



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 03:09 AM EDT

PDB ID : 8TTI / pdb_00008tti
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 : 4-5-2 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

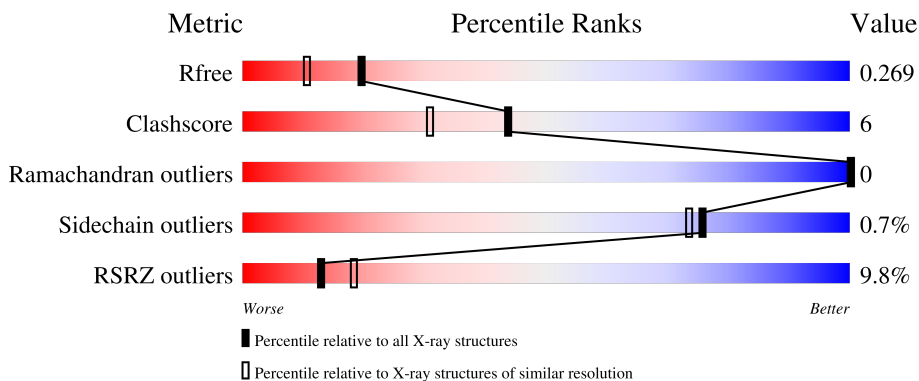
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	 5% 88% 11%
1	B	529	 7% 86% 12%
1	C	529	 10% 85% 13%
1	D	529	 17% 82% 16%

2 Entry composition [i](#)

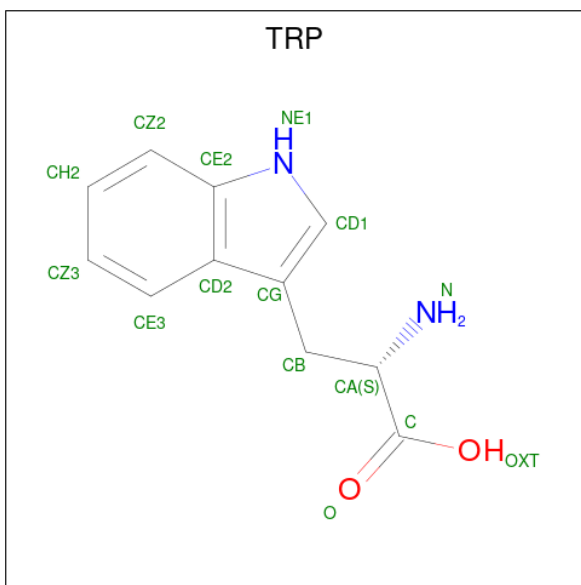
There are 5 unique types of molecules in this entry. The entry contains 18157 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: TRP) (formula: $C_{11}H_{12}N_2O_2$) (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 (CCD ID: SO4) (formula: O₄S).

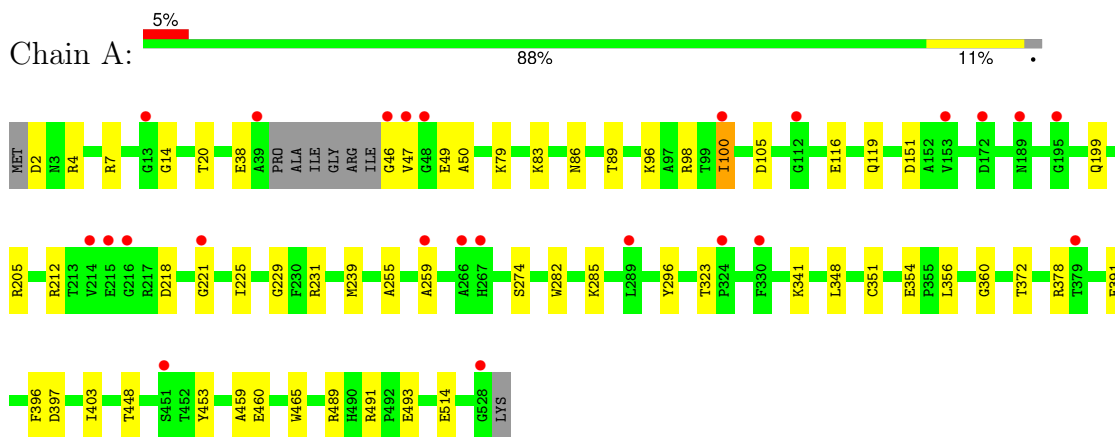


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total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

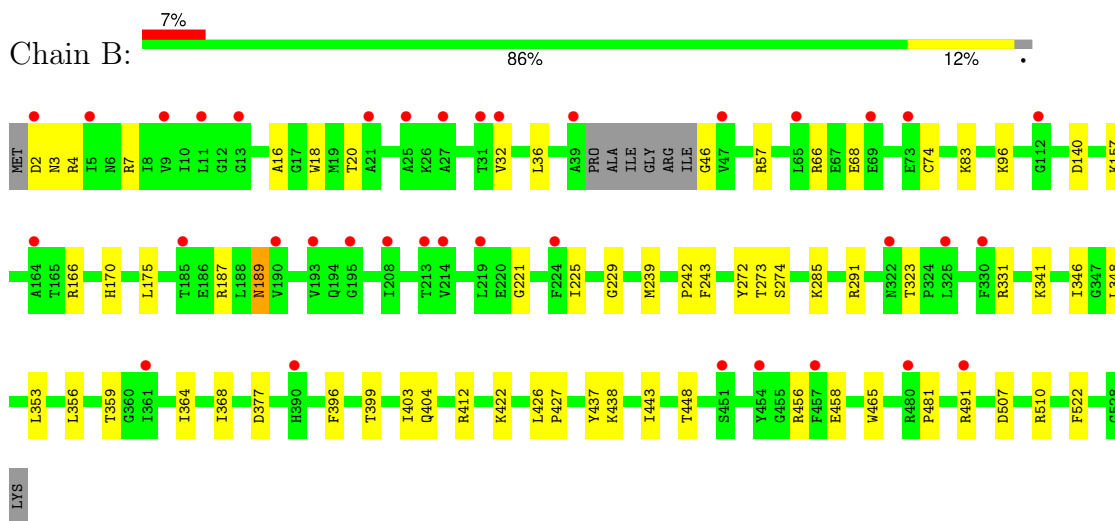
3 Residue-property plots [i](#)

