



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 01:28 am BST

PDB ID : 3ETR  
Title : Crystal structure of xanthine oxidase in complex with lumazine  
Authors : Paufl, J.M.; Cao, H.; Hille, R.  
Deposited on : 2008-10-08  
Resolution : 2.20 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

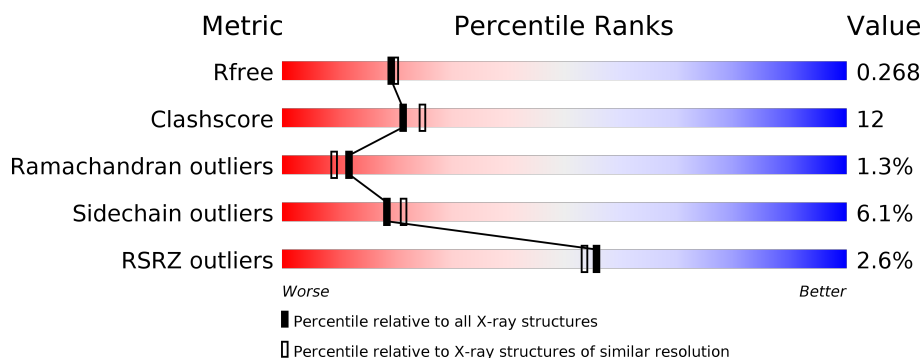
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	164	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>20%</div> <div>• •</div> </div> </div>
1	L	164	<div> <div>6%</div> <div> <div></div> <div>84%</div> <div>12%</div> <div>• •</div> </div> </div>
2	B	305	<div> <div>%</div> <div> <div></div> <div>77%</div> <div>18%</div> <div>• •</div> </div> </div>
2	M	305	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>18%</div> <div>•</div> </div> </div>
3	C	755	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>20%</div> <div>• •</div> </div> </div>
3	N	755	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>22%</div> <div>• •</div> </div> </div>

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
7	MOS	N	1327	-	-	X	-
8	LUZ	N	1	-	-	X	-

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 20307 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/oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	164	Total	C	N	O	S	0	0	0
			1255	788	225	230	12			
1	L	164	Total	C	N	O	S	0	0	0
			1255	788	225	230	12			

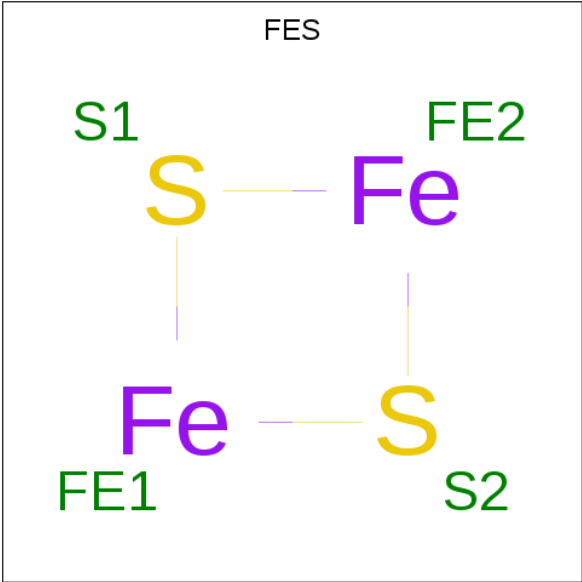
- Molecule 2 is a protein called Xanthine dehydrogenase/oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	305	Total	C	N	O	S	0	0	0
			2389	1539	402	435	13			
2	M	305	Total	C	N	O	S	0	0	0
			2389	1539	402	435	13			

- Molecule 3 is a protein called Xanthine dehydrogenase/oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	755	Total	C	N	O	S	0	0	0
			5823	3680	1003	1105	35			
3	N	745	Total	C	N	O	S	0	0	0
			5761	3643	992	1093	33			

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



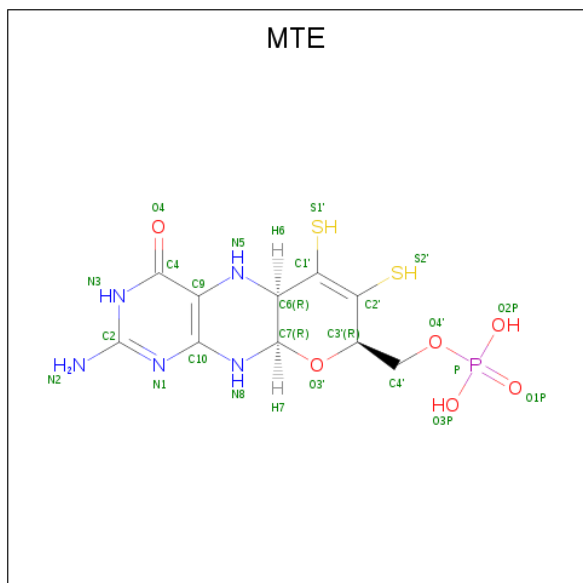
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			4	2	2		
4	A	1	Total	Fe	S	0	0
			4	2	2		
4	L	1	Total	Fe	S	0	0
			4	2	2		
4	L	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



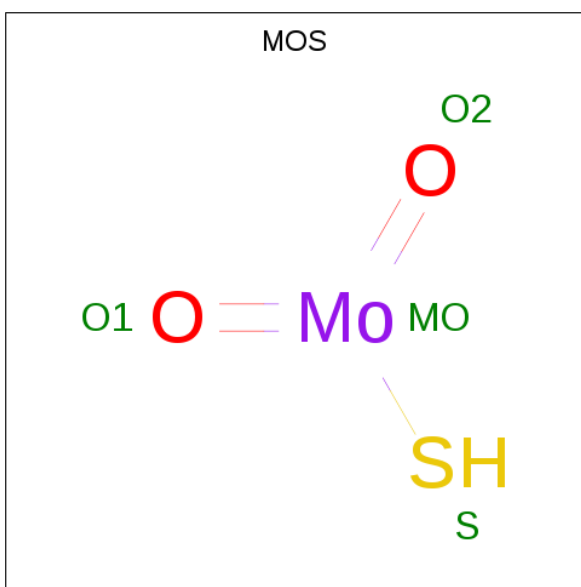
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	M	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 6 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 (three-letter code: MTE) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>6</sub>P S<sub>2</sub>).



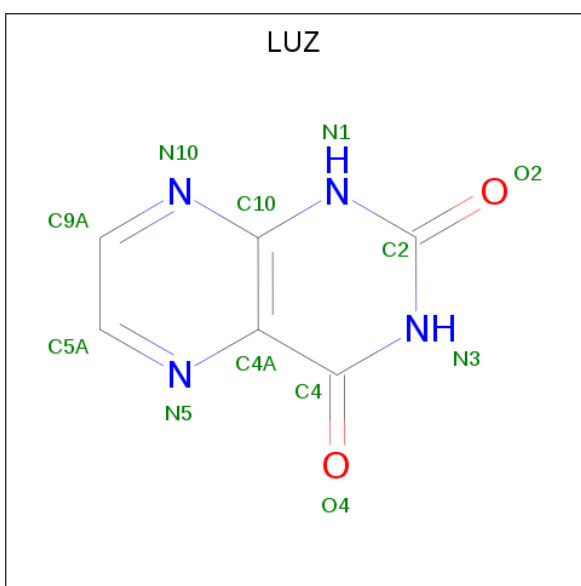
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	C	1	Total 24	C 10	N 5	O 6	P 1	S 2	0	0
6	N	1	Total 24	C 10	N 5	O 6	P 1	S 2	0	0

- Molecule 7 is DIOXOTHIOMOLYBDENUM(VI) ION (three-letter code: MOS) (formula: HMoO<sub>2</sub>S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	Mo	O	S	0	0
			4	1	2	1		
7	N	1	Total	Mo	O	S	0	0
			4	1	2	1		

- Molecule 8 is pteridine-2,4(1H,3H)-dione (three-letter code: LUZ) (formula:  $C_6H_4N_4O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	1	Total	C	N	O	0	0
			12	6	4	2		
8	N	1	Total	C	N	O	0	0
			12	6	4	2		

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	1	Total 1	Ca 1	0	0

- Molecule 10 is water.

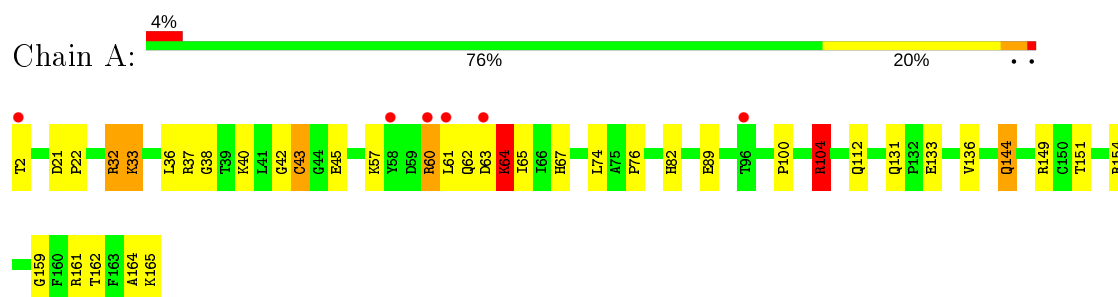
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	101	Total 101	O 101	0	0
10	B	171	Total 171	O 171	0	0
10	C	368	Total 368	O 368	0	0
10	L	116	Total 116	O 116	0	0
10	M	128	Total 128	O 128	0	0
10	N	348	Total 348	O 348	0	0



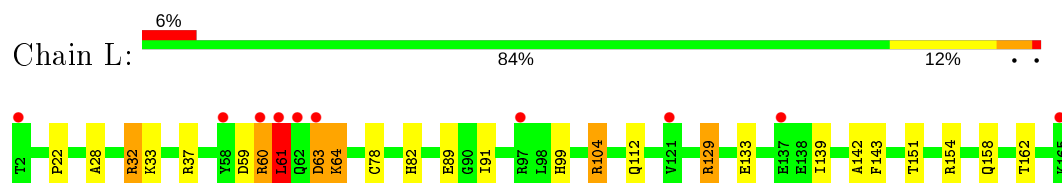
### 3 Residue-property plots [i](#)

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

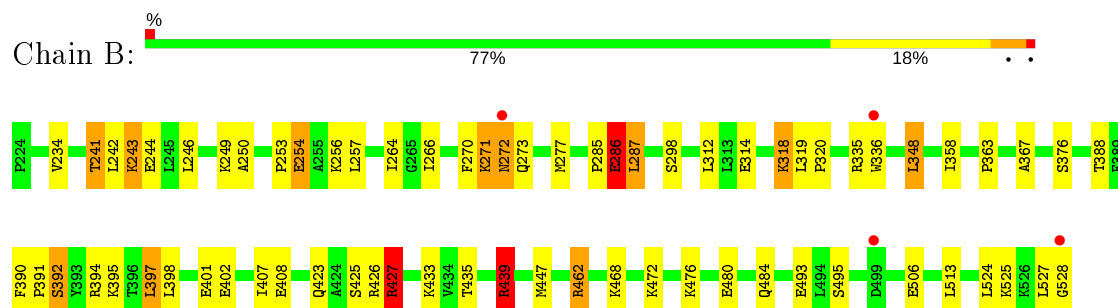
- Molecule 1: Xanthine dehydrogenase/oxidase



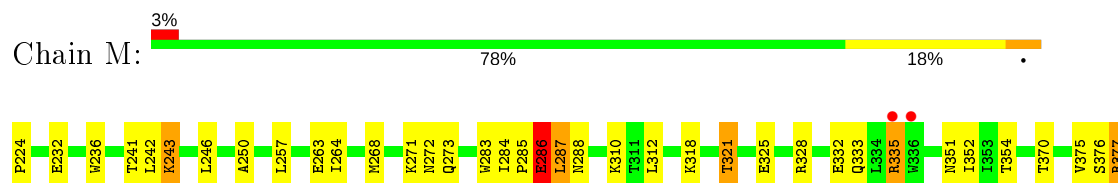
- Molecule 1: Xanthine dehydrogenase/oxidase

