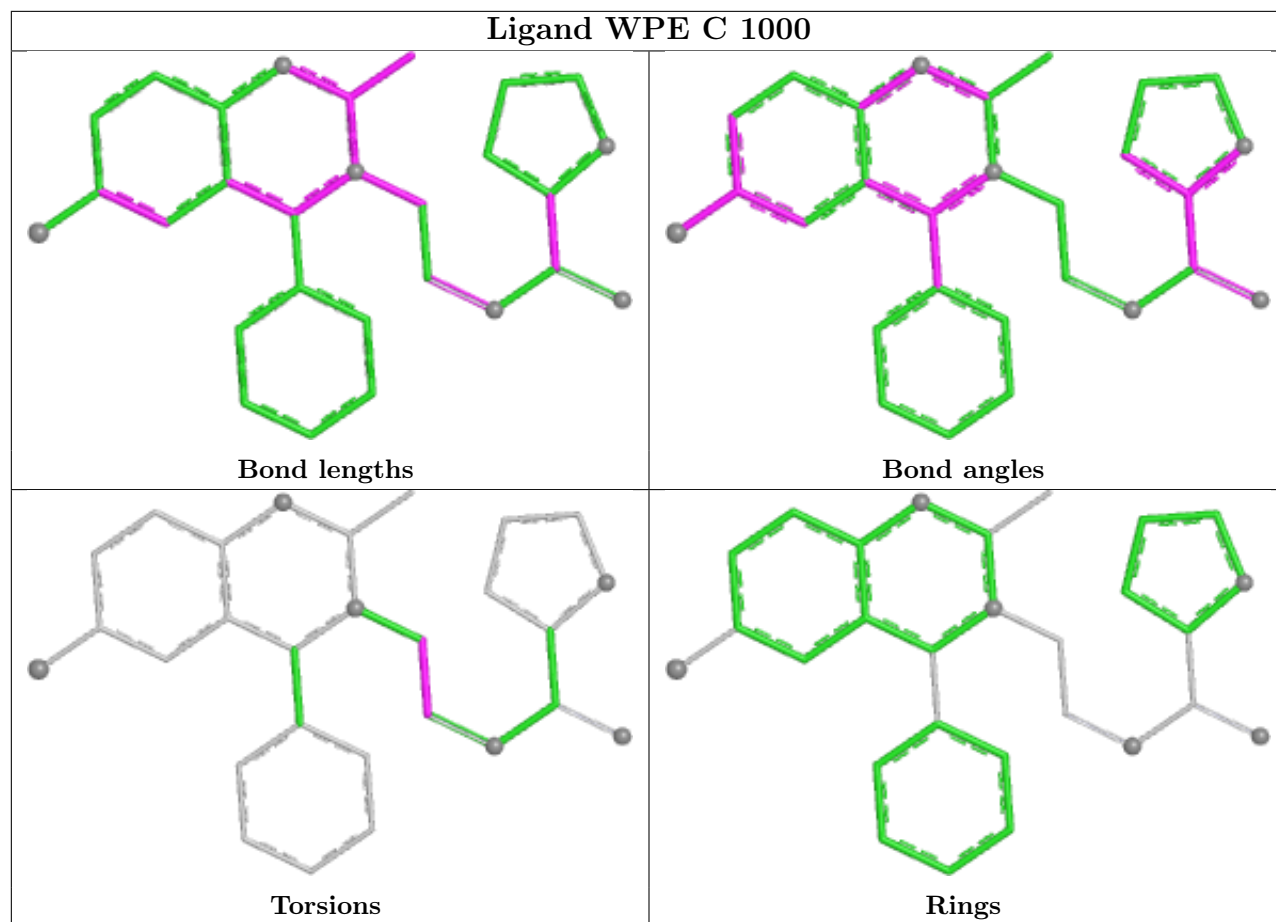
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

