



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:37 PM UTC

PDB ID : 6U0P / pdb_00006u0p
Title : Crystal structure of PieE, the flavin-dependent monooxygenase involved in the biosynthesis of piericidin A1
Authors : Shi, R.; Manenda, M.; Picard, M.-E.
Deposited on : 2019-08-14
Resolution : 2.02 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:

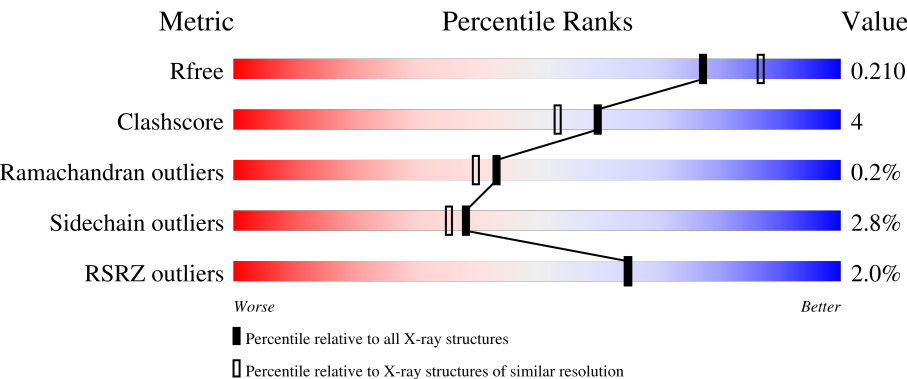
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.02 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	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

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	2% 87% 10%
1	B	601	2% 83% 13%
1	C	601	% 87% 9%
1	D	601	3% 87% 9%
1	E	601	2% 84% 11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	601	2% 87% 8% . .

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 29588 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	581	Total	C	N	O	S	0	0	0
			4434	2770	830	824	10			
1	B	579	Total	C	N	O	S	0	0	0
			4423	2764	828	821	10			
1	C	585	Total	C	N	O	S	0	0	0
			4470	2791	840	829	10			
1	D	578	Total	C	N	O	S	0	0	0
			4416	2759	827	820	10			
1	E	579	Total	C	N	O	S	0	1	0
			4431	2768	831	822	10			
1	F	579	Total	C	N	O	S	0	0	0
			4426	2765	828	823	10			

There are 18 discrepancies between the modelled and reference sequences:

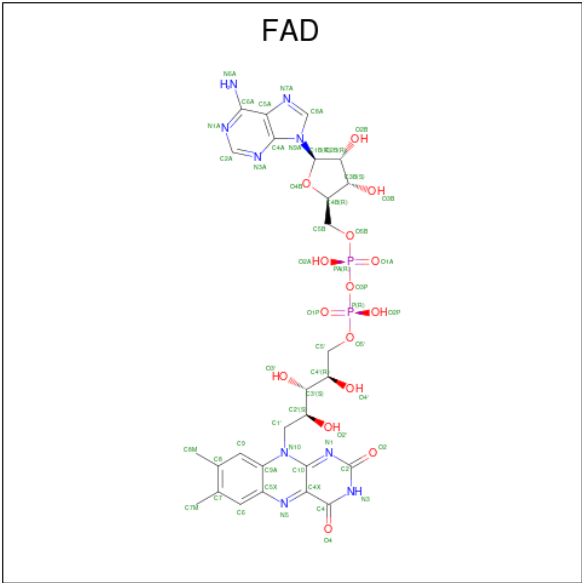
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP W0C4C9
A	-1	SER	-	expression tag	UNP W0C4C9
A	0	HIS	-	expression tag	UNP W0C4C9
B	-2	GLY	-	expression tag	UNP W0C4C9
B	-1	SER	-	expression tag	UNP W0C4C9
B	0	HIS	-	expression tag	UNP W0C4C9
C	-2	GLY	-	expression tag	UNP W0C4C9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

Continued on next page...

Continued from previous page...

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

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂) (labeled as "Ligand of Interest" by depositor).



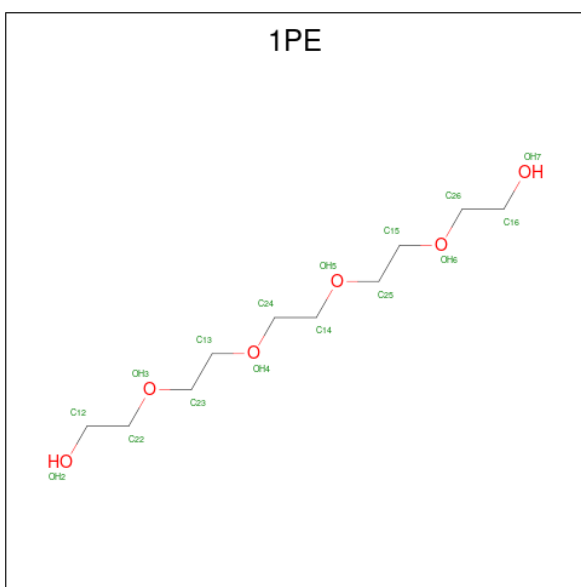
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		
3	A	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			10	6	4		
3	C	1	Total	C	O	0	0
			10	6	4		
3	C	1	Total	C	O	0	0
			10	6	4		
3	D	1	Total	C	O	0	0
			10	6	4		
3	D	1	Total	C	O	0	0
			10	6	4		
3	E	1	Total	C	O	0	0
			10	6	4		
3	E	1	Total	C	O	0	0
			10	6	4		
3	F	1	Total	C	O	0	0
			10	6	4		
3	F	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).



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

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	E	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total	C	O	0	0
			6	3	3		
6	F	1	Total	C	O	0	0
			6	3	3		
6	F	1	Total	C	O	0	0
			6	3	3		

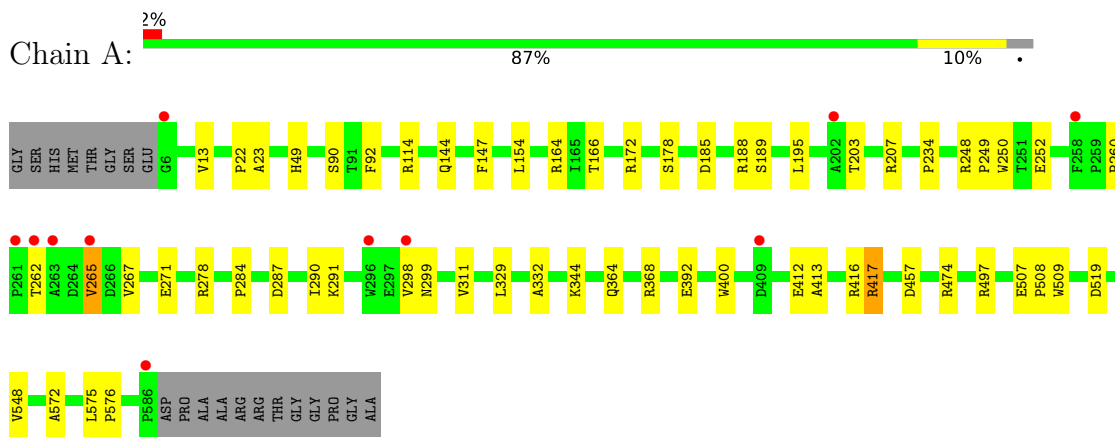
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	325	Total	O	0	0
			325	325		
7	B	362	Total	O	0	0
			362	362		
7	C	466	Total	O	0	0
			466	466		
7	D	411	Total	O	0	0
			411	411		
7	E	449	Total	O	0	0
			449	449		
7	F	329	Total	O	0	0
			329	329		

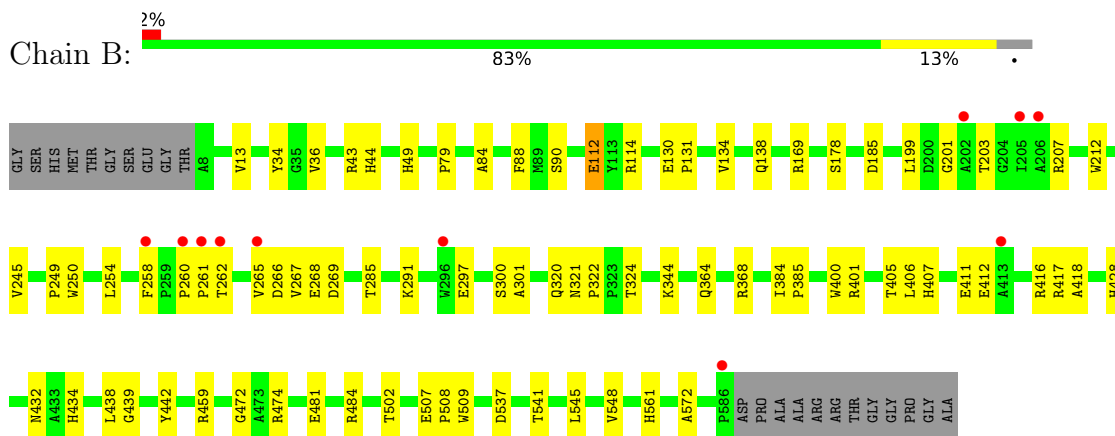
3 Residue-property plots [i](#)

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.

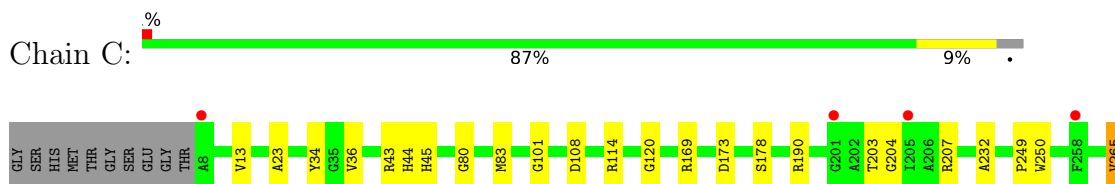
- Molecule 1: 2,4-dichlorophenol 6-monooxygenase

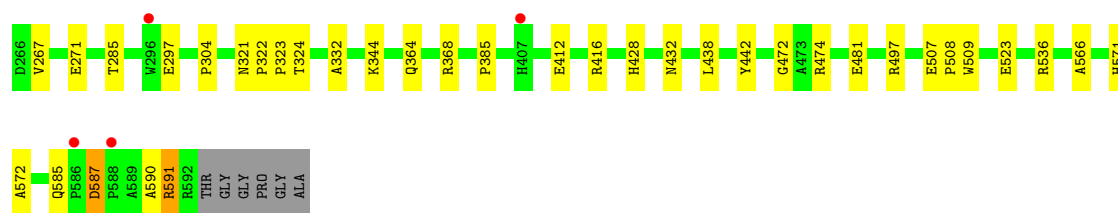


- Molecule 1: 2,4-dichlorophenol 6-monooxygenase

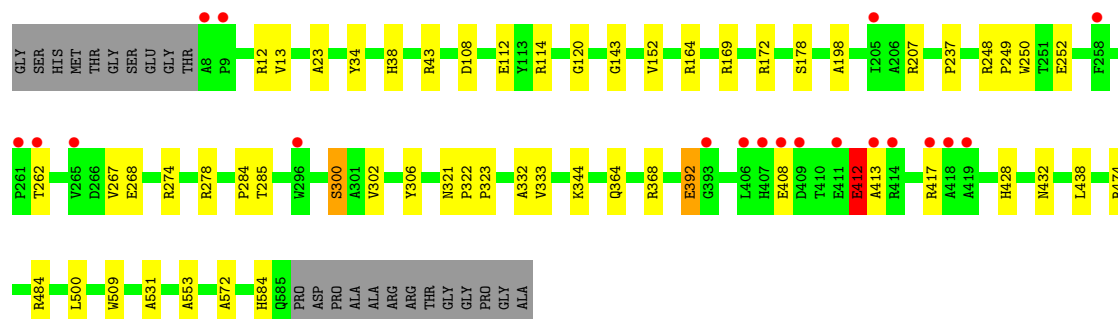
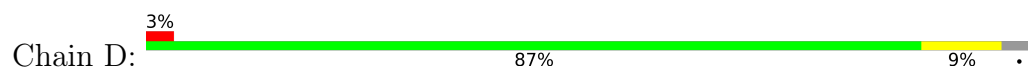


- Molecule 1: 2,4-dichlorophenol 6-monooxygenase

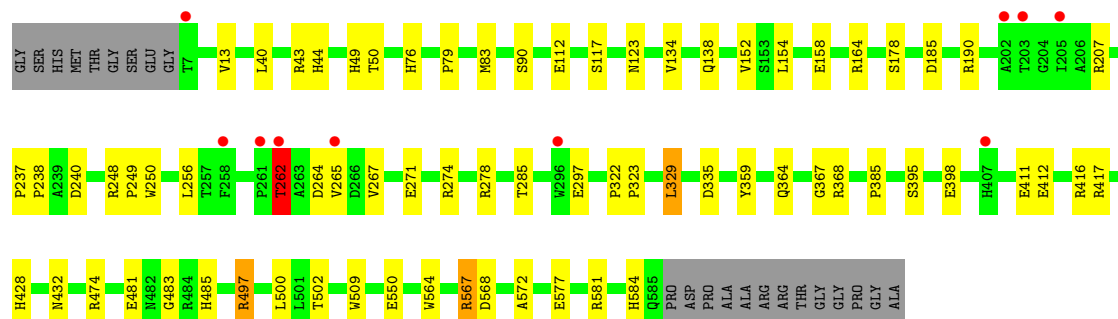
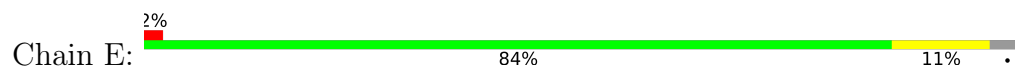