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

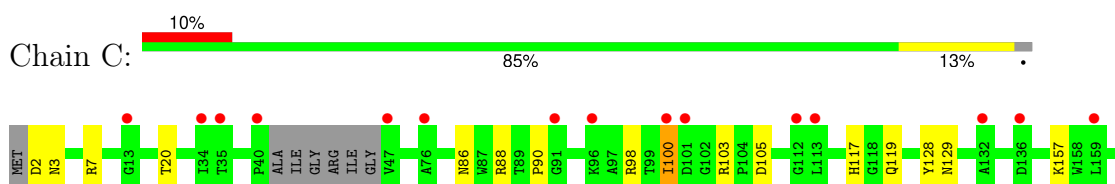
- Molecule 1: Tryptophan 6-halogenase

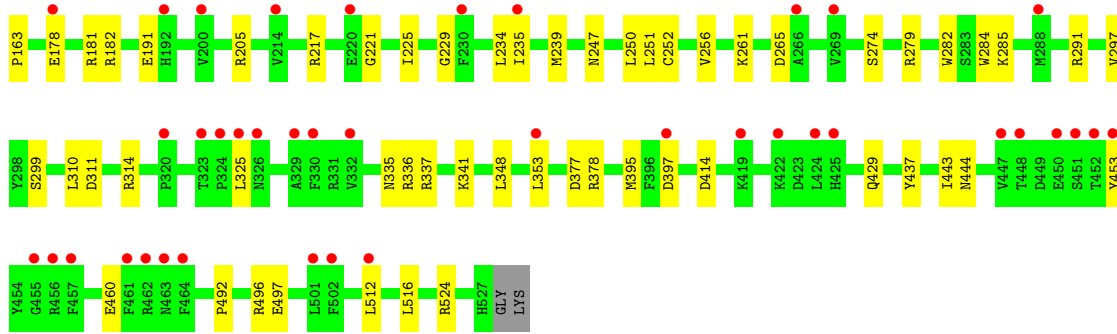


- Molecule 1: Tryptophan 6-halogenase

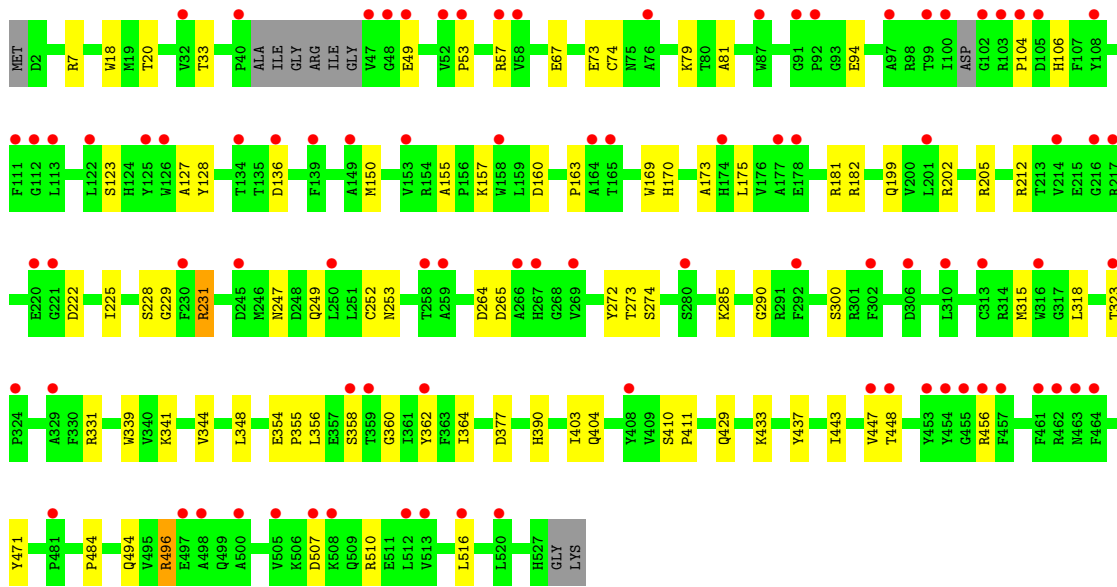


- Molecule 1: Tryptophan 6-halogenase





• 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 , 0.269	Depositor DCC
R_{free} test set	1999 reflections (1.16%)	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)	0.36 , 49.0	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	0.93	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	0.14	0/4303	0.30	0/5841
1	B	0.14	0/4314	0.30	0/5856
1	C	0.13	0/4312	0.29	0/5856
1	D	0.13	0/4269	0.27	0/5799
All	All	0.13	0/17198	0.29	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	44	0
1	B	4194	0	4035	46	0
1	C	4187	0	4023	49	0
1	D	4149	0	3979	63	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	22	1
5	D	231	0	0	27	1
All	All	18157	0	16139	202	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 (202) 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: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:81:ALA:HB3	1:D:150:MET:HE1	1.77	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: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:D:285:LYS:NZ	5:D:732:HOH:O	2.35	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:96:LYS:NZ	5:A:734:HOH:O	2.37	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: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:D:150:MET:HE3	1:D:272:TYR:HB3	1.88	0.54
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:B:448:THR:OG1	5:B:703:HOH:O	2.11	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: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:D:362:TYR:OH	5:D:709:HOH:O	2.19	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:B:239:MET:HE1	1:B:341:LYS:HD2	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:PRO:O	5:D:712:HOH:O	2.20	0.49
1:A:239:MET:HE1	1:A:341:LYS:HD2	1.93	0.49
1:B:229:GLY:HA2	1:B:348:LEU:HB2	1.95	0.49
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:341:LYS:NZ	5:D:749:HOH:O	2.48	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:170:HIS:NE2	1:D:273:THR:OG1	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:331:ARG:NH1	5:D:734:HOH:O	2.37	0.44
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:395:MET:HE2	1:C:395:MET:HB3	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:D:222:ASP:CG	5:D:736:HOH:O	2.64	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	428 (100%)	2 (0%)	81	79
1	B	431/436 (99%)	428 (99%)	3 (1%)	76	73
1	C	432/436 (99%)	428 (99%)	4 (1%)	70	67
1	D	425/436 (98%)	422 (99%)	3 (1%)	76	73
All	All	1718/1744 (98%)	1706 (99%)	12 (1%)	76	73

