



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:06 AM UTC

PDB ID : 4C5O / pdb_00004c5o
Title : Flavin monooxygenase from *Stenotrophomonas maltophilia*. Q193R H194T mutant
Authors : Jensen, C.N.; Ali, S.T.; Allen, M.J.; Grogan, G.
Deposited on : 2013-09-13
Resolution : 2.60 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:

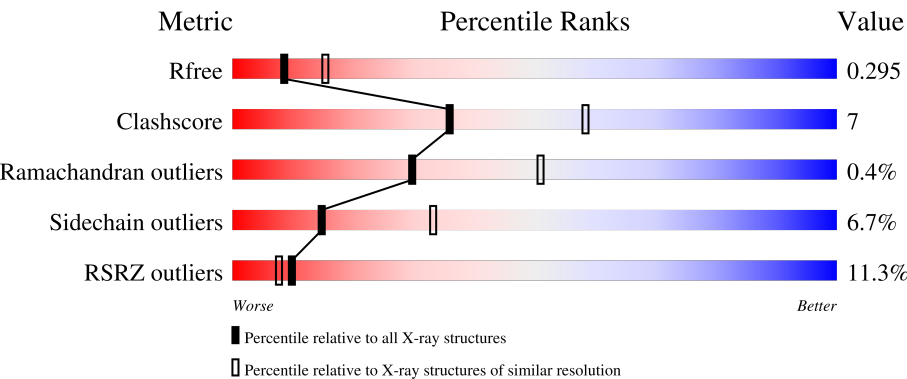
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	357	42% 78% 13% • 8%
1	B	357	19% 77% 15% • 8%
1	C	357	2% 77% 14% • 8%
1	D	357	5% 76% 15% • 7%
1	E	357	4% 78% 13% • 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	357	
1	G	357	
1	H	357	

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	SO4	F	1357	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20137 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 FLAVIN MONOOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	0	0
			2256	1444	392	414	6			
1	B	330	Total	C	N	O	S	0	0	0
			2388	1533	414	434	7			
1	C	330	Total	C	N	O	S	0	0	0
			2475	1588	436	443	8			
1	D	333	Total	C	N	O	S	0	0	0
			2495	1599	438	451	7			
1	E	330	Total	C	N	O	S	0	0	0
			2448	1574	429	437	8			
1	F	330	Total	C	N	O	S	0	0	0
			2436	1567	422	440	7			
1	G	330	Total	C	N	O	S	0	0	0
			2450	1575	432	436	7			
1	H	331	Total	C	N	O	S	0	0	0
			2494	1597	441	448	8			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	193	ARG	GLN	engineered mutation	UNP B2FRL2
A	194	THR	HIS	engineered mutation	UNP B2FRL2
B	193	ARG	GLN	engineered mutation	UNP B2FRL2
B	194	THR	HIS	engineered mutation	UNP B2FRL2
C	193	ARG	GLN	engineered mutation	UNP B2FRL2
C	194	THR	HIS	engineered mutation	UNP B2FRL2
D	193	ARG	GLN	engineered mutation	UNP B2FRL2
D	194	THR	HIS	engineered mutation	UNP B2FRL2
E	193	ARG	GLN	engineered mutation	UNP B2FRL2
E	194	THR	HIS	engineered mutation	UNP B2FRL2
F	193	ARG	GLN	engineered mutation	UNP B2FRL2
F	194	THR	HIS	engineered mutation	UNP B2FRL2
G	193	ARG	GLN	engineered mutation	UNP B2FRL2

Continued on next page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	194	THR	HIS	engineered mutation	UNP B2FRL2
H	193	ARG	GLN	engineered mutation	UNP B2FRL2
H	194	THR	HIS	engineered mutation	UNP B2FRL2

