



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 01:09 PM UTC

PDB ID : 6U0S / pdb_00006u0s
Title : Crystal structure of the flavin-dependent monooxygenase PieE in complex with FAD and substrate
Authors : Shi, R.; Manenda, M.
Deposited on : 2019-08-14
Resolution : 2.52 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

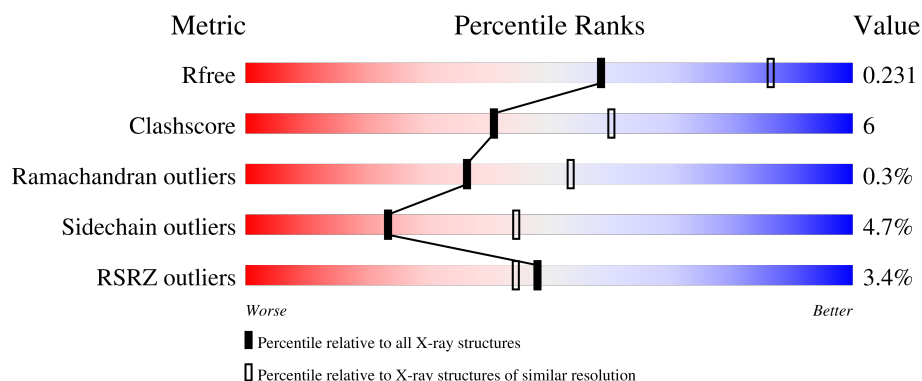
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.52 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	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (2.54-2.50)

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	601	
1	B	601	
1	C	601	
1	D	601	
1	E	601	

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Mol	Chain	Length	Quality of chain
1	F	601	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	D	603	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 27918 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 2,4-dichlorophenol 6-monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	579	Total	C	N	O	S	0	0	0
			4423	2764	828	821	10			
1	B	579	Total	C	N	O	S	0	0	0
			4423	2764	828	821	10			
1	C	580	Total	C	N	O	S	0	0	0
			4430	2768	829	823	10			
1	D	579	Total	C	N	O	S	0	0	0
			4423	2764	828	821	10			
1	E	579	Total	C	N	O	S	0	0	0
			4423	2764	828	821	10			
1	F	580	Total	C	N	O	S	0	0	0
			4427	2765	829	823	10			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP W0C4C9
A	-1	SER	-	expression tag	UNP W0C4C9
A	0	HIS	-	expression tag	UNP W0C4C9
B	-2	GLY	-	expression tag	UNP W0C4C9
B	-1	SER	-	expression tag	UNP W0C4C9
B	0	HIS	-	expression tag	UNP W0C4C9
C	-2	GLY	-	expression tag	UNP W0C4C9
C	-1	SER	-	expression tag	UNP W0C4C9
C	0	HIS	-	expression tag	UNP W0C4C9
D	-2	GLY	-	expression tag	UNP W0C4C9
D	-1	SER	-	expression tag	UNP W0C4C9
D	0	HIS	-	expression tag	UNP W0C4C9
E	-2	GLY	-	expression tag	UNP W0C4C9
E	-1	SER	-	expression tag	UNP W0C4C9
E	0	HIS	-	expression tag	UNP W0C4C9
F	-2	GLY	-	expression tag	UNP W0C4C9
F	-1	SER	-	expression tag	UNP W0C4C9

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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	HIS	-	expression tag	UNP W0C4C9

- # FAD

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

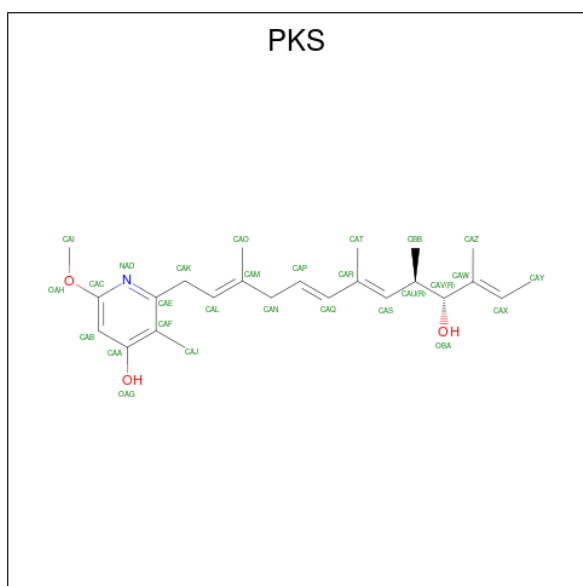
- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 3 | A | 2 | Total Cl
2 2 | 0 | 0 |
| 3 | B | 2 | Total Cl
2 2 | 0 | 0 |



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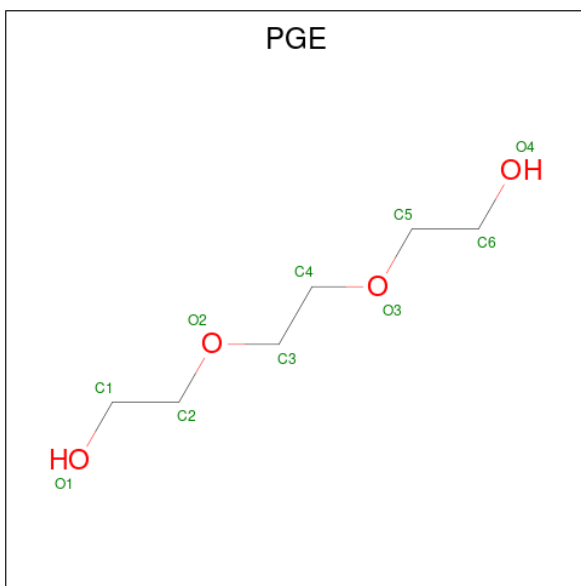
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	Cl	0	0
			1	1		
3	D	2	Total	Cl	0	0
			2	2		
3	E	2	Total	Cl	0	0
			2	2		
3	F	2	Total	Cl	0	0
			2	2		

- Molecule 4 is 2-[(2E,5E,7E,9R,10R,11E)-10-hydroxy-3,7,9,11-tetramethyltrideca-2,5,7,11-tetraen-1-yl]-6-methoxy-3-methylpyridin-4-ol (CCD ID: PKS) (formula: C₂₄H₃₅NO₃) (labeled as "Ligand of Interest" by depositor).



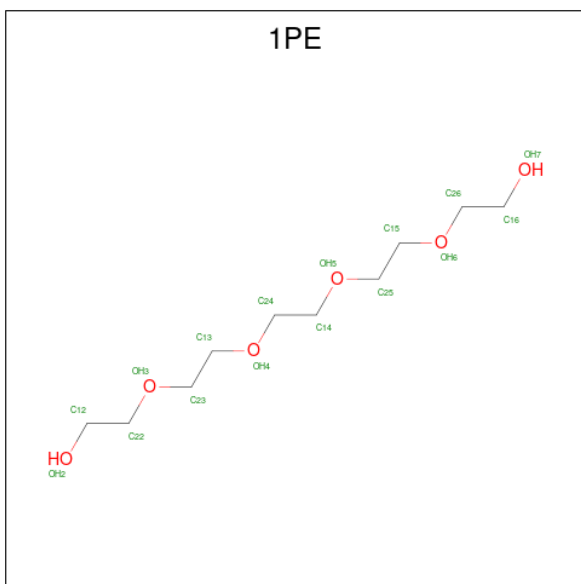
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			28	24	1	3		
4	B	1	Total	C	N	O	0	0
			28	24	1	3		
4	C	1	Total	C	N	O	0	0
			28	24	1	3		
4	D	1	Total	C	N	O	0	0
			28	24	1	3		
4	E	1	Total	C	N	O	0	0
			28	24	1	3		
4	F	1	Total	C	N	O	0	0
			28	24	1	3		

- Molecule 5 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



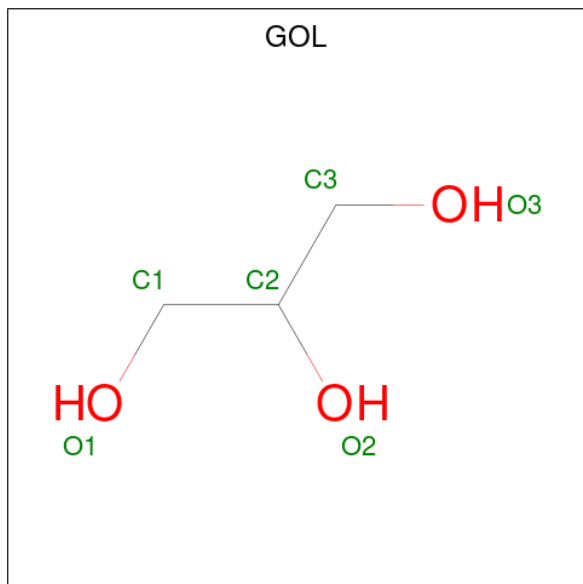
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	6	4		
5	C	1	Total	C	O	0	0
			10	6	4		
5	C	1	Total	C	O	0	0
			10	6	4		
5	E	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			16	10	6		
6	B	1	Total	C	O	0	0
			16	10	6		
6	C	1	Total	C	O	0	0
			16	10	6		
6	D	1	Total	C	O	0	0
			16	10	6		
6	E	1	Total	C	O	0	0
			16	10	6		
6	F	1	Total	C	O	0	0
			16	10	6		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	E	1	Total	C	O	0	0
			6	3	3		
7	E	1	Total	C	O	0	0
			6	3	3		

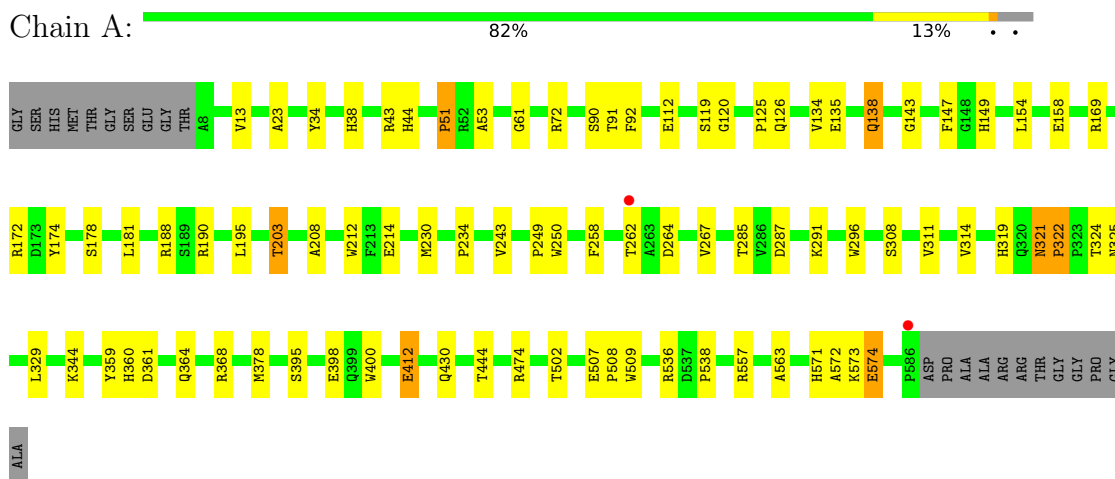
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	177	Total 177	O 177	0	0
8	B	113	Total 113	O 113	0	0
8	C	205	Total 205	O 205	0	0
8	D	88	Total 88	O 88	0	0
8	E	56	Total 56	O 56	0	0
8	F	61	Total 61	O 61	0	0

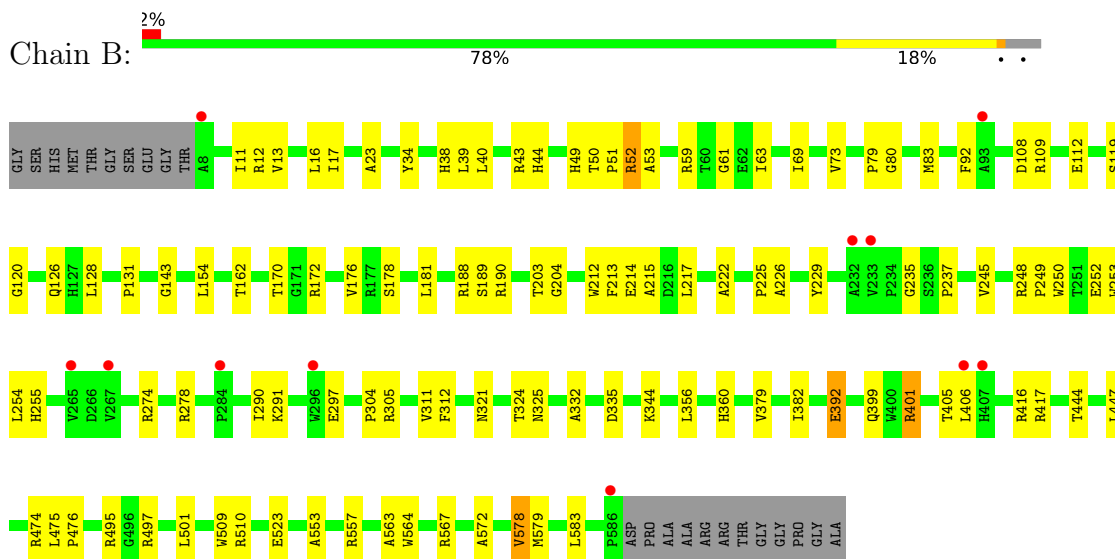
3 Residue-property plots [i](#)

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.

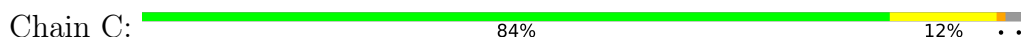
- Molecule 1: 2,4-dichlorophenol 6-monooxygenase

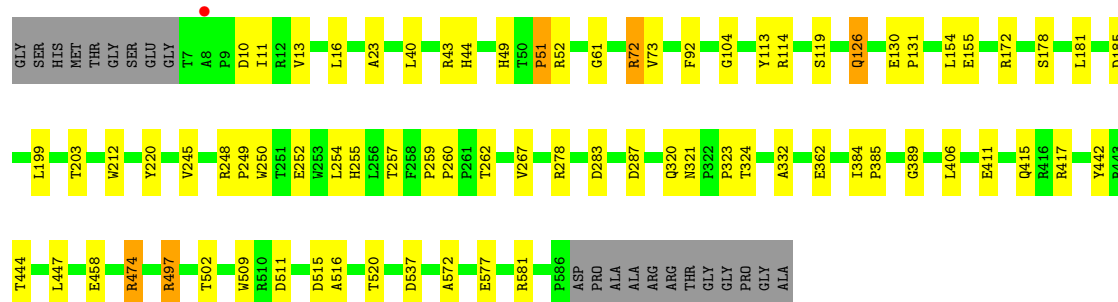


- Molecule 1: 2,4-dichlorophenol 6-monooxygenase

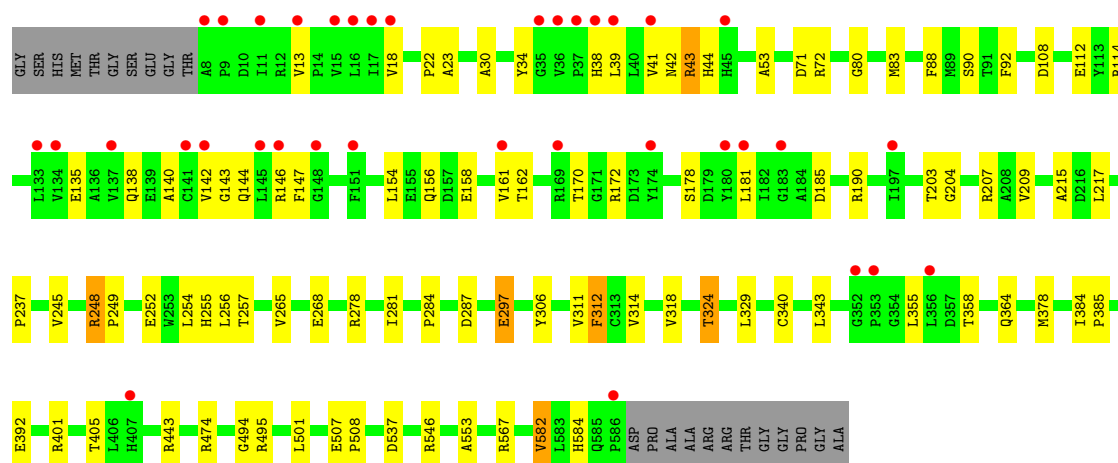
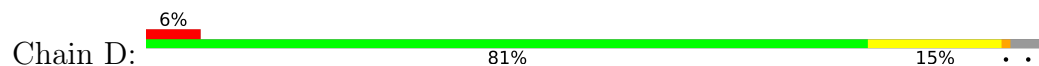


- Molecule 1: 2,4-dichlorophenol 6-monooxygenase

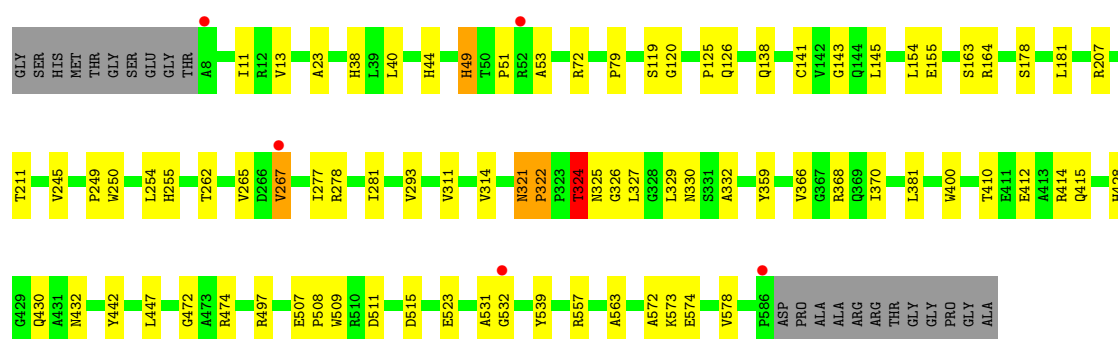
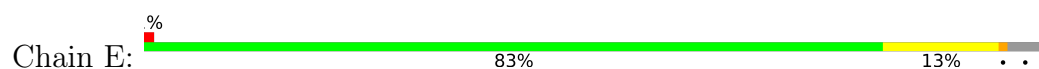




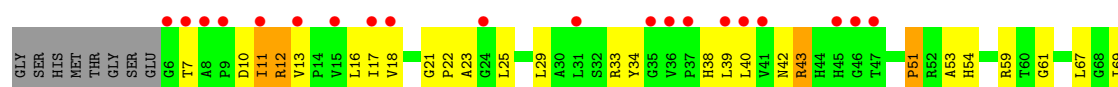
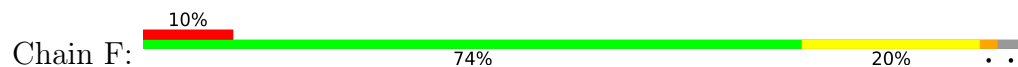
- Molecule 1: 2,4-dichlorophenol 6-monooxygenase

