



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 24, 2023 – 12:22 PM EDT

PDB ID : 8TTI
Title : Trp-6-Halogenase BorH complexed with FAD and Trp
Authors : Lingkon, K.; Bellizzi, J.J.
Deposited on : 2023-08-14
Resolution : 1.98 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
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) : 2.35

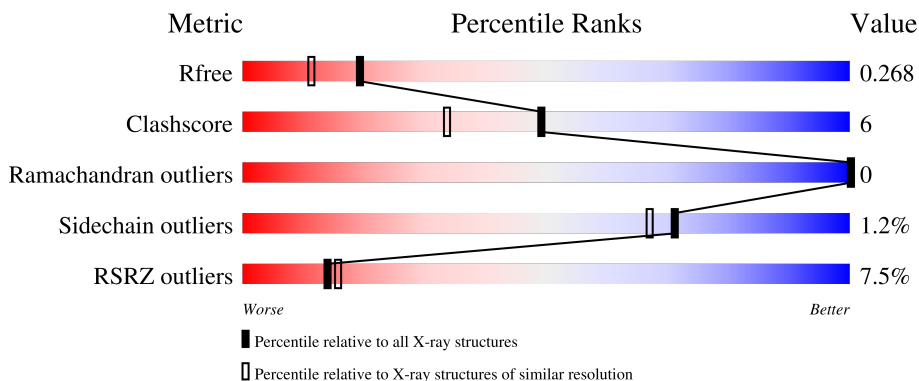
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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	529	 3% 88% 10% .
1	B	529	 4% 86% 12% .
1	C	529	 8% 85% 13% .
1	D	529	 14% 82% 15% ..

2 Entry composition [i](#)

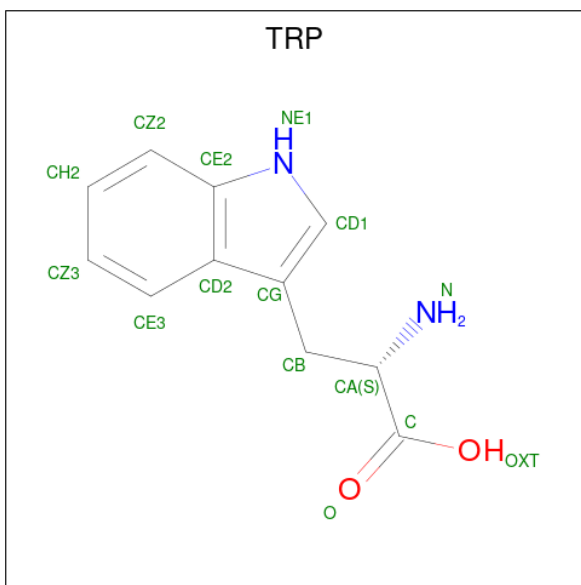
There are 5 unique types of molecules in this entry. The entry contains 18157 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Tryptophan 6-halogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	521	Total 4183	C 2667	N 736	O 758	S 22	0	1	0
1	B	521	Total 4194	C 2673	N 740	O 759	S 22	0	2	0
1	C	520	Total 4187	C 2672	N 734	O 759	S 22	0	2	0
1	D	519	Total 4149	C 2652	N 725	O 750	S 22	0	1	0

- Molecule 2 is TRYPTOPHAN (three-letter code: TRP) (formula: C₁₁H₁₂N₂O₂) (labeled as "Ligand of Interest" by depositor).



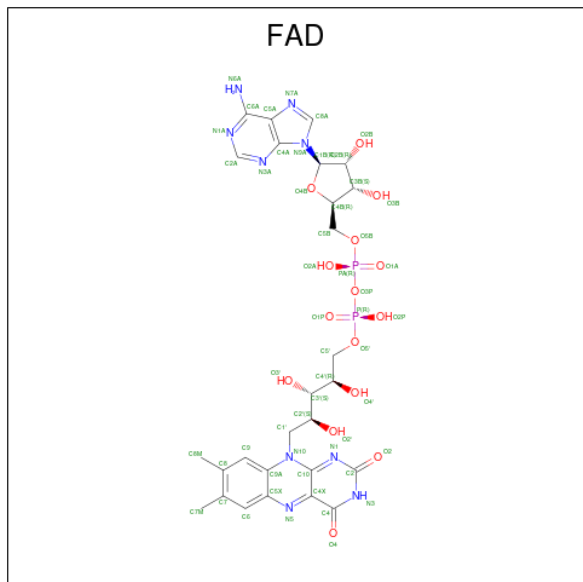
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	Total 15	C 11	N 2	O 2	0	0
2	B	1	Total 15	C 11	N 2	O 2	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



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

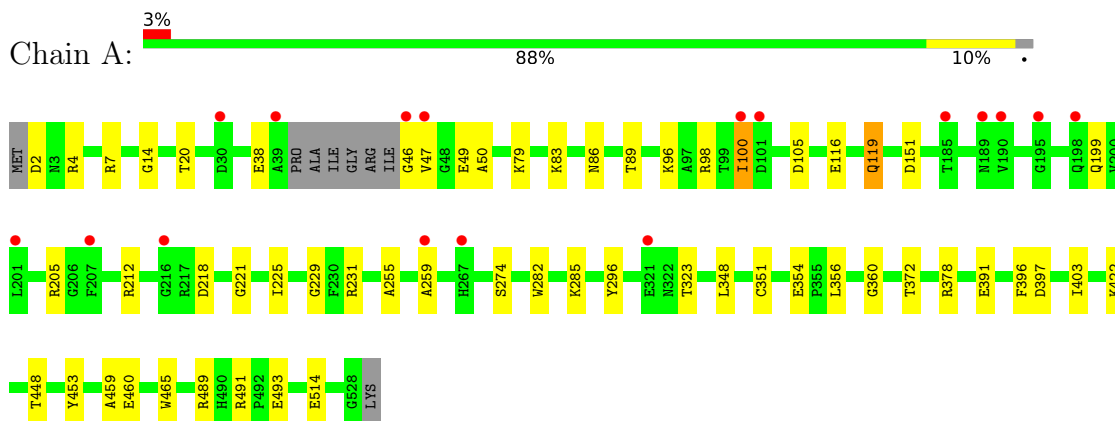
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	375	Total 375	O 375	0	0
5	B	355	Total 355	O 355	0	0
5	C	282	Total 282	O 282	0	0
5	D	231	Total 231	O 231	0	0