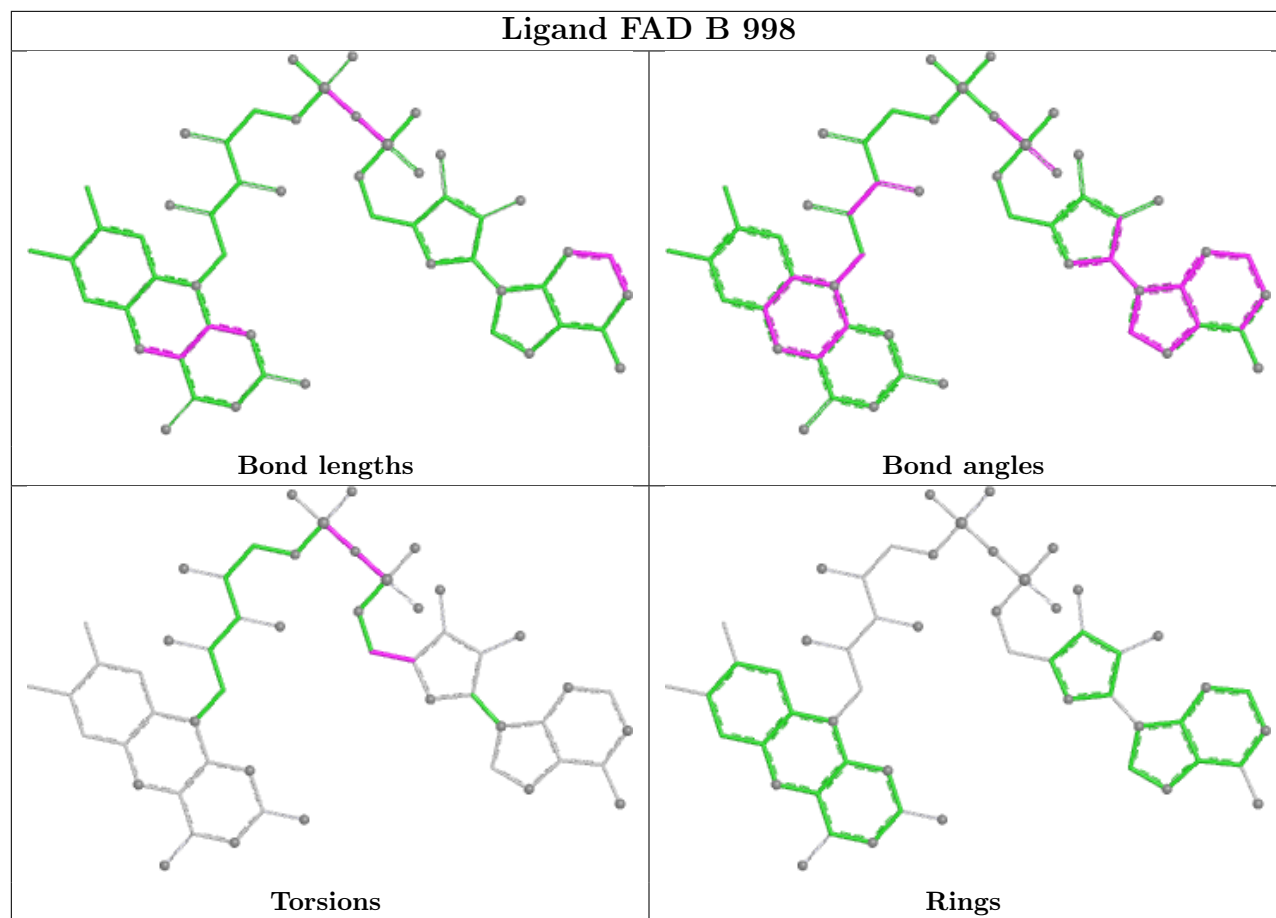
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

