



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:00 PM UTC

PDB ID : 1SEZ / pdb_00001sez
Title : Crystal Structure of Protoporphyrinogen IX Oxidase
Authors : Koch, M.; Breithaupt, C.; Kiefersauer, R.; Freigang, J.; Huber, R.; Messerschmidt, A.
Deposited on : 2004-02-19
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

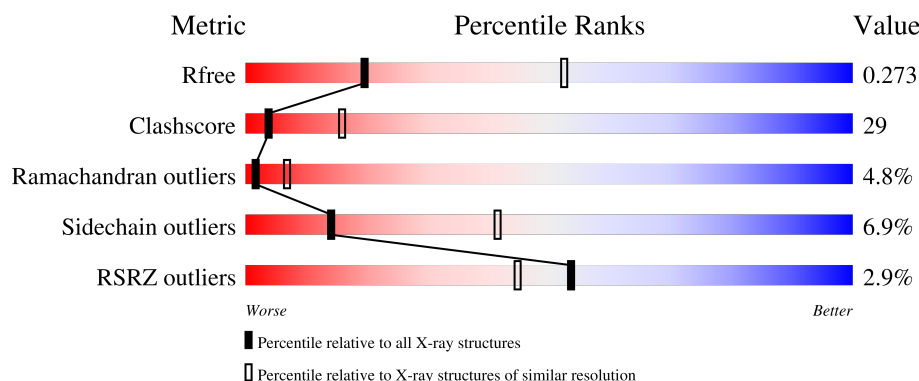
1 Overall quality at a glance

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	504	2% 52% 34% 6% 8%
1	B	504	3% 49% 38% 5% 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7295 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.

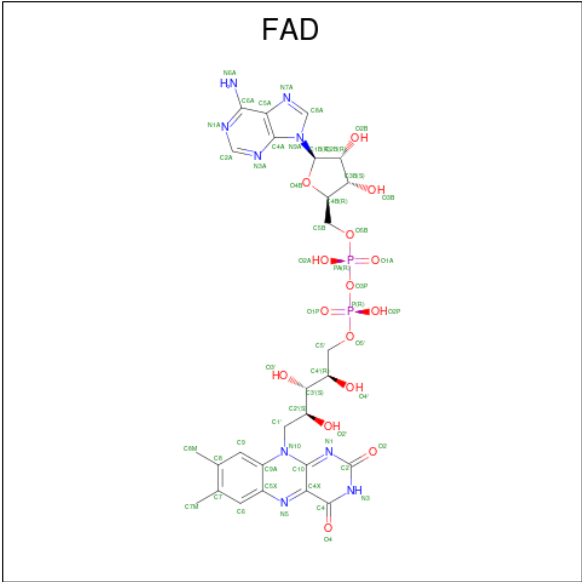
- Molecule 1 is a protein called Protoporphyrinogen oxidase, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	Se	41	0	0
			3480	2215	588	662	6	9			
1	B	465	Total	C	N	O	S	Se	165	0	0
			3480	2215	588	662	6	9			

There are 18 discrepancies between the modelled and reference sequences:

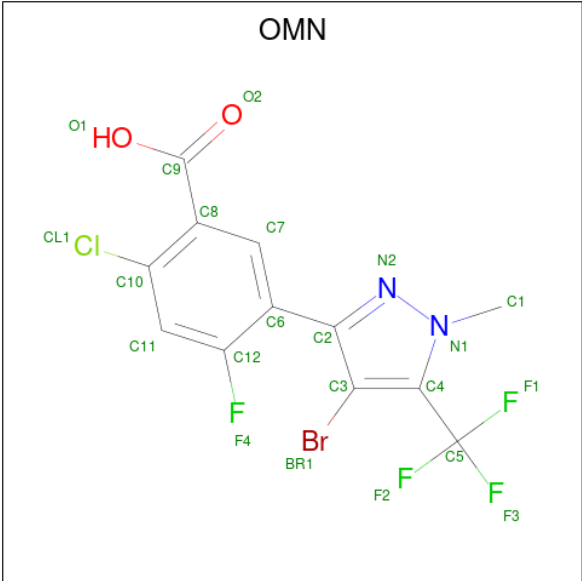
Chain	Residue	Modelled	Actual	Comment	Reference
A	69	MSE	MET	modified residue	UNP O24164
A	130	MSE	MET	modified residue	UNP O24164
A	186	MSE	MET	modified residue	UNP O24164
A	242	MSE	MET	modified residue	UNP O24164
A	302	MSE	MET	modified residue	UNP O24164
A	312	MSE	MET	modified residue	UNP O24164
A	376	MSE	MET	modified residue	UNP O24164
A	377	MSE	MET	modified residue	UNP O24164
A	456	MSE	MET	modified residue	UNP O24164
B	69	MSE	MET	modified residue	UNP O24164
B	130	MSE	MET	modified residue	UNP O24164
B	186	MSE	MET	modified residue	UNP O24164
B	242	MSE	MET	modified residue	UNP O24164
B	302	MSE	MET	modified residue	UNP O24164
B	312	MSE	MET	modified residue	UNP O24164
B	376	MSE	MET	modified residue	UNP O24164
B	377	MSE	MET	modified residue	UNP O24164
B	456	MSE	MET	modified residue	UNP O24164

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 3 is 4-BROMO-3-(5'-CARBOXY-4'-CHLORO-2'-FLUOROPHENYL)-1-METHYL-5-TRIFLUOROMETHYL-PYRAZOL (CCD ID: OMN) (formula: C₁₂H₆BrClF₄N₂O₂).



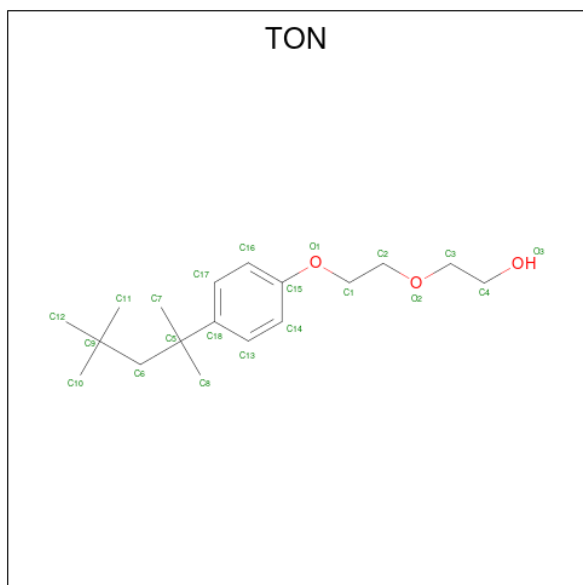
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	Br	C	Cl	F	N	O	0	0
			22	1	12	1	4	2	2		

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Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	B	1	Total	Br	C	Cl	F	N	O	0	0
			22	1	12	1	4	2	2		

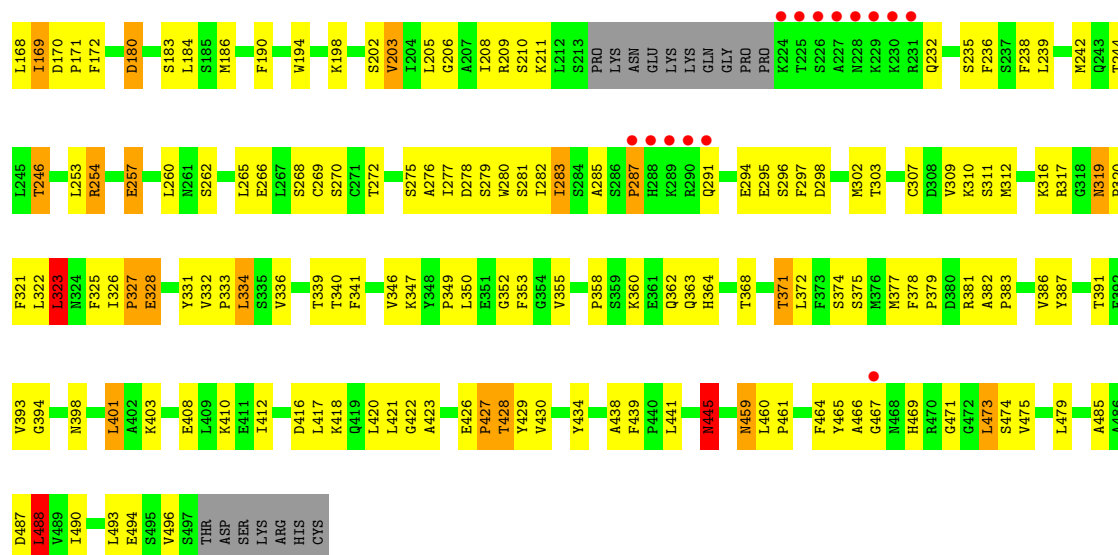
- Molecule 4 is 2-{2-[4-(1,1,3,3-TETRAMETHYLBUTYL)PHENOXY]ETHOXY}ETHANOL (CCD ID: TON) (formula: C₁₈H₃₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			21	18	3		
4	B	1	Total	C	O	0	0
			21	18	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	75	Total	O	0	0
			75	75		
5	B	68	Total	O	0	0
			68	68		



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	119.09Å 147.25Å 127.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.73 – 2.90 19.73 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.6 (19.73-2.90) 99.1 (19.73-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.62 (at 2.88Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.227 , 0.293 0.220 , 0.273	Depositor DCC
R_{free} test set	1209 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	77.2	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 45.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7295	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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: TON, OMN, FAD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.51	0/3539	1.00	16/4781 (0.3%)
1	B	0.49	0/3539	1.04	20/4781 (0.4%)
All	All	0.50	0/7078	1.02	36/9562 (0.4%)