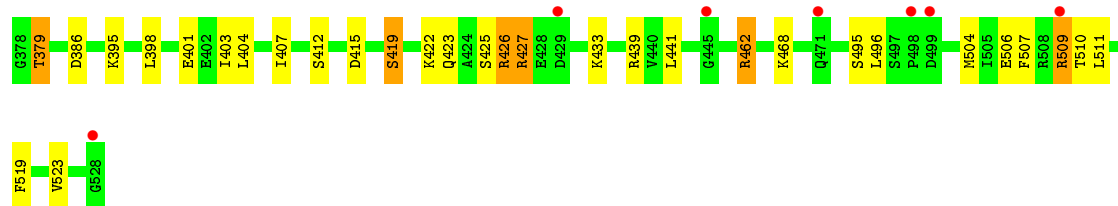


- Molecule 2: Xanthine dehydrogenase/oxidase

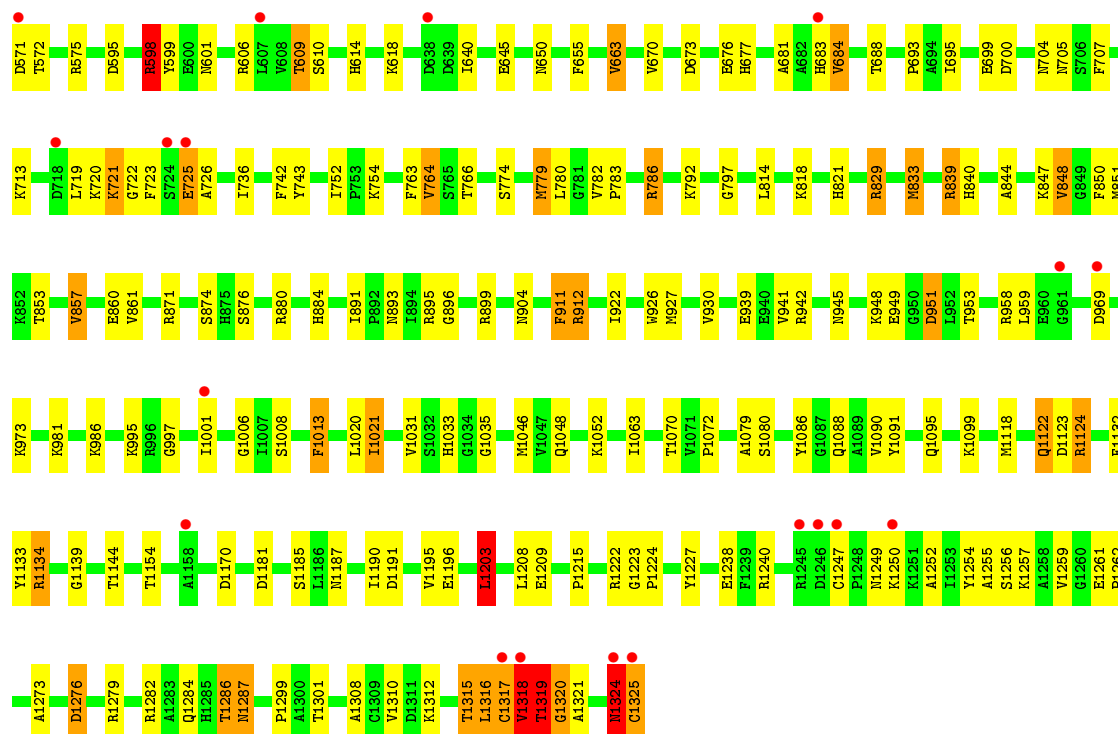
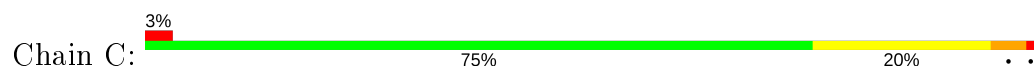


- Molecule 2: Xanthine dehydrogenase/oxidase

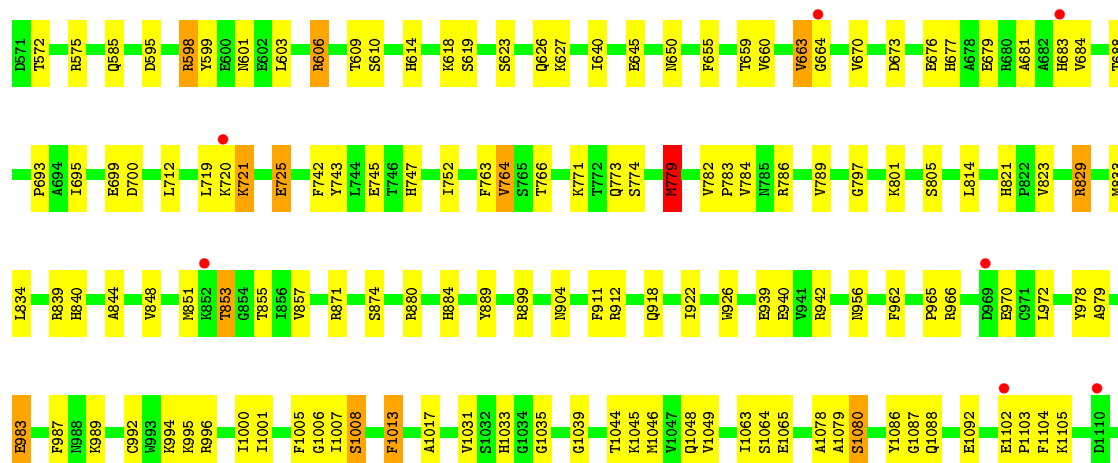
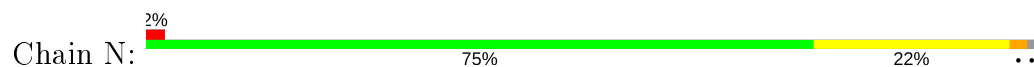


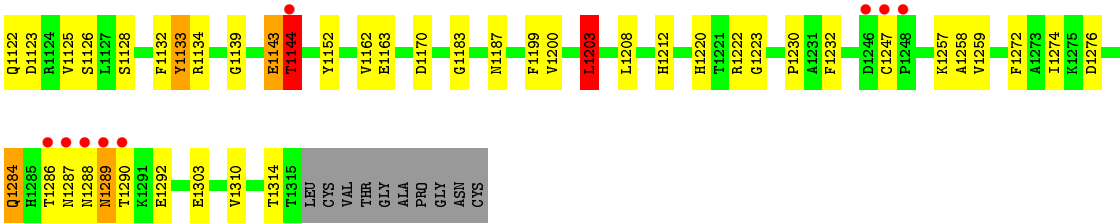


• Molecule 3: Xanthine dehydrogenase/oxidase



• Molecule 3: Xanthine dehydrogenase/oxidase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	133.19 Å 73.49 Å 146.50 Å 90.00° 98.68° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 26.42 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.7 (50.00-2.20) 98.8 (26.42-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.20	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.53 (at 2.20 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.197 , 0.267 0.199 , 0.268	Depositor DCC
$R_{free}$ test set	7052 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.1	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 51.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	20307	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MOS, LUZ, FES, CA, FAD, 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	0.99	0/1277	0.96	5/1723 (0.3%)
1	L	0.87	0/1277	0.87	3/1723 (0.2%)
2	B	0.93	1/2438 (0.0%)	0.92	5/3290 (0.2%)
2	M	0.82	0/2438	0.86	3/3290 (0.1%)
3	C	0.94	2/5951 (0.0%)	0.98	18/8061 (0.2%)
3	N	0.92	5/5888 (0.1%)	0.94	10/7974 (0.1%)
All	All	0.92	8/19269 (0.0%)	0.94	44/26061 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
3	C	0	3
All	All	0	5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	664	GLY	N-CA	5.95	1.54	1.46
3	N	725	GLU	CB-CG	5.88	1.63	1.52
3	N	745	GLU	CB-CG	5.54	1.62	1.52
3	C	1324	ASN	CB-CG	5.53	1.63	1.51
3	N	992	CYS	CB-SG	-5.36	1.73	1.81
3	N	1133	TYR	CD1-CE1	5.20	1.47	1.39
2	B	286	GLU	CG-CD	5.15	1.59	1.51
3	C	699	GLU	CG-CD	5.12	1.59	1.51

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	839	ARG	NE-CZ-NH2	-11.56	114.52	120.30
3	C	839	ARG	NE-CZ-NH2	-11.12	114.74	120.30
2	B	439	ARG	NE-CZ-NH2	-10.69	114.95	120.30
3	N	839	ARG	NE-CZ-NH1	9.69	125.15	120.30
3	N	779	MET	CG-SD-CE	-9.49	85.02	100.20
3	N	829	ARG	NE-CZ-NH2	-9.34	115.63	120.30
3	N	606	ARG	NE-CZ-NH2	-9.21	115.69	120.30
3	C	1203	LEU	CA-CB-CG	8.59	135.06	115.30
3	N	1203	LEU	CA-CB-CG	8.42	134.66	115.30
3	C	942	ARG	NE-CZ-NH1	8.20	124.40	120.30
1	L	61	LEU	CA-CB-CG	7.90	133.47	115.30
1	L	32	ARG	NE-CZ-NH1	7.23	123.92	120.30
3	C	942	ARG	NE-CZ-NH2	-7.23	116.69	120.30
3	N	829	ARG	NE-CZ-NH1	7.08	123.84	120.30
3	C	663	VAL	C-N-CA	-7.01	107.58	122.30
3	C	829	ARG	NE-CZ-NH2	-6.79	116.91	120.30
3	C	839	ARG	NE-CZ-NH1	6.58	123.59	120.30
3	C	1315	THR	C-N-CA	-6.38	105.76	121.70
3	C	1325	CYS	CA-CB-SG	6.20	125.17	114.00
3	C	1021	ILE	CG1-CB-CG2	-5.95	98.30	111.40
1	A	32	ARG	NE-CZ-NH1	-5.89	117.36	120.30
2	B	513	LEU	CA-CB-CG	5.84	128.72	115.30
1	L	32	ARG	NE-CZ-NH2	-5.81	117.39	120.30
3	N	606	ARG	NE-CZ-NH1	5.81	123.20	120.30
2	B	439	ARG	NE-CZ-NH1	5.80	123.20	120.30
3	C	1134	ARG	CB-CA-C	-5.69	99.01	110.40
3	C	606	ARG	NE-CZ-NH2	-5.68	117.46	120.30
3	C	1318	VAL	N-CA-C	5.63	126.20	111.00
1	A	33	LYS	CD-CE-NZ	-5.52	99.01	111.70
2	M	286	GLU	N-CA-C	-5.49	96.17	111.00
2	M	398	LEU	CA-CB-CG	5.47	127.88	115.30
3	C	598	ARG	NE-CZ-NH2	-5.43	117.58	120.30
3	N	663	VAL	C-N-CA	-5.42	110.93	122.30
2	B	398	LEU	CA-CB-CG	5.40	127.72	115.30
3	N	871	ARG	NE-CZ-NH2	-5.39	117.61	120.30
2	B	427	ARG	NE-CZ-NH2	-5.38	117.61	120.30
2	M	441	LEU	CA-CB-CG	5.37	127.66	115.30
1	A	104	ARG	NE-CZ-NH1	5.36	122.98	120.30
3	C	786	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	A	149	ARG	NE-CZ-NH2	-5.34	117.63	120.30
3	C	684	VAL	CB-CA-C	5.11	121.10	111.40
3	C	1124	ARG	NE-CZ-NH2	-5.09	117.76	120.30
3	C	833	MET	CG-SD-CE	-5.05	92.12	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	21	ASP	CB-CG-OD1	5.02	122.82	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	62	GLN	Peptide
1	A	64	LYS	Peptide
3	C	1316	LEU	Peptide
3	C	1318	VAL	Peptide
3	C	1320	GLY	Peptide

## 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	1255	0	1265	23	0
1	L	1255	0	1265	23	0
2	B	2389	0	2459	55	0
2	M	2389	0	2459	57	0
3	C	5823	0	5746	179	0
3	N	5761	0	5685	149	0
4	A	8	0	0	0	0
4	L	8	0	0	0	0
5	B	53	0	31	2	0
5	M	53	0	31	2	0
6	C	24	0	11	1	0
6	N	24	0	10	0	0
7	C	4	0	0	1	0
7	N	4	0	0	2	0
8	C	12	0	4	0	0
8	N	12	0	4	5	0
9	C	1	0	0	0	0
10	A	101	0	0	2	0
10	B	171	0	0	2	0
10	C	368	0	0	12	0
10	L	116	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	M	128	0	0	7	0
10	N	348	0	0	11	0
All	All	20307	0	18970	458	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 12.

