



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:49 AM UTC

PDB ID : 2W3R / pdb_00002w3r
Title : Crystal Structure of Xanthine Dehydrogenase (desulfo form) from Rhodobacter capsulatus in complex with hypoxanthine
Authors : Dietzel, U.; Kuper, J.; Leimkuhler, S.; Kisker, C.
Deposited on : 2008-11-14
Resolution : 2.90 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

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

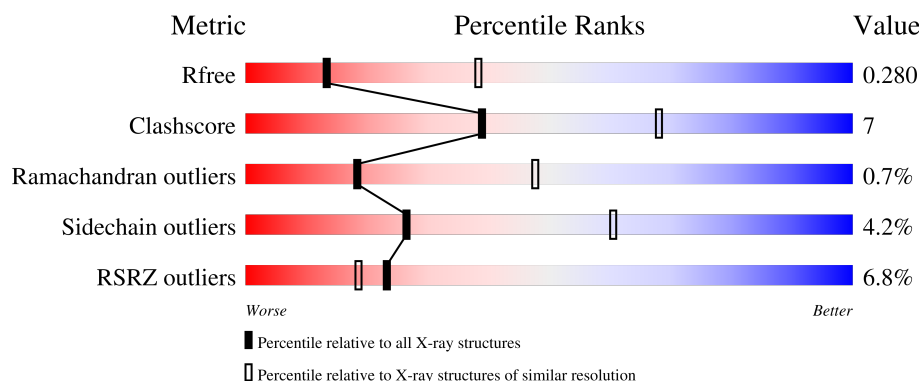
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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.



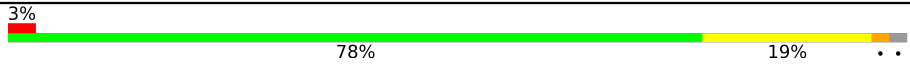
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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 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	462	13% 79% 18% .
1	C	462	20% 84% 13% ..
1	E	462	12% 78% 18% ..
1	G	462	13% 75% 21% ..
2	B	777	2% 82% 14% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	777	
2	F	777	
2	H	777	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MTE	B	1778	X	-	-	-
5	MTE	D	1778	X	-	-	-
5	MTE	F	1778	X	-	-	-
5	MTE	H	1778	X	-	-	-
8	MOM	B	1781	-	-	X	-
8	MOM	D	1781	-	-	X	-
8	MOM	F	1781	-	-	X	-
8	MOM	H	1781	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 36853 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 XANTHINE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	450	Total	C	N	O	S	0	0	0
			3376	2115	608	628	25			
1	C	450	Total	C	N	O	S	0	0	0
			3376	2115	608	628	25			
1	E	450	Total	C	N	O	S	0	0	0
			3376	2115	608	628	25			
1	G	450	Total	C	N	O	S	0	0	0
			3376	2115	608	628	25			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	TRP	LEU	conflict	UNP O54050
C	26	TRP	LEU	conflict	UNP O54050
E	26	TRP	LEU	conflict	UNP O54050
G	26	TRP	LEU	conflict	UNP O54050

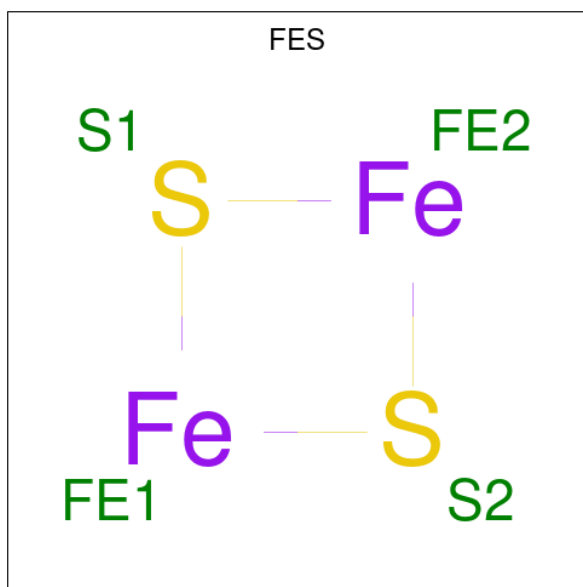
- Molecule 2 is a protein called XANTHINE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	760	Total	C	N	O	S	0	0	0
			5717	3581	1056	1054	26			
2	D	760	Total	C	N	O	S	0	0	0
			5717	3581	1056	1054	26			
2	F	760	Total	C	N	O	S	0	0	0
			5717	3581	1056	1054	26			
2	H	760	Total	C	N	O	S	0	0	0
			5717	3581	1056	1054	26			

There are 4 discrepancies between the modelled and reference sequences:

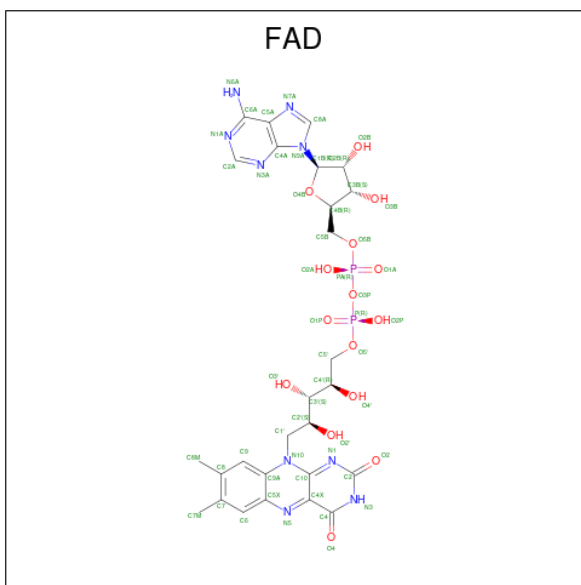
Chain	Residue	Modelled	Actual	Comment	Reference
B	772	ARG	GLY	conflict	UNP O54051
D	772	ARG	GLY	conflict	UNP O54051
F	772	ARG	GLY	conflict	UNP O54051
H	772	ARG	GLY	conflict	UNP O54051

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



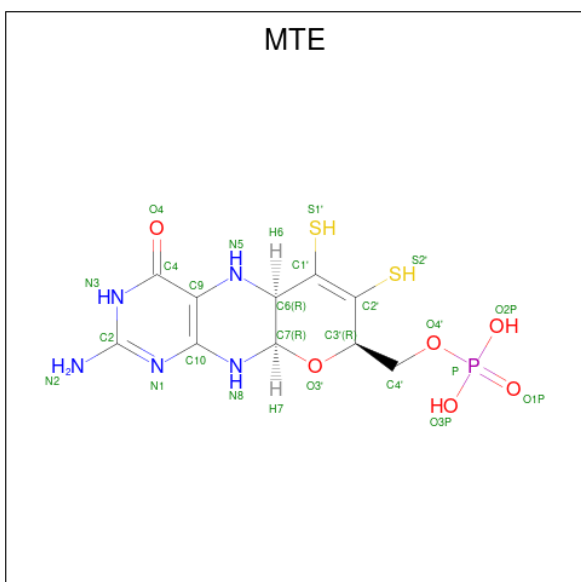
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	C	1	Total	Fe	S	0	0
			4	2	2		
3	C	1	Total	Fe	S	0	0
			4	2	2		
3	E	1	Total	Fe	S	0	0
			4	2	2		
3	E	1	Total	Fe	S	0	0
			4	2	2		
3	G	1	Total	Fe	S	0	0
			4	2	2		
3	G	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
4	C	1	Total 53	C 27	N 9	O 15	P 2	0	0
4	E	1	Total 53	C 27	N 9	O 15	P 2	0	0
4	G	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 5 is PHOSPHONIC ACIDMONO-(2-AMINO-5,6-DIMERCAPTO-4-OXO-3,7,8A, 9,10,10A-HEXAHYDRO-4H-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-7-YLMETHYL) ESTER (CCD ID: MTE) (formula: $C_{10}H_{14}N_5O_6PS_2$).

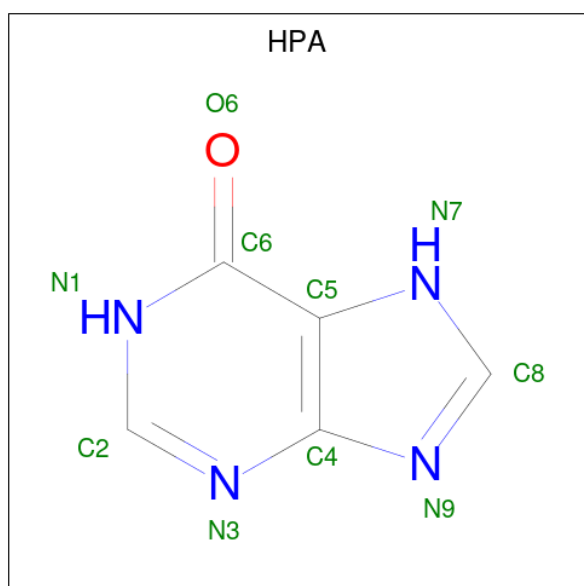


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	S	
			24	10	5	6	1	2	0
5	D	1	Total	C	N	O	P	S	
			24	10	5	6	1	2	0
5	F	1	Total	C	N	O	P	S	
			24	10	5	6	1	2	0
5	H	1	Total	C	N	O	P	S	
			24	10	5	6	1	2	0

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Ca	0	0
			1	1		
6	D	1	Total	Ca	0	0
			1	1		
6	F	1	Total	Ca	0	0
			1	1		
6	H	1	Total	Ca	0	0
			1	1		

- Molecule 7 is HYPOXANTHINE (CCD ID: HPA) (formula: C₅H₄N₄O).



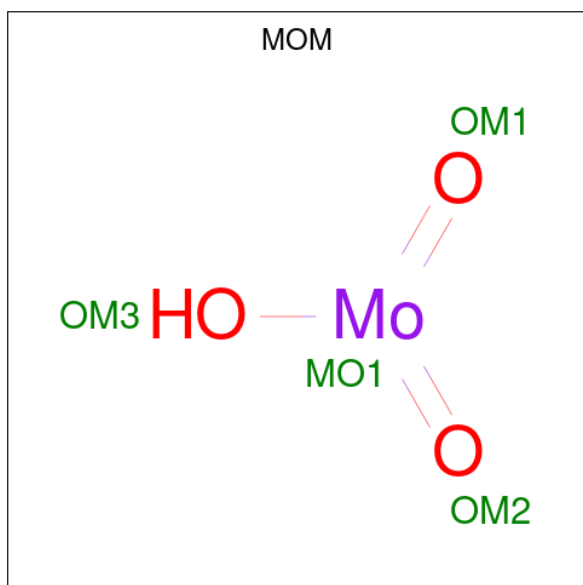
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			10	5	4	1		
7	D	1	Total	C	N	O	0	0
			10	5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	F	1	Total	C	N	O	0	0
			10	5	4	1		
7	H	1	Total	C	N	O	0	0
			10	5	4	1		

- Molecule 8 is HYDROXY(DIOXO)MOLYBDENUM (CCD ID: MOM) (formula: HMoO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Mo	O	0	0
			4	1	3		
8	D	1	Total	Mo	O	0	0
			4	1	3		
8	F	1	Total	Mo	O	0	0
			4	1	3		
8	H	1	Total	Mo	O	0	0
			4	1	3		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	6	Total	O	0	0
			6	6		
9	B	15	Total	O	0	0
			15	15		
9	C	10	Total	O	0	0
			10	10		

Continued on next page...

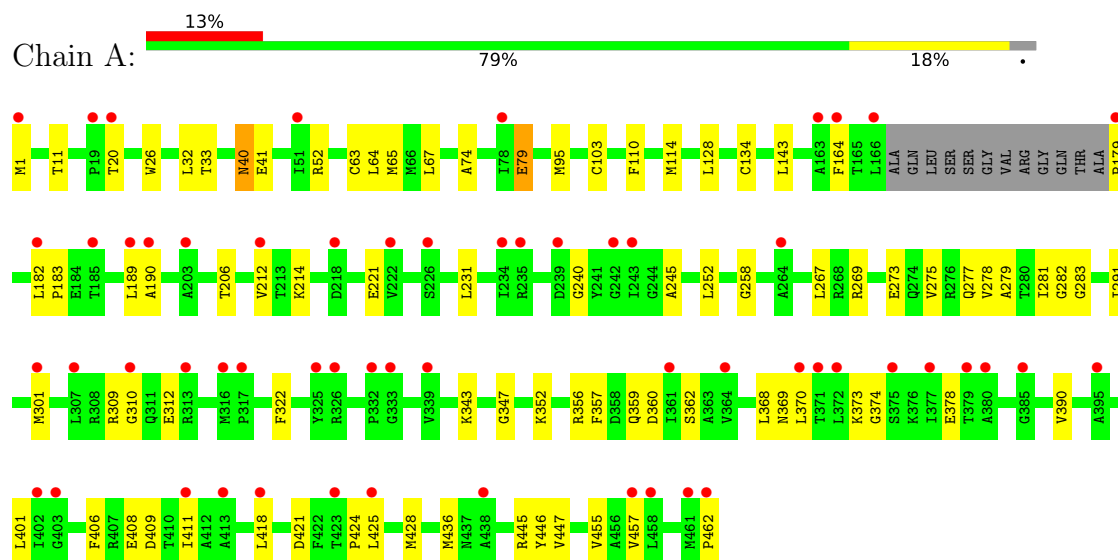
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	16	Total 16	O 16	0	0
9	E	2	Total 2	O 2	0	0
9	F	11	Total 11	O 11	0	0
9	G	5	Total 5	O 5	0	0
9	H	16	Total 16	O 16	0	0

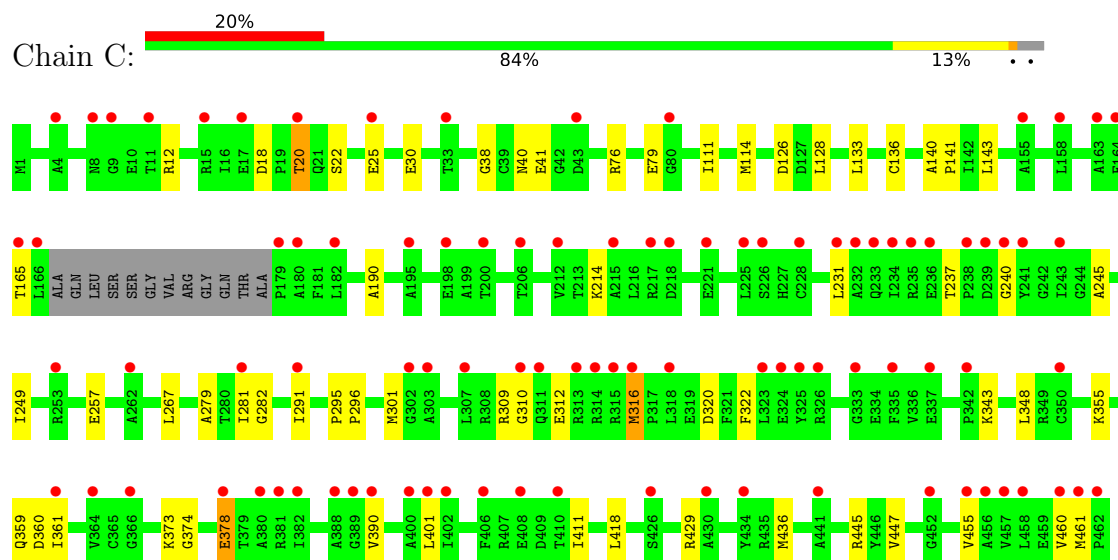
3 Residue-property plots [i](#)

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.

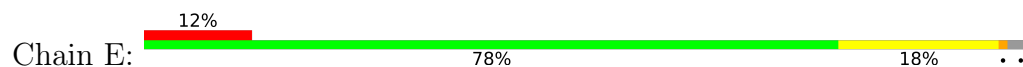
• Molecule 1: XANTHINE DEHYDROGENASE

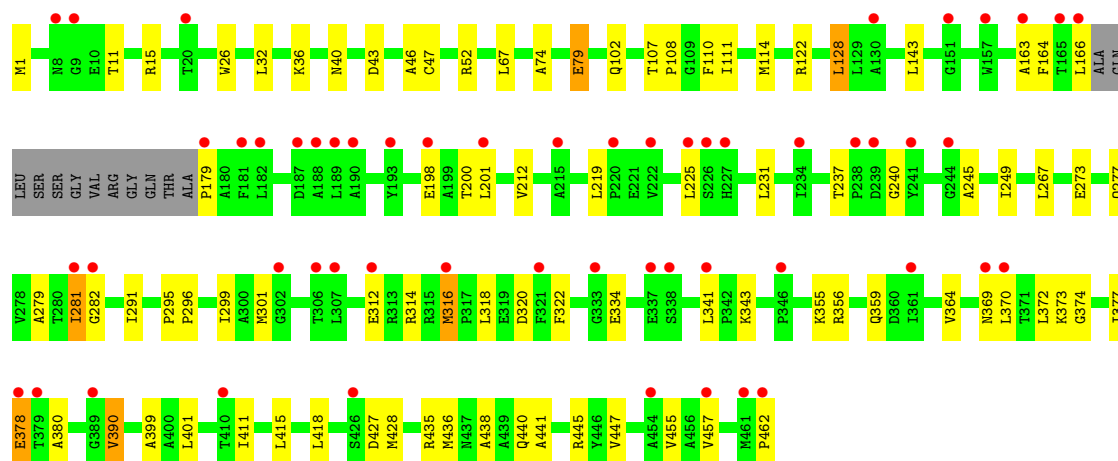


• Molecule 1: XANTHINE DEHYDROGENASE

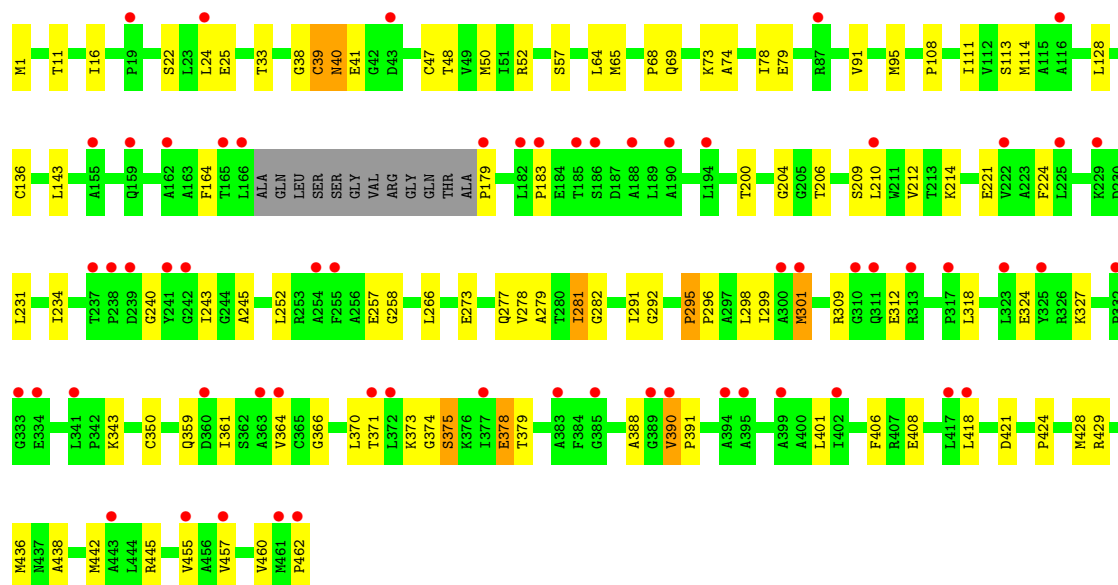
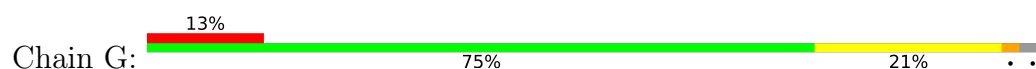