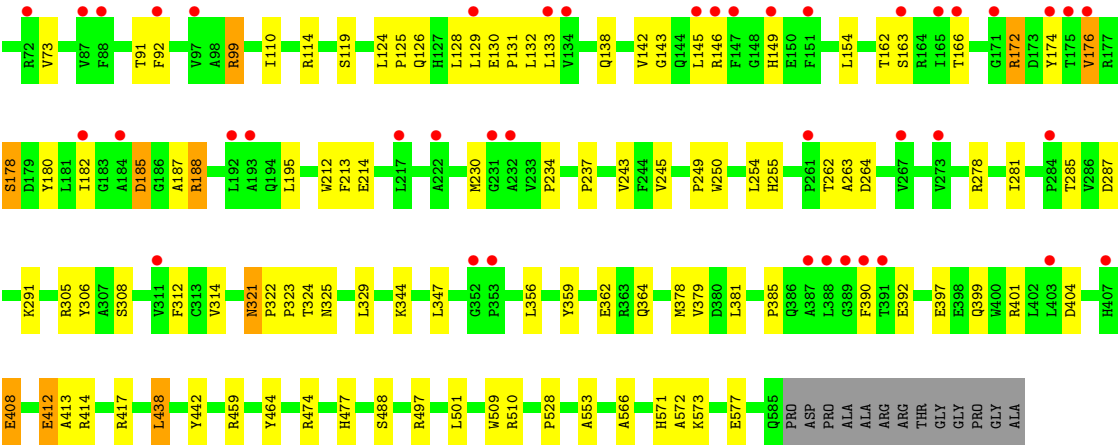


- Molecule 1: 2,4-dichlorophenol 6-monooxygenase



- Molecule 1: 2,4-dichlorophenol 6-monooxygenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	91.34Å 187.13Å 239.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.12 – 2.52 49.12 – 2.52	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.12-2.52) 100.0 (49.12-2.52)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.187 , 0.239 (Not available) , 0.231	Depositor DCC
R_{free} test set	6860 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	47.4	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	27918	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, PGE, PKS, GOL, 1PE, 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	0.60	0/4537	1.11	7/6194 (0.1%)
1	B	0.60	0/4537	1.10	3/6194 (0.0%)
1	C	0.62	0/4544	1.09	5/6204 (0.1%)
1	D	0.59	0/4537	1.10	1/6194 (0.0%)
1	E	0.57	0/4537	1.07	4/6194 (0.1%)
1	F	0.57	0/4540	1.11	2/6197 (0.0%)
All	All	0.59	0/27232	1.10	22/37177 (0.1%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	322	PRO	N-CA-CB	6.15	106.63	103.19
1	B	335	ASP	CA-CB-CG	6.10	118.70	112.60
1	E	79	PRO	CA-C-N	6.01	126.76	120.03
1	E	79	PRO	C-N-CA	6.01	126.76	120.03
1	F	185	ASP	CA-CB-CG	5.88	118.48	112.60
1	A	91	THR	CA-CB-OG1	-5.74	100.99	109.60
1	A	258	PHE	CA-CB-CG	-5.59	108.21	113.80
1	A	203	THR	CA-CB-OG1	-5.58	101.24	109.60
1	A	51	PRO	N-CA-C	5.54	121.23	113.53
1	B	79	PRO	CA-C-N	5.36	126.03	120.03
1	B	79	PRO	C-N-CA	5.36	126.03	120.03
1	C	51	PRO	N-CA-C	5.36	120.97	113.53
1	A	147	PHE	CB-CA-C	5.21	118.33	109.53
1	C	502	THR	CA-CB-OG1	-5.12	101.92	109.60
1	E	324	THR	CA-CB-OG1	-5.10	101.94	109.60
1	C	185	ASP	CA-CB-CG	5.07	117.67	112.60
1	D	537	ASP	CA-CB-CG	5.06	117.66	112.60
1	A	322	PRO	N-CA-C	-5.03	105.64	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	264	ASP	CA-CB-CG	5.02	117.62	112.60
1	E	322	PRO	N-CA-CB	5.00	105.82	103.22
1	C	515	ASP	CA-CB-CG	5.00	117.60	112.60
1	C	537	ASP	CA-CB-CG	5.00	117.60	112.60

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	4423	0	4297	47	0
1	B	4423	0	4297	63	0
1	C	4430	0	4304	40	0
1	D	4423	0	4297	66	0
1	E	4423	0	4297	42	0
1	F	4427	0	4300	86	0
2	A	53	0	31	4	0
2	B	53	0	31	4	0
2	C	53	0	31	4	0
2	D	53	0	31	14	0
2	E	53	0	31	5	0
2	F	53	0	31	8	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
3	D	2	0	0	3	0
3	E	2	0	0	0	0
3	F	2	0	0	1	0
4	A	28	0	0	1	0
4	B	28	0	0	0	0
4	C	28	0	0	0	0
4	D	28	0	0	1	0
4	E	28	0	0	0	0
4	F	28	0	0	1	0
5	A	10	0	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	20	0	28	0	0
5	E	10	0	14	0	0
6	A	16	0	22	2	0
6	B	16	0	22	2	0
6	C	16	0	22	2	0
6	D	16	0	22	0	0
6	E	16	0	22	3	0
6	F	16	0	22	0	0
7	A	12	0	16	1	0
7	D	12	0	16	1	0
7	E	12	0	16	0	0
8	A	177	0	0	5	0
8	B	113	0	0	3	0
8	C	205	0	0	4	0
8	D	88	0	0	4	0
8	E	56	0	0	2	0
8	F	61	0	0	3	0
All	All	27918	0	26214	347	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (347) 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:F:53:ALA:HB2	2:F:601:FAD:O2'	1.71	0.91
1:C:44:HIS:HD2	2:C:702:FAD:O2B	1.54	0.90
1:C:44:HIS:CD2	2:C:702:FAD:O2B	2.27	0.88
1:F:146:ARG:HD3	1:F:149:HIS:CE1	2.09	0.88
1:F:34:TYR:HB3	1:F:344:LYS:HD2	1.58	0.86
1:F:10:ASP:OD2	1:F:174:TYR:HB2	1.76	0.84
1:B:44:HIS:HD2	2:B:601:FAD:O2B	1.59	0.82
1:B:44:HIS:CD2	2:B:601:FAD:O2B	2.37	0.77
1:F:237:PRO:HB3	1:F:392:GLU:HG3	1.66	0.76
1:B:112:GLU:HG3	8:B:784:HOH:O	1.88	0.72
1:F:23:ALA:HB1	1:F:314:VAL:HG23	1.71	0.70
1:B:38:HIS:CE1	1:B:143:GLY:HA3	2.27	0.70
1:F:10:ASP:OD2	1:F:174:TYR:CB	2.40	0.70
1:D:329:LEU:HB3	2:D:602:FAD:O2	1.91	0.69
1:F:54:HIS:NE2	4:F:603:PKS:OAG	2.25	0.69
1:B:204:GLY:HA2	1:B:297:GLU:CG	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:THR:HB	8:A:702:HOH:O	1.92	0.69
1:C:114:ARG:HD3	8:C:889:HOH:O	1.92	0.69
1:D:248:ARG:HB2	1:D:252:GLU:HB3	1.75	0.68
1:B:237:PRO:HB3	1:B:392:GLU:HG2	1.75	0.67
1:F:53:ALA:HB2	2:F:601:FAD:C2'	2.25	0.67
1:A:53:ALA:HB2	2:A:601:FAD:H2'	1.77	0.67
1:F:38:HIS:CE1	1:F:143:GLY:HA3	2.30	0.67
1:F:195:LEU:HD22	1:F:308:SER:HB3	1.77	0.67
1:F:510:ARG:HH22	1:F:528:PRO:HG3	1.60	0.66
1:B:204:GLY:HA2	1:B:297:GLU:HG2	1.76	0.66
1:F:187:ALA:C	1:F:188:ARG:HG2	2.20	0.66
1:B:38:HIS:NE2	1:B:143:GLY:HA3	2.10	0.65
1:F:43:ARG:H	2:F:601:FAD:C2A	2.09	0.65
1:D:112:GLU:HG3	8:D:759:HOH:O	1.96	0.65
1:B:579:MET:O	1:B:583:LEU:HD12	1.96	0.65
1:F:91:THR:HB	1:F:281:ILE:O	1.97	0.64
1:F:408:GLU:O	1:F:417:ARG:NH2	2.31	0.64
1:D:401:ARG:O	1:D:405:THR:HG23	1.97	0.64
1:F:51:PRO:HD3	1:F:212:TRP:CE3	2.34	0.63
1:E:329:LEU:HB3	2:E:601:FAD:O2	1.98	0.63
1:F:324:THR:O	1:F:325:ASN:HB2	1.98	0.63
1:C:248:ARG:HB2	1:C:252:GLU:HB3	1.81	0.62
1:D:181:LEU:HD22	1:D:311:VAL:HG13	1.81	0.62
1:E:51:PRO:O	1:E:126:GLN:HB2	2.00	0.62
1:D:23:ALA:HB1	1:D:314:VAL:HG23	1.81	0.62
1:F:29:LEU:HD12	1:F:29:LEU:O	2.01	0.61
1:E:53:ALA:HB2	2:E:601:FAD:H2'	1.83	0.61
1:D:42:ASN:CG	2:D:602:FAD:O2B	2.44	0.61
1:D:204:GLY:HA2	1:D:297:GLU:HG2	1.82	0.60
1:C:73:VAL:HG12	6:C:705:1PE:H162	1.81	0.60
1:E:120:GLY:H	6:E:605:1PE:H141	1.65	0.60
1:B:245:VAL:HB	1:B:254:LEU:HB2	1.83	0.60
1:B:109:ARG:HD3	8:B:749:HOH:O	2.01	0.60
1:A:149:HIS:ND1	1:A:174:TYR:OH	2.28	0.60
1:F:125:PRO:HD2	1:F:128:LEU:HD12	1.82	0.59
1:E:245:VAL:HB	1:E:254:LEU:HB2	1.84	0.59
1:F:11:ILE:HD12	1:F:176:VAL:HG22	1.84	0.59
1:A:509:TRP:CZ3	1:A:572:ALA:HA	2.38	0.59
1:D:38:HIS:CE1	1:D:143:GLY:HA3	2.38	0.59
1:A:51:PRO:HB3	1:A:125:PRO:HB3	1.83	0.59
1:C:23:ALA:HB2	1:C:332:ALA:HB1	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:VAL:O	1:A:178:SER:HA	2.03	0.59
1:B:53:ALA:HB2	2:B:601:FAD:H2'	1.85	0.58
1:B:405:THR:O	1:B:416:ARG:NH2	2.37	0.58
1:B:61:GLY:HA3	1:B:119:SER:OG	2.04	0.58
1:F:34:TYR:HB3	1:F:344:LYS:CD	2.33	0.58
1:B:120:GLY:H	6:B:604:1PE:C15	2.17	0.58
1:F:321:ASN:HB2	1:F:322:PRO:HD2	1.86	0.58
1:A:169:ARG:HD2	1:E:400:TRP:CE2	2.39	0.57
1:C:72:ARG:HD2	8:C:959:HOH:O	2.03	0.57
1:D:42:ASN:ND2	1:D:147:PHE:CE2	2.73	0.57
1:D:237:PRO:HB3	1:D:392:GLU:HG2	1.86	0.57
1:E:277:ILE:O	1:E:281:ILE:HG13	2.04	0.57
1:A:72:ARG:NH1	1:A:135:GLU:OE1	2.38	0.57
1:B:406:LEU:O	1:B:417:ARG:NH1	2.38	0.57
1:C:73:VAL:CG1	6:C:705:1PE:H162	2.35	0.57
1:D:53:ALA:HB2	2:D:602:FAD:H2'	1.87	0.57
1:F:477:HIS:ND1	1:F:488:SER:OG	2.30	0.57
1:A:23:ALA:HB1	1:A:314:VAL:HG23	1.85	0.56
1:F:33:ARG:NE	1:F:67:LEU:O	2.38	0.56
1:F:230:MET:HG2	1:F:243:VAL:HG22	1.88	0.56
1:A:34:TYR:HB3	1:A:344:LYS:HD2	1.88	0.55
1:F:566:ALA:HB1	1:F:571:HIS:HB2	1.88	0.55
1:B:51:PRO:O	1:B:126:GLN:HB2	2.06	0.55
1:F:145:LEU:HB2	8:F:721:HOH:O	2.06	0.55
1:C:497:ARG:HD2	8:C:911:HOH:O	2.06	0.55
7:A:608:GOL:H12	1:B:108:ASP:HA	1.88	0.55
1:C:52:ARG:HH21	1:C:126:GLN:HE22	1.53	0.55
1:D:443:ARG:HG3	1:D:443:ARG:HH11	1.72	0.54
1:F:43:ARG:N	2:F:601:FAD:C2A	2.70	0.54
1:A:53:ALA:HB2	2:A:601:FAD:C2'	2.37	0.54
1:D:53:ALA:HB2	2:D:602:FAD:C2'	2.38	0.54
1:D:158:GLU:HG2	1:D:158:GLU:O	2.08	0.54
1:D:567:ARG:HH21	1:D:567:ARG:HG3	1.71	0.54
1:F:61:GLY:HA3	1:F:119:SER:OG	2.07	0.54
1:F:412:GLU:HG3	1:F:413:ALA:N	2.21	0.54
1:F:17:ILE:O	1:F:40:LEU:HA	2.08	0.54
1:D:13:VAL:O	1:D:178:SER:HA	2.07	0.54
1:C:52:ARG:NH2	1:C:126:GLN:HE22	2.06	0.53
1:E:154:LEU:C	1:E:154:LEU:HD12	2.34	0.53
1:A:134:VAL:O	1:A:138:GLN:HG2	2.08	0.53
1:F:362:GLU:HG2	1:F:442:TYR:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:ARG:HG3	1:A:169:ARG:HH21	1.74	0.53
1:F:234:PRO:HA	1:F:399:GLN:OE1	2.09	0.53
1:D:245:VAL:HB	1:D:254:LEU:HB2	1.90	0.52
1:E:13:VAL:O	1:E:178:SER:HA	2.08	0.52
1:E:181:LEU:C	1:E:181:LEU:HD23	2.34	0.52
1:D:42:ASN:C	1:D:42:ASN:OD1	2.52	0.52
1:D:324:THR:HG23	4:D:604:PKS:CAL	2.40	0.52
1:D:42:ASN:ND2	2:D:602:FAD:O2B	2.43	0.52
1:F:230:MET:SD	1:F:381:LEU:HD22	2.49	0.52
1:D:204:GLY:CA	1:D:297:GLU:HG2	2.39	0.52
1:E:507:GLU:N	1:E:508:PRO:CD	2.73	0.52
1:F:12:ARG:HD3	1:F:12:ARG:C	2.35	0.52
1:F:397:GLU:O	1:F:401:ARG:HG3	2.10	0.52
1:D:80:GLY:HA2	1:D:83:MET:HE2	1.92	0.51
1:A:181:LEU:C	1:A:181:LEU:HD23	2.35	0.51
1:E:329:LEU:HB3	2:E:601:FAD:C2	2.40	0.51
1:E:324:THR:O	1:E:325:ASN:HB2	2.10	0.51
1:F:42:ASN:OD1	2:F:601:FAD:H1B	2.10	0.51
1:A:329:LEU:HB3	2:A:601:FAD:O2	2.10	0.51
1:A:230:MET:HG2	1:A:243:VAL:HG22	1.91	0.51
1:B:222:ALA:O	1:B:225:PRO:HD3	2.11	0.51
1:C:255:HIS:CE1	1:C:257:THR:HG23	2.45	0.51
1:D:43:ARG:HD2	2:D:602:FAD:C5A	2.41	0.51
1:A:319:HIS:CE1	8:A:793:HOH:O	2.64	0.51
1:A:195:LEU:HD22	1:A:308:SER:HB3	1.93	0.51
1:A:507:GLU:N	1:A:508:PRO:CD	2.74	0.51
1:D:41:VAL:HA	1:D:146:ARG:O	2.10	0.51
1:F:385:PRO:O	1:F:390:PHE:HB2	2.11	0.51
1:B:235:GLY:N	1:B:399:GLN:OE1	2.30	0.51
1:A:212:TRP:CE2	1:A:291:LYS:HE3	2.46	0.50
1:C:411:GLU:OE1	1:C:415:GLN:NE2	2.44	0.50
1:E:120:GLY:N	6:E:605:1PE:H141	2.26	0.50
1:F:306:TYR:CE1	1:F:364:GLN:HG2	2.46	0.50
1:C:199:LEU:HD13	1:C:320:GLN:HE22	1.77	0.50
1:D:88:PHE:CE1	1:D:384:ILE:HG13	2.46	0.50
1:E:557:ARG:HG3	1:E:563:ALA:HB2	1.94	0.50
1:D:108:ASP:HA	7:D:607:GOL:H12	1.93	0.49
1:B:475:LEU:HD12	1:B:476:PRO:HD2	1.92	0.49
1:C:199:LEU:CD1	1:C:320:GLN:HE22	2.25	0.49
1:F:245:VAL:HB	1:F:254:LEU:HB2	1.94	0.49
1:A:571:HIS:O	1:A:574:GLU:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:355:LEU:O	1:D:358:THR:OG1	2.22	0.49
1:E:574:GLU:O	1:E:578:VAL:HG23	2.12	0.49
1:A:321:ASN:HB2	1:A:322:PRO:HD2	1.95	0.49
1:E:381:LEU:HD21	1:E:430:GLN:HE22	1.77	0.49
1:A:557:ARG:HG3	1:A:563:ALA:HB2	1.95	0.49
1:D:114:ARG:HD3	8:D:763:HOH:O	2.12	0.49
1:E:38:HIS:CE1	1:E:143:GLY:HA3	2.48	0.49
1:F:17:ILE:HG12	1:F:182:ILE:HD12	1.93	0.49
1:E:321:ASN:HB2	1:E:322:PRO:HD2	1.95	0.49
1:B:43:ARG:HG2	1:B:44:HIS:CD2	2.48	0.49
1:B:34:TYR:HB3	1:B:344:LYS:CD	2.42	0.48
1:D:255:HIS:HE1	1:D:257:THR:HG23	1.78	0.48
1:E:11:ILE:HD11	8:E:756:HOH:O	2.13	0.48
1:E:23:ALA:HB2	1:E:332:ALA:HB1	1.95	0.48
1:E:539:TYR:CZ	1:F:99:ARG:HD3	2.48	0.48
1:F:129:LEU:O	1:F:130:GLU:C	2.56	0.48
1:E:51:PRO:HB3	1:E:125:PRO:HB3	1.94	0.48
1:F:16:LEU:HD12	1:F:39:LEU:O	2.14	0.48
1:B:509:TRP:CZ3	1:B:572:ALA:HA	2.49	0.48
1:D:237:PRO:HB3	1:D:392:GLU:CG	2.43	0.48
1:F:11:ILE:HB	1:F:176:VAL:HG13	1.95	0.48
1:D:71:ASP:HB2	8:D:752:HOH:O	2.14	0.48
1:E:49:HIS:CD2	1:E:49:HIS:H	2.31	0.48
1:E:366:VAL:O	1:E:370:ILE:HG23	2.13	0.48
1:B:324:THR:O	1:B:325:ASN:HB2	2.13	0.47
1:B:564:TRP:CE2	1:B:578:VAL:HG21	2.48	0.47
1:F:312:PHE:CZ	1:F:356:LEU:HB3	2.49	0.47
1:F:314:VAL:HG12	1:F:359:TYR:OH	2.14	0.47
1:A:38:HIS:CE1	1:A:143:GLY:HA3	2.49	0.47
1:D:494:GLY:O	1:D:495:ARG:HB2	2.14	0.47
1:C:154:LEU:C	1:C:154:LEU:HD12	2.40	0.47
1:C:384:ILE:HB	1:C:385:PRO:CD	2.45	0.47
1:D:546:ARG:NH1	8:D:701:HOH:O	2.29	0.47
2:D:602:FAD:H1'2	3:D:603:CL:CL	2.52	0.47
1:B:49:HIS:HD2	1:B:50:THR:HG23	1.79	0.47
1:C:10:ASP:O	1:C:11:ILE:HG13	2.15	0.47
1:A:378:MET:HG3	4:A:603:PKS:CAQ	2.45	0.47
1:F:214:GLU:HG3	1:F:291:LYS:HD2	1.97	0.47
1:D:329:LEU:HB3	2:D:602:FAD:C2	2.45	0.47
1:D:312:PHE:CE1	1:D:343:LEU:HD21	2.50	0.46
1:C:509:TRP:CZ3	1:C:572:ALA:HA	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:LEU:HD12	1:B:39:LEU:O	2.16	0.46
1:B:305:ARG:HA	1:B:360:HIS:CE1	2.50	0.46
1:A:154:LEU:C	1:A:154:LEU:HD12	2.40	0.46
1:C:249:PRO:HA	1:C:250:TRP:HA	1.77	0.46
1:F:51:PRO:O	1:F:126:GLN:HB2	2.15	0.46
1:F:187:ALA:C	1:F:188:ARG:CG	2.87	0.46
1:A:61:GLY:HA3	1:A:119:SER:OG	2.15	0.46
1:D:39:LEU:HD12	1:D:144:GLN:HB3	1.96	0.46
1:D:255:HIS:CE1	1:D:257:THR:HG23	2.50	0.46
1:F:124:LEU:HD23	1:F:129:LEU:HD13	1.97	0.46
1:C:51:PRO:HD3	1:C:212:TRP:CE3	2.51	0.46
1:B:51:PRO:HD3	1:B:212:TRP:CE3	2.51	0.46
1:D:140:ALA:O	1:D:142:VAL:HG23	2.15	0.46
1:F:509:TRP:CZ3	1:F:572:ALA:HA	2.51	0.46
1:C:40:LEU:HD23	1:C:40:LEU:C	2.41	0.45
1:D:507:GLU:N	1:D:508:PRO:CD	2.79	0.45
1:B:40:LEU:C	1:B:40:LEU:HD23	2.40	0.45
1:D:209:VAL:O	1:D:256:LEU:HA	2.16	0.45
1:E:211:THR:HG23	1:E:293:VAL:HG22	1.98	0.45
1:F:129:LEU:O	1:F:132:LEU:N	2.48	0.45
1:B:501:LEU:O	1:B:553:ALA:HA	2.16	0.45
1:E:255:HIS:CG	1:E:277:ILE:HG12	2.51	0.45
1:B:226:ALA:HB3	1:B:229:TYR:CZ	2.52	0.45
1:D:43:ARG:HD2	2:D:602:FAD:N7A	2.32	0.45
1:D:278:ARG:NH2	1:D:284:PRO:O	2.49	0.45
1:E:40:LEU:HB3	1:E:145:LEU:HD23	1.99	0.45
1:B:80:GLY:HA2	1:B:83:MET:HE2	1.97	0.45
1:F:172:ARG:O	1:F:172:ARG:HG3	2.16	0.45
1:B:217:LEU:HD12	1:B:253:TRP:CE2	2.51	0.45
1:D:42:ASN:OD1	1:D:44:HIS:N	2.50	0.45
1:E:314:VAL:HG12	1:E:359:TYR:OH	2.16	0.45
1:D:582:VAL:C	1:D:584:HIS:H	2.25	0.45
1:F:130:GLU:HB2	1:F:131:PRO:HD3	1.98	0.45
1:F:323:PRO:HA	3:F:602:CL:CL	2.53	0.45
1:C:61:GLY:HA3	1:C:119:SER:OG	2.17	0.45
1:C:516:ALA:O	1:C:520:THR:HG23	2.17	0.45
1:D:43:ARG:HB3	2:D:602:FAD:C4A	2.46	0.45
1:C:362:GLU:HG2	1:C:442:TYR:HB3	1.99	0.45
1:F:249:PRO:HB3	1:F:250:TRP:CD2	2.52	0.45
1:A:51:PRO:O	1:A:126:GLN:HB2	2.17	0.44
1:A:208:ALA:HB3	1:A:296:TRP:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:605:1PE:H141	6:A:605:1PE:H132	1.78	0.44
1:B:495:ARG:HG3	8:B:789:HOH:O	2.17	0.44
2:D:602:FAD:C10	3:D:603:CL:CL	3.02	0.44
1:F:43:ARG:HB3	2:F:601:FAD:C4A	2.46	0.44
1:E:410:THR:O	1:E:414:ARG:HG3	2.16	0.44
1:F:29:LEU:HD12	1:F:29:LEU:C	2.42	0.44
1:F:459:ARG:HB3	1:F:464:TYR:CD2	2.52	0.44
1:E:44:HIS:CD2	2:E:601:FAD:O2B	2.71	0.44
1:F:497:ARG:HH11	1:F:497:ARG:HG2	1.83	0.44
1:B:213:PHE:HE1	1:B:255:HIS:HB2	1.82	0.44
1:A:112:GLU:HG3	8:A:813:HOH:O	2.18	0.44
1:F:13:VAL:O	1:F:178:SER:HA	2.18	0.44
1:F:21:GLY:O	1:F:22:PRO:C	2.60	0.44
1:F:42:ASN:ND2	8:F:703:HOH:O	2.50	0.44
1:A:314:VAL:HG12	1:A:359:TYR:OH	2.18	0.44
1:A:325:ASN:ND2	1:A:430:GLN:HA	2.32	0.44
1:A:361:ASP:HB3	1:A:444:THR:HG23	2.00	0.44
1:A:249:PRO:HA	1:A:250:TRP:HA	1.80	0.43
1:B:38:HIS:CD2	1:B:143:GLY:HA3	2.53	0.43
1:B:249:PRO:HA	1:B:250:TRP:HA	1.63	0.43
1:B:312:PHE:CZ	1:B:356:LEU:HB3	2.52	0.43
1:E:329:LEU:N	2:E:601:FAD:O2	2.50	0.43
1:A:395:SER:OG	1:A:398:GLU:HG3	2.18	0.43
1:B:69:ILE:O	1:B:73:VAL:HG23	2.18	0.43
1:B:214:GLU:HG3	1:B:291:LYS:HD2	2.00	0.43
1:E:442:TYR:O	1:E:472:GLY:HA3	2.18	0.43
1:B:557:ARG:HG3	1:B:563:ALA:HB2	2.01	0.43
1:E:509:TRP:CZ3	1:E:572:ALA:HA	2.53	0.43
1:F:59:ARG:HB2	1:F:438:LEU:HD12	2.00	0.43
1:A:44:HIS:CD2	2:A:601:FAD:O2B	2.72	0.43
1:A:319:HIS:HE1	8:A:793:HOH:O	1.98	0.43
1:B:248:ARG:HB3	1:B:252:GLU:HB3	2.01	0.43
1:B:212:TRP:CE2	1:B:291:LYS:HE3	2.53	0.43
1:D:156:GLN:HB3	1:D:161:VAL:HG22	2.00	0.43
1:F:212:TRP:CZ2	1:F:291:LYS:HE3	2.53	0.43
1:B:120:GLY:H	6:B:604:1PE:H151	1.82	0.43
1:C:259:PRO:HA	1:C:260:PRO:HD3	1.93	0.43
1:F:110:ILE:O	1:F:114:ARG:HG2	2.18	0.43
1:B:128:LEU:O	1:B:131:PRO:HD2	2.19	0.43
1:A:360:HIS:CE1	1:A:364:GLN:HG3	2.54	0.43
1:D:384:ILE:HB	1:D:385:PRO:CD	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:567:ARG:HG3	1:D:567:ARG:NH2	2.33	0.43
1:E:428:HIS:CD2	1:E:432:ASN:HD22	2.36	0.43
1:C:406:LEU:O	1:C:417:ARG:HD3	2.19	0.43
1:F:378:MET:HE2	1:F:378:MET:HB3	1.91	0.43
1:B:34:TYR:HB3	1:B:344:LYS:HD3	2.00	0.42
1:B:181:LEU:HD22	1:B:311:VAL:HG13	2.01	0.42
1:D:170:THR:HB	1:D:172:ARG:HG2	2.00	0.42
1:E:428:HIS:HD2	1:E:432:ASN:HD22	1.67	0.42
1:D:378:MET:HE2	1:D:378:MET:HB3	1.89	0.42
1:A:249:PRO:HB3	1:A:250:TRP:CE2	2.54	0.42
1:D:154:LEU:HA	1:D:162:THR:O	2.19	0.42
1:D:443:ARG:HG3	1:D:443:ARG:NH1	2.34	0.42
1:E:120:GLY:H	6:E:605:1PE:C15	2.32	0.42
1:F:25:LEU:HB3	1:F:133:LEU:HB3	2.01	0.42
1:F:51:PRO:CD	1:F:212:TRP:CE3	3.02	0.42
1:F:154:LEU:HA	1:F:162:THR:O	2.20	0.42
1:F:187:ALA:O	1:F:188:ARG:CG	2.68	0.42
1:B:11:ILE:HB	1:B:176:VAL:HG22	2.01	0.42
1:B:170:THR:OG1	1:B:172:ARG:HB2	2.19	0.42
1:C:577:GLU:O	1:C:581:ARG:HG2	2.19	0.42
1:D:53:ALA:HB2	2:D:602:FAD:O2'	2.18	0.42
1:A:234:PRO:HG2	1:A:400:TRP:CE2	2.53	0.42
1:C:245:VAL:HB	1:C:254:LEU:HB2	2.01	0.42
1:E:249:PRO:HA	1:E:250:TRP:HA	1.75	0.42
1:E:326:GLY:O	1:E:330:ASN:ND2	2.51	0.42
1:B:59:ARG:O	1:B:63:ILE:HG13	2.19	0.42
1:A:120:GLY:N	6:A:605:1PE:H241	2.35	0.42
1:A:285:THR:HG21	1:C:49:HIS:CB	2.49	0.42
1:B:23:ALA:HB2	1:B:332:ALA:HB1	2.01	0.42
1:B:34:TYR:HB3	1:B:344:LYS:HD2	2.02	0.42
1:B:52:ARG:HG3	2:B:601:FAD:C8M	2.50	0.42
1:C:323:PRO:HB3	2:C:702:FAD:C2	2.50	0.42
2:D:602:FAD:N10	3:D:603:CL:CL	2.90	0.42
1:D:42:ASN:OD1	1:D:43:ARG:N	2.52	0.42
1:E:181:LEU:HD22	1:E:311:VAL:HG13	2.01	0.42
2:C:702:FAD:H9	2:C:702:FAD:H1'1	1.94	0.41
1:D:39:LEU:CD1	1:D:144:GLN:HB3	2.50	0.41
1:D:207:ARG:NH2	1:D:265:VAL:HG12	2.34	0.41
1:D:501:LEU:O	1:D:553:ALA:HA	2.20	0.41
1:C:474:ARG:HB3	1:C:474:ARG:HH21	1.84	0.41
1:E:325:ASN:HB3	1:E:327:LEU:HG	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:22:PRO:O	1:F:23:ALA:C	2.63	0.41
1:F:149:HIS:HA	1:F:166:THR:O	2.19	0.41
1:C:389:GLY:HA2	8:C:816:HOH:O	2.20	0.41
1:F:10:ASP:C	1:F:11:ILE:HG13	2.45	0.41
1:F:180:TYR:HE2	1:F:347:LEU:HD23	1.85	0.41
1:F:214:GLU:CG	1:F:291:LYS:HD2	2.50	0.41
1:B:217:LEU:HD12	1:B:253:TRP:NE1	2.36	0.41
1:B:401:ARG:HD2	1:B:401:ARG:HA	1.90	0.41
1:F:329:LEU:HB3	2:F:601:FAD:O2	2.20	0.41
1:A:364:GLN:OE1	1:A:368:ARG:NH1	2.54	0.41
1:A:536:ARG:O	1:A:538:PRO:HD3	2.20	0.41
1:B:17:ILE:O	1:B:40:LEU:HA	2.20	0.41
1:D:217:LEU:HD21	1:D:281:ILE:HD13	2.02	0.41
1:A:234:PRO:HG2	1:A:400:TRP:CZ2	2.55	0.41
1:C:130:GLU:HB2	1:C:131:PRO:HD3	2.03	0.41
1:C:220:TYR:OH	1:C:283:ASP:OD2	2.38	0.41
1:D:83:MET:HE3	1:D:83:MET:HB2	1.89	0.41
1:D:306:TYR:CE1	1:D:364:GLN:HG2	2.55	0.41
1:E:138:GLN:NE2	8:E:706:HOH:O	2.44	0.41
1:F:18:VAL:HG12	1:F:185:ASP:HB3	2.03	0.41
1:F:213:PHE:HE2	1:F:255:HIS:HB2	1.86	0.41
1:C:13:VAL:O	1:C:178:SER:HA	2.21	0.41
1:C:51:PRO:O	1:C:52:ARG:C	2.63	0.41
1:D:18:VAL:HG12	1:D:185:ASP:HB3	2.03	0.41
1:D:22:PRO:HD2	2:D:602:FAD:O1P	2.21	0.41
1:F:10:ASP:OD2	1:F:174:TYR:HA	2.21	0.41
2:F:601:FAD:O2'	2:F:601:FAD:C9	2.69	0.41
1:B:312:PHE:CE2	1:B:356:LEU:HB3	2.55	0.41
1:B:379:VAL:O	1:B:382:ILE:HG22	2.21	0.41
1:B:304:PRO:O	1:B:360:HIS:HE1	2.04	0.40
1:D:34:TYR:CD1	1:D:34:TYR:N	2.87	0.40
1:D:248:ARG:O	1:D:249:PRO:C	2.64	0.40
1:A:181:LEU:HD22	1:A:311:VAL:HG13	2.04	0.40
1:A:412:GLU:HG2	8:A:803:HOH:O	2.21	0.40
1:B:154:LEU:HA	1:B:162:THR:O	2.22	0.40
1:C:16:LEU:HD23	1:C:181:LEU:HD12	2.03	0.40
1:C:52:ARG:HH21	1:C:126:GLN:NE2	2.17	0.40
1:F:51:PRO:HD3	1:F:212:TRP:CZ3	2.56	0.40
1:F:149:HIS:CD2	8:F:704:HOH:O	2.74	0.40
1:F:501:LEU:O	1:F:553:ALA:HA	2.21	0.40
1:F:69:ILE:O	1:F:73:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:VAL:O	1:B:178:SER:HA	2.21	0.40
1:C:104:GLY:HA3	1:C:113:TYR:CG	2.57	0.40
1:D:30:ALA:HB3	1:D:340:CYS:SG	2.61	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	577/601 (96%)	559 (97%)	17 (3%)	1 (0%)	43	62
1	B	577/601 (96%)	551 (96%)	25 (4%)	1 (0%)	43	62
1	C	578/601 (96%)	563 (97%)	15 (3%)	0	100	100
1	D	577/601 (96%)	550 (95%)	25 (4%)	2 (0%)	36	53
1	E	577/601 (96%)	549 (95%)	25 (4%)	3 (0%)	24	41
1	F	578/601 (96%)	546 (94%)	28 (5%)	4 (1%)	18	32
All	All	3464/3606 (96%)	3318 (96%)	135 (4%)	11 (0%)	36	53