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	ILE
1	A	205	ARG
1	B	4	ARG
1	B	32	VAL
1	B	189	ASN
1	C	100	ILE
1	C	256	VAL
1	C	279	ARG
1	C	325	LEU
1	D	231	ARG
1	D	265	ASP
1	D	496	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	327	GLN
1	B	192	HIS
1	B	198	GLN
1	C	236	ASN
1	D	119	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 oligosaccharides 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	0.23	0	6,6,6	0.07	0
3	SO4	D	604	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	D	602	-	4,4,4	0.23	0	6,6,6	0.11	0
4	FAD	D	601	-	58,58,58	0.28	0	85,89,89	0.28	0
3	SO4	D	603	-	4,4,4	0.23	0	6,6,6	0.09	0
3	SO4	A	603	-	4,4,4	0.25	0	6,6,6	0.07	0
3	SO4	A	604	-	4,4,4	0.24	0	6,6,6	0.04	0
3	SO4	B	603	-	4,4,4	0.24	0	6,6,6	0.05	0
3	SO4	B	604	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	B	601	-	4,4,4	0.25	0	6,6,6	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	TRP	B	600	-	15,16,16	0.75	1 (6%)	18,22,22	0.82	1 (5%)
3	SO4	B	602	-	4,4,4	0.24	0	6,6,6	0.12	0
3	SO4	C	602	-	4,4,4	0.25	0	6,6,6	0.07	0
4	FAD	C	601	-	58,58,58	0.28	0	85,89,89	0.29	0
3	SO4	A	602	-	4,4,4	0.23	0	6,6,6	0.09	0
2	TRP	A	600	-	15,16,16	0.78	1 (6%)	18,22,22	0.86	1 (5%)
3	SO4	A	601	-	4,4,4	0.24	0	6,6,6	0.09	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	-	-	12/34/50/50	0/6/6/6
4	FAD	C	601	-	-	12/34/50/50	0/6/6/6
2	TRP	A	600	-	-	4/8/8/8	0/2/2/2
2	TRP	B	600	-	-	4/8/8/8	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	TRP	OXT-C	-2.29	1.23	1.30
2	B	600	TRP	OXT-C	-2.26	1.23	1.30

All (2) 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	124.08
2	B	600	TRP	OXT-C-O	-2.80	117.73	124.08

There are no chirality outliers.

All (32) 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
4	C	601	FAD	C2'-C3'-C4'-O4'
4	C	601	FAD	C2'-C3'-C4'-C5'
4	C	601	FAD	O3'-C3'-C4'-O4'

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Mol	Chain	Res	Type	Atoms
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
4	D	601	FAD	C2'-C3'-C4'-O4'
4	C	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	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	D	601	FAD	C3'-C4'-C5'-O5'
4	D	601	FAD	PA-O3P-P-O1P
4	D	601	FAD	O4'-C4'-C5'-O5'
4	C	601	FAD	C5B-O5B-PA-O1A
2	A	600	TRP	O-C-CA-CB
2	A	600	TRP	OXT-C-CA-CB
2	B	600	TRP	OXT-C-CA-CB
2	B	600	TRP	O-C-CA-CB
4	C	601	FAD	PA-O3P-P-O2P
4	D	601	FAD	PA-O3P-P-O2P

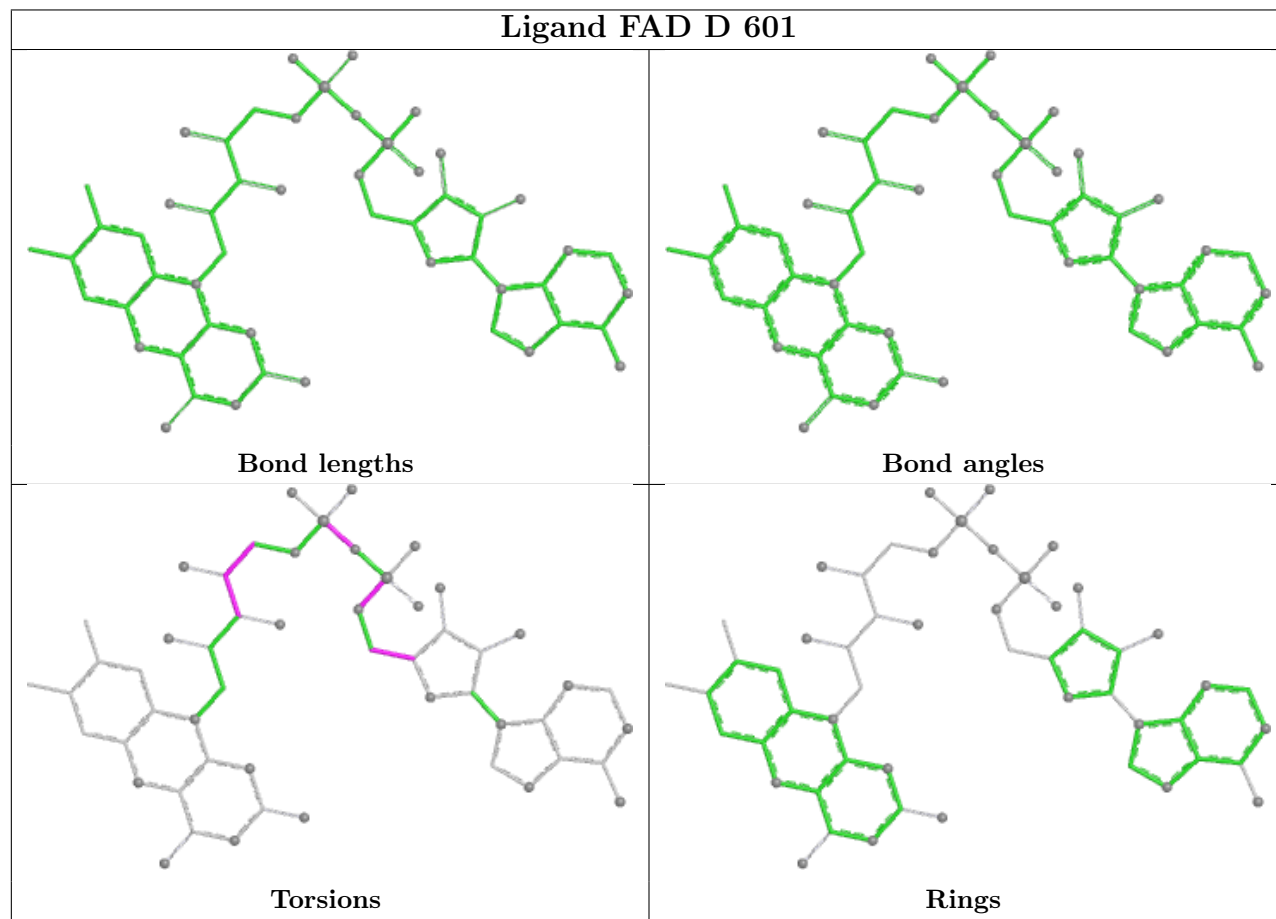
There are no ring outliers.

