



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 08:27 AM UTC

PDB ID : 1PN0 / pdb_00001pn0
Title : Phenol hydroxylase from Trichosporon cutaneum
Authors : Enroth, C.
Deposited on : 2003-06-12
Resolution : 1.70 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

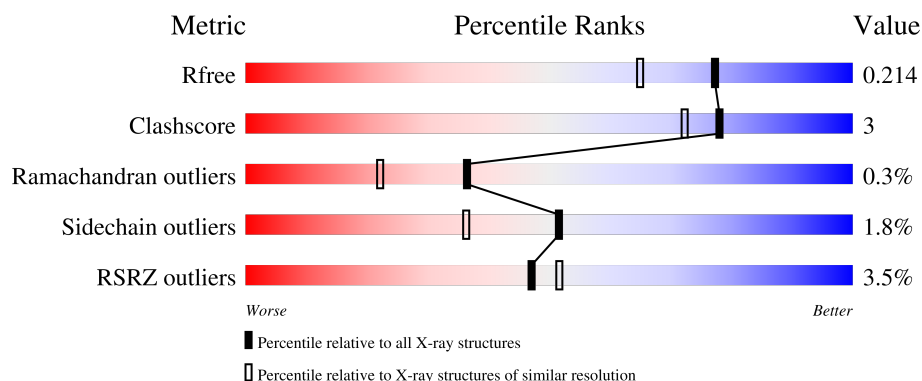
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	665	3% 91% 7% ..
1	B	665	2% 92% 6% ..
1	C	665	5% 91% 7% .
1	D	665	4% 92% 6% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23772 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 Phenol 2-monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	652	Total	C	N	O	S	15	0	0
			5187	3259	912	992	24			
1	B	652	Total	C	N	O	S	21	0	0
			5193	3263	913	993	24			
1	C	656	Total	C	N	O	S	5	0	0
			5230	3284	923	999	24			
1	D	656	Total	C	N	O	S	5	0	0
			5230	3284	923	999	24			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	123	ARG	HIS	SEE REMARK 999	UNP P15245
A	171	GLU	ASP	SEE REMARK 999	UNP P15245
A	172	ASP	HIS	SEE REMARK 999	UNP P15245
A	186	GLY	SER	SEE REMARK 999	UNP P15245
A	189	ARG	HIS	SEE REMARK 999	UNP P15245
A	265	ARG	PRO	SEE REMARK 999	UNP P15245
A	405	GLN	HIS	SEE REMARK 999	UNP P15245
A	406	PRO	ALA	SEE REMARK 999	UNP P15245
A	532	ALA	SER	SEE REMARK 999	UNP P15245
A	544	ARG	LEU	SEE REMARK 999	UNP P15245
A	549	GLY	VAL	SEE REMARK 999	UNP P15245
A	550	ALA	SER	SEE REMARK 999	UNP P15245
B	123	ARG	HIS	SEE REMARK 999	UNP P15245
B	171	GLU	ASP	SEE REMARK 999	UNP P15245
B	172	ASP	HIS	SEE REMARK 999	UNP P15245
B	186	GLY	SER	SEE REMARK 999	UNP P15245
B	189	ARG	HIS	SEE REMARK 999	UNP P15245
B	265	ARG	PRO	SEE REMARK 999	UNP P15245
B	405	GLN	HIS	SEE REMARK 999	UNP P15245
B	406	PRO	ALA	SEE REMARK 999	UNP P15245
B	532	ALA	SER	SEE REMARK 999	UNP P15245

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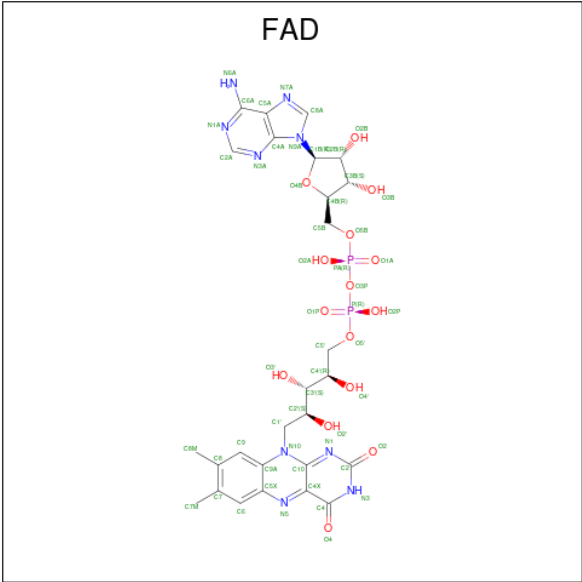
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Chain	Residue	Modelled	Actual	Comment	Reference
B	544	ARG	LEU	SEE REMARK 999	UNP P15245
B	549	GLY	VAL	SEE REMARK 999	UNP P15245
B	550	ALA	SER	SEE REMARK 999	UNP P15245
C	123	ARG	HIS	SEE REMARK 999	UNP P15245
C	171	GLU	ASP	SEE REMARK 999	UNP P15245
C	172	ASP	HIS	SEE REMARK 999	UNP P15245
C	186	GLY	SER	SEE REMARK 999	UNP P15245
C	189	ARG	HIS	SEE REMARK 999	UNP P15245
C	265	ARG	PRO	SEE REMARK 999	UNP P15245
C	405	GLN	HIS	SEE REMARK 999	UNP P15245
C	406	PRO	ALA	SEE REMARK 999	UNP P15245
C	532	ALA	SER	SEE REMARK 999	UNP P15245
C	544	ARG	LEU	SEE REMARK 999	UNP P15245
C	549	GLY	VAL	SEE REMARK 999	UNP P15245
C	550	ALA	SER	SEE REMARK 999	UNP P15245
D	123	ARG	HIS	SEE REMARK 999	UNP P15245
D	171	GLU	ASP	SEE REMARK 999	UNP P15245
D	172	ASP	HIS	SEE REMARK 999	UNP P15245
D	186	GLY	SER	SEE REMARK 999	UNP P15245
D	189	ARG	HIS	SEE REMARK 999	UNP P15245
D	265	ARG	PRO	SEE REMARK 999	UNP P15245
D	405	GLN	HIS	SEE REMARK 999	UNP P15245
D	406	PRO	ALA	SEE REMARK 999	UNP P15245
D	532	ALA	SER	SEE REMARK 999	UNP P15245
D	544	ARG	LEU	SEE REMARK 999	UNP P15245
D	549	GLY	VAL	SEE REMARK 999	UNP P15245
D	550	ALA	SER	SEE REMARK 999	UNP P15245

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

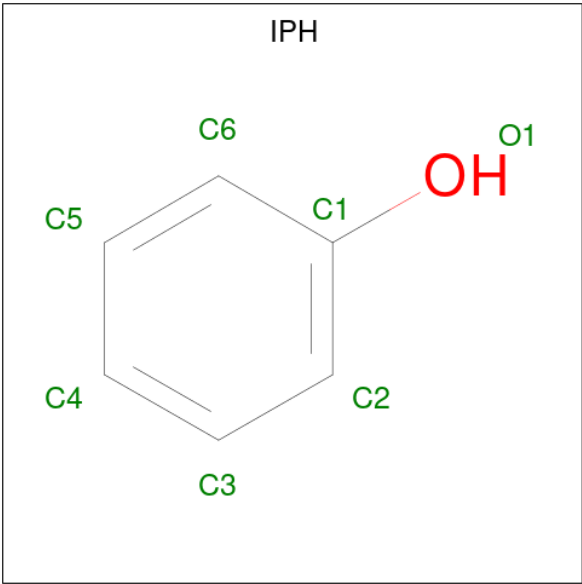
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0
2	B	1	Total Cl 1 1	0	0
2	C	1	Total Cl 1 1	0	0
2	D	1	Total Cl 1 1	0	0

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

- Molecule 4 is PHENOL (CCD ID: IPH) (formula: C₆H₆O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 6 1	0	0
4	B	1	Total C O 7 6 1	0	0
4	C	1	Total C O 7 6 1	0	0
4	D	1	Total C O 7 6 1	0	0