- # FAD

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		

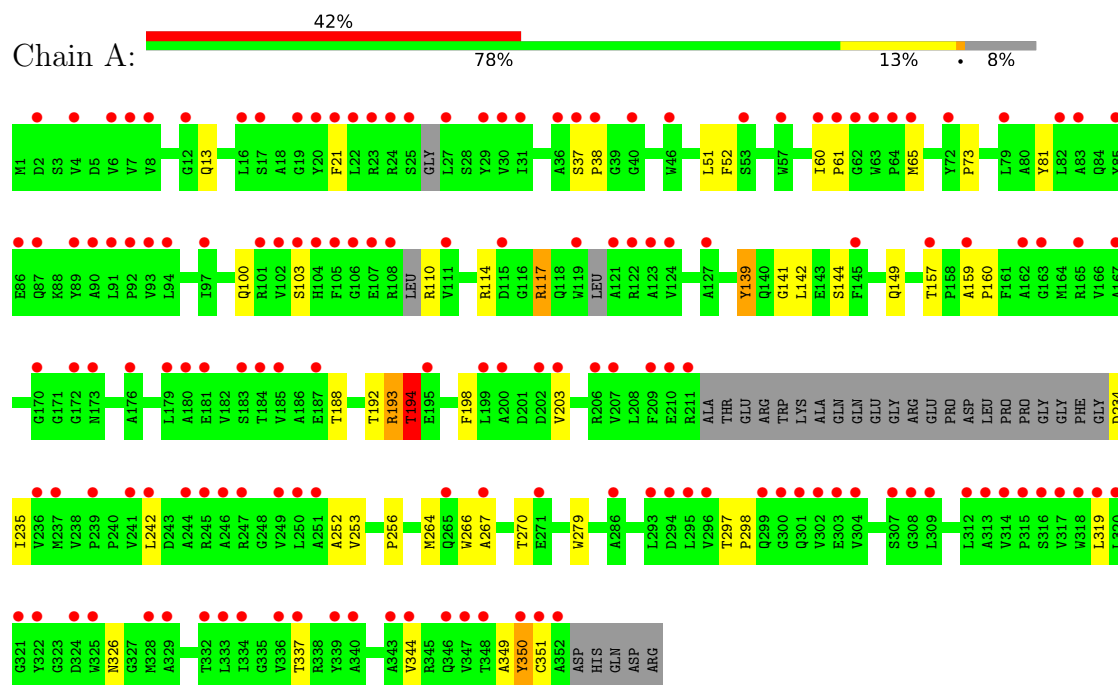
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total 5	O 5	0	0
4	B	4	Total 4	O 4	0	0
4	C	18	Total 18	O 18	0	0
4	D	12	Total 12	O 12	0	0
4	E	13	Total 13	O 13	0	0
4	F	18	Total 18	O 18	0	0
4	G	15	Total 15	O 15	0	0
4	H	21	Total 21	O 21	0	0