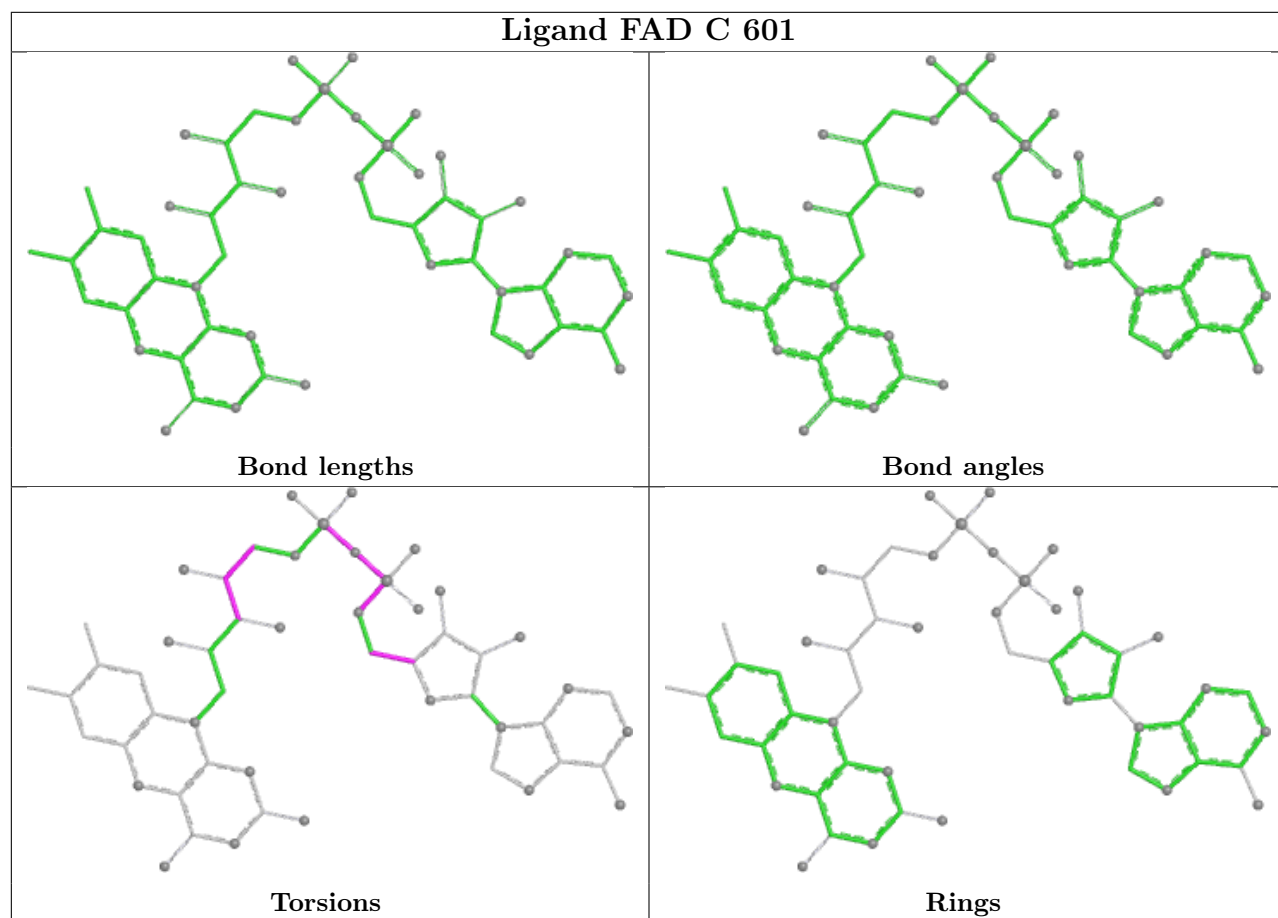
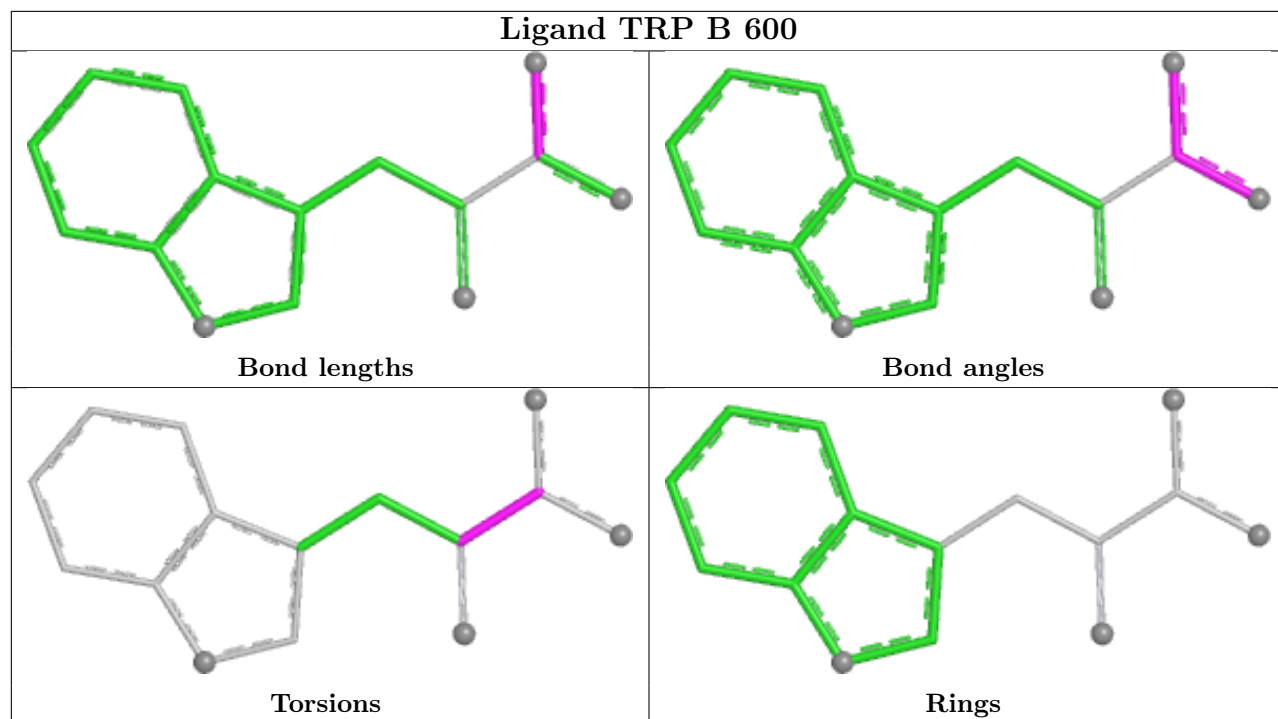
3 monomers are involved in 5 short contacts:

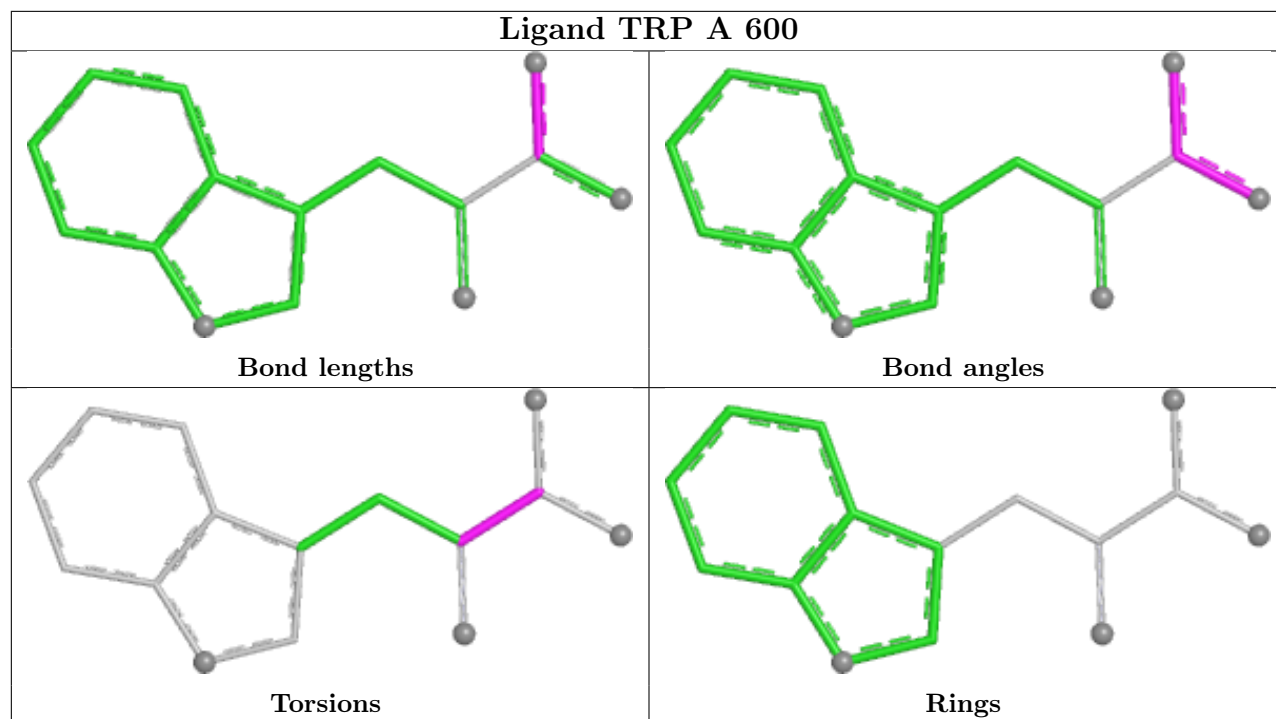
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	601	FAD	3	0
4	C	601	FAD	1	0
3	A	602	SO4	1	0

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%)	0.57	24 (4%) 37 47	17, 35, 56, 76	1 (0%)
1	B	521/529 (98%)	0.69	36 (6%) 23 30	19, 38, 65, 82	2 (0%)
1	C	520/529 (98%)	1.01	55 (10%) 11 15	23, 46, 68, 91	2 (0%)
1	D	519/529 (98%)	1.20	88 (16%) 4 5	26, 52, 74, 88	1 (0%)
All	All	2081/2116 (98%)	0.87	203 (9%) 13 18	17, 42, 68, 91	6 (0%)