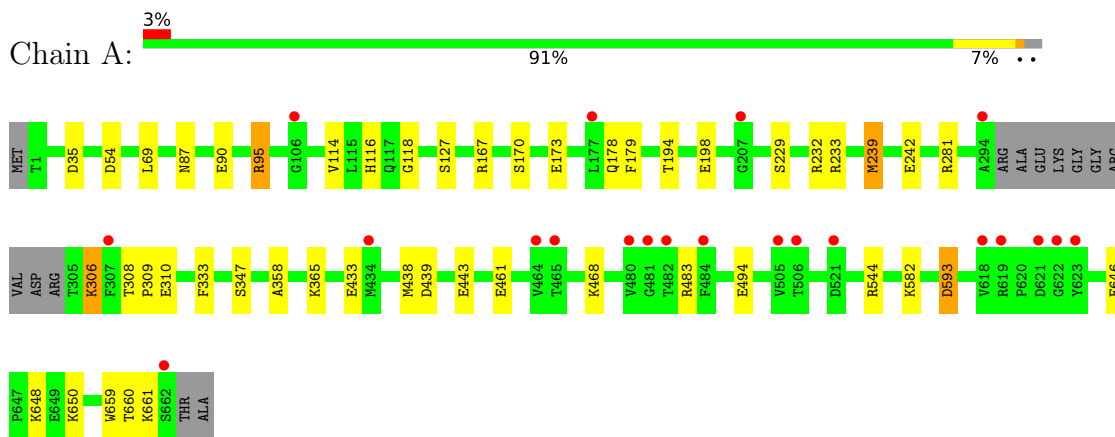
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	668	Total O 668 668	0	0
5	B	686	Total O 686 686	0	0
5	C	674	Total O 674 674	0	0
5	D	660	Total O 660 660	0	0

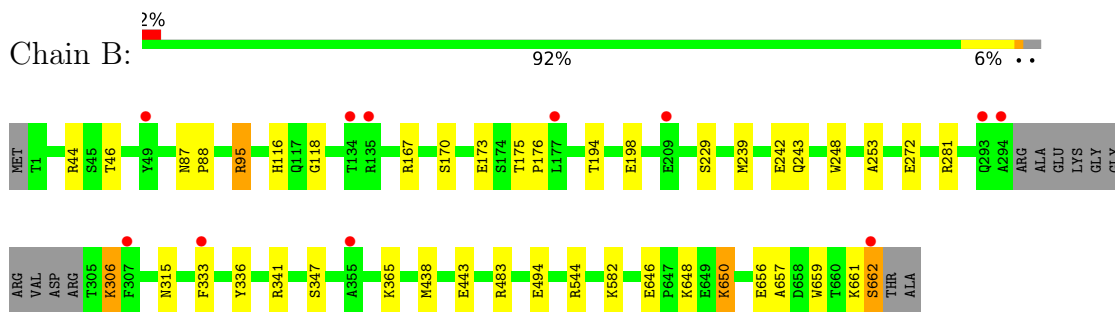
3 Residue-property plots [i](#)

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

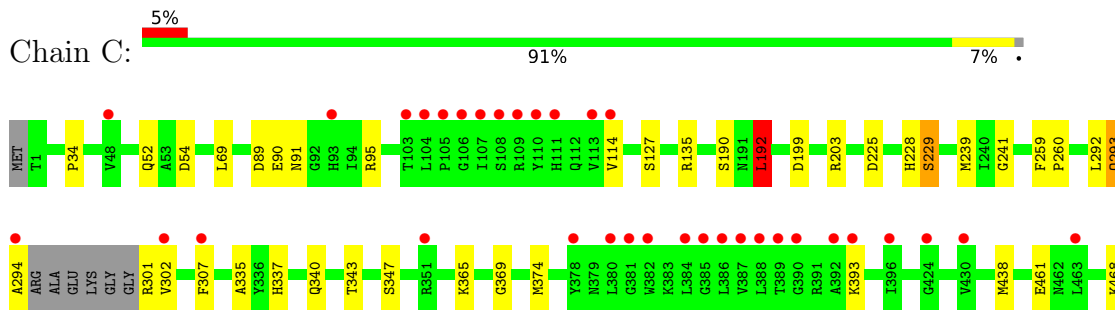
- Molecule 1: Phenol 2-monooxygenase



- Molecule 1: Phenol 2-monooxygenase

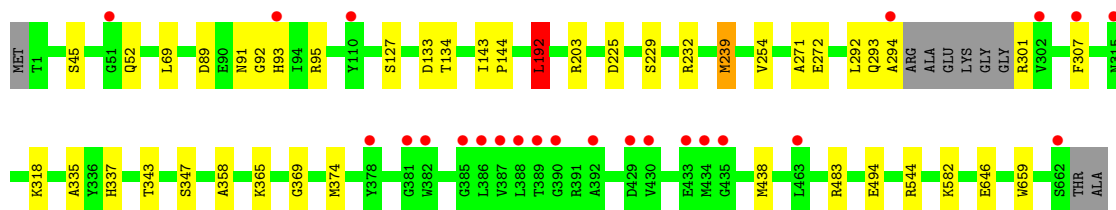
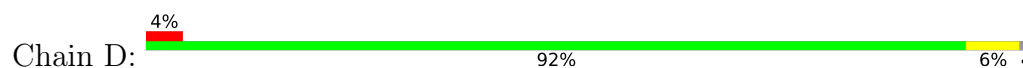


- Molecule 1: Phenol 2-monooxygenase





- Molecule 1: Phenol 2-monooxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	100.00Å 150.95Å 114.96Å 90.00° 114.63° 90.00°	Depositor
Resolution (Å)	19.96 – 1.70 19.96 – 1.70	Depositor EDS
% Data completeness (in resolution range)	86.1 (19.96-1.70) 86.1 (19.96-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.02	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.157 , 0.180 (Not available) , 0.214	Depositor DCC
R_{free} test set	14784 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	21.7	Xtriage
Anisotropy	0.947	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 60.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.013 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	23772	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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, IPH, CL

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	0.62	0/5302	0.92	3/7171 (0.0%)
1	B	0.65	0/5308	0.94	5/7178 (0.1%)
1	C	0.68	1/5345 (0.0%)	0.91	3/7227 (0.0%)
1	D	0.65	2/5345 (0.0%)	0.91	5/7227 (0.1%)
All	All	0.65	3/21300 (0.0%)	0.92	16/28803 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	374	MET	SD-CE	-8.85	1.57	1.79
1	D	374	MET	SD-CE	-6.92	1.62	1.79
1	D	203	ARG	CG-CD	5.86	1.70	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	306	LYS	CA-C-N	-13.92	103.57	123.05
1	B	306	LYS	C-N-CA	-13.92	103.57	123.05
1	B	306	LYS	O-C-N	11.55	137.95	122.59
1	A	306	LYS	CA-C-N	10.89	136.19	120.95
1	A	306	LYS	C-N-CA	10.89	136.19	120.95
1	A	306	LYS	O-C-N	-7.21	113.01	122.59
1	D	203	ARG	CB-CG-CD	7.02	127.46	111.30
1	D	225	ASP	N-CA-C	6.02	119.37	112.57
1	D	192	LEU	N-CA-C	-6.01	105.44	112.89
1	C	192	LEU	N-CA-C	-5.94	105.52	112.89
1	D	254	VAL	N-CA-C	-5.62	102.44	107.56
1	C	225	ASP	N-CA-C	5.55	119.05	112.72
1	B	253	ALA	CA-C-N	-5.32	118.98	122.60
1	B	253	ALA	C-N-CA	-5.32	118.98	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	643	ILE	N-CA-C	5.12	115.66	111.62
1	D	203	ARG	CG-CD-NE	5.07	123.16	112.00

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	5187	0	5055	38	1
1	B	5193	0	5071	32	1
1	C	5230	0	5110	23	0
1	D	5230	0	5110	25	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	53	0	31	0	0
3	B	53	0	31	0	0
3	C	53	0	31	1	0
3	D	53	0	31	1	0
4	A	7	0	6	0	0
4	B	7	0	6	0	0
4	C	7	0	6	0	0
4	D	7	0	6	0	0
5	A	668	0	0	4	1
5	B	686	0	0	3	1
5	C	674	0	0	2	0
5	D	660	0	0	0	0
All	All	23772	0	20494	118	2

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 3.