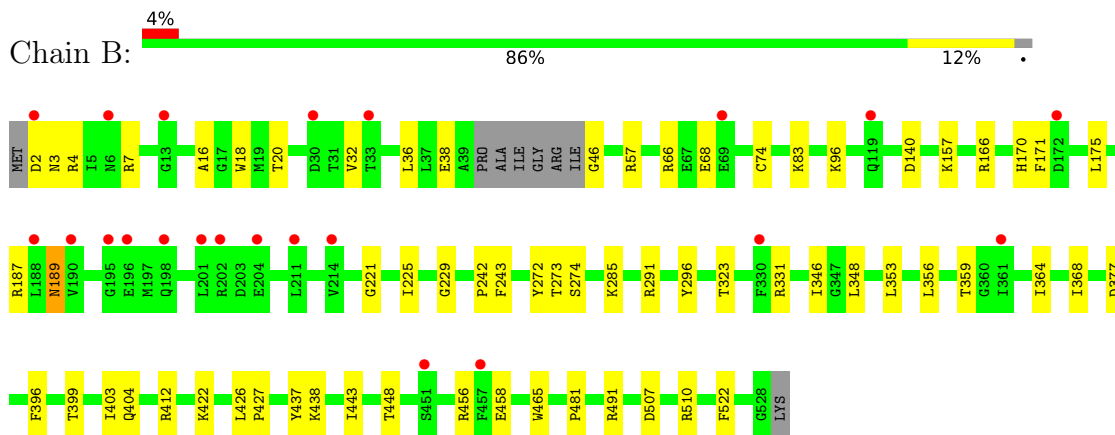
3 Residue-property plots

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

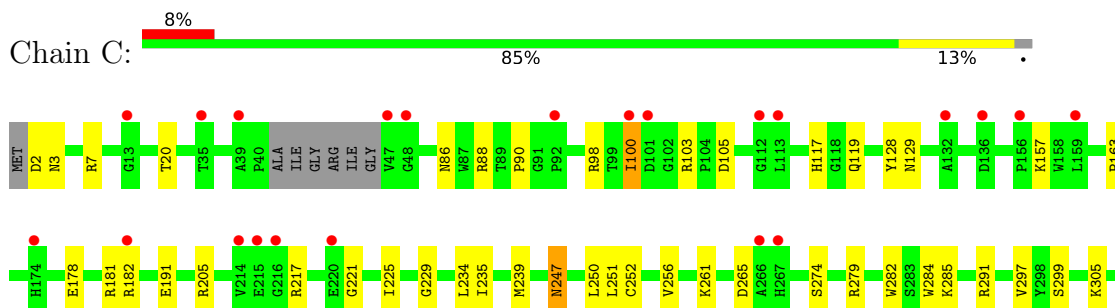
- Molecule 1: Tryptophan 6-halogenase

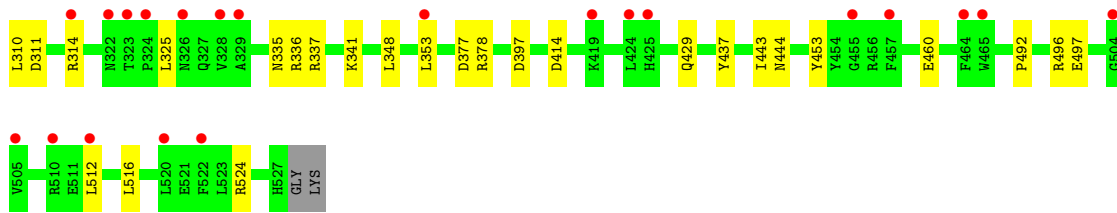


- Molecule 1: Tryptophan 6-halogenase

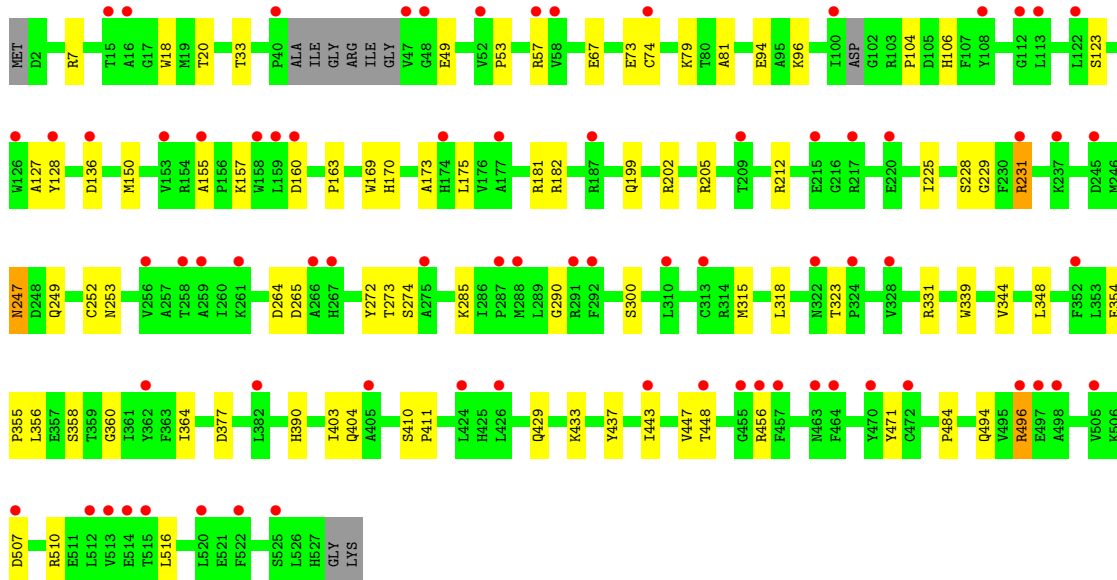
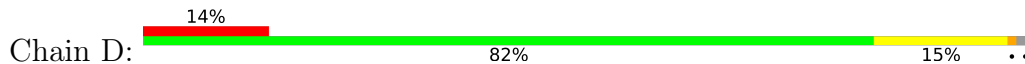


- Molecule 1: Tryptophan 6-halogenase





● Molecule 1: Tryptophan 6-halogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.68Å 157.41Å 112.83Å 90.00° 104.06° 90.00°	Depositor
Resolution (Å)	54.72 – 1.98 54.72 – 1.98	Depositor EDS
% Data completeness (in resolution range)	93.9 (54.72-1.98) 93.9 (54.72-1.98)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 1.98Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.229 , 0.270 0.228 , 0.268	Depositor DCC
R_{free} test set	1989 reflections (1.22%)	wwPDB-VP
Wilson B-factor (Å ²)	30.9	Xtrriage
Anisotropy	0.459	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 51.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18157	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.25% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, SO4

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	0.26	0/4303	0.50	0/5841
1	B	0.26	0/4314	0.50	0/5856
1	C	0.26	0/4312	0.50	0/5856
1	D	0.26	0/4269	0.49	0/5799
All	All	0.26	0/17198	0.50	0/23352

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	4183	0	4022	43	0
1	B	4194	0	4035	45	0
1	C	4187	0	4023	49	0
1	D	4149	0	3979	59	0
2	A	15	0	9	0	0
2	B	15	0	9	0	0
3	A	20	0	0	1	0
3	B	25	0	0	0	0
3	C	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	15	0	0	0	0
4	C	53	0	31	1	0
4	D	53	0	31	3	0
5	A	375	0	0	26	4
5	B	355	0	0	17	4
5	C	282	0	0	23	1
5	D	231	0	0	23	1
All	All	18157	0	16139	196	6

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 6.