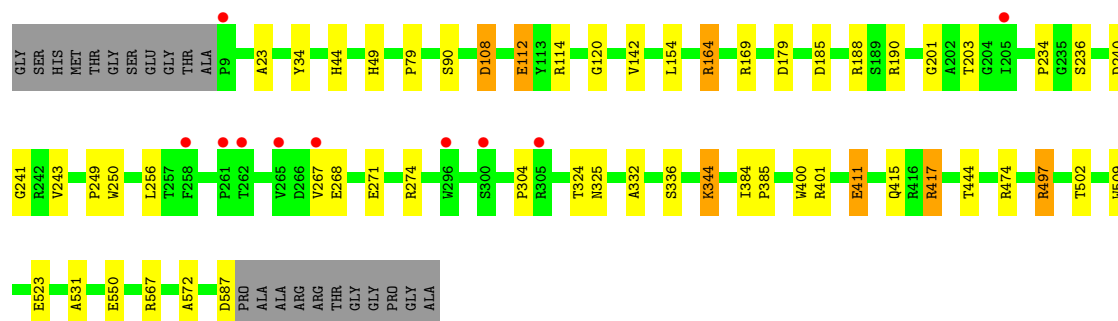
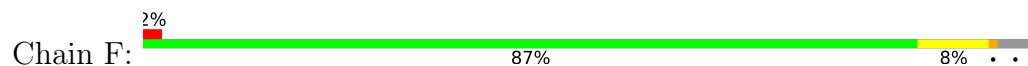
• Molecule 1: 2,4-dichlorophenol 6-monooxygenase



• 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	91.57Å 187.41Å 241.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.34 – 2.02 49.34 – 2.02	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.34-2.02) 99.8 (49.34-2.02)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.170 , 0.204 0.179 , 0.210	Depositor DCC
R_{free} test set	13453 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	29.6	Xtriage
Anisotropy	0.441	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	29588	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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: 1PE, FAD, GOL, CL, PGE

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	1.15	0/4548	1.30	7/6209 (0.1%)
1	B	1.13	4/4537 (0.1%)	1.29	8/6194 (0.1%)
1	C	1.12	2/4585 (0.0%)	1.30	4/6259 (0.1%)
1	D	1.10	1/4529 (0.0%)	1.31	4/6182 (0.1%)
1	E	1.12	4/4547 (0.1%)	1.31	14/6206 (0.2%)
1	F	1.12	3/4540 (0.1%)	1.31	11/6197 (0.2%)
All	All	1.12	14/27286 (0.1%)	1.30	48/37247 (0.1%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	367	GLY	C-O	7.47	1.32	1.23
1	B	561	HIS	CE1-NE2	7.31	1.39	1.32
1	B	434	HIS	CE1-NE2	6.36	1.39	1.32
1	E	564	TRP	C-O	6.23	1.31	1.23
1	B	439	GLY	C-O	5.91	1.29	1.24
1	E	50	THR	N-CA	5.39	1.49	1.46
1	C	36	VAL	N-CA	5.38	1.50	1.46
1	F	531	ALA	C-O	5.37	1.30	1.23
1	F	112	GLU	CD-OE1	5.36	1.35	1.25
1	E	485	HIS	CE1-NE2	5.29	1.37	1.32
1	F	336	SER	C-O	5.29	1.30	1.24
1	D	531	ALA	C-O	5.20	1.29	1.23
1	B	36	VAL	N-CA	5.15	1.50	1.46
1	C	304	PRO	C-O	-5.14	1.18	1.24

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	587	ASP	CB-CA-C	7.62	117.71	110.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	335	ASP	CA-CB-CG	6.65	119.25	112.60
1	F	411	GLU	CA-C-N	6.55	131.61	121.19
1	F	411	GLU	C-N-CA	6.55	131.61	121.19
1	D	412	GLU	CA-C-N	6.49	129.81	120.79
1	D	412	GLU	C-N-CA	6.49	129.81	120.79
1	F	185	ASP	CA-CB-CG	6.42	119.02	112.60
1	E	322	PRO	N-CA-C	-6.21	103.12	110.70
1	E	79	PRO	CA-C-N	6.15	126.92	120.03
1	E	79	PRO	C-N-CA	6.15	126.92	120.03
1	B	481	GLU	CB-CA-C	6.07	119.48	110.14
1	F	79	PRO	CA-C-N	5.98	126.73	120.03
1	F	79	PRO	C-N-CA	5.98	126.73	120.03
1	D	300	SER	CB-CA-C	5.97	119.25	111.42
1	F	304	PRO	N-CA-C	-5.89	106.50	113.86
1	F	201	GLY	CA-C-O	-5.85	118.10	122.37
1	B	201	GLY	CA-C-O	-5.73	118.18	122.37
1	B	185	ASP	CA-CB-CG	5.62	118.22	112.60
1	B	79	PRO	CA-C-N	5.59	126.29	120.03
1	B	79	PRO	C-N-CA	5.59	126.29	120.03
1	E	577	GLU	CB-CG-CD	5.53	122.00	112.60
1	C	585	GLN	CB-CA-C	5.52	118.93	109.82
1	F	240	ASP	CA-C-N	5.47	125.17	119.92
1	F	240	ASP	C-N-CA	5.47	125.17	119.92
1	A	185	ASP	CA-CB-CG	5.47	118.07	112.60
1	D	333	VAL	N-CA-C	-5.44	105.20	110.42
1	C	438	LEU	N-CA-CB	-5.40	103.71	110.90
1	E	411	GLU	CA-C-N	5.39	127.78	120.44
1	E	411	GLU	C-N-CA	5.39	127.78	120.44
1	E	359	TYR	N-CA-C	-5.38	105.11	110.97
1	A	519	ASP	CA-CB-CG	5.35	117.95	112.60
1	E	185	ASP	CA-CB-CG	5.33	117.93	112.60
1	A	416	ARG	N-CA-C	-5.32	105.38	111.07
1	E	278	ARG	N-CA-C	-5.32	105.65	111.82
1	A	147	PHE	CA-C-O	-5.31	115.55	121.81
1	A	166	THR	CA-CB-OG1	-5.21	101.78	109.60
1	B	548	VAL	CA-C-O	-5.21	116.53	121.64
1	B	112	GLU	CB-CG-CD	5.20	121.44	112.60
1	A	548	VAL	CA-C-O	-5.17	116.27	121.49
1	F	142	VAL	N-CA-C	-5.13	107.74	111.90
1	A	291	LYS	N-CA-C	-5.07	107.75	114.04
1	E	240	ASP	CA-C-N	5.06	124.78	119.92
1	E	240	ASP	C-N-CA	5.06	124.78	119.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	117	SER	O-C-N	-5.05	117.89	121.83
1	E	584	HIS	CA-C-O	-5.05	115.99	121.84
1	B	537	ASP	CA-CB-CG	5.01	117.61	112.60
1	C	101	GLY	CA-C-O	-5.00	117.01	121.41
1	F	411	GLU	O-C-N	5.00	127.23	122.03

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4434	0	4307	27	0
1	B	4423	0	4297	45	0
1	C	4470	0	4344	39	0
1	D	4416	0	4290	41	0
1	E	4431	0	4310	43	0
1	F	4426	0	4297	35	0
2	A	53	0	31	0	0
2	B	53	0	31	1	0
2	C	53	0	31	2	0
2	D	53	0	31	1	0
2	E	53	0	31	1	0
2	F	53	0	31	1	0
3	A	20	0	28	1	0
3	B	20	0	28	1	0
3	C	20	0	28	3	0
3	D	20	0	28	1	0
3	E	20	0	28	2	0
3	F	20	0	28	1	0
4	A	16	0	22	0	0
4	B	16	0	22	2	0
4	C	16	0	22	4	0
4	D	16	0	22	2	0
4	E	16	0	22	0	0
4	F	16	0	22	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	2	0	0	0	0
5	B	1	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
5	E	2	0	0	0	0
5	F	1	0	0	0	0
6	A	12	0	16	1	0
6	B	24	0	32	3	0
6	C	12	0	16	1	0
6	D	24	0	32	4	0
6	E	18	0	24	4	0
6	F	12	0	16	2	0
7	A	325	0	0	2	0
7	B	362	0	0	10	0
7	C	466	0	0	8	0
7	D	411	0	0	10	0
7	E	449	0	0	10	0
7	F	329	0	0	10	0
All	All	29588	0	26467	230	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 4.