All (118) 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:D:544:ARG:NE	1:D:646:GLU:OE2	1.96	0.98
1:A:95:ARG:HH11	1:A:95:ARG:HG3	1.25	0.97
1:B:95:ARG:HH11	1:B:95:ARG:HG3	1.27	0.97
1:A:646:GLU:OE1	1:A:650:LYS:HE2	1.70	0.92
1:A:87:ASN:O	1:A:95:ARG:HD3	1.72	0.90
1:B:87:ASN:O	1:B:95:ARG:HD3	1.73	0.88
1:B:95:ARG:HH11	1:B:95:ARG:CG	1.94	0.80
1:A:544:ARG:NE	1:A:646:GLU:OE2	2.13	0.79
1:B:544:ARG:NE	1:B:646:GLU:OE2	2.14	0.79
1:B:656:GLU:OE1	5:B:938:HOH:O	2.03	0.77
1:A:95:ARG:HH11	1:A:95:ARG:CG	1.99	0.76
1:D:307:PHE:CE1	1:D:335:ALA:HB2	2.25	0.72
1:D:544:ARG:HE	1:D:646:GLU:CD	1.98	0.69
1:B:239:MET:HB3	1:B:341:ARG:HB3	1.77	0.67
1:B:116:HIS:HD2	1:B:118:GLY:H	1.42	0.66
1:C:307:PHE:CE1	1:C:335:ALA:HB2	2.30	0.65
1:C:393:LYS:NZ	5:C:6555:HOH:O	2.32	0.59
1:D:192:LEU:O	1:D:301:ARG:NH1	2.32	0.59
1:B:242:GLU:HG3	1:B:243:GLN:N	2.18	0.58
1:A:116:HIS:HD2	1:A:118:GLY:H	1.50	0.58
1:A:660:THR:OG1	1:A:661:LYS:HE2	2.02	0.58
1:A:438:MET:HA	1:A:438:MET:HE2	1.85	0.57
1:A:95:ARG:CG	1:A:95:ARG:NH1	2.65	0.56
1:C:461:GLU:OE1	1:C:468:LYS:HG3	2.05	0.56
1:D:89:ASP:OD1	1:D:92:GLY:N	2.38	0.56
1:B:87:ASN:O	1:B:95:ARG:CD	2.49	0.56
1:A:242:GLU:HG2	5:A:6439:HOH:O	2.05	0.56
1:A:646:GLU:OE1	1:A:650:LYS:CE	2.49	0.55
1:B:661:LYS:O	1:B:662:SER:C	2.50	0.55
1:D:192:LEU:HD22	1:D:337:HIS:CD2	2.41	0.55
1:D:438:MET:HA	1:D:438:MET:HE2	1.88	0.55
1:D:369:GLY:HA3	3:D:6041:FAD:H1'2	1.87	0.55
1:A:95:ARG:HD3	1:A:95:ARG:N	2.22	0.55
1:B:95:ARG:CG	1:B:95:ARG:NH1	2.63	0.54
1:A:170:SER:OG	1:A:173:GLU:HG3	2.07	0.54
1:C:293:GLN:O	1:C:294:ALA:HB2	2.07	0.54
1:C:369:GLY:HA3	3:C:6031:FAD:H1'2	1.89	0.54
1:A:593:ASP:OD1	5:A:6310:HOH:O	2.18	0.53
1:A:648:LYS:HG3	5:A:6288:HOH:O	2.07	0.53
1:D:544:ARG:CZ	1:D:646:GLU:OE2	2.57	0.53
1:D:89:ASP:OD1	1:D:91:ASN:N	2.42	0.53
1:B:438:MET:HA	1:B:438:MET:HE2	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:239:MET:HG3	1:D:343:THR:HG22	1.91	0.52
1:B:648:LYS:HG3	5:B:932:HOH:O	2.10	0.52
1:B:443:GLU:HA	1:B:443:GLU:OE1	2.08	0.52
1:A:544:ARG:HE	1:A:646:GLU:CD	2.17	0.52
1:C:89:ASP:C	1:C:89:ASP:OD1	2.53	0.52
1:C:534:TYR:OH	1:C:637:ASP:OD1	2.27	0.51
1:A:308:THR:HB	1:A:309:PRO:HD2	1.93	0.51
1:B:582:LYS:HA	1:B:659:TRP:CE2	2.46	0.51
1:C:438:MET:HE2	1:C:438:MET:HA	1.93	0.51
1:C:601:LYS:HE2	5:C:6704:HOH:O	2.11	0.50
1:A:95:ARG:HD3	1:A:95:ARG:H	1.77	0.50
1:A:95:ARG:HG3	1:A:95:ARG:NH1	2.07	0.49
1:D:292:LEU:HD11	1:D:307:PHE:CZ	2.47	0.49
1:D:292:LEU:HD12	1:D:307:PHE:CE2	2.47	0.49
1:A:232:ARG:CZ	1:A:239:MET:HG2	2.43	0.48
1:C:199:ASP:O	1:C:203:ARG:HG2	2.13	0.48
1:D:582:LYS:HA	1:D:659:TRP:CE2	2.49	0.48
1:A:54:ASP:O	1:A:114:VAL:HA	2.14	0.48
1:A:582:LYS:HA	1:A:659:TRP:CE2	2.49	0.48
1:A:87:ASN:O	1:A:95:ARG:CD	2.52	0.47
1:C:292:LEU:HD12	1:C:307:PHE:CE2	2.49	0.47
1:C:582:LYS:HA	1:C:659:TRP:CE2	2.49	0.47
1:B:116:HIS:HB3	1:B:281:ARG:NH2	2.30	0.47
1:D:239:MET:HG3	1:D:343:THR:CG2	2.44	0.47
1:B:116:HIS:HD2	1:B:118:GLY:N	2.11	0.46
1:C:192:LEU:HD22	1:C:337:HIS:CD2	2.50	0.46
1:A:308:THR:HB	1:A:310:GLU:OE1	2.15	0.46
1:A:310:GLU:H	1:A:310:GLU:CD	2.24	0.46
1:B:544:ARG:HE	1:B:646:GLU:CD	2.19	0.46
1:A:232:ARG:HD3	1:A:358:ALA:O	2.16	0.45
1:B:194:THR:O	1:B:198:GLU:HG3	2.17	0.45
1:B:167:ARG:NH1	5:B:747:HOH:O	2.36	0.45
1:B:650:LYS:HB2	1:B:650:LYS:HE2	1.47	0.45
1:D:133:ASP:O	1:D:134:THR:OG1	2.21	0.44
1:B:95:ARG:HD3	1:B:95:ARG:H	1.82	0.44
1:A:178:GLN:HG2	1:A:179:PHE:CE1	2.53	0.44
1:A:194:THR:O	1:A:198:GLU:HG3	2.17	0.44
1:A:167:ARG:HH12	1:A:173:GLU:CD	2.26	0.44
1:D:232:ARG:HD3	1:D:358:ALA:O	2.18	0.44
1:B:656:GLU:HG2	1:B:657:ALA:O	2.18	0.43
1:A:116:HIS:HB3	1:A:281:ARG:NH2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:GLN:HG2	1:A:179:PHE:CD1	2.53	0.43
1:B:87:ASN:HB2	1:B:88:PRO:CD	2.48	0.43
1:D:292:LEU:CD1	1:D:307:PHE:CE2	3.01	0.43
1:D:544:ARG:NH2	1:D:646:GLU:OE2	2.51	0.43
1:A:439:ASP:O	1:A:443:GLU:HG3	2.18	0.43
1:A:116:HIS:HD2	1:A:118:GLY:N	2.14	0.43
1:D:89:ASP:OD2	1:D:93:HIS:HB2	2.19	0.42
1:B:95:ARG:HD3	1:B:95:ARG:N	2.35	0.42
1:C:292:LEU:HD11	1:C:307:PHE:CZ	2.54	0.42
1:D:293:GLN:HA	1:D:294:ALA:HA	1.66	0.42
1:B:170:SER:OG	1:B:173:GLU:HG3	2.19	0.42
1:C:241:GLY:HA3	1:C:340:GLN:O	2.19	0.42
1:C:54:ASP:O	1:C:114:VAL:HA	2.19	0.42
1:D:69:LEU:HD21	1:D:127:SER:HB2	2.01	0.42
1:D:271:ALA:C	1:D:272:GLU:HG2	2.44	0.42
1:A:308:THR:HB	1:A:309:PRO:CD	2.50	0.41
1:C:89:ASP:OD1	1:C:91:ASN:N	2.53	0.41
1:A:544:ARG:HG3	1:A:646:GLU:HG2	2.01	0.41
1:B:248:TRP:HB2	1:B:336:TYR:CZ	2.56	0.41
1:B:544:ARG:HG3	1:B:646:GLU:HG2	2.01	0.41
1:A:461:GLU:OE1	1:A:468:LYS:HG3	2.21	0.41
1:A:35:ASP:OD1	5:A:6086:HOH:O	2.22	0.41
1:C:228:HIS:O	1:C:229:SER:C	2.64	0.41
1:C:239:MET:HG3	1:C:343:THR:HG22	2.02	0.41
1:A:69:LEU:HD21	1:A:127:SER:HB2	2.03	0.40
1:C:34:PRO:O	1:C:135:ARG:NH2	2.49	0.40
1:C:69:LEU:HD21	1:C:127:SER:HB2	2.03	0.40
1:B:544:ARG:HE	1:B:646:GLU:CG	2.35	0.40
1:D:143:ILE:HA	1:D:144:PRO:HD3	1.97	0.40
1:B:44:ARG:HD2	1:B:46:THR:O	2.21	0.40
1:B:175:THR:HA	1:B:176:PRO:HD3	1.86	0.40
1:C:190:SER:HB2	1:C:335:ALA:O	2.21	0.40
1:C:259:PHE:HA	1:C:260:PRO:HD3	1.93	0.40
1:B:242:GLU:CG	1:B:243:GLN:N	2.84	0.40
1:D:192:LEU:O	1:D:301:ARG:NH2	2.54	0.40