All (196) 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:49:GLU:OE2	5:A:701:HOH:O	1.92	0.87
1:D:494:GLN:OE1	5:D:702:HOH:O	1.93	0.86
1:D:127:ALA:O	5:D:701:HOH:O	1.92	0.86
1:A:372:THR:OG1	5:A:702:HOH:O	1.94	0.85
1:D:323:THR:O	5:D:703:HOH:O	1.96	0.81
1:B:323:THR:O	5:B:701:HOH:O	1.99	0.79
1:D:456:ARG:NH2	5:D:707:HOH:O	2.17	0.78
1:D:136:ASP:O	5:D:704:HOH:O	2.03	0.77
1:A:489:ARG:NH1	5:A:713:HOH:O	2.17	0.77
3:A:602:SO4:O2	5:A:704:HOH:O	2.03	0.76
1:A:218:ASP:O	5:A:703:HOH:O	2.02	0.76
1:D:57:ARG:HG2	5:D:712:HOH:O	1.85	0.76
1:C:2:ASP:N	5:C:709:HOH:O	2.18	0.75
1:C:182:ARG:NH1	5:C:710:HOH:O	2.20	0.75
1:C:251:LEU:O	5:C:704:HOH:O	2.03	0.75
1:D:205:ARG:NH1	5:D:713:HOH:O	2.20	0.75
1:A:259:ALA:HB2	5:A:732:HOH:O	1.85	0.74
1:C:88:ARG:NH1	5:C:711:HOH:O	2.21	0.74
1:C:128:TYR:OH	5:C:705:HOH:O	2.05	0.73
1:D:228:SER:O	5:D:705:HOH:O	2.07	0.73
1:A:514:GLU:OE1	5:A:705:HOH:O	2.07	0.71
1:D:437:TYR:HB2	1:D:443:ILE:HD11	1.73	0.71
1:B:68:GLU:O	5:B:702:HOH:O	2.10	0.70
1:A:151:ASP:O	5:A:706:HOH:O	2.09	0.69
1:D:354:GLU:OE2	5:D:706:HOH:O	2.10	0.69
1:A:38:GLU:HA	5:A:748:HOH:O	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:GLN:OE1	5:A:708:HOH:O	2.10	0.69
1:A:465:TRP:O	5:A:707:HOH:O	2.11	0.68
1:A:397:ASP:OD2	5:A:709:HOH:O	2.11	0.67
1:B:359:THR:HG21	1:B:399:THR:HG21	1.76	0.67
1:D:507:ASP:OD1	1:D:510:ARG:NH2	2.27	0.67
1:B:448:THR:OG1	5:B:703:HOH:O	2.11	0.67
1:A:323:THR:O	5:A:711:HOH:O	2.13	0.67
1:D:7:ARG:NH2	5:D:715:HOH:O	2.21	0.67
1:B:166:ARG:O	5:B:704:HOH:O	2.13	0.66
1:B:465:TRP:O	5:B:705:HOH:O	2.13	0.66
1:A:218:ASP:OD2	5:A:710:HOH:O	2.13	0.66
1:C:299:SER:OG	5:C:704:HOH:O	2.13	0.66
1:C:437:TYR:HB2	1:C:443:ILE:HD11	1.78	0.66
1:C:397:ASP:OD2	5:C:706:HOH:O	2.12	0.66
1:C:444:ASN:ND2	5:C:702:HOH:O	2.00	0.66
1:C:119:GLN:NE2	5:C:723:HOH:O	2.29	0.65
1:D:170:HIS:HE2	1:D:273:THR:HG1	1.42	0.65
1:D:79:LYS:NZ	1:D:358:SER:OG	2.29	0.65
1:C:129:ASN:O	5:C:707:HOH:O	2.14	0.65
1:B:57:ARG:NE	5:B:706:HOH:O	2.15	0.65
1:C:496:ARG:NH1	5:C:725:HOH:O	2.31	0.64
1:A:83:LYS:NZ	5:A:726:HOH:O	2.29	0.64
1:A:391:GLU:OE2	5:A:712:HOH:O	2.15	0.64
1:C:178:GLU:OE2	1:C:181:ARG:NH2	2.31	0.63
1:B:66:ARG:HG3	1:B:68:GLU:H	1.63	0.62
1:B:7:ARG:HB2	1:B:221:GLY:HA2	1.81	0.62
1:D:81:ALA:HB3	1:D:150:MET:HE1	1.80	0.61
1:B:491:ARG:NH1	5:B:719:HOH:O	2.32	0.61
1:B:274:SER:HB2	1:B:285:LYS:HB3	1.82	0.61
1:C:217:ARG:HA	5:C:718:HOH:O	2.00	0.61
1:B:189:ASN:ND2	5:B:722:HOH:O	2.34	0.60
1:C:247:ASN:ND2	1:C:250:LEU:O	2.34	0.60
1:C:90:PRO:HB3	1:C:414:ASP:HB3	1.82	0.60
1:A:491:ARG:NH1	1:A:493:GLU:OE2	2.35	0.59
1:B:291:ARG:NH1	5:B:713:HOH:O	2.28	0.59
1:A:2:ASP:O	1:A:378:ARG:NH2	2.36	0.58
1:A:20:THR:HG21	1:A:225:ILE:HG21	1.85	0.58
1:A:199:GLN:OE1	1:A:212:ARG:NH1	2.36	0.58
1:C:348:LEU:HG	4:C:601:FAD:H5'2	1.85	0.58
1:B:356:LEU:HB3	1:B:403:ILE:HD12	1.84	0.57
1:C:492:PRO:HD2	5:C:915:HOH:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:311:ASP:O	5:C:708:HOH:O	2.17	0.57
1:D:157:LYS:HG2	1:D:163:PRO:HA	1.86	0.57
1:D:247:ASN:ND2	5:D:708:HOH:O	2.36	0.57
1:C:265:ASP:OD1	1:C:524:ARG:NH2	2.38	0.57
1:A:4:ARG:O	1:A:378:ARG:NH1	2.38	0.57
1:D:199:GLN:HB2	1:D:212:ARG:HB3	1.85	0.57
1:D:150:MET:HE3	1:D:272:TYR:HB3	1.86	0.56
1:A:229:GLY:HA2	1:A:348:LEU:HB2	1.87	0.56
1:A:14:GLY:N	5:A:735:HOH:O	2.37	0.56
1:C:429:GLN:HG3	5:C:715:HOH:O	2.05	0.55
1:B:437:TYR:HB2	1:B:443:ILE:HD11	1.89	0.55
1:A:47:VAL:HA	5:A:732:HOH:O	2.05	0.55
1:D:249:GLN:NE2	1:D:404:GLN:OE1	2.38	0.55
1:C:397:ASP:N	5:C:703:HOH:O	2.40	0.55
1:D:20:THR:HG21	1:D:225:ILE:HG21	1.89	0.55
1:A:274:SER:HB2	1:A:285:LYS:HB3	1.90	0.54
1:A:7:ARG:HB2	1:A:221:GLY:HA2	1.89	0.54
1:C:2:ASP:O	1:C:378:ARG:NH2	2.40	0.54
1:B:412:ARG:O	1:B:422:LYS:HE2	2.09	0.53
1:D:377:ASP:OD2	5:D:710:HOH:O	2.19	0.53
1:D:390:HIS:HB2	5:D:833:HOH:O	2.09	0.53
1:D:252:CYS:O	5:D:708:HOH:O	2.18	0.53
1:B:16:ALA:HA	1:B:364:ILE:HD13	1.90	0.52
1:A:96:LYS:NZ	5:A:734:HOH:O	2.37	0.52
1:D:212:ARG:NH2	5:D:730:HOH:O	2.34	0.52
1:D:73:GLU:OE1	1:D:182:ARG:NH2	2.39	0.52
1:D:231:ARG:NE	5:D:741:HOH:O	2.42	0.52
1:A:231:ARG:NH2	5:A:742:HOH:O	2.39	0.52
1:C:274:SER:HB2	1:C:285:LYS:HB3	1.92	0.52
1:B:438:LYS:HA	1:B:481:PRO:HA	1.91	0.51
1:B:426:LEU:HD12	1:B:427:PRO:HD2	1.91	0.51
1:C:86:ASN:HB3	1:C:98:ARG:NH2	2.26	0.51
1:D:356:LEU:HB3	1:D:403:ILE:HD12	1.93	0.51
1:C:310:LEU:HD22	1:C:314:ARG:HH12	1.76	0.51
1:C:103:ARG:NH1	5:C:740:HOH:O	2.44	0.50
1:D:104:PRO:HB2	1:D:106:HIS:CE1	2.47	0.50
1:B:46:GLY:N	5:B:736:HOH:O	2.43	0.50
1:B:18:TRP:CZ2	1:B:36:LEU:HD22	2.47	0.50
1:B:456:ARG:HH21	1:B:458:GLU:HB2	1.76	0.49
1:D:53:PRO:O	5:D:712:HOH:O	2.20	0.49
1:B:229:GLY:HA2	1:B:348:LEU:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:GLU:HG3	1:D:173:ALA:HB2	1.95	0.49
1:D:447:VAL:HG23	1:D:448:THR:HG23	1.95	0.49
1:B:346:ILE:HD13	1:B:368:ILE:HD13	1.94	0.49
1:A:282:TRP:NE1	1:A:354:GLU:OE1	2.30	0.49
1:B:187:ARG:NH1	5:B:738:HOH:O	2.45	0.49
1:D:411:PRO:HA	5:D:830:HOH:O	2.13	0.49
1:B:68:GLU:OE1	5:B:707:HOH:O	2.20	0.49
1:D:231:ARG:NH2	5:D:747:HOH:O	2.45	0.49
1:A:514:GLU:HA	5:A:771:HOH:O	2.13	0.48
1:D:202:ARG:NH2	5:D:749:HOH:O	2.46	0.48
1:D:128:TYR:HA	1:D:484:PRO:HB3	1.96	0.47
1:D:318:LEU:HB3	1:D:323:THR:HG21	1.96	0.47
1:B:170:HIS:NE2	1:B:273:THR:OG1	2.46	0.47
1:D:7:ARG:HG2	1:D:33:THR:OG1	2.14	0.47
1:D:160:ASP:OD1	1:D:160:ASP:N	2.47	0.47
1:A:89:THR:O	1:A:98:ARG:NH2	2.46	0.47
1:C:157:LYS:HB3	1:C:163:PRO:HA	1.97	0.47
1:B:364:ILE:O	1:B:368:ILE:HG12	2.14	0.47
1:A:351:CYS:HB2	1:A:396:PHE:CE2	2.50	0.47
1:B:20:THR:HG21	1:B:225:ILE:HG21	1.97	0.47
1:D:274:SER:HB2	1:D:285:LYS:HB3	1.97	0.47
1:B:140:ASP:OD1	1:B:140:ASP:N	2.47	0.47
1:D:253:ASN:ND2	1:D:300:SER:OG	2.46	0.46
1:D:496:ARG:HD2	1:D:496:ARG:HA	1.76	0.46
1:C:20:THR:HG21	1:C:225:ILE:HG21	1.98	0.46
1:D:429:GLN:OE1	1:D:433:LYS:HE2	2.15	0.46
1:C:7:ARG:HB2	1:C:221:GLY:HA2	1.98	0.46
1:C:512:LEU:O	1:C:516:LEU:HB2	2.16	0.46
1:B:166:ARG:HD3	5:B:969:HOH:O	2.16	0.46
1:D:339:TRP:CG	1:D:344:VAL:HG22	2.51	0.45
1:B:74[A]:CYS:HA	1:B:175:LEU:HB3	1.98	0.45
1:D:212:ARG:NH1	5:D:730:HOH:O	2.49	0.45
1:B:2:ASP:HA	5:B:718:HOH:O	2.16	0.45
1:A:459:ALA:O	5:A:714:HOH:O	2.21	0.45
1:C:100:ILE:HD11	1:C:105:ASP:HA	1.99	0.45
1:B:507:ASP:OD1	1:B:510:ARG:NH2	2.50	0.45
1:A:46:GLY:N	5:A:765:HOH:O	2.49	0.45
1:A:453:TYR:CZ	1:A:460:GLU:HG3	2.52	0.45
1:B:291:ARG:NH1	5:B:746:HOH:O	2.50	0.44
1:C:305:LYS:NZ	5:C:751:HOH:O	2.49	0.44
1:D:331:ARG:NH1	5:D:734:HOH:O	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:CYS:HB3	1:C:297:VAL:HG12	2.00	0.44
1:D:18:TRP:CZ2	1:D:181:ARG:HG3	2.53	0.44
1:D:229:GLY:HA2	1:D:348:LEU:HB2	2.00	0.44
1:D:67:GLU:OE2	1:D:169:TRP:NE1	2.36	0.44
1:C:229:GLY:HA2	1:C:348:LEU:HB2	2.00	0.43
1:A:448:THR:HG21	1:D:448:THR:HG21	2.00	0.43
1:C:3:ASN:O	1:C:377:ASP:HB2	2.18	0.43
1:A:356:LEU:HD23	1:A:403:ILE:HG23	1.99	0.43
1:B:74[B]:CYS:HA	1:B:175:LEU:HB3	1.99	0.43
1:C:261:LYS:HA	1:C:291:ARG:HB3	2.00	0.43
1:D:364:ILE:HD11	4:D:601:FAD:H5'1	2.00	0.43
1:C:453:TYR:CZ	1:C:460:GLU:HG3	2.53	0.43
1:B:404:GLN:HG3	5:B:931:HOH:O	2.18	0.42
1:D:123:SER:HB2	1:D:471:TYR:CD2	2.54	0.42
1:B:353:LEU:HG	1:B:396:PHE:CE1	2.54	0.42
1:B:3:ASN:O	1:B:377:ASP:HB2	2.19	0.42
1:B:243:PHE:CZ	1:B:331:ARG:HG2	2.53	0.42
1:D:94:GLU:HA	1:D:315:MET:HG3	2.01	0.42
1:D:360:GLY:HA3	4:D:601:FAD:N1	2.34	0.42
1:C:335:ASN:HB3	5:C:701:HOH:O	2.18	0.42
1:C:336:ARG:N	5:C:701:HOH:O	2.52	0.42
1:A:100:ILE:HG23	5:A:725:HOH:O	2.19	0.42
1:D:74[B]:CYS:HA	1:D:175:LEU:HB3	2.02	0.42
1:C:205:ARG:NH1	5:C:724:HOH:O	2.31	0.41
1:A:360:GLY:N	5:A:754:HOH:O	2.53	0.41
1:C:234:LEU:O	1:C:239:MET:HG2	2.20	0.41
1:C:250:LEU:HD12	1:C:353:LEU:HD22	2.01	0.41
1:C:191:GLU:OE2	1:C:217:ARG:NH2	2.46	0.41
1:A:98:ARG:O	1:A:105:ASP:N	2.44	0.41
1:C:282:TRP:CZ3	1:C:284:TRP:HB3	2.55	0.41
1:A:86:ASN:HB3	1:A:98:ARG:NH2	2.36	0.41
1:B:456:ARG:NH2	1:B:458:GLU:H	2.19	0.41
1:A:50:ALA:HB1	1:A:79:LYS:HD2	2.02	0.41
1:A:116:GLU:O	5:A:715:HOH:O	2.22	0.41
1:D:264:ASP:OD2	1:D:290:GLY:N	2.49	0.41
1:B:157:LYS:HE3	1:B:522:PHE:CZ	2.55	0.41
1:C:337:ARG:O	5:C:701:HOH:O	2.20	0.41
1:D:355:PRO:HG3	4:D:601:FAD:C6	2.51	0.41
1:A:255:ALA:HA	1:A:296:TYR:O	2.22	0.40
1:B:96:LYS:HE2	1:B:96:LYS:HB2	1.87	0.40
1:B:242:PRO:HA	5:B:789:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:341:LYS:HE3	5:C:952:HOH:O	2.21	0.40
1:D:155:ALA:O	1:D:516:LEU:HD13	2.21	0.40
1:D:410:SER:O	5:D:716:HOH:O	2.22	0.40
1:C:117:HIS:NE2	1:C:497:GLU:HB2	2.36	0.40
1:C:235:ILE:HD13	1:C:335:ASN:ND2	2.37	0.40
1:B:83:LYS:HD3	1:B:272:TYR:CE1	2.57	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:709:HOH:O	5:C:905:HOH:O[1_455]	1.83	0.37
5:D:772:HOH:O	5:D:838:HOH:O[1_455]	2.02	0.18
5:A:746:HOH:O	5:B:847:HOH:O[1_545]	2.17	0.03
5:A:952:HOH:O	5:B:890:HOH:O[1_545]	2.17	0.03
5:A:1002:HOH:O	5:B:990:HOH:O[1_445]	2.18	0.02
5:A:1075:HOH:O	5:B:1045:HOH:O[1_445]	2.18	0.02