• Molecule 1: XANTHINE DEHYDROGENASE

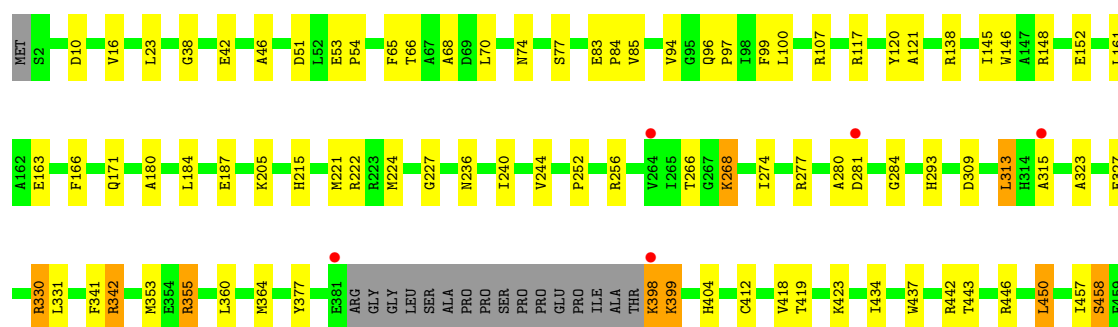
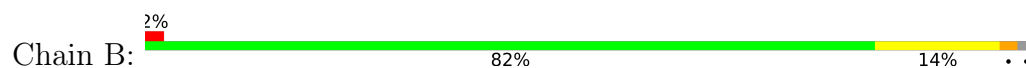


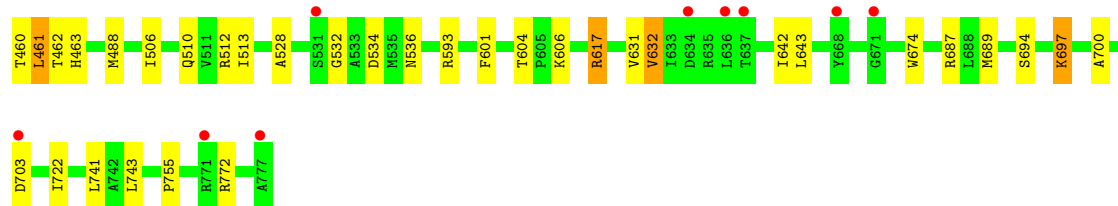


• Molecule 1: XANTHINE DEHYDROGENASE

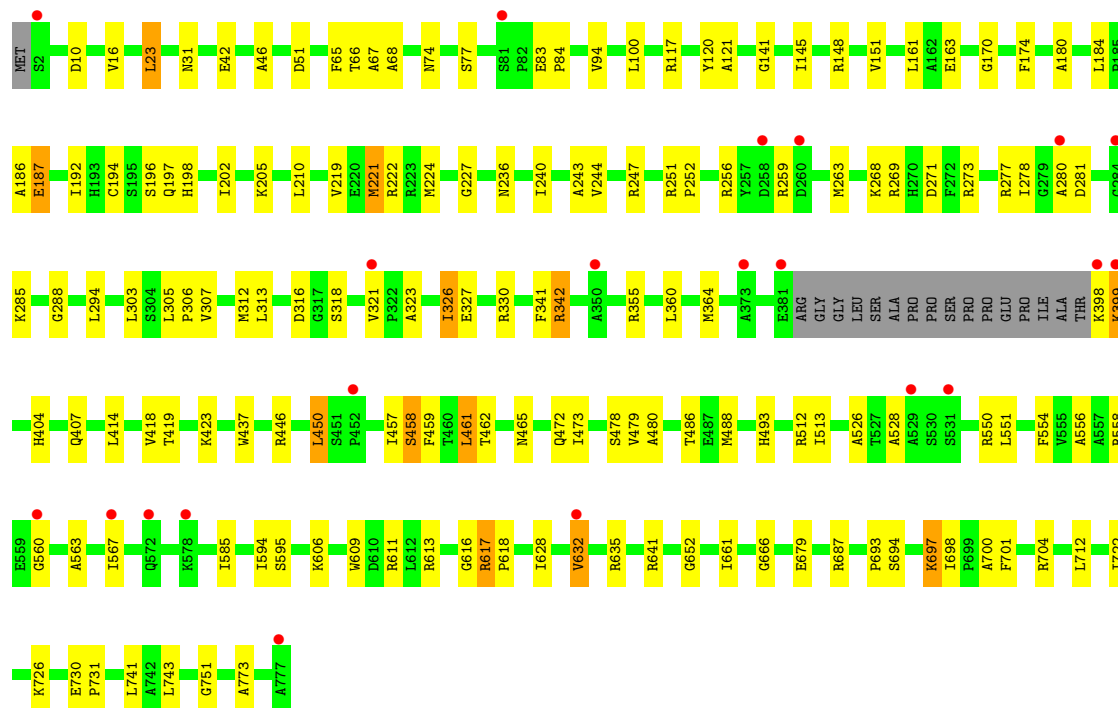
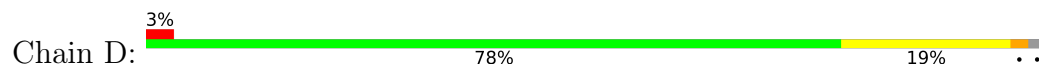


• Molecule 2: XANTHINE DEHYDROGENASE

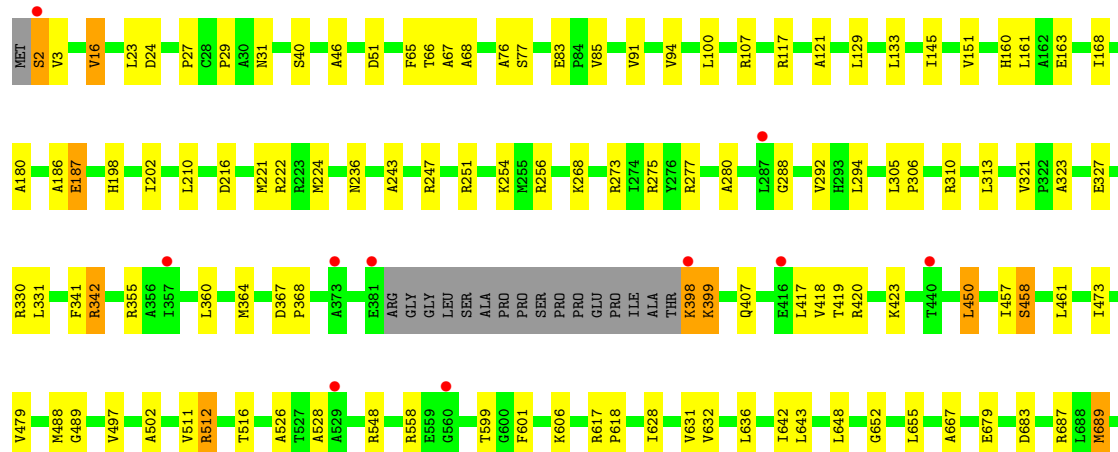
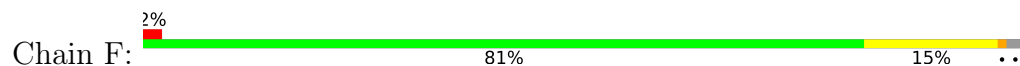


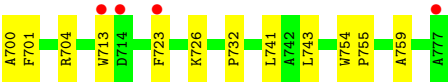


● Molecule 2: XANTHINE DEHYDROGENASE

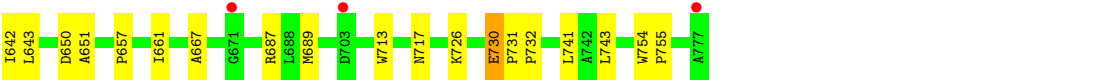
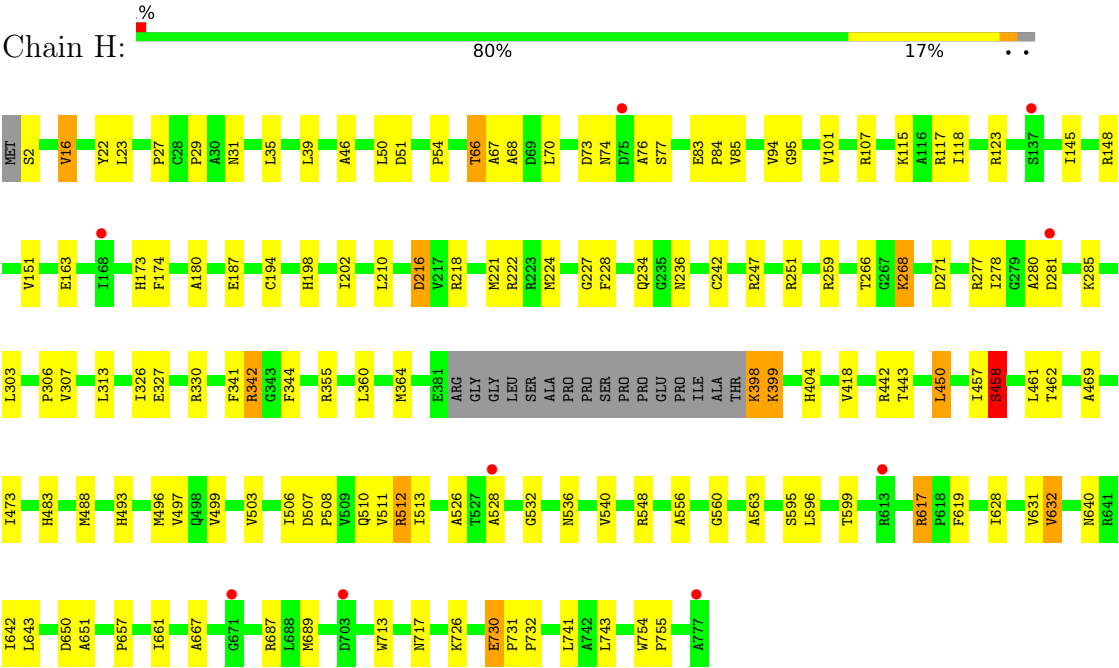


● Molecule 2: XANTHINE DEHYDROGENASE





● Molecule 2: XANTHINE DEHYDROGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	92.77Å 139.94Å 158.04Å 109.33° 106.15° 101.05°	Depositor
Resolution (Å)	51.23 – 2.90 51.23 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.2 (51.23-2.90) 98.2 (51.23-2.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.5.0055	Depositor
R, R_{free}	0.240 , 0.281 0.240 , 0.280	Depositor DCC
R_{free} test set	7476 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	53.6	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	36853	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.80% 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: CA, MOM, FAD, HPA, FES, MTE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.44	0/3439	0.81	2/4659 (0.0%)
1	C	0.43	0/3439	0.79	0/4659
1	E	0.45	0/3439	0.81	0/4659
1	G	0.46	0/3439	0.81	3/4659 (0.1%)
2	B	0.44	0/5845	0.81	1/7942 (0.0%)
2	D	0.42	0/5845	0.81	1/7942 (0.0%)
2	F	0.43	0/5845	0.80	0/7942
2	H	0.45	0/5845	0.81	1/7942 (0.0%)
All	All	0.44	0/37136	0.81	8/50404 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	462	THR	N-CA-C	6.22	119.04	111.82
2	H	462	THR	N-CA-C	5.85	118.41	111.33
2	B	462	THR	N-CA-C	5.69	117.48	111.28
1	G	258	GLY	CA-C-N	5.56	125.03	119.24
1	G	258	GLY	C-N-CA	5.56	125.03	119.24
1	G	295	PRO	N-CA-C	5.39	117.28	110.70
1	A	258	GLY	CA-C-N	5.07	124.51	119.24
1	A	258	GLY	C-N-CA	5.07	124.51	119.24