All (2) 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)
1:A:233:ARG:NH2	1:B:272:GLU:OE2[2_746]	2.15	0.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:6078:HOH:O	5:B:733:HOH:O[1_454]	2.17	0.03

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	648/665 (97%)	631 (97%)	15 (2%)	2 (0%)	36	22
1	B	648/665 (97%)	633 (98%)	14 (2%)	1 (0%)	43	28
1	C	652/665 (98%)	637 (98%)	13 (2%)	2 (0%)	36	22
1	D	652/665 (98%)	636 (98%)	14 (2%)	2 (0%)	36	22
All	All	2600/2660 (98%)	2537 (98%)	56 (2%)	7 (0%)	36	22

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	306	LYS
1	C	52	GLN
1	D	52	GLN
1	A	229	SER
1	C	229	SER
1	D	229	SER
1	B	229	SER

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	560/571 (98%)	550 (98%)	10 (2%)	51	36
1	B	562/571 (98%)	552 (98%)	10 (2%)	51	36
1	C	566/571 (99%)	555 (98%)	11 (2%)	50	34
1	D	566/571 (99%)	557 (98%)	9 (2%)	55	41
All	All	2254/2284 (99%)	2214 (98%)	40 (2%)	51	36

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	GLU
1	A	95	ARG
1	A	239	MET
1	A	333	PHE
1	A	347	SER
1	A	365	LYS
1	A	433	GLU
1	A	483	ARG
1	A	494	GLU
1	A	593	ASP
1	B	95	ARG
1	B	306	LYS
1	B	315	ASN
1	B	333	PHE
1	B	347	SER
1	B	365	LYS
1	B	483	ARG
1	B	494	GLU
1	B	650	LYS
1	B	662	SER
1	C	90	GLU
1	C	95	ARG
1	C	192	LEU
1	C	293	GLN
1	C	301	ARG
1	C	302	VAL
1	C	347	SER
1	C	365	LYS
1	C	483	ARG
1	C	494	GLU
1	C	637	ASP
1	D	45	SER
1	D	95	ARG

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Mol	Chain	Res	Type
1	D	192	LEU
1	D	239	MET
1	D	318	LYS
1	D	347	SER
1	D	365	LYS
1	D	483	ARG
1	D	494	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	66	ASN
1	A	116	HIS
1	A	315	ASN
1	A	337	HIS
1	A	449	ASN
1	B	116	HIS
1	B	409	GLN
1	B	416	HIS
1	B	449	ASN
1	B	572	HIS
1	C	66	ASN
1	C	337	HIS
1	C	449	ASN
1	C	584	GLN
1	C	604	GLN
1	D	66	ASN
1	D	243	GLN
1	D	337	HIS
1	D	449	ASN
1	D	539	ASN
1	D	584	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	IPH	B	6022	-	7,7,7	0.52	0	8,8,8	1.32	1 (12%)
4	IPH	D	6042	-	7,7,7	0.83	0	8,8,8	0.55	0
3	FAD	A	6011	-	58,58,58	1.05	6 (10%)	85,89,89	1.51	15 (17%)
4	IPH	C	6032	-	7,7,7	0.79	0	8,8,8	0.73	0
3	FAD	C	6031	-	58,58,58	1.18	6 (10%)	85,89,89	1.52	11 (12%)
3	FAD	B	6021	-	58,58,58	1.12	7 (12%)	85,89,89	1.52	13 (15%)
3	FAD	D	6041	-	58,58,58	1.25	7 (12%)	85,89,89	1.59	14 (16%)
4	IPH	A	6012	-	7,7,7	0.75	0	8,8,8	1.34	1 (12%)

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	IPH	B	6022	-	-	-	0/1/1/1
4	IPH	D	6042	-	-	-	0/1/1/1
3	FAD	A	6011	-	-	4/34/50/50	0/6/6/6
4	IPH	C	6032	-	-	-	0/1/1/1
3	FAD	C	6031	-	-	4/34/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FAD	B	6021	-	-	3/34/50/50	0/6/6/6
3	FAD	D	6041	-	-	1/34/50/50	0/6/6/6
4	IPH	A	6012	-	-	-	0/1/1/1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	6031	FAD	C4X-N5	4.07	1.39	1.30
3	C	6031	FAD	P-O3P	3.59	1.63	1.59
3	D	6041	FAD	PA-O3P	3.59	1.63	1.59
3	D	6041	FAD	P-O3P	3.49	1.63	1.59
3	A	6011	FAD	C4X-N5	3.40	1.38	1.30
3	D	6041	FAD	C4X-N5	3.30	1.37	1.30
3	B	6021	FAD	C4X-N5	3.28	1.37	1.30
3	C	6031	FAD	C10-N1	3.17	1.39	1.33
3	B	6021	FAD	C10-N1	3.07	1.39	1.33
3	D	6041	FAD	C10-N1	2.81	1.38	1.33
3	D	6041	FAD	C2A-N1A	2.68	1.38	1.33
3	D	6041	FAD	C2A-N3A	2.52	1.38	1.33
3	B	6021	FAD	C8A-N7A	2.48	1.36	1.31
3	D	6041	FAD	C8A-N7A	2.45	1.36	1.31
3	C	6031	FAD	C2A-N3A	2.44	1.38	1.33
3	B	6021	FAD	C2A-N1A	2.41	1.38	1.33
3	B	6021	FAD	PA-O3P	2.37	1.62	1.59
3	A	6011	FAD	C2A-N1A	2.36	1.38	1.33
3	B	6021	FAD	C2A-N3A	2.35	1.38	1.33
3	A	6011	FAD	C2A-N3A	2.31	1.38	1.33
3	A	6011	FAD	P-O3P	2.14	1.61	1.59
3	A	6011	FAD	C10-N1	2.08	1.37	1.33
3	A	6011	FAD	C8A-N7A	2.03	1.35	1.31
3	B	6021	FAD	C5A-N7A	-2.01	1.35	1.39
3	C	6031	FAD	C5A-N7A	-2.01	1.35	1.39
3	C	6031	FAD	C2A-N1A	2.00	1.37	1.33