All (458) 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)
3:C:1317:CYS:HB3	3:C:1318:VAL:CB	1.42	1.50
3:C:1317:CYS:HB2	3:C:1319:THR:N	1.09	1.40
3:C:1317:CYS:HB3	3:C:1318:VAL:CA	1.46	1.37
3:C:1317:CYS:CB	3:C:1319:THR:N	2.00	1.24
3:C:618:LYS:HB2	10:C:1551:HOH:O	1.40	1.21
3:C:1317:CYS:CB	3:C:1318:VAL:C	2.10	1.19
3:C:1317:CYS:CB	3:C:1318:VAL:CA	2.20	1.17
2:B:285:PRO:O	2:B:286:GLU:HB2	1.43	1.17
3:C:1317:CYS:HB2	3:C:1318:VAL:C	1.66	1.14
3:C:1312:LYS:HD3	3:C:1318:VAL:HG21	1.29	1.13
2:B:286:GLU:O	2:B:287:LEU:HB2	1.39	1.11
2:M:404:LEU:HD21	2:M:407:ILE:HD11	1.32	1.11
2:M:286:GLU:O	2:M:288:ASN:N	1.85	1.09
3:C:1315:THR:HG21	3:C:1324:ASN:HA	1.31	1.08
3:C:1317:CYS:SG	3:C:1318:VAL:HG12	1.96	1.06
3:C:1317:CYS:CB	3:C:1318:VAL:CB	2.34	1.04
3:N:725:GLU:HG3	3:N:851:MET:HE1	1.42	1.02
3:C:829:ARG:HG3	3:C:833:MET:HE2	1.38	1.01
2:B:243:LYS:HD3	2:B:243:LYS:H	1.25	1.01
3:N:779:MET:SD	10:N:1380:HOH:O	2.18	1.00
3:C:1317:CYS:HB3	3:C:1318:VAL:HB	1.38	0.98
2:B:243:LYS:N	2:B:243:LYS:HD3	1.77	0.98
10:M:674:HOH:O	3:N:683:HIS:HB2	1.64	0.98
3:C:1317:CYS:HB3	3:C:1318:VAL:C	1.77	0.97
2:M:243:LYS:HD3	2:M:243:LYS:H	1.30	0.96
2:M:325:GLU:HB2	2:M:412:SER:OG	1.63	0.96
3:N:1046:MET:HE1	3:N:1087:GLY:N	1.80	0.95
7:N:1327:MOS:O1	8:N:1:LUZ:H9A	1.66	0.95
2:B:285:PRO:O	2:B:286:GLU:CB	2.13	0.94
3:N:782:VAL:HG12	3:N:783:PRO:HD2	1.47	0.94
3:N:1046:MET:HE1	3:N:1086:TYR:C	1.87	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1317:CYS:CB	3:C:1318:VAL:HB	1.99	0.93
2:M:243:LYS:HD3	2:M:243:LYS:N	1.84	0.92
3:C:1286:THR:O	3:C:1325:CYS:C	2.07	0.92
3:N:779:MET:CG	10:N:1380:HOH:O	2.18	0.91
3:N:833:MET:HE3	3:N:1222:ARG:C	1.91	0.91
3:C:833:MET:HE3	3:C:1222:ARG:O	1.72	0.90
2:B:241:THR:HG23	2:B:243:LYS:HG2	1.52	0.89
3:N:833:MET:HE3	3:N:1223:GLY:N	1.87	0.89
3:N:983:GLU:HG3	10:N:1596:HOH:O	1.73	0.88
2:B:314:GLU:O	2:B:318:LYS:HD2	1.73	0.88
3:N:833:MET:HE3	3:N:1223:GLY:CA	2.04	0.88
3:C:926:TRP:HZ3	3:C:927:MET:HE2	1.38	0.88
3:N:1046:MET:CE	3:N:1086:TYR:C	2.41	0.87
3:C:829:ARG:CG	3:C:833:MET:HE2	2.04	0.86
2:B:286:GLU:O	2:B:287:LEU:CB	2.16	0.85
2:M:509:ARG:HH11	2:M:509:ARG:HG2	1.37	0.85
3:C:884:HIS:HE1	3:C:1006:GLY:H	1.22	0.85
2:M:257:LEU:O	5:M:606:FAD:H2B	1.76	0.85
3:N:833:MET:HE3	3:N:1223:GLY:HA2	1.57	0.85
3:C:1317:CYS:HB3	3:C:1318:VAL:CG1	2.06	0.85
3:C:1312:LYS:CD	3:C:1318:VAL:HG21	2.07	0.85
3:N:782:VAL:HG12	3:N:783:PRO:CD	2.08	0.84
1:L:32:ARG:NH2	10:L:614:HOH:O	2.10	0.84
3:N:695:ILE:H	3:N:904:ASN:HD22	1.25	0.83
3:C:1324:ASN:OD1	10:C:1570:HOH:O	1.96	0.82
3:C:1317:CYS:HB2	3:C:1319:THR:H	1.01	0.82
2:B:272:ASN:ND2	3:C:683:HIS:CE1	2.48	0.82
2:B:243:LYS:CD	2:B:243:LYS:H	1.82	0.82
3:C:1079:ALA:N	7:C:1327:MOS:O1	2.13	0.81
3:C:1282:ARG:HA	3:C:1286:THR:HG23	1.61	0.81
3:N:720:LYS:O	3:N:721:LYS:HB2	1.78	0.81
2:M:496:LEU:H	2:M:509:ARG:NH2	1.79	0.81
3:N:1046:MET:HE2	3:N:1086:TYR:HB3	1.63	0.80
2:B:348:LEU:HD13	2:B:407:ILE:HD13	1.63	0.80
3:C:1317:CYS:CB	3:C:1319:THR:H	1.78	0.80
3:C:695:ILE:HG23	3:C:700:ASP:HB3	1.65	0.79
3:C:833:MET:HE1	3:C:1223:GLY:HA2	1.64	0.79
2:B:527:LEU:O	2:B:528:GLY:O	1.99	0.79
3:C:1095:GLN:O	3:C:1099:LYS:HG2	1.84	0.78
1:A:32:ARG:NH2	10:A:688:HOH:O	2.14	0.78
3:C:1088:GLN:HG2	3:C:1133:TYR:CD1	2.19	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:695:ILE:H	3:C:904:ASN:HD22	1.30	0.77
3:N:851:MET:CE	3:N:857:VAL:HG21	2.14	0.77
3:C:601:ASN:HB2	3:C:821:HIS:HD2	1.49	0.77
3:N:829:ARG:HG2	3:N:833:MET:HE1	1.67	0.76
3:C:829:ARG:CG	3:C:833:MET:CE	2.63	0.76
3:N:764:VAL:HG22	3:N:766:THR:HG22	1.67	0.76
3:N:779:MET:HG2	10:N:1380:HOH:O	1.83	0.76
2:B:447:MET:HG2	2:B:527:LEU:HD13	1.68	0.75
2:M:243:LYS:CD	2:M:243:LYS:H	2.00	0.75
1:A:32:ARG:NE	10:A:688:HOH:O	2.00	0.75
3:C:926:TRP:CZ3	3:C:927:MET:HE2	2.22	0.75
3:C:1249:ASN:O	3:C:1255:ALA:HA	1.87	0.75
3:N:782:VAL:CG1	3:N:783:PRO:HD2	2.15	0.75
1:A:131:GLN:HE21	1:A:133:GLU:H	1.32	0.75
3:C:829:ARG:HG2	3:C:833:MET:HE1	1.68	0.74
2:M:241:THR:HB	2:M:243:LYS:HE2	1.68	0.74
3:C:829:ARG:HG2	3:C:833:MET:CE	2.17	0.74
3:C:880:ARG:O	3:C:884:HIS:HD2	1.70	0.74
3:C:884:HIS:CE1	3:C:1006:GLY:H	2.06	0.73
3:C:1118:MET:O	3:C:1122:GLN:HG2	1.88	0.73
3:C:726:ALA:HA	3:C:851:MET:CE	2.18	0.72
3:C:713:LYS:HD2	3:C:895:ARG:NH1	2.05	0.72
3:C:1315:THR:CG2	3:C:1324:ASN:HA	2.16	0.72
3:C:1046:MET:HE1	3:C:1086:TYR:C	2.10	0.72
3:C:1046:MET:HE2	3:C:1090:VAL:HG21	1.71	0.72
3:C:1134:ARG:NH1	3:N:1123:ASP:O	2.23	0.71
3:C:1276:ASP:OD2	10:C:1620:HOH:O	2.08	0.71
7:N:1327:MOS:O1	8:N:1:LUZ:C9A	2.39	0.71
3:N:699:GLU:OE2	10:N:1518:HOH:O	2.09	0.70
2:B:241:THR:HG22	2:B:244:GLU:H	1.56	0.70
3:N:833:MET:CE	3:N:1223:GLY:HA2	2.20	0.70
3:C:598:ARG:NH2	10:C:1694:HOH:O	2.23	0.70
2:B:480:GLU:O	2:B:484:GLN:HG2	1.92	0.70
3:C:926:TRP:HZ3	3:C:927:MET:CE	2.04	0.70
1:L:143:PHE:HB3	3:N:1232:PHE:CE1	2.27	0.70
3:N:640:ILE:HG12	3:N:779:MET:HE1	1.74	0.69
2:M:509:ARG:HG2	2:M:509:ARG:NH1	2.05	0.69
3:C:609:THR:HG22	10:C:1337:HOH:O	1.92	0.69
2:B:391:PRO:HG3	2:B:397:LEU:CD1	2.22	0.69
3:N:851:MET:HE3	3:N:857:VAL:HG21	1.74	0.68
3:C:1312:LYS:O	3:C:1317:CYS:HA	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1048:GLN:HE22	3:C:1187:ASN:HD22	1.40	0.68
3:C:764:VAL:HG22	3:C:766:THR:HG22	1.76	0.68
2:B:241:THR:CG2	2:B:243:LYS:HG2	2.24	0.68
2:M:404:LEU:CD2	2:M:407:ILE:HD11	2.16	0.68
3:N:782:VAL:CG1	3:N:783:PRO:CD	2.70	0.68
3:C:571:ASP:OD1	3:C:1052:LYS:HD2	1.92	0.68
3:C:953:THR:HG22	3:C:959:LEU:HD21	1.77	0.67
3:N:1102:GLU:HB3	3:N:1103:PRO:HD3	1.75	0.67
3:C:700:ASP:O	3:C:704:ASN:ND2	2.24	0.67
1:A:63:ASP:OD1	1:A:64:LYS:N	2.25	0.67
2:M:286:GLU:C	2:M:288:ASN:H	1.93	0.66
1:L:32:ARG:NH1	3:N:676:GLU:OE2	2.28	0.66
2:B:241:THR:CG2	2:B:244:GLU:H	2.08	0.66
2:M:285:PRO:O	2:M:286:GLU:OE1	2.14	0.66
3:C:726:ALA:HA	3:C:851:MET:HE1	1.76	0.66
3:C:782:VAL:CG1	3:C:786:ARG:HG3	2.25	0.66
3:C:833:MET:HE3	3:C:1222:ARG:C	2.16	0.66
3:C:871:ARG:NH2	10:C:1431:HOH:O	2.29	0.66
1:A:159:GLY:O	1:A:162:THR:HG22	1.97	0.65
3:C:1286:THR:HG22	3:C:1310:VAL:O	1.97	0.65
3:N:853:THR:HG22	3:N:855:THR:H	1.60	0.65
3:C:871:ARG:NE	10:C:1431:HOH:O	1.88	0.64
2:M:285:PRO:O	2:M:286:GLU:HB2	1.97	0.64
3:N:1046:MET:HE2	3:N:1086:TYR:CB	2.28	0.64
3:C:1317:CYS:SG	3:C:1318:VAL:CG1	2.81	0.64
3:C:720:LYS:O	3:C:721:LYS:HB2	1.98	0.64
3:C:752:ILE:CD1	3:C:763:PHE:HE1	2.11	0.64
3:N:1046:MET:CE	3:N:1086:TYR:CB	2.76	0.63
3:N:673:ASP:OD2	3:N:677:HIS:HD2	1.81	0.63
3:C:926:TRP:CZ3	3:C:927:MET:CE	2.80	0.63
1:L:129:ARG:HH11	1:L:129:ARG:HG3	1.64	0.63
1:L:22:PRO:HB3	2:M:236:TRP:HB2	1.81	0.63
2:M:386:ASP:HB2	10:M:683:HOH:O	1.99	0.63
3:N:1289:ASN:O	3:N:1292:GLU:HB2	1.98	0.62
3:N:884:HIS:HE1	3:N:1006:GLY:H	1.47	0.62
3:C:995:LYS:NZ	3:C:1284:GLN:HE21	1.97	0.62
3:N:773:GLN:HG2	3:N:784:VAL:HG13	1.80	0.62
2:B:391:PRO:HG3	2:B:397:LEU:HD12	1.82	0.61
2:M:333:GLN:O	2:M:422:LYS:NZ	2.32	0.61
3:C:610:SER:O	3:C:663:VAL:O	2.19	0.61
1:L:112:GLN:HB3	3:N:1039:GLY:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:764:VAL:HG22	3:N:766:THR:CG2	2.31	0.61
3:N:829:ARG:CG	3:N:833:MET:HE1	2.29	0.60
3:C:1317:CYS:CA	3:C:1318:VAL:HB	2.31	0.60
3:C:782:VAL:HG12	3:C:786:ARG:HG3	1.83	0.60
3:C:572:THR:O	3:C:575:ARG:HB2	2.01	0.60
3:C:618:LYS:HE2	3:C:688:THR:HG21	1.83	0.60
3:C:1046:MET:CE	3:C:1086:TYR:O	2.50	0.60
3:N:1143:GLU:O	3:N:1144:THR:HG23	2.02	0.60
3:C:1317:CYS:CB	3:C:1318:VAL:HG12	2.31	0.60
3:C:723:PHE:CZ	3:C:847:LYS:HD2	2.36	0.60
3:C:1282:ARG:CA	3:C:1286:THR:HG23	2.32	0.59
2:B:272:ASN:HD22	3:C:683:HIS:CE1	2.18	0.59
3:N:1046:MET:CE	3:N:1087:GLY:N	2.57	0.59
2:B:524:LEU:O	2:B:528:GLY:N	2.35	0.59
2:B:427:ARG:O	2:B:427:ARG:HG2	2.03	0.59
1:A:36:LEU:HD22	1:A:89:GLU:HG3	1.85	0.58
2:M:285:PRO:O	2:M:286:GLU:CB	2.50	0.58
3:C:844:ALA:HB2	3:C:922:ILE:HD13	1.84	0.58
3:N:1289:ASN:OD1	10:N:1520:HOH:O	2.16	0.58
3:N:1286:THR:HG22	3:N:1310:VAL:HB	1.85	0.58
3:C:1317:CYS:CB	3:C:1318:VAL:CG1	2.78	0.57
3:C:848:VAL:HG21	3:C:926:TRP:HB2	1.86	0.57
3:N:966:ARG:O	3:N:970:GLU:HB2	2.04	0.57
2:M:496:LEU:N	2:M:509:ARG:NH2	2.51	0.57
3:C:1185:SER:OG	3:C:1191:ASP:OD2	2.21	0.57
3:C:1046:MET:HE2	3:C:1090:VAL:CG2	2.34	0.57
2:M:242:LEU:O	2:M:246:LEU:HG	2.05	0.57
3:N:851:MET:HE2	3:N:857:VAL:HG21	1.85	0.57
3:N:725:GLU:HB2	10:N:1338:HOH:O	2.03	0.57
3:N:1007:ILE:HD12	3:N:1258:ALA:HB3	1.87	0.56
3:N:833:MET:CE	3:N:1222:ARG:C	2.71	0.56
2:M:519:PHE:O	2:M:523:VAL:HG23	2.05	0.56
3:N:1102:GLU:OE1	3:N:1105:LYS:HE2	2.05	0.56
3:N:994:LYS:O	3:N:995:LYS:HD3	2.06	0.56
1:A:112:GLN:HG3	1:A:151:THR:HG22	1.86	0.56
1:L:32:ARG:HG2	3:N:598:ARG:NH2	2.21	0.56
3:C:1317:CYS:HB2	3:C:1319:THR:CA	2.23	0.56
3:C:719:LEU:HD11	3:C:895:ARG:HB3	1.86	0.56
2:M:264:ILE:O	2:M:268:MET:HG3	2.05	0.56
3:N:995:LYS:NZ	3:N:1284:GLN:HE21	2.04	0.56
2:B:484:GLN:HA	3:C:1318:VAL:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:981:LYS:HD2	10:C:1644:HOH:O	2.06	0.55
2:M:426:ARG:HG2	10:M:613:HOH:O	2.05	0.55
2:B:271:LYS:O	2:B:271:LYS:HG3	2.05	0.55
3:C:1046:MET:CE	3:C:1086:TYR:C	2.75	0.55
3:C:726:ALA:HA	3:C:851:MET:HE3	1.87	0.55
3:N:1044:THR:O	3:N:1048:GLN:HG3	2.07	0.55
3:C:1282:ARG:HA	3:C:1286:THR:CG2	2.33	0.55
2:M:495:SER:HA	2:M:509:ARG:HH22	1.71	0.55
3:C:1048:GLN:NE2	3:C:1187:ASN:HD22	2.05	0.55
3:C:953:THR:CG2	3:C:959:LEU:HD21	2.37	0.55
1:L:112:GLN:HG3	1:L:151:THR:HG22	1.89	0.55
2:M:462:ARG:NH1	10:M:712:HOH:O	2.36	0.55
3:N:610:SER:O	3:N:663:VAL:O	2.26	0.54
3:C:601:ASN:HB2	3:C:821:HIS:CD2	2.37	0.54
3:C:725:GLU:O	3:C:725:GLU:HG3	2.06	0.54
3:N:1064:SER:O	3:N:1065:GLU:HB3	2.08	0.54
2:M:504:MET:HG2	3:N:1303:GLU:CD	2.28	0.54
3:C:571:ASP:OD1	3:C:1052:LYS:CD	2.55	0.54
1:L:60:ARG:O	1:L:61:LEU:HB3	2.06	0.54
3:N:1289:ASN:O	3:N:1292:GLU:CB	2.56	0.54
1:L:143:PHE:HB3	3:N:1232:PHE:CD1	2.43	0.53
3:N:833:MET:HE3	3:N:1222:ARG:O	2.09	0.53
3:C:833:MET:CE	3:C:1223:GLY:HA2	2.37	0.53
3:C:640:ILE:HG23	3:C:779:MET:HE2	1.90	0.53
3:C:1046:MET:CE	3:C:1090:VAL:CG2	2.87	0.53
3:C:880:ARG:O	3:C:884:HIS:CD2	2.58	0.53
3:N:572:THR:HA	3:N:575:ARG:HD3	1.91	0.53
1:A:63:ASP:O	1:A:64:LYS:O	2.27	0.52
3:C:1046:MET:HE1	3:C:1086:TYR:O	2.07	0.52
3:C:1247:CYS:SG	3:C:1247:CYS:O	2.67	0.52
3:C:695:ILE:HG23	3:C:700:ASP:CB	2.39	0.52
3:C:1252:ALA:HB3	3:C:1256:SER:O	2.10	0.52
3:C:764:VAL:HG22	3:C:766:THR:CG2	2.39	0.52
1:L:60:ARG:O	1:L:61:LEU:CB	2.56	0.52
3:N:747:HIS:ND1	3:N:805:SER:HA	2.25	0.52
3:C:1046:MET:HE1	3:C:1086:TYR:HB3	1.92	0.52
2:B:264:ILE:HD11	5:B:606:FAD:H3B	1.91	0.52
2:B:484:GLN:NE2	3:C:1318:VAL:HA	2.25	0.52