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	518/529 (98%)	502 (97%)	16 (3%)	0	100	100
1	B	519/529 (98%)	504 (97%)	15 (3%)	0	100	100
1	C	518/529 (98%)	506 (98%)	12 (2%)	0	100	100
1	D	514/529 (97%)	496 (96%)	18 (4%)	0	100	100
All	All	2069/2116 (98%)	2008 (97%)	61 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	430/436 (99%)	426 (99%)	4 (1%)	78	77
1	B	431/436 (99%)	425 (99%)	6 (1%)	67	62
1	C	432/436 (99%)	427 (99%)	5 (1%)	71	67
1	D	425/436 (98%)	420 (99%)	5 (1%)	71	67
All	All	1718/1744 (98%)	1698 (99%)	20 (1%)	71	67

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	ILE
1	A	119	GLN
1	A	205	ARG
1	A	422	LYS
1	B	4	ARG
1	B	32	VAL
1	B	38	GLU
1	B	171	PHE
1	B	189	ASN
1	B	296	TYR
1	C	100	ILE
1	C	247	ASN
1	C	256	VAL
1	C	279	ARG
1	C	325	LEU
1	D	96	LYS
1	D	231	ARG
1	D	247	ASN
1	D	265	ASP
1	D	496	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	192	HIS
1	D	106	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