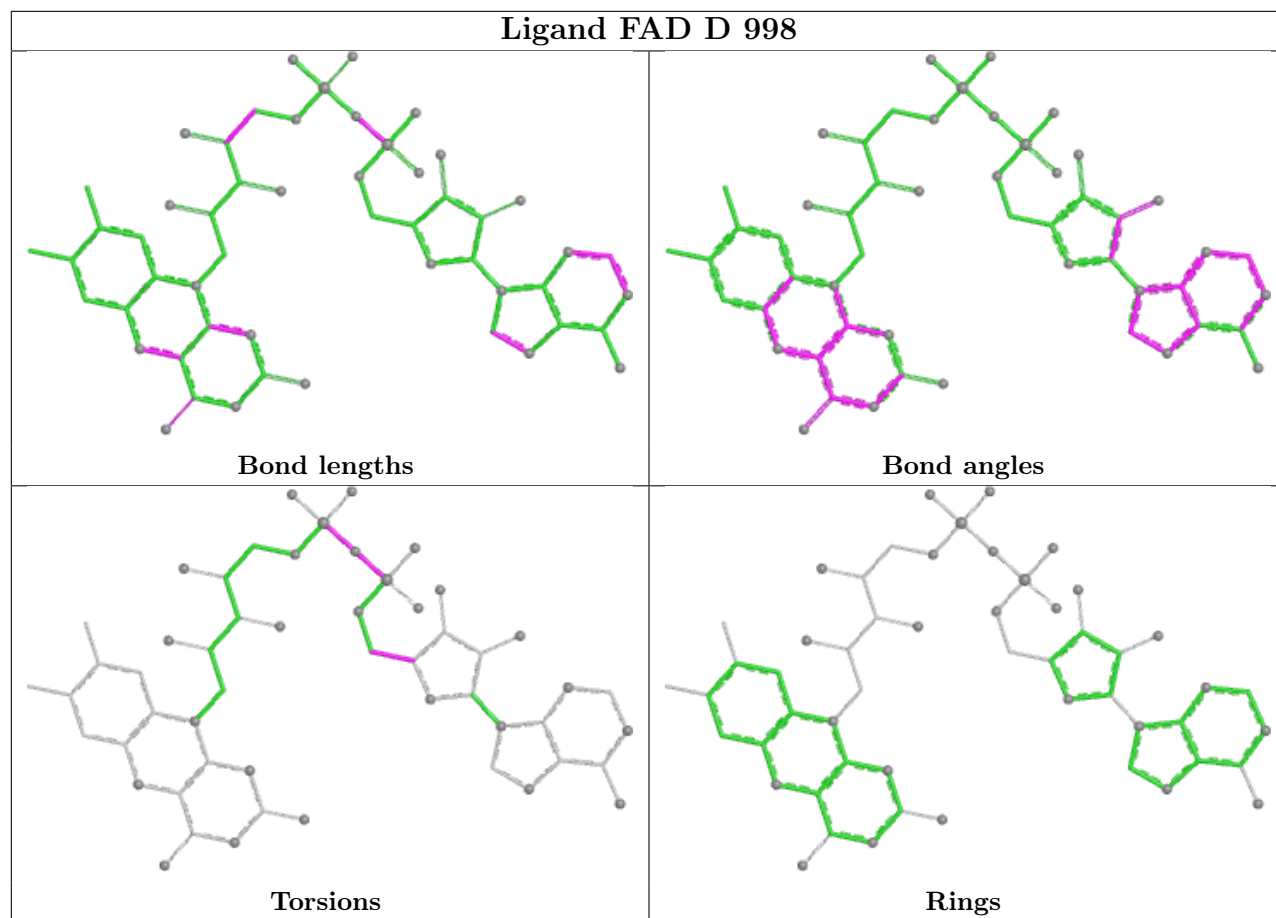


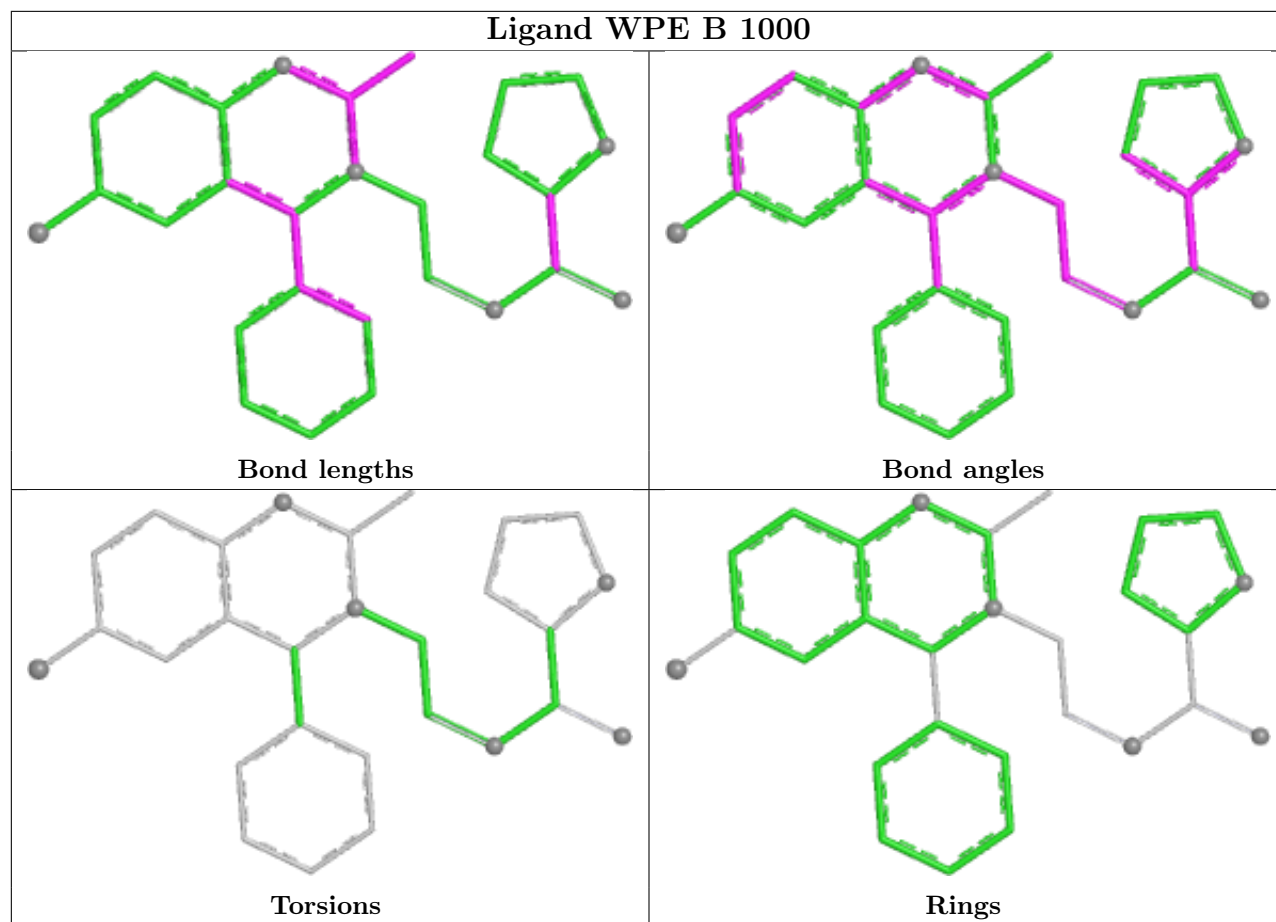


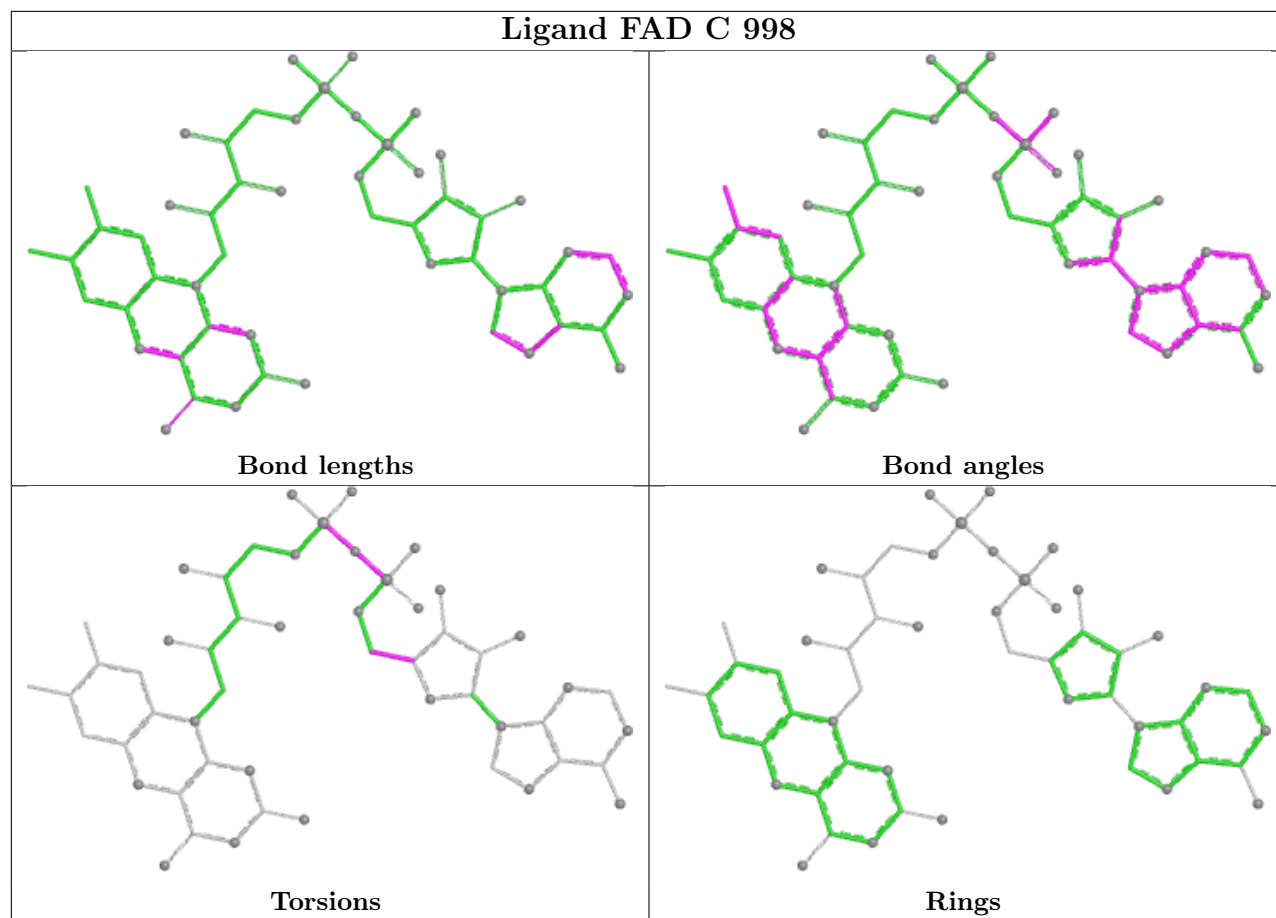












5.7 Other polymers [i](#)

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	490/495 (98%)	-0.67	0 100 100	12, 20, 36, 51	2 (0%)
1	B	486/495 (98%)	-0.19	8 (1%) 70 73	15, 27, 48, 60	2 (0%)
1	C	484/495 (97%)	-0.15	10 (2%) 63 66	14, 27, 56, 68	4 (0%)
1	D	489/495 (98%)	-0.59	1 (0%) 91 92	12, 23, 36, 56	4 (0%)
All	All	1949/1980 (98%)	-0.40	19 (0%) 79 81	12, 24, 49, 68	12 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	146	ALA	3.1
1	D	486	LYS	3.1
1	B	488	PRO	2.7
1	C	350	PHE	2.6
1	C	7	LEU	2.5
1	B	319	VAL	2.4
1	C	346	VAL	2.4
1	C	4	ALA	2.3
1	C	349	VAL	2.3
1	B	23	ALA	2.3
1	B	153	ALA	2.3
1	C	26	LEU	2.2
1	B	4	ALA	2.1
1	C	348	THR	2.1
1	B	28	GLY	2.1
1	B	350	PHE	2.1
1	C	8	VAL	2.1
1	C	345	LEU	2.0