3:C:1250:LYS:HB3	10:C:1667:HOH:O	2.09	0.52
3:N:1046:MET:CE	3:N:1086:TYR:HB3	2.36	0.51
1:A:164:ALA:O	1:A:165:LYS:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:627:LYS:NZ	10:N:1581:HOH:O	2.42	0.51
2:M:370:THR:CG2	2:M:407:ILE:HG23	2.41	0.51
3:N:752:ILE:CD1	3:N:763:PHE:HE1	2.22	0.51
3:C:719:LEU:CD1	3:C:895:ARG:HB3	2.41	0.51
2:M:509:ARG:NH1	2:M:509:ARG:CG	2.73	0.51
3:N:1046:MET:HE1	3:N:1086:TYR:CB	2.41	0.51
1:A:32:ARG:HH12	3:C:676:GLU:CD	2.13	0.51
2:M:462:ARG:NE	10:M:675:HOH:O	2.43	0.51
3:N:1104:PHE:CZ	3:N:1125:VAL:HG21	2.45	0.51
3:C:1318:VAL:N	3:C:1320:GLY:H	2.09	0.50
2:M:283:TRP:HB2	10:M:607:HOH:O	2.11	0.50
3:N:1046:MET:HE3	3:N:1086:TYR:O	2.11	0.50
3:N:889:TYR:OH	3:N:942:ARG:CD	2.59	0.50
3:C:1249:ASN:ND2	3:C:1257:LYS:HG2	2.27	0.50
2:M:510:THR:HG21	3:N:1314:THR:HG22	1.92	0.50
3:N:645:GLU:HG2	3:N:650:ASN:OD1	2.11	0.50
3:N:918:GLN:O	3:N:922:ILE:HG13	2.11	0.50
3:N:884:HIS:CE1	3:N:1006:GLY:H	2.26	0.50
1:A:37:ARG:HD3	3:C:595:ASP:O	2.11	0.50
3:N:1031:VAL:HB	3:N:1063:ILE:HG12	1.93	0.50
3:C:912:ARG:HG3	6:C:1326:MTE:S1'	2.51	0.50
3:N:1288:ASN:O	3:N:1289:ASN:C	2.50	0.50
2:B:392:SER:OG	2:B:395:LYS:HD3	2.12	0.50
3:C:1046:MET:HE1	3:C:1086:TYR:CB	2.42	0.50
3:N:1033:HIS:HD2	3:N:1035:GLY:H	1.59	0.50
3:N:655:PHE:HE1	3:N:814:LEU:HD23	1.77	0.50
2:B:363:PRO:HG2	2:B:435:THR:HG23	1.93	0.49
3:N:1088:GLN:HG2	3:N:1133:TYR:CD1	2.47	0.49
2:B:472:LYS:NZ	2:B:472:LYS:HB3	2.28	0.49
2:M:419:SER:HB2	2:M:519:PHE:CD1	2.47	0.49
3:C:670:VAL:HG11	3:C:681:ALA:HB3	1.95	0.49
3:C:941:VAL:O	3:C:945:ASN:ND2	2.44	0.49
3:N:663:VAL:HG12	3:N:834:LEU:HD11	1.94	0.49
3:N:782:VAL:HG11	3:N:786:ARG:HG3	1.95	0.49
3:C:640:ILE:HG23	3:C:779:MET:CE	2.42	0.49
3:N:1048:GLN:HE22	3:N:1187:ASN:HD22	1.58	0.49
3:N:1046:MET:HE3	3:N:1086:TYR:C	2.30	0.49
3:N:840:HIS:HE1	3:N:874:SER:OG	1.95	0.49
3:C:860:GLU:HA	3:C:895:ARG:O	2.12	0.49
3:C:861:VAL:O	3:C:896:GLY:HA2	2.12	0.49
2:B:423:GLN:HG2	2:B:425:SER:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1080:SER:HB3	3:N:1258:ALA:HB1	1.94	0.49
2:M:250:ALA:HA	2:M:401:GLU:HG2	1.95	0.48
2:M:419:SER:HB2	2:M:519:PHE:HD1	1.79	0.48
3:C:1259:VAL:O	3:C:1259:VAL:HG22	2.13	0.48
1:L:63:ASP:O	1:L:64:LYS:O	2.32	0.48
1:L:28:ALA:O	1:L:32:ARG:HB2	2.13	0.48
2:M:264:ILE:HD11	5:M:606:FAD:H3B	1.95	0.48
3:N:1152:TYR:CE1	3:N:1257:LYS:HG2	2.49	0.48
3:N:1286:THR:CG2	3:N:1310:VAL:HB	2.44	0.48
3:C:1046:MET:HE3	3:C:1086:TYR:O	2.13	0.47
3:C:752:ILE:CD1	3:C:763:PHE:CE1	2.96	0.47
2:B:388:THR:O	2:B:397:LEU:HD13	2.14	0.47
2:B:271:LYS:CG	2:B:273:GLN:HG2	2.44	0.47
2:B:468:LYS:HB2	2:B:493:GLU:CD	2.35	0.47
1:A:43:CYS:HA	3:C:829:ARG:HB2	1.95	0.47
3:N:670:VAL:HG11	3:N:681:ALA:HB3	1.96	0.47
1:A:100:PRO:O	1:A:104:ARG:HG3	2.15	0.47
3:C:779:MET:HG3	3:C:780:LEU:N	2.29	0.47
2:B:250:ALA:HA	2:B:401:GLU:HG2	1.97	0.47
2:M:423:GLN:HG2	2:M:425:SER:H	1.78	0.47
2:M:325:GLU:HB2	2:M:412:SER:HG	1.76	0.47
3:N:829:ARG:HG2	3:N:833:MET:CE	2.43	0.47
3:C:1072:PRO:HG3	3:N:1128:SER:HB2	1.97	0.47
3:N:766:THR:HA	3:N:801:LYS:HB3	1.96	0.47
3:C:1316:LEU:O	3:C:1317:CYS:O	2.33	0.47
3:C:571:ASP:CG	3:C:1052:LYS:HD2	2.35	0.47
2:B:376:SER:HB3	2:B:402:GLU:HG2	1.97	0.47
3:C:851:MET:C	3:C:853:THR:H	2.19	0.47
3:C:891:ILE:HG22	3:C:893:ASN:O	2.15	0.46
2:B:271:LYS:HG3	2:B:273:GLN:HG2	1.97	0.46
2:B:358:ILE:HD12	2:B:426:ARG:HD2	1.96	0.46
2:B:390:PHE:HB3	10:B:623:HOH:O	2.14	0.46
3:N:1102:GLU:OE1	3:N:1102:GLU:HA	2.15	0.46
2:M:376:SER:HB3	2:M:379:THR:HG23	1.97	0.46
3:N:880:ARG:O	3:N:884:HIS:HD2	1.98	0.46
3:C:1132:PHE:CD1	3:N:1126:SER:HB2	2.51	0.46
1:L:91:ILE:O	1:L:99:HIS:HB2	2.16	0.46
3:C:1124:ARG:HB3	3:N:1134:ARG:HG3	1.98	0.46
3:N:585:GLN:NE2	10:N:1409:HOH:O	2.49	0.46
3:C:850:PHE:CD1	3:C:930:VAL:HG13	2.51	0.45
2:B:390:PHE:O	2:B:462:ARG:HD2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:911:PHE:O	3:C:912:ARG:C	2.55	0.45
2:M:495:SER:CA	2:M:509:ARG:HH22	2.28	0.45
3:N:1079:ALA:HB2	8:N:1:LUZ:N5	2.31	0.45
3:N:699:GLU:OE1	10:N:1490:HOH:O	2.21	0.45
2:B:257:LEU:O	5:B:606:FAD:H2B	2.16	0.45
3:C:673:ASP:OD2	3:C:677:HIS:HD2	1.99	0.45
3:C:655:PHE:HE1	3:C:814:LEU:HD23	1.81	0.45
3:N:606:ARG:HD3	3:N:679:GLU:HA	1.98	0.45
3:N:1092:GLU:OE1	3:N:1092:GLU:HA	2.17	0.45
3:N:764:VAL:HG13	3:N:789:VAL:HG13	1.99	0.45
3:N:989:LYS:HD2	10:N:1515:HOH:O	2.15	0.45
3:N:1183:GLY:HA2	3:N:1247:CYS:O	2.17	0.45
3:N:1212:HIS:CD2	3:N:1220:HIS:HD2	2.35	0.45
3:C:1013:PHE:CD1	3:C:1013:PHE:C	2.89	0.45
3:C:1088:GLN:HG2	3:C:1133:TYR:CE1	2.51	0.45
3:C:850:PHE:N	3:C:850:PHE:CD2	2.85	0.45
2:M:495:SER:HA	2:M:509:ARG:NH2	2.31	0.45
3:N:1046:MET:CE	3:N:1086:TYR:O	2.64	0.45
1:L:139:ILE:O	1:L:142:ALA:HB3	2.16	0.45
3:N:610:SER:HB2	3:N:660:VAL:HG11	1.98	0.45
3:C:705:ASN:HA	3:C:707:PHE:CE1	2.51	0.44
2:B:242:LEU:O	2:B:246:LEU:HG	2.18	0.44
3:C:782:VAL:HG12	3:C:786:ARG:CG	2.47	0.44
3:N:1200:VAL:O	3:N:1230:PRO:HG2	2.17	0.44
3:C:1209:GLU:HB3	3:C:1227:TYR:CZ	2.52	0.44
2:M:272:ASN:ND2	3:N:683:HIS:CE1	2.86	0.44
2:M:439:ARG:NH1	10:M:718:HOH:O	2.51	0.44
1:A:136:VAL:HG21	1:A:161:ARG:HH21	1.82	0.44
1:A:74:LEU:O	1:A:76:PRO:HD3	2.17	0.44
3:N:1290:THR:C	3:N:1292:GLU:H	2.20	0.44
3:N:782:VAL:HG12	3:N:783:PRO:N	2.32	0.44
3:C:1282:ARG:NH1	3:C:1308:ALA:O	2.48	0.44
3:N:1078:ALA:HB1	8:N:1:LUZ:C9A	2.47	0.44
3:C:645:GLU:HG2	3:C:650:ASN:OD1	2.16	0.44
2:M:352:ILE:CD1	2:M:407:ILE:HG12	2.48	0.43
3:C:1261:GLU:N	3:C:1262:PRO:CD	2.81	0.43
2:M:263:GLU:CD	2:M:354:THR:HG21	2.39	0.43
3:C:1287:ASN:HB2	10:C:1613:HOH:O	2.19	0.43
1:L:22:PRO:HA	1:L:78:CYS:SG	2.58	0.43
2:B:241:THR:HG22	2:B:244:GLU:CB	2.47	0.43
2:B:298:SER:HA	2:B:408:GLU:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:321:THR:O	2:M:328:ARG:NH2	2.51	0.43
3:C:1238:GLU:OE1	3:C:1240:ARG:NE	2.50	0.43
3:C:995:LYS:HZ1	3:C:1284:GLN:HE21	1.65	0.43
3:C:655:PHE:HE1	3:C:814:LEU:CD2	2.32	0.43
1:L:63:ASP:HB3	1:L:64:LYS:H	1.64	0.43
3:N:1017:ALA:HB1	3:N:1086:TYR:CD2	2.54	0.43
3:N:1199:PHE:CE2	3:N:1203:LEU:HD23	2.54	0.43
1:A:38:GLY:O	1:A:40:LYS:HE2	2.19	0.43
1:L:59:ASP:O	1:L:63:ASP:O	2.37	0.43
1:A:144:GLN:HE22	2:B:336:TRP:HA	1.83	0.43
3:N:619:SER:HG	3:N:688:THR:HG1	1.64	0.43
2:B:254:GLU:OE2	2:B:254:GLU:N	2.52	0.42
2:B:319:LEU:HB3	2:B:320:PRO:HD2	2.01	0.42
3:C:1079:ALA:O	3:C:1080:SER:HB2	2.19	0.42
1:L:104:ARG:HA	1:L:104:ARG:HD3	1.65	0.42
1:L:37:ARG:HD3	3:N:595:ASP:O	2.19	0.42
3:N:1033:HIS:CD2	3:N:1035:GLY:H	2.37	0.42
3:C:1279:ARG:HD3	10:C:1502:HOH:O	2.18	0.42
3:C:1091:TYR:O	3:C:1095:GLN:HG2	2.19	0.42
2:B:241:THR:HG22	2:B:244:GLU:HB2	2.01	0.42
3:N:987:PHE:CD2	3:N:996:ARG:HG3	2.54	0.42
3:C:1031:VAL:HB	3:C:1063:ILE:HG12	2.00	0.42
3:N:623:SER:HA	3:N:626:GLN:HE21	1.84	0.42
3:N:695:ILE:HG23	3:N:700:ASP:HB3	2.01	0.42
3:N:603:LEU:HB2	3:N:823:VAL:HG22	2.01	0.42
1:A:104:ARG:NE	1:A:162:THR:HG21	2.35	0.42
3:C:754:LYS:HD3	3:C:754:LYS:HA	1.65	0.42
3:C:851:MET:C	3:C:853:THR:N	2.72	0.42
3:N:972:LEU:HD23	3:N:1000:ILE:HD13	2.01	0.42
3:N:1017:ALA:O	3:N:1132:PHE:HA	2.19	0.42
2:B:527:LEU:O	2:B:528:GLY:C	2.58	0.42
3:C:997:GLY:HA3	3:C:1273:ALA:O	2.19	0.42
2:M:377:ARG:HE	2:M:377:ARG:HB3	1.19	0.42
2:M:370:THR:HG21	2:M:407:ILE:HG23	2.01	0.42
3:N:833:MET:CE	3:N:1222:ARG:O	2.67	0.42
3:N:1259:VAL:HG22	3:N:1259:VAL:O	2.20	0.42
3:C:1203:LEU:HD13	10:C:1338:HOH:O	2.19	0.42
1:L:61:LEU:C	1:L:63:ASP:H	2.23	0.42
1:A:45:GLU:CD	3:C:1224:PRO:HD2	2.39	0.42
3:N:1007:ILE:O	3:N:1008:SER:CB	2.67	0.41
3:N:782:VAL:CG1	3:N:786:ARG:HG3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1191:ASP:O	3:C:1195:VAL:HG23	2.20	0.41
3:C:1052:LYS:HG2	3:C:1254:TYR:CZ	2.55	0.41
2:M:271:LYS:HG2	2:M:273:GLN:HG2	2.02	0.41
3:N:978:TYR:O	3:N:979:ALA:C	2.59	0.41
2:B:254:GLU:CD	2:B:254:GLU:H	2.23	0.41
2:B:266:ILE:O	2:B:270:PHE:HB2	2.20	0.41
3:C:1124:ARG:CB	3:N:1134:ARG:HG3	2.50	0.41
3:C:1154:THR:HG23	3:C:1181:ASP:O	2.20	0.41
3:C:720:LYS:O	3:C:721:LYS:CB	2.68	0.41
3:N:1162:VAL:HG21	3:N:1274:ILE:HG13	2.02	0.41
3:N:1079:ALA:HA	8:N:1:LUZ:H5A	2.02	0.41
3:C:782:VAL:HG12	3:C:783:PRO:HD2	2.03	0.41
3:C:840:HIS:HE1	3:C:874:SER:OG	2.03	0.41
3:N:1046:MET:CE	3:N:1087:GLY:CA	2.98	0.41
1:A:42:GLY:O	3:C:829:ARG:HD2	2.19	0.41
2:B:249:LYS:NZ	2:B:253:PRO:O	2.54	0.41
3:C:948:LYS:HB2	3:C:951:ASP:OD1	2.21	0.41
2:M:395:LYS:HB3	2:M:395:LYS:HE2	1.81	0.41
3:N:1045:LYS:O	3:N:1049:VAL:HG23	2.21	0.41
3:N:829:ARG:CG	3:N:833:MET:CE	2.97	0.41
3:N:844:ALA:HB2	3:N:922:ILE:HD13	2.02	0.41
3:C:969:ASP:O	3:C:973:LYS:HD2	2.21	0.41
1:L:60:ARG:NH2	2:M:224:PRO:HD3	2.35	0.41
3:C:1046:MET:CE	3:C:1090:VAL:HG21	2.44	0.41
2:M:284:ILE:HB	2:M:287:LEU:HD12	2.03	0.41
3:N:1013:PHE:CD1	3:N:1013:PHE:C	2.94	0.41
2:B:367:ALA:O	2:B:439:ARG:HD3	2.21	0.41
3:N:614:HIS:HD2	3:N:693:PRO:O	2.03	0.41
3:N:771:LYS:HD3	3:N:771:LYS:HA	1.82	0.41
3:C:1033:HIS:HD2	3:C:1035:GLY:H	1.68	0.41
3:N:962:PHE:CE2	3:N:965:PRO:HD3	2.56	0.41
3:C:1020:LEU:C	3:C:1021:ILE:HD12	2.41	0.41
1:A:154:ARG:NE	3:C:1196:GLU:OE2	2.47	0.41
3:C:884:HIS:HE1	3:C:1006:GLY:N	2.03	0.41
2:M:427:ARG:HG2	2:M:427:ARG:O	2.20	0.41
2:M:507:PHE:CZ	2:M:511:LEU:HD11	2.56	0.41
3:N:1001:ILE:CD1	3:N:1272:PHE:CD1	3.04	0.41
3:C:614:HIS:HD2	3:C:693:PRO:O	2.04	0.41
2:M:423:GLN:NE2	2:M:504:MET:HE3	2.36	0.41
3:N:994:LYS:HD3	3:N:1163:GLU:OE1	2.21	0.41
1:A:22:PRO:HG2	2:B:234:VAL:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ILE:HG22	1:A:67:HIS:CE1	2.56	0.40
2:B:394:ARG:HD3	10:B:761:HOH:O	2.20	0.40
3:C:1299:PRO:HG2	3:C:1301:THR:HG23	2.03	0.40
3:C:599:TYR:HA	3:N:599:TYR:HA	2.04	0.40
3:N:1001:ILE:HD11	3:N:1272:PHE:CD1	2.56	0.40
3:N:1046:MET:CE	3:N:1087:GLY:HA2	2.52	0.40
3:N:655:PHE:HE1	3:N:814:LEU:CD2	2.34	0.40
3:C:1020:LEU:HD23	3:C:1070:THR:HB	2.02	0.40
3:N:725:GLU:HG3	3:N:851:MET:CE	2.30	0.40
3:N:884:HIS:HE1	3:N:1005:PHE:HA	1.86	0.40
3:N:601:ASN:HB2	3:N:821:HIS:CD2	2.56	0.40
2:B:241:THR:HG22	2:B:244:GLU:HG3	2.04	0.40
3:C:722:GLY:O	3:C:857:VAL:CG1	2.70	0.40
1:L:154:ARG:NH1	1:L:158:GLN:OE1	2.55	0.40
2:M:287:LEU:HD21	2:M:403:ILE:HD12	2.02	0.40
3:N:1048:GLN:NE2	3:N:1187:ASN:HD22	2.19	0.40
2:M:232:GLU:OE1	3:N:677:HIS:HE1	2.05	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	162/164 (99%)	151 (93%)	7 (4%)	4 (2%)	5	3
1	L	162/164 (99%)	152 (94%)	8 (5%)	2 (1%)	13	10
2	B	303/305 (99%)	284 (94%)	17 (6%)	2 (1%)	22	22
2	M	303/305 (99%)	284 (94%)	15 (5%)	4 (1%)	12	9
3	C	753/755 (100%)	702 (93%)	41 (5%)	10 (1%)	12	9
3	N	743/755 (98%)	701 (94%)	33 (4%)	9 (1%)	13	10
All	All	2426/2448 (99%)	2274 (94%)	121 (5%)	31 (1%)	12	9