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	6031	FAD	N3A-C2A-N1A	-7.19	117.70	128.58
3	B	6021	FAD	N3A-C2A-N1A	-6.84	118.22	128.58
3	D	6041	FAD	N3A-C2A-N1A	-6.59	118.60	128.58
3	A	6011	FAD	N3A-C2A-N1A	-5.95	119.57	128.58
3	B	6021	FAD	N9A-C8A-N7A	-4.58	107.44	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	6041	FAD	N9A-C8A-N7A	-4.46	107.61	113.94
3	D	6041	FAD	C5A-C4A-N3A	-3.93	121.31	126.72
3	D	6041	FAD	C2A-N3A-C4A	3.74	120.96	111.83
3	A	6011	FAD	N9A-C8A-N7A	-3.64	108.77	113.94
3	C	6031	FAD	N9A-C8A-N7A	-3.44	109.05	113.94
3	A	6011	FAD	C5A-C4A-N3A	-3.42	122.01	126.72
3	C	6031	FAD	C2A-N3A-C4A	3.40	120.12	111.83
3	A	6011	FAD	C5X-C9A-N10	3.37	121.02	117.97
3	B	6021	FAD	C5A-N7A-C8A	3.26	108.57	103.45
3	C	6031	FAD	C5A-C4A-N3A	-3.25	122.24	126.72
3	B	6021	FAD	C2A-N3A-C4A	3.21	119.66	111.83
3	B	6021	FAD	C5X-C9A-N10	3.13	120.80	117.97
3	D	6041	FAD	C5A-N7A-C8A	3.12	108.35	103.45
3	B	6021	FAD	C5A-C4A-N3A	-3.07	122.49	126.72
3	A	6011	FAD	C4-N3-C2	-3.02	120.28	125.64
3	D	6041	FAD	C4-N3-C2	-2.98	120.34	125.64
3	D	6041	FAD	C4X-C4-N3	2.91	120.65	113.25
3	A	6011	FAD	C2A-N3A-C4A	2.90	118.91	111.83
3	A	6011	FAD	C4X-C10-N10	2.89	120.62	116.48
3	C	6031	FAD	C5A-N7A-C8A	2.87	107.95	103.45
3	D	6041	FAD	C4A-N9A-C8A	2.81	108.68	105.74
3	D	6041	FAD	N3A-C4A-N9A	2.77	131.87	127.17
3	D	6041	FAD	C4'-C3'-C2'	-2.71	109.06	113.57
3	C	6031	FAD	C2A-N1A-C6A	2.70	123.17	118.73
3	A	6011	FAD	C5A-N7A-C8A	2.70	107.70	103.45
3	C	6031	FAD	C5X-C9A-N10	2.68	120.39	117.97
3	C	6031	FAD	C9A-C5X-N5	-2.60	119.69	122.45
4	B	6022	IPH	C4-C3-C2	-2.59	117.04	120.24
3	D	6041	FAD	O4-C4-C4X	-2.58	119.73	126.53
3	A	6011	FAD	C9A-C5X-N5	-2.56	119.73	122.45
3	C	6031	FAD	C4X-C4-N3	2.56	119.76	113.25
3	B	6021	FAD	C9A-C5X-N5	-2.56	119.74	122.45
3	C	6031	FAD	N3A-C4A-N9A	2.47	131.37	127.17
3	D	6041	FAD	C5X-C9A-N10	2.46	120.19	117.97
3	A	6011	FAD	C10-C4X-N5	-2.45	119.81	124.81
3	B	6021	FAD	C4A-N9A-C8A	2.37	108.23	105.74
3	A	6011	FAD	N3A-C4A-N9A	2.37	131.19	127.17
3	B	6021	FAD	C2A-N1A-C6A	2.32	122.53	118.73
3	D	6041	FAD	C4X-C10-N10	2.27	119.73	116.48
3	B	6021	FAD	C4X-C10-N10	2.26	119.72	116.48
3	A	6011	FAD	C4A-N9A-C8A	2.25	108.10	105.74
3	A	6011	FAD	C4X-C4-N3	2.24	118.97	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	6031	FAD	C4-N3-C2	-2.17	121.79	125.64
3	B	6021	FAD	O2P-P-O5'	2.16	117.34	107.57
4	A	6012	IPH	C4-C3-C2	-2.10	117.65	120.24
3	A	6011	FAD	C4-C4X-C10	2.09	120.51	116.93
3	A	6011	FAD	O2P-P-O3P	2.05	112.81	107.27
3	B	6021	FAD	C4'-C3'-C2'	-2.05	110.16	113.57
3	D	6041	FAD	C4X-C10-N1	-2.03	119.60	124.59
3	B	6021	FAD	C4X-C4-N3	2.03	118.42	113.25

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	6011	FAD	C5'-O5'-P-O3P
3	B	6021	FAD	C5'-O5'-P-O3P
3	C	6031	FAD	PA-O3P-P-O5'
3	D	6041	FAD	PA-O3P-P-O5'
3	A	6011	FAD	C5'-O5'-P-O1P
3	B	6021	FAD	C5'-O5'-P-O1P
3	C	6031	FAD	O2'-C2'-C3'-C4'
3	C	6031	FAD	O2'-C2'-C3'-O3'
3	C	6031	FAD	C1'-C2'-C3'-O3'
3	A	6011	FAD	O4B-C4B-C5B-O5B
3	A	6011	FAD	P-O3P-PA-O2A
3	B	6021	FAD	P-O3P-PA-O2A

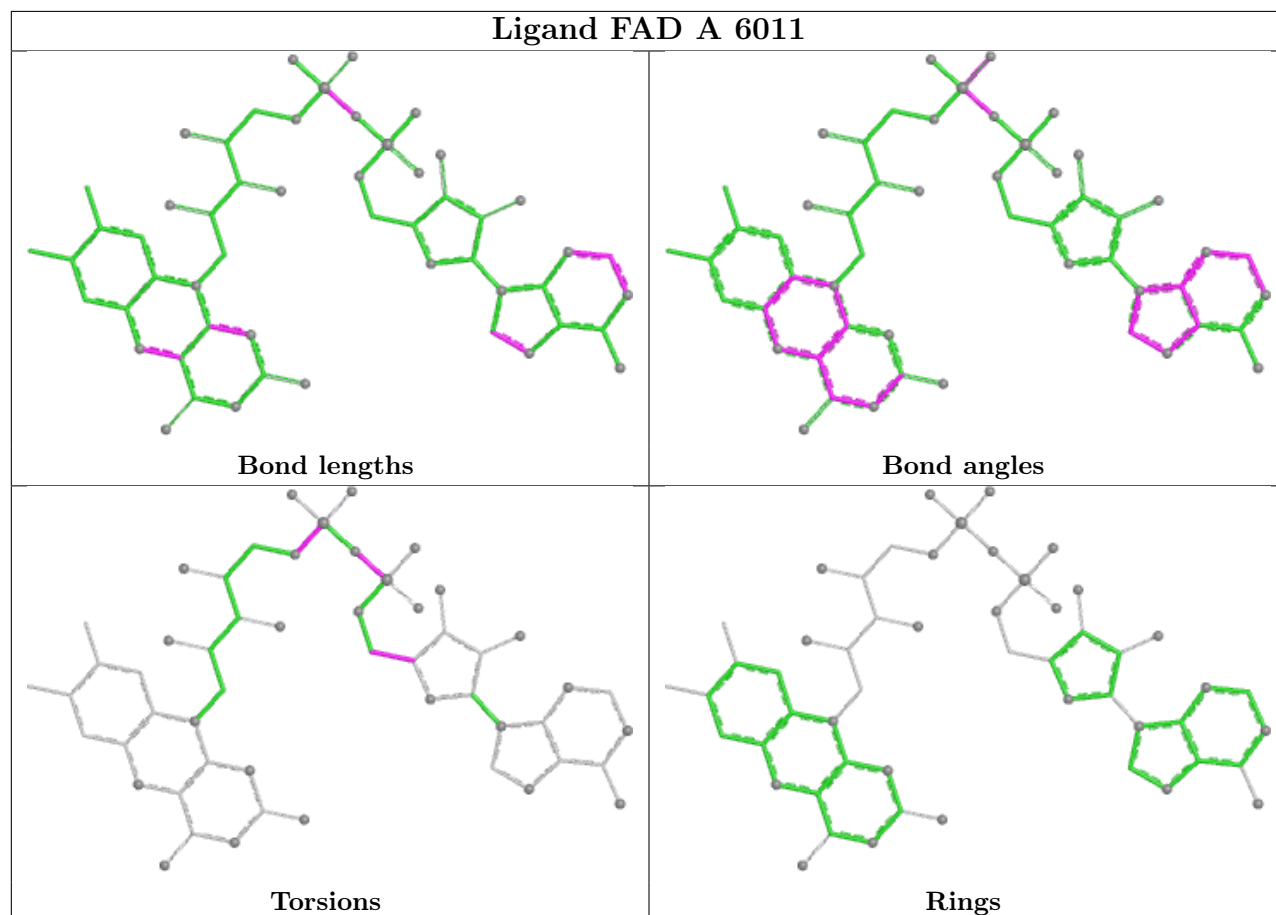
There are no ring outliers.