All (230) 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:502:THR:HB	7:F:716:HOH:O	1.51	1.09
1:A:114:ARG:HD3	7:A:773:HOH:O	1.59	1.01
6:D:609:GOL:H11	7:D:960:HOH:O	1.67	0.94
1:E:502:THR:HB	7:E:809:HOH:O	1.69	0.93
4:C:604:1PE:H262	7:C:924:HOH:O	1.75	0.86
1:D:114:ARG:HD3	7:D:953:HOH:O	1.75	0.84
1:F:114:ARG:HD3	7:F:799:HOH:O	1.77	0.82
1:C:481:GLU:OE1	1:C:536:ARG:NH1	2.13	0.82
1:E:581:ARG:HD3	7:E:800:HOH:O	1.81	0.80
1:C:590:ALA:O	1:C:591:ARG:HB3	1.81	0.79
1:E:385:PRO:HD3	3:E:603:PGE:H2	1.62	0.79
1:A:144:GLN:HB2	3:A:602:PGE:H2	1.66	0.78
1:E:271:GLU:OE1	1:E:274[B]:ARG:NH2	2.17	0.77
1:A:49:HIS:HB2	1:E:285:THR:HG21	1.66	0.76
1:F:120:GLY:H	4:F:605:1PE:H251	1.49	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:HIS:ND1	7:B:702:HOH:O	2.19	0.74
1:B:412:GLU:OE1	1:B:416:ARG:NE	2.20	0.74
1:D:412:GLU:HA	7:D:1001:HOH:O	1.89	0.73
1:E:329:LEU:HD13	1:E:329:LEU:C	2.15	0.72
1:C:285:THR:HG21	1:E:49:HIS:HB2	1.72	0.71
1:E:152:VAL:HG11	1:E:164:ARG:NH1	2.06	0.71
1:B:114:ARG:HD3	7:B:787:HOH:O	1.91	0.69
1:D:500:LEU:HD11	1:D:553:ALA:HB1	1.75	0.68
1:F:44:HIS:CD2	2:F:602:FAD:O2B	2.47	0.68
1:C:587:ASP:HB3	1:C:590:ALA:HB2	1.75	0.67
1:C:120:GLY:H	4:C:604:1PE:H251	1.58	0.67
1:C:323:PRO:HG2	6:C:607:GOL:H31	1.76	0.67
1:D:484:ARG:HH12	6:D:610:GOL:H31	1.59	0.67
1:B:459:ARG:O	7:B:701:HOH:O	2.12	0.66
1:C:173:ASP:OD1	7:C:701:HOH:O	2.12	0.66
1:E:112:GLU:HG3	7:E:977:HOH:O	1.94	0.65
1:C:412:GLU:OE1	1:C:416:ARG:NE	2.28	0.65
1:C:114:ARG:HD2	7:C:967:HOH:O	1.95	0.65
1:D:428:HIS:HD2	1:D:432:ASN:HD22	1.44	0.64
1:F:411:GLU:OE1	1:F:415:GLN:NE2	2.30	0.64
1:E:567:ARG:HD3	7:E:770:HOH:O	1.97	0.63
1:D:364:GLN:OE1	1:D:368:ARG:NH1	2.32	0.63
1:E:329:LEU:HD13	1:E:329:LEU:O	1.99	0.63
1:B:368:ARG:HD2	7:B:1031:HOH:O	1.98	0.62
4:B:604:1PE:H262	7:B:932:HOH:O	1.99	0.62
1:A:207:ARG:NH2	1:A:265:VAL:HG12	2.14	0.62
1:B:428:HIS:HD2	1:B:432:ASN:HD22	1.46	0.62
1:F:241:GLY:HA3	3:F:604:PGE:H3	1.82	0.62
1:D:152:VAL:HG11	1:D:164:ARG:HH12	1.65	0.61
4:F:605:1PE:H262	7:F:887:HOH:O	1.99	0.61
1:E:44:HIS:ND1	2:E:601:FAD:O2B	2.33	0.61
1:B:13:VAL:O	1:B:178:SER:HA	2.01	0.61
4:B:604:1PE:C26	7:B:932:HOH:O	2.49	0.61
1:D:108:ASP:OD1	7:D:701:HOH:O	2.17	0.60
1:C:364:GLN:OE1	1:C:368:ARG:NH1	2.34	0.59
1:B:169:ARG:NH2	7:B:706:HOH:O	2.30	0.59
1:B:484:ARG:NH1	6:B:609:GOL:H11	2.17	0.59
1:D:112:GLU:HG3	7:D:994:HOH:O	2.02	0.58
1:D:413:ALA:O	1:D:417:ARG:HG3	2.03	0.58
1:C:285:THR:HG21	1:E:49:HIS:CB	2.33	0.58
1:C:44:HIS:CD2	2:C:601:FAD:O2B	2.57	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:HIS:ND1	7:C:706:HOH:O	2.32	0.57
1:F:179:ASP:OD2	7:F:701:HOH:O	2.17	0.57
1:E:329:LEU:C	1:E:329:LEU:CD1	2.78	0.57
1:C:509:TRP:CZ3	1:C:572:ALA:HA	2.40	0.57
1:E:497:ARG:HD2	7:E:1044:HOH:O	2.04	0.57
1:D:169:ARG:HD3	1:F:400:TRP:CE2	2.39	0.57
1:B:502:THR:HB	7:B:741:HOH:O	2.04	0.56
1:B:112:GLU:HG3	7:B:905:HOH:O	2.05	0.56
1:D:323:PRO:HB2	6:D:607:GOL:H32	1.88	0.56
1:B:49:HIS:HB2	1:D:285:THR:HG21	1.86	0.56
1:E:323:PRO:HG2	6:E:607:GOL:H12	1.86	0.56
1:F:154:LEU:HD12	1:F:154:LEU:C	2.31	0.56
1:E:395:SER:OG	1:E:398:GLU:HG3	2.06	0.56
1:B:34:TYR:HB3	1:B:344:LYS:HD2	1.89	0.55
1:A:49:HIS:HB2	1:E:285:THR:CG2	2.36	0.55
1:C:204:GLY:HA2	1:C:297:GLU:HG3	1.88	0.55
1:C:120:GLY:H	4:C:604:1PE:C25	2.20	0.55
1:F:120:GLY:H	4:F:605:1PE:C25	2.19	0.55
1:E:417:ARG:NH2	1:F:550:GLU:OE2	2.38	0.54
1:E:550:GLU:OE2	1:F:417:ARG:NH2	2.41	0.54
1:B:49:HIS:CB	1:D:285:THR:HG21	2.38	0.54
1:B:84:ALA:O	6:B:606:GOL:O2	2.26	0.54
1:E:152:VAL:HG11	1:E:164:ARG:HH12	1.71	0.54
1:D:428:HIS:CD2	1:D:432:ASN:HD22	2.26	0.53
1:C:590:ALA:O	1:C:591:ARG:CB	2.57	0.52
7:D:1011:HOH:O	3:E:602:PGE:H6	2.08	0.52
1:A:49:HIS:CB	1:E:285:THR:HG21	2.36	0.52
1:B:265:VAL:HG13	1:B:265:VAL:O	2.10	0.52
1:A:188:ARG:O	1:A:189:SER:C	2.52	0.52
1:A:13:VAL:O	1:A:178:SER:HA	2.10	0.52
1:F:384:ILE:HB	1:F:385:PRO:CD	2.40	0.52
1:D:274:ARG:NH1	1:D:278:ARG:HD2	2.25	0.52
1:C:120:GLY:N	4:C:604:1PE:H251	2.25	0.52
4:D:604:1PE:H142	7:D:1054:HOH:O	2.10	0.52
1:A:260:PRO:C	1:A:262:THR:H	2.18	0.51
4:F:605:1PE:H151	7:F:991:HOH:O	2.11	0.51
1:B:134:VAL:O	1:B:138:GLN:HG2	2.11	0.51
1:D:412:GLU:HG3	1:D:413:ALA:N	2.22	0.51
1:C:428:HIS:HD2	1:C:432:ASN:HD22	1.57	0.51
1:A:23:ALA:HB2	1:A:332:ALA:HB1	1.91	0.51
1:D:13:VAL:O	1:D:178:SER:HA	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:587:ASP:OD1	1:F:587:ASP:C	2.54	0.51
1:E:509:TRP:CZ3	1:E:572:ALA:HA	2.46	0.50
1:D:34:TYR:HB3	1:D:344:LYS:HD2	1.93	0.50
1:B:266:ASP:HB3	1:B:269:ASP:HB2	1.92	0.50
1:D:120:GLY:H	4:D:604:1PE:C25	2.24	0.50
1:A:329:LEU:C	1:A:329:LEU:HD13	2.36	0.50
1:E:412:GLU:OE1	1:E:416:ARG:NE	2.44	0.50
1:B:285:THR:HG21	1:F:49:HIS:HB2	1.94	0.50
1:F:23:ALA:HB2	1:F:332:ALA:HB1	1.93	0.50
1:A:234:PRO:HG2	1:A:400:TRP:CZ2	2.46	0.50
1:B:428:HIS:CD2	1:B:432:ASN:HD22	2.29	0.50
1:D:509:TRP:CZ3	1:D:572:ALA:HA	2.47	0.50
1:D:152:VAL:HG11	1:D:164:ARG:NH1	2.26	0.49
1:E:154:LEU:C	1:E:154:LEU:HD12	2.37	0.49
3:C:602:PGE:O4	7:C:702:HOH:O	2.20	0.49
1:D:321:ASN:HB2	1:D:322:PRO:HD2	1.94	0.49
1:B:44:HIS:ND1	2:B:601:FAD:O2B	2.43	0.49
1:C:232:ALA:HB2	3:C:603:PGE:H12	1.95	0.49
1:F:34:TYR:HB3	1:F:344:LYS:HD3	1.93	0.49
1:E:428:HIS:HD2	1:E:432:ASN:HD22	1.59	0.49
1:F:509:TRP:CZ3	1:F:572:ALA:HA	2.48	0.49
1:A:248:ARG:HB2	1:A:252:GLU:HB3	1.94	0.48
1:C:442:TYR:O	1:C:472:GLY:HA3	2.13	0.48
1:D:237:PRO:HB3	1:D:392:GLU:HG3	1.96	0.47
1:E:265:VAL:O	1:E:265:VAL:HG23	2.14	0.47
6:E:608:GOL:H11	7:E:815:HOH:O	2.13	0.47
1:A:22:PRO:HG2	1:A:329:LEU:HD23	1.96	0.47
1:B:364:GLN:OE1	1:B:368:ARG:NH1	2.46	0.47
1:E:481:GLU:HG2	1:E:483:GLY:O	2.14	0.47
1:B:199:LEU:HB3	1:B:301:ALA:HB1	1.95	0.47
1:D:408:GLU:HB2	1:D:413:ALA:HB2	1.96	0.47
1:E:76:HIS:CE1	7:E:804:HOH:O	2.66	0.47
1:A:457:ASP:O	6:A:608:GOL:O1	2.32	0.47
1:E:13:VAL:O	1:E:178:SER:HA	2.14	0.47
1:B:384:ILE:HB	1:B:385:PRO:CD	2.45	0.47
1:E:262:THR:O	1:E:262:THR:OG1	2.31	0.47
6:E:608:GOL:H31	7:F:964:HOH:O	2.15	0.47
1:C:321:ASN:HB2	1:C:322:PRO:HD2	1.97	0.47
1:D:198:ALA:HA	7:D:715:HOH:O	2.15	0.47
1:F:120:GLY:N	4:F:605:1PE:H251	2.24	0.47
1:E:364:GLN:OE1	1:E:368:ARG:NH1	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:271:GLU:OE1	1:F:271:GLU:HA	2.15	0.46
1:B:207:ARG:HD3	1:B:261:PRO:HA	1.96	0.46
1:C:34:TYR:HB3	1:C:344:LYS:HD2	1.97	0.46
1:D:43:ARG:NH1	2:D:601:FAD:N7A	2.63	0.46
1:A:364:GLN:OE1	1:A:368:ARG:NH1	2.49	0.46
1:B:249:PRO:HB3	1:B:250:TRP:CE2	2.50	0.46
1:E:581:ARG:CD	7:E:800:HOH:O	2.52	0.46
6:F:601:GOL:C1	7:F:762:HOH:O	2.62	0.46
1:B:509:TRP:CZ3	1:B:572:ALA:HA	2.51	0.46
1:E:40:LEU:C	1:E:40:LEU:HD23	2.41	0.46
1:A:507:GLU:N	1:A:508:PRO:HD2	2.31	0.46
1:C:536:ARG:NH2	7:C:709:HOH:O	2.43	0.46
1:B:212:TRP:CE2	1:B:291:LYS:HE3	2.51	0.45
1:A:249:PRO:HA	1:A:250:TRP:HA	1.72	0.45
1:C:80:GLY:HA2	1:C:83:MET:HE2	1.99	0.45
1:D:509:TRP:CE2	1:D:553:ALA:HB2	2.51	0.45
1:B:400:TRP:CE2	1:F:169:ARG:HD3	2.51	0.45
1:B:88:PHE:CE1	1:B:384:ILE:HG13	2.52	0.45
1:C:368:ARG:HD3	7:C:961:HOH:O	2.17	0.45
3:D:602:PGE:H42	7:D:1024:HOH:O	2.17	0.45
1:E:83:MET:SD	1:E:123:ASN:HB2	2.57	0.45
1:F:164:ARG:HB3	1:F:164:ARG:CZ	2.45	0.45
1:B:249:PRO:HA	1:B:250:TRP:HA	1.75	0.44
1:D:306:TYR:CE1	1:D:364:GLN:HG2	2.51	0.44
6:E:608:GOL:C1	7:E:815:HOH:O	2.65	0.44
1:C:13:VAL:O	1:C:178:SER:HA	2.17	0.44
1:C:587:ASP:CB	1:C:590:ALA:HB2	2.47	0.44
1:F:384:ILE:HB	1:F:385:PRO:HD3	1.98	0.44
1:B:285:THR:HG21	1:F:49:HIS:CB	2.47	0.44
1:D:278:ARG:NH2	1:D:284:PRO:O	2.48	0.44
1:F:274:ARG:HG2	1:F:274:ARG:HH11	1.82	0.44
1:E:265:VAL:O	1:E:265:VAL:CG2	2.66	0.44
1:E:249:PRO:HA	1:E:250:TRP:HA	1.71	0.44
1:A:509:TRP:CZ3	1:A:572:ALA:HA	2.52	0.44
1:C:385:PRO:HD3	3:C:603:PGE:H2	2.00	0.44
1:A:154:LEU:C	1:A:154:LEU:HD12	2.43	0.43
1:D:38:HIS:CE1	1:D:143:GLY:HA3	2.53	0.43
1:F:249:PRO:HA	1:F:250:TRP:HA	1.80	0.43
1:A:195:LEU:HD11	1:A:311:VAL:CG1	2.48	0.43
1:B:484:ARG:HH12	6:B:609:GOL:H11	1.82	0.43
1:B:418:ALA:O	7:B:703:HOH:O	2.21	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:484:ARG:HH12	6:D:610:GOL:C3	2.28	0.43
1:F:154:LEU:HD12	1:F:154:LEU:O	2.19	0.43
1:F:243:VAL:HB	1:F:256:LEU:HB2	2.01	0.43
1:B:541:THR:HG22	1:B:545:LEU:HD12	1.99	0.43
1:F:411:GLU:OE2	1:F:411:GLU:HA	2.19	0.43
1:F:108:ASP:HA	6:F:601:GOL:H12	2.00	0.43
1:B:258:PHE:N	1:B:258:PHE:CD2	2.87	0.42
1:B:300:SER:HA	1:B:320:GLN:O	2.19	0.42
1:B:385:PRO:HD3	3:B:603:PGE:H52	2.01	0.42
1:C:566:ALA:HB1	1:C:571:HIS:HB2	2.01	0.42
1:D:23:ALA:HB2	1:D:332:ALA:HB1	2.00	0.42
1:D:207:ARG:HB2	1:D:207:ARG:HH11	1.83	0.42
1:E:248:ARG:NH2	7:E:730:HOH:O	2.52	0.42
1:C:207:ARG:NH2	1:C:265:VAL:HG13	2.35	0.42
1:A:234:PRO:HG2	1:A:400:TRP:CH2	2.55	0.42
1:C:507:GLU:N	1:C:508:PRO:CD	2.82	0.42
1:C:23:ALA:HB2	1:C:332:ALA:HB1	2.01	0.42
1:B:321:ASN:HB2	1:B:322:PRO:HD2	2.01	0.42
1:C:43:ARG:NH2	2:C:601:FAD:N7A	2.68	0.42
1:F:169:ARG:HG3	7:F:827:HOH:O	2.20	0.42
1:B:401:ARG:O	1:B:405:THR:HG23	2.20	0.42
1:F:234:PRO:HG2	1:F:400:TRP:CZ2	2.55	0.42
1:F:324:THR:O	1:F:325:ASN:HB2	2.20	0.41
1:C:249:PRO:HB3	1:C:250:TRP:CE2	2.55	0.41
1:C:285:THR:CG2	1:E:49:HIS:HB2	2.46	0.41
1:C:428:HIS:CD2	1:C:432:ASN:HD22	2.37	0.41
1:D:249:PRO:HA	1:D:250:TRP:HA	1.81	0.41
1:D:302:VAL:HG11	1:D:368:ARG:HG2	2.01	0.41
1:F:497:ARG:HD2	7:F:848:HOH:O	2.19	0.41
1:B:406:LEU:O	1:B:417:ARG:HD3	2.21	0.41
1:A:278:ARG:NH2	1:A:284:PRO:O	2.53	0.41
1:C:169:ARG:HG2	7:C:857:HOH:O	2.20	0.41
1:A:207:ARG:NH2	1:A:265:VAL:CG1	2.81	0.41
1:A:575:LEU:HB3	1:A:576:PRO:HD3	2.03	0.41
1:F:112:GLU:HG3	7:F:936:HOH:O	2.20	0.41
1:A:114:ARG:CD	7:A:773:HOH:O	2.40	0.41
1:D:408:GLU:O	1:D:417:ARG:NH2	2.53	0.41
1:B:245:VAL:HB	1:B:254:LEU:HB2	2.02	0.41
1:C:321:ASN:HB2	1:C:322:PRO:CD	2.51	0.41
1:D:584:HIS:HD2	7:D:1053:HOH:O	2.04	0.41
1:B:130:GLU:HB2	1:B:131:PRO:HD3	2.04	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:134:VAL:O	1:E:138:GLN:HG2	2.21	0.41
1:D:500:LEU:HD12	1:D:500:LEU:HA	1.92	0.40
1:A:413:ALA:O	1:A:417:ARG:HB2	2.21	0.40
1:E:568:ASP:C	1:E:568:ASP:OD1	2.65	0.40
1:B:507:GLU:N	1:B:508:PRO:CD	2.84	0.40
1:D:248:ARG:HB2	1:D:252:GLU:HB3	2.04	0.40
1:B:442:TYR:O	1:B:472:GLY:HA3	2.21	0.40
1:D:438:LEU:HD12	1:D:438:LEU:HA	1.89	0.40
1:E:237:PRO:HA	1:E:238:PRO:HD3	1.95	0.40
1:E:500:LEU:CD2	1:E:509:TRP:HB3	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	579/601 (96%)	566 (98%)	12 (2%)	1 (0%)	43	40
1	B	577/601 (96%)	563 (98%)	12 (2%)	2 (0%)	36	31
1	C	583/601 (97%)	574 (98%)	8 (1%)	1 (0%)	43	40
1	D	576/601 (96%)	566 (98%)	10 (2%)	0	100	100
1	E	578/601 (96%)	569 (98%)	7 (1%)	2 (0%)	36	31
1	F	577/601 (96%)	565 (98%)	11 (2%)	1 (0%)	43	40
All	All	3470/3606 (96%)	3403 (98%)	60 (2%)	7 (0%)	43	40

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	591	ARG
1	A	90	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	90	SER
1	E	262	THR
1	F	90	SER
1	E	90	SER
1	B	260	PRO

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	448/460 (97%)	431 (96%)	17 (4%)	29	23
1	B	447/460 (97%)	437 (98%)	10 (2%)	45	45
1	C	451/460 (98%)	441 (98%)	10 (2%)	45	45
1	D	446/460 (97%)	437 (98%)	9 (2%)	48	48
1	E	448/460 (97%)	435 (97%)	13 (3%)	37	34
1	F	448/460 (97%)	432 (96%)	16 (4%)	31	26
All	All	2688/2760 (97%)	2613 (97%)	75 (3%)	38	35