17 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	SO4	B	605	-	4,4,4	0.13	0	6,6,6	0.06	0
3	SO4	D	604	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	A	602	-	4,4,4	0.13	0	6,6,6	0.06	0
3	SO4	C	602	-	4,4,4	0.15	0	6,6,6	0.11	0
2	TRP	B	600	-	14,16,16	0.84	1 (7%)	16,22,22	1.17	2 (12%)
3	SO4	A	604	-	4,4,4	0.14	0	6,6,6	0.07	0
4	FAD	D	601	-	53,58,58	0.45	0	68,89,89	0.49	1 (1%)
2	TRP	A	600	-	14,16,16	0.86	1 (7%)	16,22,22	1.15	2 (12%)
3	SO4	A	601	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	D	602	-	4,4,4	0.13	0	6,6,6	0.09	0
3	SO4	D	603	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	B	603	-	4,4,4	0.14	0	6,6,6	0.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FAD	C	601	-	53,58,58	0.44	0	68,89,89	0.51	2 (2%)
3	SO4	B	601	-	4,4,4	0.14	0	6,6,6	0.18	0
3	SO4	B	602	-	4,4,4	0.14	0	6,6,6	0.08	0
3	SO4	A	603	-	4,4,4	0.15	0	6,6,6	0.05	0
3	SO4	B	604	-	4,4,4	0.14	0	6,6,6	0.05	0

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	FAD	D	601	-	-	11/30/50/50	0/6/6/6
2	TRP	B	600	-	-	3/7/8/8	0/2/2/2
2	TRP	A	600	-	-	4/7/8/8	0/2/2/2
4	FAD	C	601	-	-	13/30/50/50	0/6/6/6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	TRP	OXT-C	-2.20	1.23	1.30
2	B	600	TRP	OXT-C	-2.17	1.23	1.30

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	TRP	OXT-C-O	-2.81	117.70	124.09
2	B	600	TRP	OXT-C-O	-2.80	117.73	124.09
4	C	601	FAD	C5A-C6A-N6A	2.44	124.06	120.35
4	D	601	FAD	C5A-C6A-N6A	2.29	123.84	120.35
4	C	601	FAD	P-O3P-PA	-2.15	125.46	132.83
2	B	600	TRP	OXT-C-CA	2.12	120.62	113.38
2	A	600	TRP	OXT-C-CA	2.09	120.50	113.38

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	601	FAD	C5B-O5B-PA-O3P
4	C	601	FAD	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
4	C	601	FAD	C3B-C4B-C5B-O5B
4	C	601	FAD	C2'-C3'-C4'-O4'
4	C	601	FAD	C2'-C3'-C4'-C5'
4	C	601	FAD	O3'-C3'-C4'-O4'
4	C	601	FAD	O3'-C3'-C4'-C5'
4	C	601	FAD	C3'-C4'-C5'-O5'
4	C	601	FAD	O4'-C4'-C5'-O5'
4	D	601	FAD	C5B-O5B-PA-O1A
4	D	601	FAD	C5B-O5B-PA-O3P
4	D	601	FAD	O4B-C4B-C5B-O5B
4	D	601	FAD	C3B-C4B-C5B-O5B
2	A	600	TRP	OXT-C-CA-N
2	B	600	TRP	OXT-C-CA-N
4	D	601	FAD	O3'-C3'-C4'-O4'
4	D	601	FAD	C2'-C3'-C4'-O4'
4	D	601	FAD	O3'-C3'-C4'-C5'
4	D	601	FAD	C2'-C3'-C4'-C5'
2	A	600	TRP	O-C-CA-N
2	B	600	TRP	O-C-CA-N
4	C	601	FAD	P-O3P-PA-O5B
4	C	601	FAD	C5'-O5'-P-O3P
4	D	601	FAD	PA-O3P-P-O1P
4	C	601	FAD	C5B-O5B-PA-O1A
4	D	601	FAD	C3'-C4'-C5'-O5'
4	D	601	FAD	O4'-C4'-C5'-O5'
2	A	600	TRP	OXT-C-CA-CB
2	A	600	TRP	O-C-CA-CB
4	C	601	FAD	C5'-O5'-P-O1P
2	B	600	TRP	OXT-C-CA-CB

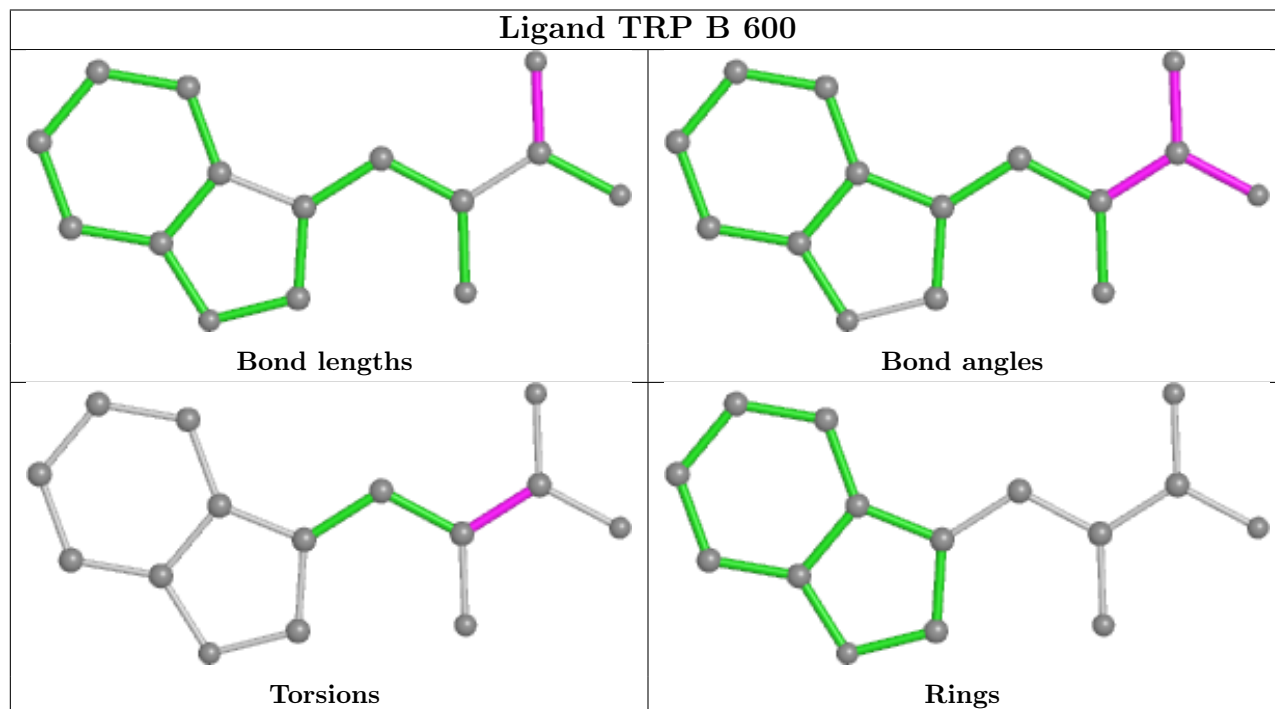
There are no ring outliers.