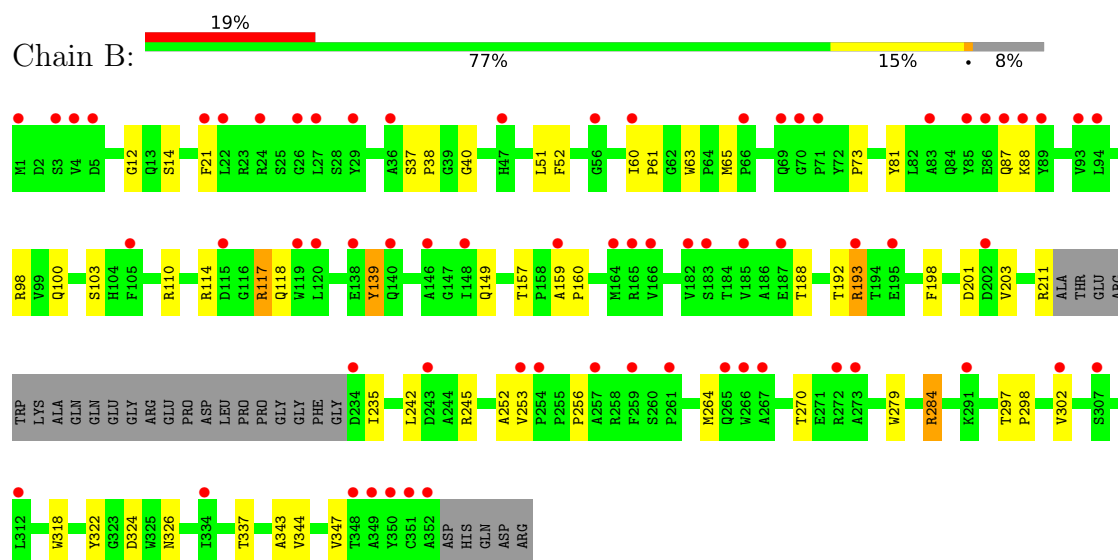
3 Residue-property plots

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

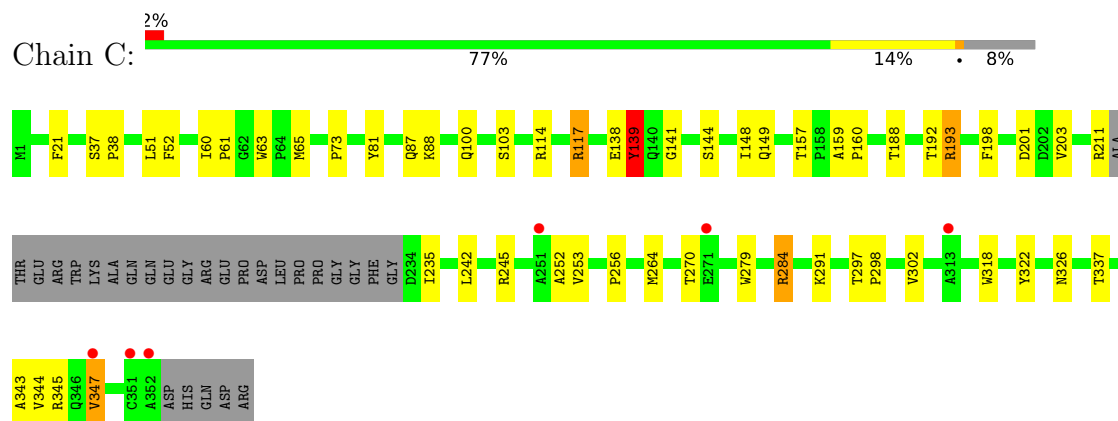
• Molecule 1: FLAVIN MONOOXYGENASE



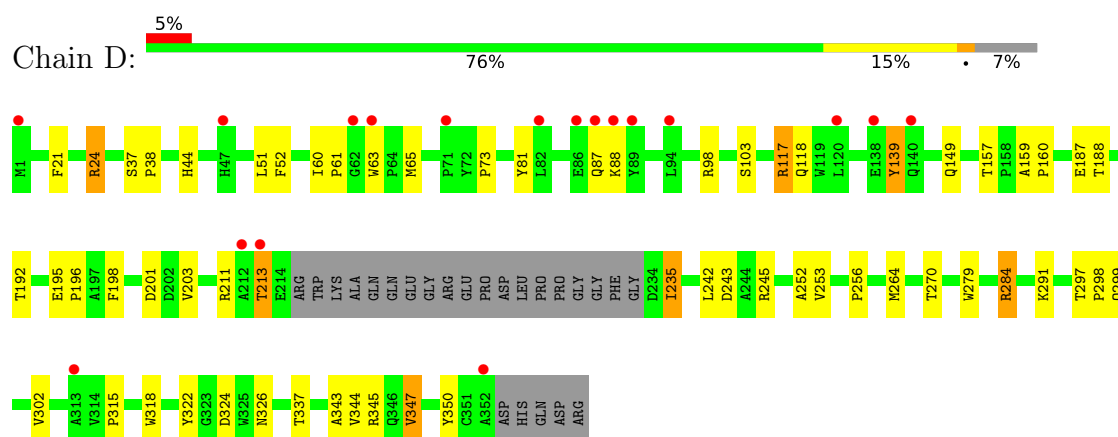
• Molecule 1: FLAVIN MONOOXYGENASE



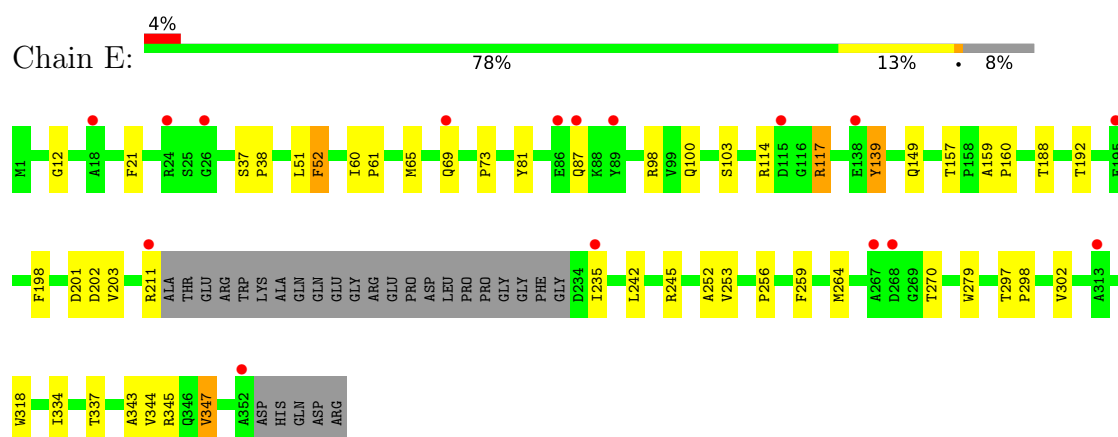
- Molecule 1: FLAVIN MONOOXYGENASE



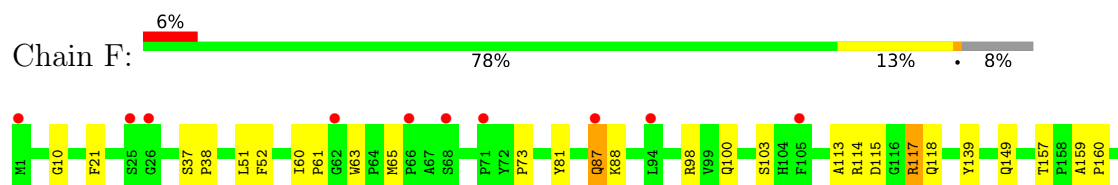
- Molecule 1: FLAVIN MONOOXYGENASE

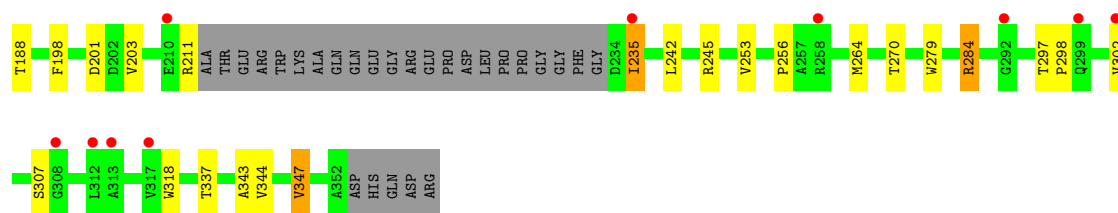


- Molecule 1: FLAVIN MONOOXYGENASE

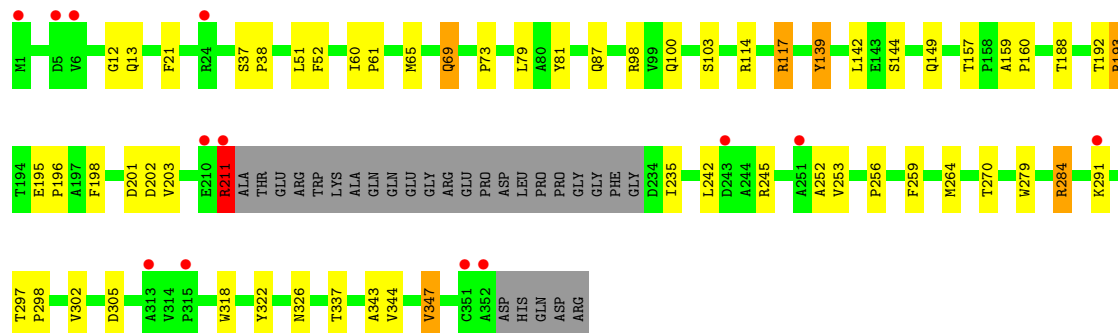
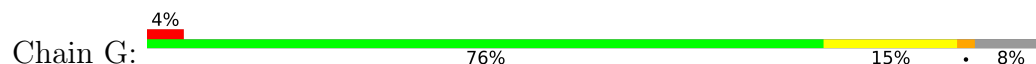


- Molecule 1: FLAVIN MONOOXYGENASE

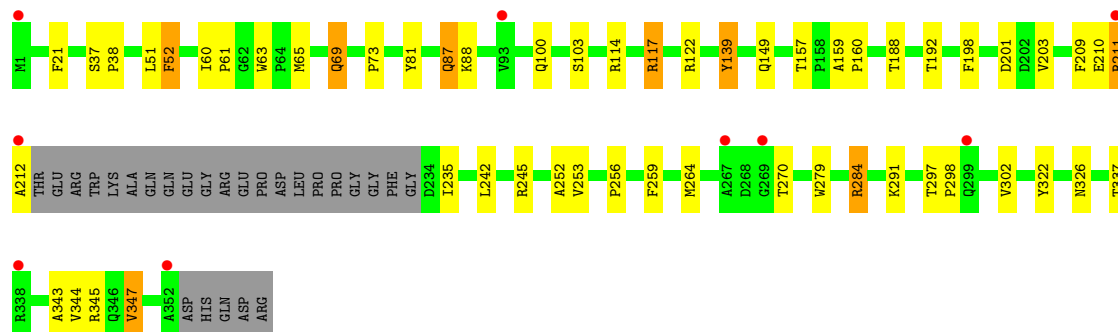
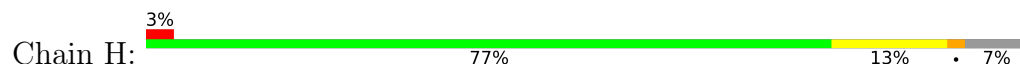




● Molecule 1: FLAVIN MONOOXYGENASE



● Molecule 1: FLAVIN MONOOXYGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	170.54Å 170.54Å 101.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	147.69 – 2.60 147.69 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.2 (147.69-2.60) 97.2 (147.69-2.60)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0033	Depositor
R, R_{free}	0.255 , 0.295 0.258 , 0.295	Depositor DCC
R_{free} test set	6415 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	46.4	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 35.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.039 for -h,-k,l 0.057 for h,-h-k,-l 0.044 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	20137	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 71.77 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.4807e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: SO4, FAD