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	115	ASP	N-CA-C	-11.98	98.30	113.16
1	B	488	LEU	N-CA-C	-9.41	100.12	111.69
1	A	382	ALA	N-CA-C	9.26	116.47	108.13
1	B	51	LYS	N-CA-C	-8.75	102.61	113.20
1	A	51	LYS	N-CA-C	-8.68	102.70	113.20
1	B	382	ALA	N-CA-C	8.10	115.42	108.13
1	B	211	LYS	N-CA-C	-7.76	103.33	114.12
1	A	488	LEU	N-CA-C	-7.38	102.19	112.45
1	B	374	SER	N-CA-C	7.04	119.61	111.02
1	B	426	GLU	CA-C-N	6.60	128.09	119.84
1	B	426	GLU	C-N-CA	6.60	128.09	119.84
1	A	287	PRO	N-CA-C	-6.60	105.26	113.84
1	A	287	PRO	N-CA-CB	6.52	110.00	103.48
1	B	287	PRO	N-CA-CB	6.40	109.97	103.25
1	B	72	SER	N-CA-C	-6.38	105.25	113.16
1	A	72	SER	N-CA-C	-6.25	105.41	113.16
1	B	232	GLN	N-CA-C	-6.23	104.48	111.28
1	A	426	GLU	CA-C-N	6.00	127.34	119.84
1	A	426	GLU	C-N-CA	6.00	127.34	119.84
1	A	374	SER	N-CA-C	5.87	118.18	111.02
1	B	471	GLY	N-CA-C	5.85	121.05	113.27
1	A	469	HIS	N-CA-C	-5.85	106.00	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	180	ASP	CA-C-N	5.62	126.87	119.84
1	B	180	ASP	C-N-CA	5.62	126.87	119.84
1	B	401	LEU	N-CA-C	-5.61	107.08	114.04
1	A	347	LYS	N-CA-C	5.60	117.83	111.11
1	A	492	TYR	N-CA-C	-5.49	106.26	113.12
1	B	319	ASN	CA-C-N	5.34	126.51	119.84
1	B	319	ASN	C-N-CA	5.34	126.51	119.84
1	A	460	LEU	CA-C-N	5.28	125.20	119.76
1	A	460	LEU	C-N-CA	5.28	125.20	119.76
1	B	439	PHE	CA-C-N	5.16	125.32	119.90
1	B	439	PHE	C-N-CA	5.16	125.32	119.90
1	B	291	GLN	CB-CA-C	-5.16	110.21	117.23
1	A	447	ASP	N-CA-C	-5.11	105.89	111.82
1	A	162	LYS	N-CA-C	5.03	116.84	111.36

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	3480	0	3367	199	0
1	B	3480	0	3367	194	0
2	A	53	0	31	2	0
2	B	53	0	31	2	0
3	A	22	0	5	0	0
3	B	22	0	5	0	0
4	A	21	0	30	2	0
4	B	21	0	30	1	0
5	A	75	0	0	14	0
5	B	68	0	0	15	0
All	All	7295	0	6866	391	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 29.