All (203) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	112	GLY	5.6
1	D	457	PHE	5.4
1	D	47	VAL	4.6
1	D	245	ASP	4.2
1	B	330	PHE	4.1
1	A	39	ALA	4.1
1	A	259	ALA	4.1
1	B	361	ILE	4.0
1	B	214	VAL	4.0
1	C	47	VAL	4.0
1	D	100	ILE	4.0
1	C	13	GLY	3.9
1	C	324	PRO	3.9
1	D	214	VAL	3.8
1	C	329	ALA	3.7
1	D	455	GLY	3.7
1	D	498	ALA	3.6
1	A	195	GLY	3.6
1	C	457	PHE	3.4
1	A	214	VAL	3.4
1	B	47	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	111	PHE	3.3
1	D	177	ALA	3.3
1	D	258	THR	3.3
1	A	100	ILE	3.3
1	C	214	VAL	3.3
1	B	39	ALA	3.2
1	C	462	ARG	3.2
1	D	112	GLY	3.2
1	B	193	VAL	3.1
1	D	48	GLY	3.1
1	A	189	ASN	3.1
1	C	40	PRO	3.1
1	B	69	GLU	3.1
1	D	40	PRO	3.1
1	A	46	GLY	3.1
1	C	136	ASP	3.0
1	C	512	LEU	3.0
1	C	447	VAL	3.0
1	D	447	VAL	3.0
1	A	451	SER	3.0
1	D	358	SER	2.9
1	D	97	ALA	2.9
1	C	132	ALA	2.9
1	D	102	GLY	2.9
1	D	323	THR	2.8
1	C	76	ALA	2.8
1	A	330	PHE	2.8
1	C	464	PHE	2.8
1	C	325	LEU	2.8
1	D	49	GLU	2.8
1	A	47	VAL	2.8
1	C	326	ASN	2.7
1	D	461	PHE	2.7
1	A	267	HIS	2.7
1	D	92	PRO	2.7
1	B	454	TYR	2.7
1	B	457	PHE	2.7
1	D	178	GLU	2.7
1	D	32	VAL	2.7
1	D	53	PRO	2.6
1	B	11	LEU	2.6
1	D	362	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	422	LYS	2.6
1	C	502	PHE	2.6
1	A	221	GLY	2.6
1	D	463	ASN	2.6
1	C	461	PHE	2.6
1	D	302	PHE	2.6
1	D	464	PHE	2.6
1	D	310	LEU	2.6
1	D	456	ARG	2.6
1	D	216	GLY	2.6
1	C	452	THR	2.6
1	B	65	LEU	2.5
1	B	13	GLY	2.5
1	D	266	ALA	2.5
1	C	353	LEU	2.5
1	D	126	TRP	2.5
1	D	267	HIS	2.5
1	C	323	THR	2.5
1	C	332	VAL	2.5
1	D	134	THR	2.5
1	D	453	TYR	2.5
1	B	219	LEU	2.5
1	C	501	LEU	2.5
1	D	113	LEU	2.5
1	B	451	SER	2.5
1	B	185	THR	2.5
1	B	2	ASP	2.5
1	C	455	GLY	2.4
1	C	453	TYR	2.4
1	D	512	LEU	2.4
1	D	520	LEU	2.4
1	C	100	ILE	2.4
1	D	76	ALA	2.4
1	D	99	THR	2.4
1	B	9	VAL	2.4
1	D	153	VAL	2.4
1	B	195	GLY	2.4
1	C	220	GLU	2.4
1	D	516	LEU	2.4
1	D	165	THR	2.4
1	D	481	PRO	2.4
1	C	397	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	136	ASP	2.4
1	C	448	THR	2.4
1	B	27	ALA	2.4
1	D	158	TRP	2.4
1	A	172	ASP	2.3
1	D	105	ASP	2.3
1	D	306	ASP	2.3
1	B	480[A]	ARG	2.3
1	B	208	ILE	2.3
1	C	425[A]	HIS	2.3
1	A	216	GLY	2.3
1	A	528	GLY	2.3
1	D	52	VAL	2.3
1	D	250	LEU	2.3
1	D	230	PHE	2.3
1	B	21	ALA	2.3
1	D	462	ARG	2.3
1	A	215	GLU	2.3
1	D	125	TYR	2.3
1	D	139	PHE	2.3
1	D	454	TYR	2.3
1	A	324	PRO	2.3
1	D	149	ALA	2.3
1	D	217	ARG	2.3
1	C	101	ASP	2.3
1	D	497	GLU	2.3
1	D	507	ASP	2.3
1	B	322	ASN	2.3
1	C	192	HIS	2.3
1	D	91	GLY	2.2
1	D	408	TYR	2.2
1	B	190	VAL	2.2
1	D	505	VAL	2.2
1	D	57	ARG	2.2
1	D	313	CYS	2.2
1	B	325	LEU	2.2
1	C	450	GLU	2.2
1	D	280	SER	2.2
1	A	266	ALA	2.2
1	B	25	ALA	2.2
1	D	259	ALA	2.2
1	C	200	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	320	PRO	2.2
1	D	108	TYR	2.2
1	B	5	ILE	2.2
1	C	288	MET	2.2
1	C	419	LYS	2.2
1	D	87	TRP	2.2
1	C	463	ASN	2.2
1	C	178	GLU	2.2
1	A	379	THR	2.2
1	B	31	THR	2.2
1	B	213	THR	2.2
1	D	359	THR	2.2
1	A	289	LEU	2.2
1	C	91	GLY	2.2
1	C	113	LEU	2.2
1	D	329	ALA	2.2
1	C	456	ARG	2.2
1	D	103	ARG	2.2
1	C	230	PHE	2.1
1	C	330	PHE	2.1
1	C	96	LYS	2.1
1	D	324	PRO	2.1
1	B	224	PHE	2.1
1	C	34	ILE	2.1
1	B	491	ARG	2.1
1	D	513	VAL	2.1
1	D	220	GLU	2.1
1	B	390	HIS	2.1
1	D	122	LEU	2.1
1	D	201	LEU	2.1
1	C	266	ALA	2.1
1	D	448	THR	2.1
1	D	508	LYS	2.1
1	A	13	GLY	2.1
1	A	48	GLY	2.1
1	B	112	GLY	2.1
1	A	153	VAL	2.1
1	D	58	VAL	2.1
1	D	316	TRP	2.1
1	B	164	ALA	2.1
1	D	164	ALA	2.1
1	D	500	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	451	SER	2.0
1	C	35	THR	2.0
1	A	112	GLY	2.0
1	D	174	HIS	2.0
1	B	32	VAL	2.0
1	D	269	VAL	2.0
1	C	159	LEU	2.0
1	C	424	LEU	2.0
1	B	73	GLU	2.0
1	C	235	ILE	2.0
1	D	292	PHE	2.0
1	D	221	GLY	2.0
1	D	104	PRO	2.0
1	C	269	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