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	PHE
1	A	164	ARG
1	A	172	ARG
1	A	203	THR
1	A	265	VAL
1	A	267	VAL
1	A	271	GLU
1	A	287	ASP
1	A	290	ILE
1	A	298	VAL
1	A	299	ASN
1	A	344	LYS
1	A	392	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	412	GLU
1	A	417	ARG
1	A	474	ARG
1	A	497	ARG
1	B	43	ARG
1	B	203	THR
1	B	262	THR
1	B	267	VAL
1	B	268	GLU
1	B	297	GLU
1	B	324	THR
1	B	411	GLU
1	B	438	LEU
1	B	474	ARG
1	C	108	ASP
1	C	190	ARG
1	C	203	THR
1	C	265	VAL
1	C	267	VAL
1	C	271	GLU
1	C	324	THR
1	C	474	ARG
1	C	497	ARG
1	C	523	GLU
1	D	12	ARG
1	D	172	ARG
1	D	262	THR
1	D	267	VAL
1	D	268	GLU
1	D	300	SER
1	D	392	GLU
1	D	412	GLU
1	D	474	ARG
1	E	43	ARG
1	E	158	GLU
1	E	190	ARG
1	E	207	ARG
1	E	256	LEU
1	E	262	THR
1	E	264	ASP
1	E	267	VAL
1	E	297	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	329	LEU
1	E	474	ARG
1	E	497	ARG
1	E	567	ARG
1	F	108	ASP
1	F	164	ARG
1	F	188	ARG
1	F	190	ARG
1	F	203	THR
1	F	236	SER
1	F	267	VAL
1	F	268	GLU
1	F	344	LYS
1	F	401	ARG
1	F	417	ARG
1	F	444	THR
1	F	474	ARG
1	F	497	ARG
1	F	523	GLU
1	F	567	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	HIS
1	A	105	ASN
1	A	127	HIS
1	A	159	HIS
1	A	299	ASN
1	A	320	GLN
1	A	325	ASN
1	A	428	HIS
1	B	58	GLN
1	B	123	ASN
1	B	159	HIS
1	B	325	ASN
1	B	415	GLN
1	B	428	HIS
1	C	44	HIS
1	C	325	ASN
1	C	428	HIS
1	C	485	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	299	ASN
1	D	320	GLN
1	D	325	ASN
1	D	415	GLN
1	D	428	HIS
1	D	430	GLN
1	E	321	ASN
1	E	325	ASN
1	E	407	HIS
1	E	428	HIS
1	E	485	HIS
1	F	44	HIS
1	F	123	ASN
1	F	325	ASN
1	F	584	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 51 ligands modelled in this entry, 10 are monoatomic - leaving 41 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
3	PGE	B	603	-	9,9,9	0.27	0	8,8,8	0.15	0
6	GOL	B	606	-	5,5,5	0.22	0	5,5,5	0.53	0
2	FAD	C	601	-	58,58,58	2.24	15 (25%)	85,89,89	1.82	23 (27%)
3	PGE	B	602	-	9,9,9	0.35	0	8,8,8	0.31	0
4	1PE	C	604	-	15,15,15	0.92	0	14,14,14	1.06	1 (7%)
6	GOL	B	608	-	5,5,5	0.15	0	5,5,5	0.45	0
2	FAD	F	602	-	58,58,58	1.92	12 (20%)	85,89,89	1.81	23 (27%)
3	PGE	E	602	-	9,9,9	0.60	0	8,8,8	0.48	0
6	GOL	B	609	-	5,5,5	0.18	0	5,5,5	0.49	0
6	GOL	E	607	-	5,5,5	0.35	0	5,5,5	0.92	0
6	GOL	A	608	-	5,5,5	0.13	0	5,5,5	0.44	0
3	PGE	D	602	-	9,9,9	0.27	0	8,8,8	0.18	0
2	FAD	E	601	-	58,58,58	1.84	11 (18%)	85,89,89	1.84	21 (24%)
2	FAD	A	601	-	58,58,58	1.90	10 (17%)	85,89,89	1.93	24 (28%)
4	1PE	B	604	-	15,15,15	0.76	0	14,14,14	0.67	0
4	1PE	D	604	-	15,15,15	0.78	0	14,14,14	0.74	0
6	GOL	F	601	-	5,5,5	0.22	0	5,5,5	0.48	0
6	GOL	A	607	-	5,5,5	0.30	0	5,5,5	0.55	0
4	1PE	E	604	-	15,15,15	0.89	0	14,14,14	1.02	2 (14%)
4	1PE	F	605	-	15,15,15	0.84	0	14,14,14	0.81	0
3	PGE	F	604	-	9,9,9	0.47	0	8,8,8	0.28	0
3	PGE	E	603	-	9,9,9	0.52	0	8,8,8	0.43	0
3	PGE	D	603	-	9,9,9	0.39	0	8,8,8	0.21	0
6	GOL	E	609	-	5,5,5	0.19	0	5,5,5	0.51	0
3	PGE	F	603	-	9,9,9	0.28	0	8,8,8	0.28	0
6	GOL	C	607	-	5,5,5	0.40	0	5,5,5	0.99	0
6	GOL	D	608	-	5,5,5	0.14	0	5,5,5	0.46	0
6	GOL	D	607	-	5,5,5	0.22	0	5,5,5	0.50	0
6	GOL	D	609	-	5,5,5	0.27	0	5,5,5	0.59	0
6	GOL	E	608	-	5,5,5	0.23	0	5,5,5	0.59	0
3	PGE	A	602	-	9,9,9	0.56	0	8,8,8	0.40	0
3	PGE	C	602	-	9,9,9	0.14	0	8,8,8	0.12	0
4	1PE	A	604	-	15,15,15	0.70	0	14,14,14	0.48	0
6	GOL	B	607	-	5,5,5	0.39	0	5,5,5	0.98	0
6	GOL	F	607	-	5,5,5	0.22	0	5,5,5	0.53	0
2	FAD	B	601	-	58,58,58	2.08	13 (22%)	85,89,89	2.11	21 (24%)
2	FAD	D	601	-	58,58,58	2.13	12 (20%)	85,89,89	1.72	22 (25%)
6	GOL	C	608	-	5,5,5	0.18	0	5,5,5	0.46	0
3	PGE	C	603	-	9,9,9	0.45	0	8,8,8	0.37	0
6	GOL	D	610	-	5,5,5	0.27	0	5,5,5	1.04	0
3	PGE	A	603	-	9,9,9	0.37	0	8,8,8	0.16	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PGE	B	603	-	-	4/7/7/7	-
6	GOL	B	606	-	-	4/4/4/4	-
2	FAD	C	601	-	-	1/34/50/50	0/6/6/6
3	PGE	B	602	-	-	6/7/7/7	-
4	1PE	C	604	-	-	7/13/13/13	-
6	GOL	B	608	-	-	4/4/4/4	-
2	FAD	F	602	-	-	4/34/50/50	0/6/6/6
3	PGE	E	602	-	-	6/7/7/7	-
6	GOL	B	609	-	-	0/4/4/4	-
6	GOL	E	607	-	-	1/4/4/4	-
6	GOL	A	608	-	-	4/4/4/4	-
3	PGE	D	602	-	-	5/7/7/7	-
2	FAD	E	601	-	-	3/34/50/50	0/6/6/6
2	FAD	A	601	-	-	6/34/50/50	0/6/6/6
4	1PE	B	604	-	-	7/13/13/13	-
4	1PE	D	604	-	-	6/13/13/13	-
6	GOL	F	601	-	-	2/4/4/4	-
6	GOL	A	607	-	-	2/4/4/4	-
4	1PE	E	604	-	-	9/13/13/13	-
4	1PE	F	605	-	-	5/13/13/13	-
3	PGE	F	604	-	-	5/7/7/7	-
3	PGE	E	603	-	-	4/7/7/7	-
3	PGE	D	603	-	-	5/7/7/7	-
6	GOL	E	609	-	-	4/4/4/4	-
3	PGE	F	603	-	-	1/7/7/7	-
6	GOL	C	607	-	-	4/4/4/4	-
6	GOL	D	608	-	-	2/4/4/4	-
6	GOL	D	607	-	-	2/4/4/4	-
6	GOL	D	609	-	-	2/4/4/4	-
6	GOL	E	608	-	-	3/4/4/4	-
3	PGE	A	602	-	-	3/7/7/7	-
3	PGE	C	602	-	-	2/7/7/7	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	1PE	A	604	-	-	5/13/13/13	-
6	GOL	B	607	-	-	0/4/4/4	-
6	GOL	F	607	-	-	2/4/4/4	-
2	FAD	B	601	-	-	1/34/50/50	0/6/6/6
2	FAD	D	601	-	-	1/34/50/50	0/6/6/6
6	GOL	C	608	-	-	4/4/4/4	-
3	PGE	C	603	-	-	3/7/7/7	-
6	GOL	D	610	-	-	0/4/4/4	-
3	PGE	A	603	-	-	2/7/7/7	-

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	FAD	P-O3P	6.76	1.66	1.59
2	C	601	FAD	C9A-C5X	6.50	1.51	1.41
2	F	602	FAD	C9A-C5X	6.49	1.51	1.41
2	E	601	FAD	C5A-C4A	6.39	1.50	1.39
2	C	601	FAD	PA-O3P	6.31	1.66	1.59
2	B	601	FAD	C9A-C5X	6.29	1.51	1.41
2	A	601	FAD	C9A-C5X	6.19	1.51	1.41
2	B	601	FAD	C5A-C4A	6.06	1.49	1.39
2	C	601	FAD	P-O3P	5.83	1.65	1.59
2	D	601	FAD	C5A-C4A	5.81	1.49	1.39
2	D	601	FAD	C9A-C5X	5.65	1.50	1.41
2	A	601	FAD	P-O3P	5.58	1.65	1.59
2	F	602	FAD	P-O3P	5.48	1.65	1.59
2	B	601	FAD	PA-O3P	5.42	1.65	1.59
2	D	601	FAD	PA-O3P	5.37	1.65	1.59
2	C	601	FAD	C5A-C4A	5.04	1.48	1.39
2	E	601	FAD	C9A-C5X	5.03	1.49	1.41
2	A	601	FAD	C5A-C4A	4.98	1.48	1.39
2	B	601	FAD	P-O3P	4.91	1.64	1.59
2	C	601	FAD	C8-C7	4.63	1.52	1.40
2	F	602	FAD	C8-C7	4.54	1.51	1.40
2	D	601	FAD	C8-C7	4.47	1.51	1.40
2	C	601	FAD	C8A-N7A	4.37	1.40	1.31
2	B	601	FAD	C8-C7	4.36	1.51	1.40
2	E	601	FAD	P-O3P	4.29	1.64	1.59
2	E	601	FAD	C8-C7	4.11	1.50	1.40
2	F	602	FAD	PA-O3P	3.89	1.63	1.59
2	F	602	FAD	C5A-C4A	3.81	1.45	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	FAD	C4X-N5	3.77	1.38	1.30
2	E	601	FAD	C5'-C4'	3.77	1.56	1.51
2	D	601	FAD	C4A-N9A	-3.76	1.29	1.37
2	F	602	FAD	C4X-N5	3.64	1.38	1.30
2	A	601	FAD	C8-C7	3.63	1.49	1.40
2	A	601	FAD	PA-O3P	3.48	1.63	1.59
2	A	601	FAD	C8A-N7A	3.46	1.38	1.31
2	A	601	FAD	C5A-C6A	3.38	1.50	1.41
2	D	601	FAD	C4X-N5	3.29	1.37	1.30
2	B	601	FAD	C4X-N5	3.29	1.37	1.30
2	D	601	FAD	C8A-N7A	3.27	1.38	1.31
2	B	601	FAD	C5A-C6A	3.24	1.50	1.41
2	E	601	FAD	C8A-N7A	3.22	1.37	1.31
2	E	601	FAD	C4-N3	-3.22	1.32	1.38
2	A	601	FAD	C4X-N5	3.17	1.37	1.30
2	B	601	FAD	C8A-N7A	3.15	1.37	1.31
2	F	602	FAD	C5A-C6A	3.12	1.49	1.41
2	E	601	FAD	C4X-N5	2.87	1.37	1.30
2	C	601	FAD	C10-N10	2.82	1.43	1.37
2	D	601	FAD	C4-N3	-2.81	1.33	1.38
2	C	601	FAD	C2A-N3A	2.71	1.38	1.33
2	B	601	FAD	C10-N10	2.68	1.43	1.37
2	B	601	FAD	C2A-N3A	2.59	1.38	1.33
2	C	601	FAD	C4A-N3A	-2.57	1.29	1.34
2	C	601	FAD	C5A-C6A	2.46	1.47	1.41
2	D	601	FAD	C5A-N7A	-2.46	1.34	1.39
2	C	601	FAD	C5A-N7A	-2.44	1.34	1.39
2	C	601	FAD	C2A-N1A	2.39	1.38	1.33
2	B	601	FAD	C4X-C10	2.35	1.51	1.44
2	C	601	FAD	C4X-C10	2.34	1.51	1.44
2	F	602	FAD	C4-N3	-2.30	1.34	1.38
2	D	601	FAD	C10-N10	2.30	1.42	1.37
2	B	601	FAD	C4A-N9A	-2.27	1.33	1.37
2	A	601	FAD	C4A-N9A	-2.26	1.33	1.37
2	D	601	FAD	C4X-C10	2.25	1.50	1.44
2	B	601	FAD	C10-N1	2.17	1.37	1.33
2	F	602	FAD	O2-C2	2.15	1.28	1.24
2	A	601	FAD	C2A-N1A	2.13	1.37	1.33
2	E	601	FAD	C4X-C10	2.12	1.50	1.44
2	F	602	FAD	C4X-C10	2.09	1.50	1.44
2	F	602	FAD	C10-N1	2.09	1.37	1.33
2	E	601	FAD	C5A-C6A	2.08	1.46	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	601	FAD	C10-N1	2.06	1.37	1.33
2	F	602	FAD	C8A-N7A	2.05	1.35	1.31
2	C	601	FAD	C10-N1	2.01	1.37	1.33