All (391) 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:69:MSE:HE2	1:A:242:MSE:HE1	1.44	1.00
1:B:69:MSE:HE1	1:B:238:PHE:HE1	1.25	0.99
1:B:309:VAL:HA	1:B:312:MSE:HE3	1.47	0.95
1:A:496:VAL:HG23	1:A:497:SER:H	1.32	0.95
1:B:69:MSE:HE1	1:B:238:PHE:CE1	2.06	0.90
1:A:69:MSE:HE1	1:A:238:PHE:HE1	1.35	0.90
1:A:69:MSE:HE1	1:A:238:PHE:CE1	2.11	0.86
1:A:410:LYS:HG3	1:A:430:VAL:HG21	1.60	0.84
1:A:316:LYS:HG3	1:A:317:ARG:H	1.45	0.81
1:A:309:VAL:HA	1:A:312:MSE:HE3	1.62	0.81
1:A:460:LEU:HB2	5:A:652:HOH:O	1.81	0.81
1:A:253:LEU:HD22	1:A:257:GLU:HG2	1.64	0.79
1:B:265:LEU:HD11	1:B:285:ALA:HB2	1.65	0.78
1:B:346:VAL:HG21	1:B:387:TYR:HD1	1.46	0.78
1:A:460:LEU:HD22	5:A:652:HOH:O	1.82	0.77
1:A:209:ARG:HG2	1:A:209:ARG:HH11	1.50	0.77
1:B:69:MSE:HE2	1:B:242:MSE:HE1	1.67	0.76
1:A:69:MSE:HE2	1:A:242:MSE:CE	2.16	0.75
1:B:114:ILE:HD13	1:B:114:ILE:O	1.85	0.74
1:A:265:LEU:HD11	1:A:285:ALA:HB2	1.68	0.74
1:B:410:LYS:HG3	1:B:430:VAL:HG21	1.69	0.74
1:A:360:LYS:O	1:A:363:GLN:HG2	1.88	0.73
1:A:340:THR:O	1:A:428:THR:HB	1.89	0.73
1:A:69:MSE:HG2	1:A:70:THR:N	2.03	0.73
1:A:251:LYS:HE2	1:A:251:LYS:HA	1.69	0.73
1:B:69:MSE:HG2	1:B:70:THR:N	2.03	0.73
1:A:325:PHE:H	1:A:325:PHE:HD2	1.37	0.72
1:A:410:LYS:HE2	1:A:427:PRO:HD2	1.72	0.72
1:A:100:ILE:HD11	1:A:109:LEU:HD13	1.71	0.71
1:B:334:LEU:HD23	1:B:334:LEU:O	1.91	0.71
1:B:310:LYS:HE3	1:B:311:SER:HB3	1.72	0.71
1:A:310:LYS:HE3	1:A:311:SER:HB3	1.72	0.71
1:A:242:MSE:HG2	5:A:660:HOH:O	1.90	0.70
1:B:332:VAL:HG23	1:B:441:LEU:HD13	1.72	0.70
1:A:340:THR:O	1:A:427:PRO:O	2.09	0.70
1:B:50:GLY:N	5:B:651:HOH:O	2.25	0.69
1:B:76:VAL:O	1:B:80:ILE:HG12	1.93	0.69
1:A:323:LEU:HA	1:A:325:PHE:CE2	2.28	0.69
1:A:331:TYR:OH	1:A:469:HIS:HE1	1.75	0.69
1:B:331:TYR:OH	1:B:469:HIS:HE1	1.76	0.68
1:B:340:THR:O	1:B:427:PRO:O	2.10	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:LEU:HD22	1:A:377:MSE:HE1	1.74	0.68
1:B:198:LYS:HD3	1:B:198:LYS:C	2.19	0.68
1:A:411:GLU:HB2	5:A:650:HOH:O	1.95	0.67
1:A:496:VAL:HG23	1:A:497:SER:N	2.08	0.67
1:B:494:GLU:O	1:B:496:VAL:HG23	1.94	0.67
1:A:35:HIS:O	1:A:35:HIS:ND1	2.27	0.67
1:B:340:THR:O	1:B:428:THR:HB	1.95	0.67
1:A:314:ILE:HD11	1:A:460:LEU:CD2	2.26	0.66
1:A:314:ILE:HD11	1:A:460:LEU:HD23	1.77	0.66
1:B:310:LYS:C	1:B:310:LYS:HD2	2.20	0.66
1:A:49:GLY:HA2	1:A:246:THR:HG21	1.78	0.66
1:B:49:GLY:HA2	5:B:651:HOH:O	1.97	0.65
1:B:418:LYS:HA	1:B:423:ALA:H	1.60	0.65
1:A:334:LEU:O	1:A:334:LEU:HD23	1.96	0.65
1:B:15:ARG:HB2	1:B:297:PHE:HA	1.79	0.65
1:B:336:VAL:HG23	5:B:644:HOH:O	1.95	0.65
1:A:316:LYS:HE2	1:A:321:PHE:HD1	1.60	0.65
1:A:228:ASN:HA	5:A:620:HOH:O	1.97	0.65
1:B:398:ASN:HD22	1:B:401:LEU:HD22	1.63	0.64
1:A:17:ALA:HB3	1:A:300:VAL:HG22	1.79	0.64
1:A:398:ASN:ND2	1:A:401:LEU:HB2	2.12	0.64
1:A:383:PRO:O	1:A:386:VAL:HG12	1.98	0.63
1:B:334:LEU:HD22	1:B:438:ALA:CB	2.29	0.63
1:A:76:VAL:O	1:A:80:ILE:HG12	1.99	0.63
1:B:410:LYS:HE2	1:B:427:PRO:HD2	1.81	0.63
1:B:35:HIS:O	1:B:35:HIS:ND1	2.32	0.63
1:A:403:LYS:HG2	1:A:434:TYR:CZ	2.35	0.62
1:B:332:VAL:CG2	1:B:441:LEU:HD13	2.28	0.62
1:A:198:LYS:HD3	1:A:198:LYS:C	2.23	0.62
1:B:340:THR:HG22	1:B:429:TYR:HB3	1.80	0.62
1:A:281:SER:HA	1:A:295:GLU:O	2.00	0.62
1:A:100:ILE:CG1	1:A:109:LEU:HD13	2.30	0.61
1:A:332:VAL:HG23	1:A:441:LEU:HD13	1.80	0.61
1:B:326:ILE:HD12	1:B:328:GLU:N	2.15	0.61
1:B:171:PRO:HG3	1:B:358:PRO:HG3	1.81	0.61
1:A:340:THR:HG22	1:A:429:TYR:HB3	1.82	0.61
1:B:281:SER:HA	1:B:295:GLU:O	2.00	0.61
1:A:334:LEU:HD22	1:A:438:ALA:CB	2.30	0.61
1:A:310:LYS:HD2	1:A:310:LYS:C	2.25	0.61
1:A:334:LEU:HD23	1:A:334:LEU:C	2.26	0.61
1:B:360:LYS:O	1:B:363:GLN:HG2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:GLN:HG3	1:A:62:TRP:CH2	2.36	0.61
1:A:100:ILE:CD1	1:A:109:LEU:HD13	2.31	0.61
1:B:403:LYS:HG2	1:B:434:TYR:CZ	2.37	0.60
1:B:102:ARG:C	1:B:104:GLY:H	2.09	0.60
1:B:334:LEU:HD22	1:B:438:ALA:HB2	1.83	0.60
1:B:253:LEU:HA	5:B:636:HOH:O	2.01	0.60
1:A:16:VAL:HG13	1:A:299:ALA:HB3	1.85	0.59
1:A:410:LYS:CE	1:A:427:PRO:HD2	2.31	0.59
1:A:356:LEU:HD11	4:A:603:TON:H31	1.82	0.59
1:A:316:LYS:HG3	1:A:317:ARG:N	2.15	0.59
1:B:57:GLN:HG3	1:B:58:ASP:OD1	2.03	0.59
1:A:326:ILE:HD12	1:A:326:ILE:O	2.02	0.59
1:B:183:SER:O	1:B:184:LEU:HD12	2.02	0.59
1:A:209:ARG:HG2	1:A:209:ARG:NH1	2.16	0.59
1:A:96:ASN:O	1:A:96:ASN:CG	2.46	0.58
1:A:103:ASN:C	1:A:103:ASN:OD1	2.46	0.58
1:A:427:PRO:C	1:A:429:TYR:H	2.11	0.58
1:B:131:LEU:O	1:B:134:PRO:HD2	2.03	0.58
1:B:445:ASN:C	1:B:445:ASN:HD22	2.10	0.58
1:A:70:THR:HG22	1:A:71:GLU:N	2.18	0.58
1:B:109:LEU:HD12	1:B:110:PRO:HD2	1.84	0.58
1:B:106:PRO:HG2	1:B:350:LEU:HD11	1.84	0.58
1:B:283:ILE:HD12	1:B:283:ILE:N	2.18	0.58
1:B:427:PRO:C	1:B:429:TYR:H	2.11	0.58
1:A:66:ALA:HA	2:A:600:FAD:N5	2.19	0.58
1:B:340:THR:O	1:B:340:THR:HG23	2.03	0.58
1:B:79:LEU:HD12	1:B:479:LEU:HD21	1.86	0.57
1:A:266:GLU:CB	1:A:283:ILE:HD13	2.34	0.57
1:A:332:VAL:CG2	1:A:441:LEU:HD13	2.35	0.57
1:B:49:GLY:CA	5:B:651:HOH:O	2.52	0.57
1:B:334:LEU:HD23	1:B:334:LEU:C	2.30	0.57
1:A:19:ILE:O	1:A:303:THR:HB	2.05	0.57
1:A:398:ASN:HD22	1:A:401:LEU:HD22	1.70	0.57
1:B:48:ALA:O	1:B:49:GLY:C	2.48	0.57
1:A:334:LEU:HD22	1:A:438:ALA:HB2	1.85	0.57
1:B:66:ALA:HA	2:B:610:FAD:N5	2.20	0.57
1:B:169:ILE:C	1:B:169:ILE:HD12	2.30	0.57
1:B:459:ASN:O	1:B:461:PRO:HD3	2.05	0.57
1:A:170:ASP:HB3	1:A:171:PRO:HD3	1.87	0.56
1:B:39:VAL:HG12	1:B:40:THR:N	2.19	0.56
1:A:79:LEU:HD12	1:A:479:LEU:HD21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:GLU:HB3	5:B:624:HOH:O	2.04	0.56
1:B:398:ASN:ND2	1:B:401:LEU:HD22	2.21	0.56
1:A:48:ALA:O	1:A:49:GLY:C	2.48	0.55
1:A:183:SER:O	1:A:184:LEU:HD12	2.06	0.55
1:B:464:PHE:CD2	1:B:488:LEU:HD23	2.40	0.55
1:B:23:VAL:HG13	1:B:24:SER:N	2.21	0.55
1:B:102:ARG:HD3	1:B:167:TYR:CE2	2.41	0.55
1:B:244:THR:HG22	5:B:629:HOH:O	2.07	0.55
1:B:327:PRO:O	1:B:328:GLU:C	2.49	0.55
1:A:69:MSE:HE2	1:A:242:MSE:SE	2.57	0.55
1:B:368:THR:HG23	1:B:416:ASP:OD1	2.07	0.55
1:A:169:ILE:HD12	1:A:169:ILE:C	2.32	0.55
1:B:347:LYS:C	1:B:349:PRO:HD3	2.32	0.55
1:B:372:LEU:HD22	1:B:377:MSE:HE1	1.89	0.55
1:A:346:VAL:HG21	1:A:387:TYR:HD1	1.72	0.54
1:B:302:MSE:HB3	1:B:465:TYR:HA	1.89	0.54
1:B:13:ALA:HB3	5:B:616:HOH:O	2.08	0.54
1:B:123:SER:O	1:B:127:LYS:HG3	2.07	0.54
1:B:88:LYS:NZ	5:B:614:HOH:O	2.37	0.54
1:B:323:LEU:HB2	1:B:326:ILE:CG2	2.37	0.54
1:A:445:ASN:C	1:A:445:ASN:HD22	2.13	0.54
1:B:133:GLU:N	1:B:134:PRO:CD	2.70	0.54
1:A:368:THR:HG23	1:A:416:ASP:OD1	2.07	0.54
1:B:353:PHE:O	1:B:377:MSE:HE2	2.07	0.54
1:A:86:ARG:HH11	1:A:89:GLN:HE22	1.54	0.54
1:B:49:GLY:HA2	1:B:246:THR:HG21	1.90	0.54
1:A:71:GLU:O	1:A:71:GLU:HG3	2.08	0.54
1:B:70:THR:HG22	1:B:71:GLU:N	2.21	0.54
1:B:398:ASN:ND2	1:B:401:LEU:HB2	2.23	0.54
1:A:419:GLN:HG2	5:A:655:HOH:O	2.08	0.53
1:A:325:PHE:N	1:A:325:PHE:CD2	2.75	0.53
1:A:346:VAL:HG12	1:A:349:PRO:HG3	1.89	0.53
1:A:283:ILE:N	1:A:283:ILE:HD12	2.23	0.53
1:B:14:LYS:HD2	1:B:298:ASP:OD2	2.07	0.53
1:B:309:VAL:O	1:B:312:MSE:HB2	2.08	0.53
1:A:73:GLU:HB2	1:A:76:VAL:HG23	1.91	0.53
1:A:251:LYS:HE2	1:A:251:LYS:CA	2.38	0.53
1:A:411:GLU:CB	5:A:650:HOH:O	2.54	0.53
1:B:266:GLU:CB	1:B:283:ILE:HD13	2.39	0.52
1:B:346:VAL:HG21	1:B:387:TYR:CD1	2.37	0.52
1:B:372:LEU:HB3	1:B:377:MSE:HE1	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:GLN:NE2	1:A:97:LYS:HD2	2.24	0.52
1:B:96:ASN:CG	1:B:96:ASN:O	2.51	0.52
1:A:171:PRO:HG3	1:A:358:PRO:HG3	1.92	0.52
1:A:294:GLU:HG2	1:A:295:GLU:N	2.24	0.52
1:B:170:ASP:HB3	1:B:171:PRO:HD3	1.91	0.52
1:B:346:VAL:HG12	1:B:349:PRO:HG3	1.91	0.52
1:A:15:ARG:HD2	5:A:613:HOH:O	2.10	0.52
1:B:383:PRO:O	1:B:386:VAL:HG12	2.09	0.52
1:B:386:VAL:HG22	1:B:387:TYR:N	2.24	0.52
1:A:79:LEU:HD12	1:A:479:LEU:HD11	1.91	0.52
1:A:168:LEU:O	1:A:171:PRO:HD2	2.09	0.51
1:A:294:GLU:O	1:A:295:GLU:HG3	2.09	0.51
1:B:119:SER:HB3	5:B:659:HOH:O	2.09	0.51
1:B:254:ARG:O	1:B:257:GLU:HB2	2.10	0.51
1:A:104:GLY:O	1:A:105:THR:HG23	2.09	0.51
1:A:187:HIS:HD1	1:A:194:TRP:CD1	2.28	0.51
1:A:134:PRO:HB3	1:A:205:LEU:HD13	1.92	0.51
1:B:445:ASN:C	1:B:445:ASN:ND2	2.68	0.51
1:B:473:LEU:H	1:B:473:LEU:HD12	1.76	0.51
1:A:253:LEU:HB3	1:A:257:GLU:HB3	1.93	0.51
1:B:340:THR:O	1:B:340:THR:CG2	2.58	0.51
1:B:372:LEU:HB3	1:B:377:MSE:CE	2.41	0.51
1:A:420:LEU:HD23	5:A:655:HOH:O	2.10	0.51
1:A:39:VAL:HG12	1:A:40:THR:N	2.25	0.50
1:A:372:LEU:HB3	1:A:377:MSE:CE	2.41	0.50
1:B:15:ARG:HB3	1:B:297:PHE:CD2	2.46	0.50
1:A:168:LEU:C	1:A:171:PRO:HD2	2.37	0.50
1:B:341:PHE:O	1:B:386:VAL:HG23	2.10	0.50
1:A:114:ILE:HD11	1:B:208:ILE:HG22	1.94	0.50
1:A:269:CYS:HB3	1:A:280:TRP:CD2	2.46	0.50
1:A:323:LEU:HA	1:A:325:PHE:HE2	1.74	0.50
1:A:340:THR:O	1:A:340:THR:HG23	2.10	0.50