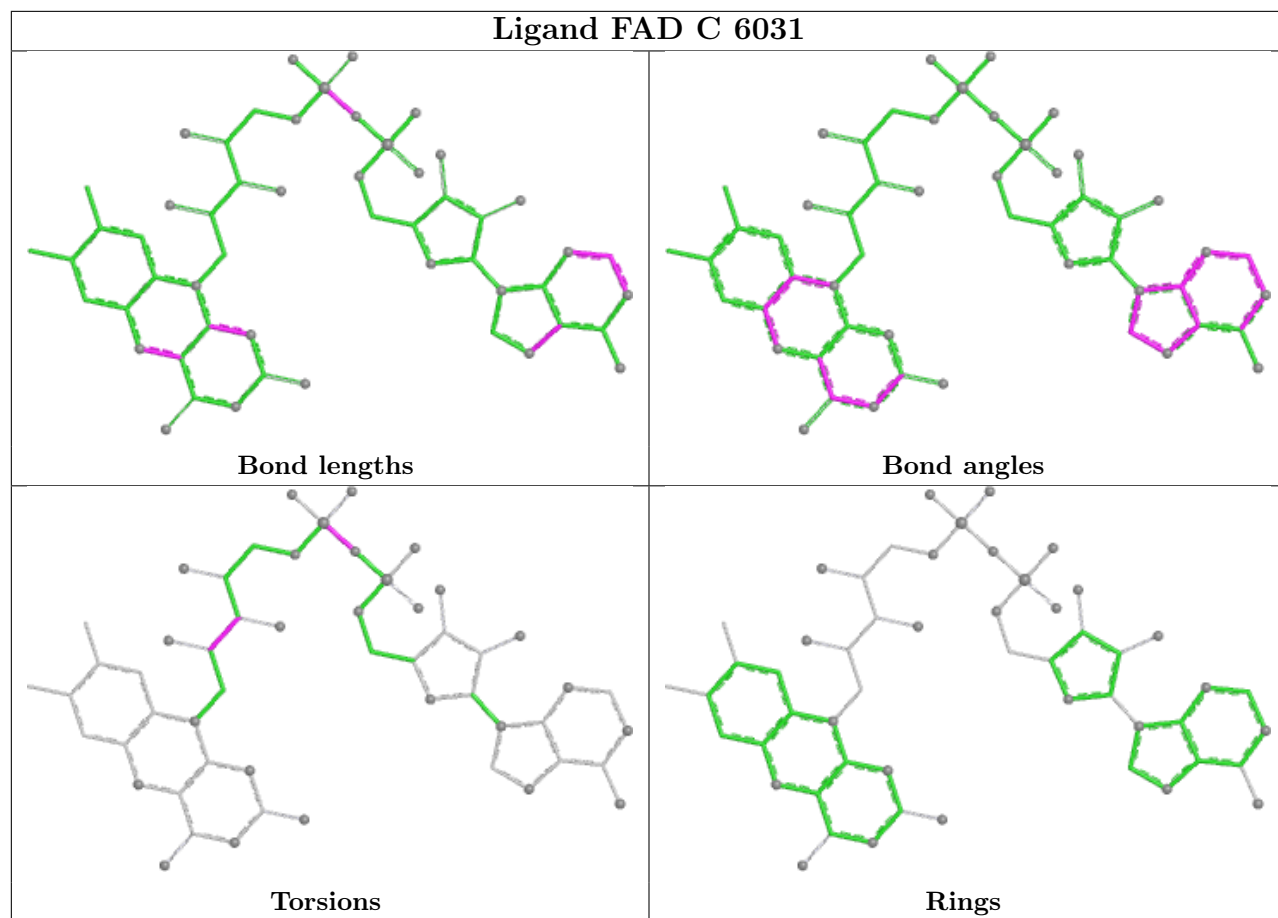
2 monomers are involved in 2 short contacts:

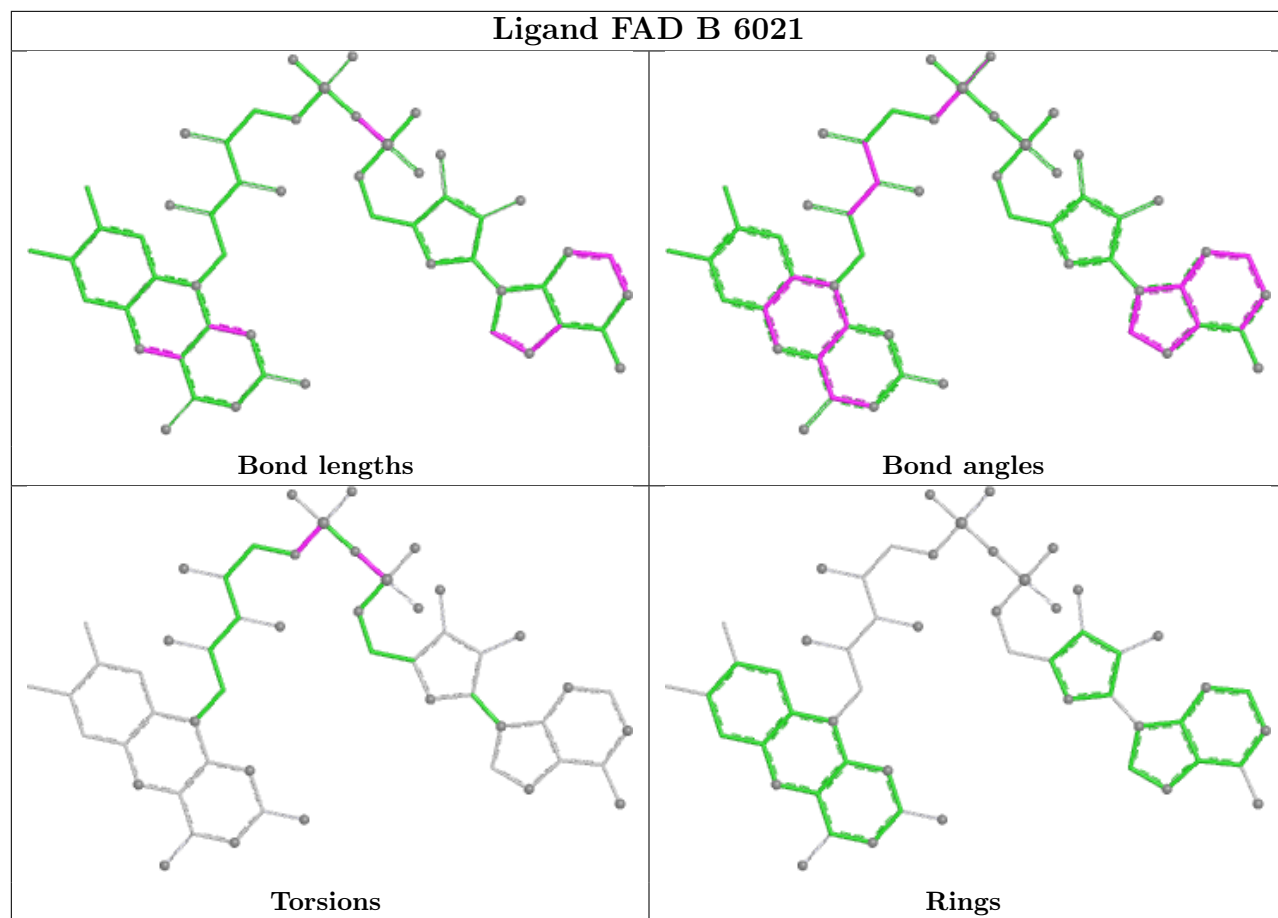
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	6031	FAD	1	0
3	D	6041	FAD	1	0