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	3376	0	3367	47	0
1	C	3376	0	3367	36	0
1	E	3376	0	3367	50	0
1	G	3376	0	3367	60	0
2	B	5717	0	5631	67	0
2	D	5717	0	5630	92	0
2	F	5717	0	5631	77	0
2	H	5717	0	5631	85	0
3	A	8	0	0	0	0
3	C	8	0	0	0	0
3	E	8	0	0	0	0
3	G	8	0	0	1	0
4	A	53	0	31	5	0
4	C	53	0	31	3	0
4	E	53	0	31	3	0
4	G	53	0	31	4	0
5	B	24	0	8	1	0
5	D	24	0	8	1	0
5	F	24	0	8	1	0
5	H	24	0	8	2	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
6	H	1	0	0	0	0
7	B	10	0	4	2	0
7	D	10	0	4	1	0
7	F	10	0	4	1	0
7	H	10	0	4	0	0
8	B	4	0	0	2	0
8	D	4	0	0	2	0
8	F	4	0	0	2	0
8	H	4	0	0	2	0
9	A	6	0	0	0	0
9	B	15	0	0	1	0
9	C	10	0	0	1	0
9	D	16	0	0	0	0
9	E	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	F	11	0	0	0	0
9	G	5	0	0	0	0
9	H	16	0	0	1	0
All	All	36853	0	36163	494	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 (494) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ALA:HB1	1:A:310:GLY:HA2	1.53	0.91
1:A:445:ARG:HG3	1:A:455:VAL:HG11	1.56	0.86
2:F:31:ASN:HB2	2:F:251:ARG:HD3	1.62	0.82
1:G:136:CYS:HB2	3:G:1463:FES:S2	2.21	0.81
1:E:445:ARG:HG3	1:E:455:VAL:HG11	1.61	0.80
1:C:445:ARG:HG3	1:C:455:VAL:HG11	1.64	0.80
2:F:221:MET:HE2	2:F:224:MET:HE2	1.66	0.78
1:C:240:GLY:HA2	1:C:343:LYS:HG2	1.65	0.78
2:D:94:VAL:HG11	2:D:687:ARG:HG2	1.66	0.77
2:B:205:LYS:HG3	2:B:236:ASN:OD1	1.85	0.76
1:A:359:GLN:HE22	4:A:1465:FAD:H6	1.49	0.75
2:F:94:VAL:HG11	2:F:687:ARG:HG2	1.66	0.75
1:G:240:GLY:HA2	1:G:343:LYS:HG2	1.71	0.73
1:E:32:LEU:HD22	1:E:79:GLU:HG3	1.69	0.72
2:F:65:PHE:HB2	2:F:100:LEU:HB3	1.71	0.72
2:B:94:VAL:HG11	2:B:687:ARG:HG2	1.72	0.72
1:C:411:ILE:HG13	1:C:447:VAL:HG21	1.71	0.72
2:H:163:GLU:HG2	2:H:277:ARG:HG2	1.72	0.72
1:A:41:GLU:HG3	1:A:214:LYS:HE3	1.70	0.71
2:B:224:MET:HE3	2:B:488:MET:HB3	1.72	0.71
2:B:399:LYS:HD2	2:B:399:LYS:H	1.54	0.71
1:G:445:ARG:HG3	1:G:455:VAL:HG11	1.72	0.70
2:F:360:LEU:HG	2:F:364:MET:HE3	1.73	0.70
2:D:606:LYS:O	2:D:617:ARG:HD2	1.92	0.69
2:D:163:GLU:HG2	2:D:277:ARG:HG2	1.74	0.69
1:E:295:PRO:HB2	1:E:296:PRO:HD3	1.75	0.69
2:F:145:ILE:HG12	2:F:327:GLU:HG3	1.75	0.69
2:D:74:ASN:O	2:D:84:PRO:HA	1.92	0.68
1:A:373:LYS:HB2	1:A:378:GLU:HG3	1.76	0.68
1:A:322:PHE:HB3	1:A:390:VAL:HG23	1.77	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:407:GLN:OE1	2:D:618:PRO:HD2	1.95	0.67
2:H:148:ARG:HD2	2:H:404:HIS:HA	1.76	0.67
2:H:173:HIS:HA	2:H:341:PHE:CZ	2.30	0.67
1:A:309:ARG:HB3	1:A:312:GLU:HB2	1.76	0.66
2:F:51:ASP:HB3	2:F:117:ARG:HB2	1.78	0.66
1:C:359:GLN:O	1:C:359:GLN:HG3	1.94	0.66
2:D:360:LEU:HG	2:D:364:MET:HE3	1.77	0.66
2:F:163:GLU:HG2	2:F:277:ARG:HG2	1.77	0.66
1:G:428:MET:HE3	2:H:689:MET:HB3	1.76	0.65
2:B:528:ALA:HA	5:B:1778:MTE:S2'	2.37	0.65
8:B:1781:MOM:MO1	8:B:1781:MOM:OM1	1.68	0.65
2:B:274:ILE:HG12	2:B:293:HIS:HD2	1.63	0.64
8:F:1781:MOM:OM1	8:F:1781:MOM:MO1	1.68	0.64
2:B:148:ARG:HD2	2:B:404:HIS:HA	1.80	0.64
2:F:399:LYS:H	2:F:399:LYS:HD2	1.62	0.64
2:H:399:LYS:H	2:H:399:LYS:HD2	1.62	0.63
8:H:1781:MOM:OM1	8:H:1781:MOM:MO1	1.70	0.63
2:H:457:ILE:O	2:H:458:SER:HB2	1.98	0.63
2:D:224:MET:HE3	2:D:488:MET:HB3	1.81	0.63
8:D:1781:MOM:OM1	8:D:1781:MOM:MO1	1.69	0.63
2:H:51:ASP:HB3	2:H:117:ARG:HB2	1.81	0.63
2:H:280:ALA:HB2	2:H:360:LEU:HD21	1.80	0.62
8:H:1781:MOM:MO1	8:H:1781:MOM:OM3	1.70	0.62
2:F:27:PRO:HB2	2:H:29:PRO:HG3	1.82	0.62
2:H:224:MET:HE3	2:H:488:MET:HB3	1.81	0.62
1:C:41:GLU:HG3	1:C:214:LYS:HE3	1.80	0.62
2:D:419:THR:O	2:D:423:LYS:HG2	1.98	0.62
2:H:66:THR:HG22	2:H:68:ALA:H	1.63	0.62
1:A:428:MET:HE3	2:B:689:MET:HB3	1.81	0.62
2:F:280:ALA:HB2	2:F:360:LEU:HD21	1.81	0.62
8:F:1781:MOM:MO1	8:F:1781:MOM:OM3	1.70	0.62
1:A:240:GLY:HA2	1:A:343:LYS:HG2	1.82	0.61
2:F:3:VAL:HG13	2:F:655:LEU:HD23	1.80	0.61
1:G:299:ILE:HG13	1:G:318:LEU:HD23	1.82	0.61
8:B:1781:MOM:MO1	8:B:1781:MOM:OM3	1.70	0.61
1:G:279:ALA:HB1	4:G:1465:FAD:H4'	1.82	0.61
1:C:401:LEU:HD11	1:C:411:ILE:HD13	1.82	0.61
2:F:473:ILE:HG12	2:F:479:VAL:HG22	1.82	0.61
1:A:1:MET:HE1	1:A:182:LEU:HD13	1.82	0.61
1:A:269:ARG:HH21	1:A:357:PHE:HA	1.66	0.61
1:G:460:VAL:HG11	2:H:632:VAL:HG11	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:418:VAL:HG13	2:D:450:LEU:HD11	1.83	0.61
1:A:11:THR:HG22	1:A:164:PHE:HE1	1.66	0.60
8:D:1781:MOM:MO1	8:D:1781:MOM:OM3	1.70	0.60
1:C:279:ALA:HB1	4:C:1465:FAD:H4'	1.82	0.60
1:G:374:GLY:O	1:G:375:SER:HB3	2.00	0.60
1:E:279:ALA:HB1	4:E:1465:FAD:H4'	1.84	0.60
2:H:23:LEU:HD13	2:H:194:CYS:HA	1.84	0.60
2:D:399:LYS:H	2:D:399:LYS:HD2	1.67	0.59
2:D:528:ALA:HA	5:D:1778:MTE:S2'	2.43	0.59
1:G:418:LEU:HA	1:G:421:ASP:HB2	1.85	0.59
1:E:356:ARG:HH21	1:E:359:GLN:HB3	1.68	0.59
1:C:237:THR:HG23	1:C:240:GLY:H	1.66	0.59
2:D:174:PHE:HZ	2:D:693:PRO:HG3	1.68	0.59
2:B:66:THR:HG22	2:B:68:ALA:H	1.67	0.59
2:H:77:SER:HB2	2:H:83:GLU:HB3	1.84	0.59
1:G:22:SER:OG	1:G:25:GLU:HG2	2.02	0.58
1:C:373:LYS:HB2	1:C:378:GLU:CG	2.34	0.58
1:G:371:THR:HB	1:G:379:THR:H	1.69	0.58
2:D:51:ASP:HB3	2:D:117:ARG:HB2	1.86	0.58
2:D:661:ILE:HD11	2:D:712:LEU:HG	1.84	0.58
2:F:683:ASP:HB3	2:F:689:MET:CE	2.33	0.58
2:D:23:LEU:HD22	2:D:180:ALA:HB1	1.85	0.58
2:H:218:ARG:HD2	9:H:2009:HOH:O	2.04	0.58
1:A:52:ARG:HB3	1:A:74:ALA:HB3	1.86	0.58
2:B:74:ASN:O	2:B:84:PRO:HA	2.04	0.58
2:B:281:ASP:HB3	2:B:284:GLY:H	1.69	0.57
1:E:418:LEU:HB3	1:E:436:MET:HE1	1.87	0.57
2:B:360:LEU:HG	2:B:364:MET:HE3	1.86	0.57
1:A:252:LEU:HD23	1:A:267:LEU:HD11	1.87	0.57
2:H:398:LYS:HA	2:H:398:LYS:HE3	1.84	0.57
2:B:755:PRO:O	2:B:772:ARG:HD2	2.05	0.56
2:F:31:ASN:HB2	2:F:251:ARG:CD	2.33	0.56
1:E:240:GLY:HA2	1:E:343:LYS:HG2	1.87	0.56
2:F:407:GLN:OE1	2:F:618:PRO:HD2	2.05	0.56
1:G:373:LYS:HB2	1:G:378:GLU:CG	2.36	0.56
2:F:288:GLY:HA2	2:F:323:ALA:O	2.05	0.56
2:D:280:ALA:HB2	2:D:360:LEU:HD21	1.87	0.56
1:C:445:ARG:HG3	1:C:455:VAL:CG1	2.34	0.56
1:G:41:GLU:HG3	1:G:214:LYS:HE3	1.87	0.56
1:A:418:LEU:HA	1:A:421:ASP:HB2	1.87	0.56
1:C:38:GLY:O	2:D:259:ARG:HD2	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:LEU:HD22	1:A:79:GLU:HG3	1.88	0.55
1:C:316:MET:HG3	1:C:320:ASP:HB2	1.88	0.55
1:A:64:LEU:HD13	1:A:206:THR:HG22	1.88	0.55
2:H:360:LEU:HG	2:H:364:MET:HE3	1.88	0.55
2:B:419:THR:O	2:B:423:LYS:HG2	2.07	0.55
1:E:322:PHE:HB3	1:E:390:VAL:HG23	1.89	0.54
2:D:77:SER:HB2	2:D:83:GLU:HB3	1.89	0.54
1:A:455:VAL:HG13	2:B:443:THR:HG21	1.88	0.54
1:A:347:GLY:O	1:A:369:ASN:HA	2.06	0.54
2:B:461:LEU:H	7:B:1780:HPA:H8	1.72	0.54
2:D:459:PHE:HB2	2:D:465:ASN:ND2	2.23	0.54
2:F:77:SER:HB2	2:F:83:GLU:HB3	1.90	0.54
1:G:266:LEU:HD13	1:G:350:CYS:HB3	1.89	0.54
2:B:280:ALA:HB2	2:B:360:LEU:HD21	1.89	0.54
1:E:111:ILE:HA	1:E:114:MET:HE3	1.90	0.54
2:H:74:ASN:O	2:H:84:PRO:HA	2.08	0.54
2:H:631:VAL:HG12	2:H:642:ILE:HA	1.90	0.54
1:E:299:ILE:HG13	1:E:318:LEU:HD23	1.89	0.54
2:B:446:ARG:HG2	2:B:632:VAL:HG12	1.90	0.53
2:D:202:ILE:HD13	2:D:236:ASN:HD22	1.72	0.53
1:C:373:LYS:HB2	1:C:378:GLU:HG2	1.90	0.53
1:C:22:SER:OG	1:C:25:GLU:HG2	2.09	0.53
2:F:221:MET:HE1	2:F:224:MET:HG3	1.89	0.53
1:E:370:LEU:HD23	1:E:380:ALA:HA	1.90	0.53
2:B:606:LYS:O	2:B:617:ARG:HD2	2.09	0.53
2:D:31:ASN:HB2	2:D:251:ARG:HD3	1.90	0.53
1:E:110:PHE:HB3	1:E:114:MET:HE2	1.89	0.53
2:B:205:LYS:HB3	2:B:240:ILE:HD11	1.91	0.53
2:D:66:THR:HG22	2:D:68:ALA:H	1.73	0.53
2:D:730:GLU:H	2:D:731:PRO:CD	2.22	0.53
2:F:224:MET:HE3	2:F:488:MET:HB3	1.91	0.53
2:F:461:LEU:H	7:F:1780:HPA:H8	1.73	0.53
2:F:46:ALA:HB3	2:F:121:ALA:HB3	1.91	0.52
2:H:499:VAL:O	2:H:503:VAL:HG23	2.09	0.52
1:E:462:PRO:HA	2:F:643:LEU:HD22	1.92	0.52
2:H:67:ALA:HA	2:H:70:LEU:HD12	1.91	0.52
1:C:249:ILE:HG23	1:C:267:LEU:HD22	1.90	0.52
1:G:309:ARG:HB3	1:G:312:GLU:HB2	1.91	0.52
2:B:221:MET:HE2	2:B:224:MET:HE2	1.92	0.52
2:H:632:VAL:HG13	2:H:643:LEU:HD11	1.92	0.52
9:C:2009:HOH:O	2:D:641:ARG:HD2	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:65:MET:HE2	1:G:278:VAL:HG11	1.92	0.52
1:A:418:LEU:HB3	1:A:436:MET:HE1	1.92	0.52
2:F:341:PHE:O	2:F:342:ARG:C	2.53	0.52
1:G:388:ALA:C	1:G:390:VAL:H	2.17	0.51
2:B:274:ILE:HG12	2:B:293:HIS:CD2	2.45	0.51
2:D:450:LEU:HB2	2:D:628:ILE:HG12	1.90	0.51
1:G:48:THR:HG21	1:G:113:SER:OG	2.10	0.51
1:G:234:ILE:HG12	1:G:243:ILE:HG23	1.92	0.51
2:B:51:ASP:HB3	2:B:117:ARG:HB2	1.91	0.51
2:F:528:ALA:HA	5:F:1778:MTE:S2'	2.51	0.51
1:A:245:ALA:HB1	1:A:282:GLY:HA3	1.92	0.51
1:E:52:ARG:HB3	1:E:74:ALA:HB3	1.93	0.51
2:B:65:PHE:HB2	2:B:100:LEU:HB3	1.92	0.51
2:H:667:ALA:HB3	2:H:732:PRO:HB2	1.93	0.51
1:C:411:ILE:HG13	1:C:447:VAL:CG2	2.39	0.51
2:D:273:ARG:HD2	2:D:294:LEU:HD12	1.93	0.51
4:E:1465:FAD:H2'	4:E:1465:FAD:N1	2.25	0.51
1:G:370:LEU:HD12	1:G:406:PHE:HE1	1.76	0.51
1:A:40:ASN:HD22	1:A:63:CYS:HB2	1.76	0.50
2:D:42:GLU:HG3	2:D:120:TYR:CG	2.46	0.50
2:D:550:ARG:NH1	2:D:595:SER:HB3	2.26	0.50
2:D:730:GLU:N	2:D:731:PRO:CD	2.74	0.50
2:B:145:ILE:HG12	2:B:327:GLU:HG3	1.94	0.50
2:D:312:MET:HE3	2:D:326:ILE:HB	1.94	0.50
2:F:310:ARG:NH2	2:F:458:SER:O	2.45	0.50
1:G:52:ARG:HB3	1:G:74:ALA:HB3	1.92	0.50
2:H:496:MET:HE2	2:H:496:MET:HA	1.93	0.50
2:F:210:LEU:HD22	2:F:247:ARG:HD2	1.94	0.50
2:B:399:LYS:H	2:B:399:LYS:CD	2.24	0.49
1:E:373:LYS:HB2	1:E:378:GLU:HG2	1.94	0.49
2:H:341:PHE:O	2:H:342:ARG:C	2.54	0.49
2:D:170:GLY:N	2:D:271:ASP:HB3	2.28	0.49
1:A:110:PHE:HB3	1:A:114:MET:HE2	1.94	0.49
2:B:418:VAL:HG13	2:B:450:LEU:HD11	1.93	0.49
2:D:701:PHE:O	2:D:704:ARG:HG2	2.12	0.49
2:F:418:VAL:HG13	2:F:450:LEU:HD11	1.94	0.49
2:D:288:GLY:HA2	2:D:323:ALA:O	2.13	0.49
2:F:66:THR:HG22	2:F:68:ALA:H	1.77	0.49
2:F:305:LEU:HB3	2:F:306:PRO:CD	2.42	0.49
1:G:298:LEU:HD23	1:G:301:MET:HE3	1.95	0.49
2:H:210:LEU:HD22	2:H:247:ARG:HD2	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:266:THR:O	2:H:268:LYS:HE2	2.13	0.49
2:B:513:ILE:HG22	9:B:2012:HOH:O	2.13	0.49
4:C:1465:FAD:H2'	4:C:1465:FAD:N1	2.27	0.49
2:D:341:PHE:HD2	2:D:342:ARG:N	2.11	0.49
2:D:457:ILE:O	2:D:458:SER:CB	2.61	0.49
1:A:370:LEU:HD12	1:A:406:PHE:HE1	1.77	0.49
1:A:445:ARG:HG3	1:A:455:VAL:CG1	2.36	0.49
2:D:184:LEU:HD23	2:D:252:PRO:HB3	1.95	0.49
2:F:129:LEU:HD23	2:F:331:LEU:HD12	1.95	0.49
2:H:198:HIS:ND1	2:H:526:ALA:HB2	2.28	0.49
2:B:166:PHE:HB3	2:B:355:ARG:NH2	2.28	0.48
2:B:266:THR:O	2:B:268:LYS:HE2	2.12	0.48
1:A:411:ILE:HG13	1:A:447:VAL:HG21	1.95	0.48
2:F:419:THR:O	2:F:423:LYS:HG2	2.12	0.48
1:G:373:LYS:HB2	1:G:378:GLU:HG2	1.95	0.48
1:E:316:MET:HG3	1:E:320:ASP:HB2	1.93	0.48
1:C:136:CYS:O	2:D:666:GLY:HA3	2.13	0.48
2:H:457:ILE:O	2:H:458:SER:CB	2.62	0.48
1:C:322:PHE:HB3	1:C:390:VAL:HG23	1.96	0.48
1:E:245:ALA:HB1	1:E:282:GLY:HA3	1.96	0.48
1:G:243:ILE:HG21	1:G:252:LEU:HD13	1.95	0.48
1:C:133:LEU:HD13	2:D:698:ILE:HD11	1.95	0.48
2:D:461:LEU:HB2	7:D:1780:HPA:H8	1.95	0.48
1:G:11:THR:HG22	1:G:164:PHE:HE1	1.78	0.48
2:D:148:ARG:HD2	2:D:404:HIS:HA	1.95	0.47
1:E:1:MET:HB2	1:E:179:PRO:HD2	1.96	0.47
2:B:341:PHE:O	2:B:342:ARG:C	2.56	0.47
2:F:216:ASP:OD1	2:H:512:ARG:HD2	2.14	0.47
2:F:683:ASP:HB3	2:F:689:MET:HE1	1.95	0.47
1:G:111:ILE:HD11	2:H:16:VAL:HG22	1.96	0.47
2:H:94:VAL:HG11	2:H:687:ARG:HG2	1.96	0.47
2:H:556:ALA:HB2	2:H:563:ALA:HA	1.96	0.47
1:A:95:MET:SD	1:A:114:MET:HE1	2.54	0.47
2:D:192:ILE:HB	2:D:219:VAL:HG22	1.96	0.47
2:D:551:LEU:HD22	2:D:585:ILE:HG22	1.96	0.47
1:E:212:VAL:O	2:F:107:ARG:NH1	2.47	0.47
2:B:171:GLN:NE2	2:B:674:TRP:HB2	2.30	0.47
2:B:360:LEU:HG	2:B:364:MET:CE	2.43	0.47
2:D:65:PHE:HB2	2:D:100:LEU:HB3	1.96	0.47
2:F:606:LYS:O	2:F:617:ARG:HD2	2.14	0.47
2:F:652:GLY:HA3	2:F:726:LYS:HG3	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:102:GLN:HB3	2:F:489:GLY:O	2.15	0.47
1:E:428:MET:HE3	2:F:689:MET:HG3	1.95	0.47
4:G:1465:FAD:N1	4:G:1465:FAD:H2'	2.29	0.47
2:B:77:SER:HB2	2:B:83:GLU:HB3	1.97	0.47
1:C:322:PHE:HB3	1:C:390:VAL:CG2	2.45	0.47
1:E:356:ARG:NH2	1:E:359:GLN:HB3	2.30	0.47
2:H:145:ILE:HG12	2:H:327:GLU:HG3	1.97	0.47
2:D:31:ASN:O	2:D:251:ARG:HD2	2.15	0.47
2:F:398:LYS:HE3	2:F:398:LYS:HA	1.96	0.47
1:G:234:ILE:HG23	1:G:243:ILE:HG12	1.97	0.47
2:B:601:PHE:CG	2:D:595:SER:HB2	2.50	0.47
1:C:126:ASP:OD1	2:D:704:ARG:NH1	2.47	0.47
1:A:26:TRP:CD1	1:A:67:LEU:HD11	2.50	0.46
1:A:352:LYS:HG3	1:A:362:SER:OG	2.14	0.46
1:E:364:VAL:HG21	1:E:438:ALA:HB3	1.97	0.46
1:G:366:GLY:HA3	1:G:442:MET:SD	2.56	0.46
1:E:200:THR:HG21	1:E:219:LEU:HD13	1.98	0.46
1:G:50:MET:HE3	1:G:57:SER:HB2	1.97	0.46
2:H:173:HIS:HA	2:H:341:PHE:CE1	2.49	0.46
2:D:437:TRP:CE3	2:D:446:ARG:HG3	2.50	0.46
1:E:26:TRP:CD1	1:E:67:LEU:HD11	2.51	0.46
1:E:249:ILE:HG23	1:E:267:LEU:HD22	1.98	0.46
2:F:450:LEU:HB2	2:F:628:ILE:HG12	1.97	0.46
2:B:446:ARG:HG2	2:B:632:VAL:CG1	2.46	0.46
1:E:163:ALA:HA	1:E:166:LEU:HD12	1.96	0.46
2:F:275:ARG:HB3	2:F:292:VAL:HB	1.96	0.46
1:G:212:VAL:O	2:H:107:ARG:NH1	2.49	0.46
2:H:221:MET:HE1	2:H:224:MET:HG3	1.96	0.46
2:D:23:LEU:HD13	2:D:194:CYS:HA	1.97	0.46
2:F:29:PRO:HG3	2:H:27:PRO:HB2	1.96	0.46
2:F:76:ALA:HB2	2:F:85:VAL:HG22	1.97	0.46
2:H:202:ILE:HD13	2:H:236:ASN:HD22	1.80	0.46
2:B:377:TYR:HB2	2:B:412:CYS:SG	2.56	0.46
1:C:355:LYS:HE2	2:D:679:GLU:OE1	2.16	0.46
2:F:701:PHE:O	2:F:704:ARG:HG2	2.15	0.46
1:G:245:ALA:HB1	1:G:282:GLY:HA3	1.98	0.46
2:H:281:ASP:HB2	2:H:285:LYS:O	2.16	0.46
1:A:424:PRO:HG2	1:A:436:MET:HB2	1.97	0.46
2:B:23:LEU:HD22	2:B:180:ALA:HB1	1.97	0.46
4:A:1465:FAD:H9	4:A:1465:FAD:H1'2	1.82	0.46
1:C:295:PRO:HB2	1:C:296:PRO:HD3	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:210:LEU:HD11	2:D:243:ALA:HB1	1.98	0.46
2:D:554:PHE:HB2	2:D:594:ILE:HD13	1.97	0.46
1:E:427:ASP:OD1	1:E:435:ARG:NH2	2.48	0.46
1:A:408:GLU:CD	2:B:442:ARG:HH22	2.22	0.45
2:B:700:ALA:O	2:B:703:ASP:HB2	2.15	0.45
2:H:528:ALA:HA	5:H:1778:MTE:S2'	2.56	0.45
1:A:445:ARG:HE	1:A:455:VAL:HG12	1.81	0.45
2:B:42:GLU:HG3	2:B:120:TYR:CG	2.50	0.45
2:D:194:CYS:SG	2:D:196:SER:HB3	2.56	0.45
2:H:532:GLY:O	2:H:536:ASN:HB2	2.16	0.45
1:C:361:ILE:HD11	1:C:429:ARG:CZ	2.46	0.45
2:D:269:ARG:NH2	2:D:341:PHE:CD2	2.84	0.45
2:D:694:SER:O	2:D:697:LYS:HE2	2.16	0.45
2:H:497:VAL:HG13	2:H:511:VAL:HB	1.99	0.45
2:B:38:GLY:HA3	2:B:99:PHE:CE2	2.52	0.45
2:D:145:ILE:HG12	2:D:327:GLU:HG3	1.97	0.45
1:E:240:GLY:HA3	1:E:341:LEU:O	2.16	0.45
1:E:355:LYS:HE2	2:F:679:GLU:OE1	2.16	0.45
1:G:41:GLU:HA	1:G:210:LEU:HD21	1.98	0.45
1:A:183:PRO:HG3	1:A:189:LEU:HD13	1.98	0.45
2:D:197:GLN:HG2	2:D:224:MET:HE1	1.98	0.45
1:A:252:LEU:HB2	1:A:281:ILE:HD11	1.98	0.45
4:E:1465:FAD:H9	4:E:1465:FAD:H1'2	1.77	0.45
2:F:512:ARG:NH1	2:H:216:ASP:OD2	2.50	0.45
1:G:370:LEU:HD12	1:G:406:PHE:CE1	2.52	0.45
4:G:1465:FAD:H1'2	4:G:1465:FAD:H9	1.78	0.45
1:A:65:MET:CE	1:A:278:VAL:HG11	2.47	0.45
2:H:31:ASN:O	2:H:251:ARG:HD2	2.17	0.45
2:H:631:VAL:HG21	2:H:743:LEU:HD12	1.99	0.45
1:G:24:LEU:HD13	1:G:47:CYS:HB2	1.98	0.44
2:H:228:PHE:HA	5:H:1778:MTE:HN5	1.81	0.44
1:A:212:VAL:O	2:B:107:ARG:NH1	2.50	0.44
2:B:46:ALA:HB3	2:B:121:ALA:HB3	1.99	0.44
2:B:184:LEU:HD23	2:B:252:PRO:HB3	1.99	0.44
1:G:455:VAL:HG13	2:H:443:THR:HG21	1.97	0.44
2:D:174:PHE:CZ	2:D:693:PRO:HG3	2.51	0.44
2:D:730:GLU:H	2:D:731:PRO:HD3	1.82	0.44
2:H:717:ASN:HD22	2:H:726:LYS:HG2	1.83	0.44
2:B:146:TRP:CZ3	2:B:313:LEU:HD13	2.53	0.44
2:B:457:ILE:O	2:B:458:SER:CB	2.66	0.44
2:D:472:GLN:HB2	2:D:480:ALA:HB3	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:36:LYS:O	1:E:47:CYS:HB3	2.18	0.44
1:E:373:LYS:HB2	1:E:378:GLU:CG	2.48	0.44
1:E:399:ALA:C	1:E:401:LEU:H	2.25	0.44
2:F:273:ARG:HD2	2:F:294:LEU:HD12	1.98	0.44
2:F:700:ALA:O	2:F:701:PHE:C	2.60	0.44
1:G:390:VAL:HG22	1:G:391:PRO:HD2	2.00	0.44
2:H:730:GLU:H	2:H:731:PRO:CD	2.31	0.44
1:C:111:ILE:HA	1:C:114:MET:HE3	1.99	0.44
2:D:341:PHE:O	2:D:342:ARG:C	2.60	0.44
1:G:364:VAL:HG21	1:G:438:ALA:HB3	2.00	0.44
2:H:306:PRO:HB2	2:H:344:PHE:HE2	1.81	0.44
2:H:754:TRP:HA	2:H:755:PRO:HD3	1.84	0.44
4:A:1465:FAD:N1	4:A:1465:FAD:H2'	2.32	0.44
2:F:420:ARG:HE	2:F:713:TRP:HZ3	1.65	0.44
2:F:2:SER:N	2:F:502:ALA:HB2	2.32	0.44
2:F:202:ILE:HD13	2:F:236:ASN:HD22	1.83	0.44
2:B:434:ILE:HG23	2:B:446:ARG:HB2	1.98	0.44
2:D:457:ILE:O	2:D:458:SER:HB2	2.18	0.44
2:F:24:ASP:OD2	2:F:254:LYS:NZ	2.50	0.44
2:H:730:GLU:H	2:H:731:PRO:HD2	1.82	0.44
1:A:279:ALA:HB1	4:A:1465:FAD:H4'	1.98	0.44
2:B:461:LEU:HD12	2:B:463:HIS:CE1	2.52	0.44
2:F:23:LEU:HD22	2:F:180:ALA:HB1	2.00	0.44
1:G:78:ILE:HG21	1:G:108:PRO:HB3	2.00	0.44
1:G:273:GLU:O	1:G:277:GLN:HG2	2.18	0.44
1:G:408:GLU:OE1	2:H:442:ARG:NH2	2.50	0.44
2:H:22:TYR:O	2:H:23:LEU:C	2.61	0.44
1:E:281:ILE:H	1:E:281:ILE:HG13	1.52	0.43
1:G:183:PRO:HD2	1:G:224:PHE:O	2.18	0.43
1:G:359:GLN:O	1:G:359:GLN:HG3	2.18	0.43
1:A:1:MET:HB2	1:A:179:PRO:HG2	2.00	0.43
1:A:462:PRO:HA	2:B:643:LEU:HB3	2.00	0.43
2:D:221:MET:HE2	2:D:486:THR:HB	2.00	0.43
2:D:473:ILE:HG12	2:D:479:VAL:HG22	2.00	0.43
1:G:292:GLY:HA2	4:G:1465:FAD:O2	2.18	0.43
4:C:1465:FAD:N1	4:C:1465:FAD:C2'	2.81	0.43
2:D:318:SER:HB3	2:D:414:LEU:CD1	2.49	0.43
2:D:700:ALA:O	2:D:701:PHE:C	2.61	0.43
1:E:111:ILE:HD11	2:F:16:VAL:HG22	1.99	0.43
1:G:1:MET:HB2	1:G:179:PRO:HG2	2.00	0.43
2:D:305:LEU:HB3	2:D:306:PRO:CD	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:301:MET:HB3	1:C:348:LEU:HD22	1.99	0.43
2:F:601:PHE:CG	2:H:595:SER:HB2	2.54	0.43
2:D:210:LEU:HD22	2:D:247:ARG:HD2	2.00	0.43
2:D:305:LEU:HB3	2:D:306:PRO:HD3	2.00	0.43
1:E:415:LEU:HD22	1:E:440:GLN:HB3	2.01	0.43
2:F:133:LEU:HD13	2:F:331:LEU:HD21	2.01	0.43
2:F:667:ALA:HB3	2:F:732:PRO:HB2	2.00	0.43
1:G:252:LEU:HD22	1:G:281:ILE:HG12	2.00	0.43
2:F:168:ILE:HA	2:F:759:ALA:HB3	2.00	0.43
2:B:163:GLU:HG2	2:B:277:ARG:HG2	2.00	0.43
2:B:215:HIS:ND1	2:D:478:SER:HB2	2.33	0.43
2:D:198:HIS:ND1	2:D:526:ALA:HB2	2.34	0.43
2:F:3:VAL:HG21	2:F:723:PHE:CE1	2.54	0.43
1:G:16:ILE:HD13	1:G:68:PRO:HG3	2.00	0.43
1:C:76:ARG:HA	1:C:76:ARG:HD3	1.87	0.43
2:D:66:THR:HG22	2:D:67:ALA:N	2.34	0.43
2:D:493:HIS:CG	2:D:513:ILE:HG12	2.54	0.43
2:F:210:LEU:HD11	2:F:243:ALA:HB1	2.01	0.43
2:H:39:LEU:HB3	2:H:95:GLY:HA2	2.01	0.43
2:F:77:SER:HB2	2:F:83:GLU:CB	2.48	0.43
2:F:367:ASP:HA	2:F:368:PRO:HD3	1.92	0.43
1:G:371:THR:HB	1:G:378:GLU:HB2	2.00	0.43
2:B:506:ILE:HD12	2:B:510:GLN:HB2	2.01	0.42
1:E:301:MET:HA	1:E:369:ASN:HD22	1.84	0.42
1:G:324:GLU:HB2	1:G:327:LYS:HB3	2.01	0.42
2:H:632:VAL:O	2:H:640:ASN:HA	2.19	0.42
2:H:651:ALA:C	2:H:726:LYS:HB2	2.45	0.42
2:H:657:PRO:O	2:H:661:ILE:HG12	2.19	0.42
2:D:661:ILE:CD1	2:D:712:LEU:HG	2.50	0.42
2:F:40:SER:HB2	2:F:91:VAL:HG11	2.00	0.42
2:H:221:MET:HE2	2:H:224:MET:HE2	2.01	0.42
2:H:418:VAL:HG13	2:H:450:LEU:HD11	2.00	0.42
2:D:46:ALA:HB3	2:D:121:ALA:HB3	2.00	0.42
1:A:356:ARG:HH21	1:A:359:GLN:HB3	1.84	0.42
2:B:96:GLN:HA	2:B:97:PRO:HD3	1.95	0.42
1:A:273:GLU:O	1:A:277:GLN:HG2	2.19	0.42
2:B:398:LYS:HE3	2:B:398:LYS:HA	2.00	0.42
1:C:140:ALA:N	1:C:141:PRO:HD2	2.33	0.42
2:H:50:LEU:HD12	2:H:118:ILE:HG12	2.00	0.42
2:B:53:GLU:HB3	2:B:54:PRO:HD3	2.01	0.42
1:E:11:THR:HG22	1:E:164:PHE:HE1	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:107:THR:HB	1:E:108:PRO:HD3	2.02	0.42
2:F:160:HIS:HB3	2:F:364:MET:HE2	2.02	0.42
1:G:39:CYS:O	1:G:40:ASN:HB2	2.19	0.42
1:G:424:PRO:HG2	1:G:436:MET:HB2	2.01	0.42
2:H:650:ASP:HA	2:H:713:TRP:HB3	2.01	0.42
1:G:69:GLN:O	1:G:73:LYS:HE2	2.19	0.42
2:H:76:ALA:HB2	2:H:85:VAL:HG22	2.02	0.42
2:B:138:ARG:HA	2:B:331:LEU:HA	2.00	0.42
1:C:418:LEU:HB3	1:C:436:MET:HE1	2.02	0.42
2:D:281:ASP:HB2	2:D:285:LYS:O	2.19	0.42
1:E:295:PRO:HB2	1:E:296:PRO:CD	2.47	0.42
1:C:445:ARG:CG	1:C:455:VAL:HG11	2.42	0.42
2:F:66:THR:HG22	2:F:67:ALA:N	2.34	0.42
1:G:204:GLY:HA3	1:G:278:VAL:O	2.19	0.42
1:G:209:SER:O	1:G:212:VAL:HG12	2.20	0.42
2:H:35:LEU:HA	2:H:101:VAL:O	2.20	0.42
2:H:506:ILE:HD12	2:H:510:GLN:HB2	2.01	0.42
1:A:368:LEU:HB2	1:A:446:TYR:CD1	2.55	0.42
2:B:437:TRP:CE3	2:B:446:ARG:HG3	2.55	0.42
1:E:273:GLU:OE2	1:E:277:GLN:NE2	2.51	0.42
2:F:497:VAL:HG13	2:F:511:VAL:HB	2.01	0.42
1:G:64:LEU:HD13	1:G:206:THR:HG22	2.02	0.42
1:G:298:LEU:HB2	1:G:318:LEU:HD22	2.01	0.42
1:A:40:ASN:ND2	1:A:63:CYS:HB2	2.35	0.41
1:A:283:GLY:HA2	4:A:1465:FAD:C8A	2.50	0.41
2:D:556:ALA:HB2	2:D:563:ALA:HA	2.01	0.41
2:H:23:LEU:HD22	2:H:180:ALA:HB1	2.01	0.41
2:H:278:ILE:HG12	2:H:360:LEU:HD22	2.02	0.41
2:H:450:LEU:HB2	2:H:628:ILE:HG12	2.02	0.41
2:H:493:HIS:CG	2:H:513:ILE:HG12	2.55	0.41
1:E:372:LEU:HD23	1:E:377:ILE:HA	2.01	0.41
2:H:617:ARG:HD3	2:H:619:PHE:O	2.20	0.41
2:B:315:ALA:O	2:B:353:MET:HE2	2.21	0.41
2:D:281:ASP:N	2:D:285:LYS:O	2.49	0.41
1:E:36:LYS:HB2	1:E:46:ALA:HB1	2.02	0.41
2:F:186:ALA:O	2:F:187:GLU:C	2.62	0.41
2:F:599:THR:HG23	2:H:599:THR:HG23	2.02	0.41
2:H:536:ASN:O	2:H:540:VAL:HG23	2.20	0.41
1:C:12:ARG:NH2	1:C:30:GLU:OE1	2.53	0.41
1:C:18:ASP:OD2	1:C:20:THR:HG22	2.20	0.41
1:E:314:ARG:HD3	1:E:334:GLU:OE1	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:46:ALA:HB2	2:H:123:ARG:NH2	2.36	0.41
2:H:469:ALA:HA	2:H:483:HIS:HA	2.03	0.41
1:E:122:ARG:HB3	1:E:128:LEU:HD21	2.01	0.41
2:H:473:ILE:HB	2:H:596:LEU:HB3	2.02	0.41
1:A:110:PHE:HE1	1:A:134:CYS:HB2	1.85	0.41
2:D:186:ALA:O	2:D:187:GLU:C	2.63	0.41
1:E:411:ILE:HG13	1:E:447:VAL:HG21	2.02	0.41
2:F:221:MET:CE	2:F:224:MET:HG3	2.51	0.41
2:F:417:LEU:HG	2:F:648:LEU:HD23	2.02	0.41
2:B:309:ASP:OD1	2:B:330:ARG:NH2	2.50	0.41
1:C:190:ALA:HB1	1:C:310:GLY:HA2	2.02	0.41
1:C:360:ASP:OD1	2:D:697:LYS:HE3	2.20	0.41
2:D:321:VAL:HG12	2:D:323:ALA:O	2.21	0.41
1:E:441:ALA:HB1	2:F:636:LEU:HB3	2.02	0.41
2:H:360:LEU:HG	2:H:364:MET:CE	2.50	0.41
1:A:360:ASP:OD1	2:B:697:LYS:HE3	2.20	0.41
2:B:532:GLY:O	2:B:536:ASN:HB2	2.20	0.41
2:D:259:ARG:HG3	2:D:263:MET:HE3	2.01	0.41
2:D:280:ALA:HB3	2:D:364:MET:HE1	2.02	0.41
2:D:751:GLY:HA3	2:D:773:ALA:O	2.21	0.41
1:E:312:GLU:H	1:E:312:GLU:HG2	1.68	0.41
2:B:70:LEU:HD23	2:B:244:VAL:HG11	2.01	0.41
2:D:316:ASP:HB3	2:D:404:HIS:ND1	2.36	0.41
2:D:652:GLY:HA3	2:D:726:LYS:HG3	2.02	0.41
1:E:201:LEU:HD22	1:E:225:LEU:HD21	2.02	0.41
2:F:457:ILE:O	2:F:458:SER:CB	2.68	0.41
1:G:361:ILE:HD11	1:G:429:ARG:CZ	2.50	0.41
1:G:462:PRO:HA	2:H:643:LEU:HD22	2.03	0.41
1:C:245:ALA:HB1	1:C:282:GLY:HA3	2.03	0.41
2:D:609:TRP:HA	2:D:616:GLY:HA3	2.02	0.41
1:G:38:GLY:O	2:H:259:ARG:HD3	2.21	0.41
2:H:35:LEU:HD11	2:H:242:CYS:HA	2.02	0.41
2:H:174:PHE:HA	2:H:259:ARG:HH21	1.86	0.41
2:D:205:LYS:HB3	2:D:240:ILE:HD11	2.04	0.40
2:F:198:HIS:ND1	2:F:526:ALA:HB2	2.36	0.40
2:H:303:LEU:O	2:H:307:VAL:HG23	2.21	0.40
2:B:631:VAL:HG12	2:B:642:ILE:HA	2.03	0.40
2:B:694:SER:O	2:B:697:LYS:HE2	2.21	0.40
2:F:754:TRP:HA	2:F:755:PRO:HD3	1.88	0.40
2:H:54:PRO:HB2	2:H:115:LYS:HB3	2.03	0.40
2:B:148:ARG:O	2:B:323:ALA:HA	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:460:THR:H	7:B:1780:HPA:HN7	1.70	0.40
2:D:236:ASN:HD22	2:D:236:ASN:HA	1.68	0.40
2:F:321:VAL:HG12	2:F:323:ALA:O	2.21	0.40
2:F:631:VAL:HG12	2:F:642:ILE:HA	2.02	0.40
1:G:95:MET:HG3	1:G:114:MET:HE1	2.03	0.40
1:G:295:PRO:HB2	1:G:296:PRO:HD3	2.03	0.40
1:C:460:VAL:HG11	2:D:632:VAL:HG11	2.02	0.40
2:D:303:LEU:O	2:D:307:VAL:HG23	2.21	0.40
1:E:401:LEU:HD11	1:E:411:ILE:HD13	2.03	0.40
1:A:206:THR:HG21	1:A:275:VAL:HG13	2.02	0.40
2:D:278:ILE:HG12	2:D:360:LEU:HD22	2.03	0.40
2:D:305:LEU:HD21	2:D:611:ARG:NE	2.35	0.40
2:H:507:ASP:HA	2:H:508:PRO:HD2	1.93	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	446/462 (96%)	415 (93%)	29 (6%)	2 (0%)	30	59
1	C	446/462 (96%)	425 (95%)	19 (4%)	2 (0%)	30	59
1	E	446/462 (96%)	416 (93%)	29 (6%)	1 (0%)	43	72
1	G	446/462 (96%)	415 (93%)	27 (6%)	4 (1%)	14	41
2	B	756/777 (97%)	722 (96%)	28 (4%)	6 (1%)	16	44
2	D	756/777 (97%)	725 (96%)	24 (3%)	7 (1%)	14	41
2	F	756/777 (97%)	721 (95%)	32 (4%)	3 (0%)	30	59
2	H	756/777 (97%)	711 (94%)	38 (5%)	7 (1%)	14	41
All	All	4808/4956 (97%)	4550 (95%)	226 (5%)	32 (1%)	18	48