1:A:51:LYS:HB2	2:A:600:FAD:O4'	2.12	0.50
1:A:113:PRO:HB3	5:A:678:HOH:O	2.12	0.50
1:B:69:MSE:HE3	1:B:236:PHE:CE1	2.47	0.50
1:B:102:ARG:C	1:B:104:GLY:N	2.70	0.50
1:A:133:GLU:N	1:A:134:PRO:CD	2.75	0.49
1:B:347:LYS:O	1:B:349:PRO:HD3	2.12	0.49
1:A:33:LYS:C	1:A:35:HIS:H	2.19	0.49
1:B:155:PHE:CD1	1:B:186:MSE:HG2	2.48	0.49
1:A:62:TRP:HE1	1:A:64:GLU:HG2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:ASP:O	1:A:458:LYS:HG3	2.12	0.49
1:B:340:THR:CG2	1:B:428:THR:HG22	2.42	0.49
1:B:88:LYS:HD3	5:B:654:HOH:O	2.11	0.49
1:A:407:THR:O	5:A:650:HOH:O	2.20	0.49
1:A:26:LEU:HB3	1:A:249:ILE:HG21	1.93	0.49
1:B:362:GLN:C	1:B:364:HIS:H	2.20	0.49
1:A:362:GLN:C	1:A:364:HIS:H	2.21	0.49
1:B:69:MSE:HE2	1:B:242:MSE:CE	2.40	0.49
1:B:410:LYS:CE	1:B:427:PRO:HD2	2.42	0.49
1:A:276:ALA:O	1:A:277:ILE:C	2.54	0.49
1:A:100:ILE:HG13	1:A:109:LEU:HD13	1.95	0.48
1:A:316:LYS:HG2	1:A:319:ASN:O	2.13	0.48
1:A:474:SER:O	1:A:475:VAL:C	2.56	0.48
1:B:66:ALA:O	1:B:242:MSE:HG3	2.14	0.48
1:B:86:ARG:HH11	1:B:89:GLN:HE22	1.61	0.48
1:B:294:GLU:O	1:B:295:GLU:HG3	2.13	0.48
1:B:496:VAL:HG12	1:B:496:VAL:O	2.13	0.48
1:A:316:LYS:HE2	1:A:321:PHE:CD1	2.46	0.48
1:B:110:PRO:HG2	1:B:116:LEU:HD12	1.95	0.48
1:B:282:ILE:O	1:B:294:GLU:HA	2.13	0.48
1:A:104:GLY:N	1:A:361:GLU:OE1	2.47	0.48
1:A:151:SER:HA	1:A:184:LEU:O	2.13	0.48
1:B:164:VAL:O	1:B:168:LEU:HB2	2.13	0.48
1:A:52:LEU:HD23	1:A:66:ALA:HB3	1.95	0.48
1:B:68:THR:OG1	1:B:235:SER:HB2	2.14	0.48
1:A:253:LEU:CD2	1:A:257:GLU:HG2	2.39	0.47
1:A:340:THR:CG2	1:A:428:THR:HG22	2.44	0.47
1:B:69:MSE:CG	1:B:70:THR:N	2.75	0.47
1:A:78:PHE:CD1	1:A:78:PHE:C	2.92	0.47
1:A:236:PHE:CD1	1:A:236:PHE:C	2.92	0.47
1:B:62:TRP:HE1	1:B:64:GLU:HG2	1.78	0.47
1:A:54:SER:H	1:A:243:GLN:HB2	1.79	0.47
1:A:411:GLU:CG	5:A:650:HOH:O	2.62	0.47
1:A:202:SER:OG	1:A:205:LEU:HB2	2.14	0.47
1:B:22:GLY:HA2	1:B:50:GLY:HA3	1.97	0.47
1:B:15:ARG:HH11	1:B:15:ARG:HG2	1.79	0.47
1:B:270:SER:OG	1:B:279:SER:HB3	2.14	0.47
1:A:302:MSE:HB3	1:A:465:TYR:HA	1.96	0.47
1:B:19:ILE:O	1:B:303:THR:HB	2.15	0.47
1:B:294:GLU:HG2	1:B:295:GLU:N	2.30	0.47
1:A:187:HIS:ND1	1:A:194:TRP:CD1	2.83	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:ILE:O	1:A:294:GLU:HA	2.15	0.47
1:A:427:PRO:O	1:A:429:TYR:N	2.47	0.47
1:B:323:LEU:HA	5:B:619:HOH:O	2.14	0.47
1:B:420:LEU:C	1:B:421:LEU:HD23	2.40	0.47
1:A:316:LYS:CG	1:A:317:ARG:N	2.76	0.47
1:A:259:ARG:NH1	1:A:295:GLU:OE2	2.48	0.46
1:B:371:THR:HB	1:B:391:THR:OG1	2.14	0.46
1:A:306:LEU:H	1:A:469:HIS:CE1	2.33	0.46
1:B:36:GLY:O	1:B:37:LEU:C	2.59	0.46
1:B:172:PHE:HA	4:B:605:TON:H32	1.98	0.46
1:B:202:SER:OG	1:B:205:LEU:HB2	2.15	0.46
1:B:260:LEU:C	1:B:262:SER:H	2.23	0.46
1:B:479:LEU:HD23	1:B:479:LEU:C	2.40	0.46
1:A:103:ASN:HA	1:A:364:HIS:CD2	2.51	0.46
1:A:316:LYS:CG	1:A:317:ARG:H	2.15	0.46
1:B:23:VAL:CG1	1:B:24:SER:N	2.78	0.46
1:B:268:SER:HB2	1:B:281:SER:OG	2.16	0.46
1:A:33:LYS:HD2	1:A:253:LEU:HD23	1.98	0.46
1:A:340:THR:O	1:A:340:THR:CG2	2.64	0.46
1:A:372:LEU:HB3	1:A:377:MSE:HE1	1.98	0.46
1:B:52:LEU:CD2	1:B:66:ALA:HB3	2.46	0.46
1:B:242:MSE:HE2	1:B:475:VAL:HG21	1.98	0.46
1:B:155:PHE:HD2	1:B:156:PHE:N	2.14	0.46
1:B:70:THR:CG2	1:B:71:GLU:N	2.78	0.46
1:B:408:GLU:O	1:B:412:ILE:HG12	2.15	0.46
1:B:339:THR:HB	1:B:427:PRO:HB3	1.97	0.46
1:B:202:SER:O	1:B:203:VAL:C	2.59	0.45
1:B:427:PRO:O	1:B:428:THR:HB	2.16	0.45
1:A:52:LEU:CD2	1:A:66:ALA:HB3	2.47	0.45
1:A:310:LYS:HD2	1:A:311:SER:N	2.31	0.45
1:A:393:VAL:HG12	1:A:394:GLY:N	2.30	0.45
1:B:321:PHE:CZ	1:B:459:ASN:ND2	2.84	0.45
1:A:448:SER:HA	1:A:451:ASP:OD2	2.16	0.45
1:B:151:SER:HA	1:B:184:LEU:O	2.17	0.45
1:B:168:LEU:O	1:B:171:PRO:HD2	2.16	0.45
1:A:69:MSE:CG	1:A:70:THR:N	2.78	0.45
1:B:49:GLY:C	5:B:651:HOH:O	2.55	0.45
1:B:64:GLU:O	1:B:336:VAL:HG21	2.16	0.45
1:B:487:ASP:HA	1:B:490:ILE:HB	1.98	0.45
1:B:168:LEU:C	1:B:171:PRO:HD2	2.42	0.45
1:B:326:ILE:HD12	1:B:328:GLU:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:LYS:CG	1:A:311:SER:N	2.80	0.45
1:B:78:PHE:CD1	1:B:78:PHE:C	2.96	0.44
1:A:35:HIS:O	1:A:35:HIS:CG	2.71	0.44
1:B:418:LYS:HA	1:B:423:ALA:N	2.31	0.44
1:A:187:HIS:HD1	1:A:194:TRP:CG	2.35	0.44
1:A:340:THR:CG2	1:A:429:TYR:HB3	2.48	0.44
1:A:496:VAL:O	1:A:497:SER:HB2	2.18	0.44
1:B:39:VAL:CG1	1:B:40:THR:N	2.81	0.44
1:B:418:LYS:O	1:B:422:GLY:N	2.49	0.44
1:A:316:LYS:HD2	1:A:319:ASN:ND2	2.33	0.44
1:A:398:ASN:ND2	1:A:401:LEU:HD22	2.30	0.44
1:A:70:THR:CG2	1:A:71:GLU:N	2.80	0.44
1:B:14:LYS:HG2	1:B:37:LEU:HD22	1.99	0.44
1:B:417:LEU:HA	1:B:417:LEU:HD23	1.79	0.44
1:A:100:ILE:O	1:A:107:VAL:HG12	2.18	0.44
1:B:294:GLU:CG	1:B:295:GLU:N	2.81	0.44
1:B:393:VAL:HG12	1:B:394:GLY:N	2.33	0.44
1:A:48:ALA:HB2	1:A:258:LEU:HD21	1.99	0.43
1:A:269:CYS:HB3	1:A:280:TRP:CE3	2.54	0.43
1:B:86:ARG:NH2	5:B:653:HOH:O	2.51	0.43
1:B:269:CYS:HB3	1:B:280:TRP:CE3	2.53	0.43
1:A:59:GLY:O	1:A:383:PRO:HD3	2.18	0.43
1:A:172:PHE:HA	4:A:603:TON:H32	2.00	0.43
1:A:326:ILE:O	1:A:326:ILE:CG1	2.66	0.43
1:A:339:THR:HB	1:A:427:PRO:HB3	1.99	0.43
1:A:57:GLN:O	1:A:59:GLY:N	2.52	0.43
1:A:322:LEU:O	1:A:325:PHE:HE2	2.01	0.43
1:B:114:ILE:HD13	1:B:114:ILE:C	2.43	0.43
1:B:115:ASP:O	1:B:119:SER:HB3	2.18	0.43
1:B:494:GLU:C	1:B:496:VAL:N	2.73	0.43
1:A:294:GLU:CG	1:A:295:GLU:N	2.80	0.43
1:B:155:PHE:C	1:B:155:PHE:CD2	2.96	0.43
1:B:494:GLU:C	1:B:496:VAL:H	2.26	0.43
1:A:209:ARG:NH1	1:B:114:ILE:HD12	2.33	0.43
1:A:408:GLU:O	1:A:412:ILE:HG12	2.18	0.43
1:B:459:ASN:O	1:B:461:PRO:CD	2.67	0.43
1:A:280:TRP:O	1:A:296:SER:HA	2.19	0.43
1:B:69:MSE:CE	1:B:242:MSE:HE1	2.45	0.43
1:B:137:TRP:C	1:B:202:SER:HB3	2.44	0.43
1:B:474:SER:O	1:B:475:VAL:C	2.62	0.43
1:B:73:GLU:HB2	1:B:76:VAL:HG23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:GLU:OE1	1:A:204:ILE:HB	2.18	0.42
1:A:162:LYS:NZ	1:A:166:ASP:OD1	2.44	0.42
1:A:202:SER:CB	5:A:659:HOH:O	2.65	0.42
1:A:242:MSE:HE2	1:A:475:VAL:HG21	2.01	0.42
1:A:137:TRP:C	1:A:202:SER:HB3	2.44	0.42
1:B:427:PRO:O	1:B:429:TYR:N	2.52	0.42
1:A:310:LYS:HG3	1:A:311:SER:N	2.34	0.42
1:A:445:ASN:C	1:A:445:ASN:ND2	2.70	0.42
1:B:48:ALA:O	1:B:49:GLY:O	2.36	0.42
1:B:323:LEU:HB2	1:B:326:ILE:HG23	2.01	0.42
1:A:374:SER:HB2	1:A:388:LEU:O	2.20	0.42
1:B:69:MSE:HE2	1:B:242:MSE:SE	2.70	0.42
1:B:168:LEU:HD23	1:B:168:LEU:HA	1.80	0.42
1:A:79:LEU:CD1	1:A:479:LEU:HD21	2.50	0.42
1:B:88:LYS:O	1:B:238:PHE:HA	2.20	0.42
1:B:112:ASN:HA	1:B:113:PRO:HD3	1.93	0.42
1:A:486:ALA:O	1:A:490:ILE:HG13	2.20	0.42
1:A:355:VAL:HG23	1:A:373:PHE:CZ	2.55	0.41
1:A:391:THR:HG21	1:A:413:VAL:HG22	2.01	0.41
1:B:99:TYR:HB2	1:B:355:VAL:HG22	2.01	0.41
1:B:307:CYS:HB3	1:B:331:TYR:CE1	2.55	0.41
1:B:427:PRO:C	1:B:429:TYR:N	2.76	0.41
1:A:22:GLY:HA2	1:A:50:GLY:HA3	2.02	0.41
1:A:309:VAL:O	1:A:312:MSE:HB2	2.20	0.41
1:A:336:VAL:HG22	1:A:392:PHE:CE2	2.55	0.41
1:B:186:MSE:HE3	1:B:190:PHE:HB2	2.03	0.41
1:A:116:LEU:HD12	1:A:116:LEU:HA	1.93	0.41
1:A:131:LEU:O	1:A:134:PRO:HD2	2.21	0.41
1:B:280:TRP:O	1:B:296:SER:HA	2.21	0.41
1:A:52:LEU:HD22	1:A:242:MSE:HB3	2.01	0.41
1:A:326:ILE:HG22	5:A:609:HOH:O	2.21	0.41
1:A:378:PHE:HB2	1:A:381:ARG:HG3	2.02	0.41
1:A:417:LEU:HD23	1:A:417:LEU:HA	1.82	0.41
1:B:464:PHE:HD2	1:B:488:LEU:HD23	1.82	0.41
1:A:206:GLY:O	1:A:207:ALA:C	2.64	0.41
1:B:206:GLY:O	1:B:209:ARG:N	2.53	0.41
1:A:164:VAL:O	1:A:168:LEU:HB2	2.20	0.41
1:A:441:LEU:HD12	1:A:441:LEU:HA	1.71	0.41
1:B:238:PHE:O	1:B:239:LEU:C	2.63	0.41
1:B:310:LYS:C	1:B:310:LYS:CD	2.89	0.41
1:B:378:PHE:HB2	1:B:381:ARG:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:LYS:C	1:A:231:ARG:N	2.77	0.41
1:B:95:GLN:O	1:B:352:GLY:HA2	2.20	0.41
1:B:466:ALA:HB2	1:B:485:ALA:HB2	2.03	0.41
1:B:102:ARG:HD3	1:B:167:TYR:CD2	2.55	0.40
1:B:119:SER:CB	5:B:659:HOH:O	2.68	0.40
1:B:148:SER:N	1:B:194:TRP:HH2	2.18	0.40
1:B:205:LEU:HA	1:B:205:LEU:HD12	1.84	0.40
1:B:333:PRO:O	1:B:334:LEU:HB3	2.20	0.40
1:B:340:THR:CG2	1:B:429:TYR:HB3	2.49	0.40
1:B:441:LEU:HD12	1:B:441:LEU:HA	1.75	0.40
1:A:57:GLN:HG3	1:A:62:TRP:CZ3	2.56	0.40
1:A:326:ILE:O	1:A:326:ILE:CD1	2.68	0.40
1:B:375:SER:O	1:B:379:PRO:HA	2.20	0.40
1:A:88:LYS:O	1:A:238:PHE:HA	2.21	0.40
1:A:183:SER:C	1:A:184:LEU:HD12	2.46	0.40
1:A:269:CYS:HA	1:A:279:SER:O	2.21	0.40
1:A:303:THR:O	1:A:303:THR:CG2	2.69	0.40
1:A:99:TYR:HB2	1:A:355:VAL:HG22	2.03	0.40
1:A:168:LEU:HA	1:A:168:LEU:HD23	1.89	0.40
1:A:306:LEU:HD12	1:A:306:LEU:HA	1.70	0.40
1:B:20:GLY:HA2	2:B:610:FAD:H1B	2.02	0.40
1:B:183:SER:C	1:B:184:LEU:HD12	2.47	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	459/504 (91%)	391 (85%)	50 (11%)	18 (4%)	2	10
1	B	459/504 (91%)	373 (81%)	60 (13%)	26 (6%)	1	4
All	All	918/1008 (91%)	764 (83%)	110 (12%)	44 (5%)	2	7