1	C	32	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 95th 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	WPE	C	1000	28/28	0.87	0.14	40,49,82,83	0
6	MPD	A	1494	8/8	0.88	0.10	34,39,41,43	0
7	MRD	D	1492	8/8	0.91	0.10	39,42,44,44	0
3	WPE	B	1000	28/28	0.93	0.10	29,33,62,63	0
5	CL	B	1494	1/1	0.94	0.07	33,33,33,33	0
5	CL	D	1491	1/1	0.94	0.09	36,36,36,36	0
4	NA	B	1489	1/1	0.95	0.07	37,37,37,37	0
5	CL	B	1492	1/1	0.95	0.09	40,40,40,40	0
4	NA	A	1489	1/1	0.95	0.06	26,26,26,26	0
5	CL	C	1491	1/1	0.96	0.11	42,42,42,42	0
5	CL	D	1488	1/1	0.96	0.06	32,32,32,32	0
5	CL	D	1490	1/1	0.96	0.08	39,39,39,39	0
3	WPE	D	1000	28/28	0.96	0.08	17,25,60,61	0
4	NA	C	1487	1/1	0.96	0.04	26,26,26,26	0
5	CL	C	1488	1/1	0.96	0.07	39,39,39,39	0
2	FAD	B	998	53/53	0.97	0.06	15,24,37,39	0
2	FAD	C	998	53/53	0.97	0.05	16,26,36,38	0
3	WPE	A	1000	28/28	0.97	0.07	15,24,53,54	0