All (137) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	FAD	C5A-C4A-N3A	-6.55	117.69	126.72
2	A	601	FAD	C4A-N9A-C8A	5.96	112.00	105.74
2	B	601	FAD	C2A-N3A-C4A	5.61	125.53	111.83
2	C	601	FAD	C5A-C4A-N3A	-5.44	119.22	126.72
2	B	601	FAD	C4A-C5A-N7A	-5.43	104.37	110.58
2	B	601	FAD	N3A-C2A-N1A	-5.21	120.70	128.58
2	E	601	FAD	N3A-C2A-N1A	-5.07	120.91	128.58
2	A	601	FAD	N9A-C8A-N7A	-4.74	107.21	113.94
2	F	602	FAD	C4A-N9A-C8A	4.71	110.68	105.74
2	F	602	FAD	C4-C4X-N5	4.65	124.64	118.21
2	F	602	FAD	C5A-C4A-N3A	-4.61	120.36	126.72
2	E	601	FAD	C5A-C4A-N3A	-4.58	120.41	126.72
2	B	601	FAD	N3A-C4A-N9A	4.50	134.83	127.17
2	A	601	FAD	C4A-N9A-C1B	-4.50	116.10	126.63
2	A	601	FAD	C4-C4X-N5	4.39	124.28	118.21
2	E	601	FAD	C2A-N3A-C4A	4.37	122.50	111.83
2	C	601	FAD	C2A-N3A-C4A	4.30	122.34	111.83
2	B	601	FAD	C4-C4X-N5	4.28	124.11	118.21
2	D	601	FAD	N3A-C2A-N1A	-4.25	122.15	128.58
2	A	601	FAD	C4A-C5A-N7A	-4.11	105.88	110.58
2	F	602	FAD	N3A-C4A-N9A	4.10	134.13	127.17
2	E	601	FAD	C4A-N9A-C8A	4.09	110.03	105.74
2	F	602	FAD	C2A-N3A-C4A	3.97	121.53	111.83
2	E	601	FAD	C4-C4X-N5	3.95	123.67	118.21
2	E	601	FAD	C4A-C5A-N7A	-3.93	106.09	110.58
2	D	601	FAD	O5'-P-O1P	3.93	124.50	108.94
2	D	601	FAD	C4A-N9A-C8A	3.92	109.85	105.74
2	B	601	FAD	C5A-N7A-C8A	3.90	109.58	103.45
2	E	601	FAD	N3A-C4A-N9A	3.89	133.79	127.17
2	C	601	FAD	N3A-C4A-N9A	3.88	133.76	127.17
2	B	601	FAD	C6A-C5A-N7A	3.83	139.47	132.09
2	F	602	FAD	N9A-C8A-N7A	-3.82	108.51	113.94
2	A	601	FAD	C5A-N7A-C8A	3.71	109.28	103.45
2	E	601	FAD	C5A-N7A-C8A	3.65	109.18	103.45
2	B	601	FAD	O5'-P-O1P	3.64	123.35	108.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	FAD	N3A-C2A-N1A	-3.62	123.10	128.58
2	D	601	FAD	C4-C4X-N5	3.49	123.03	118.21
2	E	601	FAD	N9A-C8A-N7A	-3.48	108.99	113.94
2	F	602	FAD	N3A-C2A-N1A	-3.45	123.36	128.58
2	A	601	FAD	C6A-C5A-N7A	3.44	138.72	132.09
2	B	601	FAD	C4A-N9A-C8A	3.41	109.32	105.74
2	A	601	FAD	O5'-P-O1P	3.38	122.34	108.94
2	B	601	FAD	N9A-C8A-N7A	-3.33	109.21	113.94
2	E	601	FAD	C6A-C5A-N7A	3.32	138.49	132.09
2	C	601	FAD	C4-C4X-N5	3.32	122.79	118.21
2	C	601	FAD	C4A-C5A-N7A	-3.30	106.81	110.58
2	A	601	FAD	C4'-C3'-C2'	-3.29	108.09	113.57
2	F	602	FAD	C4A-C5A-N7A	-3.29	106.82	110.58
2	C	601	FAD	C4A-N9A-C8A	3.29	109.19	105.74
2	A	601	FAD	C5A-C4A-N3A	-3.27	122.21	126.72
2	D	601	FAD	C2A-N1A-C6A	3.26	124.09	118.73
2	C	601	FAD	N9A-C8A-N7A	-3.25	109.33	113.94
2	F	602	FAD	C5A-N7A-C8A	3.22	108.50	103.45
2	A	601	FAD	C2A-N3A-C4A	3.19	119.63	111.83
2	C	601	FAD	C4X-C4-N3	3.16	121.30	113.25
2	A	601	FAD	N3A-C2A-N1A	-3.15	123.81	128.58
2	B	601	FAD	C4X-C4-N3	3.15	121.26	113.25
2	C	601	FAD	C5X-C9A-N10	3.13	120.80	117.97
2	E	601	FAD	C4X-C4-N3	3.12	121.18	113.25
2	F	602	FAD	O3P-PA-O1A	3.03	119.83	110.70
2	D	601	FAD	C4A-N9A-C1B	-2.99	119.63	126.63
2	A	601	FAD	C4X-C4-N3	2.94	120.73	113.25
2	A	601	FAD	N3A-C4A-N9A	2.93	132.15	127.17
2	C	601	FAD	N6A-C6A-N1A	2.89	124.83	118.38
2	B	601	FAD	C10-N1-C2	2.86	123.04	116.85
2	F	602	FAD	C4X-C4-N3	2.84	120.48	113.25
2	A	601	FAD	C2B-C3B-C4B	2.84	108.09	102.61
2	D	601	FAD	N6A-C6A-N1A	2.84	124.69	118.38
2	D	601	FAD	O2P-P-O3P	-2.83	99.63	107.27
2	D	601	FAD	O3'-C3'-C2'	-2.82	102.52	108.93
2	B	601	FAD	O4-C4-C4X	-2.81	119.11	126.53
2	D	601	FAD	C2A-N3A-C4A	2.81	118.69	111.83
2	F	602	FAD	C4A-N9A-C1B	-2.78	120.14	126.63
2	D	601	FAD	C5A-C4A-N3A	-2.76	122.91	126.72
2	C	601	FAD	C5A-N7A-C8A	2.72	107.73	103.45
2	B	601	FAD	C4-N3-C2	-2.71	120.83	125.64
2	A	601	FAD	C4X-C10-N10	2.65	120.27	116.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	FAD	C8M-C8-C7	2.63	126.12	120.76
2	A	601	FAD	C10-N1-C2	2.62	122.52	116.85
2	D	601	FAD	O3P-P-O1P	-2.61	102.85	110.70
2	C	601	FAD	O4-C4-C4X	-2.59	119.69	126.53
4	E	604	1PE	OH5-C25-C15	2.58	122.12	110.35
2	C	601	FAD	C5A-C6A-N6A	-2.58	116.90	123.29
2	B	601	FAD	C4'-C3'-C2'	-2.57	109.29	113.57
2	D	601	FAD	C4X-C4-N3	2.57	119.80	113.25
2	C	601	FAD	C4X-C10-N1	-2.57	118.29	124.59
2	B	601	FAD	C4X-C10-N1	-2.52	118.41	124.59
2	E	601	FAD	O4-C4-C4X	-2.51	119.91	126.53
2	D	601	FAD	N3A-C4A-N9A	2.49	131.40	127.17
2	E	601	FAD	C2A-N1A-C6A	2.49	122.82	118.73
2	F	602	FAD	C6A-C5A-N7A	2.49	136.88	132.09
2	F	602	FAD	C4-C4X-C10	-2.46	112.70	116.93
2	F	602	FAD	O5'-P-O1P	2.46	118.68	108.94
2	C	601	FAD	C4-N3-C2	-2.45	121.29	125.64
2	C	601	FAD	C8M-C8-C9	-2.45	115.26	119.57
2	D	601	FAD	C8M-C8-C7	2.40	125.66	120.76
2	C	601	FAD	C9-C9A-N10	-2.36	118.68	121.85
4	C	604	1PE	C25-OH5-C14	2.36	123.58	113.26
2	E	601	FAD	C4A-N9A-C1B	-2.33	121.18	126.63
2	E	601	FAD	O4B-C1B-N9A	2.33	112.57	108.09
2	C	601	FAD	C10-N1-C2	2.33	121.89	116.85
2	C	601	FAD	C9A-C5X-N5	-2.32	120.00	122.45
2	D	601	FAD	O4-C4-C4X	-2.32	120.42	126.53
2	D	601	FAD	O3'-C3'-C4'	2.31	114.18	108.93
2	D	601	FAD	C8M-C8-C9	-2.30	115.53	119.57
2	B	601	FAD	O2B-C2B-C1B	-2.29	102.22	110.10
2	E	601	FAD	C5X-C9A-N10	2.26	120.01	117.97
2	A	601	FAD	O4B-C1B-N9A	2.26	112.43	108.09
2	F	602	FAD	N6A-C6A-N1A	2.26	123.40	118.38
2	F	602	FAD	C4'-C3'-C2'	-2.26	109.82	113.57
2	F	602	FAD	C5A-C6A-N6A	-2.25	117.72	123.29
2	F	602	FAD	O2A-PA-O3P	-2.24	101.20	107.27
2	D	601	FAD	C10-N1-C2	2.23	121.67	116.85
2	F	602	FAD	C8M-C8-C7	2.22	125.30	120.76
2	D	601	FAD	C4A-C5A-N7A	-2.22	108.05	110.58
2	D	601	FAD	C4X-C10-N1	-2.19	119.22	124.59
4	E	604	1PE	OH6-C26-C16	2.18	119.73	110.11
2	D	601	FAD	N9A-C8A-N7A	-2.17	110.86	113.94
2	A	601	FAD	C4-N3-C2	-2.17	121.80	125.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	FAD	C1B-N9A-C8A	2.17	131.90	127.09
2	A	601	FAD	C1'-N10-C9A	2.16	124.82	120.63
2	B	601	FAD	C2B-C3B-C4B	2.15	106.76	102.61
2	E	601	FAD	C4X-C10-N1	-2.14	119.34	124.59
2	E	601	FAD	C10-N1-C2	2.12	121.44	116.85
2	E	601	FAD	C1'-N10-C9A	2.11	124.72	120.63
2	E	601	FAD	O3B-C3B-C4B	-2.10	105.04	111.08
2	E	601	FAD	O5'-P-O1P	2.09	117.21	108.94
2	F	602	FAD	O4-C4-C4X	-2.08	121.03	126.53
2	C	601	FAD	O5'-P-O1P	2.08	117.19	108.94
2	F	602	FAD	C9A-C5X-N5	-2.07	120.26	122.45
2	A	601	FAD	O4-C4-C4X	-2.07	121.08	126.53
2	F	602	FAD	C10-N1-C2	2.06	121.32	116.85
2	B	601	FAD	O3'-C3'-C4'	2.05	113.60	108.93
2	C	601	FAD	O2'-C2'-C3'	2.04	114.03	109.25
2	A	601	FAD	C9A-N10-C10	-2.04	117.64	120.75
2	B	601	FAD	C4X-C10-N10	2.03	119.39	116.48
2	A	601	FAD	C4X-C10-N1	-2.03	119.61	124.59

There are no chirality outliers.

All (141) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FAD	C5'-O5'-P-O2P
2	A	601	FAD	C5'-O5'-P-O3P
2	B	601	FAD	C5'-O5'-P-O2P
2	D	601	FAD	C5'-O5'-P-O2P
2	E	601	FAD	C5'-O5'-P-O2P
2	E	601	FAD	C5'-O5'-P-O3P
6	A	607	GOL	C1-C2-C3-O3
6	B	606	GOL	C1-C2-C3-O3
6	B	608	GOL	O1-C1-C2-C3
6	C	607	GOL	O1-C1-C2-C3
6	C	607	GOL	C1-C2-C3-O3
6	C	608	GOL	O1-C1-C2-O2
6	C	608	GOL	O1-C1-C2-C3
6	D	609	GOL	C1-C2-C3-O3
6	E	608	GOL	O1-C1-C2-O2
6	E	608	GOL	O1-C1-C2-C3
6	E	609	GOL	O1-C1-C2-C3
6	F	601	GOL	O1-C1-C2-O2
6	F	601	GOL	O1-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	F	607	GOL	O1-C1-C2-C3
4	D	604	1PE	C23-C13-OH4-C24
3	F	604	PGE	O2-C3-C4-O3
3	C	603	PGE	O2-C3-C4-O3
4	B	604	1PE	OH5-C14-C24-OH4
4	E	604	1PE	OH6-C15-C25-OH5
4	E	604	1PE	OH5-C14-C24-OH4
4	D	604	1PE	OH4-C13-C23-OH3
6	B	606	GOL	O1-C1-C2-O2
6	C	607	GOL	O1-C1-C2-O2
3	D	602	PGE	O1-C1-C2-O2
3	D	602	PGE	O3-C5-C6-O4
3	D	603	PGE	O3-C5-C6-O4
4	C	604	1PE	OH7-C16-C26-OH6
4	D	604	1PE	OH6-C15-C25-OH5
3	B	603	PGE	O2-C3-C4-O3
3	A	602	PGE	O2-C3-C4-O3
4	F	605	1PE	OH4-C13-C23-OH3
3	B	602	PGE	O3-C5-C6-O4
3	C	602	PGE	O3-C5-C6-O4
3	E	602	PGE	O1-C1-C2-O2
3	E	602	PGE	O3-C5-C6-O4
3	E	603	PGE	O1-C1-C2-O2
4	D	604	1PE	OH2-C12-C22-OH3
4	E	604	1PE	OH7-C16-C26-OH6
4	C	604	1PE	OH5-C14-C24-OH4
6	A	608	GOL	O1-C1-C2-C3
6	A	608	GOL	C1-C2-C3-O3
6	B	606	GOL	O1-C1-C2-C3
6	B	608	GOL	C1-C2-C3-O3
6	C	608	GOL	C1-C2-C3-O3
6	D	607	GOL	O1-C1-C2-C3
6	D	608	GOL	O1-C1-C2-C3
3	A	602	PGE	O1-C1-C2-O2
4	B	604	1PE	OH2-C12-C22-OH3
6	A	607	GOL	O2-C2-C3-O3
6	A	608	GOL	O1-C1-C2-O2
6	B	606	GOL	O2-C2-C3-O3
6	B	608	GOL	O1-C1-C2-O2
6	E	609	GOL	O1-C1-C2-O2
6	F	607	GOL	O1-C1-C2-O2
4	E	604	1PE	OH4-C13-C23-OH3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	F	604	PGE	O1-C1-C2-O2
3	A	602	PGE	C4-C3-O2-C2
4	B	604	1PE	OH6-C15-C25-OH5
3	B	603	PGE	O1-C1-C2-O2
3	D	603	PGE	O1-C1-C2-O2
3	F	604	PGE	O3-C5-C6-O4
4	B	604	1PE	OH4-C13-C23-OH3
3	E	603	PGE	O3-C5-C6-O4
4	A	604	1PE	OH7-C16-C26-OH6
4	E	604	1PE	OH2-C12-C22-OH3
6	A	608	GOL	O2-C2-C3-O3
6	C	608	GOL	O2-C2-C3-O3
6	D	609	GOL	O2-C2-C3-O3
4	C	604	1PE	C25-C15-OH6-C26
4	C	604	1PE	C23-C13-OH4-C24
3	B	602	PGE	O1-C1-C2-O2
4	F	605	1PE	OH7-C16-C26-OH6
4	A	604	1PE	OH4-C13-C23-OH3
4	A	604	1PE	C15-C25-OH5-C14
6	B	608	GOL	O2-C2-C3-O3
6	D	607	GOL	O1-C1-C2-O2
4	F	605	1PE	C23-C13-OH4-C24
4	E	604	1PE	C23-C13-OH4-C24
3	E	602	PGE	C3-C4-O3-C5
3	B	602	PGE	C1-C2-O2-C3
4	E	604	1PE	C25-C15-OH6-C26
3	F	604	PGE	C3-C4-O3-C5
3	C	602	PGE	C3-C4-O3-C5
3	D	603	PGE	C6-C5-O3-C4
4	E	604	1PE	C15-C25-OH5-C14
4	C	604	1PE	OH4-C13-C23-OH3
3	D	602	PGE	O2-C3-C4-O3
2	F	602	FAD	O4'-C4'-C5'-O5'
3	D	603	PGE	C4-C3-O2-C2
3	D	602	PGE	C6-C5-O3-C4
3	E	603	PGE	C1-C2-O2-C3
3	F	603	PGE	C3-C4-O3-C5
3	D	603	PGE	O2-C3-C4-O3
3	E	603	PGE	C6-C5-O3-C4
4	D	604	1PE	OH5-C14-C24-OH4
4	F	605	1PE	C12-C22-OH3-C23
4	B	604	1PE	C16-C26-OH6-C15

Continued on next page...