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	262	THR
1	F	263	ALA
1	E	532	GLY
1	F	7	THR
1	A	90	SER
1	B	215	ALA
1	D	90	SER
1	D	215	ALA
1	E	531	ALA

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Mol	Chain	Res	Type
1	F	51	PRO
1	E	267	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	447/460 (97%)	428 (96%)	19 (4%)	26	49
1	B	447/460 (97%)	426 (95%)	21 (5%)	23	44
1	C	448/460 (97%)	429 (96%)	19 (4%)	26	49
1	D	447/460 (97%)	431 (96%)	16 (4%)	31	55
1	E	447/460 (97%)	423 (95%)	24 (5%)	20	39
1	F	447/460 (97%)	421 (94%)	26 (6%)	18	36
All	All	2683/2760 (97%)	2558 (95%)	125 (5%)	23	44

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

Mol	Chain	Res	Type
1	A	43	ARG
1	A	92	PHE
1	A	138	GLN
1	A	158	GLU
1	A	172	ARG
1	A	188	ARG
1	A	190	ARG
1	A	203	THR
1	A	214	GLU
1	A	262	THR
1	A	264	ASP
1	A	267	VAL
1	A	287	ASP
1	A	321	ASN
1	A	324	THR
1	A	412	GLU

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Mol	Chain	Res	Type
1	A	474	ARG
1	A	573	LYS
1	A	574	GLU
1	B	12	ARG
1	B	52	ARG
1	B	92	PHE
1	B	188	ARG
1	B	189	SER
1	B	190	ARG
1	B	203	THR
1	B	274	ARG
1	B	278	ARG
1	B	290	ILE
1	B	321	ASN
1	B	392	GLU
1	B	401	ARG
1	B	444	THR
1	B	447	LEU
1	B	474	ARG
1	B	497	ARG
1	B	510	ARG
1	B	523	GLU
1	B	567	ARG
1	B	578	VAL
1	C	43	ARG
1	C	72	ARG
1	C	92	PHE
1	C	126	GLN
1	C	155	GLU
1	C	172	ARG
1	C	203	THR
1	C	262	THR
1	C	267	VAL
1	C	278	ARG
1	C	287	ASP
1	C	321	ASN
1	C	324	THR
1	C	444	THR
1	C	447	LEU
1	C	458	GLU
1	C	474	ARG
1	C	497	ARG

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Mol	Chain	Res	Type
1	C	511	ASP
1	D	43	ARG
1	D	72	ARG
1	D	92	PHE
1	D	135	GLU
1	D	138	GLN
1	D	190	ARG
1	D	203	THR
1	D	248	ARG
1	D	268	GLU
1	D	287	ASP
1	D	297	GLU
1	D	312	PHE
1	D	318	VAL
1	D	324	THR
1	D	474	ARG
1	D	582	VAL
1	E	49	HIS
1	E	72	ARG
1	E	119	SER
1	E	141	CYS
1	E	155	GLU
1	E	163	SER
1	E	164	ARG
1	E	207	ARG
1	E	262	THR
1	E	265	VAL
1	E	267	VAL
1	E	278	ARG
1	E	321	ASN
1	E	324	THR
1	E	368	ARG
1	E	412	GLU
1	E	415	GLN
1	E	447	LEU
1	E	474	ARG
1	E	497	ARG
1	E	511	ASP
1	E	515	ASP
1	E	523	GLU
1	E	573	LYS
1	F	11	ILE

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Mol	Chain	Res	Type
1	F	12	ARG
1	F	43	ARG
1	F	92	PHE
1	F	99	ARG
1	F	138	GLN
1	F	142	VAL
1	F	163	SER
1	F	172	ARG
1	F	176	VAL
1	F	178	SER
1	F	188	ARG
1	F	278	ARG
1	F	285	THR
1	F	287	ASP
1	F	305	ARG
1	F	321	ASN
1	F	379	VAL
1	F	404	ASP
1	F	408	GLU
1	F	412	GLU
1	F	414	ARG
1	F	438	LEU
1	F	474	ARG
1	F	573	LYS
1	F	577	GLU

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

Mol	Chain	Res	Type
1	A	44	HIS
1	A	49	HIS
1	A	123	ASN
1	A	325	ASN
1	A	415	GLN
1	A	485	HIS
1	B	44	HIS
1	B	49	HIS
1	B	123	ASN
1	B	325	ASN
1	B	430	GLN
1	B	485	HIS
1	C	44	HIS

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Mol	Chain	Res	Type
1	C	45	HIS
1	C	123	ASN
1	C	126	GLN
1	C	138	GLN
1	C	299	ASN
1	C	320	GLN
1	C	325	ASN
1	C	360	HIS
1	C	485	HIS
1	D	325	ASN
1	D	415	GLN
1	D	485	HIS
1	D	585	GLN
1	E	44	HIS
1	E	49	HIS
1	E	159	HIS
1	E	321	ASN
1	E	325	ASN
1	E	428	HIS
1	E	430	GLN
1	E	485	HIS
1	E	561	HIS
1	F	81	HIS
1	F	223	HIS
1	F	270	HIS
1	F	325	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 39 ligands modelled in this entry, 11 are monoatomic - leaving 28 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
2	FAD	B	601	-	58,58,58	1.75	11 (18%)	85,89,89	1.73	22 (25%)
4	PKS	B	603	-	28,28,28	2.03	8 (28%)	33,37,37	2.06	10 (30%)
6	1PE	A	605	-	15,15,15	0.53	0	14,14,14	0.47	0
6	1PE	B	604	-	15,15,15	0.59	0	14,14,14	0.41	0
7	GOL	E	608	-	5,5,5	0.15	0	5,5,5	0.51	0
2	FAD	C	702	-	58,58,58	2.12	16 (27%)	85,89,89	1.75	19 (22%)
2	FAD	A	601	-	58,58,58	2.05	13 (22%)	85,89,89	1.90	24 (28%)
5	PGE	E	604	-	9,9,9	0.34	0	8,8,8	0.18	0
4	PKS	F	603	-	28,28,28	2.10	7 (25%)	33,37,37	2.18	8 (24%)
6	1PE	E	605	-	15,15,15	0.60	0	14,14,14	0.48	0
6	1PE	F	604	-	15,15,15	0.66	0	14,14,14	0.39	0
6	1PE	D	605	-	15,15,15	0.60	0	14,14,14	0.30	0
2	FAD	F	601	-	58,58,58	1.83	11 (18%)	85,89,89	1.89	19 (22%)
7	GOL	D	601	-	5,5,5	0.18	0	5,5,5	0.47	0
5	PGE	C	704	-	9,9,9	0.28	0	8,8,8	0.16	0
4	PKS	C	703	-	28,28,28	2.32	9 (32%)	33,37,37	2.24	12 (36%)
2	FAD	D	602	-	58,58,58	1.83	12 (20%)	85,89,89	1.69	21 (24%)
7	GOL	A	607	-	5,5,5	0.13	0	5,5,5	0.33	0
6	1PE	C	705	-	15,15,15	0.68	0	14,14,14	0.61	0
5	PGE	C	701	-	9,9,9	0.31	0	8,8,8	0.16	0
4	PKS	A	603	-	28,28,28	2.50	10 (35%)	33,37,37	2.25	15 (45%)
7	GOL	A	608	-	5,5,5	0.11	0	5,5,5	0.25	0
7	GOL	D	607	-	5,5,5	0.12	0	5,5,5	0.39	0
2	FAD	E	601	-	58,58,58	1.92	11 (18%)	85,89,89	1.80	25 (29%)
7	GOL	E	607	-	5,5,5	0.16	0	5,5,5	0.54	0
5	PGE	A	604	-	9,9,9	0.27	0	8,8,8	0.18	0
4	PKS	D	604	-	28,28,28	2.37	10 (35%)	33,37,37	1.76	6 (18%)
4	PKS	E	603	-	28,28,28	2.08	8 (28%)	33,37,37	2.22	8 (24%)