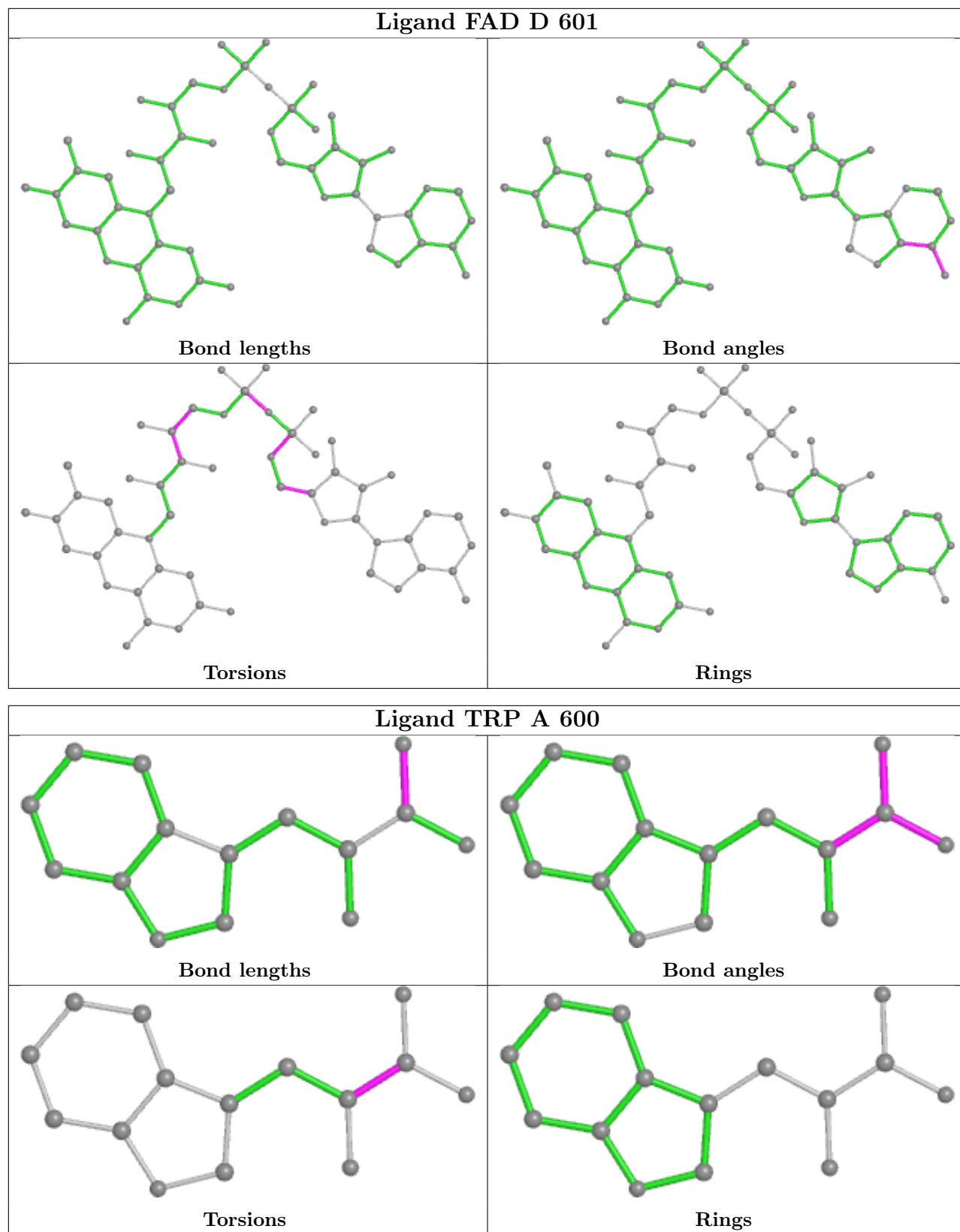
3 monomers are involved in 5 short contacts:

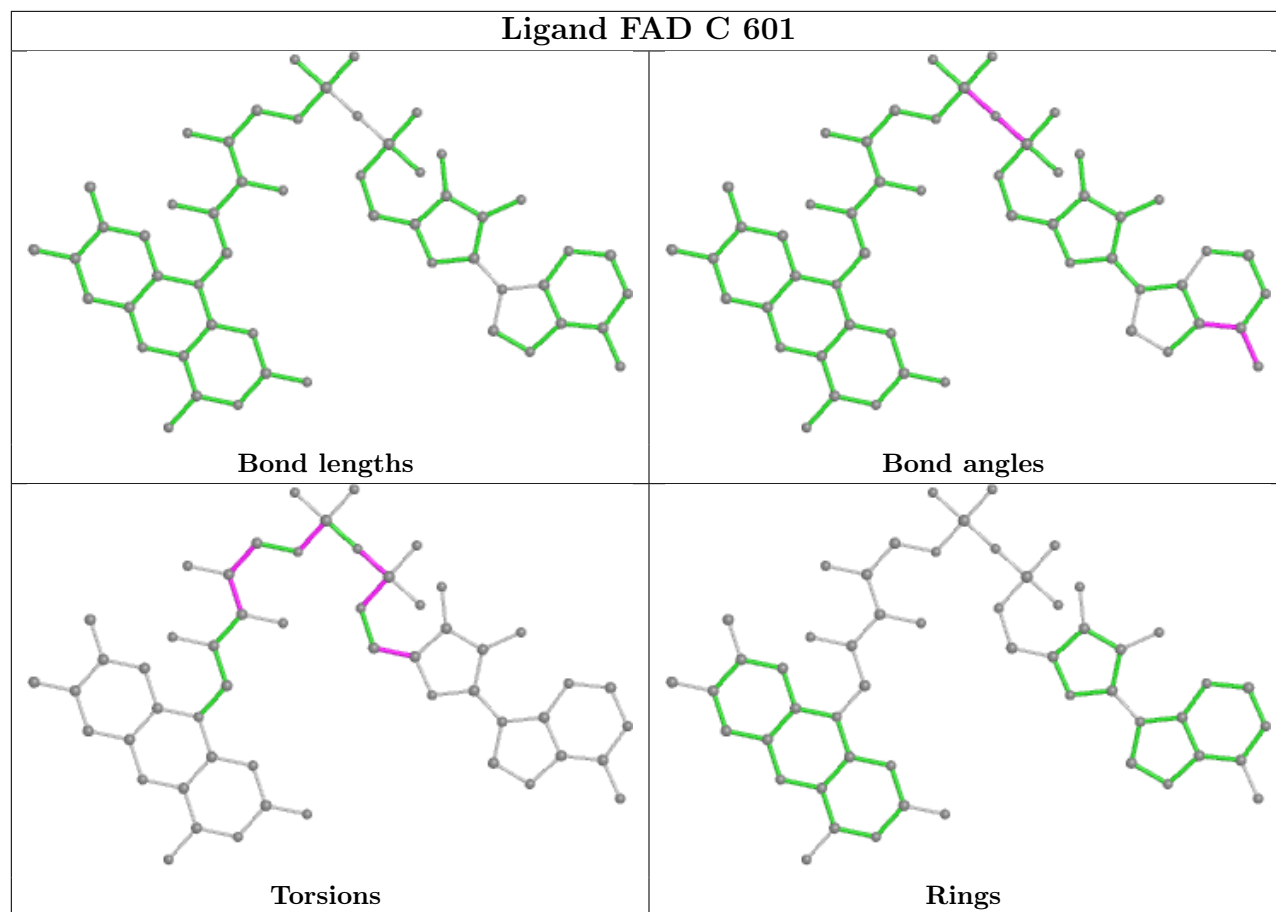
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	SO4	1	0
4	D	601	FAD	3	0
4	C	601	FAD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	521/529 (98%)	0.54	17 (3%) 46 49	17, 35, 56, 76	0
1	B	521/529 (98%)	0.60	22 (4%) 36 38	19, 38, 65, 82	0
1	C	520/529 (98%)	0.84	43 (8%) 11 12	23, 46, 68, 91	0
1	D	519/529 (98%)	0.98	75 (14%) 2 2	26, 52, 74, 88	0
All	All	2081/2116 (98%)	0.74	157 (7%) 14 16	17, 42, 68, 91	0