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	LYS
3	C	1321	ALA
3	C	1324	ASN
1	L	61	LEU
1	L	64	LYS
2	M	287	LEU
3	N	1008	SER
3	N	1287	ASN
1	A	60	ARG
1	A	61	LEU
3	C	721	LYS
3	C	1008	SER
3	C	1317	CYS
3	C	1318	VAL
3	C	1319	THR
2	M	286	GLU
3	N	721	LYS
3	N	912	ARG
3	N	1289	ASN
3	C	912	ARG
2	M	321	THR
1	A	43	CYS
2	M	335	ARG
2	B	286	GLU
2	B	287	LEU
3	N	1144	THR
3	C	1139	GLY
3	N	956	ASN
3	C	797	GLY
3	N	1139	GLY
3	N	797	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	137/137 (100%)	129 (94%)	8 (6%)	20	23
1	L	137/137 (100%)	127 (93%)	10 (7%)	14	15
2	B	261/261 (100%)	240 (92%)	21 (8%)	12	12
2	M	261/261 (100%)	242 (93%)	19 (7%)	14	15
3	C	631/631 (100%)	594 (94%)	37 (6%)	19	23
3	N	624/631 (99%)	594 (95%)	30 (5%)	25	32
All	All	2051/2058 (100%)	1926 (94%)	125 (6%)	18	21