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	0.83	1/2318 (0.0%)	0.97	4/3187 (0.1%)
1	B	0.84	0/2457	0.96	4/3377 (0.1%)
1	C	0.90	0/2546	0.93	1/3483 (0.0%)
1	D	0.89	0/2566	0.96	3/3512 (0.1%)
1	E	0.89	0/2519	0.94	1/3451 (0.0%)
1	F	0.90	1/2507 (0.0%)	0.95	1/3439 (0.0%)
1	G	0.88	0/2521	0.94	3/3454 (0.1%)
1	H	0.92	0/2565	0.94	3/3508 (0.1%)
All	All	0.88	2/19999 (0.0%)	0.95	20/27411 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	194	THR	CA-C	5.59	1.60	1.52
1	F	10	GLY	CA-C	-5.17	1.48	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	211	ARG	N-CA-C	8.59	135.06	111.00
1	B	193	ARG	CA-CB-CG	8.02	130.13	114.10
1	A	193	ARG	N-CA-C	-7.62	92.78	107.57
1	B	193	ARG	CB-CG-CD	-7.42	94.23	111.30
1	D	213	THR	N-CA-C	-6.72	105.23	113.50
1	B	193	ARG	N-CA-CB	-6.33	100.56	110.30
1	H	69	GLN	CB-CA-C	5.95	120.97	110.85
1	G	69	GLN	CB-CA-C	5.86	120.81	110.85
1	A	139	TYR	N-CA-C	5.74	123.02	110.80
1	F	118	GLN	N-CA-CB	-5.69	100.93	111.52
1	A	110	ARG	CA-CB-CG	5.65	125.40	114.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	139	TYR	N-CA-C	5.59	122.71	110.80
1	E	139	TYR	N-CA-C	5.40	122.31	110.80
1	D	24	ARG	CB-CG-CD	5.39	123.69	111.30
1	H	139	TYR	N-CA-C	5.36	122.22	110.80
1	H	291	LYS	N-CA-C	-5.32	102.52	110.23
1	B	139	TYR	N-CA-C	5.28	122.04	110.80
1	A	194	THR	N-CA-C	5.16	121.78	110.80
1	C	139	TYR	N-CA-C	5.13	121.74	110.80
1	D	139	TYR	N-CA-C	5.09	121.63	110.80

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	2256	0	2032	34	0
1	B	2388	0	2265	36	0
1	C	2475	0	2413	34	0
1	D	2495	0	2425	37	0
1	E	2448	0	2370	30	0
1	F	2436	0	2339	31	0
1	G	2450	0	2375	40	0
1	H	2494	0	2434	42	0
2	A	53	0	31	4	0
2	B	53	0	31	4	0
2	C	53	0	31	0	0
2	D	53	0	31	1	0
2	E	53	0	31	2	0
2	F	53	0	31	0	0
2	G	53	0	31	4	0
2	H	53	0	31	2	0
3	A	15	0	0	1	0
3	B	20	0	0	2	0
3	C	25	0	0	1	0
3	D	30	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	15	0	0	2	0
3	F	20	0	0	3	0
3	G	20	0	0	2	0
3	H	20	0	0	1	0
4	A	5	0	0	1	0
4	B	4	0	0	1	0
4	C	18	0	0	0	0
4	D	12	0	0	1	0
4	E	13	0	0	0	0
4	F	18	0	0	1	0
4	G	15	0	0	0	0
4	H	21	0	0	0	0
All	All	20137	0	18901	284	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 7.