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	458	SER
2	D	187	GLU
2	D	458	SER
2	F	187	GLU
2	F	458	SER
2	H	458	SER
2	B	342	ARG
2	B	722	ILE
1	C	165	THR
2	F	342	ARG
1	G	221	GLU
1	G	378	GLU
2	H	187	GLU
2	H	342	ARG
2	B	227	GLY
2	D	342	ARG
1	E	374	GLY
1	G	375	SER
2	B	593	ARG
2	D	141	GLY
2	H	227	GLY
1	A	221	GLU
2	B	187	GLU
2	D	227	GLY
1	G	39	CYS
2	H	234	GLN
2	D	722	ILE
2	H	730	GLU
2	D	560	GLY
1	A	374	GLY
1	C	374	GLY
2	H	560	GLY

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	339/347 (98%)	325 (96%)	14 (4%)	27	61
1	C	339/347 (98%)	325 (96%)	14 (4%)	27	61
1	E	339/347 (98%)	324 (96%)	15 (4%)	25	59
1	G	339/347 (98%)	324 (96%)	15 (4%)	25	59
2	B	571/584 (98%)	548 (96%)	23 (4%)	28	62
2	D	571/584 (98%)	543 (95%)	28 (5%)	22	54
2	F	571/584 (98%)	550 (96%)	21 (4%)	30	64
2	H	571/584 (98%)	548 (96%)	23 (4%)	28	62
All	All	3640/3724 (98%)	3487 (96%)	153 (4%)	26	60