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
2	FAD	B	601	-	-	11/34/50/50	0/6/6/6
4	PKS	B	603	-	-	4/27/27/27	0/1/1/1
6	1PE	A	605	-	-	7/13/13/13	-
6	1PE	B	604	-	-	10/13/13/13	-
7	GOL	E	608	-	-	4/4/4/4	-
2	FAD	C	702	-	-	9/34/50/50	0/6/6/6
2	FAD	A	601	-	-	7/34/50/50	0/6/6/6
5	PGE	E	604	-	-	3/7/7/7	-
4	PKS	F	603	-	-	8/27/27/27	0/1/1/1
6	1PE	E	605	-	-	12/13/13/13	-
6	1PE	F	604	-	-	10/13/13/13	-
6	1PE	D	605	-	-	9/13/13/13	-
2	FAD	F	601	-	-	7/34/50/50	0/6/6/6
7	GOL	D	601	-	-	4/4/4/4	-
5	PGE	C	704	-	-	3/7/7/7	-
4	PKS	C	703	-	-	8/27/27/27	0/1/1/1
2	FAD	D	602	-	-	8/34/50/50	0/6/6/6
7	GOL	A	607	-	-	4/4/4/4	-
6	1PE	C	705	-	-	7/13/13/13	-
5	PGE	C	701	-	-	4/7/7/7	-
4	PKS	A	603	-	-	8/27/27/27	0/1/1/1
7	GOL	A	608	-	-	4/4/4/4	-
7	GOL	D	607	-	-	4/4/4/4	-
2	FAD	E	601	-	-	5/34/50/50	0/6/6/6
7	GOL	E	607	-	-	0/4/4/4	-
5	PGE	A	604	-	-	5/7/7/7	-
4	PKS	D	604	-	-	10/27/27/27	0/1/1/1
4	PKS	E	603	-	-	9/27/27/27	0/1/1/1

All (126) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	603	PKS	CAK-CAE	9.15	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	703	PKS	CAK-CAE	7.69	1.57	1.51
4	D	604	PKS	CAK-CAE	7.41	1.57	1.51
2	C	702	FAD	C9A-C5X	6.98	1.52	1.41
2	C	702	FAD	PA-O3P	6.49	1.66	1.59
4	F	603	PKS	CAK-CAE	6.44	1.56	1.51
2	A	601	FAD	PA-O3P	6.25	1.66	1.59
4	E	603	PKS	CAK-CAE	6.21	1.56	1.51
2	D	602	FAD	C9A-C5X	6.08	1.50	1.41
2	E	601	FAD	C9A-C5X	5.95	1.50	1.41
2	E	601	FAD	PA-O3P	5.87	1.65	1.59
2	B	601	FAD	C9A-C5X	5.79	1.50	1.41
2	A	601	FAD	C9A-C5X	5.75	1.50	1.41
2	F	601	FAD	C9A-C5X	5.72	1.50	1.41
2	B	601	FAD	C5A-C4A	5.38	1.48	1.39
2	D	602	FAD	C5A-C4A	5.31	1.48	1.39
2	A	601	FAD	C5A-C4A	5.27	1.48	1.39
2	C	702	FAD	C5A-C4A	5.12	1.48	1.39
2	E	601	FAD	C5A-C4A	5.11	1.48	1.39
2	A	601	FAD	C8-C7	4.99	1.53	1.40
2	F	601	FAD	C5A-C4A	4.99	1.48	1.39
4	B	603	PKS	OAH-CAC	4.89	1.43	1.35
2	E	601	FAD	P-O3P	4.88	1.64	1.59
4	F	603	PKS	OAH-CAC	4.65	1.42	1.35
2	F	601	FAD	PA-O3P	4.54	1.64	1.59
4	D	604	PKS	CAQ-CAR	4.42	1.55	1.46
2	E	601	FAD	C8-C7	4.37	1.51	1.40
4	E	603	PKS	CAQ-CAR	4.32	1.55	1.46
4	D	604	PKS	OAH-CAC	4.23	1.42	1.35
4	C	703	PKS	OAH-CAC	4.11	1.41	1.35
2	D	602	FAD	PA-O3P	4.07	1.63	1.59
2	F	601	FAD	C8-C7	4.03	1.50	1.40
2	D	602	FAD	C8-C7	4.03	1.50	1.40
2	C	702	FAD	C8-C7	4.03	1.50	1.40
2	B	601	FAD	C8-C7	4.03	1.50	1.40
4	A	603	PKS	OAH-CAC	4.02	1.41	1.35
4	C	703	PKS	CAQ-CAR	3.99	1.54	1.46
2	A	601	FAD	C10-N10	3.97	1.45	1.37
4	B	603	PKS	CAK-CAE	3.76	1.54	1.51
2	D	602	FAD	C10-N10	3.76	1.45	1.37
2	F	601	FAD	C5A-C6A	3.64	1.51	1.41
4	B	603	PKS	CAQ-CAR	3.63	1.53	1.46
2	A	601	FAD	C5A-C6A	3.61	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	702	FAD	P-O3P	3.59	1.63	1.59
2	C	702	FAD	C10-N10	3.57	1.45	1.37
2	E	601	FAD	C10-N10	3.57	1.45	1.37
2	B	601	FAD	C5A-C6A	3.54	1.50	1.41
2	F	601	FAD	P-O3P	3.53	1.63	1.59
4	A	603	PKS	CAQ-CAR	3.53	1.53	1.46
4	F	603	PKS	CAQ-CAR	3.43	1.53	1.46
2	D	602	FAD	P-O3P	3.39	1.63	1.59
2	E	601	FAD	C5A-C6A	3.27	1.50	1.41
2	F	601	FAD	C10-N10	3.21	1.44	1.37
2	C	702	FAD	C5A-C6A	3.18	1.49	1.41
2	C	702	FAD	C1'-C2'	3.18	1.57	1.52
2	B	601	FAD	C10-N10	3.13	1.44	1.37
2	A	601	FAD	C4X-C10	3.09	1.53	1.44
4	B	603	PKS	CAC-NAD	3.04	1.38	1.33
4	C	703	PKS	CAA-CAF	-3.01	1.36	1.40
2	A	601	FAD	C4X-N5	2.94	1.37	1.30
2	B	601	FAD	PA-O3P	2.93	1.62	1.59
2	A	601	FAD	P-O3P	2.88	1.62	1.59
2	F	601	FAD	C4X-N5	2.88	1.37	1.30
4	A	603	PKS	CAA-CAF	-2.85	1.37	1.40
2	D	602	FAD	C4X-N5	2.85	1.36	1.30
2	D	602	FAD	C5A-C6A	2.82	1.48	1.41
4	A	603	PKS	CAF-CAE	2.79	1.42	1.39
2	A	601	FAD	C8A-N7A	2.78	1.37	1.31
4	D	604	PKS	CAB-CAC	2.77	1.43	1.38
2	F	601	FAD	C8A-N7A	2.73	1.36	1.31
2	B	601	FAD	C9A-N10	2.71	1.45	1.41
4	B	603	PKS	OAG-CAA	2.67	1.41	1.36
4	C	703	PKS	CAS-CAR	2.67	1.41	1.34
4	A	603	PKS	CAL-CAM	2.64	1.39	1.33
2	D	602	FAD	C8A-N7A	2.62	1.36	1.31
2	C	702	FAD	C4-N3	-2.62	1.34	1.38
2	A	601	FAD	C9A-N10	2.58	1.45	1.41
2	E	601	FAD	C4X-N5	2.58	1.36	1.30
2	F	601	FAD	C4-N3	-2.57	1.34	1.38
2	A	601	FAD	C10-N1	2.56	1.38	1.33
2	C	702	FAD	C4X-N5	2.55	1.36	1.30
2	B	601	FAD	C8A-N7A	2.53	1.36	1.31
4	E	603	PKS	CAB-CAC	2.51	1.42	1.38
4	B	603	PKS	CAL-CAM	2.49	1.38	1.33
2	E	601	FAD	C8A-N7A	2.49	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	604	PKS	CAT-CAR	2.47	1.55	1.50
4	E	603	PKS	OAG-CAA	2.46	1.41	1.36
4	E	603	PKS	OAH-CAC	2.45	1.39	1.35
4	D	604	PKS	CAA-CAF	-2.44	1.37	1.40
2	C	702	FAD	C8A-N7A	2.43	1.36	1.31
2	C	702	FAD	C4X-C10	2.43	1.51	1.44
4	D	604	PKS	CAK-CAL	2.41	1.56	1.50
2	B	601	FAD	C4X-C10	2.39	1.51	1.44
4	A	603	PKS	CAC-NAD	2.35	1.37	1.33
2	E	601	FAD	C4X-C10	2.35	1.51	1.44
2	D	602	FAD	C10-N1	2.33	1.37	1.33
4	E	603	PKS	CAT-CAR	2.32	1.55	1.50
4	C	703	PKS	OAG-CAA	2.31	1.41	1.36
2	C	702	FAD	C9A-N10	2.30	1.45	1.41
4	C	703	PKS	CAL-CAM	2.29	1.38	1.33
2	B	601	FAD	C4X-N5	2.28	1.35	1.30
4	E	603	PKS	CAK-CAL	2.28	1.55	1.50
4	C	703	PKS	CAT-CAR	2.25	1.55	1.50
4	D	604	PKS	CAL-CAM	2.24	1.38	1.33
4	F	603	PKS	CAB-CAC	2.22	1.42	1.38
4	D	604	PKS	CAC-NAD	2.21	1.36	1.33
2	C	702	FAD	C2'-C3'	2.20	1.57	1.53
4	B	603	PKS	CAT-CAR	2.19	1.55	1.50
2	D	602	FAD	C5A-N7A	-2.19	1.35	1.39
4	E	603	PKS	CAL-CAM	2.19	1.38	1.33
2	E	601	FAD	C4-N3	-2.19	1.34	1.38
2	C	702	FAD	C5X-N5	-2.18	1.35	1.39
4	B	603	PKS	CAA-CAF	-2.13	1.37	1.40
4	A	603	PKS	CAZ-CAW	2.10	1.54	1.50
2	F	601	FAD	C4X-C10	2.10	1.50	1.44
2	D	602	FAD	C4X-C10	2.09	1.50	1.44
4	A	603	PKS	CAT-CAR	2.09	1.55	1.50
2	B	601	FAD	C10-N1	2.09	1.37	1.33
4	C	703	PKS	CAU-CAS	2.08	1.55	1.51
4	F	603	PKS	CAA-CAF	-2.07	1.37	1.40
2	C	702	FAD	C10-N1	2.07	1.37	1.33
4	D	604	PKS	CAS-CAR	2.04	1.39	1.34
4	F	603	PKS	CAT-CAR	2.03	1.55	1.50
2	A	601	FAD	C5'-C4'	2.03	1.54	1.51
4	F	603	PKS	OAG-CAA	2.03	1.40	1.36
4	A	603	PKS	CAV-CAW	2.01	1.57	1.51

All (189) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	601	FAD	C5A-C4A-N3A	-7.24	116.74	126.72
4	C	703	PKS	CAP-CAQ-CAR	-7.07	115.20	125.89
4	F	603	PKS	CAK-CAL-CAM	-6.78	117.71	127.42
4	E	603	PKS	CAP-CAQ-CAR	-6.63	115.87	125.89
4	B	603	PKS	CAK-CAL-CAM	-5.62	119.36	127.42
2	B	601	FAD	C5A-C4A-N3A	-5.59	119.01	126.72
2	D	602	FAD	C5A-C4A-N3A	-5.33	119.38	126.72
4	E	603	PKS	CAE-CAK-CAL	-5.21	103.23	112.07
2	C	702	FAD	C5A-C4A-N3A	-5.10	119.69	126.72
2	F	601	FAD	N3A-C4A-N9A	5.04	135.74	127.17
4	B	603	PKS	CAE-CAK-CAL	-5.02	103.56	112.07
2	A	601	FAD	C5A-C4A-N3A	-4.99	119.84	126.72
2	F	601	FAD	C4A-C5A-N7A	-4.74	105.17	110.58
4	F	603	PKS	CAP-CAQ-CAR	-4.62	118.90	125.89
2	D	602	FAD	N3A-C4A-N9A	4.59	134.98	127.17
2	E	601	FAD	N3A-C2A-N1A	-4.42	121.89	128.58
2	F	601	FAD	C2A-N3A-C4A	4.38	122.52	111.83
4	A	603	PKS	CAF-CAE-NAD	-4.35	119.28	123.84
2	E	601	FAD	C4A-N9A-C8A	4.35	110.30	105.74
2	A	601	FAD	C4A-C5A-N7A	-4.34	105.62	110.58
4	E	603	PKS	CAK-CAL-CAM	-4.33	121.22	127.42
2	B	601	FAD	N3A-C4A-N9A	4.32	134.51	127.17
4	F	603	PKS	CAB-CAC-NAD	-4.28	119.16	124.16
4	D	604	PKS	CAK-CAL-CAM	-4.16	121.46	127.42
2	C	702	FAD	C4A-C5A-N7A	-4.15	105.84	110.58
4	A	603	PKS	CAJ-CAF-CAA	-4.14	115.67	120.75
2	F	601	FAD	C4-C4X-N5	4.13	123.91	118.21
2	E	601	FAD	C5A-C4A-N3A	-4.07	121.11	126.72
4	C	703	PKS	CAB-CAC-NAD	-4.06	119.42	124.16
4	D	604	PKS	CAA-CAF-CAE	4.02	119.47	116.51
4	A	603	PKS	CAE-CAK-CAL	-3.99	105.30	112.07
2	A	601	FAD	N3A-C4A-N9A	3.97	133.92	127.17
4	D	604	PKS	CAE-CAK-CAL	-3.89	105.46	112.07
2	C	702	FAD	N3A-C4A-N9A	3.88	133.77	127.17
2	A	601	FAD	C4A-N9A-C8A	3.83	109.76	105.74
4	F	603	PKS	CAE-CAK-CAL	-3.83	105.58	112.07
2	B	601	FAD	C4A-C5A-N7A	-3.79	106.25	110.58
2	E	601	FAD	N3A-C4A-N9A	3.77	133.59	127.17
2	A	601	FAD	C7M-C7-C8	3.76	128.44	120.76
2	E	601	FAD	C2A-N3A-C4A	3.76	121.01	111.83
2	B	601	FAD	O4-C4-C4X	-3.72	116.72	126.53
4	E	603	PKS	CAA-CAF-CAE	3.71	119.25	116.51
2	A	601	FAD	C7M-C7-C6	-3.67	113.10	119.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	FAD	C2A-N3A-C4A	3.66	120.77	111.83
2	B	601	FAD	C2A-N3A-C4A	3.62	120.67	111.83
4	C	703	PKS	CAF-CAE-NAD	-3.60	120.07	123.84
4	B	603	PKS	CAB-CAC-NAD	-3.57	119.99	124.16
4	A	603	PKS	CAO-CAM-CAN	3.56	122.73	115.03
2	C	702	FAD	C2A-N3A-C4A	3.56	120.52	111.83
2	E	601	FAD	C4X-C10-N1	-3.49	116.02	124.59
2	A	601	FAD	O4B-C1B-N9A	3.48	114.77	108.09
2	D	602	FAD	C4X-C10-N1	-3.43	116.18	124.59
2	C	702	FAD	C4X-C10-N1	-3.43	116.18	124.59
2	D	602	FAD	C2A-N3A-C4A	3.40	120.14	111.83
2	C	702	FAD	C9A-N10-C10	-3.39	115.59	120.75
2	A	601	FAD	C5A-N7A-C8A	3.38	108.76	103.45
4	A	603	PKS	CAJ-CAF-CAE	3.37	125.61	122.70
2	A	601	FAD	C4X-C10-N1	-3.35	116.37	124.59
2	C	702	FAD	C4'-C3'-C2'	3.30	119.06	113.57
2	A	601	FAD	N3A-C2A-N1A	-3.28	123.61	128.58
4	D	604	PKS	CAP-CAQ-CAR	-3.27	120.95	125.89
4	C	703	PKS	CAN-CAM-CAL	-3.26	112.71	121.14
4	B	603	PKS	CAA-CAF-CAE	3.24	118.90	116.51
2	B	601	FAD	C4X-C10-N1	-3.23	116.67	124.59
2	A	601	FAD	C6A-C5A-N7A	3.22	138.30	132.09
2	C	702	FAD	C5A-N7A-C8A	3.18	108.45	103.45
2	D	602	FAD	N3A-C2A-N1A	-3.18	123.77	128.58
2	F	601	FAD	C5A-N7A-C8A	3.18	108.44	103.45
2	F	601	FAD	C4X-C10-N1	-3.16	116.85	124.59
4	B	603	PKS	CAO-CAM-CAN	3.16	121.85	115.03
2	E	601	FAD	O4B-C1B-N9A	3.13	114.10	108.09
4	A	603	PKS	CAN-CAM-CAL	-3.13	113.04	121.14
2	E	601	FAD	C4A-C5A-N7A	-3.12	107.01	110.58
4	B	603	PKS	CAZ-CAW-CAX	-3.10	115.65	123.52
2	E	601	FAD	C6A-C5A-N7A	3.09	138.06	132.09
2	A	601	FAD	C4-N3-C2	-3.09	120.15	125.64
2	C	702	FAD	C1'-C2'-C3'	3.08	118.00	109.66
2	F	601	FAD	C9A-N10-C10	-3.07	116.07	120.75
2	A	601	FAD	N9A-C8A-N7A	-3.04	109.62	113.94
2	E	601	FAD	C2A-N1A-C6A	3.04	123.72	118.73
4	D	604	PKS	CAF-CAE-NAD	-3.04	120.67	123.84
4	E	603	PKS	CAF-CAE-NAD	-3.03	120.67	123.84
2	C	702	FAD	C4A-N9A-C8A	3.00	108.89	105.74
2	B	601	FAD	C4-N3-C2	-3.00	120.32	125.64
2	E	601	FAD	C4-N3-C2	-3.00	120.32	125.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	603	PKS	CAA-CAF-CAE	2.99	118.72	116.51
4	C	703	PKS	CAT-CAR-CAQ	-2.99	113.53	118.09
2	D	602	FAD	C4A-C5A-N7A	-2.98	107.17	110.58
2	D	602	FAD	C4A-N9A-C8A	2.98	108.87	105.74
2	A	601	FAD	N3-C2-N1	2.97	125.82	119.50
4	F	603	PKS	CAO-CAM-CAN	2.97	121.44	115.03
2	D	602	FAD	C4-C4X-N5	2.96	122.29	118.21
4	C	703	PKS	CAJ-CAF-CAE	-2.93	120.18	122.70
4	C	703	PKS	CAO-CAM-CAN	2.88	121.25	115.03
2	E	601	FAD	N9A-C8A-N7A	-2.85	109.89	113.94
4	B	603	PKS	CAZ-CAW-CAV	2.85	121.93	115.85
2	C	702	FAD	N3A-C2A-N1A	-2.84	124.29	128.58
2	F	601	FAD	N3A-C2A-N1A	-2.82	124.31	128.58
4	C	703	PKS	CAA-CAF-CAE	2.82	118.59	116.51
2	B	601	FAD	O2'-C2'-C3'	-2.82	102.65	109.25
2	F	601	FAD	C9A-C5X-N5	-2.81	119.47	122.45
4	A	603	PKS	CAP-CAQ-CAR	-2.80	121.66	125.89
4	E	603	PKS	CAO-CAM-CAN	2.80	121.08	115.03
2	F	601	FAD	C6A-C5A-N7A	2.79	137.47	132.09
4	C	703	PKS	CAC-NAD-CAE	2.78	121.55	117.63
2	C	702	FAD	C5X-C9A-N10	2.76	120.46	117.97
2	C	702	FAD	C4X-C10-N10	2.74	120.41	116.48
2	F	601	FAD	C10-C4X-N5	-2.72	119.25	124.81
2	D	602	FAD	C4-N3-C2	-2.71	120.83	125.64
2	B	601	FAD	C4A-N9A-C8A	2.70	108.58	105.74
2	B	601	FAD	C5A-N7A-C8A	2.70	107.69	103.45
4	A	603	PKS	CAB-CAC-NAD	-2.70	121.01	124.16
2	D	602	FAD	C2B-C1B-N9A	2.69	119.98	113.30
4	F	603	PKS	CAF-CAE-NAD	-2.67	121.05	123.84
2	E	601	FAD	C4-C4X-N5	2.64	121.85	118.21
2	D	602	FAD	C10-N1-C2	2.63	122.55	116.85
2	E	601	FAD	C4A-N9A-C1B	-2.63	120.47	126.63
2	A	601	FAD	O2-C2-N3	-2.63	113.55	118.58
2	C	702	FAD	N9A-C8A-N7A	-2.58	110.28	113.94
2	B	601	FAD	C9A-N10-C10	-2.57	116.83	120.75
2	E	601	FAD	C5A-N7A-C8A	2.56	107.48	103.45
2	E	601	FAD	O4B-C4B-C3B	2.56	110.23	105.15
2	D	602	FAD	C4X-C4-N3	2.54	119.72	113.25
2	B	601	FAD	N3A-C2A-N1A	-2.52	124.77	128.58
2	B	601	FAD	C6A-C5A-N7A	2.52	136.94	132.09
2	B	601	FAD	N3-C2-N1	2.51	124.83	119.50
2	C	702	FAD	C10-N1-C2	2.50	122.26	116.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	601	FAD	C10-N1-C2	2.50	122.26	116.85
2	C	702	FAD	O4'-C4'-C3'	2.48	115.06	109.25
2	D	602	FAD	O4-C4-C4X	-2.47	120.02	126.53
2	A	601	FAD	N10-C10-N1	2.45	125.73	118.51
4	A	603	PKS	CAT-CAR-CAQ	2.45	121.83	118.09
2	C	702	FAD	C6A-C5A-N7A	2.45	136.81	132.09
2	E	601	FAD	C10-N1-C2	2.44	122.12	116.85
2	E	601	FAD	C4X-C4-N3	2.43	119.44	113.25
2	D	602	FAD	C9A-C5X-N5	-2.41	119.90	122.45
2	A	601	FAD	C4X-C4-N3	2.40	119.37	113.25
4	C	703	PKS	CAK-CAE-NAD	2.40	120.89	116.24
2	F	601	FAD	C3B-C2B-C1B	2.40	106.00	101.46
2	B	601	FAD	N10-C10-N1	2.37	125.49	118.51
4	A	603	PKS	CAC-NAD-CAE	2.37	120.97	117.63
4	F	603	PKS	CAC-NAD-CAE	2.36	120.97	117.63
2	A	601	FAD	C4-C4X-N5	2.34	121.44	118.21
2	D	602	FAD	O2B-C2B-C1B	-2.34	102.05	110.10
2	F	601	FAD	C4X-C4-N3	2.30	119.11	113.25
2	D	602	FAD	C5A-N7A-C8A	2.30	107.06	103.45
4	E	603	PKS	CAU-CAS-CAR	-2.28	119.63	126.72
2	D	602	FAD	N10-C10-N1	2.27	125.19	118.51
2	A	601	FAD	O4-C4-C4X	-2.26	120.56	126.53
2	B	601	FAD	O4-C4-N3	2.25	124.35	120.11
2	E	601	FAD	C10-C4X-N5	-2.24	120.23	124.81
2	A	601	FAD	C2A-N1A-C6A	2.23	122.40	118.73
2	E	601	FAD	C5X-N5-C4X	2.23	121.70	118.09
2	F	601	FAD	C4-N3-C2	-2.23	121.68	125.64
2	B	601	FAD	C4X-C4-N3	2.23	118.93	113.25
2	E	601	FAD	N3-C2-N1	2.20	124.17	119.50
2	D	602	FAD	C10-C4X-N5	-2.19	120.34	124.81
2	E	601	FAD	O3P-P-O1P	2.18	117.27	110.70
2	F	601	FAD	O2A-PA-O3P	-2.18	101.39	107.27
2	B	601	FAD	C6-C5X-C9A	2.17	122.03	119.05
2	E	601	FAD	O4-C4-C4X	-2.16	120.83	126.53
2	B	601	FAD	C3B-C2B-C1B	2.16	105.55	101.46
4	A	603	PKS	CAZ-CAW-CAX	-2.14	118.08	123.52
4	A	603	PKS	OBA-CAV-CAU	-2.12	104.67	108.10
2	B	601	FAD	C4'-C3'-C2'	-2.12	110.05	113.57
2	A	601	FAD	C4A-N9A-C1B	-2.12	121.69	126.63
2	F	601	FAD	O2'-C2'-C3'	-2.12	104.30	109.25
2	C	702	FAD	O3'-C3'-C4'	-2.11	104.13	108.93
2	D	602	FAD	C9A-N10-C10	-2.10	117.55	120.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	602	FAD	O2P-P-O1P	2.10	122.19	112.44
2	D	602	FAD	C2A-N1A-C6A	2.09	122.17	118.73
4	D	604	PKS	CAJ-CAF-CAE	-2.09	120.91	122.70
4	E	603	PKS	CAJ-CAF-CAE	-2.09	120.91	122.70
2	A	601	FAD	C10-C4X-N5	-2.09	120.55	124.81
2	A	601	FAD	O3'-C3'-C4'	2.08	113.65	108.93
4	B	603	PKS	CAP-CAQ-CAR	-2.08	122.75	125.89
4	C	703	PKS	OAH-CAC-CAB	2.06	124.48	118.04
2	B	601	FAD	N9A-C8A-N7A	-2.06	111.01	113.94
4	A	603	PKS	CAY-CAX-CAW	-2.06	121.76	126.45
2	B	601	FAD	O2A-PA-O1A	2.05	121.99	112.44
4	A	603	PKS	CBB-CAU-CAS	-2.05	106.60	110.08
4	B	603	PKS	CAF-CAE-NAD	-2.05	121.70	123.84
2	E	601	FAD	N10-C10-N1	2.05	124.54	118.51
2	E	601	FAD	C4X-C10-N10	2.05	119.41	116.48
4	C	703	PKS	CAZ-CAW-CAV	2.04	120.21	115.85
4	B	603	PKS	CAY-CAX-CAW	-2.03	121.83	126.45
4	F	603	PKS	CAZ-CAW-CAV	2.03	120.18	115.85
2	F	601	FAD	N9A-C8A-N7A	-2.02	111.07	113.94
2	C	702	FAD	C6-C5X-C9A	2.02	121.82	119.05