All (284) 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:H:210:GLU:C	1:H:212:ALA:HB3	1.59	1.27
1:H:210:GLU:O	1:H:212:ALA:HB3	1.52	1.10
1:H:210:GLU:C	1:H:212:ALA:CB	2.40	0.94
1:A:266:TRP:O	1:D:315:PRO:HG2	1.68	0.92
1:D:117:ARG:HG3	1:D:117:ARG:HH11	1.39	0.86
1:H:117:ARG:HG3	1:H:117:ARG:HH11	1.41	0.85
1:B:117:ARG:HH11	1:B:117:ARG:HG3	1.42	0.85
1:F:117:ARG:HG3	1:F:117:ARG:HH11	1.40	0.85
1:F:87:GLN:HE22	1:G:202:ASP:HB3	1.43	0.84
1:H:211:ARG:N	1:H:212:ALA:HB3	1.94	0.82
1:G:117:ARG:HG3	1:G:117:ARG:HH11	1.42	0.82
1:C:117:ARG:HG3	1:C:117:ARG:HH11	1.45	0.81
1:E:117:ARG:HG3	1:E:117:ARG:HH11	1.45	0.81
1:A:267:ALA:O	1:D:315:PRO:HD2	1.81	0.81
1:A:117:ARG:HG3	1:A:117:ARG:HH11	1.45	0.80
1:A:193:ARG:O	1:A:194:THR:OG1	2.01	0.78
1:H:198:PHE:CE1	1:H:235:ILE:HD11	2.21	0.75
1:D:198:PHE:CE1	1:D:235:ILE:HD11	2.23	0.74
1:H:211:ARG:CA	1:H:212:ALA:HB3	2.16	0.73
1:H:210:GLU:O	1:H:212:ALA:CB	2.33	0.73
1:B:193:ARG:CZ	1:B:193:ARG:HB3	2.09	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:THR:HG22	1:A:159:ALA:H	1.55	0.72
1:B:198:PHE:CE1	1:B:235:ILE:HD11	2.24	0.71
1:F:198:PHE:CE1	1:F:235:ILE:HD11	2.25	0.71
1:A:198:PHE:CE1	1:A:235:ILE:HD11	2.26	0.71
1:G:198:PHE:CE1	1:G:235:ILE:HD11	2.25	0.70
1:C:198:PHE:CE1	1:C:235:ILE:HD11	2.27	0.70
1:E:198:PHE:CE1	1:E:235:ILE:HD11	2.27	0.69
1:A:60:ILE:HB	1:A:61:PRO:HD2	1.76	0.68
1:B:60:ILE:HB	1:B:61:PRO:HD2	1.75	0.68
1:D:284:ARG:HG2	1:D:284:ARG:HH11	1.59	0.68
1:D:60:ILE:HB	1:D:61:PRO:HD2	1.76	0.67
1:C:60:ILE:HB	1:C:61:PRO:HD2	1.76	0.67
1:H:284:ARG:HG2	1:H:284:ARG:HH11	1.59	0.67
1:E:60:ILE:HB	1:E:61:PRO:HD2	1.76	0.66
1:C:157:THR:HG22	1:C:159:ALA:H	1.60	0.66
1:B:284:ARG:HG2	1:B:284:ARG:HH11	1.60	0.66
1:H:209:PHE:O	1:H:212:ALA:HB2	1.96	0.66
1:G:60:ILE:HB	1:G:61:PRO:HD2	1.77	0.65
1:H:60:ILE:HB	1:H:61:PRO:HD2	1.77	0.65
1:E:157:THR:HG22	1:E:159:ALA:H	1.62	0.64
1:F:284:ARG:HG2	1:F:284:ARG:HH11	1.62	0.64
1:F:60:ILE:HB	1:F:61:PRO:HD2	1.78	0.64
1:G:284:ARG:HG2	1:G:284:ARG:HH11	1.63	0.63
1:H:149:GLN:HE21	1:H:279:TRP:HE1	1.47	0.62
1:C:149:GLN:HE21	1:C:279:TRP:HE1	1.47	0.62
1:D:157:THR:HG22	1:D:159:ALA:H	1.64	0.62
1:D:149:GLN:HE21	1:D:279:TRP:HE1	1.48	0.61
1:E:149:GLN:HE21	1:E:279:TRP:HE1	1.49	0.61
1:A:319:LEU:CB	1:A:326:ASN:HD21	2.14	0.61
1:B:149:GLN:HE21	1:B:279:TRP:HE1	1.49	0.61
1:G:149:GLN:HE21	1:G:279:TRP:HE1	1.49	0.61
1:D:117:ARG:HG3	1:D:117:ARG:NH1	2.13	0.61
1:C:193:ARG:HG2	1:C:193:ARG:HH11	1.65	0.61
1:H:211:ARG:HA	1:H:212:ALA:HB3	1.83	0.61
1:F:157:THR:HG22	1:F:159:ALA:H	1.66	0.60
1:G:157:THR:HG22	1:G:159:ALA:H	1.66	0.60
1:A:149:GLN:HE21	1:A:279:TRP:HE1	1.49	0.60
1:B:14:SER:HB2	4:B:2001:HOH:O	2.02	0.60