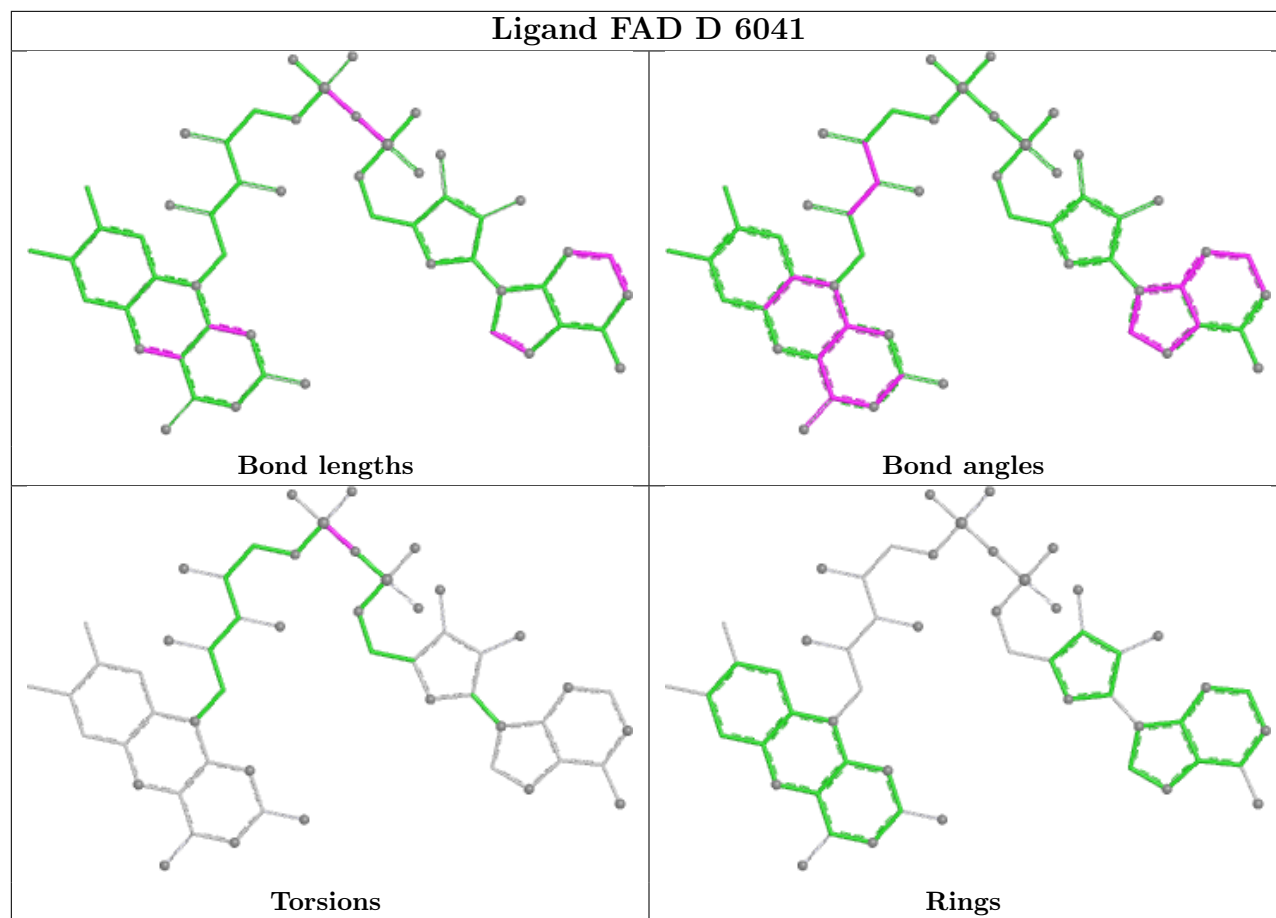
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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	650/665 (97%)	0.01	21 (3%)	50	54	3, 9, 25, 40	1 (0%)
1	B	650/665 (97%)	-0.14	11 (1%)	69	73	3, 9, 23, 40	1 (0%)
1	C	656/665 (98%)	0.11	35 (5%)	32	35	3, 9, 26, 44	1 (0%)
1	D	656/665 (98%)	-0.05	24 (3%)	45	49	3, 9, 25, 40	1 (0%)
All	All	2612/2660 (98%)	-0.02	91 (3%)	47	52	3, 9, 25, 44	4 (0%)

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	110	TYR	6.0
1	C	385	GLY	4.7
1	C	106	GLY	4.4
1	C	294	ALA	4.3
1	C	389	THR	4.3
1	A	662	SER	4.3
1	D	294	ALA	4.2
1	A	480	VAL	4.1
1	C	107	ILE	3.8
1	B	662	SER	3.8
1	C	386	LEU	3.7
1	A	506	THR	3.7
1	A	621	ASP	3.6
1	C	387	VAL	3.4
1	D	307	PHE	3.4
1	B	177	LEU	3.3
1	C	109	ARG	3.3
1	D	385	GLY	3.3
1	C	113	VAL	3.2
1	C	108	SER	3.1
1	C	388	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	392	ALA	3.1
1	C	105	PRO	3.0
1	D	382	TRP	3.0
1	B	294	ALA	3.0
1	A	623	TYR	2.9
1	C	463	LEU	2.9
1	A	481	GLY	2.9
1	C	307	PHE	2.9
1	C	111	HIS	2.9
1	D	388	LEU	2.9
1	C	103	THR	2.8
1	B	307	PHE	2.8
1	A	505	VAL	2.8
1	C	104	LEU	2.8
1	A	207	GLY	2.8
1	A	482	THR	2.8
1	B	49	TYR	2.7
1	A	622	GLY	2.7
1	D	662	SER	2.7
1	D	386	LEU	2.7
1	D	389	THR	2.7
1	C	430	VAL	2.6
1	C	390	GLY	2.6
1	C	396	ILE	2.6
1	A	307	PHE	2.6
1	A	464	VAL	2.6
1	A	521	ASP	2.5
1	C	382	TRP	2.5
1	C	662	SER	2.5
1	C	381	GLY	2.4
1	D	302	VAL	2.4
1	D	463	LEU	2.4
1	D	434	MET	2.4
1	D	381	GLY	2.4
1	C	384	LEU	2.4
1	A	484	PHE	2.4
1	D	430	VAL	2.3
1	D	315	ASN	2.3
1	C	93	HIS	2.3
1	D	110	TYR	2.3
1	B	134	THR	2.3
1	A	177	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	429	ASP	2.2
1	D	378	TYR	2.2
1	D	390	GLY	2.2
1	D	392	ALA	2.2
1	B	209	GLU	2.2
1	C	424	GLY	2.2
1	A	619	ARG	2.2
1	D	93	HIS	2.2
1	A	618	VAL	2.1
1	C	393	LYS	2.1
1	D	387	VAL	2.1
1	A	106	GLY	2.1
1	D	51	GLY	2.1
1	D	435	GLY	2.1
1	B	333	PHE	2.1
1	A	294	ALA	2.0
1	B	355	ALA	2.0
1	A	434	MET	2.0
1	C	48	VAL	2.0
1	C	114	VAL	2.0
1	C	302	VAL	2.0
1	C	351	ARG	2.0
1	C	380	LEU	2.0
1	A	465	THR	2.0
1	D	433	GLU	2.0
1	B	293	GLN	2.0
1	B	135	ARG	2.0
1	C	378	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

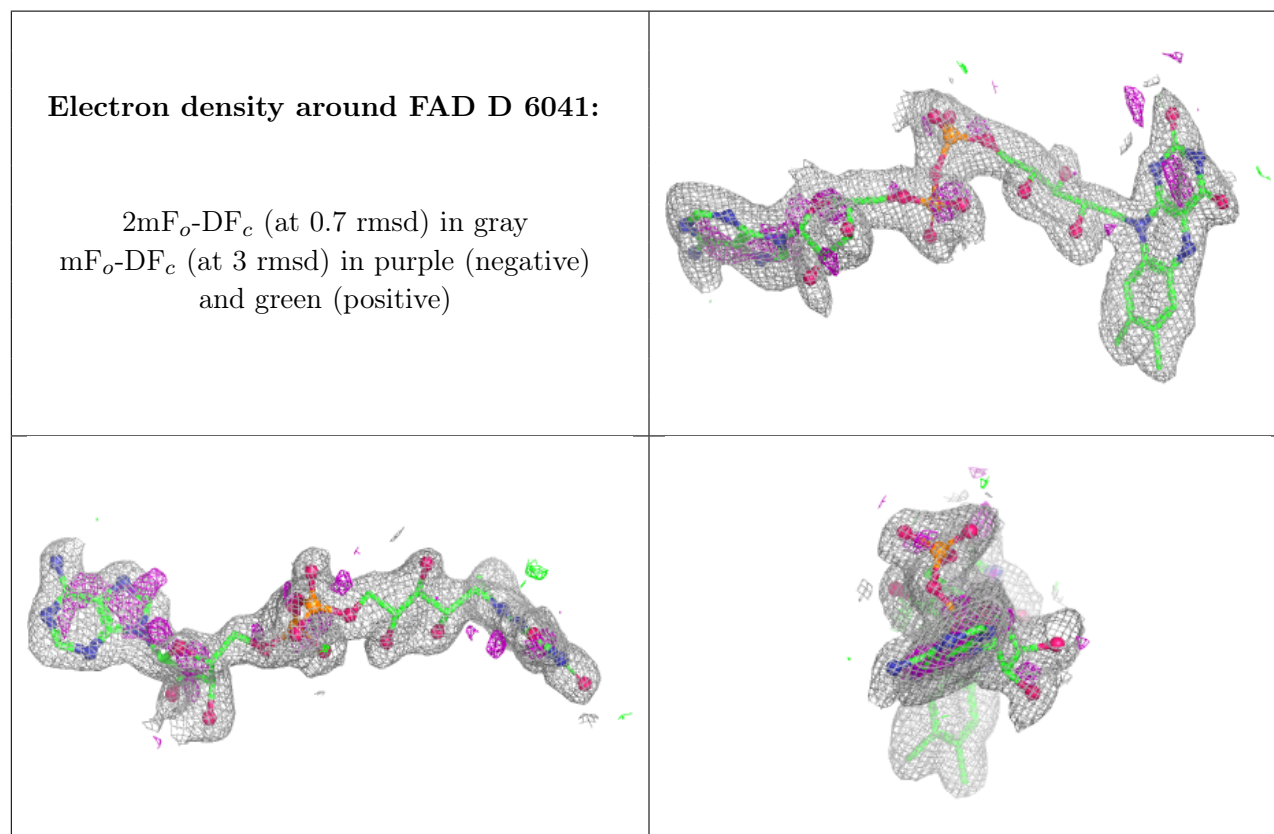
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