There are no chirality outliers.

All (184) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FAD	C1'-C2'-C3'-O3'
2	A	601	FAD	C1'-C2'-C3'-C4'
2	A	601	FAD	O4'-C4'-C5'-O5'
2	B	601	FAD	C5B-O5B-PA-O2A
2	B	601	FAD	C1'-C2'-C3'-O3'
2	B	601	FAD	C1'-C2'-C3'-C4'
2	B	601	FAD	O4'-C4'-C5'-O5'
2	C	702	FAD	O4'-C4'-C5'-O5'
2	C	702	FAD	PA-O3P-P-O5'
2	D	602	FAD	O4'-C4'-C5'-O5'
2	D	602	FAD	C5'-O5'-P-O1P
2	D	602	FAD	C5'-O5'-P-O2P
2	D	602	FAD	C5'-O5'-P-O3P
2	E	601	FAD	C5'-O5'-P-O3P
4	A	603	PKS	CAP-CAQ-CAR-CAS
4	A	603	PKS	CAP-CAQ-CAR-CAT
4	C	703	PKS	CAM-CAN-CAP-CAQ

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Mol	Chain	Res	Type	Atoms
4	C	703	PKS	CAO-CAM-CAN-CAP
4	E	603	PKS	NAD-CAC-OAH-CAI
4	E	603	PKS	CAS-CAU-CAV-CAW
4	E	603	PKS	CAM-CAN-CAP-CAQ
4	E	603	PKS	CAO-CAM-CAN-CAP
4	F	603	PKS	OBA-CAV-CAW-CAZ
4	F	603	PKS	CAM-CAN-CAP-CAQ
7	A	607	GOL	C1-C2-C3-O3
7	A	608	GOL	O1-C1-C2-C3
7	A	608	GOL	C1-C2-C3-O3
7	D	601	GOL	O1-C1-C2-C3
7	D	607	GOL	O1-C1-C2-O2
7	D	607	GOL	C1-C2-C3-O3
7	E	608	GOL	C1-C2-C3-O3
4	E	603	PKS	CAL-CAM-CAN-CAP
4	E	603	PKS	CAB-CAC-OAH-CAI
4	F	603	PKS	CAB-CAC-OAH-CAI
4	B	603	PKS	NAD-CAC-OAH-CAI
4	F	603	PKS	NAD-CAC-OAH-CAI
2	B	601	FAD	O2'-C2'-C3'-O3'
4	A	603	PKS	CAL-CAM-CAN-CAP
4	C	703	PKS	CAL-CAM-CAN-CAP
6	A	605	1PE	OH4-C13-C23-OH3
5	C	701	PGE	O2-C3-C4-O3
6	C	705	1PE	OH6-C15-C25-OH5
4	B	603	PKS	CAB-CAC-OAH-CAI
4	C	703	PKS	CAB-CAC-OAH-CAI
6	D	605	1PE	OH4-C13-C23-OH3
4	A	603	PKS	CAO-CAM-CAN-CAP
6	C	705	1PE	OH5-C14-C24-OH4
6	D	605	1PE	OH5-C14-C24-OH4
6	E	605	1PE	OH6-C15-C25-OH5
4	B	603	PKS	CAP-CAQ-CAR-CAT
4	C	703	PKS	CAP-CAQ-CAR-CAT
4	D	604	PKS	CAP-CAQ-CAR-CAT
4	F	603	PKS	CAP-CAQ-CAR-CAT
4	B	603	PKS	CAP-CAQ-CAR-CAS
4	C	703	PKS	CAP-CAQ-CAR-CAS
4	D	604	PKS	CAP-CAQ-CAR-CAS
4	F	603	PKS	CAP-CAQ-CAR-CAS
6	D	605	1PE	OH6-C15-C25-OH5
2	B	601	FAD	O2'-C2'-C3'-C4'

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Mol	Chain	Res	Type	Atoms
7	E	608	GOL	O1-C1-C2-O2
6	F	604	1PE	OH4-C13-C23-OH3
4	C	703	PKS	NAD-CAC-OAH-CAI
5	E	604	PGE	O1-C1-C2-O2
6	F	604	1PE	OH2-C12-C22-OH3
2	C	702	FAD	C2'-C3'-C4'-C5'
6	F	604	1PE	OH5-C14-C24-OH4
6	B	604	1PE	OH4-C13-C23-OH3
2	A	601	FAD	O2'-C2'-C3'-O3'
2	C	702	FAD	C2'-C3'-C4'-O4'
5	A	604	PGE	O1-C1-C2-O2
6	D	605	1PE	OH7-C16-C26-OH6
6	E	605	1PE	OH2-C12-C22-OH3
6	F	604	1PE	OH7-C16-C26-OH6
6	F	604	1PE	OH6-C15-C25-OH5
6	E	605	1PE	OH5-C14-C24-OH4
7	A	607	GOL	O1-C1-C2-C3
7	D	601	GOL	C1-C2-C3-O3
7	D	607	GOL	O1-C1-C2-C3
7	E	608	GOL	O1-C1-C2-C3
6	D	605	1PE	OH2-C12-C22-OH3
5	E	604	PGE	O2-C3-C4-O3
7	A	607	GOL	O2-C2-C3-O3
7	A	608	GOL	O1-C1-C2-O2
7	D	601	GOL	O2-C2-C3-O3
7	E	608	GOL	O2-C2-C3-O3
6	B	604	1PE	OH6-C15-C25-OH5
2	E	601	FAD	O4'-C4'-C5'-O5'
5	E	604	PGE	O3-C5-C6-O4
6	A	605	1PE	OH2-C12-C22-OH3
6	C	705	1PE	OH2-C12-C22-OH3
5	C	704	PGE	O2-C3-C4-O3
5	C	701	PGE	O1-C1-C2-O2
2	C	702	FAD	O3'-C3'-C4'-C5'
2	D	602	FAD	C3'-C4'-C5'-O5'
2	E	601	FAD	C3'-C4'-C5'-O5'
4	A	603	PKS	NAD-CAC-OAH-CAI
5	C	704	PGE	O3-C5-C6-O4
7	A	607	GOL	O1-C1-C2-O2
7	A	608	GOL	O2-C2-C3-O3
7	D	601	GOL	O1-C1-C2-O2
7	D	607	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
6	E	605	1PE	C13-C23-OH3-C22
4	D	604	PKS	OBA-CAV-CAW-CAZ
4	A	603	PKS	CAB-CAC-OAH-CAI
5	C	704	PGE	C6-C5-O3-C4
2	C	702	FAD	O3'-C3'-C4'-O4'
2	D	602	FAD	PA-O3P-P-O5'
2	C	702	FAD	O2'-C2'-C3'-C4'
6	E	605	1PE	C25-C15-OH6-C26
6	F	604	1PE	C16-C26-OH6-C15
5	A	604	PGE	C6-C5-O3-C4
4	E	603	PKS	CAP-CAQ-CAR-CAT
4	E	603	PKS	CAP-CAQ-CAR-CAS
6	D	605	1PE	C16-C26-OH6-C15
6	B	604	1PE	C15-C25-OH5-C14
6	A	605	1PE	C16-C26-OH6-C15
2	A	601	FAD	O2'-C2'-C3'-C4'
6	E	605	1PE	C14-C24-OH4-C13
6	B	604	1PE	C12-C22-OH3-C23
6	B	604	1PE	C23-C13-OH4-C24
6	B	604	1PE	C25-C15-OH6-C26
4	A	603	PKS	CAU-CAV-CAW-CAZ
4	C	703	PKS	CAU-CAV-CAW-CAZ
4	D	604	PKS	CAU-CAV-CAW-CAZ
4	F	603	PKS	CAU-CAV-CAW-CAZ
6	C	705	1PE	C25-C15-OH6-C26
6	D	605	1PE	C14-C24-OH4-C13
2	E	601	FAD	C2B-C1B-N9A-C8A
2	F	601	FAD	C2B-C1B-N9A-C8A
2	D	602	FAD	P-O3P-PA-O1A
4	D	604	PKS	CAU-CAV-CAW-CAX
4	F	603	PKS	CAU-CAV-CAW-CAX
6	E	605	1PE	C24-C14-OH5-C25
6	F	604	1PE	C14-C24-OH4-C13
6	E	605	1PE	C16-C26-OH6-C15
6	B	604	1PE	C24-C14-OH5-C25
6	E	605	1PE	OH7-C16-C26-OH6
5	C	701	PGE	C3-C4-O3-C5
6	F	604	1PE	C15-C25-OH5-C14
6	C	705	1PE	C16-C26-OH6-C15
2	B	601	FAD	O4B-C4B-C5B-O5B
2	B	601	FAD	C5'-O5'-P-O2P
6	A	605	1PE	OH6-C15-C25-OH5

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Mol	Chain	Res	Type	Atoms
6	A	605	1PE	C14-C24-OH4-C13
6	E	605	1PE	C12-C22-OH3-C23
6	B	604	1PE	C13-C23-OH3-C22
6	D	605	1PE	C13-C23-OH3-C22
6	F	604	1PE	C24-C14-OH5-C25
5	C	701	PGE	C6-C5-O3-C4
2	F	601	FAD	C2B-C1B-N9A-C4A
4	D	604	PKS	NAD-CAC-OAH-CAI
2	E	601	FAD	O4B-C1B-N9A-C8A
6	D	605	1PE	C24-C14-OH5-C25
6	E	605	1PE	C23-C13-OH4-C24
2	F	601	FAD	PA-O3P-P-O5'
5	A	604	PGE	O3-C5-C6-O4
5	A	604	PGE	C3-C4-O3-C5
2	F	601	FAD	C1'-C2'-C3'-O3'
2	F	601	FAD	O3'-C3'-C4'-C5'
2	C	702	FAD	O2'-C2'-C3'-O3'
2	B	601	FAD	C2B-C1B-N9A-C8A
4	D	604	PKS	CBB-CAU-CAV-OBA
4	E	603	PKS	CBB-CAU-CAV-OBA
6	A	605	1PE	OH5-C14-C24-OH4
6	C	705	1PE	C24-C14-OH5-C25
6	C	705	1PE	OH4-C13-C23-OH3
4	D	604	PKS	CAB-CAC-OAH-CAI
2	A	601	FAD	C3'-C4'-C5'-O5'
2	B	601	FAD	C3'-C4'-C5'-O5'
2	D	602	FAD	P-O3P-PA-O2A
4	D	604	PKS	CAS-CAU-CAV-CAW
6	F	604	1PE	C13-C23-OH3-C22
2	F	601	FAD	O4B-C1B-N9A-C8A
6	A	605	1PE	C25-C15-OH6-C26
2	F	601	FAD	O4B-C4B-C5B-O5B
4	A	603	PKS	CAU-CAV-CAW-CAX
6	B	604	1PE	C16-C26-OH6-C15
2	B	601	FAD	C3B-C4B-C5B-O5B
6	E	605	1PE	OH4-C13-C23-OH3
6	B	604	1PE	OH5-C14-C24-OH4
5	A	604	PGE	O2-C3-C4-O3
2	C	702	FAD	P-O3P-PA-O2A
4	D	604	PKS	CAO-CAM-CAN-CAP
2	A	601	FAD	O4B-C4B-C5B-O5B

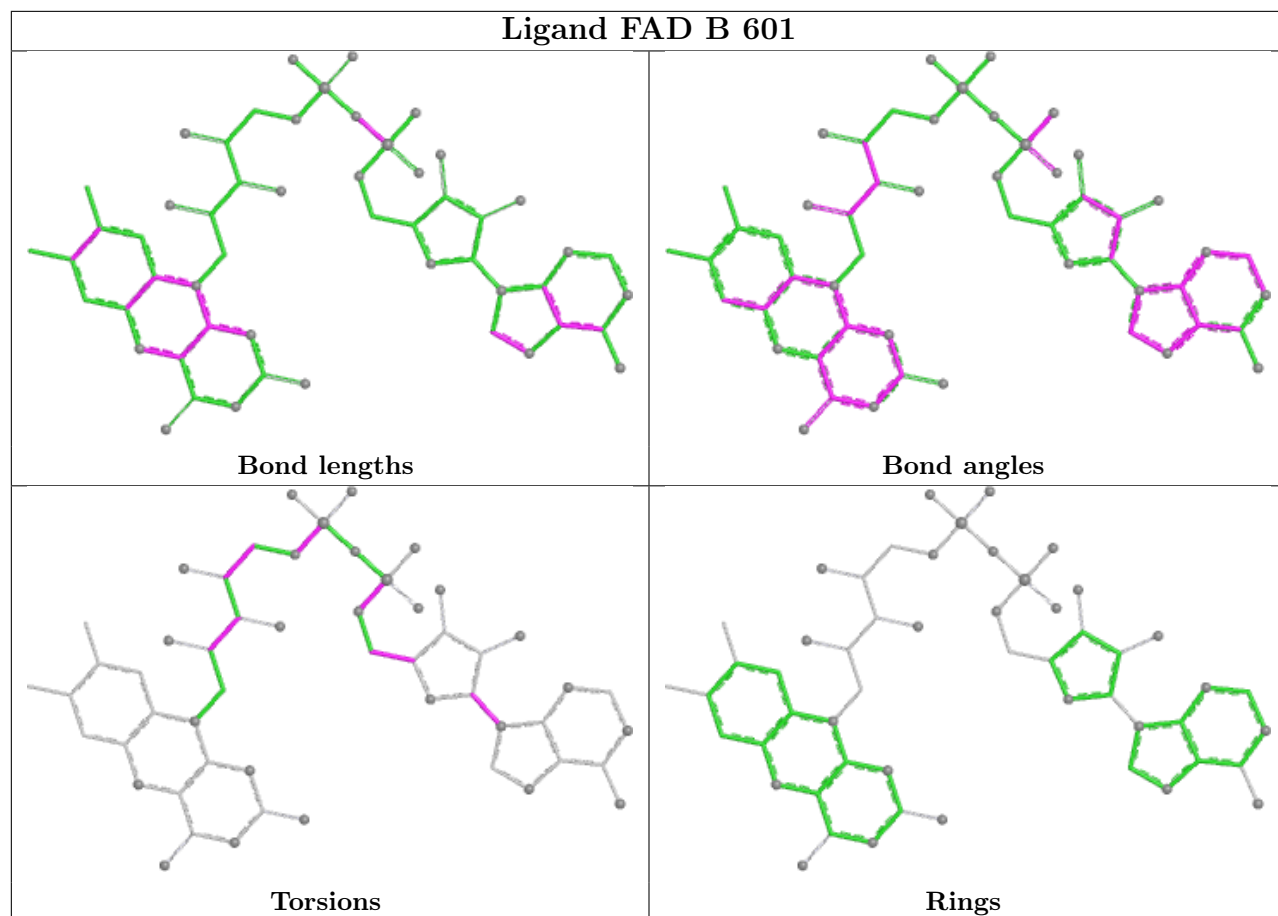
There are no ring outliers.