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	ASP
1	A	210	SER
1	A	211	LYS
1	A	272	THR
1	A	275	SER
1	A	276	ALA
1	A	496	VAL
1	B	114	ILE
1	B	150	GLU
1	B	275	SER
1	B	276	ALA
1	B	287	PRO
1	B	320	PRO
1	B	323	LEU
1	B	328	GLU
1	A	316	LYS
1	A	317	ARG
1	B	37	LEU
1	B	49	GLY
1	B	210	SER
1	B	272	THR
1	B	278	ASP
1	A	212	LEU
1	A	229	LYS
1	A	427	PRO
1	B	203	VAL
1	B	254	ARG
1	B	322	LEU
1	B	459	ASN
1	A	155	PHE
1	A	288	HIS
1	B	113	PRO
1	B	316	LYS
1	A	278	ASP
1	B	277	ILE
1	B	317	ARG
1	B	327	PRO
1	A	228	ASN
1	B	325	PHE
1	B	427	PRO
1	B	445	ASN
1	A	277	ILE

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Mol	Chain	Res	Type
1	A	49	GLY
1	B	467	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	362/423 (86%)	337 (93%)	25 (7%)	14	41
1	B	362/423 (86%)	337 (93%)	25 (7%)	14	41
All	All	724/846 (86%)	674 (93%)	50 (7%)	14	41

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	VAL
1	A	45	GLU
1	A	58	ASP
1	A	69	MSE
1	A	102	ARG
1	A	103	ASN
1	A	113	PRO
1	A	120	ASN
1	A	137	TRP
1	A	169	ILE
1	A	180	ASP
1	A	209	ARG
1	A	246	THR
1	A	257	GLU
1	A	303	THR
1	A	319	ASN
1	A	323	LEU
1	A	325	PHE
1	A	334	LEU
1	A	371	THR
1	A	428	THR

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Mol	Chain	Res	Type
1	A	445	ASN
1	A	460	LEU
1	A	473	LEU
1	A	488	LEU
1	B	45	GLU
1	B	58	ASP
1	B	69	MSE
1	B	102	ARG
1	B	105	THR
1	B	114	ILE
1	B	115	ASP
1	B	120	ASN
1	B	126	SER
1	B	137	TRP
1	B	169	ILE
1	B	180	ASP
1	B	246	THR
1	B	257	GLU
1	B	283	ILE
1	B	319	ASN
1	B	323	LEU
1	B	334	LEU
1	B	371	THR
1	B	428	THR
1	B	445	ASN
1	B	460	LEU
1	B	473	LEU
1	B	488	LEU
1	B	493	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	129	GLN
1	A	149	HIS
1	A	319	ASN
1	A	362	GLN
1	A	398	ASN
1	A	445	ASN
1	A	469	HIS
1	B	89	GLN

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Mol	Chain	Res	Type
1	B	398	ASN
1	B	445	ASN
1	B	459	ASN
1	B	469	HIS

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](#)

6 ligands are modelled in this entry.

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$
3	OMN	B	604	-	22,23,23	2.03	4 (18%)	30,36,36	2.08	7 (23%)
3	OMN	A	601	-	22,23,23	2.08	5 (22%)	30,36,36	2.26	7 (23%)
2	FAD	B	610	-	58,58,58	1.18	4 (6%)	85,89,89	1.02	3 (3%)
4	TON	B	605	-	21,21,21	1.91	5 (23%)	29,29,29	1.06	0
2	FAD	A	600	-	58,58,58	1.32	5 (8%)	85,89,89	1.05	5 (5%)
4	TON	A	603	-	21,21,21	1.91	8 (38%)	29,29,29	1.11	2 (6%)

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
3	OMN	B	604	-	-	4/14/14/14	0/2/2/2
3	OMN	A	601	-	-	2/14/14/14	0/2/2/2
2	FAD	B	610	-	-	2/34/50/50	0/6/6/6
4	TON	B	605	-	-	8/19/19/19	0/1/1/1
2	FAD	A	600	-	-	0/34/50/50	0/6/6/6
4	TON	A	603	-	-	10/19/19/19	0/1/1/1

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	OMN	C2-N2	5.78	1.42	1.33
3	B	604	OMN	C2-N2	5.40	1.42	1.33
3	A	601	OMN	C6-C12	5.28	1.45	1.38
2	A	600	FAD	C4X-N5	4.91	1.41	1.30
3	B	604	OMN	C5-C4	4.41	1.56	1.49
2	B	610	FAD	C4X-N5	4.33	1.40	1.30
4	B	605	TON	C5-C18	4.08	1.60	1.53
4	A	603	TON	C5-C18	3.91	1.59	1.53
3	B	604	OMN	C6-C12	3.87	1.44	1.38
2	A	600	FAD	P-O3P	-3.53	1.55	1.59
4	A	603	TON	C17-C18	3.22	1.44	1.39
3	A	601	OMN	C8-C10	3.06	1.43	1.39
2	A	600	FAD	C9A-C5X	2.89	1.45	1.41
4	B	605	TON	C17-C18	2.85	1.44	1.39
4	B	605	TON	C13-C18	2.80	1.44	1.39
2	B	610	FAD	C2A-N1A	2.79	1.38	1.33
3	A	601	OMN	C5-C4	2.74	1.54	1.49
3	B	604	OMN	C8-C10	2.72	1.43	1.39
4	B	605	TON	C14-C13	2.50	1.42	1.38
2	A	600	FAD	C10-N1	2.49	1.38	1.33
4	A	603	TON	O1-C15	2.45	1.43	1.37
2	B	610	FAD	C9A-C5X	2.42	1.45	1.41
2	B	610	FAD	C10-N1	2.36	1.38	1.33
2	A	600	FAD	C2A-N1A	2.31	1.38	1.33
4	A	603	TON	C16-C15	2.27	1.43	1.38
4	A	603	TON	C17-C16	2.25	1.42	1.38
4	A	603	TON	C13-C18	2.25	1.43	1.39
4	A	603	TON	C14-C15	2.11	1.42	1.38
4	B	605	TON	C6-C9	2.07	1.61	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	603	TON	C6-C9	2.04	1.61	1.55
3	A	601	OMN	C11-C12	2.01	1.41	1.37