All (153) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	THR
1	A	33	THR
1	A	40	ASN
1	A	79	GLU
1	A	103	CYS
1	A	128	LEU
1	A	143	LEU
1	A	231	LEU
1	A	291	ILE
1	A	301	MET
1	A	401	LEU
1	A	409	ASP
1	A	425	LEU
1	A	457	VAL
2	B	10	ASP
2	B	16	VAL
2	B	85	VAL
2	B	152	GLU
2	B	161	LEU
2	B	222	ARG
2	B	256	ARG
2	B	268	LYS
2	B	313	LEU
2	B	330	ARG
2	B	355	ARG
2	B	398	LYS
2	B	399	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	450	LEU
2	B	461	LEU
2	B	512	ARG
2	B	534	ASP
2	B	604	THR
2	B	617	ARG
2	B	632	VAL
2	B	697	LYS
2	B	741	LEU
2	B	743	LEU
1	C	20	THR
1	C	40	ASN
1	C	79	GLU
1	C	128	LEU
1	C	143	LEU
1	C	231	LEU
1	C	257	GLU
1	C	281	ILE
1	C	291	ILE
1	C	309	ARG
1	C	312	GLU
1	C	316	MET
1	C	378	GLU
1	C	461	MET
2	D	10	ASP
2	D	16	VAL
2	D	23	LEU
2	D	151	VAL
2	D	161	LEU
2	D	221	MET
2	D	222	ARG
2	D	244	VAL
2	D	256	ARG
2	D	268	LYS
2	D	313	LEU
2	D	326	ILE
2	D	330	ARG
2	D	355	ARG
2	D	398	LYS
2	D	399	LYS
2	D	450	LEU
2	D	461	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	512	ARG
2	D	558	ARG
2	D	567	ILE
2	D	613	ARG
2	D	617	ARG
2	D	632	VAL
2	D	635	ARG
2	D	697	LYS
2	D	741	LEU
2	D	743	LEU
1	E	15	ARG
1	E	40	ASN
1	E	43	ASP
1	E	79	GLU
1	E	128	LEU
1	E	143	LEU
1	E	198	GLU
1	E	231	LEU
1	E	237	THR
1	E	281	ILE
1	E	291	ILE
1	E	316	MET
1	E	378	GLU
1	E	390	VAL
1	E	457	VAL
2	F	2	SER
2	F	16	VAL
2	F	151	VAL
2	F	161	LEU
2	F	222	ARG
2	F	256	ARG
2	F	268	LYS
2	F	313	LEU
2	F	330	ARG
2	F	355	ARG
2	F	398	LYS
2	F	399	LYS
2	F	450	LEU
2	F	512	ARG
2	F	516	THR
2	F	548	ARG
2	F	558	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	632	VAL
2	F	689	MET
2	F	741	LEU
2	F	743	LEU
1	G	33	THR
1	G	40	ASN
1	G	79	GLU
1	G	91	VAL
1	G	128	LEU
1	G	143	LEU
1	G	200	THR
1	G	231	LEU
1	G	257	GLU
1	G	281	ILE
1	G	291	ILE
1	G	301	MET
1	G	390	VAL
1	G	401	LEU
1	G	457	VAL
2	H	2	SER
2	H	16	VAL
2	H	66	THR
2	H	73	ASP
2	H	151	VAL
2	H	216	ASP
2	H	222	ARG
2	H	268	LYS
2	H	271	ASP
2	H	313	LEU
2	H	326	ILE
2	H	330	ARG
2	H	355	ARG
2	H	398	LYS
2	H	399	LYS
2	H	450	LEU
2	H	458	SER
2	H	461	LEU
2	H	512	ARG
2	H	548	ARG
2	H	617	ARG
2	H	632	VAL
2	H	741	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	61	ASN
1	A	118	HIS
1	A	274	GLN
1	A	359	GLN
2	B	208	HIS
2	B	293	HIS
2	B	359	HIS
2	B	441	ASN
2	B	463	HIS
2	B	715	GLN
1	C	40	ASN
1	C	98	HIS
1	C	118	HIS
2	D	19	GLN
2	D	236	ASN
2	D	338	ASN
2	D	426	ASN
2	D	441	ASN
2	D	463	HIS
1	E	40	ASN
1	E	61	ASN
1	E	328	GLN
1	E	369	ASN
1	E	437	ASN
2	F	236	ASN
2	F	293	HIS
2	F	359	HIS
2	F	426	ASN
2	F	441	ASN
2	F	463	HIS
2	F	482	ASN
1	G	40	ASN
1	G	93	GLN
2	H	72	HIS
2	H	193	HIS
2	H	234	GLN
2	H	236	ASN
2	H	293	HIS
2	H	359	HIS
2	H	426	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	441	ASN
2	H	463	HIS
2	H	640	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 4 are monoatomic - leaving 24 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	$\# Z > 2$
5	MTE	B	1778	8	21,26,26	3.96	5 (23%)	19,40,40	3.69	7 (36%)
5	MTE	F	1778	8	21,26,26	4.02	5 (23%)	19,40,40	3.33	8 (42%)
3	FES	C	1464	1	0,4,4	-	-	-		
3	FES	A	1464	1	0,4,4	-	-	-		
3	FES	E	1464	1	0,4,4	-	-	-		
3	FES	G	1463	1	0,4,4	-	-	-		
8	MOM	F	1781	5	0,3,3	-	-	-		
3	FES	G	1464	1	0,4,4	-	-	-		
4	FAD	G	1465	-	58,58,58	1.34	8 (13%)	85,89,89	1.53	14 (16%)
8	MOM	H	1781	5	0,3,3	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FES	C	1463	1	0,4,4	-	-	-		
5	MTE	H	1778	8	21,26,26	3.98	6 (28%)	19,40,40	3.22	7 (36%)
7	HPA	B	1780	-	10,11,11	1.76	1 (10%)	11,15,15	3.09	8 (72%)
7	HPA	F	1780	-	10,11,11	1.77	1 (10%)	11,15,15	3.14	8 (72%)
4	FAD	A	1465	-	58,58,58	1.27	6 (10%)	85,89,89	1.53	15 (17%)
7	HPA	H	1780	-	10,11,11	1.77	1 (10%)	11,15,15	3.20	8 (72%)
4	FAD	E	1465	-	58,58,58	1.26	6 (10%)	85,89,89	1.52	15 (17%)
3	FES	A	1463	1	0,4,4	-	-	-		
3	FES	E	1463	1	0,4,4	-	-	-		
7	HPA	D	1780	-	10,11,11	1.76	1 (10%)	11,15,15	3.16	8 (72%)
4	FAD	C	1465	-	58,58,58	1.24	5 (8%)	85,89,89	1.58	15 (17%)
8	MOM	B	1781	5	0,3,3	-	-	-		
8	MOM	D	1781	5	0,3,3	-	-	-		
5	MTE	D	1778	8	21,26,26	4.06	5 (23%)	19,40,40	3.48	7 (36%)

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
5	MTE	B	1778	8	1/1/6/8	3/6/34/34	0/3/3/3
5	MTE	F	1778	8	1/1/6/8	5/6/34/34	0/3/3/3
3	FES	C	1464	1	-	-	0/1/1/1
3	FES	A	1464	1	-	-	0/1/1/1
3	FES	E	1464	1	-	-	0/1/1/1
3	FES	G	1463	1	-	-	0/1/1/1
3	FES	G	1464	1	-	-	0/1/1/1
4	FAD	G	1465	-	-	11/34/50/50	0/6/6/6
3	FES	C	1463	1	-	-	0/1/1/1
5	MTE	H	1778	8	1/1/6/8	1/6/34/34	0/3/3/3
7	HPA	B	1780	-	-	-	0/2/2/2
7	HPA	F	1780	-	-	-	0/2/2/2
4	FAD	A	1465	-	-	10/34/50/50	0/6/6/6
7	HPA	H	1780	-	-	-	0/2/2/2
4	FAD	E	1465	-	-	9/34/50/50	0/6/6/6
3	FES	A	1463	1	-	-	0/1/1/1
3	FES	E	1463	1	-	-	0/1/1/1
7	HPA	D	1780	-	-	-	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FAD	C	1465	-	-	10/34/50/50	0/6/6/6
5	MTE	D	1778	8	1/1/6/8	5/6/34/34	0/3/3/3

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1778	MTE	C4'-C3'	-13.14	1.33	1.51
5	H	1778	MTE	C4'-C3'	-12.80	1.34	1.51
5	B	1778	MTE	C4'-C3'	-12.59	1.34	1.51
5	F	1778	MTE	C4'-C3'	-12.44	1.34	1.51
5	F	1778	MTE	C6-N5	-11.36	1.33	1.46
5	D	1778	MTE	C6-N5	-10.93	1.34	1.46
5	B	1778	MTE	C6-N5	-10.75	1.34	1.46
5	H	1778	MTE	C6-N5	-10.61	1.34	1.46
5	B	1778	MTE	C9-C10	5.28	1.47	1.38
5	H	1778	MTE	C9-C10	5.14	1.47	1.38
5	D	1778	MTE	C9-C10	5.07	1.47	1.38
5	F	1778	MTE	C9-C10	5.06	1.47	1.38
7	D	1780	HPA	C2-N3	4.80	1.38	1.30
7	H	1780	HPA	C2-N3	4.80	1.38	1.30
7	F	1780	HPA	C2-N3	4.78	1.38	1.30
7	B	1780	HPA	C2-N3	4.76	1.38	1.30
4	E	1465	FAD	C4X-N5	4.71	1.40	1.30
4	C	1465	FAD	C4X-N5	4.56	1.40	1.30
4	G	1465	FAD	C4X-N5	4.51	1.40	1.30
4	A	1465	FAD	C4X-N5	4.38	1.40	1.30
4	E	1465	FAD	C10-N1	3.88	1.41	1.33
4	C	1465	FAD	C10-N1	3.88	1.41	1.33
4	A	1465	FAD	C10-N1	3.71	1.40	1.33
4	G	1465	FAD	C10-N1	3.71	1.40	1.33
4	G	1465	FAD	PA-O3P	3.54	1.63	1.59
5	B	1778	MTE	C9-N5	3.29	1.45	1.37
5	H	1778	MTE	C9-N5	3.27	1.45	1.37
4	A	1465	FAD	C5A-N7A	-3.24	1.33	1.39
5	D	1778	MTE	C9-N5	3.16	1.45	1.37
4	E	1465	FAD	C5A-N7A	-3.15	1.33	1.39
5	F	1778	MTE	C9-N5	2.99	1.44	1.37
4	G	1465	FAD	C5A-N7A	-2.94	1.33	1.39
4	C	1465	FAD	C5A-N7A	-2.75	1.34	1.39
5	H	1778	MTE	C7-C6	-2.31	1.51	1.53
4	C	1465	FAD	C8A-N9A	-2.26	1.33	1.37
4	A	1465	FAD	C8A-N9A	-2.26	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1465	FAD	C10-N10	2.23	1.42	1.37
5	B	1778	MTE	C9-C4	2.20	1.48	1.41
4	E	1465	FAD	C8A-N9A	-2.19	1.33	1.37
5	D	1778	MTE	C9-C4	2.16	1.48	1.41
4	G	1465	FAD	O4B-C1B	2.14	1.47	1.42
4	C	1465	FAD	C4A-N9A	-2.13	1.33	1.37
4	E	1465	FAD	C4A-N9A	-2.12	1.33	1.37
4	G	1465	FAD	C4A-N9A	-2.11	1.33	1.37
4	G	1465	FAD	C10-N10	2.10	1.41	1.37
4	G	1465	FAD	C8A-N9A	-2.08	1.34	1.37
5	H	1778	MTE	C9-C4	2.07	1.48	1.41
5	F	1778	MTE	C9-C4	2.06	1.48	1.41
4	E	1465	FAD	C10-N10	2.01	1.41	1.37
4	A	1465	FAD	O4B-C1B	2.00	1.46	1.42

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1778	MTE	C7-C6-N5	12.04	119.70	107.87
5	D	1778	MTE	C7-C6-N5	11.34	119.01	107.87
5	F	1778	MTE	C7-C6-N5	11.31	118.98	107.87
5	H	1778	MTE	C7-C6-N5	10.97	118.64	107.87
5	B	1778	MTE	O4'-C4'-C3'	5.45	122.03	108.58
4	A	1465	FAD	C5A-C4A-N3A	-5.41	119.27	126.72
4	E	1465	FAD	C5A-C4A-N3A	-5.34	119.37	126.72
4	C	1465	FAD	C5A-C4A-N3A	-5.33	119.37	126.72
5	B	1778	MTE	O3'-C7-C6	5.26	112.47	108.96
5	D	1778	MTE	O3'-C7-C6	5.24	112.46	108.96
4	G	1465	FAD	C5A-C4A-N3A	-5.07	119.73	126.72
4	E	1465	FAD	N3A-C2A-N1A	-4.94	121.10	128.58
4	G	1465	FAD	N3A-C2A-N1A	-4.85	121.25	128.58
7	D	1780	HPA	N1-C2-N3	-4.81	119.96	125.50
7	H	1780	HPA	N1-C2-N3	-4.75	120.03	125.50
7	F	1780	HPA	N1-C2-N3	-4.75	120.03	125.50
4	A	1465	FAD	N3A-C2A-N1A	-4.69	121.48	128.58
5	F	1778	MTE	C2-N1-C10	4.67	121.59	113.36
7	B	1780	HPA	N1-C2-N3	-4.63	120.17	125.50
5	B	1778	MTE	C2-N1-C10	4.61	121.50	113.36
5	D	1778	MTE	C2-N1-C10	4.56	121.40	113.36
4	C	1465	FAD	N3A-C2A-N1A	-4.50	121.77	128.58
5	H	1778	MTE	C2-N1-C10	4.50	121.30	113.36
7	H	1780	HPA	C5-C6-N1	4.45	120.02	110.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	1778	MTE	O4'-C4'-C3'	4.41	119.46	108.58
5	D	1778	MTE	O4'-C4'-C3'	4.34	119.28	108.58
7	F	1780	HPA	C5-C6-N1	4.30	119.70	110.26
7	D	1780	HPA	C5-C6-N1	4.29	119.68	110.26
7	B	1780	HPA	C5-C6-N1	4.24	119.57	110.26
5	H	1778	MTE	O4'-C4'-C3'	4.12	118.76	108.58
4	A	1465	FAD	N3A-C4A-N9A	3.90	133.80	127.17
7	H	1780	HPA	C2-N1-C6	-3.87	119.78	125.09
7	B	1780	HPA	C2-N1-C6	-3.75	119.95	125.09
7	D	1780	HPA	C2-N1-C6	-3.74	119.96	125.09
4	E	1465	FAD	C2A-N3A-C4A	3.74	120.96	111.83
7	F	1780	HPA	C2-N1-C6	-3.74	119.97	125.09
4	E	1465	FAD	N3A-C4A-N9A	3.69	133.45	127.17
7	F	1780	HPA	N7-C8-N9	-3.69	108.70	112.98
7	D	1780	HPA	N7-C8-N9	-3.67	108.72	112.98
7	H	1780	HPA	N7-C8-N9	-3.67	108.72	112.98
4	C	1465	FAD	N3A-C4A-N9A	3.67	133.41	127.17
4	C	1465	FAD	C2A-N3A-C4A	3.66	120.76	111.83
4	G	1465	FAD	C2A-N3A-C4A	3.62	120.68	111.83
4	A	1465	FAD	C2A-N3A-C4A	3.60	120.61	111.83
7	B	1780	HPA	N7-C8-N9	-3.59	108.81	112.98
4	G	1465	FAD	N3A-C4A-N9A	3.56	133.23	127.17
4	C	1465	FAD	C4-N3-C2	-3.40	119.61	125.64
4	G	1465	FAD	N9A-C8A-N7A	-3.38	109.14	113.94
4	G	1465	FAD	C4-N3-C2	-3.36	119.68	125.64
4	C	1465	FAD	N9A-C8A-N7A	-3.35	109.18	113.94
4	A	1465	FAD	C4-N3-C2	-3.30	119.77	125.64
4	E	1465	FAD	C4-N3-C2	-3.27	119.83	125.64
4	A	1465	FAD	N9A-C8A-N7A	-3.27	109.30	113.94
7	D	1780	HPA	C8-N9-C4	3.26	108.51	102.89
7	H	1780	HPA	C8-N9-C4	3.25	108.51	102.89
7	H	1780	HPA	C6-C5-C4	-3.24	119.39	121.61
7	F	1780	HPA	C8-N9-C4	3.21	108.43	102.89
7	B	1780	HPA	C8-N9-C4	3.18	108.38	102.89
7	D	1780	HPA	C6-C5-C4	-3.15	119.46	121.61
7	H	1780	HPA	O6-C6-C5	-3.11	119.75	127.26
7	D	1780	HPA	O6-C6-C5	-3.11	119.77	127.26
4	E	1465	FAD	N9A-C8A-N7A	-3.09	109.55	113.94
7	F	1780	HPA	C6-C5-C4	-3.02	119.55	121.61
5	H	1778	MTE	C4-C9-N5	3.01	124.48	116.27
4	C	1465	FAD	C4A-C5A-N7A	-3.00	107.15	110.58
5	D	1778	MTE	C4-C9-N5	2.99	124.42	116.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1780	HPA	O6-C6-C5	-2.99	120.06	127.26
7	F	1780	HPA	O6-C6-C5	-2.96	120.13	127.26
7	B	1780	HPA	C6-C5-C4	-2.95	119.59	121.61
4	C	1465	FAD	C5A-N7A-C8A	2.94	108.07	103.45
7	D	1780	HPA	C2-N3-C4	2.92	120.53	113.34
7	F	1780	HPA	C2-N3-C4	2.90	120.50	113.34
4	C	1465	FAD	C10-C4X-N5	-2.90	118.90	124.81
7	B	1780	HPA	C2-N3-C4	2.87	120.43	113.34
4	E	1465	FAD	C4X-C4-N3	2.87	120.55	113.25
4	G	1465	FAD	C5A-N7A-C8A	2.85	107.93	103.45
4	A	1465	FAD	C5A-N7A-C8A	2.85	107.93	103.45
7	H	1780	HPA	C2-N3-C4	2.85	120.37	113.34
4	G	1465	FAD	C4X-C10-N10	2.84	120.54	116.48
4	C	1465	FAD	C4X-C10-N10	2.83	120.53	116.48
5	B	1778	MTE	C4-C9-N5	2.75	123.77	116.27
4	C	1465	FAD	C4X-C4-N3	2.74	120.24	113.25
4	G	1465	FAD	C4X-C4-N3	2.73	120.21	113.25
4	E	1465	FAD	C5A-N7A-C8A	2.71	107.71	103.45
4	G	1465	FAD	C4A-C5A-N7A	-2.69	107.51	110.58
4	G	1465	FAD	C10-C4X-N5	-2.65	119.39	124.81
4	A	1465	FAD	C4X-C10-N10	2.63	120.25	116.48
5	F	1778	MTE	C4-C9-N5	2.63	123.44	116.27
4	A	1465	FAD	C4X-C4-N3	2.61	119.91	113.25
4	E	1465	FAD	C4A-C5A-N7A	-2.61	107.60	110.58
4	E	1465	FAD	C4X-C10-N10	2.59	120.18	116.48
4	E	1465	FAD	C10-C4X-N5	-2.58	119.53	124.81
5	B	1778	MTE	O4-C4-C9	-2.55	121.11	127.26
4	A	1465	FAD	C4A-C5A-N7A	-2.55	107.67	110.58
4	C	1465	FAD	C4A-N9A-C8A	2.51	108.38	105.74
4	G	1465	FAD	C4A-N9A-C8A	2.50	108.37	105.74
5	F	1778	MTE	O4-C4-C9	-2.47	121.31	127.26
4	A	1465	FAD	C10-C4X-N5	-2.45	119.80	124.81
4	A	1465	FAD	O4-C4-C4X	-2.45	120.07	126.53
5	H	1778	MTE	O4-C4-C9	-2.41	121.46	127.26
4	C	1465	FAD	O4B-C1B-N9A	-2.39	103.51	108.09
5	F	1778	MTE	O3'-C7-N8	2.36	110.75	108.61
5	B	1778	MTE	C9-C4-N3	2.33	118.53	112.13
5	D	1778	MTE	C9-C4-N3	2.32	118.51	112.13
4	A	1465	FAD	C4A-N9A-C8A	2.31	108.17	105.74
5	H	1778	MTE	C9-C4-N3	2.28	118.38	112.13
5	D	1778	MTE	O4-C4-C9	-2.25	121.85	127.26
5	F	1778	MTE	C9-C4-N3	2.23	118.27	112.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1465	FAD	O4-C4-C4X	-2.23	120.64	126.53
4	E	1465	FAD	C9A-C5X-N5	-2.21	120.11	122.45
4	C	1465	FAD	O4-C4-C4X	-2.21	120.70	126.53
4	A	1465	FAD	C4X-C10-N1	-2.18	119.23	124.59
4	A	1465	FAD	C4-C4X-C10	2.16	120.63	116.93
4	G	1465	FAD	O4-C4-C4X	-2.12	120.93	126.53
4	E	1465	FAD	C4A-N9A-C8A	2.11	107.96	105.74
4	G	1465	FAD	C4X-C10-N1	-2.11	119.42	124.59
4	E	1465	FAD	C4X-C10-N1	-2.09	119.47	124.59
5	F	1778	MTE	O3'-C7-C6	2.07	110.35	108.96
4	C	1465	FAD	C4X-C10-N1	-2.06	119.54	124.59
5	H	1778	MTE	O3'-C7-C6	-2.04	107.61	108.96