15 monomers are involved in 53 short contacts:

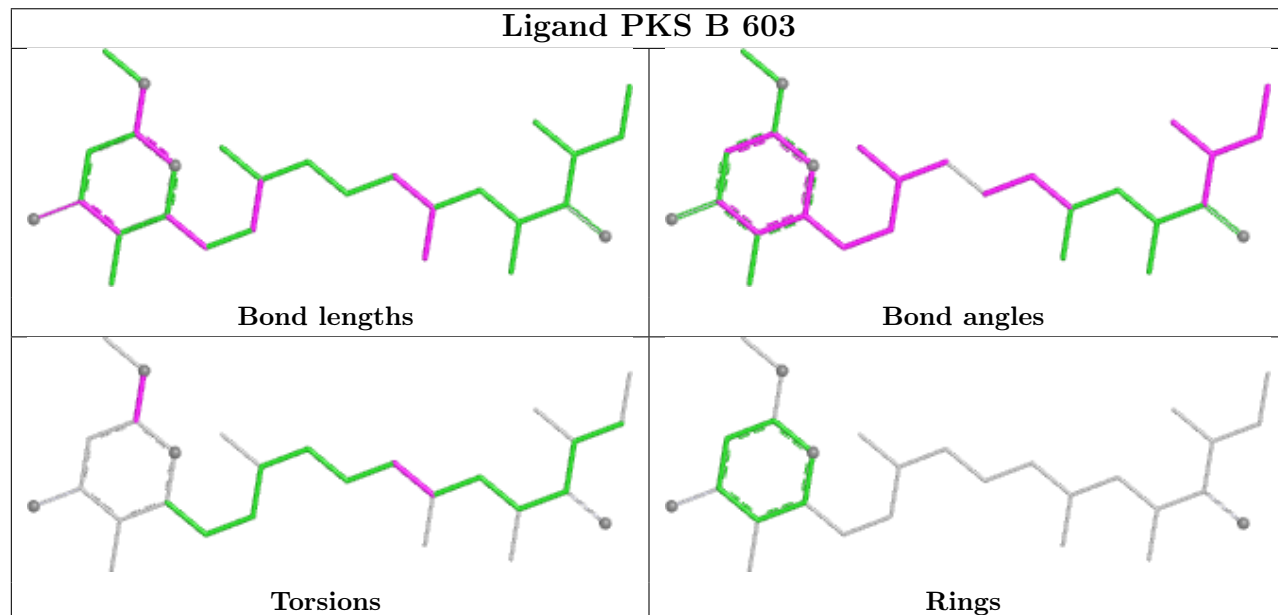
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	FAD	4	0
6	A	605	1PE	2	0
6	B	604	1PE	2	0
2	C	702	FAD	4	0
2	A	601	FAD	4	0
4	F	603	PKS	1	0
6	E	605	1PE	3	0
2	F	601	FAD	8	0
2	D	602	FAD	14	0
6	C	705	1PE	2	0
4	A	603	PKS	1	0
7	A	608	GOL	1	0
7	D	607	GOL	1	0
2	E	601	FAD	5	0
4	D	604	PKS	1	0

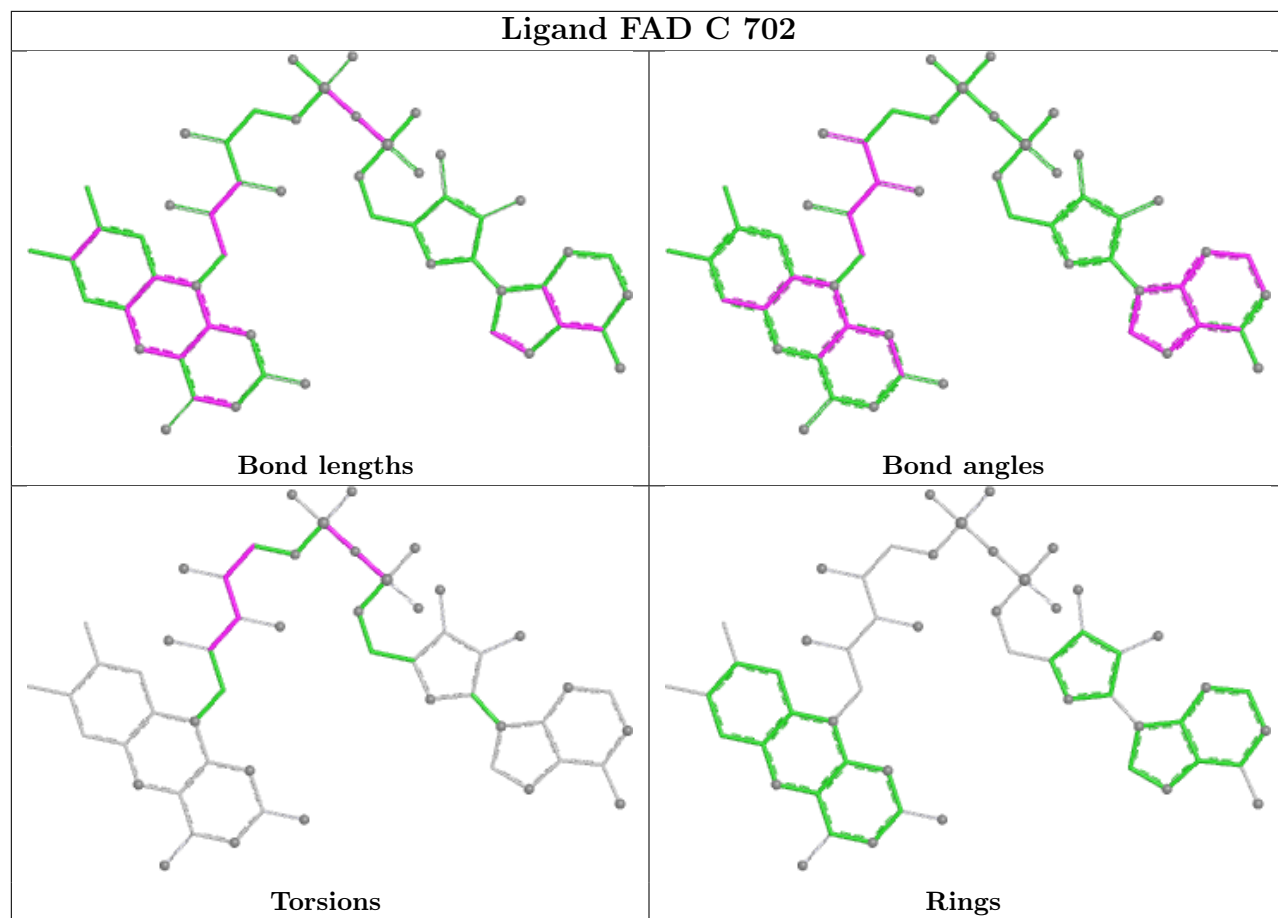
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand FAD B 601