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	33	LYS
1	A	57	LYS
1	A	60	ARG
1	A	64	LYS
1	A	82	HIS
1	A	104	ARG
1	A	144	GLN
2	B	241	THR
2	B	243	LYS
2	B	254	GLU
2	B	256	LYS
2	B	271	LYS
2	B	272	ASN
2	B	277	MET
2	B	312	LEU
2	B	318	LYS
2	B	335	ARG
2	B	348	LEU
2	B	392	SER
2	B	397	LEU
2	B	427	ARG
2	B	433	LYS
2	B	439	ARG
2	B	462	ARG
2	B	476	LYS
2	B	495	SER
2	B	506	GLU
2	B	525	LYS
3	C	598	ARG

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Mol	Chain	Res	Type
3	C	609	THR
3	C	684	VAL
3	C	725	GLU
3	C	736	ILE
3	C	742	PHE
3	C	743	TYR
3	C	764	VAL
3	C	774	SER
3	C	779	MET
3	C	792	LYS
3	C	818	LYS
3	C	839	ARG
3	C	848	VAL
3	C	857	VAL
3	C	876	SER
3	C	899	ARG
3	C	911	PHE
3	C	939	GLU
3	C	949	GLU
3	C	951	ASP
3	C	958	ARG
3	C	986	LYS
3	C	1001	ILE
3	C	1013	PHE
3	C	1122	GLN
3	C	1123	ASP
3	C	1144	THR
3	C	1170	ASP
3	C	1190	ILE
3	C	1203	LEU
3	C	1208	LEU
3	C	1215	PRO
3	C	1276	ASP
3	C	1286	THR
3	C	1287	ASN
3	C	1319	THR
1	L	33	LYS
1	L	60	ARG
1	L	61	LEU
1	L	63	ASP
1	L	82	HIS
1	L	89	GLU

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Mol	Chain	Res	Type
1	L	104	ARG
1	L	129	ARG
1	L	133	GLU
1	L	162	THR
2	M	243	LYS
2	M	310	LYS
2	M	312	LEU
2	M	318	LYS
2	M	332	GLU
2	M	335	ARG
2	M	351	ASN
2	M	375	VAL
2	M	377	ARG
2	M	379	THR
2	M	415	ASP
2	M	419	SER
2	M	426	ARG
2	M	427	ARG
2	M	433	LYS
2	M	462	ARG
2	M	468	LYS
2	M	506	GLU
2	M	509	ARG
3	N	598	ARG
3	N	609	THR
3	N	618	LYS
3	N	659	THR
3	N	684	VAL
3	N	712	LEU
3	N	719	LEU
3	N	742	PHE
3	N	743	TYR
3	N	764	VAL
3	N	774	SER
3	N	779	MET
3	N	848	VAL
3	N	853	THR
3	N	899	ARG
3	N	911	PHE
3	N	926	TRP
3	N	939	GLU
3	N	940	GLU

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Mol	Chain	Res	Type
3	N	983	GLU
3	N	1013	PHE
3	N	1080	SER
3	N	1122	GLN
3	N	1143	GLU
3	N	1144	THR
3	N	1170	ASP
3	N	1203	LEU
3	N	1208	LEU
3	N	1276	ASP
3	N	1284	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	144	GLN
1	A	146	ASN
2	B	272	ASN
2	B	351	ASN
2	B	473	GLN
2	B	484	GLN
3	C	585	GLN
3	C	614	HIS
3	C	677	HIS
3	C	683	HIS
3	C	821	HIS
3	C	840	HIS
3	C	884	HIS
3	C	904	ASN
3	C	1016	GLN
3	C	1033	HIS
3	C	1048	GLN
3	C	1212	HIS
3	C	1284	GLN
3	C	1287	ASN
1	L	131	GLN
1	L	146	ASN
2	M	272	ASN
2	M	351	ASN
3	N	585	GLN
3	N	614	HIS

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Mol	Chain	Res	Type
3	N	626	GLN
3	N	677	HIS
3	N	683	HIS
3	N	821	HIS
3	N	840	HIS
3	N	884	HIS
3	N	904	ASN
3	N	1016	GLN
3	N	1033	HIS
3	N	1048	GLN
3	N	1220	HIS
3	N	1284	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 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	$\# Z  > 2$
4	FES	L	601	1	0,4,4	0.00	-	-		
8	LUZ	N	1	-	12,13,13	1.52	2 (16%)	11,18,18	2.15	3 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	FES	A	602	1	0,4,4	0.00	-	-		
8	LUZ	C	1	-	12,13,13	1.24	1 (8%)	11,18,18	2.61	5 (45%)
5	FAD	B	606	-	51,58,58	1.51	8 (15%)	60,89,89	2.55	12 (20%)
7	MOS	C	1327	6	0,3,3	0.00	-	-		
6	MTE	C	1326	7	21,26,26	1.59	2 (9%)	21,40,40	2.55	12 (57%)
4	FES	A	601	1	0,4,4	0.00	-	-		
6	MTE	N	1326	7	21,26,26	1.34	2 (9%)	21,40,40	2.07	6 (28%)
4	FES	L	602	1	0,4,4	0.00	-	-		
7	MOS	N	1327	6	0,3,3	0.00	-	-		
5	FAD	M	606	-	51,58,58	1.56	7 (13%)	60,89,89	1.87	13 (21%)

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
4	FES	L	601	1	-	-	0/1/1/1
8	LUZ	N	1	-	-	-	0/2/2/2
4	FES	A	602	1	-	-	0/1/1/1
8	LUZ	C	1	-	-	-	0/2/2/2
5	FAD	B	606	-	-	0/30/50/50	0/6/6/6
6	MTE	C	1326	7	-	1/6/34/34	0/3/3/3
4	FES	A	601	1	-	-	0/1/1/1
6	MTE	N	1326	7	-	1/6/34/34	0/3/3/3
4	FES	L	602	1	-	-	0/1/1/1
5	FAD	M	606	-	-	0/30/50/50	0/6/6/6

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1326	MTE	C4-C9	5.66	1.49	1.41
6	N	1326	MTE	C4-C9	4.59	1.47	1.41
5	M	606	FAD	C2A-N3A	4.53	1.39	1.32
5	M	606	FAD	C4X-N5	4.52	1.39	1.33
5	M	606	FAD	C4-N3	4.18	1.40	1.33
5	B	606	FAD	C10-N1	3.99	1.38	1.33
8	N	1	LUZ	C4-N3	3.58	1.39	1.33
5	B	606	FAD	C2A-N3A	3.45	1.37	1.32
5	M	606	FAD	C10-N1	3.34	1.37	1.33
5	M	606	FAD	C5X-N5	3.20	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	606	FAD	C4X-N5	3.12	1.37	1.33
5	B	606	FAD	C9A-N10	2.95	1.42	1.38
5	B	606	FAD	C5X-N5	2.85	1.40	1.35
6	N	1326	MTE	C9-C10	2.80	1.46	1.41
5	B	606	FAD	C4-C4X	-2.77	1.36	1.41
6	C	1326	MTE	C9-C10	2.73	1.46	1.41
5	M	606	FAD	C1'-N10	2.59	1.50	1.48
5	B	606	FAD	C4X-C10	2.52	1.41	1.38
5	B	606	FAD	C2A-N1A	2.43	1.38	1.33
8	C	1	LUZ	C4A-N5	2.31	1.36	1.33
5	M	606	FAD	C2A-N1A	2.25	1.38	1.33
8	N	1	LUZ	C4A-N5	2.18	1.36	1.33

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	606	FAD	C4-N3-C2	10.01	123.59	115.14
5	B	606	FAD	C1'-N10-C9A	9.98	126.15	118.29
5	B	606	FAD	N3A-C2A-N1A	-7.45	117.03	128.68
5	M	606	FAD	N3A-C2A-N1A	-6.63	118.32	128.68
8	C	1	LUZ	C4-N3-C2	5.66	119.92	115.14
5	M	606	FAD	C4-N3-C2	5.64	119.90	115.14
6	C	1326	MTE	C4-C9-N5	5.45	123.70	119.12
6	N	1326	MTE	C4-C9-N5	4.69	123.06	119.12
5	B	606	FAD	O3'-C3'-C2'	-4.60	97.71	108.81
5	B	606	FAD	C1'-N10-C10	-4.44	114.43	118.41
8	N	1	LUZ	C4-N3-C2	4.34	118.81	115.14
5	M	606	FAD	O3'-C3'-C2'	-4.25	98.54	108.81
8	N	1	LUZ	N10-C10-N1	4.04	120.54	114.93
5	B	606	FAD	C4X-C4-N3	-3.91	118.09	123.43
6	C	1326	MTE	P-O4'-C4'	3.85	128.90	118.30
6	N	1326	MTE	C4-N3-C2	3.83	122.02	115.93
5	M	606	FAD	C4X-N5-C5X	3.78	120.55	116.77
5	M	606	FAD	C1'-N10-C9A	3.76	121.25	118.29
6	C	1326	MTE	N2-C2-N3	3.54	122.77	117.25
8	C	1	LUZ	N10-C10-N1	3.44	119.70	114.93
6	C	1326	MTE	C4-N3-C2	3.33	121.22	115.93
5	M	606	FAD	C10-C4X-N5	-3.28	118.99	121.26
6	C	1326	MTE	C4-C9-C10	3.21	117.42	114.57
8	N	1	LUZ	C4A-C4-N3	-3.13	119.15	123.43
5	M	606	FAD	C4X-C4-N3	-3.11	119.18	123.43
6	N	1326	MTE	N2-C2-N3	3.02	121.95	117.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	606	FAD	C2A-N1A-C6A	3.02	123.91	118.75
5	B	606	FAD	O3'-C3'-C4'	-3.00	101.58	108.81
5	B	606	FAD	C4X-N5-C5X	2.94	119.71	116.77
6	C	1326	MTE	O4'-P-O1P	-2.92	98.27	106.47
5	B	606	FAD	C1B-N9A-C4A	-2.85	121.63	126.64
5	M	606	FAD	C4-C4X-N5	2.83	121.83	118.60
6	N	1326	MTE	C2-N1-C10	2.83	120.88	114.54
6	C	1326	MTE	O2P-P-O1P	2.81	121.67	110.68
8	C	1	LUZ	C4-C4A-N5	2.77	121.69	118.24
6	N	1326	MTE	C7-C6-C1'	-2.76	104.35	110.53
8	C	1	LUZ	C4-C4A-C10	-2.66	118.19	119.95
6	C	1326	MTE	C2-N1-C10	2.64	120.47	114.54
5	M	606	FAD	C5X-C9A-N10	2.55	119.56	117.72
6	C	1326	MTE	N2-C2-N1	-2.43	113.48	117.25
5	M	606	FAD	O4'-C4'-C3'	2.42	114.98	109.10
5	B	606	FAD	C5X-C9A-N10	2.41	119.46	117.72
5	B	606	FAD	C2A-N1A-C6A	2.24	122.59	118.75
8	C	1	LUZ	C4A-C4-N3	-2.24	120.36	123.43
6	C	1326	MTE	O3'-C7-C6	-2.24	107.47	108.96
5	M	606	FAD	C6-C5X-N5	2.15	121.42	119.05
6	C	1326	MTE	O3'-C7-N8	-2.13	106.37	108.57
6	C	1326	MTE	C9-C4-N3	-2.13	117.96	124.01
5	M	606	FAD	C1B-N9A-C4A	-2.13	122.91	126.64
5	B	606	FAD	C6-C5X-C9A	2.10	121.80	119.05
6	N	1326	MTE	C10-N8-C7	-2.01	119.74	123.67

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	1326	MTE	C3'-C4'-O4'-P
6	N	1326	MTE	C3'-C4'-O4'-P

There are no ring outliers.