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	1778	MTE	C3'
5	D	1778	MTE	C3'
5	F	1778	MTE	C3'
5	H	1778	MTE	C3'

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1465	FAD	N10-C1'-C2'-O2'
4	A	1465	FAD	N10-C1'-C2'-C3'
4	A	1465	FAD	C2'-C3'-C4'-O4'
4	A	1465	FAD	C2'-C3'-C4'-C5'
4	A	1465	FAD	O3'-C3'-C4'-O4'
4	A	1465	FAD	O3'-C3'-C4'-C5'
4	C	1465	FAD	C2'-C1'-N10-C10
4	C	1465	FAD	N10-C1'-C2'-O2'
4	C	1465	FAD	N10-C1'-C2'-C3'
4	C	1465	FAD	C2'-C3'-C4'-O4'
4	C	1465	FAD	C2'-C3'-C4'-C5'
4	C	1465	FAD	O3'-C3'-C4'-O4'
4	C	1465	FAD	O3'-C3'-C4'-C5'
4	C	1465	FAD	C3'-C4'-C5'-O5'
4	C	1465	FAD	O4'-C4'-C5'-O5'
4	E	1465	FAD	N10-C1'-C2'-O2'
4	E	1465	FAD	N10-C1'-C2'-C3'
4	E	1465	FAD	C2'-C3'-C4'-O4'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	E	1465	FAD	C2'-C3'-C4'-C5'
4	E	1465	FAD	O3'-C3'-C4'-O4'
4	E	1465	FAD	O3'-C3'-C4'-C5'
4	E	1465	FAD	C3'-C4'-C5'-O5'
4	E	1465	FAD	O4'-C4'-C5'-O5'
4	G	1465	FAD	N10-C1'-C2'-O2'
4	G	1465	FAD	N10-C1'-C2'-C3'
4	G	1465	FAD	C2'-C3'-C4'-C5'
4	G	1465	FAD	C3'-C4'-C5'-O5'
5	B	1778	MTE	O3'-C3'-C4'-O4'
5	D	1778	MTE	O3'-C3'-C4'-O4'
5	D	1778	MTE	C4'-O4'-P-O2P
5	D	1778	MTE	C4'-O4'-P-O3P
5	F	1778	MTE	C4'-O4'-P-O2P
5	F	1778	MTE	C4'-O4'-P-O3P
5	H	1778	MTE	O3'-C3'-C4'-O4'
4	G	1465	FAD	O3'-C3'-C4'-O4'
4	G	1465	FAD	C2'-C3'-C4'-O4'
4	G	1465	FAD	O3'-C3'-C4'-C5'
4	A	1465	FAD	O4'-C4'-C5'-O5'
4	G	1465	FAD	O4'-C4'-C5'-O5'
4	A	1465	FAD	C3'-C4'-C5'-O5'
5	D	1778	MTE	C4'-O4'-P-O1P
5	F	1778	MTE	C4'-O4'-P-O1P
5	B	1778	MTE	C3'-C4'-O4'-P
5	F	1778	MTE	O3'-C3'-C4'-O4'
5	F	1778	MTE	C3'-C4'-O4'-P
4	A	1465	FAD	C2'-C1'-N10-C10
4	E	1465	FAD	C2'-C1'-N10-C10
4	G	1465	FAD	C2'-C1'-N10-C10
5	B	1778	MTE	C4'-O4'-P-O1P
4	C	1465	FAD	C4'-C5'-O5'-P
4	G	1465	FAD	C4'-C5'-O5'-P
4	A	1465	FAD	C4'-C5'-O5'-P
5	D	1778	MTE	C3'-C4'-O4'-P
4	G	1465	FAD	PA-O3P-P-O1P

There are no ring outliers.

16 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1778	MTE	1	0

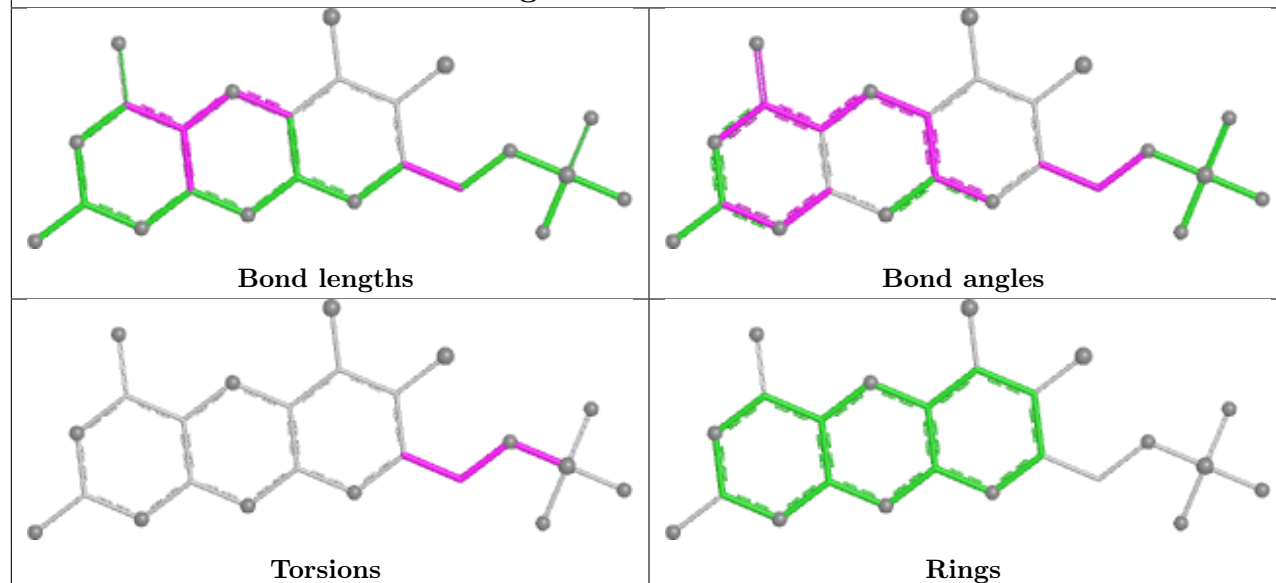
Continued on next page...

Continued from previous page...

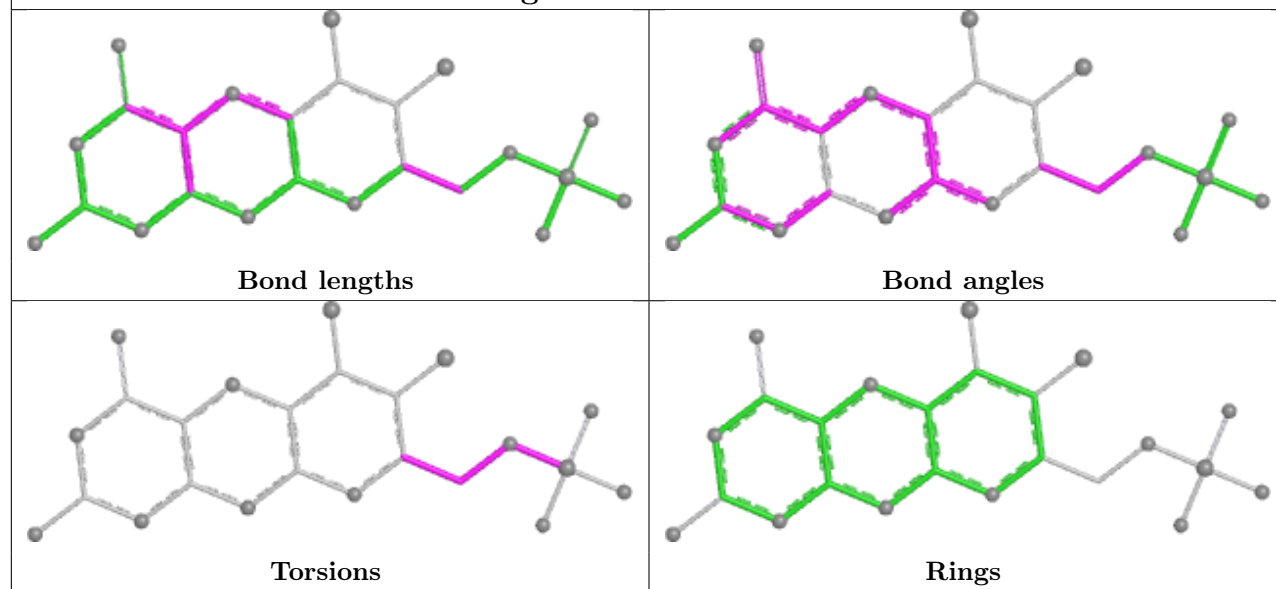
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	1778	MTE	1	0
3	G	1463	FES	1	0
8	F	1781	MOM	2	0
4	G	1465	FAD	4	0
8	H	1781	MOM	2	0
5	H	1778	MTE	2	0
7	B	1780	HPA	2	0
7	F	1780	HPA	1	0
4	A	1465	FAD	5	0
4	E	1465	FAD	3	0
7	D	1780	HPA	1	0
4	C	1465	FAD	3	0
8	B	1781	MOM	2	0
8	D	1781	MOM	2	0
5	D	1778	MTE	1	0

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.