5	CL	B	1490	1/1	0.97	0.04	27,27,27,27	0
5	CL	C	1492	1/1	0.97	0.06	34,34,34,34	0
5	CL	A	1493	1/1	0.98	0.09	35,35,35,35	0
4	NA	D	1487	1/1	0.98	0.03	33,33,33,33	0
5	CL	C	1490	1/1	0.98	0.03	24,24,24,24	0
5	CL	A	1492	1/1	0.98	0.04	26,26,26,26	0
5	CL	B	1493	1/1	0.98	0.06	33,33,33,33	0
2	FAD	A	998	53/53	0.99	0.04	8,15,18,20	0
2	FAD	D	998	53/53	0.99	0.03	11,16,19,20	0

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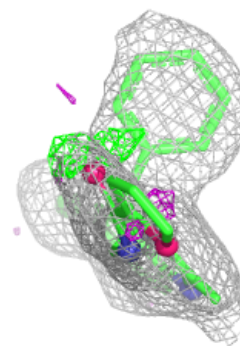
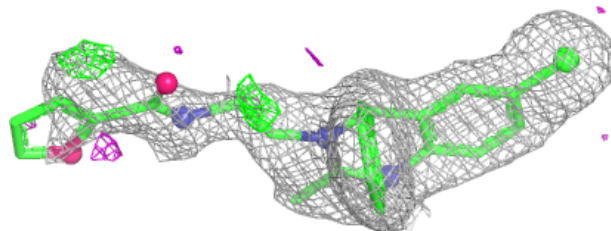
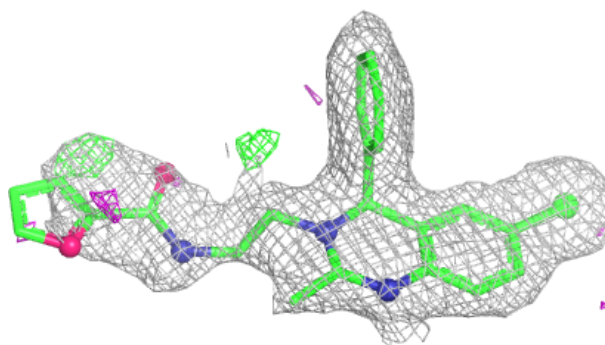
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	CL	D	1489	1/1	0.99	0.04	21,21,21,21	0
5	CL	A	1490	1/1	0.99	0.03	24,24,24,24	0
5	CL	C	1489	1/1	0.99	0.04	38,38,38,38	0
5	CL	B	1491	1/1	0.99	0.05	24,24,24,24	0
5	CL	A	1491	1/1	0.99	0.03	22,22,22,22	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.