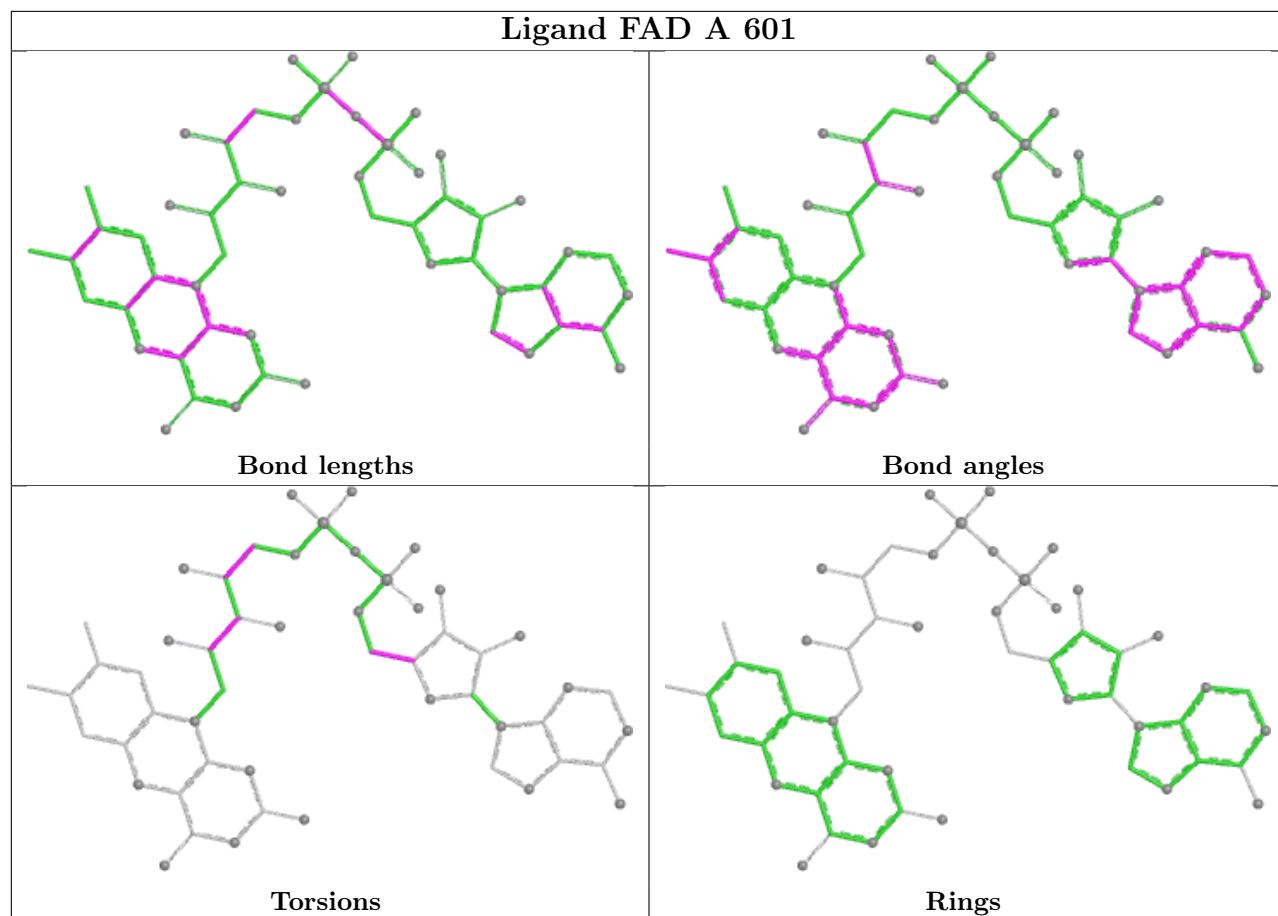


Ligand PKS B 603

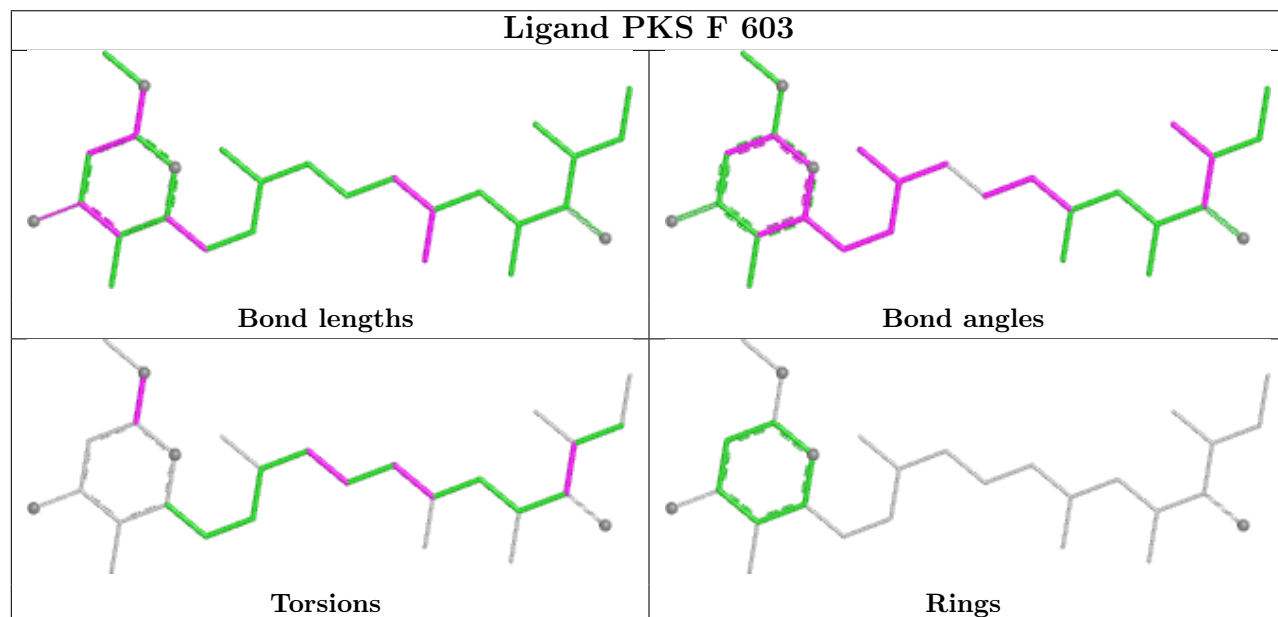




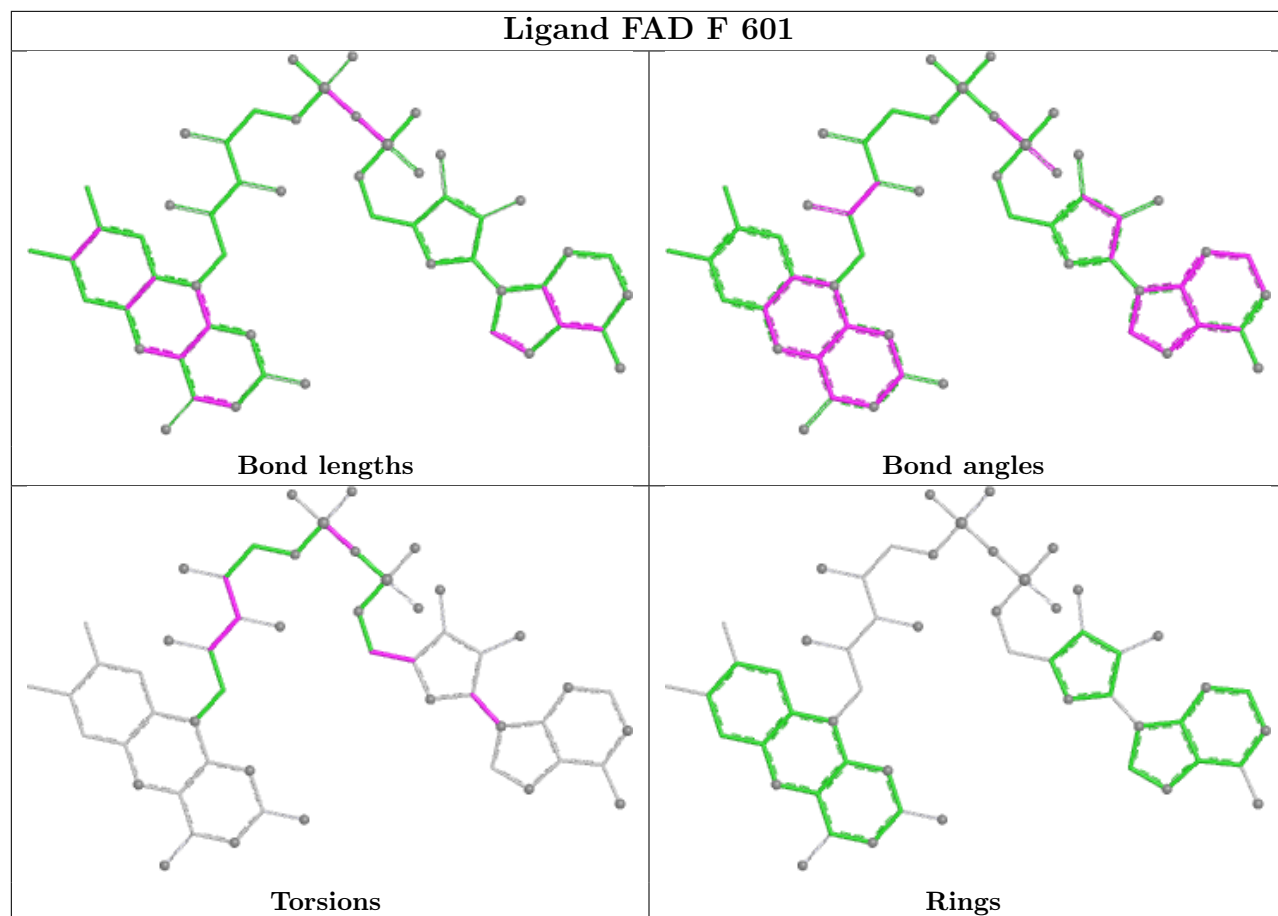
Ligand FAD A 601



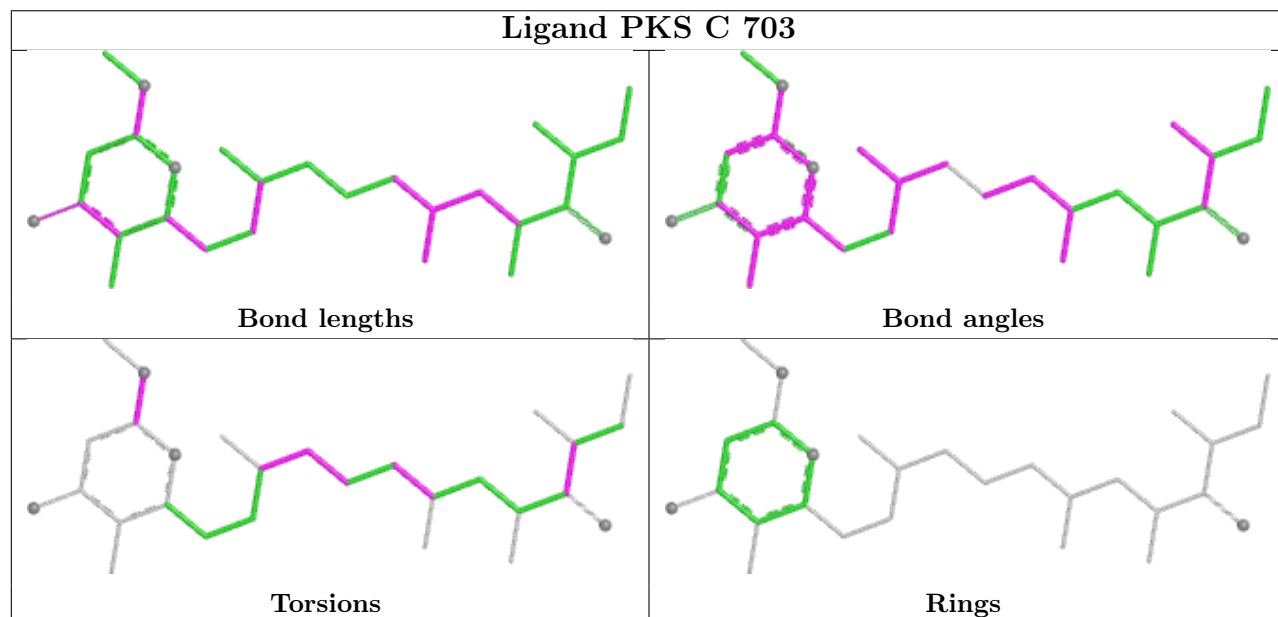
Ligand PKS F 603



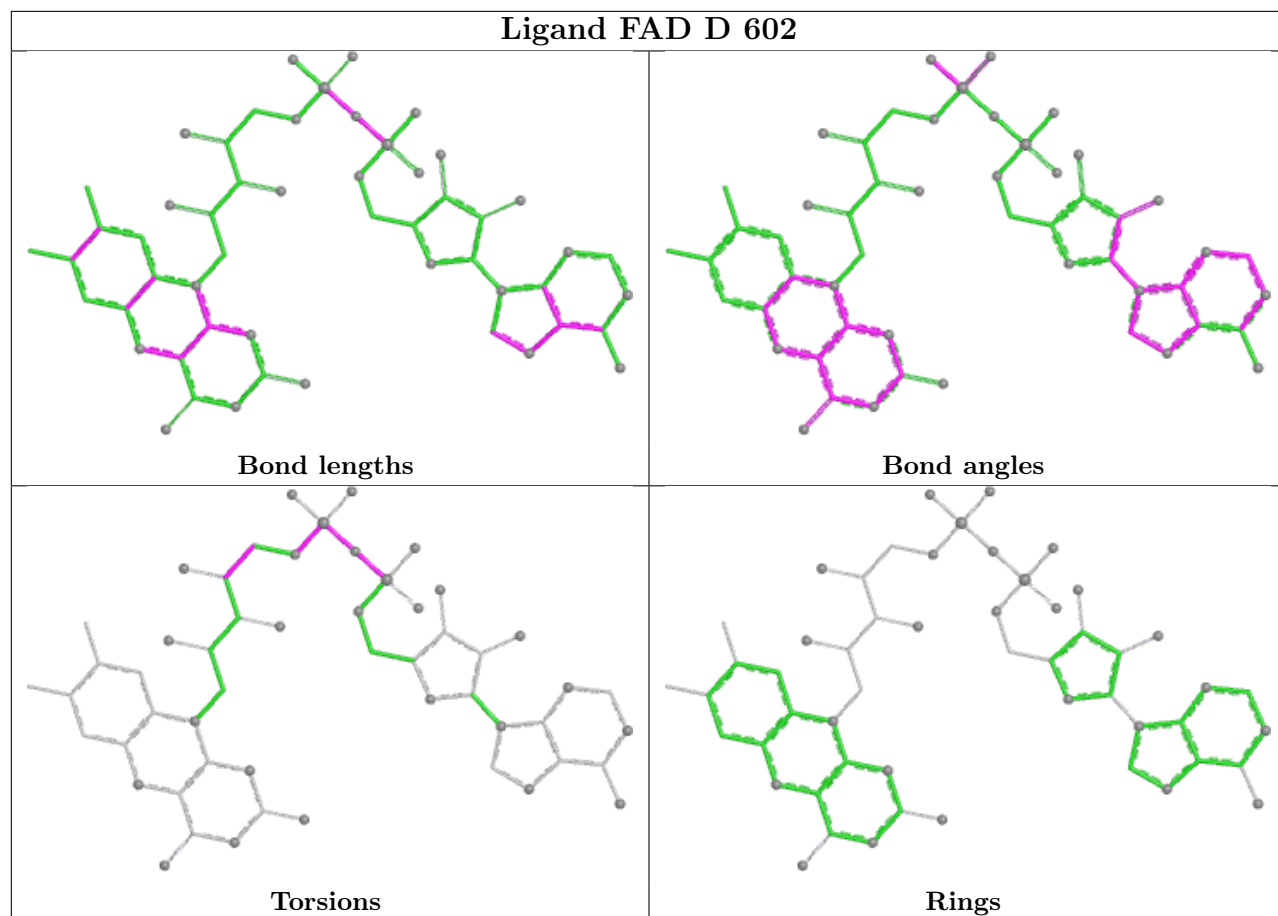
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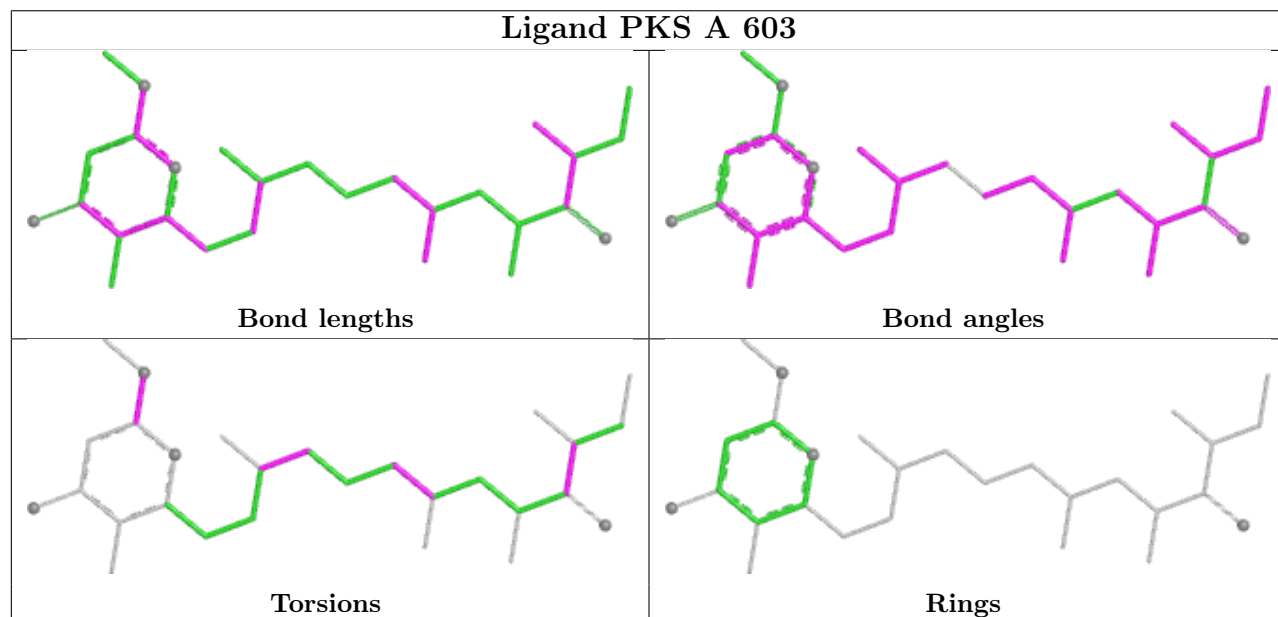
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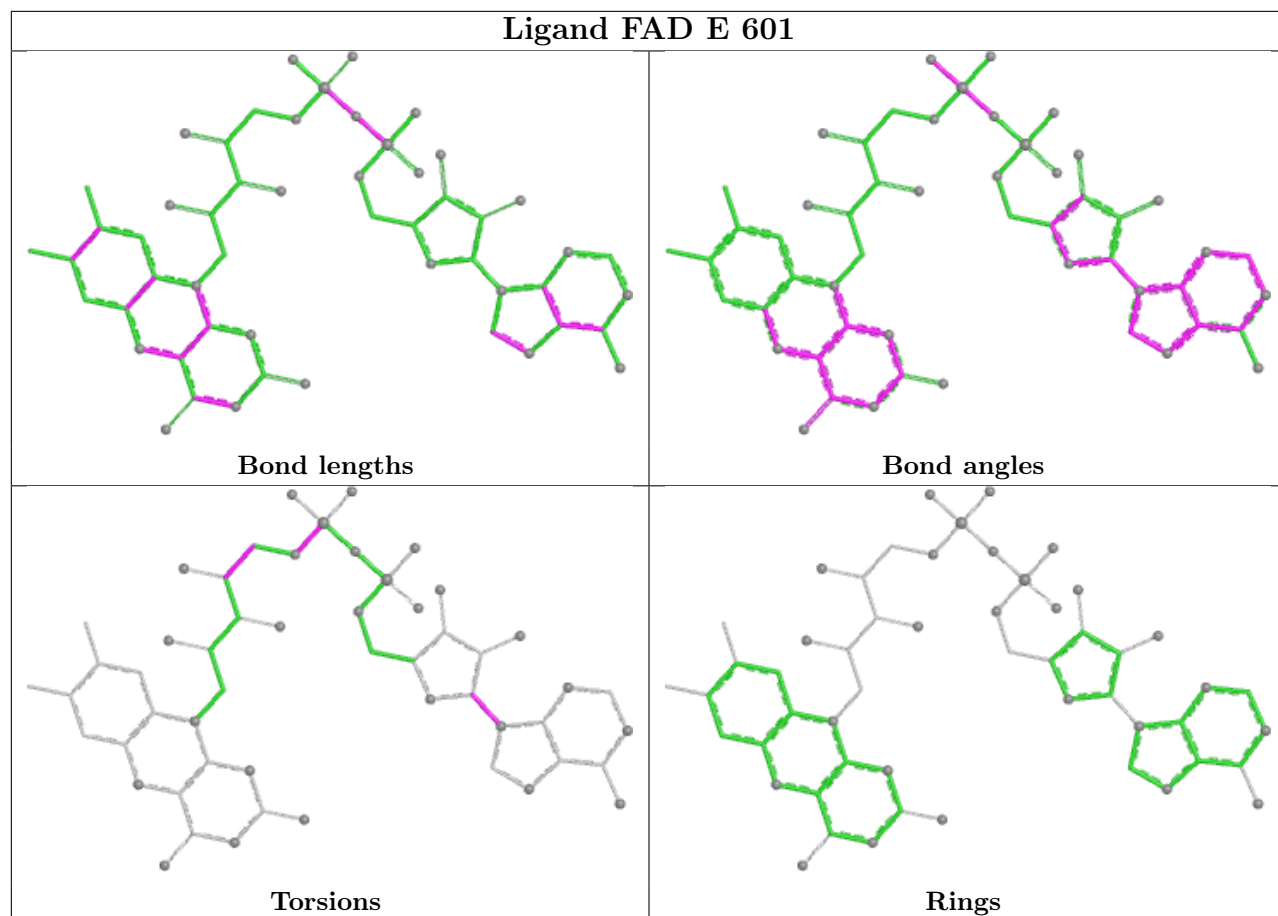
Ligand FAD D 602



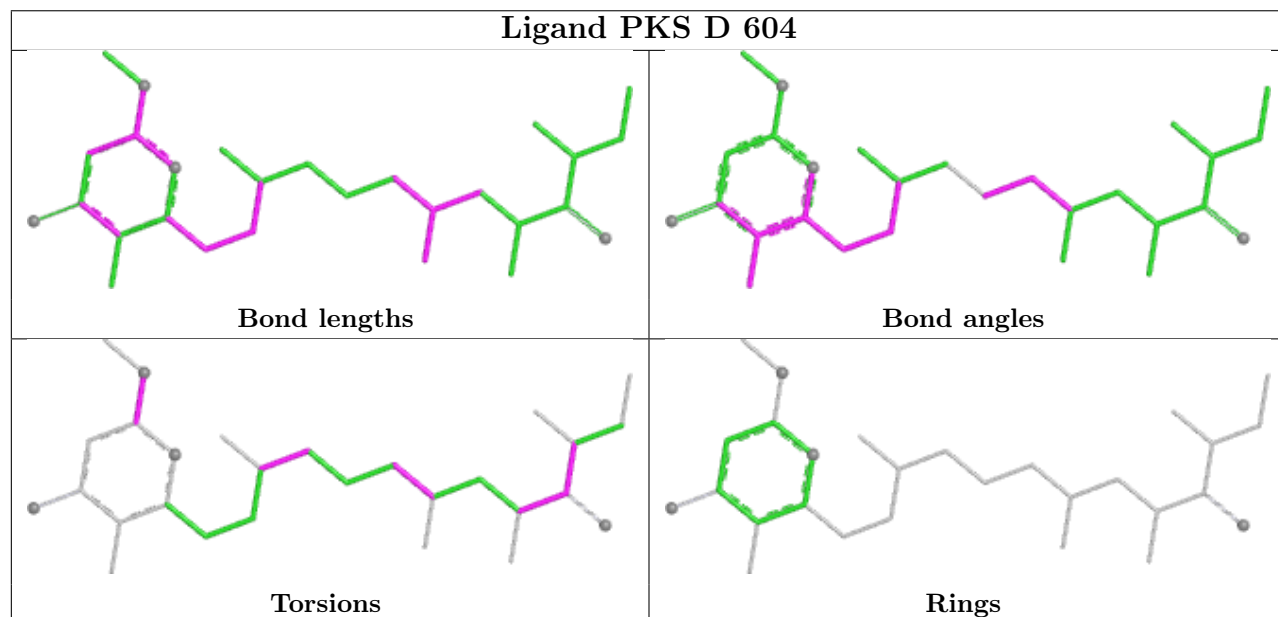
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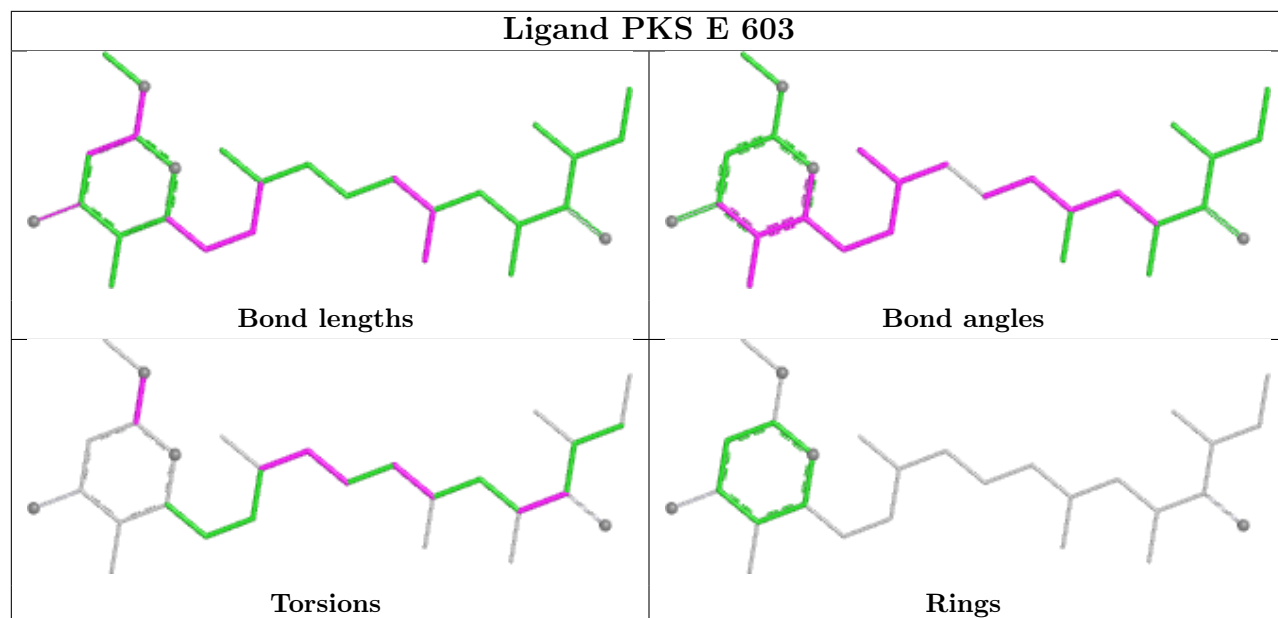


Ligand FAD E 601



Ligand PKS D 604





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	579/601 (96%)	-0.51	2 (0%) 90 88	22, 40, 69, 104	0
1	B	579/601 (96%)	-0.06	11 (1%) 66 63	24, 51, 87, 115	0
1	C	580/601 (96%)	-0.55	1 (0%) 91 90	24, 39, 70, 107	0
1	D	579/601 (96%)	0.35	36 (6%) 26 24	27, 61, 97, 137	0
1	E	579/601 (96%)	-0.07	5 (0%) 81 79	33, 55, 93, 116	0
1	F	580/601 (96%)	0.59	62 (10%) 11 9	31, 71, 111, 142	0
All	All	3476/3606 (96%)	-0.04	117 (3%) 48 44	22, 50, 95, 142	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	134	VAL	6.6
1	F	134	VAL	6.1
1	D	41	VAL	5.2
1	F	11	ILE	4.7
1	F	35	GLY	4.4
1	F	92	PHE	4.2
1	F	403	LEU	4.1
1	F	41	VAL	4.1
1	F	36	VAL	4.0
1	B	586	PRO	3.9
1	F	145	LEU	3.9
1	D	11	ILE	3.5
1	E	586	PRO	3.4
1	F	232	ALA	3.4
1	F	7	THR	3.3
1	F	163	SER	3.3
1	A	586	PRO	3.3
1	F	352	GLY	3.2
1	D	183	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	181	LEU	3.2
1	F	18	VAL	3.2
1	B	407	HIS	3.2
1	D	37	PRO	3.1
1	F	9	PRO	3.1
1	D	15	VAL	3.1
1	B	8	ALA	3.1
1	F	174	TYR	3.0
1	F	407	HIS	3.0
1	F	47	THR	3.0
1	B	232	ALA	3.0
1	F	133	LEU	3.0
1	F	388	LEU	3.0
1	F	6	GLY	3.0
1	D	586	PRO	2.9
1	D	133	LEU	2.9
1	D	174	TYR	2.9
1	D	141	CYS	2.8
1	F	171	GLY	2.8
1	F	231	GLY	2.8
1	F	39	LEU	2.8
1	F	13	VAL	2.7
1	F	166	THR	2.7
1	D	197	ILE	2.7
1	F	267	VAL	2.7
1	D	8	ALA	2.7
1	D	352	GLY	2.7
1	F	37	PRO	2.7
1	F	175	THR	2.7
1	F	97	VAL	2.7
1	D	13	VAL	2.6
1	D	142	VAL	2.6
1	D	161	VAL	2.6
1	F	8	ALA	2.6
1	D	407	HIS	2.6
1	D	9	PRO	2.6
1	F	24	GLY	2.6
1	D	356	LEU	2.5
1	D	39	LEU	2.5
1	D	36	VAL	2.5
1	F	151	PHE	2.5
1	B	265	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	261	PRO	2.4
1	F	17	ILE	2.4
1	F	182	ILE	2.4
1	F	31	LEU	2.4
1	D	35	GLY	2.4
1	E	532	GLY	2.4
1	D	16	LEU	2.4
1	F	149	HIS	2.4
1	F	273	VAL	2.4
1	E	267	VAL	2.3
1	D	353	PRO	2.3
1	F	284	PRO	2.3
1	E	52	ARG	2.3
1	D	180	TYR	2.3
1	E	8	ALA	2.3
1	F	389	GLY	2.3
1	F	147	PHE	2.3
1	F	15	VAL	2.3
1	D	45	HIS	2.3
1	D	137	VAL	2.3
1	B	284	PRO	2.3
1	F	146	ARG	2.3
1	D	145	LEU	2.2
1	F	165	ILE	2.2
1	B	267	VAL	2.2
1	C	8	ALA	2.2
1	F	222	ALA	2.2
1	D	38	HIS	2.2
1	D	146	ARG	2.2
1	F	390	PHE	2.2
1	B	296	TRP	2.2
1	D	169	ARG	2.2
1	F	72	ARG	2.2
1	B	233	VAL	2.2
1	F	176	VAL	2.2
1	F	45	HIS	2.2
1	F	192	LEU	2.2
1	F	217	LEU	2.1
1	D	18	VAL	2.1
1	F	87	VAL	2.1
1	F	387	ALA	2.1
1	A	262	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	46	GLY	2.1
1	F	129	LEU	2.1
1	F	353	PRO	2.1
1	B	93	ALA	2.1
1	F	391	THR	2.1
1	F	184	ALA	2.1
1	D	17	ILE	2.1
1	F	88	PHE	2.0
1	F	40	LEU	2.0
1	D	148	GLY	2.0
1	D	151	PHE	2.0
1	F	311	VAL	2.0
1	B	406	LEU	2.0
1	F	193	ALA	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
2	FAD	F	601	53/53	0.76	0.16	77,104,114,118	21
2	FAD	D	602	53/53	0.77	0.17	60,88,110,115	21
7	GOL	D	607	6/6	0.83	0.18	61,77,81,83	0
6	1PE	F	604	16/16	0.84	0.16	68,85,93,100	0
3	CL	F	605	1/1	0.84	0.10	83,83,83,83	0
3	CL	F	602	1/1	0.86	0.13	70,70,70,70	1
7	GOL	A	607	6/6	0.87	0.16	59,72,73,75	0
5	PGE	C	701	10/10	0.87	0.14	55,73,83,86	0
6	1PE	A	605	16/16	0.88	0.16	63,75,83,88	0