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	324	PRO	10.2
1	C	100	ILE	5.5
1	C	101	ASP	4.8
1	D	100	ILE	4.7
1	D	324	PRO	4.6
1	D	47	VAL	4.6
1	B	201	LEU	4.3
1	C	425[A]	HIS	4.3
1	D	259	ALA	4.2
1	C	47	VAL	4.2
1	C	216	GLY	4.1
1	D	313	CYS	4.1
1	D	520	LEU	4.0
1	C	520	LEU	3.9
1	C	112	GLY	3.9
1	D	40	PRO	3.8
1	C	267	HIS	3.8
1	A	195	GLY	3.7
1	D	267	HIS	3.6
1	D	159	LEU	3.6
1	C	323	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	48	GLY	3.4
1	B	361	ILE	3.4
1	D	443	ILE	3.4
1	A	189	ASN	3.4
1	C	159	LEU	3.4
1	D	155	ALA	3.3
1	B	204	GLU	3.3
1	D	322	ASN	3.2
1	D	522	PHE	3.2
1	A	39	ALA	3.1
1	D	424	LEU	3.1
1	C	522	PHE	3.1
1	D	58	VAL	3.1
1	D	498	ALA	3.1
1	D	457	PHE	3.0
1	C	424	LEU	3.0
1	C	35	THR	3.0
1	D	258	THR	3.0
1	D	525	SER	2.9
1	D	405	ALA	2.9
1	B	13	GLY	2.9
1	B	214	VAL	2.9
1	B	6	ASN	2.9
1	A	100	ILE	2.9
1	D	455	GLY	2.9
1	D	426	LEU	2.9
1	D	245	ASP	2.9
1	D	220	GLU	2.8
1	D	328	VAL	2.8
1	D	505	VAL	2.8
1	C	39	ALA	2.8
1	A	201	LEU	2.8
1	C	13	GLY	2.8
1	D	288	MET	2.8
1	B	119	GLN	2.7
1	C	182	ARG	2.7
1	D	291	ARG	2.7
1	A	47	VAL	2.7
1	B	457	PHE	2.7
1	D	160	ASP	2.7
1	D	310	LEU	2.7
1	B	330	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	321	GLU	2.6
1	C	510	ARG	2.6
1	A	30	ASP	2.6
1	C	505	VAL	2.6
1	D	507	ASP	2.6
1	C	419	LYS	2.6
1	B	190	VAL	2.6
1	C	328	VAL	2.6
1	D	108	TYR	2.6
1	B	211	LEU	2.6
1	B	198	GLN	2.6
1	D	136	ASP	2.6
1	D	512	LEU	2.5
1	C	214	VAL	2.5
1	A	46	GLY	2.5
1	B	2	ASP	2.5
1	D	513	VAL	2.5
1	D	287	PRO	2.5
1	C	465	TRP	2.5
1	C	48	GLY	2.5
1	B	202	ARG	2.5
1	B	172	ASP	2.4
1	D	187	ARG	2.4
1	A	207	PHE	2.4
1	D	128	TYR	2.4
1	B	30	ASP	2.4
1	C	455	GLY	2.4
1	B	195	GLY	2.4
1	A	259	ALA	2.4
1	D	266	ALA	2.4
1	C	156	PRO	2.4
1	C	504	GLY	2.4
1	C	353	LEU	2.4
1	D	215	GLU	2.4
1	D	74[A]	CYS	2.4
1	A	267	HIS	2.4
1	D	112	GLY	2.4
1	D	470	TYR	2.4
1	D	496	ARG	2.4
1	D	256	VAL	2.4
1	C	464	PHE	2.3
1	A	101	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	16	ALA	2.3
1	B	33	THR	2.3
1	B	188	LEU	2.3
1	C	215	GLU	2.3
1	C	132	ALA	2.2
1	D	52	VAL	2.2
1	D	515	THR	2.2
1	A	216	GLY	2.2
1	A	190	VAL	2.2
1	C	220	GLU	2.2
1	C	322	ASN	2.2
1	D	237	LYS	2.2
1	D	261	LYS	2.2
1	D	174	HIS	2.2
1	B	69	GLU	2.2
1	D	113	LEU	2.1
1	D	126	TRP	2.1
1	D	153	VAL	2.1
1	D	472	CYS	2.1
1	D	57	ARG	2.1
1	D	456	ARG	2.1
1	D	177	ALA	2.1
1	D	497	GLU	2.1
1	D	217	ARG	2.1
1	C	136	ASP	2.1
1	D	514	GLU	2.1
1	C	113	LEU	2.1
1	C	329	ALA	2.1
1	D	382	LEU	2.1
1	C	314	ARG	2.1
1	C	92	PRO	2.1
1	A	198	GLN	2.1
1	D	158	TRP	2.1
1	C	266	ALA	2.1
1	D	122	LEU	2.1
1	B	196	GLU	2.1
1	A	185	THR	2.1
1	D	209	THR	2.1
1	D	352	PHE	2.1
1	D	464	PHE	2.1
1	C	512	LEU	2.1
1	C	457	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	292	PHE	2.0
1	D	231	ARG	2.0
1	D	448	THR	2.0
1	D	463	ASN	2.0
1	B	451	SER	2.0
1	D	362	TYR	2.0
1	D	275	ALA	2.0
1	C	326	ASN	2.0
1	C	174	HIS	2.0
1	D	15	THR	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 monosaccharides 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.

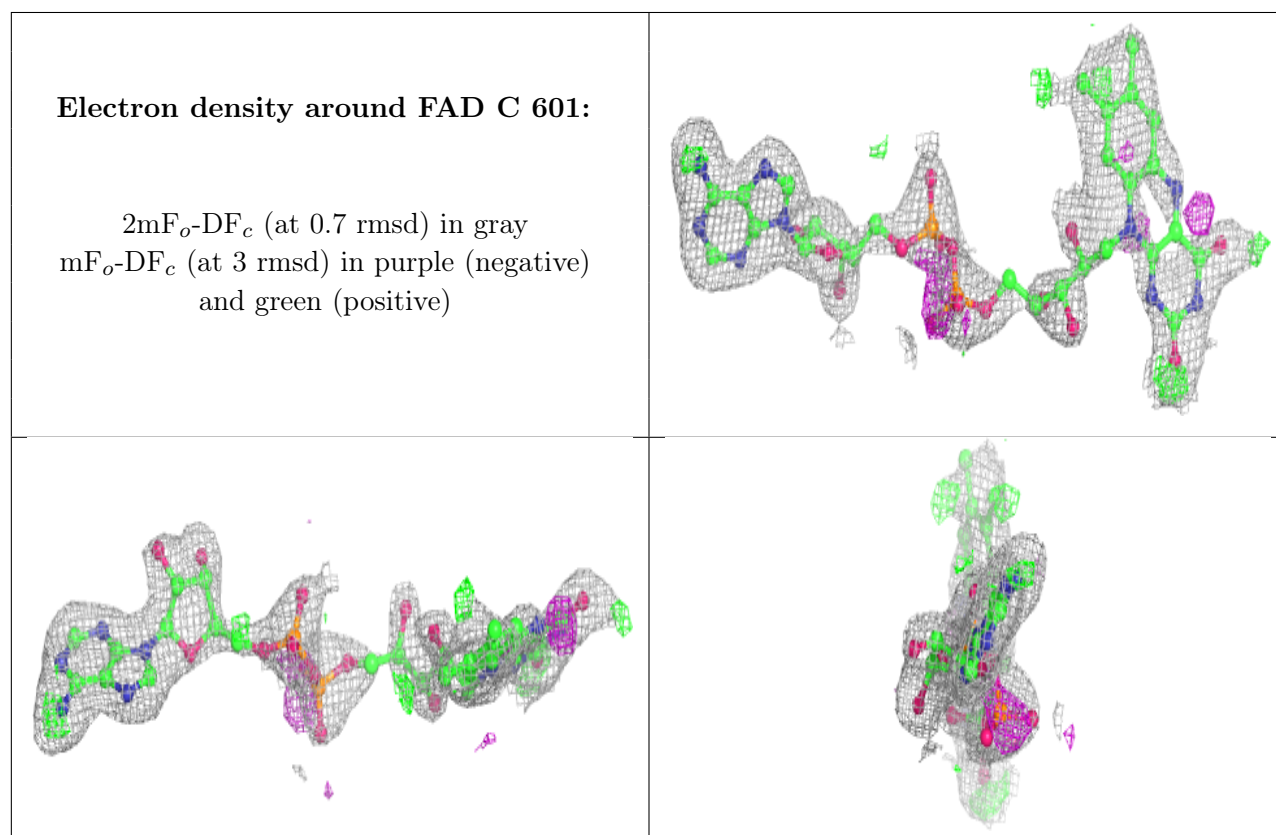
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	FAD	C	601	53/53	0.76	0.23	30,43,51,52	53
4	FAD	D	601	53/53	0.82	0.21	33,47,56,60	53
2	TRP	A	600	15/15	0.83	0.18	24,28,35,38	0
2	TRP	B	600	15/15	0.86	0.18	27,33,40,40	0
3	SO4	B	605	5/5	0.89	0.23	55,58,91,107	0
3	SO4	D	604	5/5	0.90	0.17	56,62,78,85	0
3	SO4	A	603	5/5	0.91	0.24	63,68,79,81	0
3	SO4	A	604	5/5	0.93	0.18	51,57,75,81	0
3	SO4	B	603	5/5	0.94	0.14	62,63,69,74	0
3	SO4	B	604	5/5	0.94	0.20	55,60,75,86	0
3	SO4	D	602	5/5	0.95	0.12	43,45,58,61	0
3	SO4	C	602	5/5	0.95	0.17	43,44,55,63	0
3	SO4	D	603	5/5	0.96	0.11	60,64,68,70	0