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	OMN	C3-C4-N1	9.04	110.32	104.90
3	B	604	OMN	C3-C4-N1	7.57	109.44	104.90
3	A	601	OMN	C11-C12-C6	-3.67	119.42	123.48
3	B	604	OMN	C11-C12-C6	-3.55	119.56	123.48
3	B	604	OMN	C10-C11-C12	3.40	120.98	118.42
3	A	601	OMN	C2-C3-C4	-2.97	104.50	108.10
2	A	600	FAD	O4B-C1B-C2B	-2.96	100.28	106.62
3	A	601	OMN	F2-C5-C4	-2.81	107.79	112.40
3	B	604	OMN	C2-C3-C4	-2.59	104.96	108.10
2	A	600	FAD	C9A-C5X-N5	-2.59	119.71	122.45
3	B	604	OMN	F1-C5-C4	-2.53	108.25	112.40
2	B	610	FAD	C9A-C5X-N5	-2.51	119.79	122.45
3	A	601	OMN	C1-N1-N2	2.49	123.02	119.29
3	A	601	OMN	C10-C11-C12	2.45	120.27	118.42
4	A	603	TON	C13-C14-C15	2.37	122.44	119.73
2	B	610	FAD	O4B-C1B-C2B	-2.35	101.60	106.62
2	A	600	FAD	O3P-PA-O1A	-2.34	103.66	110.70
4	A	603	TON	C9-C6-C5	2.20	132.31	123.78
3	A	601	OMN	C2-N2-N1	2.16	108.66	105.44
2	A	600	FAD	C4-C4X-N5	2.14	121.17	118.21
2	B	610	FAD	N3A-C2A-N1A	-2.13	125.36	128.58
3	B	604	OMN	C1-N1-N2	2.12	122.45	119.29
2	A	600	FAD	C4X-C10-N10	2.08	119.46	116.48
3	B	604	OMN	O1-C9-C8	2.03	121.05	115.28

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	610	FAD	N10-C1'-C2'-O2'
3	B	604	OMN	C10-C8-C9-O1
3	B	604	OMN	C10-C8-C9-O2
4	A	603	TON	C8-C5-C6-C9
4	A	603	TON	C7-C5-C6-C9
4	B	605	TON	C8-C5-C6-C9
4	B	605	TON	C7-C5-C6-C9

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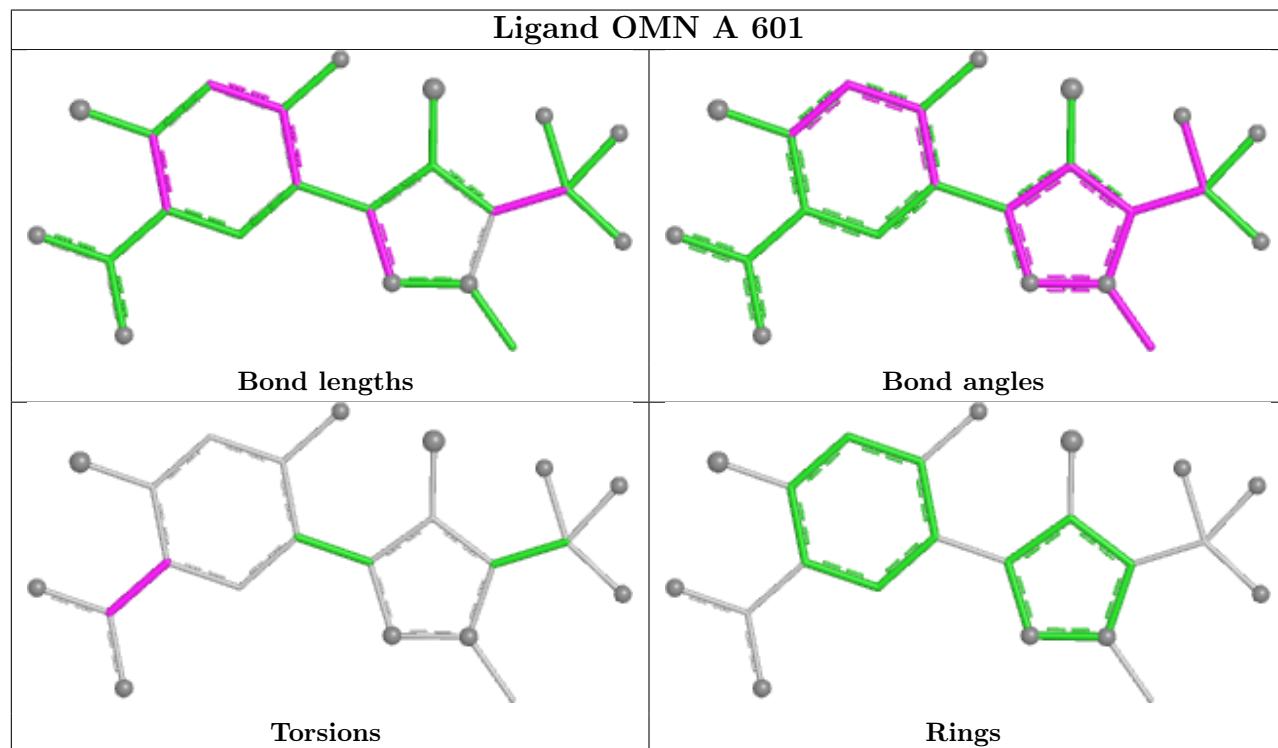
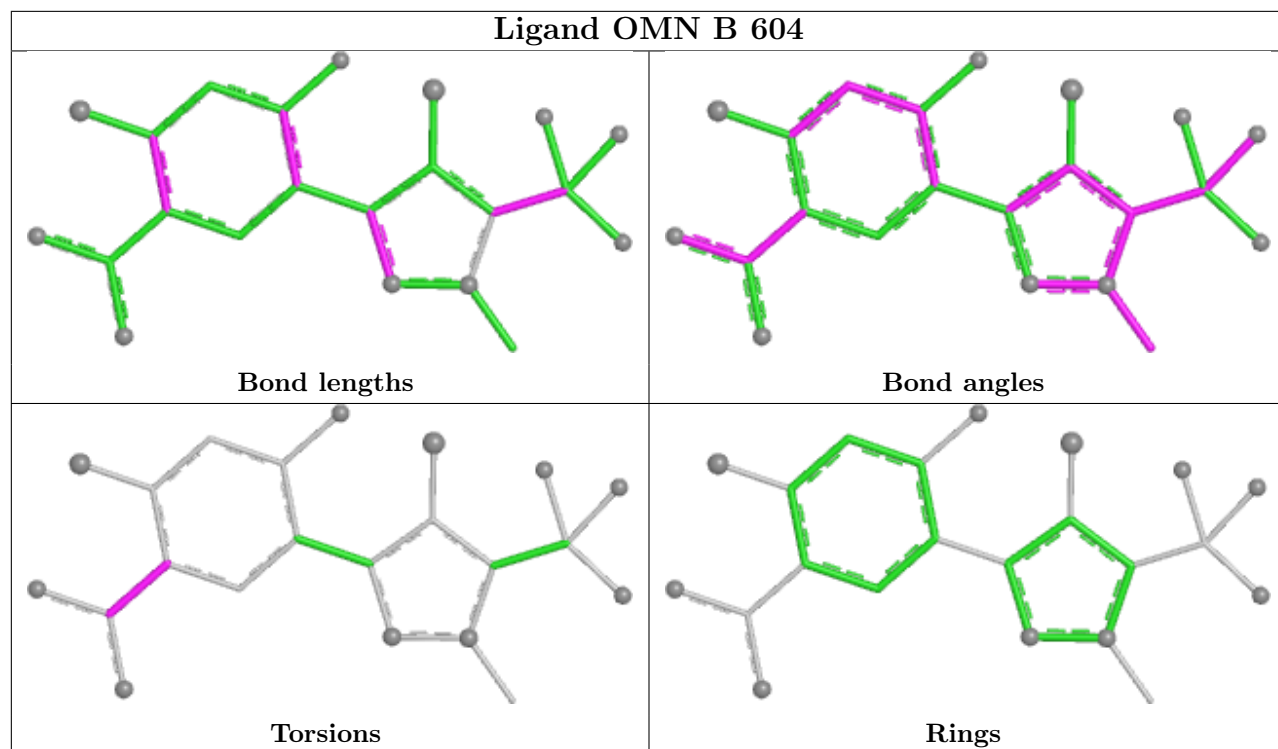
Mol	Chain	Res	Type	Atoms
4	B	605	TON	O1-C1-C2-O2
4	A	603	TON	C18-C5-C6-C9
4	B	605	TON	C18-C5-C6-C9
4	A	603	TON	O1-C1-C2-O2
4	B	605	TON	O2-C3-C4-O3
4	B	605	TON	C14-C15-O1-C1
4	A	603	TON	C14-C15-O1-C1
4	B	605	TON	C16-C15-O1-C1
4	A	603	TON	C16-C15-O1-C1
4	A	603	TON	C2-C1-O1-C15
4	B	605	TON	C2-C1-O1-C15
4	A	603	TON	C1-C2-O2-C3
3	B	604	OMN	C7-C8-C9-O1
3	B	604	OMN	C7-C8-C9-O2
2	B	610	FAD	N10-C1'-C2'-C3'
3	A	601	OMN	C7-C8-C9-O1
4	A	603	TON	C13-C18-C5-C7
3	A	601	OMN	C7-C8-C9-O2
4	A	603	TON	C17-C18-C5-C7

There are no ring outliers.