1:B:157:THR:HG22	1:B:159:ALA:H	1.67	0.59
1:C:284:ARG:HH11	1:C:284:ARG:HG2	1.66	0.59
1:F:149:GLN:HE21	1:F:279:TRP:HE1	1.50	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:GLN:NE2	2:A:1353:FAD:H4'	2.16	0.59
1:C:148:ILE:HA	3:C:1356:SO4:O1	2.03	0.58
1:D:324:ASP:N	3:D:1358:SO4:O4	2.36	0.58
1:B:284:ARG:HH11	1:B:284:ARG:CG	2.17	0.58
1:F:307:SER:O	4:F:2018:HOH:O	2.17	0.58
1:A:13:GLN:CD	2:A:1353:FAD:H4'	2.28	0.58
1:A:319:LEU:HB3	1:A:326:ASN:HD21	1.70	0.57
1:E:117:ARG:HG3	1:E:117:ARG:NH1	2.18	0.57
1:H:157:THR:HG22	1:H:159:ALA:H	1.70	0.56
1:H:284:ARG:HH11	1:H:284:ARG:CG	2.18	0.56
1:G:201:ASP:OD2	1:G:245:ARG:NH2	2.38	0.56
1:H:201:ASP:OD2	1:H:245:ARG:NH2	2.38	0.56
1:F:284:ARG:HH11	1:F:284:ARG:CG	2.18	0.56
1:C:148:ILE:HD11	1:D:118:GLN:CD	2.30	0.56
1:C:201:ASP:OD2	1:C:245:ARG:NH2	2.39	0.56
1:F:113:ALA:HB1	3:F:1357:SO4:O4	2.06	0.55
1:B:324:ASP:N	3:B:1357:SO4:O3	2.39	0.55
1:C:65:MET:HE1	1:C:73:PRO:HB3	1.89	0.55
1:C:284:ARG:HH11	1:C:284:ARG:CG	2.20	0.55
1:D:60:ILE:HB	1:D:61:PRO:CD	2.37	0.55
1:G:245:ARG:HH11	1:G:245:ARG:HG2	1.72	0.55
1:E:69:GLN:HG2	1:G:79:LEU:HD13	1.89	0.55
1:F:87:GLN:NE2	1:G:202:ASP:HB3	2.18	0.55
1:G:284:ARG:HH11	1:G:284:ARG:CG	2.20	0.55
1:B:201:ASP:OD2	1:B:245:ARG:NH2	2.40	0.55
1:F:245:ARG:HG2	1:F:245:ARG:HH11	1.72	0.54
1:D:284:ARG:HH11	1:D:284:ARG:CG	2.20	0.54
1:E:202:ASP:HB3	1:H:87:GLN:HE22	1.71	0.54
1:B:65:MET:HE1	1:B:73:PRO:HB3	1.89	0.54
1:E:192:THR:OG1	3:E:1356:SO4:O3	2.23	0.54
1:C:60:ILE:HB	1:C:61:PRO:CD	2.38	0.54
1:E:201:ASP:OD2	1:E:245:ARG:NH2	2.41	0.54
2:E:1353:FAD:N1	2:E:1353:FAD:O2'	2.39	0.54
1:D:201:ASP:OD2	1:D:245:ARG:NH2	2.41	0.53
1:F:201:ASP:OD2	1:F:245:ARG:NH2	2.41	0.53
1:H:211:ARG:CA	1:H:212:ALA:CB	2.86	0.53
1:H:60:ILE:HB	1:H:61:PRO:CD	2.38	0.53
1:A:234:ASP:N	4:A:2005:HOH:O	2.42	0.53
1:E:60:ILE:HB	1:E:61:PRO:CD	2.38	0.53
1:D:245:ARG:HH11	1:D:245:ARG:HG2	1.72	0.53
1:H:65:MET:HE1	1:H:73:PRO:HB3	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:ALA:O	1:A:351:CYS:N	2.42	0.53
1:E:98:ARG:NH1	3:E:1354:SO4:O3	2.32	0.53
1:G:65:MET:HE1	1:G:73:PRO:HB3	1.91	0.53
1:A:60:ILE:HB	1:A:61:PRO:CD	2.38	0.52
1:B:245:ARG:HH11	1:B:245:ARG:HG2	1.74	0.52
1:H:284:ARG:HG2	1:H:284:ARG:NH1	2.25	0.52
1:A:65:MET:HE1	1:A:73:PRO:HB3	1.91	0.52
1:C:117:ARG:HG3	1:C:117:ARG:NH1	2.19	0.52
1:B:60:ILE:HB	1:B:61:PRO:CD	2.37	0.52
1:F:159:ALA:HB3	1:F:160:PRO:HD3	1.92	0.52
1:E:65:MET:HE1	1:E:73:PRO:HB3	1.92	0.52
1:F:60:ILE:HB	1:F:61:PRO:CD	2.40	0.52
1:H:245:ARG:HG2	1:H:245:ARG:HH11	1.73	0.52
1:G:60:ILE:HB	1:G:61:PRO:CD	2.39	0.52
1:D:65:MET:HE1	1:D:73:PRO:HB3	1.92	0.51
1:G:98:ARG:HD2	3:G:1354:SO4:O3	2.10	0.51