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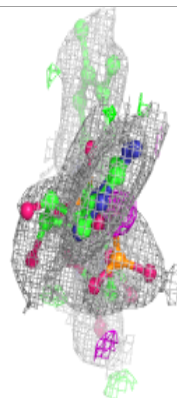
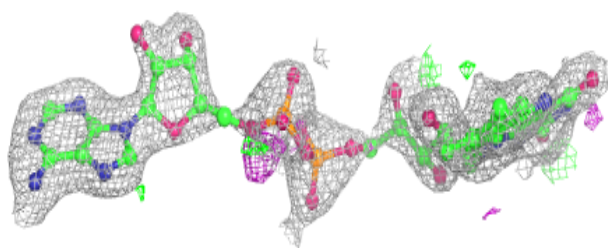
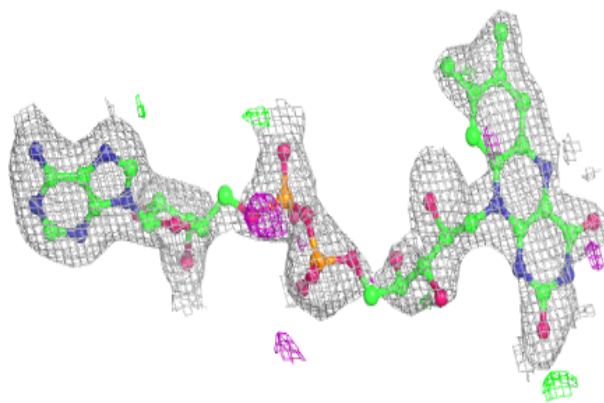
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SO4	B	602	5/5	0.96	0.10	53,57,64,67	0
3	SO4	A	602	5/5	0.98	0.21	50,58,67,72	0
3	SO4	B	601	5/5	0.98	0.08	28,33,36,38	0
3	SO4	A	601	5/5	0.98	0.07	37,37,53,57	0

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.

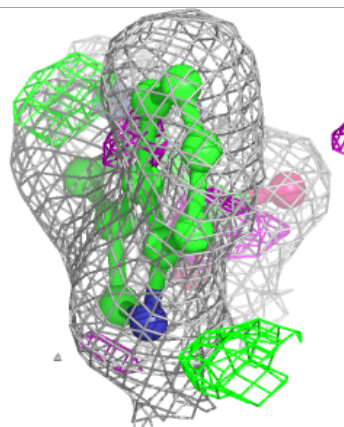
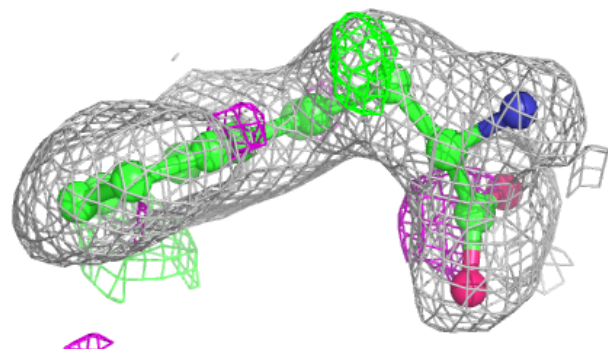
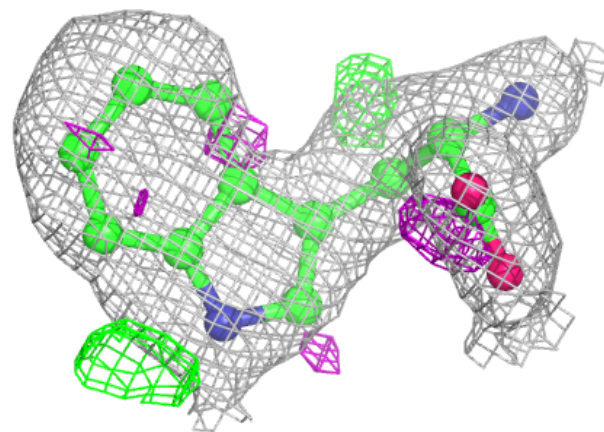


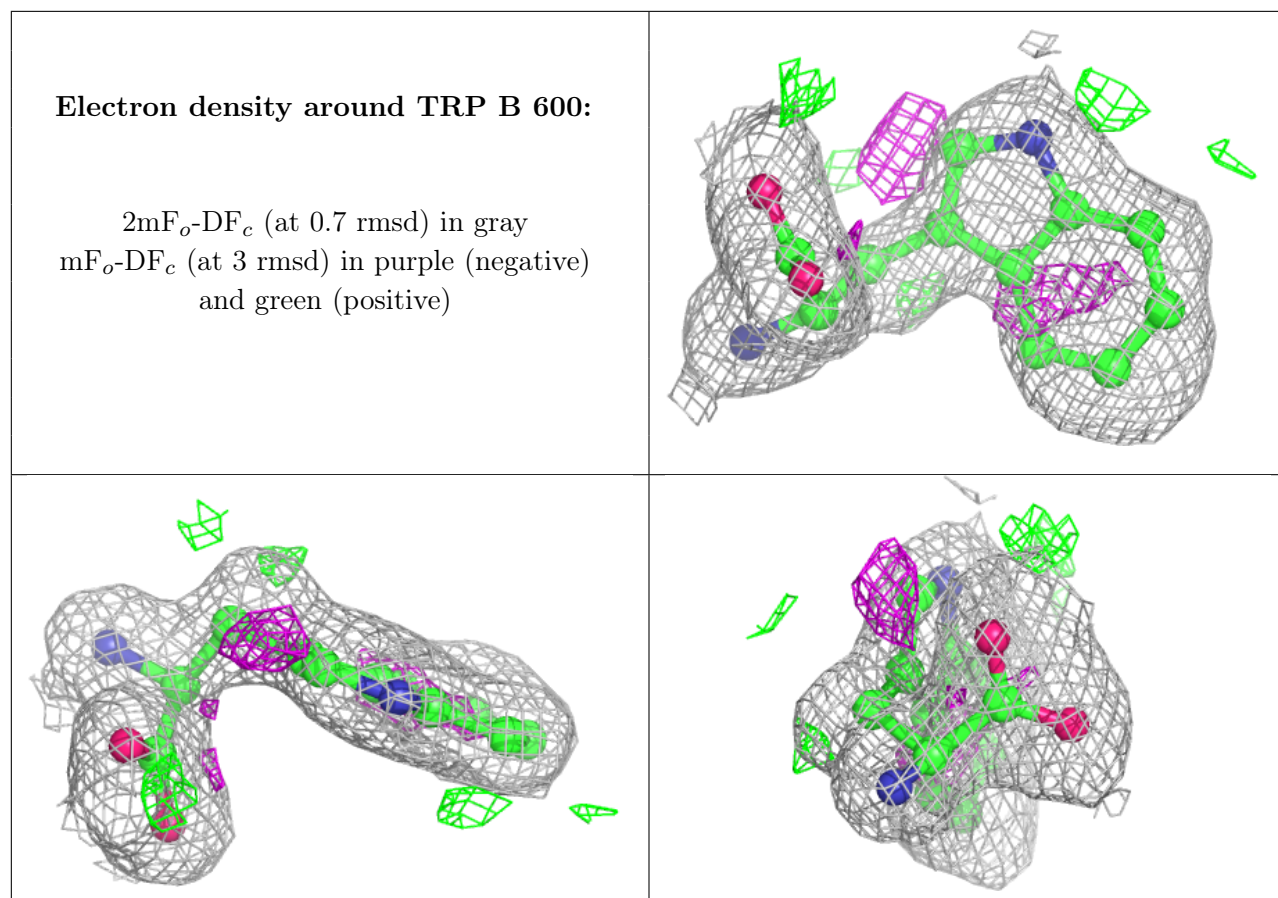
Electron density around FAD D 601:

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

**Electron density around TRP 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.