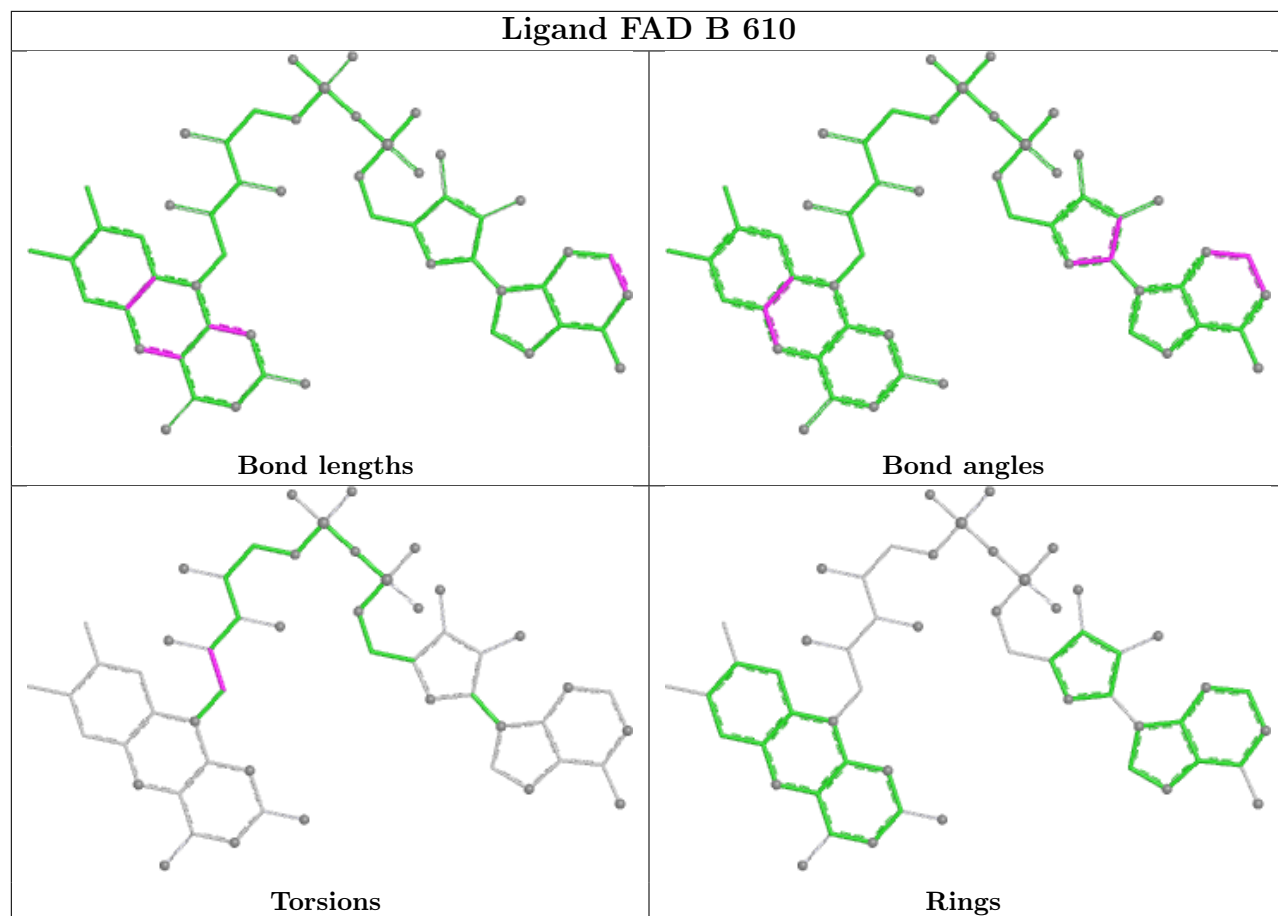
4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	610	FAD	2	0
4	B	605	TON	1	0
2	A	600	FAD	2	0
4	A	603	TON	2	0

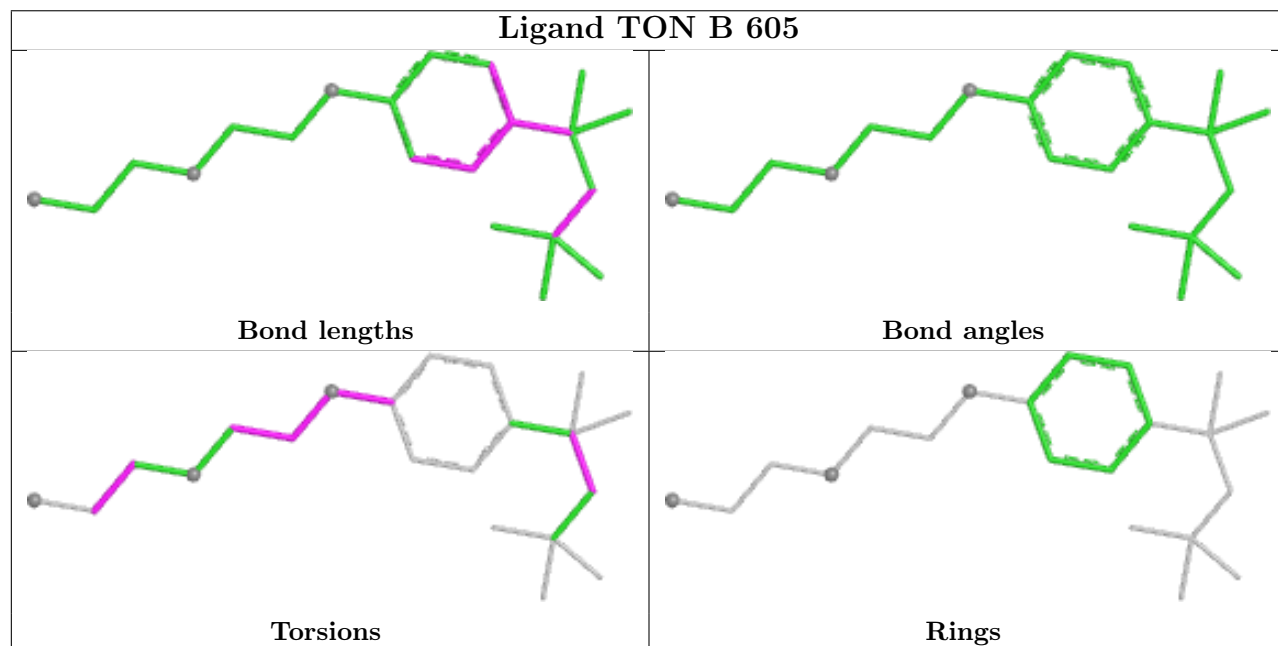
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

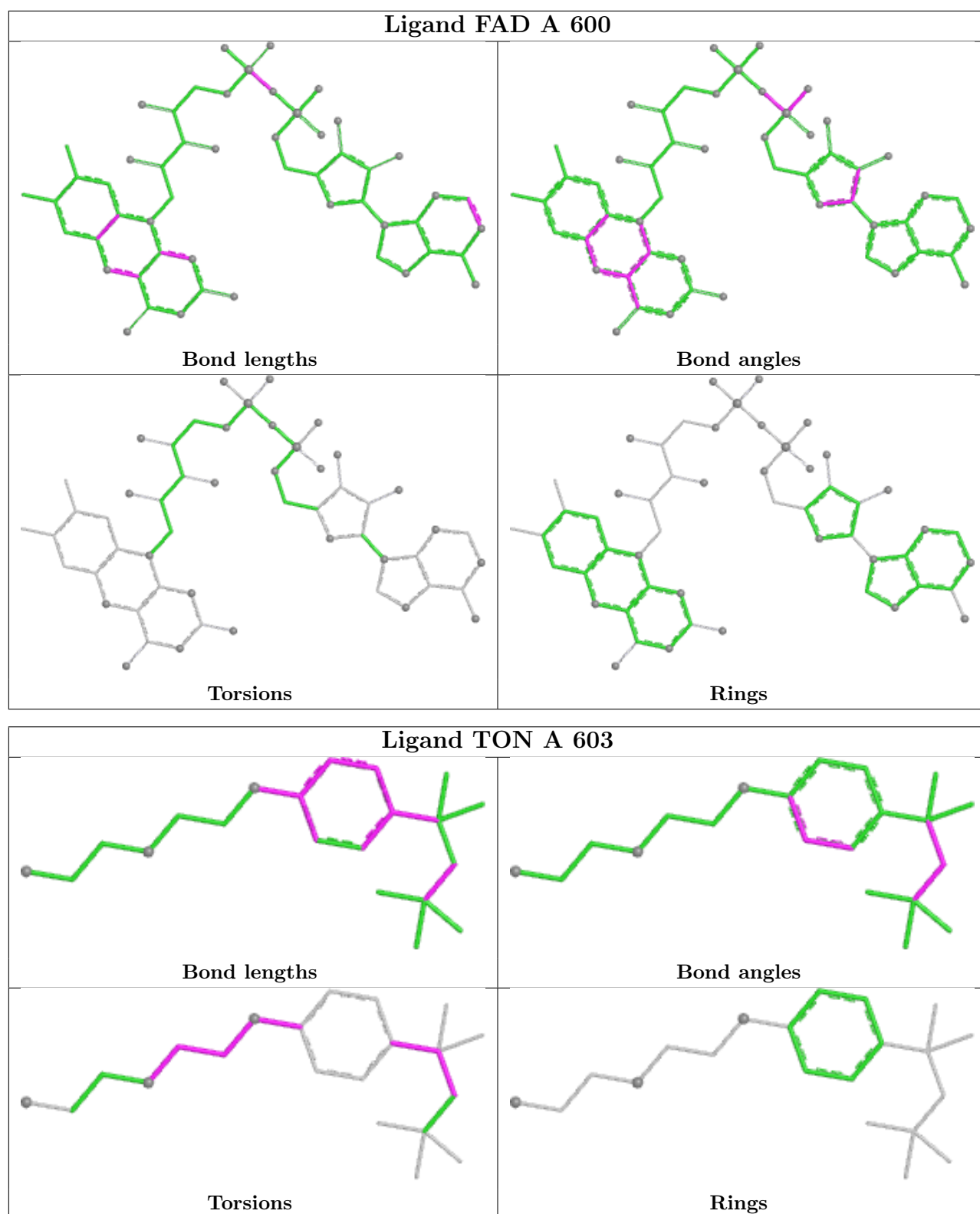


Ligand FAD B 610



Ligand TON B 605





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	455/504 (90%)	-0.10	12 (2%) 57 48	9, 61, 86, 98	25 (5%)
1	B	448/504 (88%)	0.04	14 (3%) 51 42	17, 63, 95, 100	47 (10%)
All	All	903/1008 (89%)	-0.03	26 (2%) 53 45	9, 62, 92, 100	72 (7%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	288	HIS	5.3
1	A	291	GLN	4.9
1	B	291	GLN	4.5
1	A	286	SER	4.4
1	B	290	ARG	4.4
1	B	287	PRO	4.1
1	B	230	LYS	4.0
1	A	288	HIS	4.0
1	A	290	ARG	3.8
1	A	229	LYS	3.7
1	A	289	LYS	3.5
1	B	231	ARG	3.4
1	B	225	THR	3.3
1	B	228	ASN	3.1
1	B	226	SER	2.9
1	A	227	ALA	2.7
1	A	228	ASN	2.7
1	B	227	ALA	2.6
1	B	289	LYS	2.6
1	B	224	LYS	2.4
1	A	224	LYS	2.4
1	A	287	PRO	2.2
1	B	467	GLY	2.1
1	B	229	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	50	GLY	2.0
1	A	230	LYS	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](#)