6 monomers are involved in 11 short contacts:

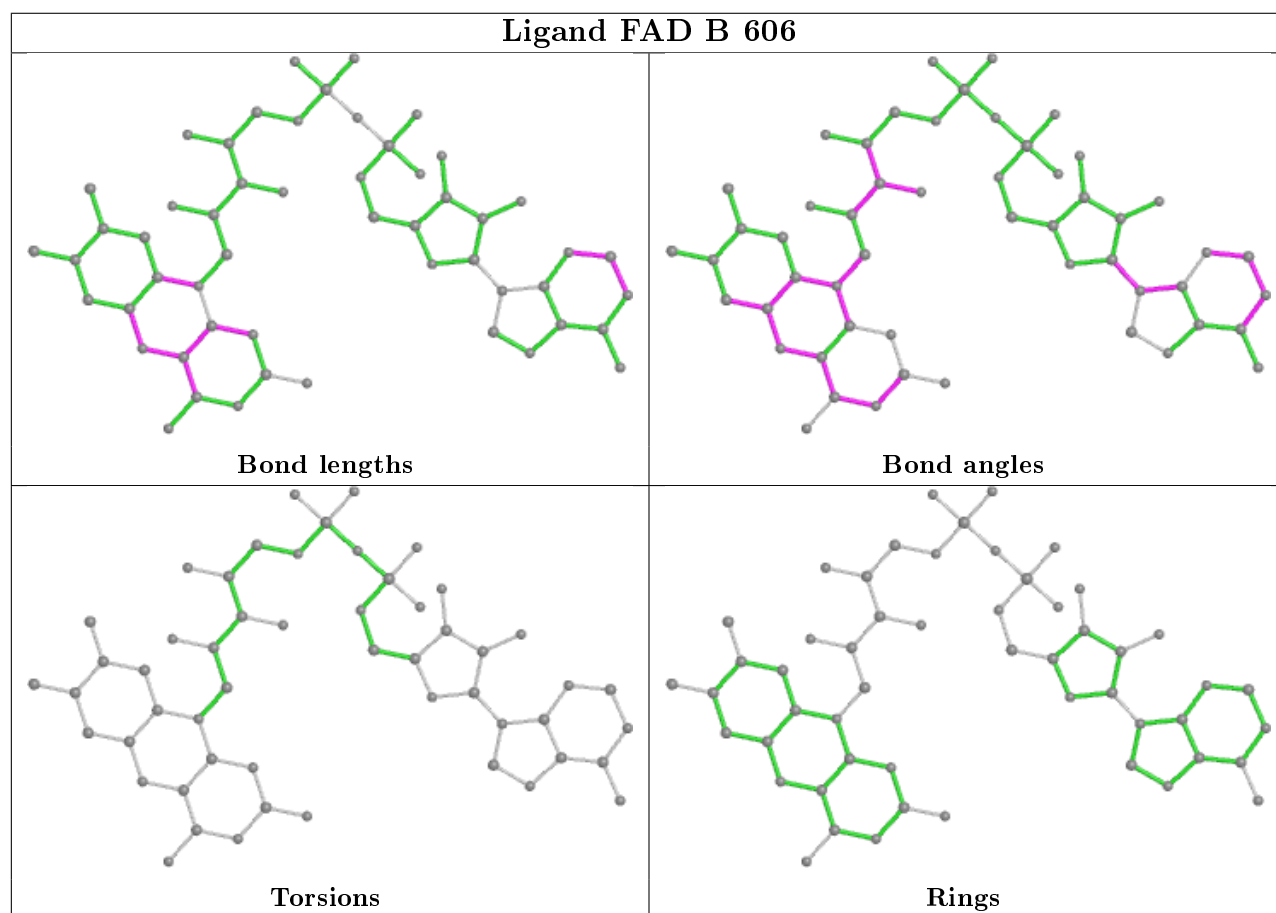
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	N	1	LUZ	5	0
5	B	606	FAD	2	0
7	C	1327	MOS	1	0
6	C	1326	MTE	1	0

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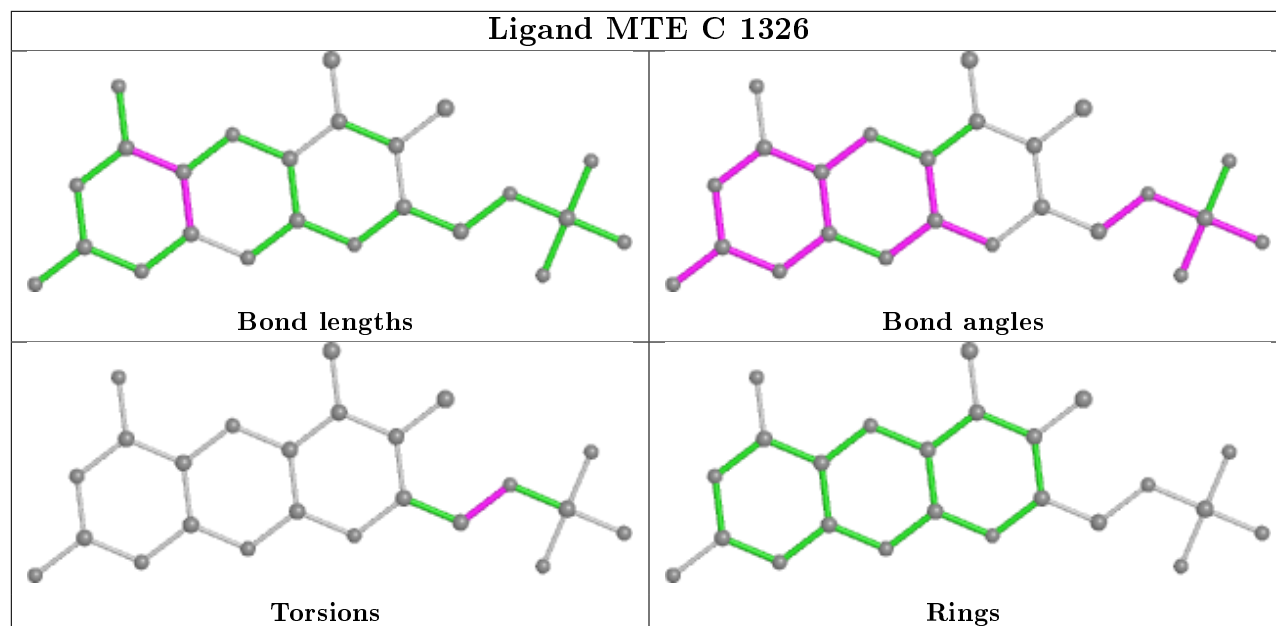
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	N	1327	MOS	2	0
5	M	606	FAD	2	0

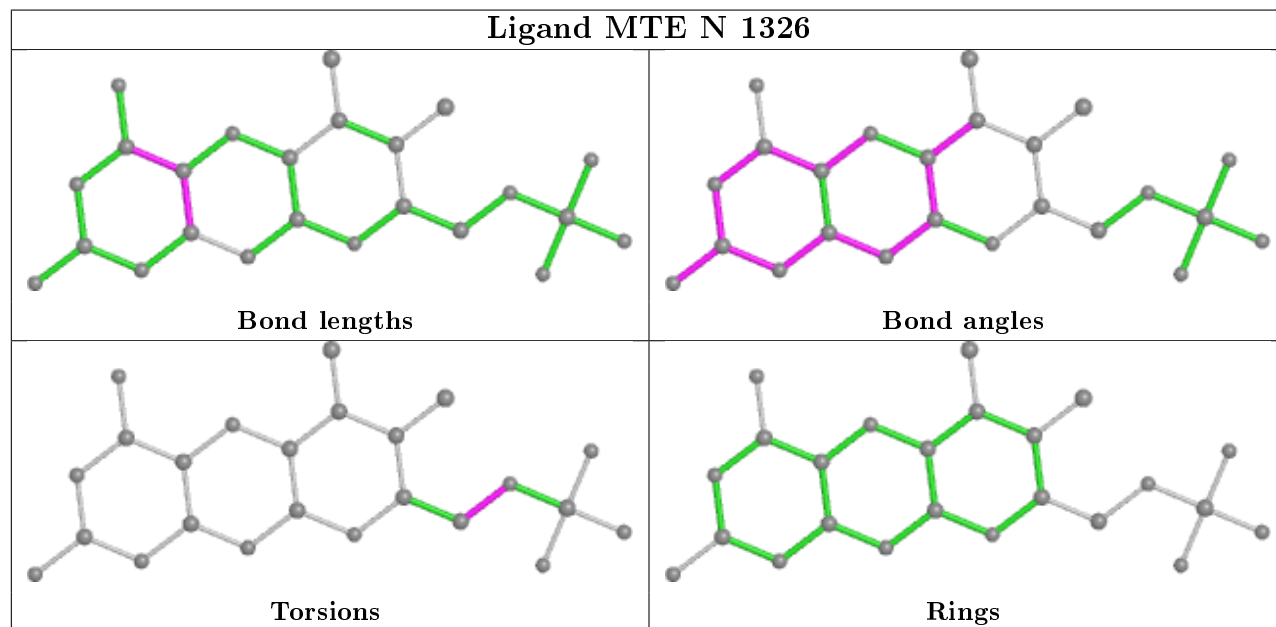
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