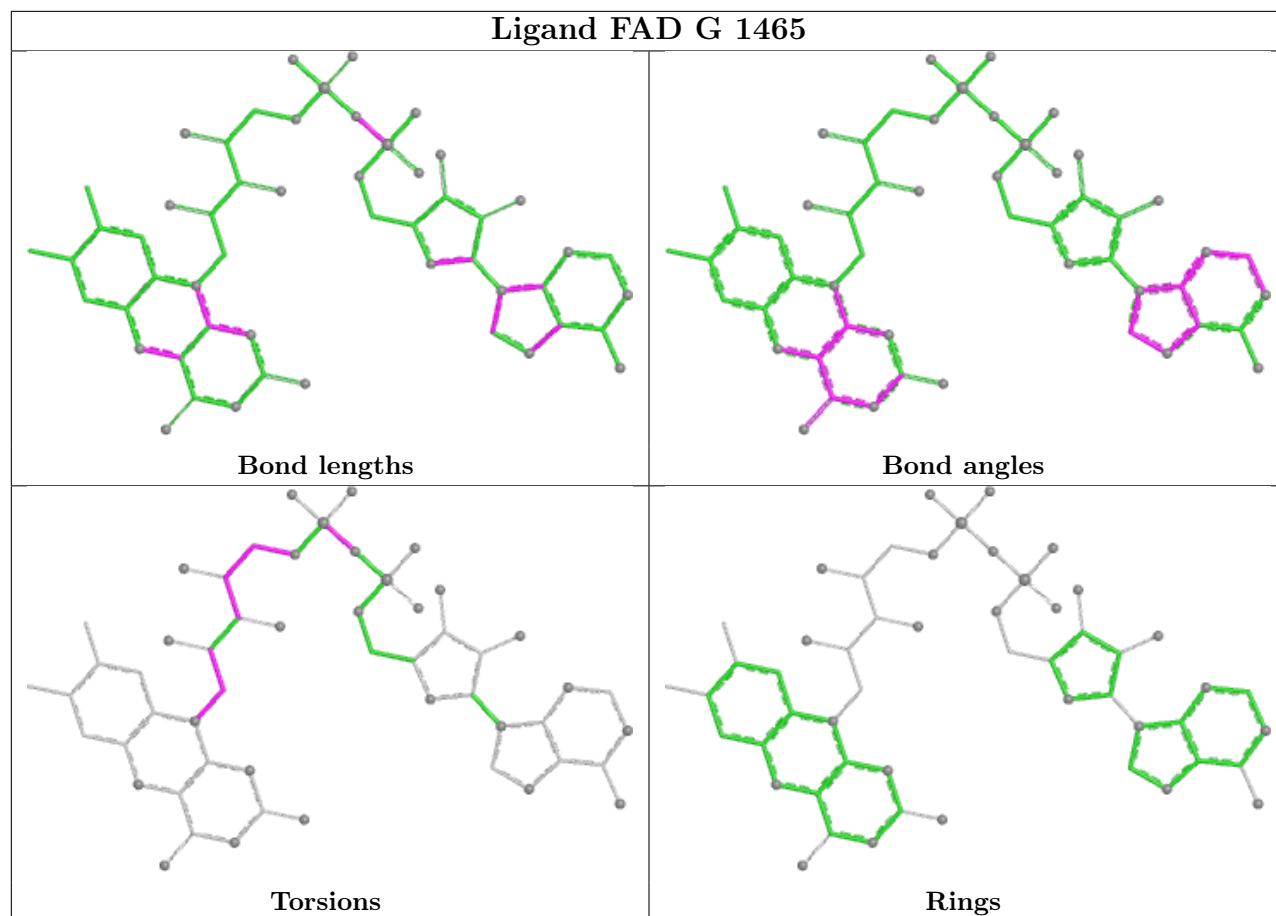
Ligand MTE B 1778



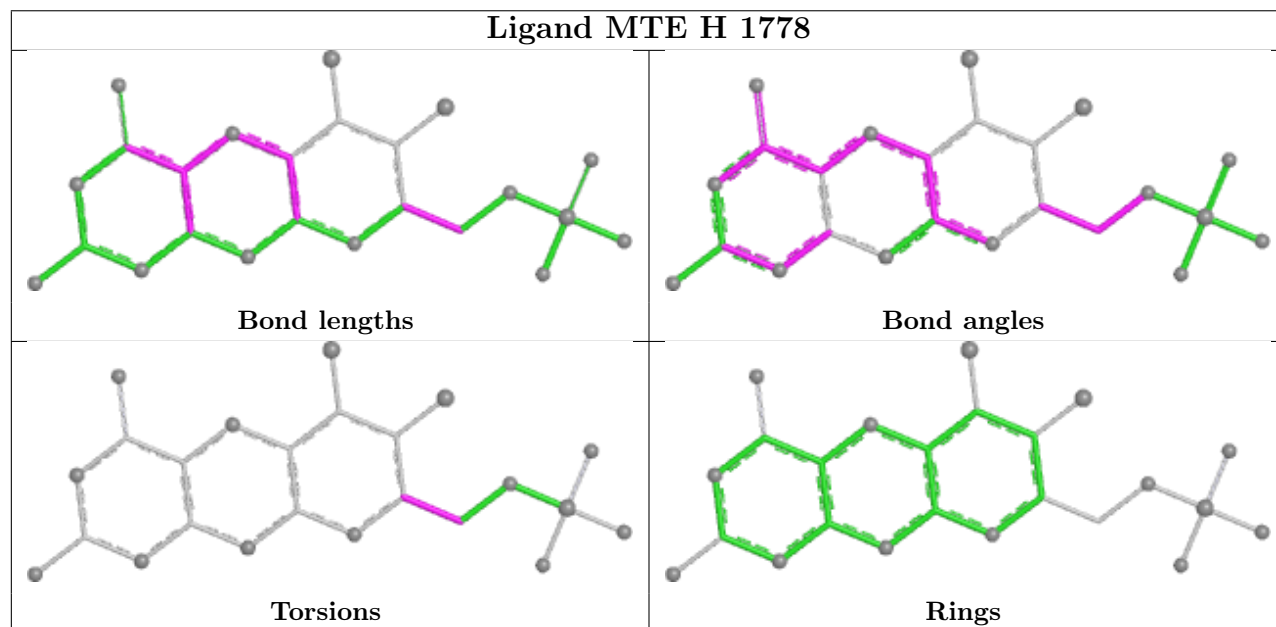
Ligand MTE F 1778

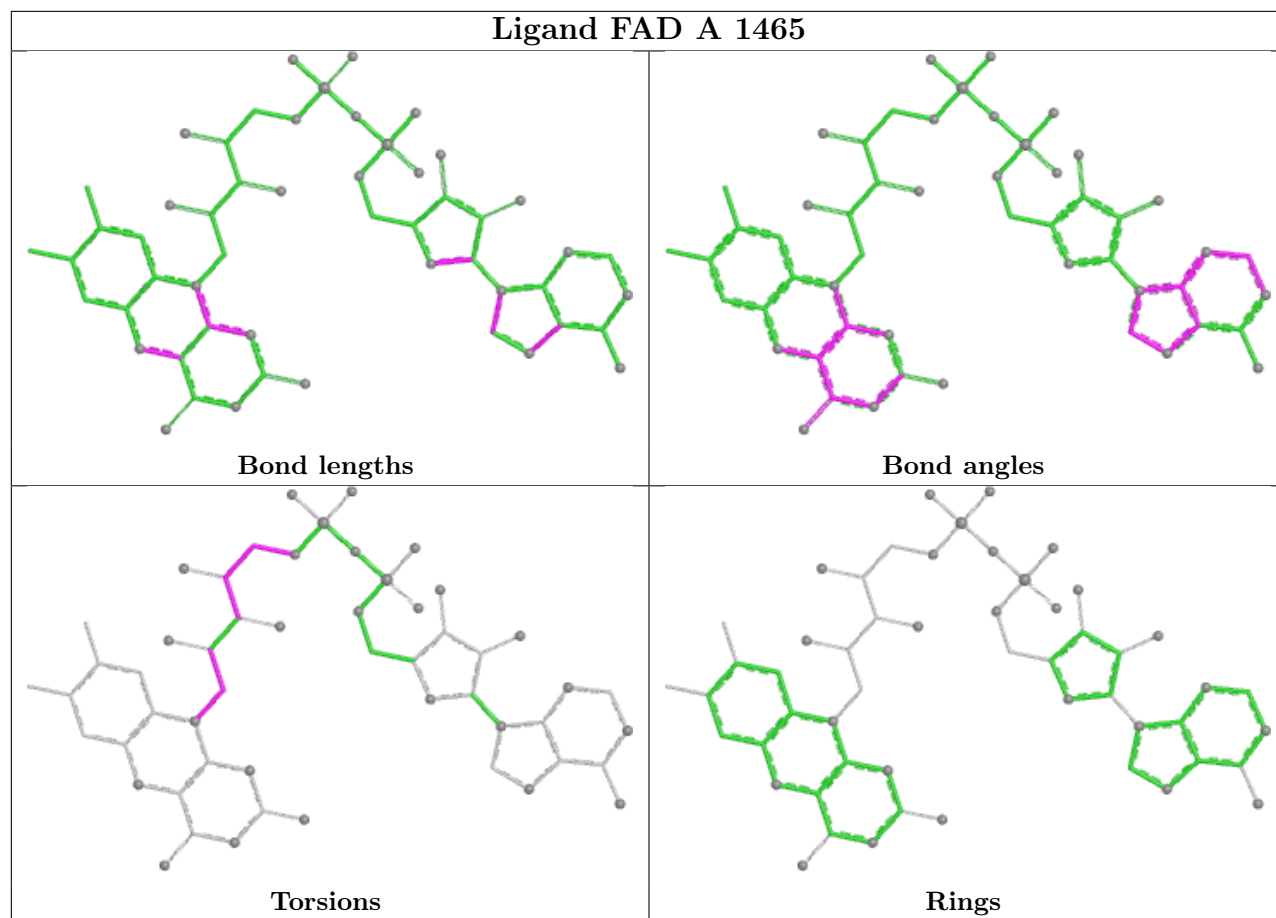


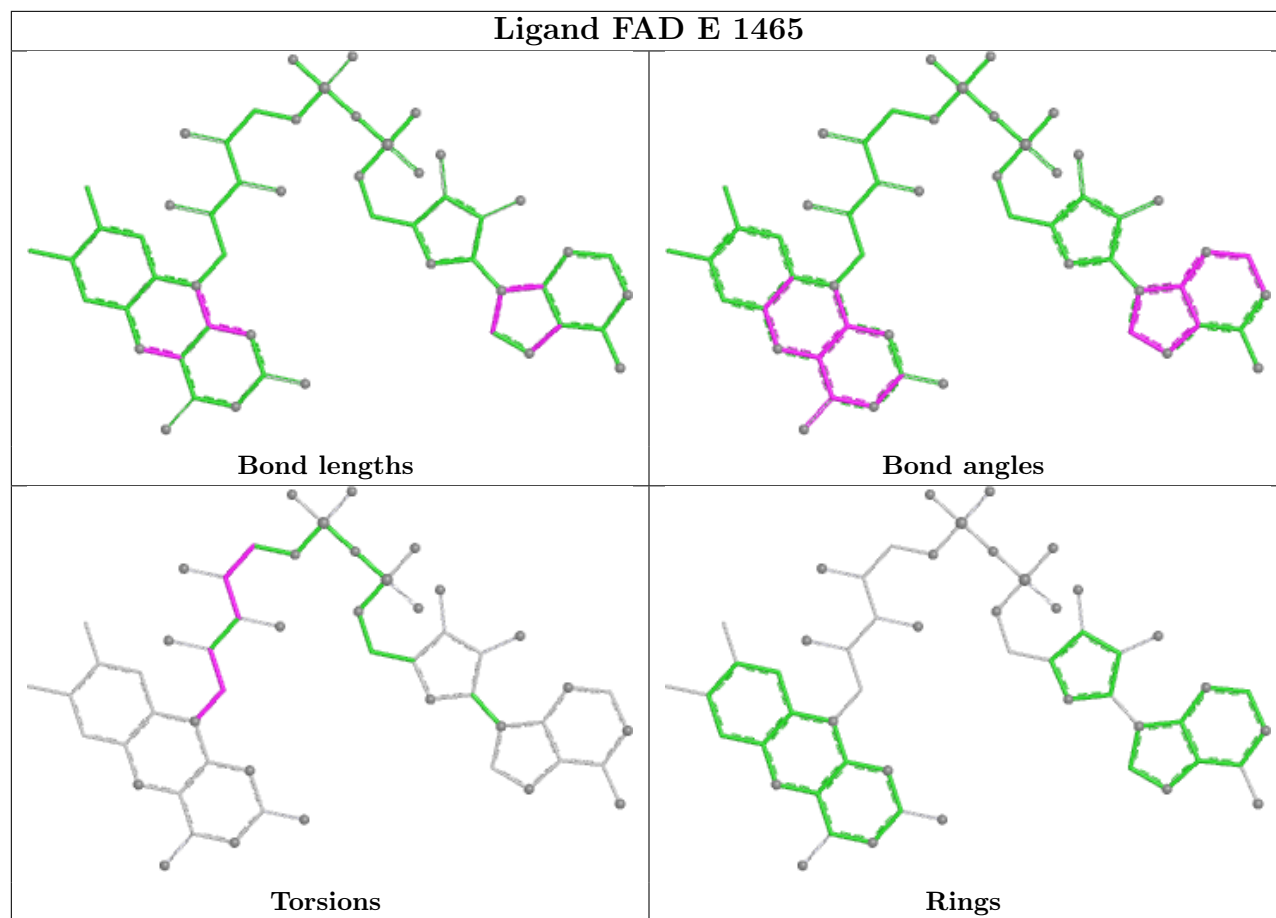
Ligand FAD G 1465

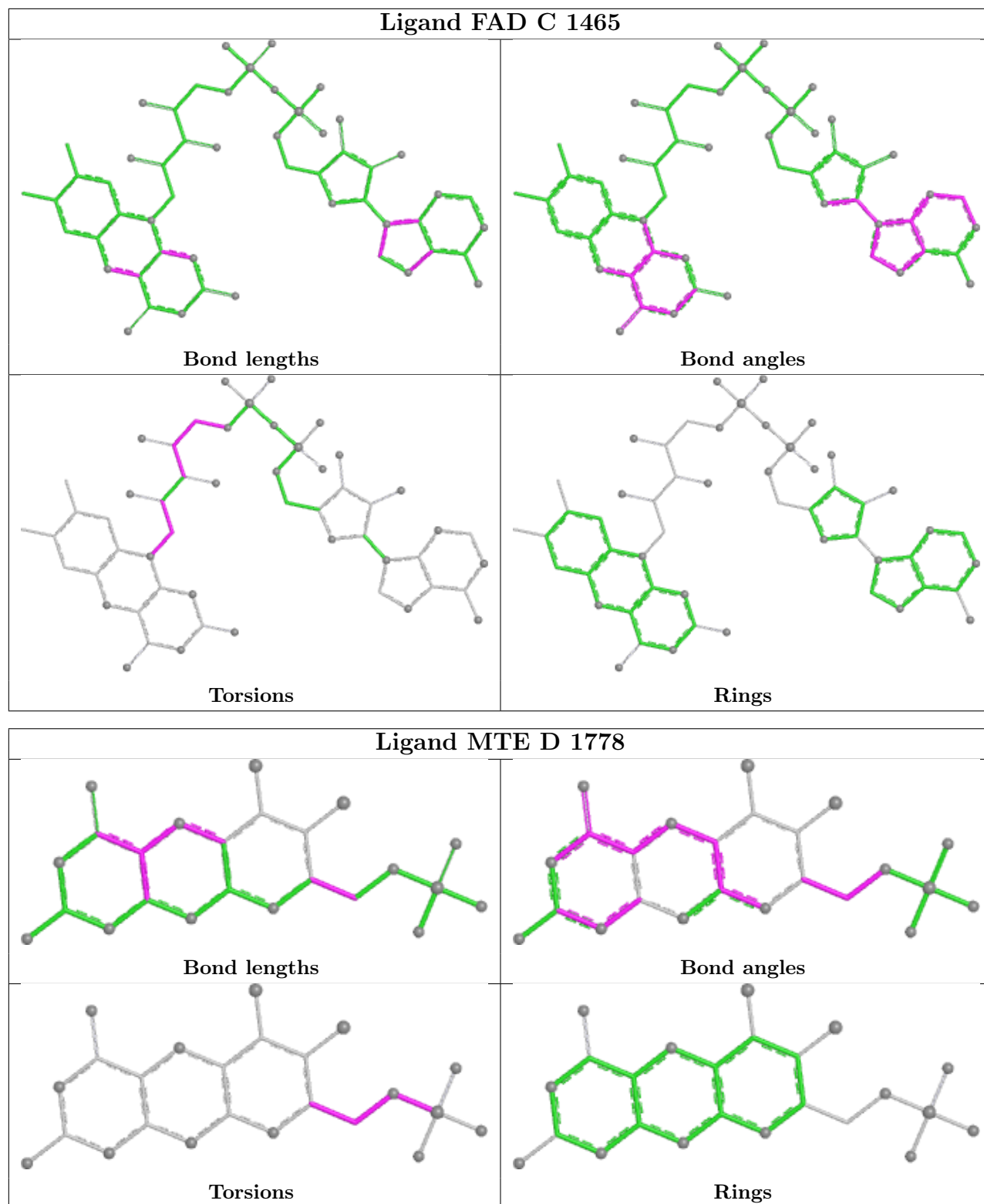


Ligand MTE H 1778









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	450/462 (97%)	1.10	58 (12%) 7 6	40, 63, 78, 79	0
1	C	450/462 (97%)	1.37	94 (20%) 2 2	40, 63, 77, 79	0
1	E	450/462 (97%)	1.16	55 (12%) 8 7	40, 63, 78, 79	0
1	G	450/462 (97%)	1.27	62 (13%) 6 5	40, 63, 78, 79	0
2	B	760/777 (97%)	0.46	14 (1%) 67 59	34, 47, 60, 65	0
2	D	760/777 (97%)	0.61	21 (2%) 55 46	34, 46, 60, 65	0
2	F	760/777 (97%)	0.57	14 (1%) 67 59	35, 46, 60, 65	0
2	H	760/777 (97%)	0.56	9 (1%) 76 69	35, 47, 60, 66	0
All	All	4840/4956 (97%)	0.80	327 (6%) 23 18	34, 51, 75, 79	0

All (327) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	166	LEU	7.9
1	C	166	LEU	5.8
1	G	166	LEU	5.5
1	A	166	LEU	5.2
2	D	560	GLY	5.0
1	G	310	GLY	4.4
1	G	333	GLY	4.3
1	E	461	MET	4.3
1	A	375	SER	4.3
1	A	332	PRO	4.3
1	A	182	LEU	4.0
1	E	179	PRO	4.0
1	C	235	ARG	4.0
1	A	461	MET	3.9
1	C	215	ALA	3.9
1	C	315	ARG	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	777	ALA	3.6
1	G	334	GLU	3.6
1	G	332	PRO	3.6
2	D	284	GLY	3.5
2	D	2	SER	3.5
2	D	777	ALA	3.5
1	C	302	GLY	3.4
1	C	461	MET	3.4
1	A	379	THR	3.4
1	G	242	GLY	3.4
1	A	364	VAL	3.3
1	A	310	GLY	3.3
1	G	241	TYR	3.2
1	E	337	GLU	3.2
1	A	380	ALA	3.2
1	A	239	ASP	3.2
1	G	182	LEU	3.2
1	C	198	GLU	3.2
1	E	338	SER	3.2
1	G	239	ASP	3.2
2	H	777	ALA	3.2
1	C	402	ILE	3.2
1	G	190	ALA	3.1
2	H	137	SER	3.1
1	G	364	VAL	3.1
1	C	324	GLU	3.1
1	E	9	GLY	3.1
1	C	17	GLU	3.1
1	C	165	THR	3.1
1	C	43	ASP	3.1
1	C	291	ILE	3.1
1	E	241	TYR	3.0
2	F	373	ALA	3.0
1	G	455	VAL	3.0
1	C	217	ARG	3.0
1	G	402	ILE	3.0
1	E	462	PRO	3.0
1	A	333	GLY	3.0
1	C	234	ILE	3.0
2	D	373	ALA	3.0
1	G	363	ALA	2.9
1	C	281	ILE	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	241	TYR	2.9
1	E	281	ILE	2.9
1	C	240	GLY	2.9
1	G	43	ASP	2.9
1	C	426	SER	2.9
1	C	228	CYS	2.9
2	F	398	LYS	2.9
2	B	531	SER	2.8
1	G	461	MET	2.8
1	C	233	GLN	2.8
1	E	321	PHE	2.8
1	G	313	ARG	2.8
1	E	181	PHE	2.8
1	E	188	ALA	2.8
1	A	78	ILE	2.8
1	C	226	SER	2.8
1	C	364	VAL	2.7
1	C	164	PHE	2.7
1	C	361	ILE	2.7
1	G	185	THR	2.7
1	C	310	GLY	2.7
1	C	179	PRO	2.7
1	C	303	ALA	2.7
1	C	325	TYR	2.7
1	A	458	LEU	2.7
2	D	398	LYS	2.7
1	G	371	THR	2.7
1	C	239	ASP	2.7
1	E	312	GLU	2.7
2	F	381	GLU	2.7
1	C	225	LEU	2.7
1	E	341	LEU	2.7
1	C	381	ARG	2.7
2	F	560	GLY	2.7
1	G	417	LEU	2.7
1	A	462	PRO	2.6
1	E	225	LEU	2.6
1	G	225	LEU	2.6
1	E	215	ALA	2.6
2	F	777	ALA	2.6
1	A	403	GLY	2.6
1	G	462	PRO	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	281	ASP	2.6
1	A	395	ALA	2.6
1	C	313	ARG	2.6
1	G	325	TYR	2.6
1	A	377	ILE	2.6
1	E	457	VAL	2.6
1	A	316	MET	2.6
1	C	4	ALA	2.6
1	E	189	LEU	2.6
1	A	190	ALA	2.6
1	G	155	ALA	2.6
2	F	529	ALA	2.6
1	A	179	PRO	2.5
1	E	198	GLU	2.5
1	A	438	ALA	2.5
1	A	317	PRO	2.5
1	C	318	LEU	2.5
1	C	408	GLU	2.5
1	E	239	ASP	2.5
2	H	703	ASP	2.5
1	C	231	LEU	2.5
1	G	179	PRO	2.5
1	G	372	LEU	2.5
1	E	234	ILE	2.5
1	E	244	GLY	2.5
1	E	361	ILE	2.5
1	C	163	ALA	2.5
1	C	458	LEU	2.5
1	G	19	PRO	2.5
1	A	234	ILE	2.5
1	A	243	ILE	2.5
1	C	452	GLY	2.5
2	D	567	ILE	2.5
1	G	395	ALA	2.5
1	E	182	LEU	2.4
1	C	462	PRO	2.4
1	A	313	ARG	2.4
1	C	15	ARG	2.4
1	E	378	GLU	2.4
1	C	20	THR	2.4
1	C	9	GLY	2.4
1	C	155	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	454	ALA	2.4
1	A	185	THR	2.4
1	A	423	THR	2.4
1	E	165	THR	2.4
1	G	183	PRO	2.4
1	E	187	ASP	2.4
1	E	302	GLY	2.4
1	G	300	ALA	2.4
1	C	11	THR	2.4
1	C	200	THR	2.4
1	G	237	THR	2.4
1	A	189	LEU	2.4
1	A	402	ILE	2.4
1	G	360	ASP	2.4
2	B	281	ASP	2.4
1	C	25	GLU	2.4
1	A	301	MET	2.4
1	A	371	THR	2.4
1	A	372	LEU	2.4
1	C	323	LEU	2.4
2	D	399	LYS	2.3
1	G	385	GLY	2.3
1	C	350	CYS	2.3
2	B	703	ASP	2.3
1	C	380	ALA	2.3
1	G	116	ALA	2.3
1	E	370	LEU	2.3
1	G	210	LEU	2.3
1	E	346	PRO	2.3
1	C	460	VAL	2.3
2	D	572	GLN	2.3
1	C	206	THR	2.3
2	B	398	LYS	2.3
1	C	337	GLU	2.3
2	B	315	ALA	2.3
2	B	381	GLU	2.3
1	E	316	MET	2.3
2	F	2	SER	2.3
1	G	390	VAL	2.3
1	A	413	ALA	2.3
1	C	232	ALA	2.3
1	C	236	GLU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	370	LEU	2.3
2	D	260	ASP	2.3
1	G	377	ILE	2.3
1	E	379	THR	2.3
1	G	87	ARG	2.3
1	A	457	VAL	2.3
1	C	80	GLY	2.3
1	C	262	ALA	2.2
1	C	400	ALA	2.2
1	E	130	ALA	2.2
1	C	307	LEU	2.2
1	A	411	ILE	2.2
1	A	20	THR	2.2
1	A	226	SER	2.2
1	E	226	SER	2.2
2	D	531	SER	2.2
1	G	323	LEU	2.2
1	A	385	GLY	2.2
1	C	366	GLY	2.2
1	C	335	PHE	2.2
1	C	180	ALA	2.2
1	E	163	ALA	2.2
2	B	636	LEU	2.2
1	E	8	ASN	2.2
1	E	227	HIS	2.2
1	G	222	VAL	2.2
1	C	33	THR	2.2
1	E	282	GLY	2.2
1	G	229	LYS	2.2
1	A	418	LEU	2.2
1	C	182	LEU	2.2
1	G	24	LEU	2.2
1	G	418	LEU	2.2
1	C	388	ALA	2.2
1	C	456	ALA	2.2
1	G	399	ALA	2.2
2	D	350	ALA	2.2
1	C	314	ARG	2.2
1	A	212	VAL	2.2
1	C	238	PRO	2.2
1	C	316	MET	2.2
1	E	151	GLY	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	307	LEU	2.2
1	A	203	ALA	2.2
2	H	613	ARG	2.1
1	A	222	VAL	2.1
1	A	339	VAL	2.1
1	C	390	VAL	2.1
1	C	457	VAL	2.1
2	D	258	ASP	2.1
2	H	75	ASP	2.1
1	C	333	GLY	2.1
2	B	671	GLY	2.1
1	A	164	PHE	2.1
1	E	157	TRP	2.1
1	A	307	LEU	2.1
1	C	158	LEU	2.1
1	E	190	ALA	2.1
1	G	162	ALA	2.1
1	G	254	ALA	2.1
2	H	528	ALA	2.1
2	B	771	ARG	2.1
1	C	243	ILE	2.1
1	G	311	GLN	2.1
1	G	301	MET	2.1
2	B	634	ASP	2.1
1	C	389	GLY	2.1
1	E	306	THR	2.1
1	E	389	GLY	2.1
2	H	671	GLY	2.1
1	E	201	LEU	2.1
1	G	341	LEU	2.1
1	A	235	ARG	2.1
1	A	325	TYR	2.1
1	A	326	ARG	2.1
1	A	51	ILE	2.1
2	D	81	SER	2.1
2	B	264	VAL	2.1
1	C	342	PRO	2.1
2	D	452	PRO	2.1
1	A	425	LEU	2.1
1	E	333	GLY	2.1
1	G	194	LEU	2.1
1	C	326	ARG	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	163	ALA	2.1
1	G	394	ALA	2.1
1	G	443	ALA	2.1
2	F	357	ILE	2.1
2	F	416	GLU	2.1
1	G	159	GLN	2.1
1	A	1	MET	2.1
1	C	212	VAL	2.1
1	E	220	PRO	2.1
1	G	238	PRO	2.1
1	C	8	ASN	2.1
1	E	369	ASN	2.1
1	C	406	PHE	2.1
1	G	255	PHE	2.1
1	E	20	THR	2.1
2	B	637	THR	2.1
1	C	430	ALA	2.1
1	G	188	ALA	2.1
1	G	383	ALA	2.1
2	F	713	TRP	2.1
1	C	221	GLU	2.1
1	C	378	GLU	2.1
1	G	186	SER	2.0
1	C	311	GLN	2.0
2	D	578	LYS	2.0
1	C	455	VAL	2.0
2	D	632	VAL	2.0
1	E	238	PRO	2.0
2	F	287	LEU	2.0
1	G	389	GLY	2.0
1	A	361	ILE	2.0
1	C	382	ILE	2.0
1	E	410	THR	2.0
1	G	165	THR	2.0
2	F	440	THR	2.0
2	H	168	ILE	2.0
1	C	195	ALA	2.0
2	D	280	ALA	2.0
2	D	529	ALA	2.0
2	D	381	GLU	2.0
1	C	434	TYR	2.0
1	E	193	TYR	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	426	SER	2.0
1	G	457	VAL	2.0
1	A	19	PRO	2.0
1	G	317	PRO	2.0
1	C	401	LEU	2.0
1	C	253	ARG	2.0
1	A	242	GLY	2.0
2	F	723	PHE	2.0
1	A	264	ALA	2.0
1	C	410	THR	2.0
1	C	441	ALA	2.0
1	A	218	ASP	2.0
1	C	218	ASP	2.0
2	F	714	ASP	2.0
2	B	668	TYR	2.0
1	E	222	VAL	2.0
2	D	321	VAL	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
7	HPA	F	1780	10/10	0.80	0.19	55,56,57,57	0
7	HPA	B	1780	10/10	0.81	0.19	57,58,58,58	0
7	HPA	D	1780	10/10	0.82	0.19	52,53,54,54	0
7	HPA	H	1780	10/10	0.83	0.15	59,59,60,60	0
4	FAD	G	1465	53/53	0.88	0.15	68,70,76,76	0
4	FAD	A	1465	53/53	0.90	0.12	58,61,68,68	0

Continued on next page...