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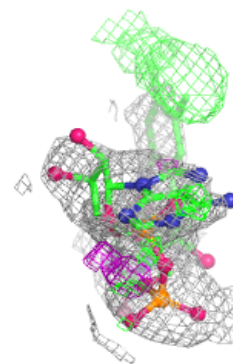
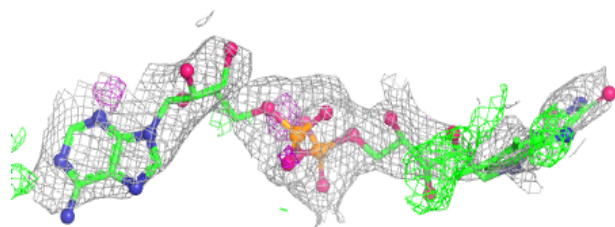
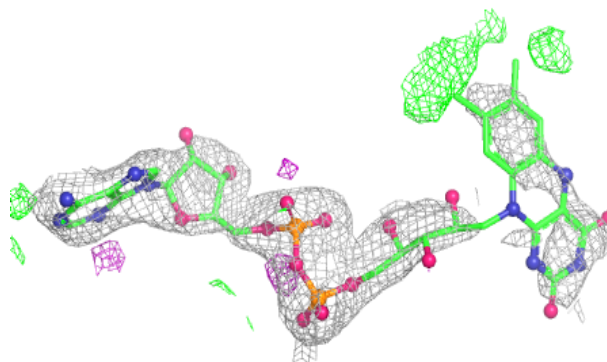
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	1PE	E	605	16/16	0.88	0.13	70,80,84,88	0
2	FAD	E	601	53/53	0.88	0.13	52,71,84,90	21
2	FAD	B	601	53/53	0.88	0.13	48,67,84,86	21
7	GOL	A	608	6/6	0.88	0.14	60,66,70,70	0
3	CL	D	606	1/1	0.88	0.10	78,78,78,78	0
7	GOL	E	607	6/6	0.88	0.13	70,78,82,86	0
7	GOL	E	608	6/6	0.88	0.13	60,74,80,80	0
3	CL	D	603	1/1	0.90	0.10	68,68,68,68	1
6	1PE	D	605	16/16	0.91	0.12	59,66,86,87	0
7	GOL	D	601	6/6	0.91	0.12	51,56,60,68	0
2	FAD	C	702	53/53	0.91	0.13	46,65,94,96	0
2	FAD	A	601	53/53	0.91	0.10	37,52,66,67	21
6	1PE	B	604	16/16	0.91	0.13	63,71,78,80	0
5	PGE	E	604	10/10	0.92	0.12	56,61,68,70	0
5	PGE	A	604	10/10	0.92	0.13	54,57,74,81	0
5	PGE	C	704	10/10	0.93	0.11	48,56,59,64	0
3	CL	B	602	1/1	0.93	0.10	63,63,63,63	1
6	1PE	C	705	16/16	0.93	0.12	57,66,82,85	0
3	CL	E	602	1/1	0.95	0.06	59,59,59,59	1
4	PKS	B	603	28/28	0.95	0.09	40,47,71,77	0
4	PKS	D	604	28/28	0.95	0.10	37,54,69,70	0
4	PKS	F	603	28/28	0.95	0.12	53,68,94,105	0
4	PKS	C	703	28/28	0.96	0.08	23,32,60,61	0
3	CL	E	606	1/1	0.96	0.09	71,71,71,71	0
4	PKS	E	603	28/28	0.96	0.08	31,41,68,70	0
4	PKS	A	603	28/28	0.96	0.08	24,41,52,64	0
3	CL	A	602	1/1	0.96	0.07	59,59,59,59	1
3	CL	A	606	1/1	0.97	0.08	64,64,64,64	0
3	CL	C	706	1/1	0.97	0.07	72,72,72,72	0
3	CL	B	605	1/1	0.98	0.12	65,65,65,65	0

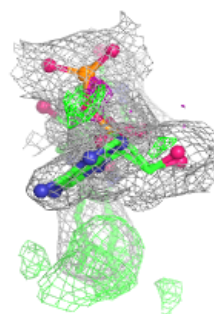
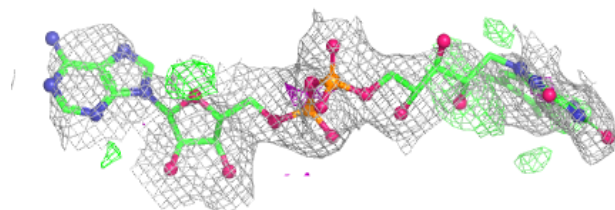
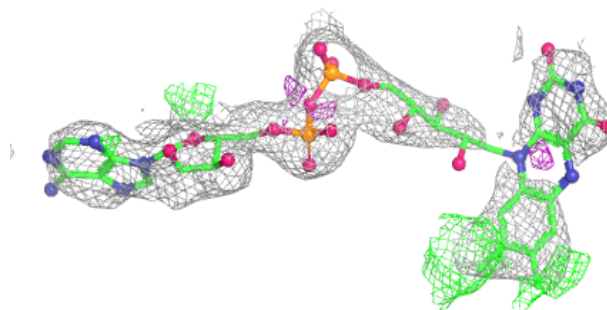
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD F 601:

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

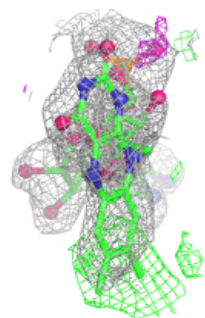
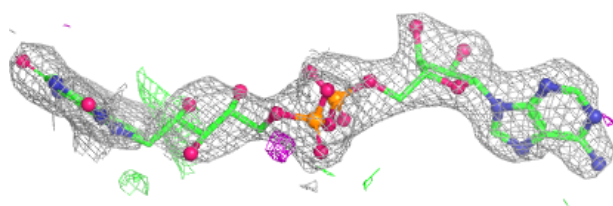
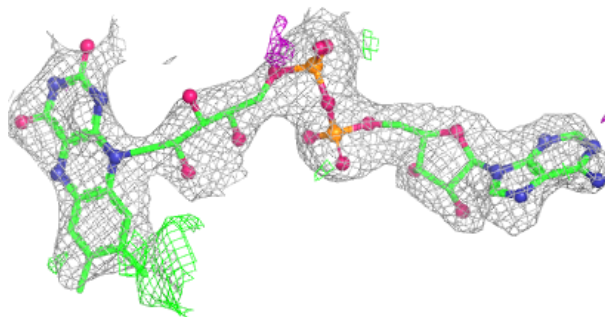
**Electron density around FAD D 602:**

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

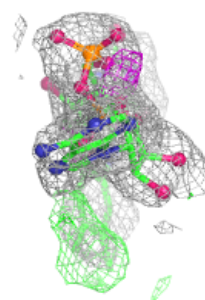
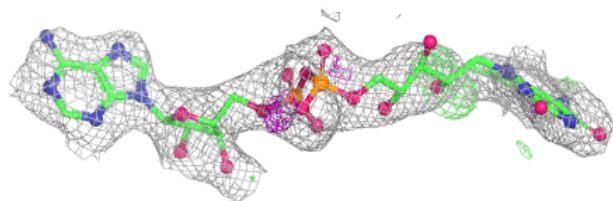
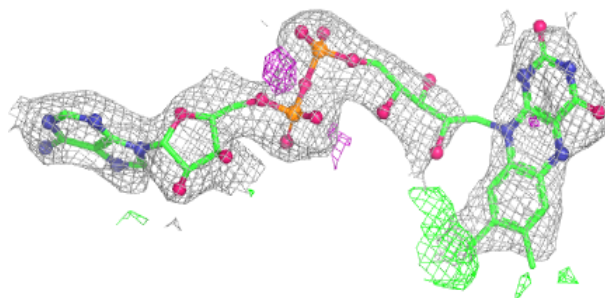


Electron density around FAD E 601:

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

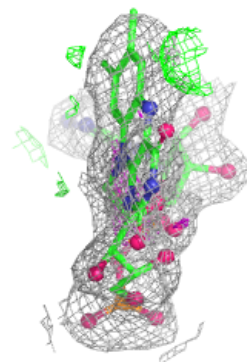
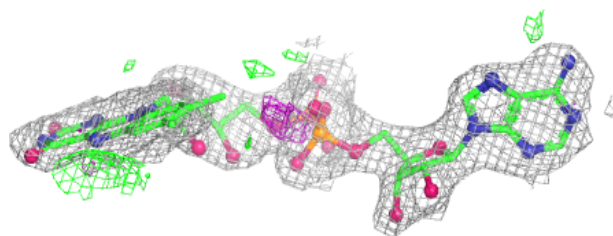
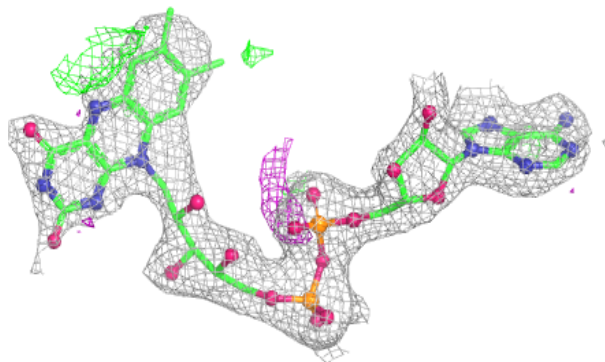
**Electron density around FAD B 601:**

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

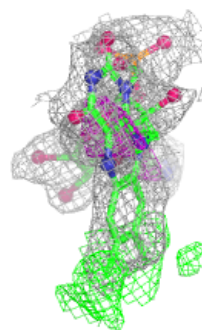
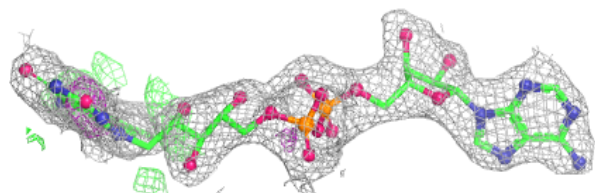
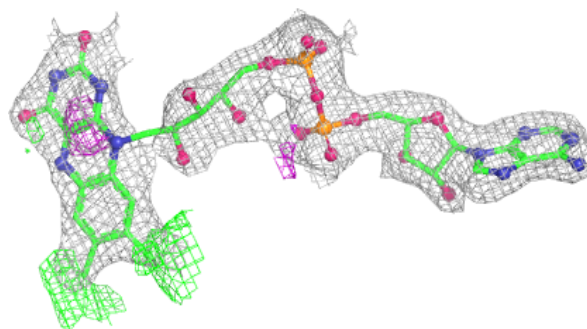


Electron density around FAD C 702:

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

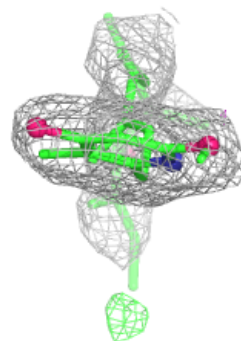
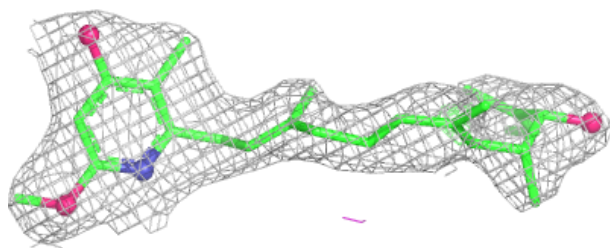
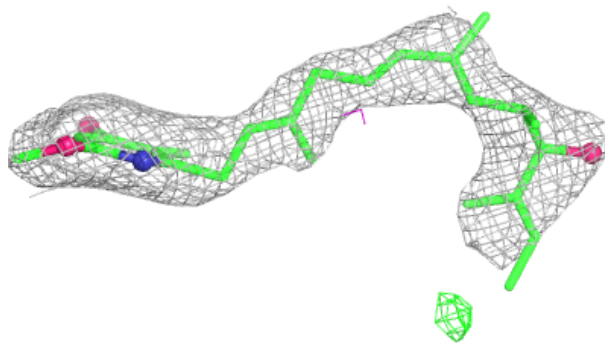
**Electron density around FAD A 601:**

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

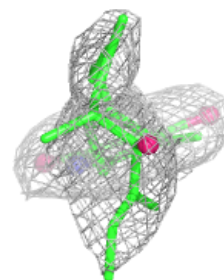
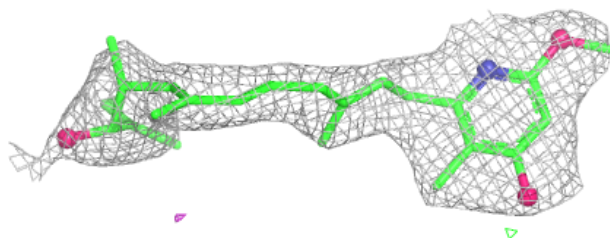
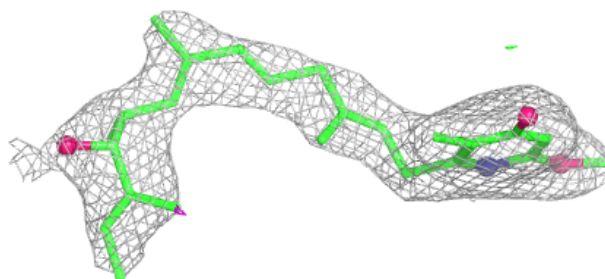


Electron density around PKS B 603:

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

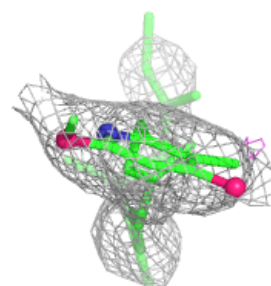
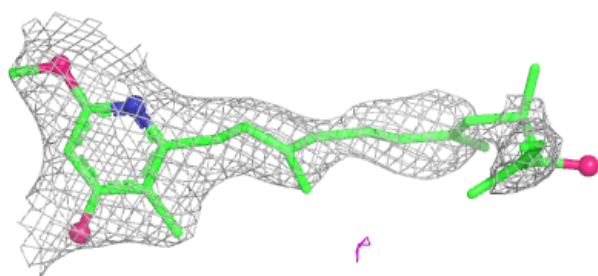
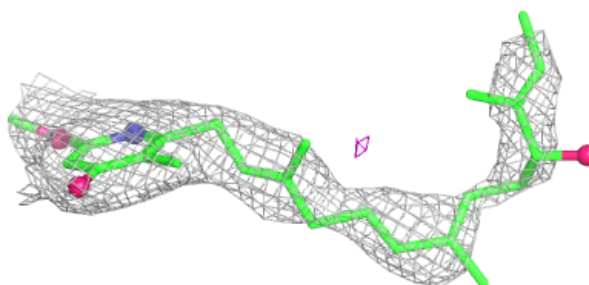
**Electron density around PKS D 604:**

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

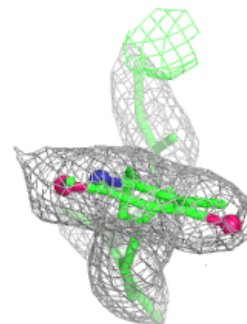
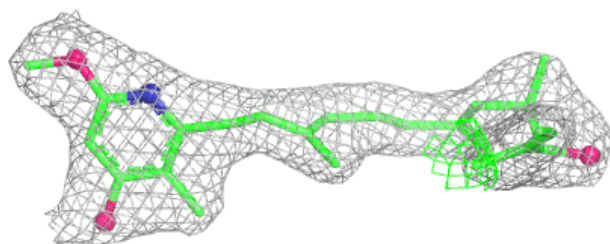
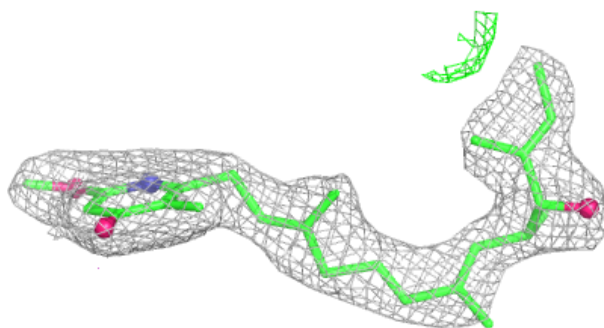


Electron density around PKS F 603:

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

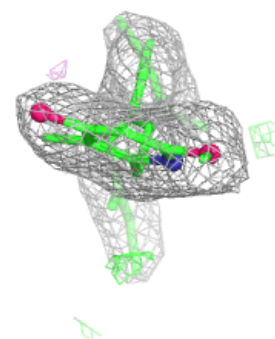
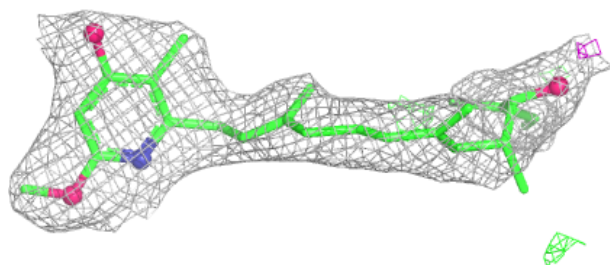
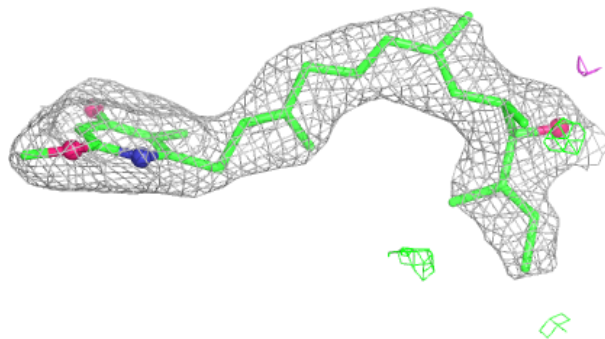
**Electron density around PKS C 703:**

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

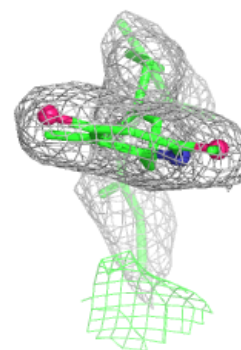
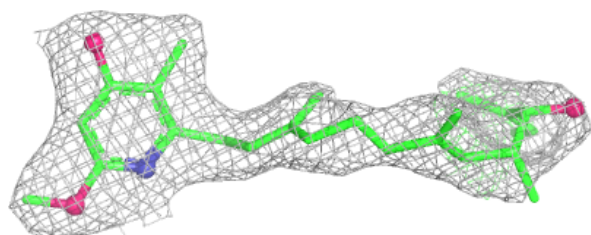
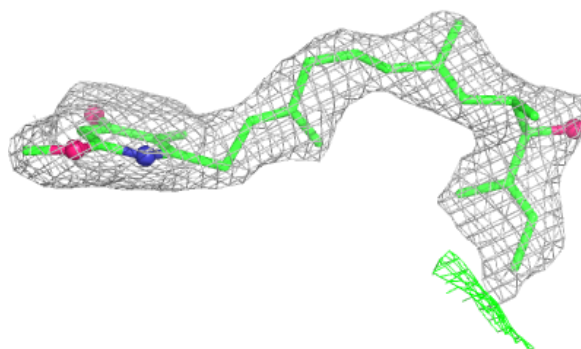


Electron density around PKS E 603:

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

**Electron density around PKS A 603:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.