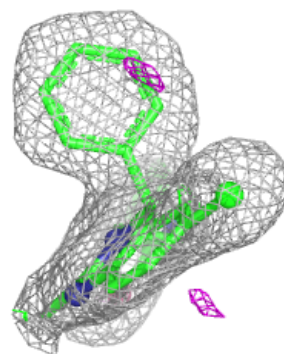
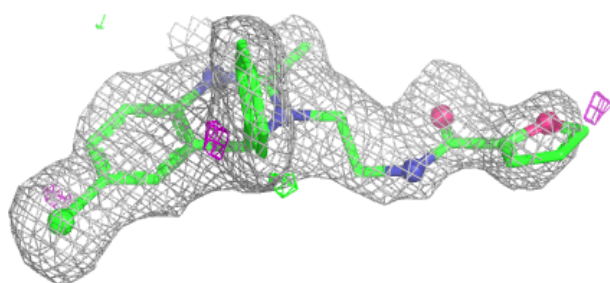
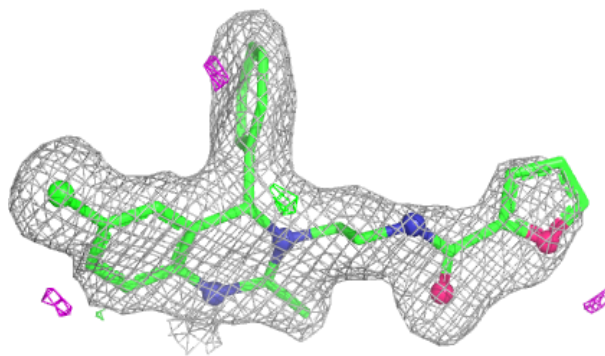
Electron density around WPE C 1000:

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

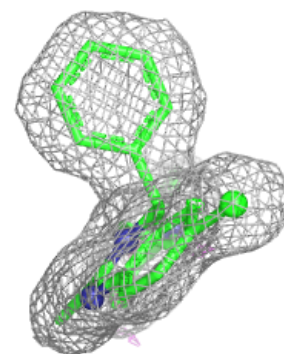
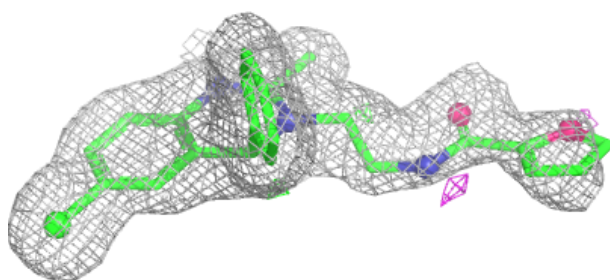
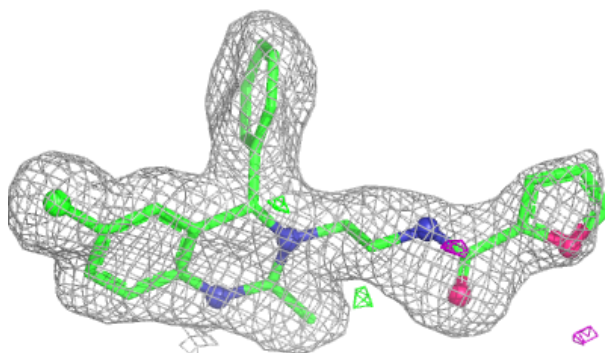


Electron density around WPE B 1000:

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

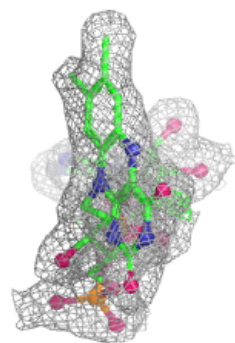
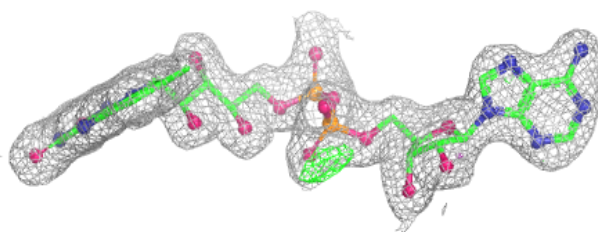
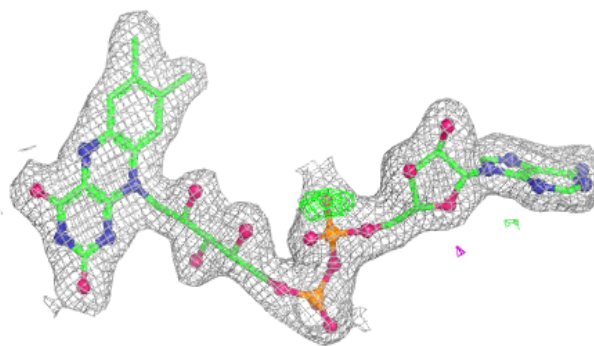
**Electron density around WPE D 1000:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

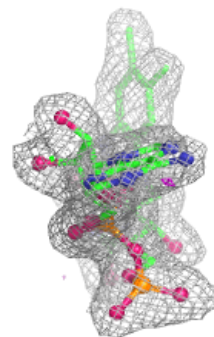
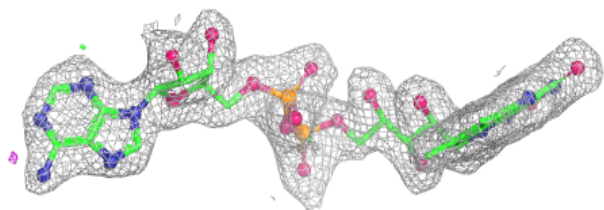
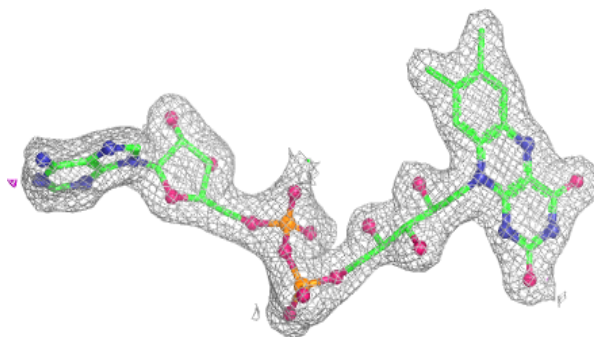


Electron density around FAD B 998:

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

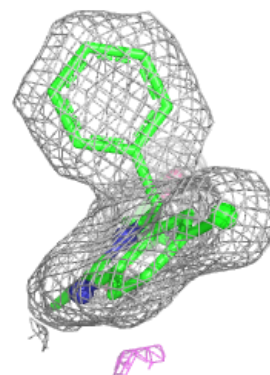
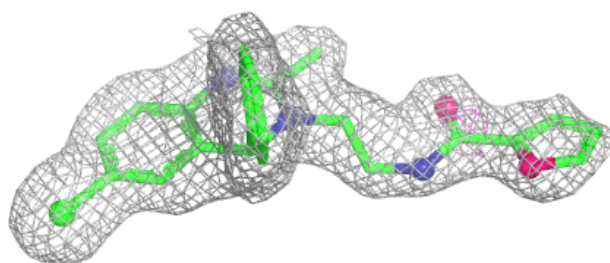
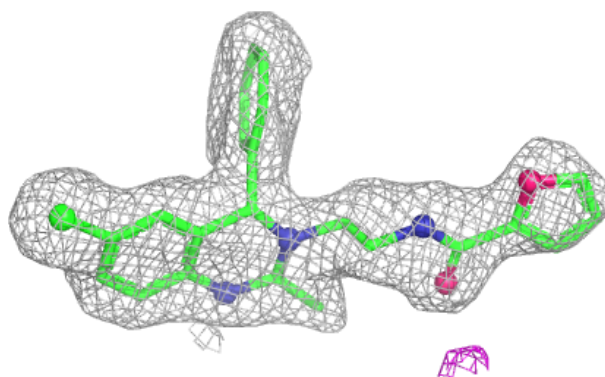
**Electron density around FAD C 998:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