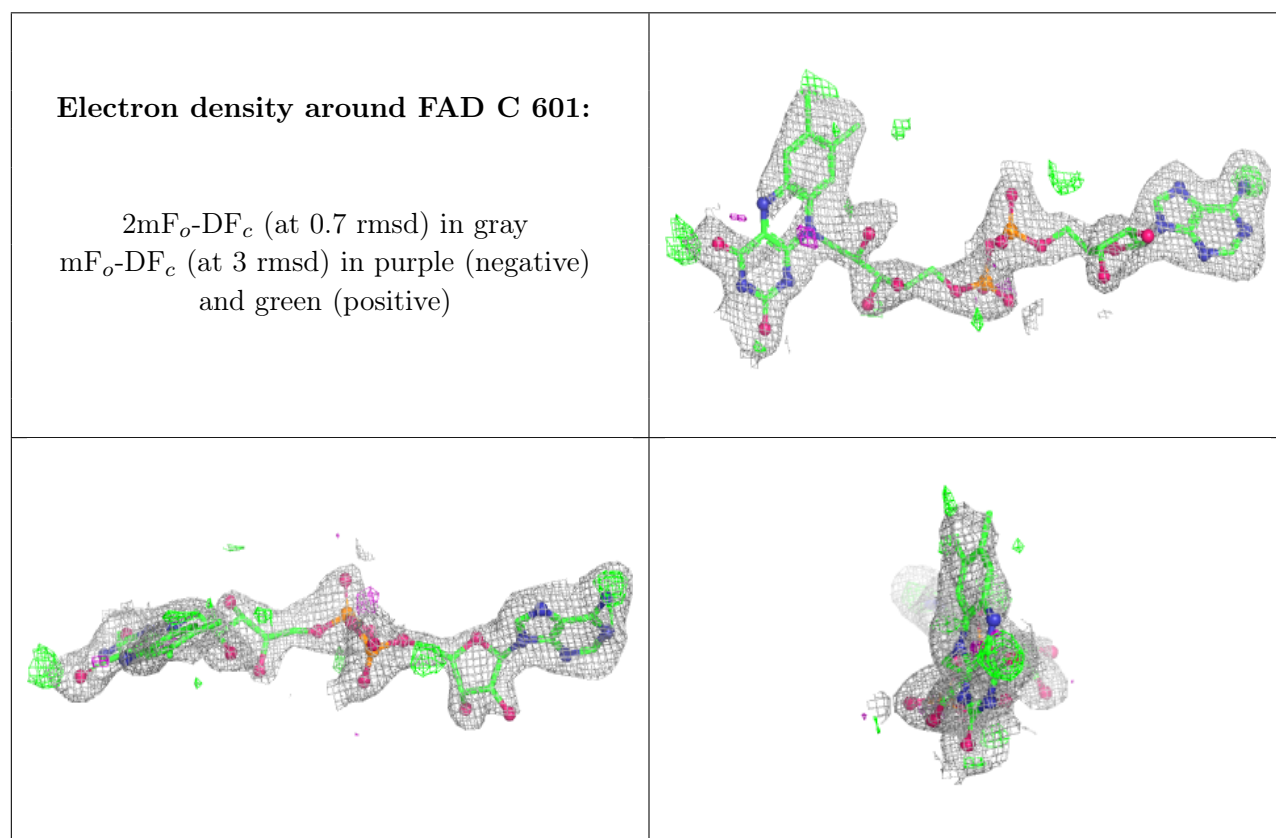
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	A	603	5/5	0.66	0.13	63,68,79,81	0
3	SO4	A	604	5/5	0.69	0.15	51,57,75,81	0
3	SO4	B	605	5/5	0.73	0.14	55,58,91,107	0
3	SO4	D	604	5/5	0.73	0.13	56,62,78,85	0
3	SO4	D	603	5/5	0.81	0.10	60,64,68,70	0
3	SO4	B	604	5/5	0.83	0.12	55,60,75,86	0
4	FAD	C	601	53/53	0.83	0.16	30,43,51,52	53
3	SO4	B	603	5/5	0.85	0.11	62,63,69,74	0
2	TRP	A	600	15/15	0.85	0.12	24,28,35,38	0