Continued from previous page...

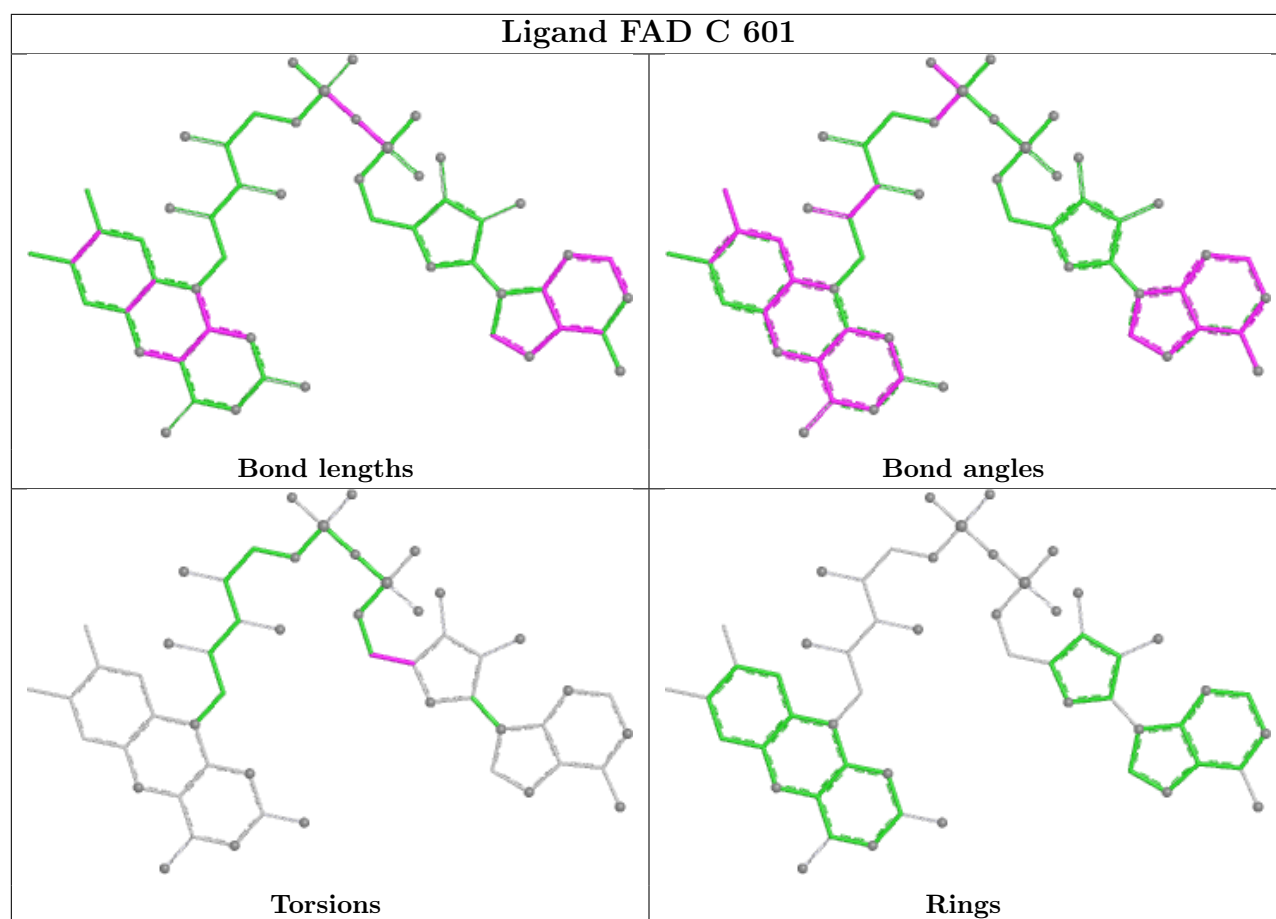
Mol	Chain	Res	Type	Atoms
4	A	604	1PE	C25-C15-OH6-C26
4	E	604	1PE	C12-C22-OH3-C23
4	D	604	1PE	C13-C23-OH3-C22
3	C	603	PGE	C4-C3-O2-C2
4	B	604	1PE	C14-C24-OH4-C13
3	A	603	PGE	O1-C1-C2-O2
4	C	604	1PE	OH2-C12-C22-OH3
3	E	602	PGE	O2-C3-C4-O3
2	F	602	FAD	C3'-C4'-C5'-O5'
6	E	609	GOL	C1-C2-C3-O3
6	C	607	GOL	O2-C2-C3-O3
6	E	609	GOL	O2-C2-C3-O3
3	D	602	PGE	C4-C3-O2-C2
6	D	608	GOL	O1-C1-C2-O2
3	B	603	PGE	C3-C4-O3-C5
3	E	602	PGE	C1-C2-O2-C3
4	C	604	1PE	C12-C22-OH3-C23
6	E	607	GOL	C1-C2-C3-O3
3	A	603	PGE	C3-C4-O3-C5
3	E	602	PGE	C4-C3-O2-C2
3	B	602	PGE	C6-C5-O3-C4
3	F	604	PGE	C6-C5-O3-C4
4	F	605	1PE	OH5-C14-C24-OH4
3	B	603	PGE	C6-C5-O3-C4
4	B	604	1PE	C15-C25-OH5-C14
3	C	603	PGE	C1-C2-O2-C3
4	A	604	1PE	C14-C24-OH4-C13
2	A	601	FAD	O4B-C1B-N9A-C8A
2	A	601	FAD	C2B-C1B-N9A-C8A
2	F	602	FAD	C2B-C1B-N9A-C8A
6	E	608	GOL	O2-C2-C3-O3
2	A	601	FAD	O4B-C4B-C5B-O5B
2	C	601	FAD	O4B-C4B-C5B-O5B
3	B	602	PGE	O2-C3-C4-O3
3	B	602	PGE	C4-C3-O2-C2
2	A	601	FAD	P-O3P-PA-O2A
2	F	602	FAD	P-O3P-PA-O2A
2	E	601	FAD	O4B-C4B-C5B-O5B

There are no ring outliers.

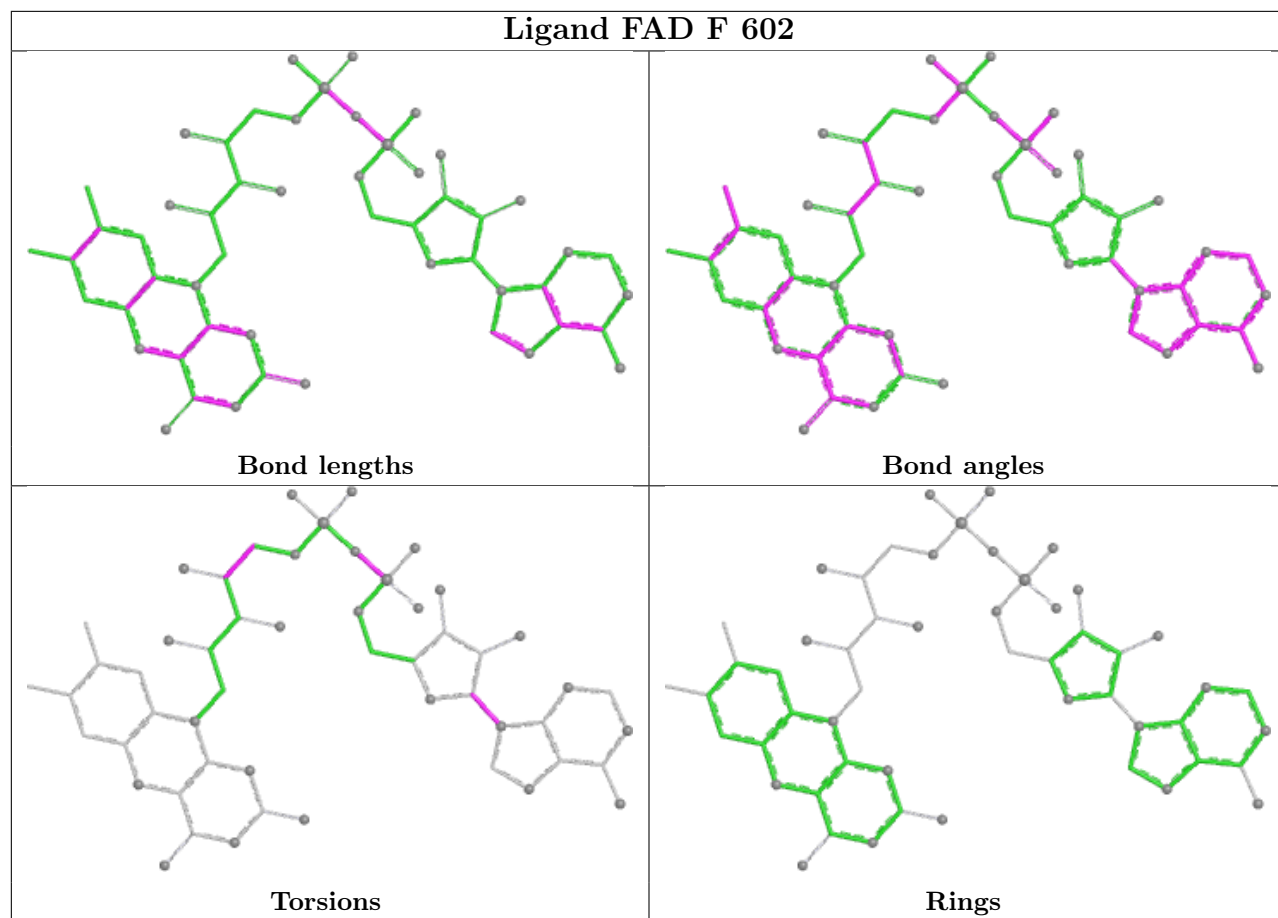
27 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	603	PGE	1	0
6	B	606	GOL	1	0
2	C	601	FAD	2	0
4	C	604	1PE	4	0
2	F	602	FAD	1	0
3	E	602	PGE	1	0
6	B	609	GOL	2	0
6	E	607	GOL	1	0
6	A	608	GOL	1	0
3	D	602	PGE	1	0
2	E	601	FAD	1	0
4	B	604	1PE	2	0
4	D	604	1PE	2	0
6	F	601	GOL	2	0
4	F	605	1PE	5	0
3	F	604	PGE	1	0
3	E	603	PGE	1	0
6	C	607	GOL	1	0
6	D	607	GOL	1	0
6	D	609	GOL	1	0
6	E	608	GOL	3	0
3	A	602	PGE	1	0
3	C	602	PGE	1	0
2	B	601	FAD	1	0
2	D	601	FAD	1	0
3	C	603	PGE	2	0
6	D	610	GOL	2	0

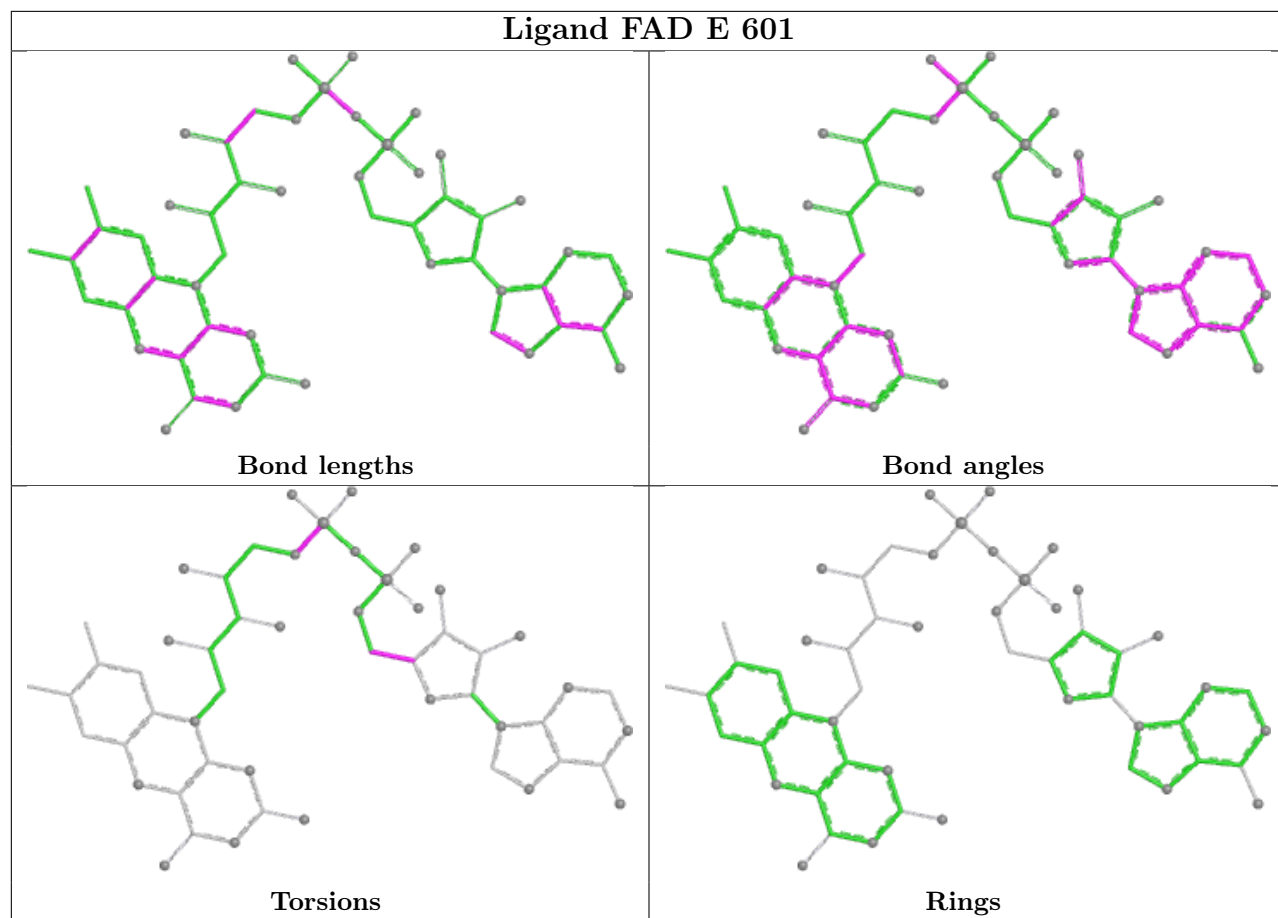
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