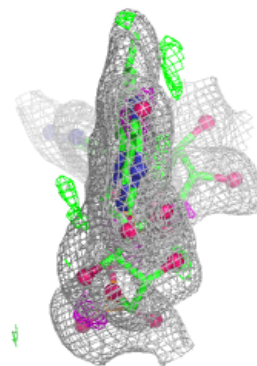
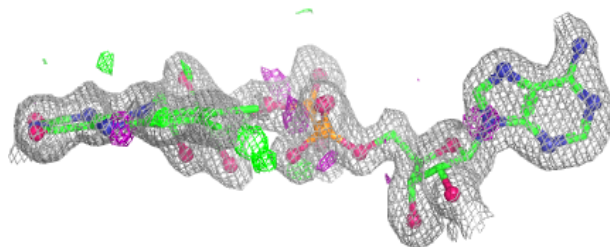
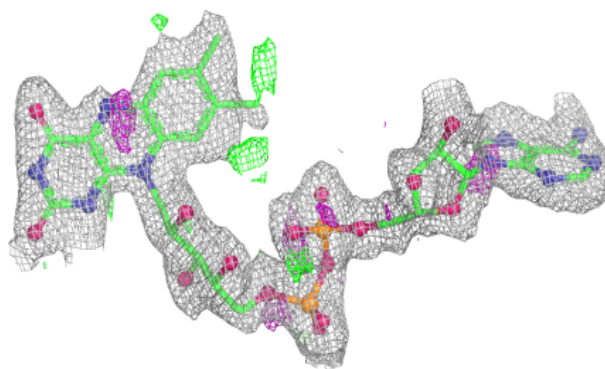
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	IPH	D	6042	7/7	0.87	0.11	29,33,35,35	0
4	IPH	A	6012	7/7	0.90	0.10	22,24,29,30	0
4	IPH	B	6022	7/7	0.92	0.11	22,27,29,30	0
3	FAD	D	6041	53/53	0.93	0.07	6,11,14,15	0
4	IPH	C	6032	7/7	0.94	0.08	23,28,31,32	0
3	FAD	B	6021	53/53	0.94	0.07	4,8,13,17	0
3	FAD	C	6031	53/53	0.95	0.06	7,11,14,15	0
2	CL	C	6003	1/1	0.96	0.10	13,13,13,13	0
3	FAD	A	6011	53/53	0.97	0.05	4,8,11,13	0
2	CL	A	6001	1/1	0.98	0.10	12,12,12,12	0
2	CL	B	6002	1/1	0.99	0.08	12,12,12,12	0
2	CL	D	6004	1/1	0.99	0.14	13,13,13,13	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.

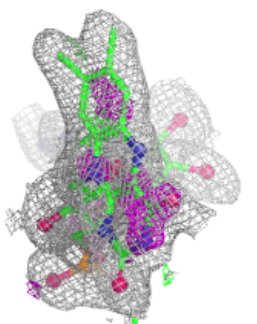
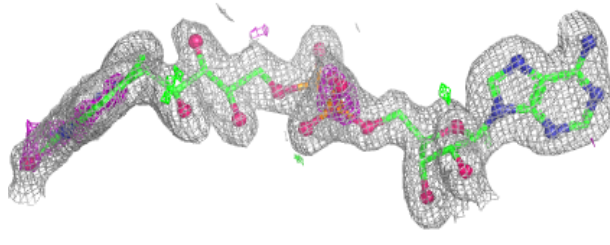
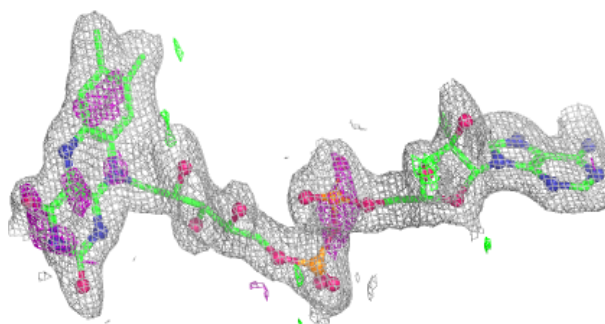


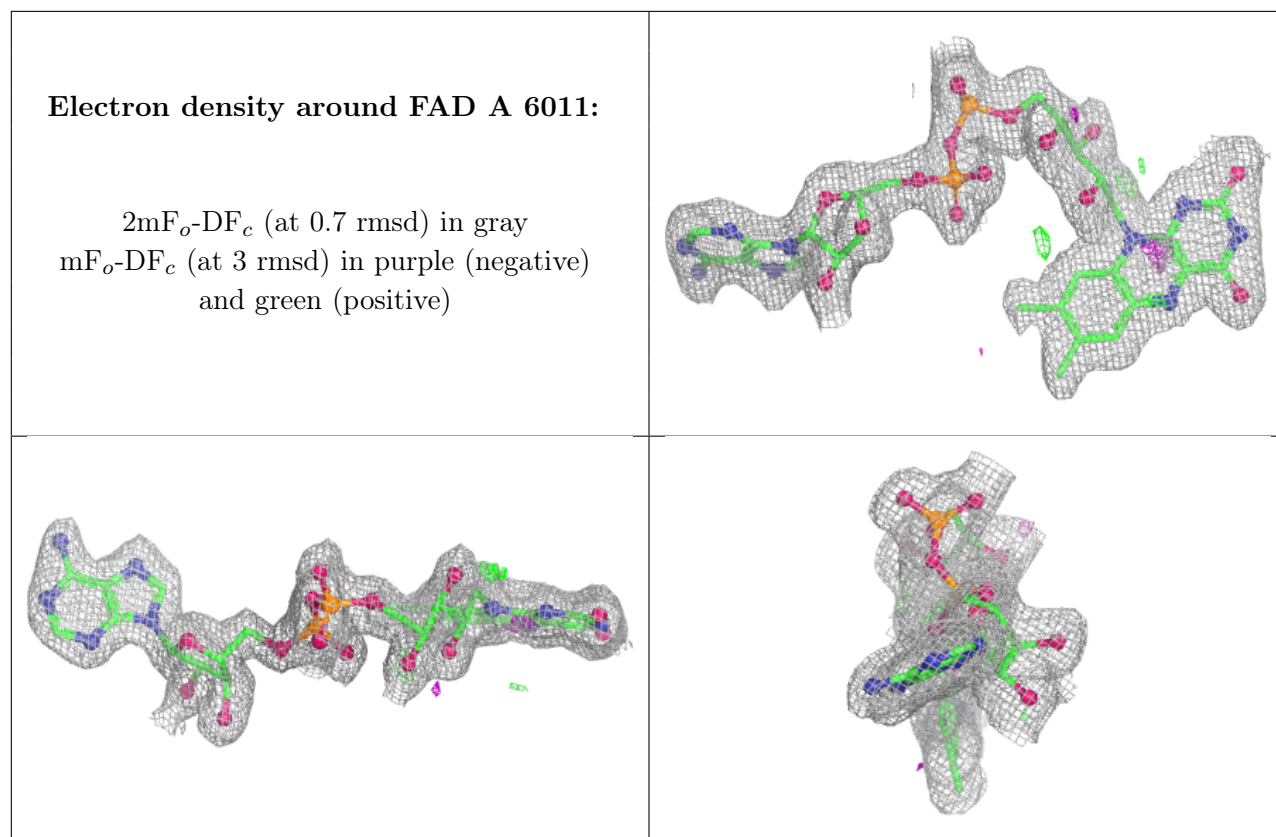
Electron density around FAD B 6021:

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

**Electron density around FAD C 6031:**

$2mF_o-DF_c$ (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.