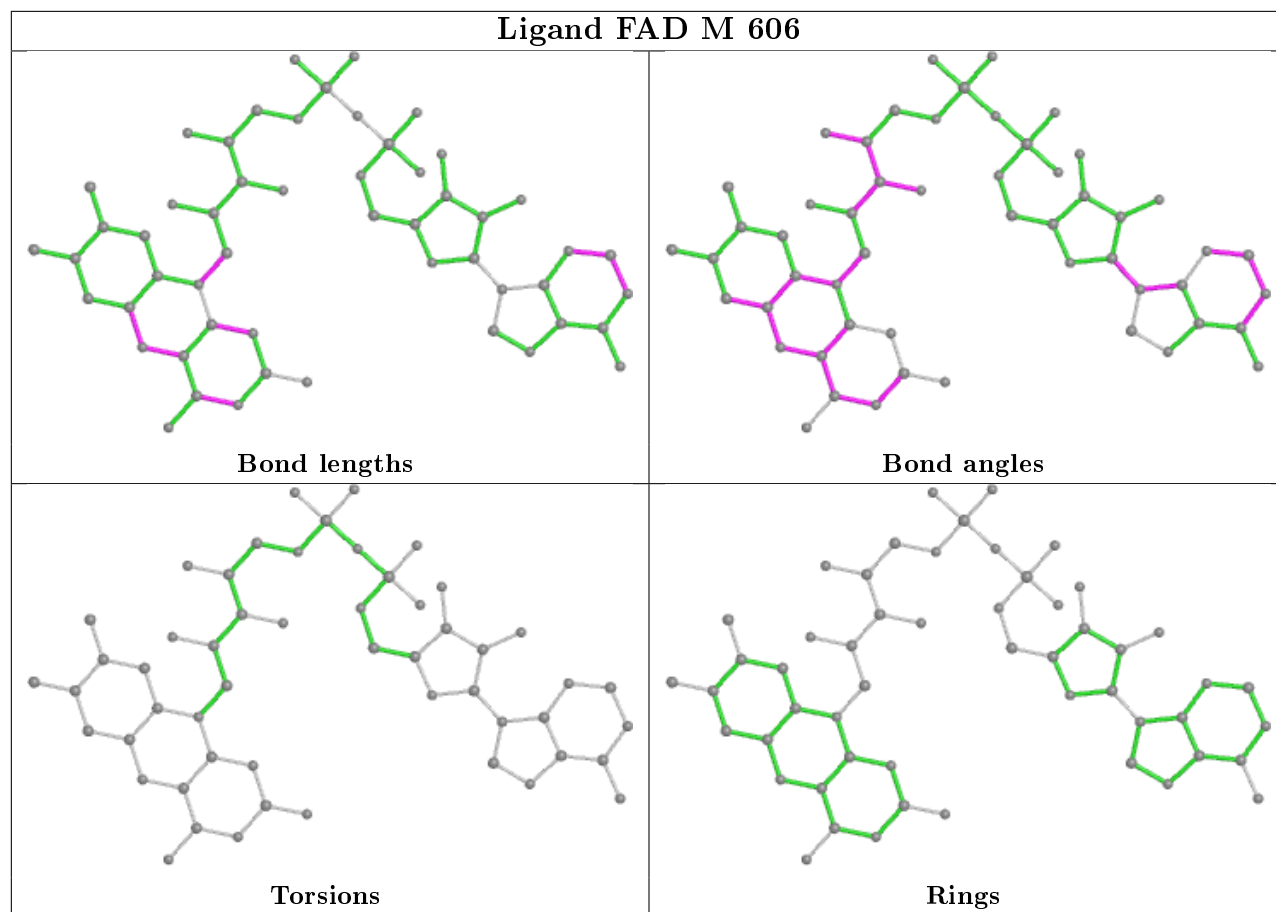


## Ligand MTE C 1326



## Ligand MTE N 1326





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	164/164 (100%)	-0.08	6 (3%) 41 39	12, 20, 40, 56	0
1	L	164/164 (100%)	0.08	10 (6%) 21 20	16, 28, 54, 67	0
2	B	305/305 (100%)	-0.05	4 (1%) 77 75	15, 27, 40, 45	0
2	M	305/305 (100%)	0.12	9 (2%) 50 48	22, 36, 49, 53	0
3	C	755/755 (100%)	-0.08	19 (2%) 57 55	11, 26, 43, 58	0
3	N	745/755 (98%)	-0.18	16 (2%) 63 61	12, 27, 43, 69	0
All	All	2438/2448 (99%)	-0.07	64 (2%) 56 53	11, 27, 45, 69	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	2	THR	5.7
3	N	1248	PRO	5.7
3	N	1288	ASN	5.2
2	M	429	ASP	4.7
1	L	60	ARG	4.4
1	L	61	LEU	4.4
1	L	58	TYR	4.2
2	M	528	GLY	4.2
2	M	499	ASP	3.8
1	A	2	THR	3.7
3	C	1318	VAL	3.6
1	A	60	ARG	3.6
3	N	852	LYS	3.4
2	M	336	TRP	3.4
1	L	97	ARG	3.3
1	A	61	LEU	3.2
3	N	1286	THR	3.1
3	C	1250	LYS	3.1
3	C	683	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
3	C	1245	ARG	3.0
2	B	272	ASN	2.9
2	M	498	PRO	2.9
1	A	96	THR	2.8
3	N	1287	ASN	2.8
3	N	683	HIS	2.8
1	A	58	TYR	2.8
3	C	1001	ILE	2.7
3	C	607	LEU	2.7
3	N	1246	ASP	2.7
3	N	969	ASP	2.7
3	C	725	GLU	2.6
2	B	499	ASP	2.6
3	C	718	ASP	2.6
3	C	724	SER	2.5
1	A	63	ASP	2.5
1	L	63	ASP	2.5
3	C	969	ASP	2.5
3	C	1324	ASN	2.4
2	M	445	GLY	2.4
2	M	471	GLN	2.4
1	L	165	LYS	2.4
3	N	1290	THR	2.4
1	L	62	GLN	2.4
2	M	335	ARG	2.4
1	L	121	VAL	2.3
3	C	1325	CYS	2.3
2	M	509	ARG	2.3
3	C	1246	ASP	2.3
3	N	1289	ASN	2.2
3	C	638	ASP	2.2
3	C	961	GLY	2.2
1	L	137	GLU	2.2
3	N	1110	ASP	2.2
3	N	1247	CYS	2.2
3	C	1158	ALA	2.2
3	N	720	LYS	2.2
3	N	1144	THR	2.2
3	C	1317	CYS	2.2
3	N	1102	GLU	2.2
3	N	664	GLY	2.1
2	B	336	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	1247	CYS	2.0
2	B	528	GLY	2.0
3	C	571	ASP	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

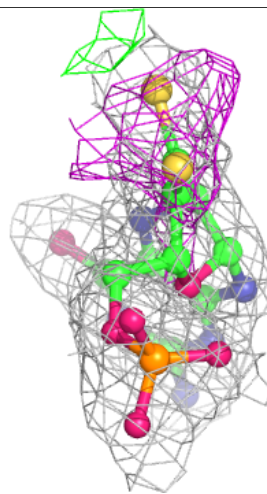
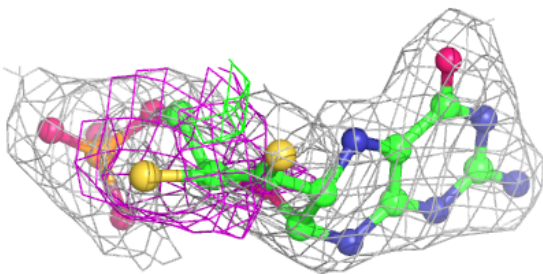
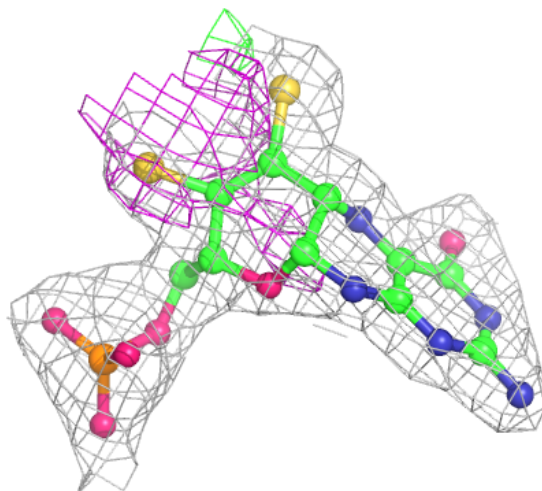
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	MOS	C	1327	4/4	0.84	0.26	22,61,61,67	0
8	LUZ	C	1	12/12	0.88	0.16	37,38,39,40	0
8	LUZ	N	1	12/12	0.89	0.15	28,31,32,32	0
6	MTE	C	1326	24/24	0.92	0.13	18,26,34,41	0
9	CA	C	1328	1/1	0.93	0.11	43,43,43,43	0
5	FAD	B	606	53/53	0.96	0.12	15,20,24,28	0
6	MTE	N	1326	24/24	0.96	0.10	26,28,31,33	0
5	FAD	M	606	53/53	0.97	0.11	19,27,36,45	0
7	MOS	N	1327	4/4	0.98	0.12	45,46,48,54	0
4	FES	A	602	4/4	0.99	0.06	13,15,16,16	0
4	FES	L	601	4/4	0.99	0.08	21,22,23,23	0
4	FES	A	601	4/4	0.99	0.08	15,16,17,17	0
4	FES	L	602	4/4	1.00	0.05	19,20,21,24	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.

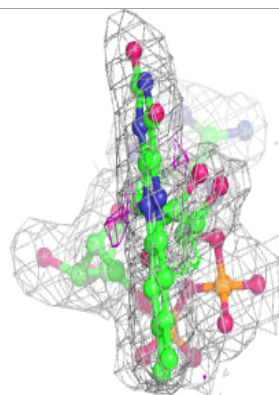
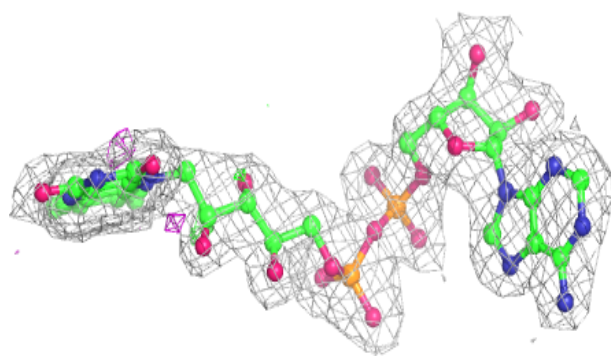
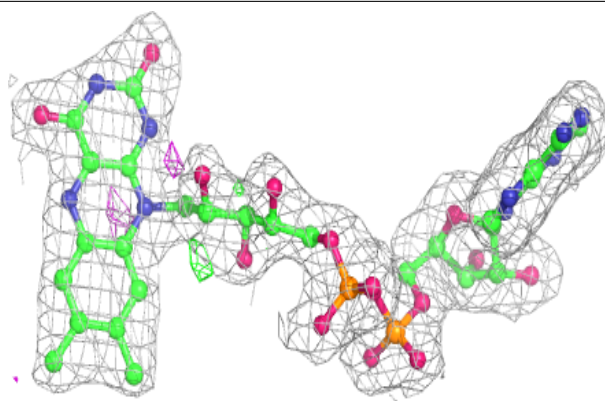
**Electron density around MTE C 1326:**

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



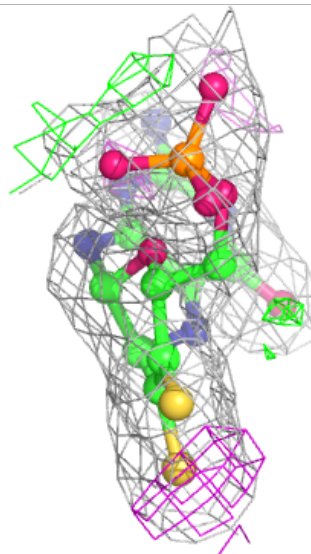
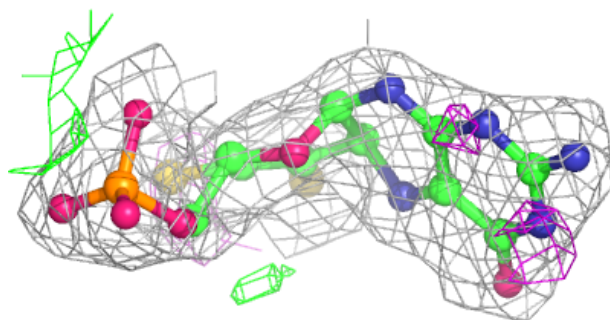
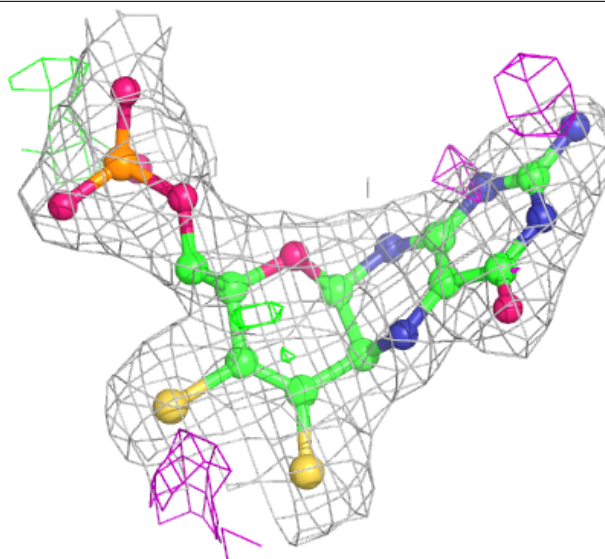
**Electron density around FAD B 606:**

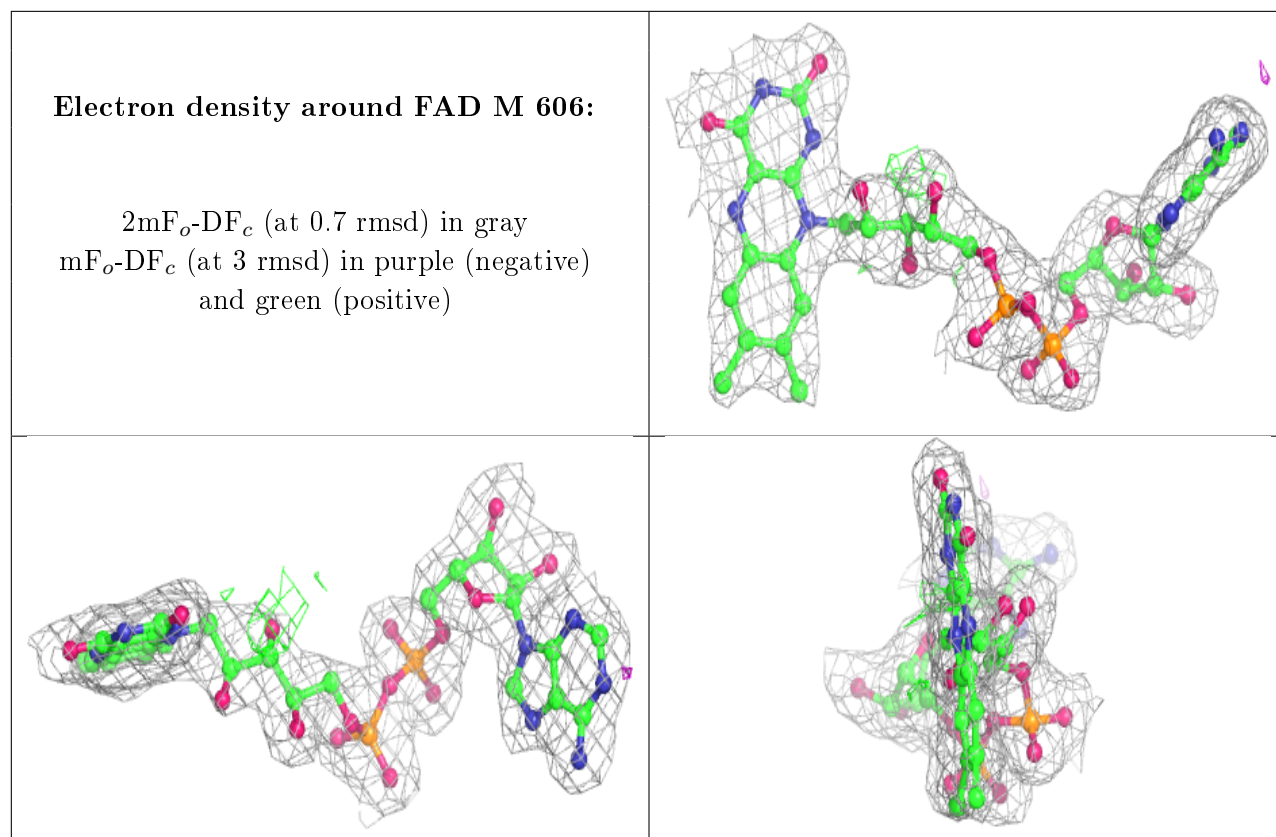
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around MTE N 1326:**

$2mF_o-DF_c$  (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.