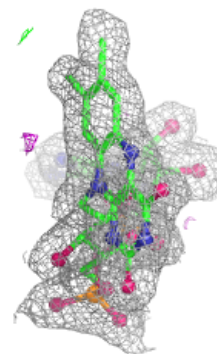
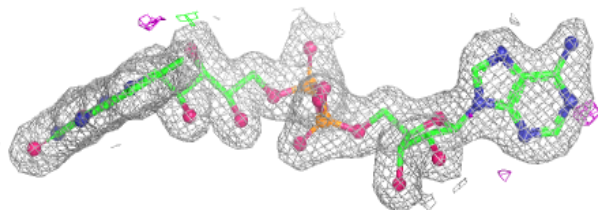
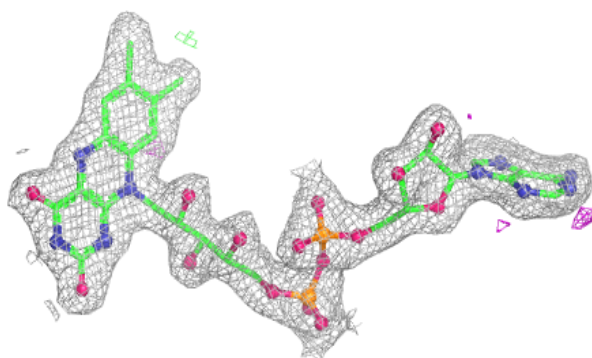


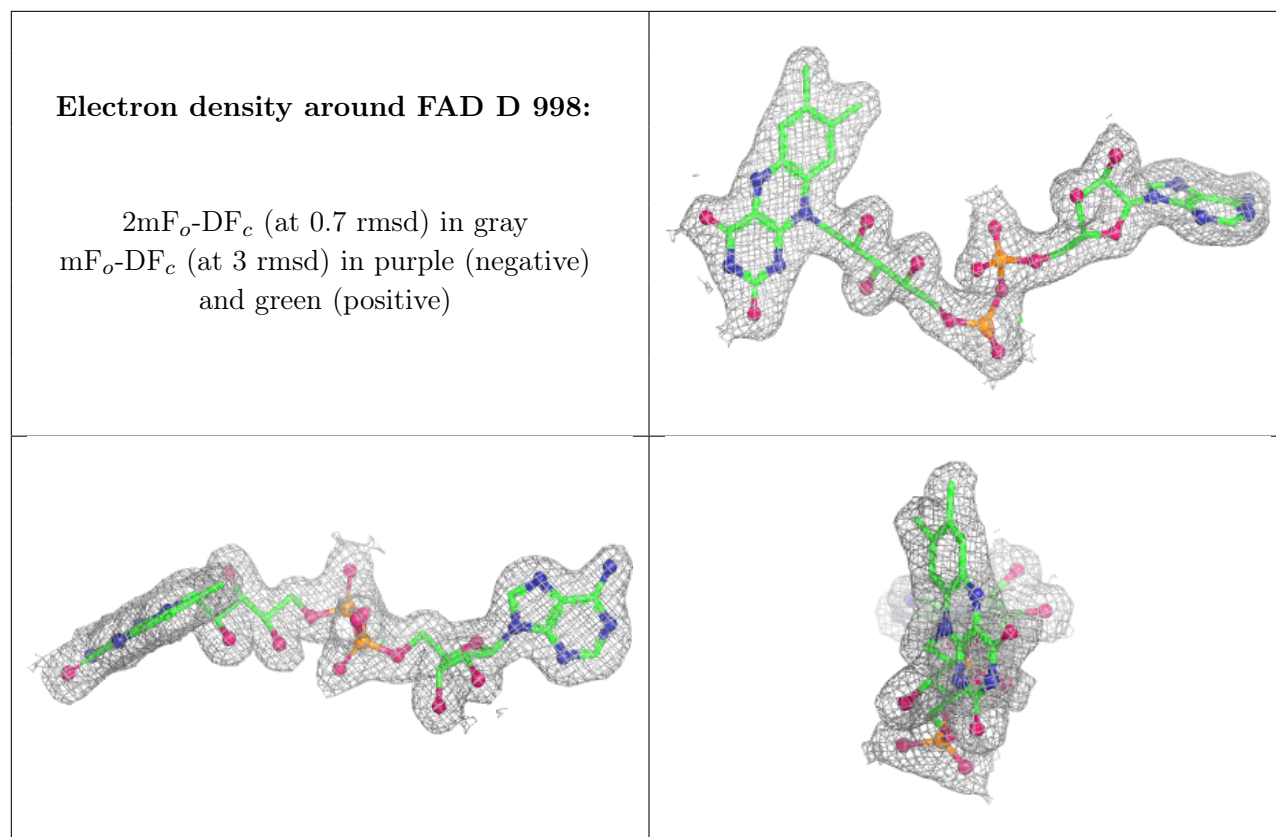
Electron density around WPE A 1000:

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

**Electron density around FAD A 998:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.