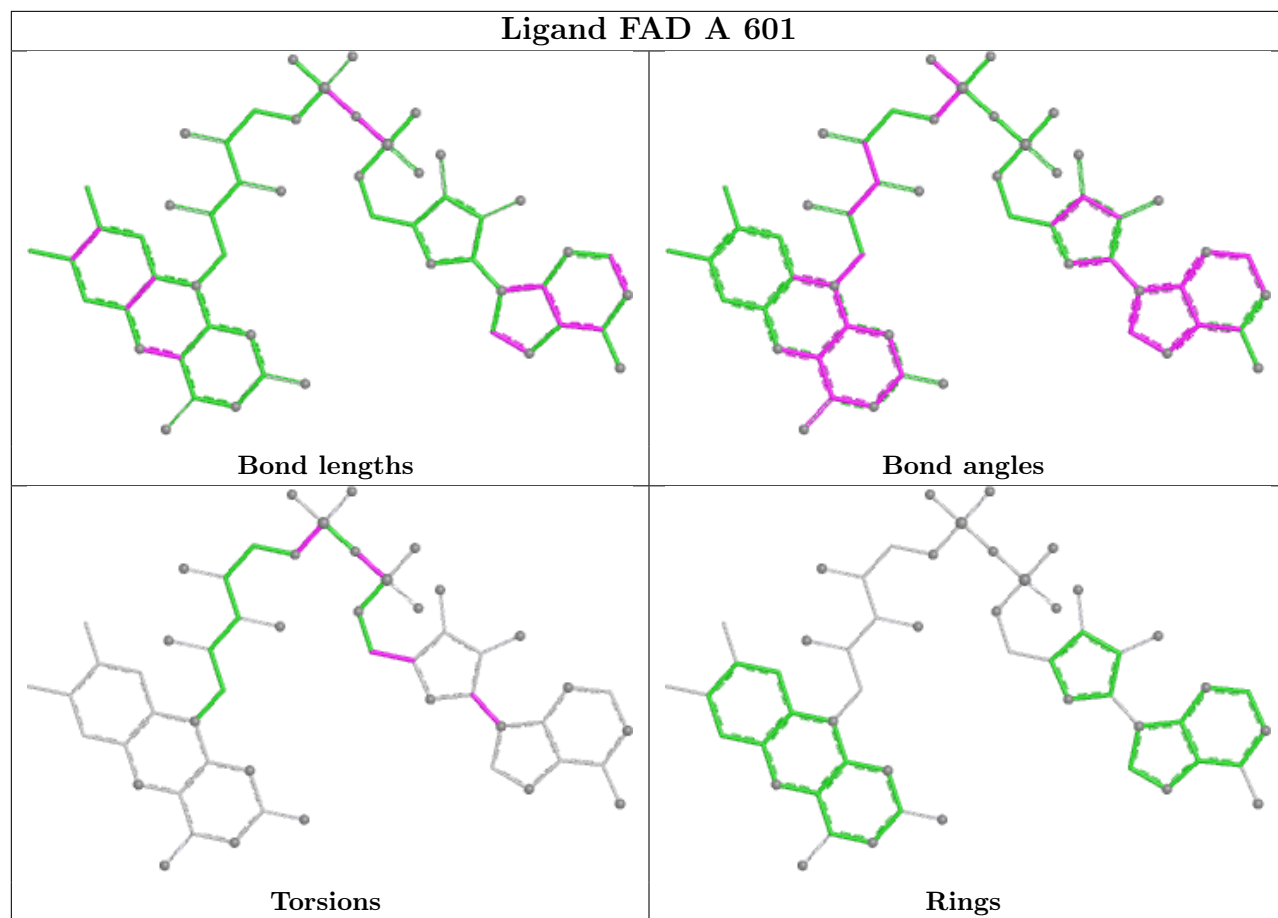


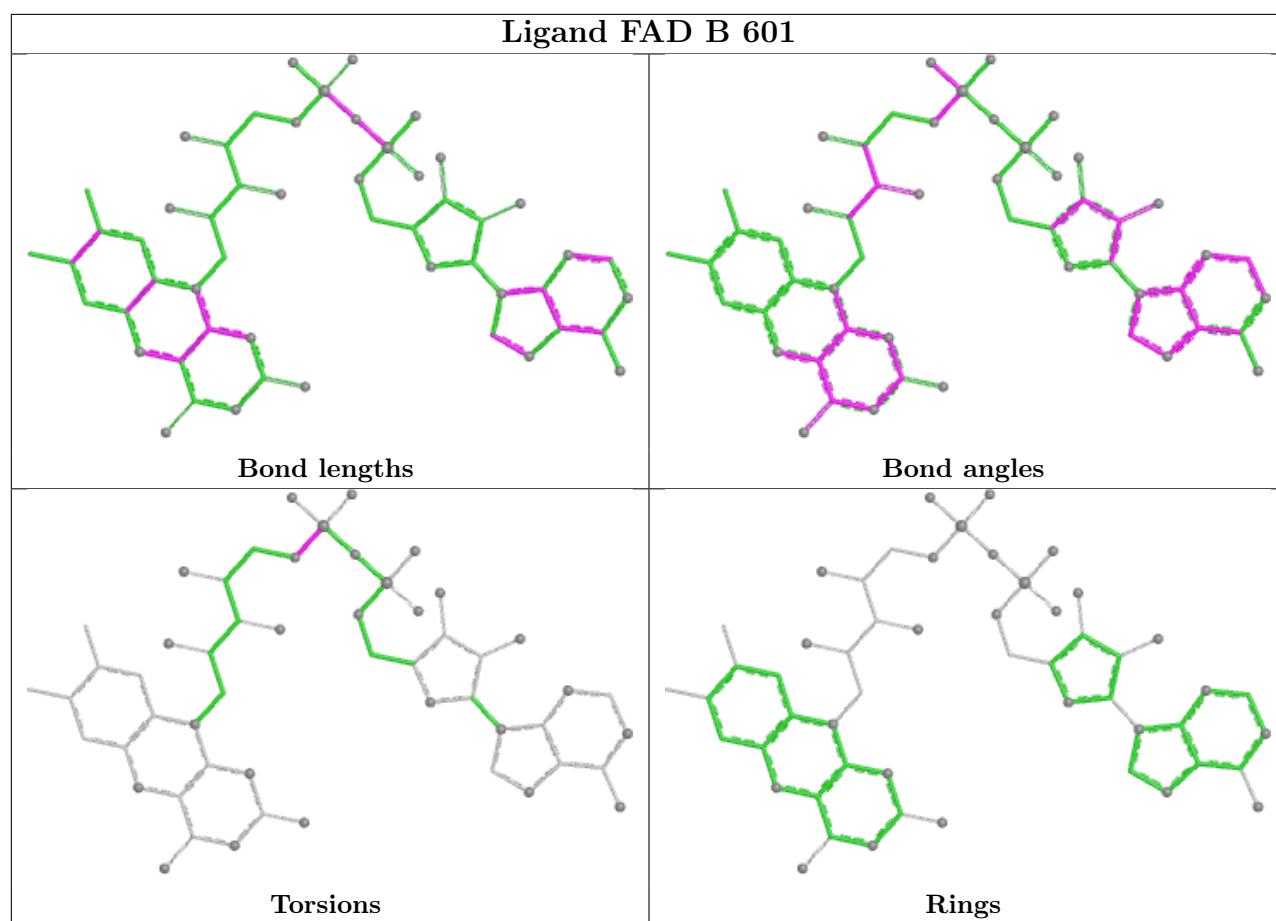
Ligand FAD F 602

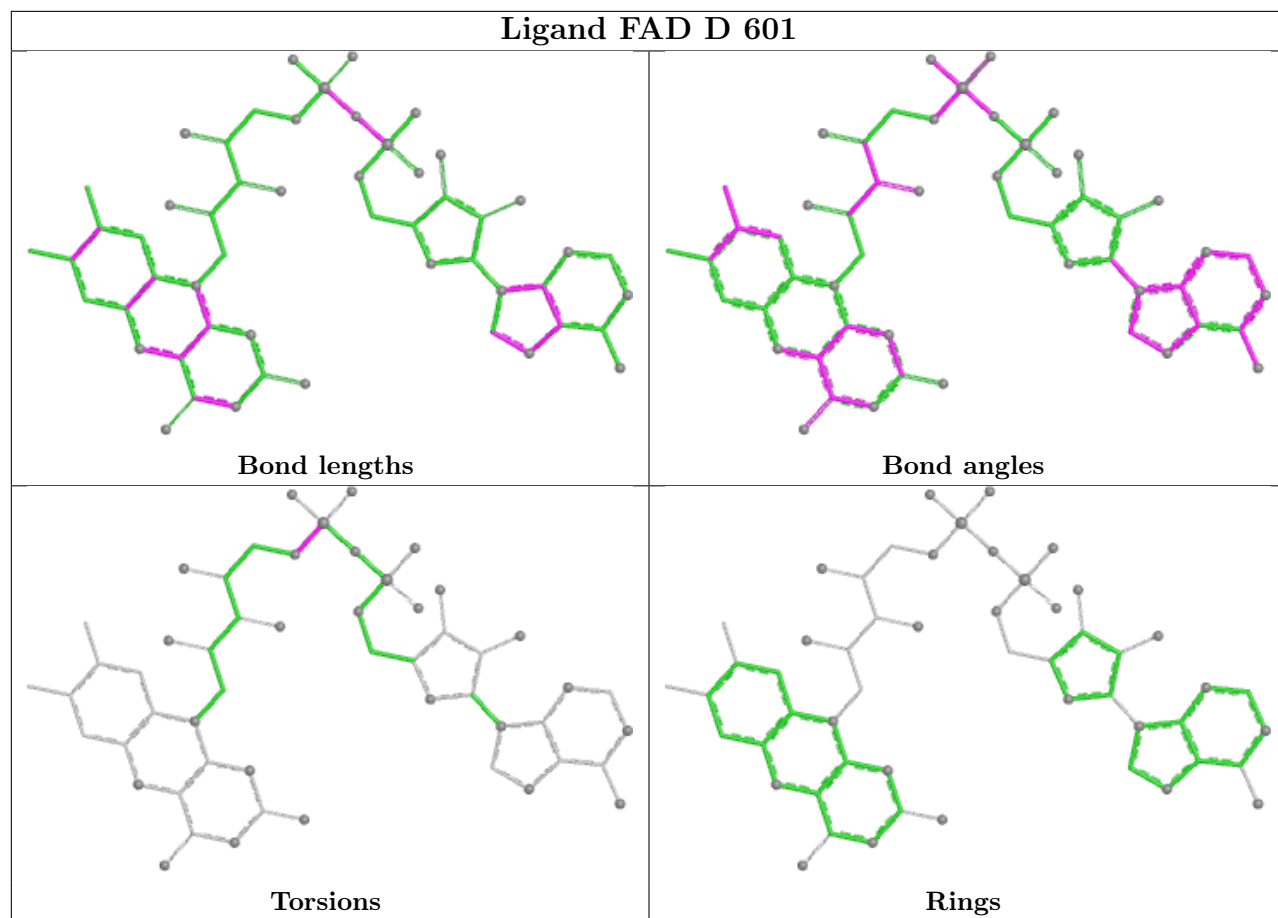


Ligand FAD E 601









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	581/601 (96%)	0.14	11 (1%) 66 66	23, 36, 63, 111	0
1	B	579/601 (96%)	0.05	11 (1%) 66 66	20, 34, 66, 109	0
1	C	585/601 (97%)	-0.30	8 (1%) 73 73	16, 28, 54, 81	0
1	D	578/601 (96%)	-0.04	19 (3%) 49 48	19, 32, 63, 95	0
1	E	579/601 (96%)	-0.20	10 (1%) 69 69	17, 30, 55, 85	1 (0%)
1	F	579/601 (96%)	0.09	10 (1%) 69 69	21, 37, 66, 92	0
All	All	3481/3606 (96%)	-0.04	69 (1%) 65 65	16, 33, 63, 111	1 (0%)