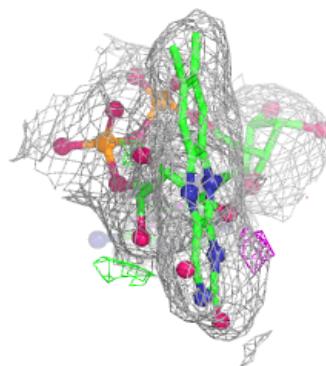
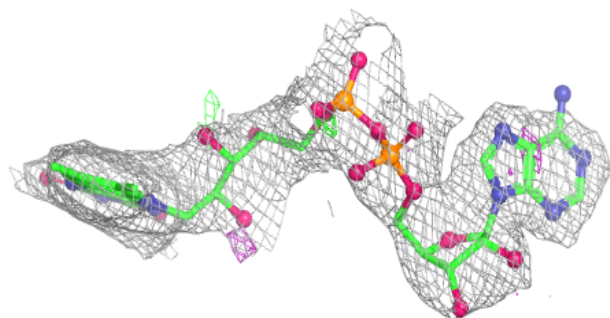
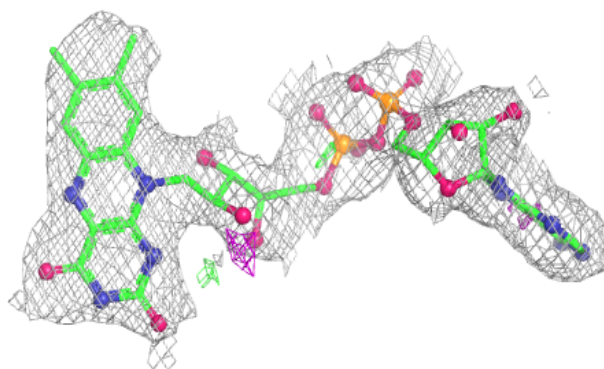
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MTE	B	1778	24/24	0.91	0.17	50,52,54,55	24
5	MTE	F	1778	24/24	0.91	0.16	39,40,42,42	24
4	FAD	E	1465	53/53	0.92	0.12	51,58,73,73	0
5	MTE	D	1778	24/24	0.93	0.15	30,35,39,39	24
5	MTE	H	1778	24/24	0.93	0.16	60,61,64,65	24
4	FAD	C	1465	53/53	0.94	0.10	32,35,44,44	0
8	MOM	H	1781	4/4	0.95	0.19	63,65,66,66	3
6	CA	H	1779	1/1	0.96	0.07	65,65,65,65	0
6	CA	B	1779	1/1	0.97	0.05	55,55,55,55	0
6	CA	D	1779	1/1	0.97	0.04	48,48,48,48	0
6	CA	F	1779	1/1	0.97	0.07	54,54,54,54	0
3	FES	E	1463	4/4	0.98	0.05	43,43,45,45	0
3	FES	E	1464	4/4	0.98	0.07	55,56,56,58	0
3	FES	G	1463	4/4	0.98	0.04	47,49,50,50	0
3	FES	A	1464	4/4	0.98	0.06	52,52,53,53	0
8	MOM	B	1781	4/4	0.98	0.18	55,55,56,58	3
3	FES	C	1464	4/4	0.98	0.07	42,42,44,46	0
3	FES	A	1463	4/4	0.99	0.04	41,42,42,43	0
3	FES	C	1463	4/4	0.99	0.06	38,40,40,41	0
8	MOM	F	1781	4/4	0.99	0.07	40,41,42,42	3
3	FES	G	1464	4/4	0.99	0.06	53,55,55,56	0
8	MOM	D	1781	4/4	1.00	0.08	38,38,39,40	3

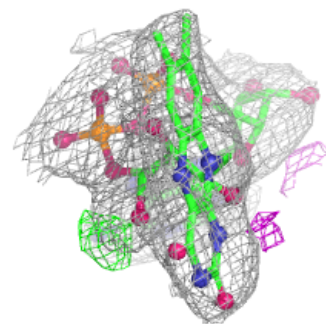
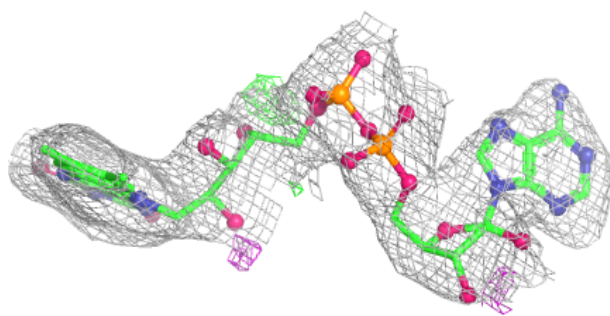
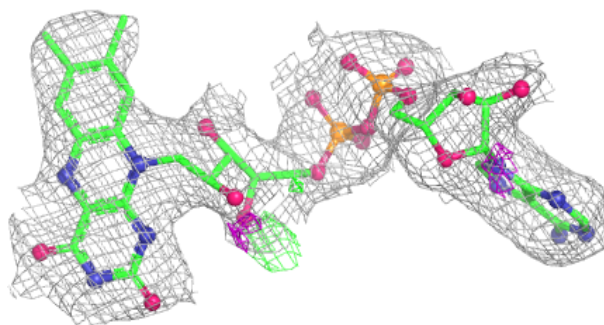
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD G 1465:

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

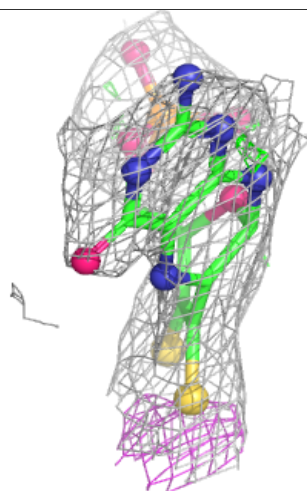
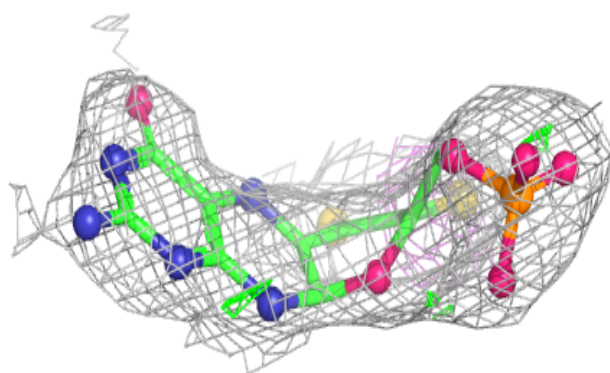
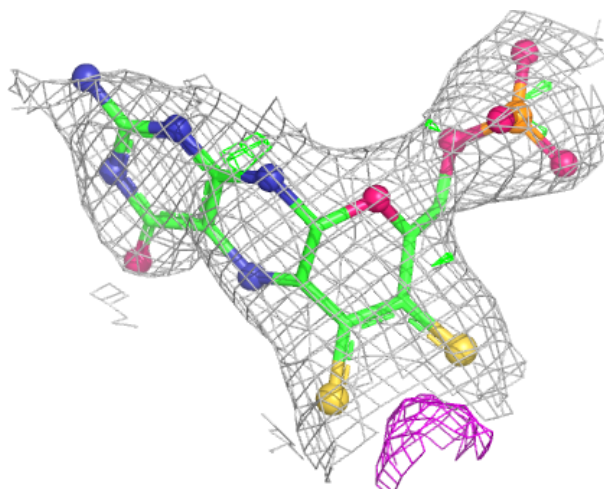
**Electron density around FAD A 1465:**

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



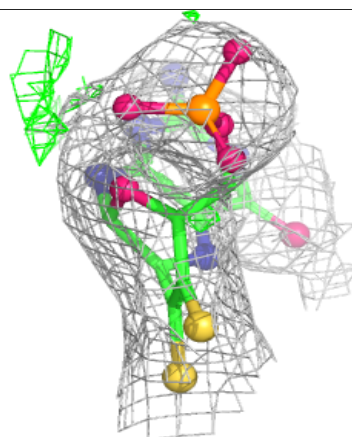
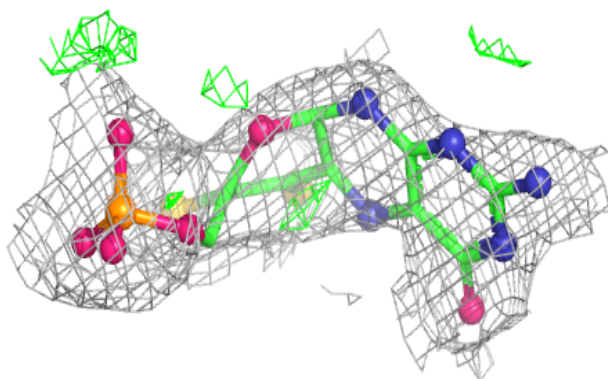
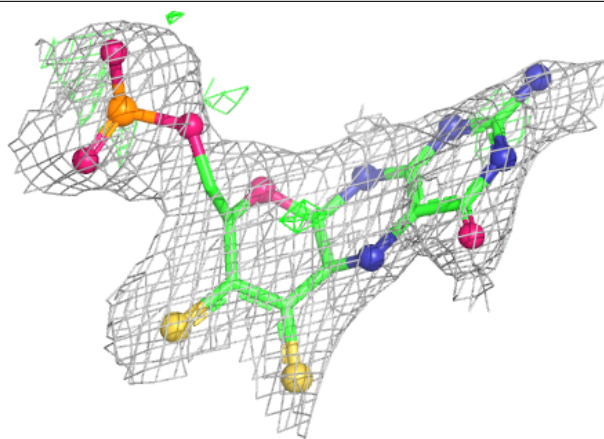
Electron density around MTE B 1778:

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

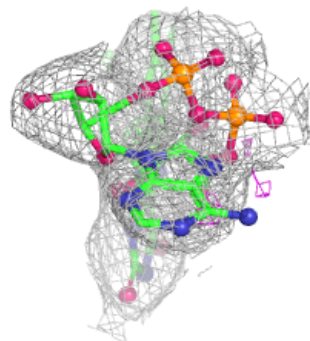
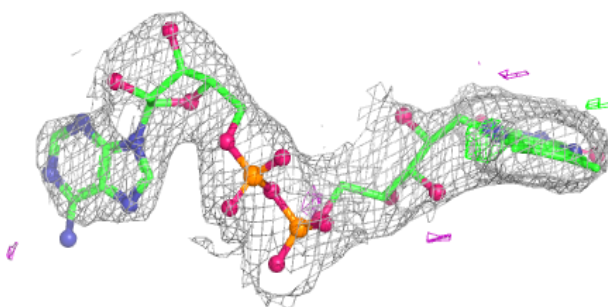
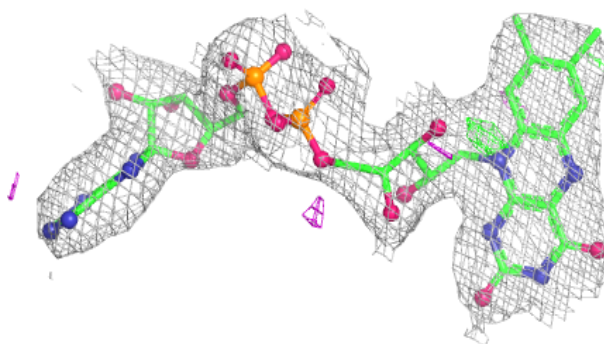


Electron density around MTE F 1778:

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

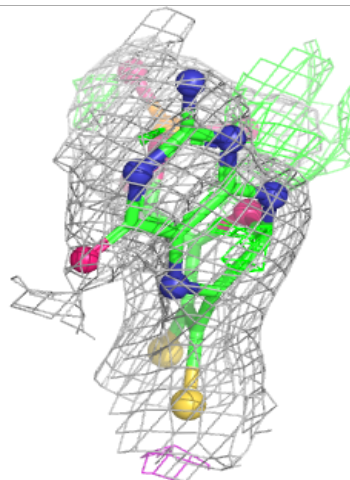
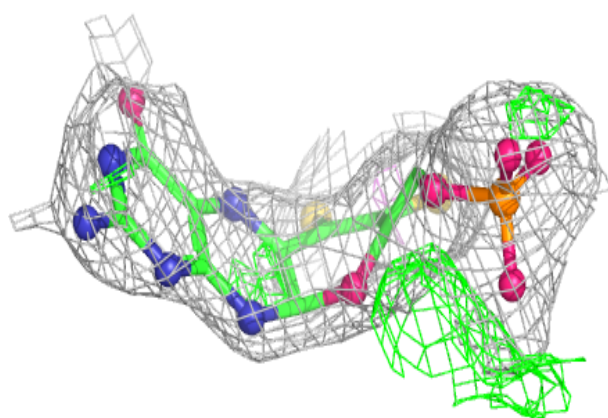
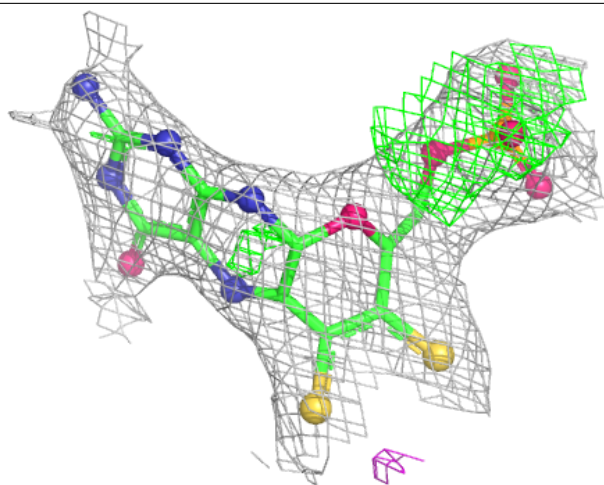
**Electron density around FAD E 1465:**

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



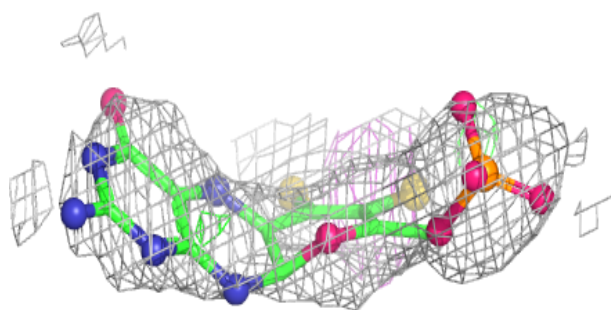
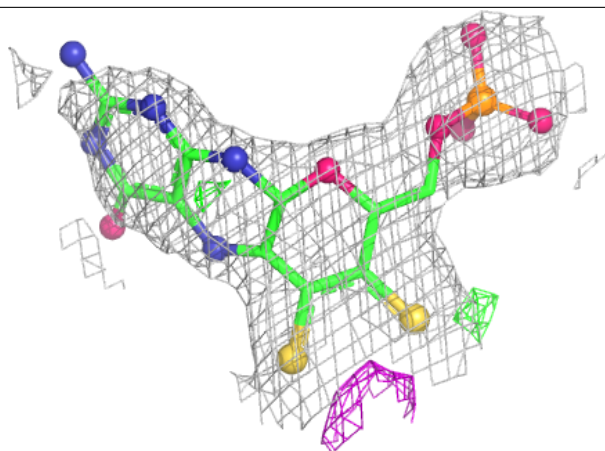
Electron density around MTE D 1778:

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

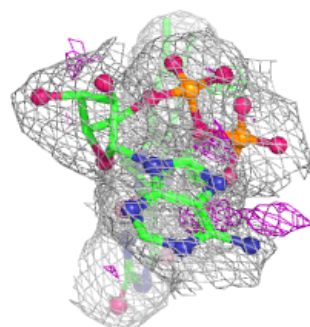
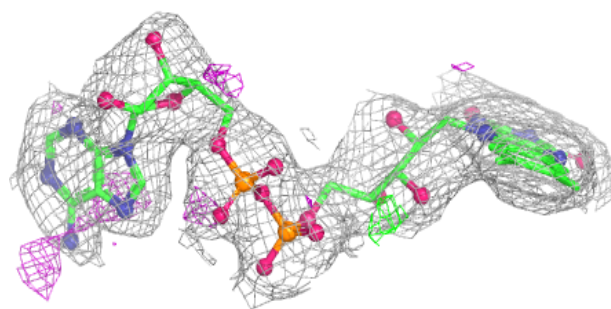
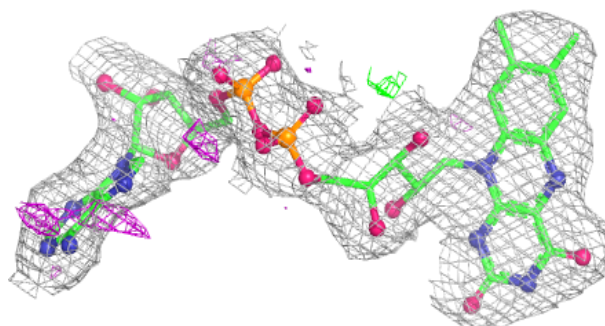


Electron density around MTE H 1778:

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

**Electron density around FAD C 1465:**

$2mF_o-DF_c$ (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.