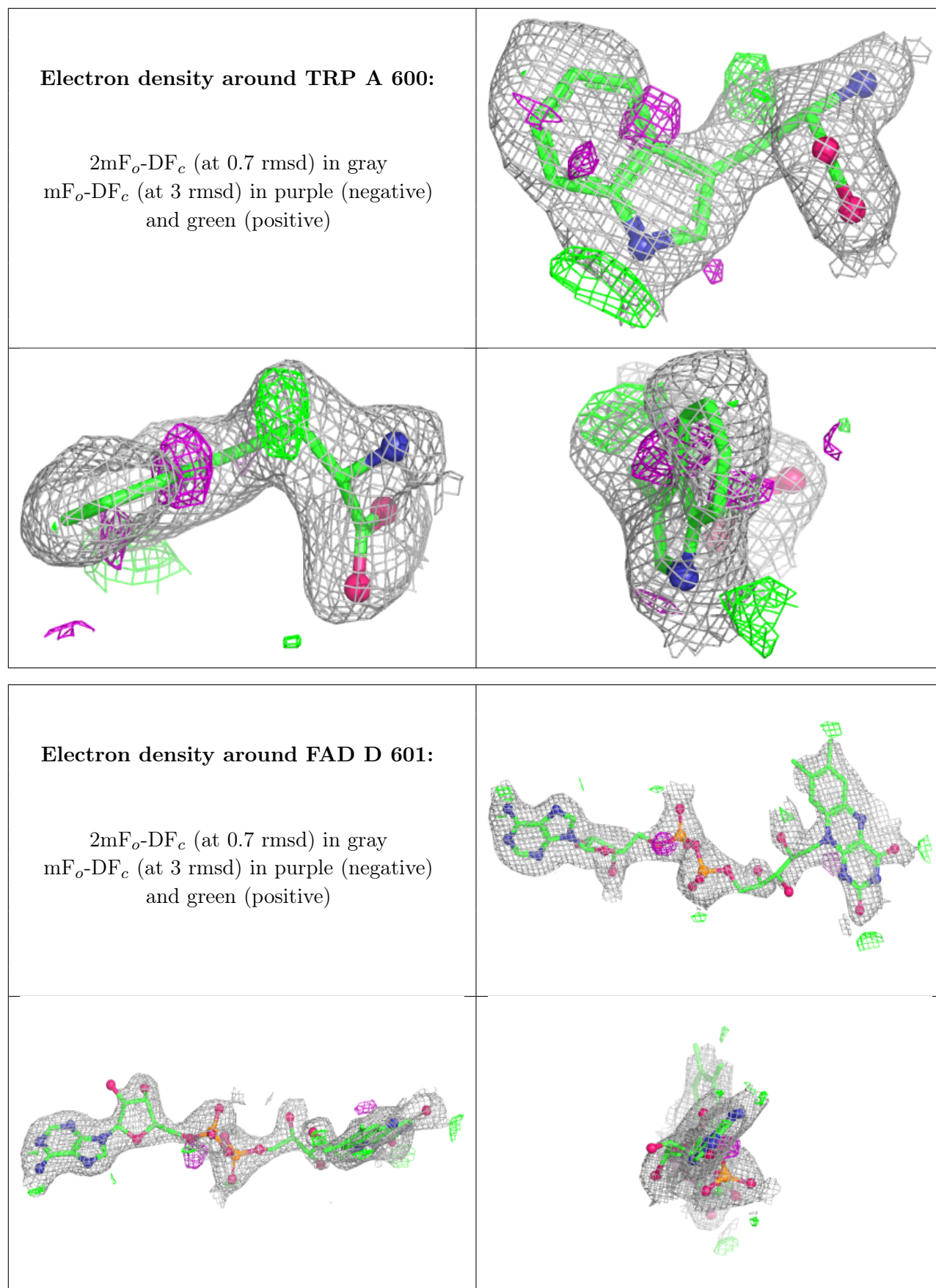
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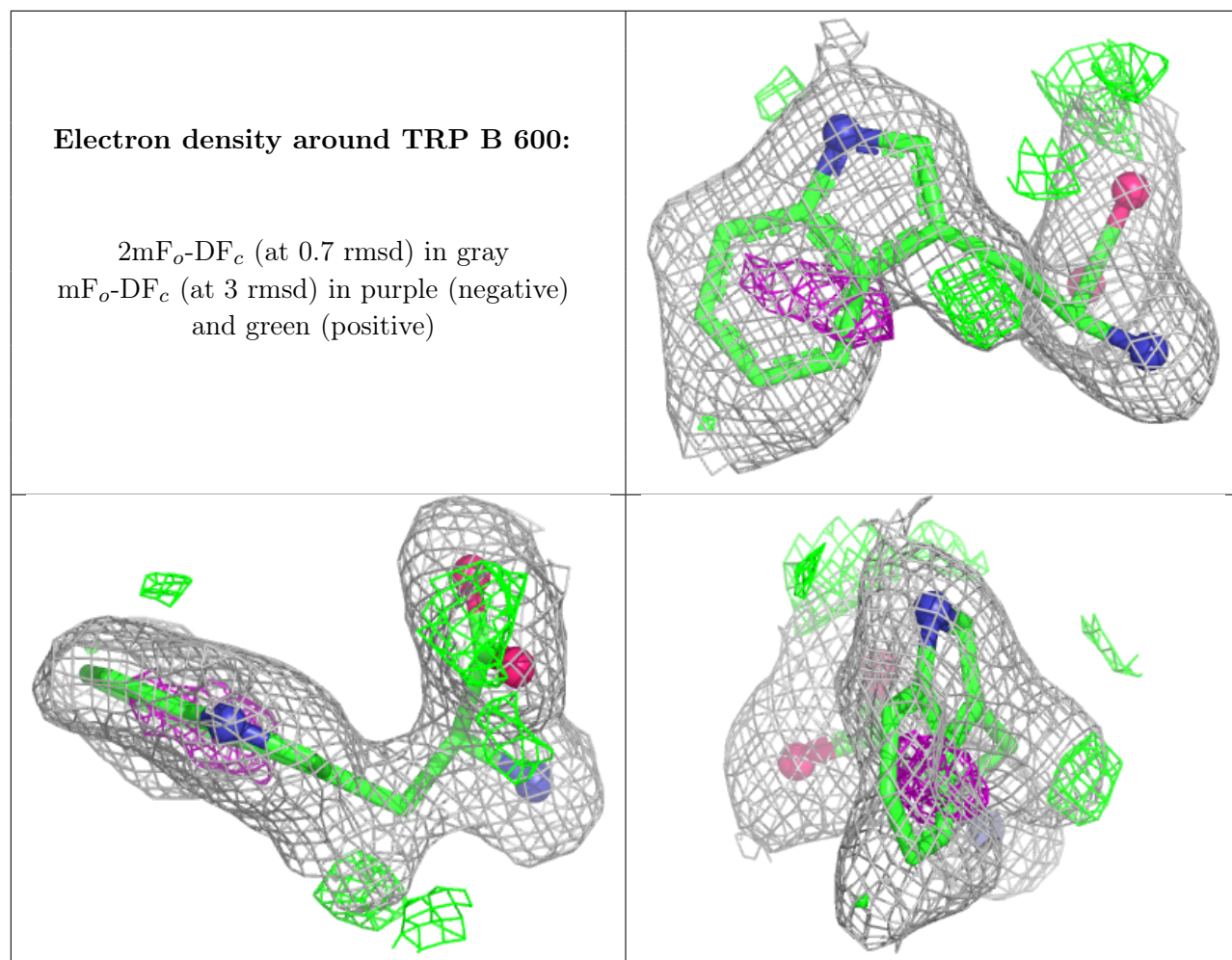
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	FAD	D	601	53/53	0.85	0.15	33,47,56,60	53
2	TRP	B	600	15/15	0.88	0.11	27,33,40,40	0
3	SO4	C	602	5/5	0.93	0.11	43,44,55,63	0
3	SO4	B	602	5/5	0.94	0.07	53,57,64,67	0
3	SO4	A	602	5/5	0.95	0.06	50,58,67,72	0
3	SO4	D	602	5/5	0.95	0.06	43,45,58,61	0
3	SO4	A	601	5/5	0.97	0.11	37,37,53,57	0
3	SO4	B	601	5/5	0.97	0.09	28,33,36,38	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.







6.5 Other polymers [i](#)

There are no such residues in this entry.