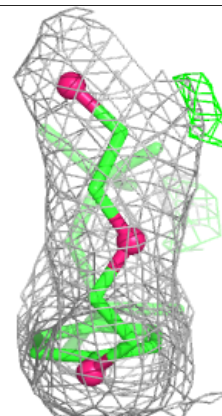
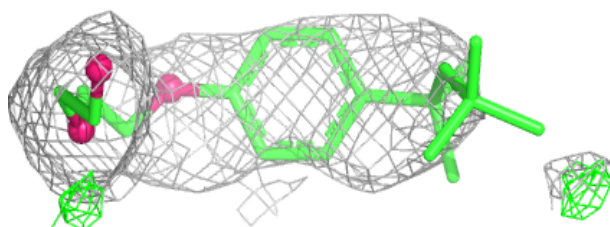
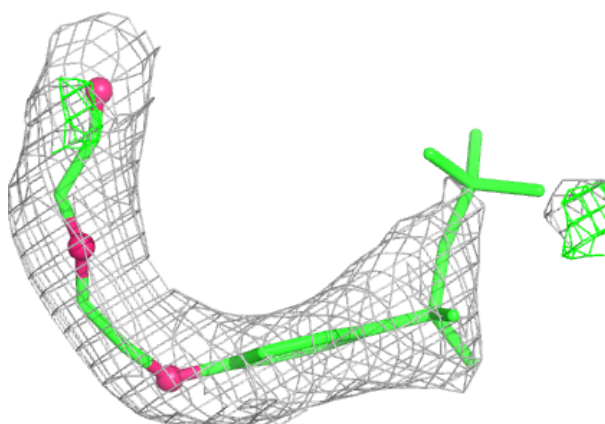
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	TON	B	605	21/21	0.76	0.15	83,86,90,91	0
4	TON	A	603	21/21	0.84	0.14	78,85,93,93	0
2	FAD	B	610	53/53	0.93	0.09	49,63,72,73	0
2	FAD	A	600	53/53	0.95	0.07	27,42,50,51	0
3	OMN	B	604	22/22	0.96	0.09	61,63,66,73	0
3	OMN	A	601	22/22	0.97	0.08	52,58,60,70	0

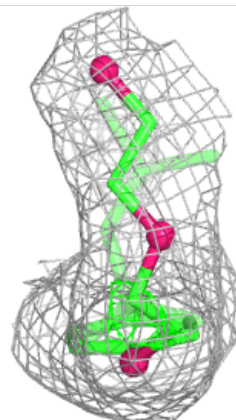
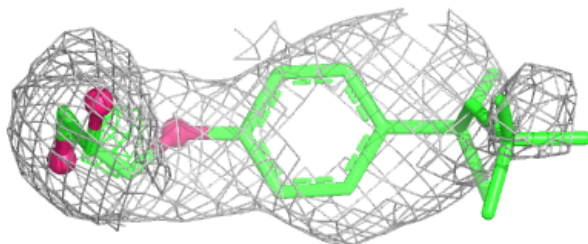
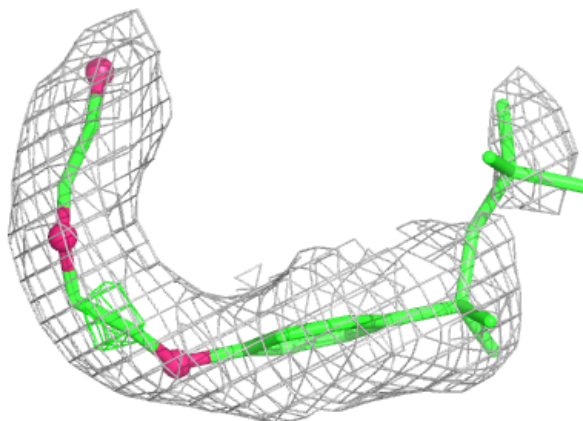
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TON B 605:

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

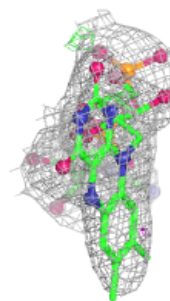
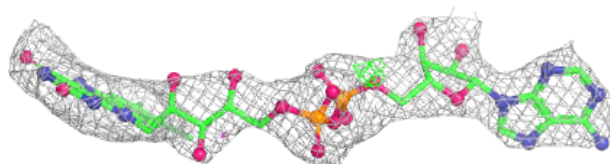
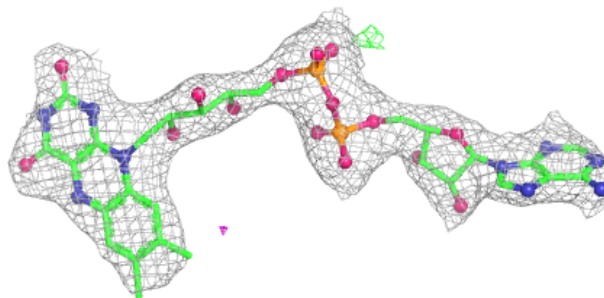
**Electron density around TON A 603:**

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

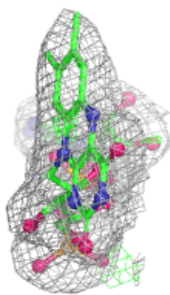
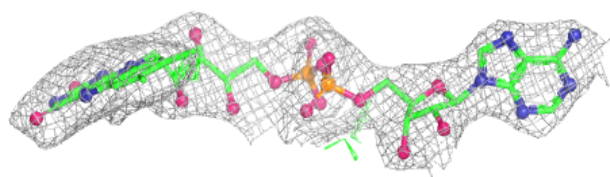
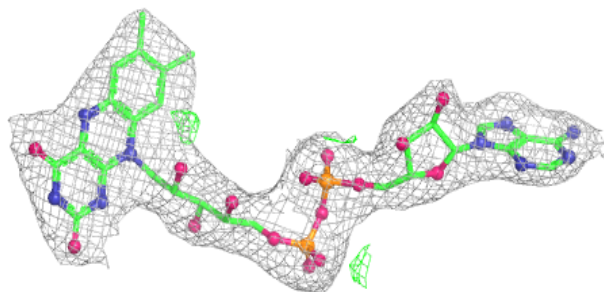


Electron density around FAD B 610:

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

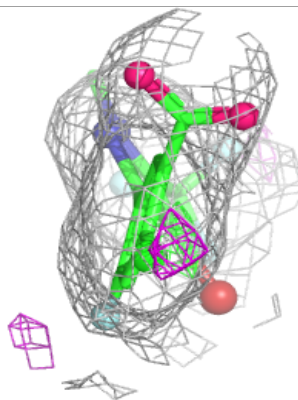
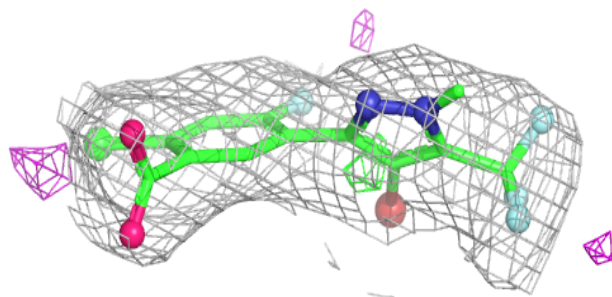
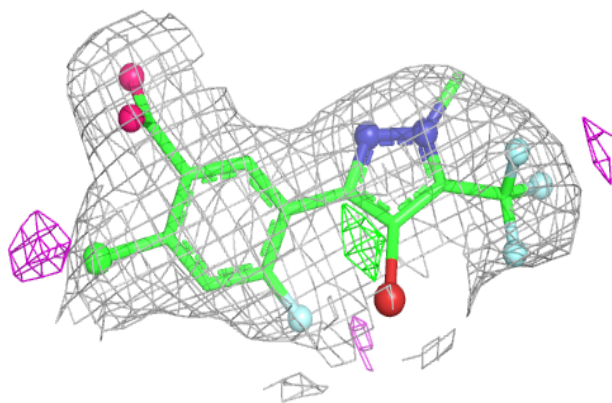
**Electron density around FAD A 600:**

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

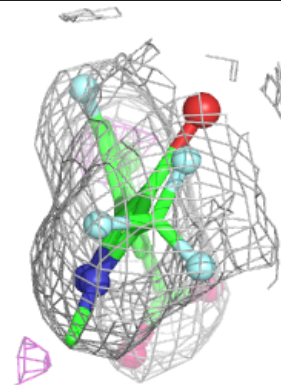
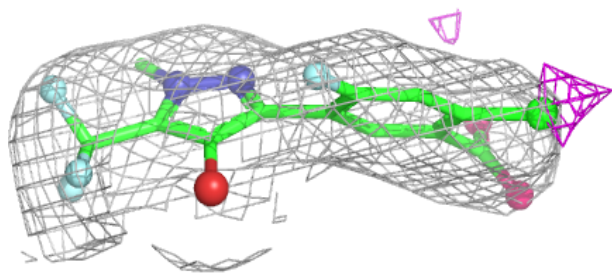
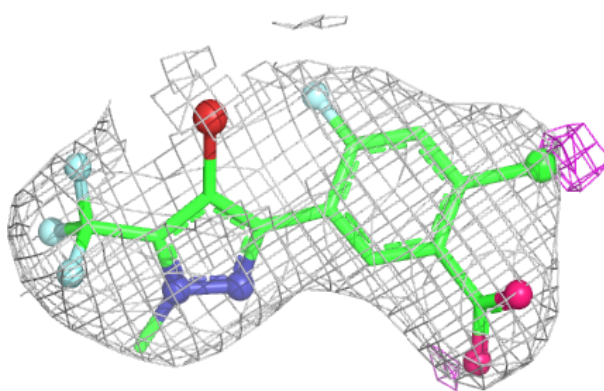


Electron density around OMN B 604:

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

**Electron density around OMN A 601:**

$2mF_o-DF_c$ (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.