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	413	ALA	4.6
1	B	296	TRP	4.4
1	A	263	ALA	3.7
1	E	296	TRP	3.7
1	C	296	TRP	3.6
1	B	262	THR	3.5
1	D	408	GLU	3.2
1	F	258	PHE	3.1
1	D	407	HIS	3.1
1	B	261	PRO	3.1
1	D	414	ARG	3.1
1	A	261	PRO	3.0
1	B	205	ILE	3.0
1	E	258	PHE	3.0
1	D	205	ILE	3.0
1	D	8	ALA	2.9
1	F	205	ILE	2.9
1	E	202	ALA	2.9
1	B	265	VAL	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	262	THR	2.8
1	B	206	ALA	2.8
1	A	262	THR	2.8
1	A	296	TRP	2.8
1	D	296	TRP	2.8
1	D	258	PHE	2.7
1	F	296	TRP	2.7
1	D	418	ALA	2.6
1	D	262	THR	2.6
1	E	262	THR	2.6
1	D	409	ASP	2.6
1	E	265	VAL	2.6
1	C	258	PHE	2.6
1	D	265	VAL	2.6
1	C	407	HIS	2.6
1	D	406	LEU	2.6
1	A	265	VAL	2.5
1	E	407	HIS	2.5
1	C	8	ALA	2.5
1	C	586	PRO	2.5
1	F	261	PRO	2.5
1	B	202	ALA	2.5
1	B	586	PRO	2.5
1	C	588	PRO	2.5
1	A	258	PHE	2.5
1	F	267	VAL	2.5
1	A	202	ALA	2.5
1	B	260	PRO	2.5
1	A	298	VAL	2.4
1	B	413	ALA	2.3
1	E	205	ILE	2.3
1	A	586	PRO	2.3
1	D	9	PRO	2.3
1	C	201	GLY	2.3
1	E	261	PRO	2.2
1	A	6	GLY	2.2
1	D	393	GLY	2.2
1	F	305	ARG	2.2
1	D	261	PRO	2.1
1	D	419	ALA	2.1
1	F	300	SER	2.1
1	F	9	PRO	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	258	PHE	2.1
1	C	205	ILE	2.1
1	F	265	VAL	2.1
1	E	203	THR	2.0
1	D	411	GLU	2.0
1	A	409	ASP	2.0
1	D	417	ARG	2.0
1	E	7	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PGE	D	603	10/10	0.75	0.21	60,68,70,71	0
6	GOL	D	610	6/6	0.77	0.19	51,55,57,61	0
3	PGE	F	604	10/10	0.78	0.19	42,56,64,65	0
3	PGE	E	603	10/10	0.79	0.20	51,56,63,64	0
3	PGE	A	603	10/10	0.80	0.17	56,61,67,69	0
3	PGE	C	603	10/10	0.81	0.17	44,53,57,62	0
4	1PE	D	604	16/16	0.82	0.17	41,53,61,62	0
4	1PE	B	604	16/16	0.82	0.16	49,56,62,62	0
6	GOL	A	608	6/6	0.83	0.11	52,58,61,64	0
4	1PE	E	604	16/16	0.83	0.16	41,51,63,67	0
6	GOL	F	601	6/6	0.83	0.14	48,50,53,57	0
4	1PE	A	604	16/16	0.84	0.15	41,54,61,61	0
6	GOL	B	609	6/6	0.84	0.17	47,57,59,63	0
6	GOL	D	608	6/6	0.84	0.14	52,62,66,66	0
3	PGE	B	603	10/10	0.84	0.16	57,60,68,71	0

Continued on next page...

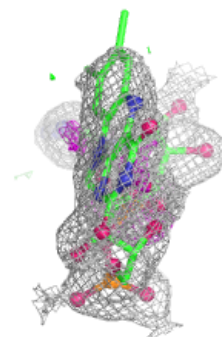
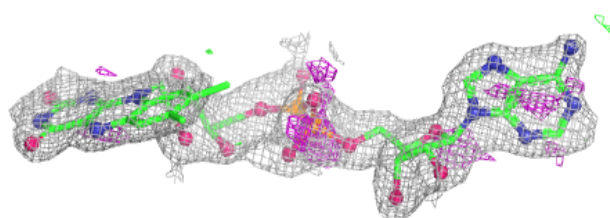
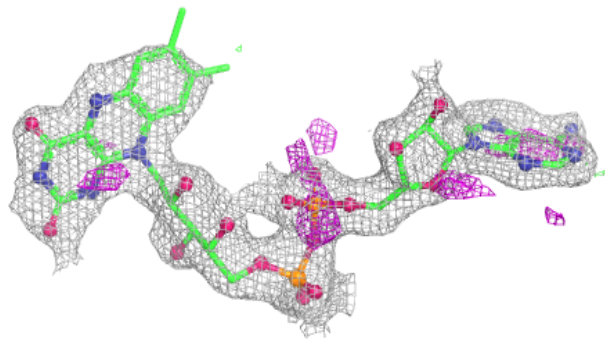
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	1PE	F	605	16/16	0.84	0.14	45,52,66,68	0
6	GOL	F	607	6/6	0.84	0.18	62,65,66,68	0
4	1PE	C	604	16/16	0.85	0.14	38,50,61,63	0
6	GOL	C	607	6/6	0.85	0.20	46,49,57,57	0
6	GOL	B	607	6/6	0.86	0.17	52,59,65,66	0
6	GOL	B	606	6/6	0.86	0.12	46,53,55,55	0
6	GOL	D	609	6/6	0.86	0.13	44,45,49,50	0
6	GOL	E	607	6/6	0.87	0.18	46,59,61,63	0
6	GOL	A	607	6/6	0.88	0.14	50,58,58,65	0
3	PGE	E	602	10/10	0.89	0.13	40,44,47,49	0
5	CL	C	606	1/1	0.89	0.12	60,60,60,60	0
6	GOL	C	608	6/6	0.89	0.13	51,53,56,57	0
6	GOL	E	609	6/6	0.89	0.14	52,56,57,65	0
6	GOL	D	607	6/6	0.89	0.17	53,58,59,62	0
3	PGE	A	602	10/10	0.89	0.14	42,48,52,52	0
6	GOL	B	608	6/6	0.90	0.12	49,54,56,58	0
6	GOL	E	608	6/6	0.91	0.10	38,48,49,52	0
5	CL	E	605	1/1	0.91	0.11	43,43,43,43	0
3	PGE	D	602	10/10	0.92	0.11	41,47,50,52	0
2	FAD	B	601	53/53	0.92	0.11	33,47,73,76	0
2	FAD	F	602	53/53	0.93	0.10	37,50,73,75	0
3	PGE	F	603	10/10	0.93	0.11	46,50,54,57	0
3	PGE	C	602	10/10	0.93	0.11	40,43,47,50	0
3	PGE	B	602	10/10	0.93	0.10	43,47,48,52	0
5	CL	F	606	1/1	0.94	0.08	51,51,51,51	0
2	FAD	A	601	53/53	0.94	0.09	30,43,64,71	0
5	CL	A	606	1/1	0.94	0.10	51,51,51,51	0
2	FAD	E	601	53/53	0.95	0.09	25,37,66,72	0
5	CL	D	606	1/1	0.95	0.09	55,55,55,55	0
5	CL	B	605	1/1	0.95	0.07	45,45,45,45	0
2	FAD	C	601	53/53	0.96	0.08	25,35,59,62	0
2	FAD	D	601	53/53	0.96	0.08	30,41,64,71	0
5	CL	A	605	1/1	0.96	0.08	48,48,48,48	0
5	CL	D	605	1/1	0.96	0.07	41,41,41,41	0
5	CL	C	605	1/1	0.97	0.06	41,41,41,41	0
5	CL	E	606	1/1	0.98	0.07	46,46,46,46	0

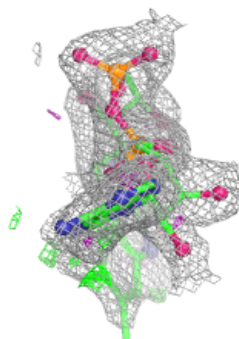
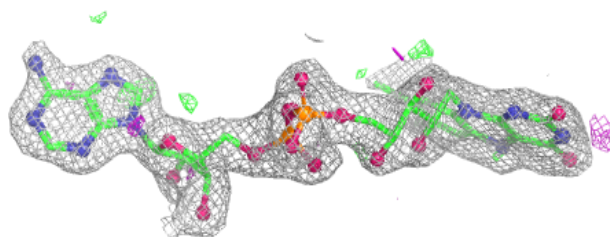
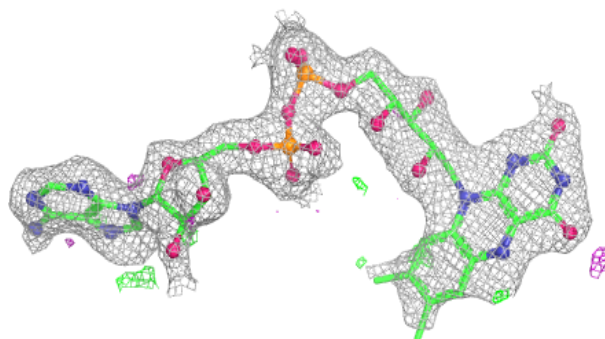
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD B 601:

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

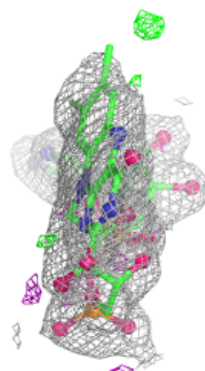
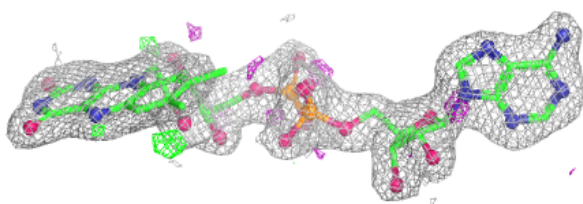
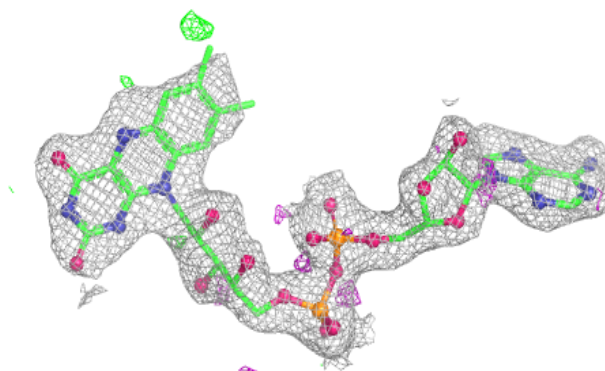
**Electron density around FAD F 602:**

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

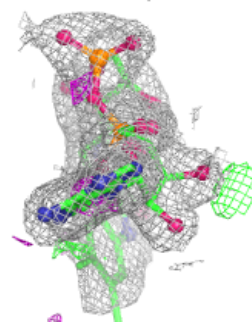
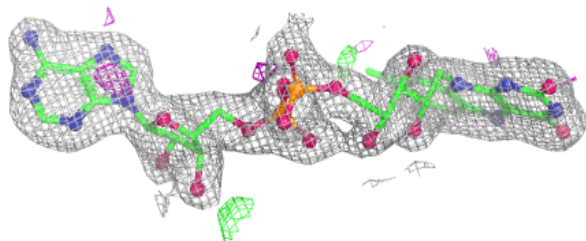
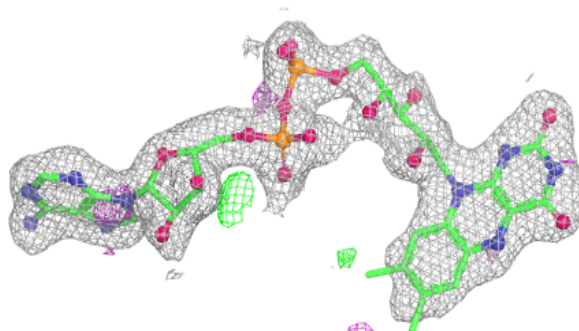


Electron density around FAD A 601:

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

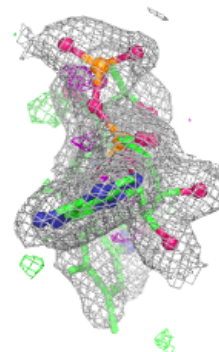
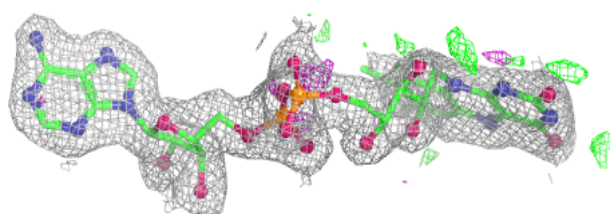
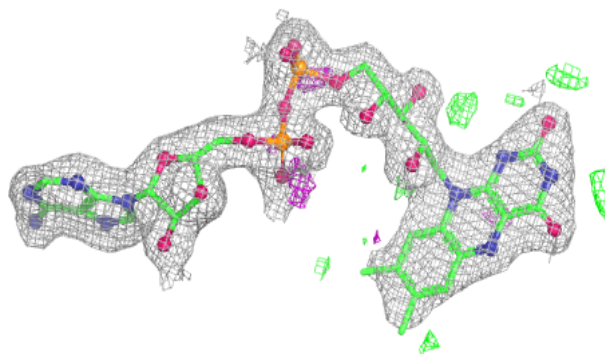
**Electron density around FAD E 601:**

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

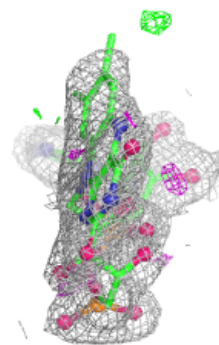
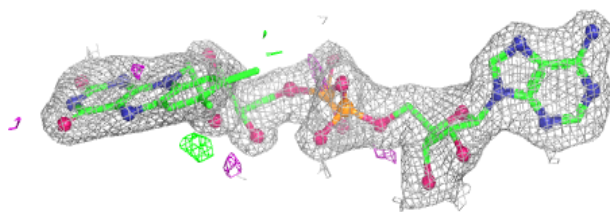
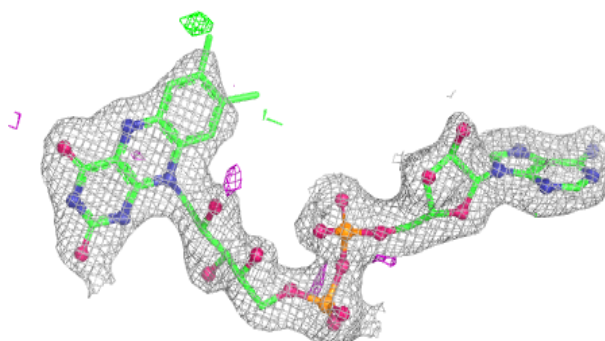


Electron density around FAD C 601:

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

**Electron density around FAD D 601:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.