1:F:65:MET:HE1	1:F:73:PRO:HB3	1.92	0.51
2:A:1353:FAD:N1	2:A:1353:FAD:O2'	2.42	0.51
1:C:193:ARG:HH11	1:C:193:ARG:CG	2.22	0.51
1:C:245:ARG:HG2	1:C:245:ARG:HH11	1.75	0.51
1:B:63:TRP:HB2	1:B:88:LYS:HE3	1.92	0.51
1:B:117:ARG:HG3	1:B:117:ARG:NH1	2.16	0.51
1:G:12:GLY:HA3	2:G:1353:FAD:H52A	1.93	0.50
1:H:63:TRP:HB2	1:H:88:LYS:HE3	1.93	0.50
1:B:193:ARG:CZ	1:B:193:ARG:CB	2.86	0.50
1:D:63:TRP:HB2	1:D:88:LYS:HE3	1.94	0.50
1:B:98:ARG:HD2	3:B:1354:SO4:O3	2.11	0.50
1:C:37:SER:HB3	1:C:38:PRO:HD2	1.94	0.50
1:D:159:ALA:HB3	1:D:160:PRO:HD3	1.94	0.50
1:E:245:ARG:HG2	1:E:245:ARG:HH11	1.76	0.50
1:G:37:SER:HB3	1:G:38:PRO:HD2	1.93	0.50
1:H:37:SER:HB3	1:H:38:PRO:HD2	1.95	0.49
1:E:202:ASP:HB3	1:H:87:GLN:NE2	2.27	0.49
1:D:37:SER:HB3	1:D:38:PRO:HD2	1.94	0.48
1:A:37:SER:HB3	1:A:38:PRO:HD2	1.95	0.48
1:A:159:ALA:HB3	1:A:160:PRO:HD3	1.96	0.48
1:E:37:SER:HB3	1:E:38:PRO:HD2	1.94	0.48
1:F:37:SER:HB3	1:F:38:PRO:HD2	1.95	0.48
1:F:117:ARG:HG3	1:F:117:ARG:NH1	2.15	0.48
1:H:211:ARG:N	1:H:212:ALA:CB	2.72	0.48
1:B:110:ARG:HE	1:B:118:GLN:NE2	2.11	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:211:ARG:HD3	1:G:211:ARG:N	2.29	0.48
1:B:343:ALA:O	1:B:347:VAL:HG13	2.14	0.48
1:C:141:GLY:O	1:C:144:SER:OG	2.28	0.47
1:F:117:ARG:HH11	1:F:117:ARG:CG	2.21	0.47
1:F:63:TRP:HB2	1:F:88:LYS:HE3	1.95	0.47
1:H:117:ARG:HG3	1:H:117:ARG:NH1	2.15	0.47
1:A:117:ARG:HG3	1:A:117:ARG:NH1	2.18	0.47
2:A:1353:FAD:H9	2:A:1353:FAD:H1'1	1.72	0.47
1:E:343:ALA:O	1:E:347:VAL:HG13	2.15	0.47
1:E:297:THR:HB	1:E:298:PRO:HD2	1.97	0.47
1:H:297:THR:HB	1:H:298:PRO:HD2	1.96	0.47
1:B:159:ALA:HB3	1:B:160:PRO:HD3	1.97	0.47
1:B:297:THR:HB	1:B:298:PRO:HD2	1.96	0.47
1:C:63:TRP:HB2	1:C:88:LYS:HE3	1.95	0.47
1:G:297:THR:HB	1:G:298:PRO:HD2	1.96	0.47
1:E:12:GLY:HA3	2:E:1353:FAD:H52A	1.97	0.47
1:F:343:ALA:O	1:F:347:VAL:HG13	2.15	0.47
1:A:61:PRO:HG3	1:A:337:THR:HG23	1.97	0.47
1:B:65:MET:HG3	1:B:81:TYR:CD2	2.50	0.46
1:D:65:MET:HG3	1:D:81:TYR:CD2	2.51	0.46
1:E:159:ALA:HB3	1:E:160:PRO:HD3	1.98	0.46
1:B:117:ARG:HH11	1:B:117:ARG:CG	2.22	0.46
1:F:297:THR:HB	1:F:298:PRO:HD2	1.98	0.46
1:H:343:ALA:O	1:H:347:VAL:HG13	2.15	0.46
1:D:44:HIS:O	3:D:1355:SO4:O3	2.33	0.46
1:F:284:ARG:HG2	1:F:284:ARG:NH1	2.29	0.46
1:G:117:ARG:HG3	1:G:117:ARG:NH1	2.16	0.46
1:A:267:ALA:HB2	1:D:350:TYR:OH	2.15	0.46
1:B:37:SER:HB3	1:B:38:PRO:HD2	1.96	0.46
1:C:322:TYR:H	1:C:326:ASN:HD22	1.64	0.46
1:D:343:ALA:O	1:D:347:VAL:HG13	2.15	0.46
1:F:21:PHE:HB2	1:F:344:VAL:HG21	1.98	0.46
1:B:40:GLY:HA2	2:B:1353:FAD:O3B	2.15	0.46
1:A:114:ARG:NH1	3:A:1354:SO4:O3	2.43	0.46
1:D:284:ARG:HG2	1:D:284:ARG:NH1	2.23	0.46
1:D:61:PRO:HG3	1:D:337:THR:HG23	1.98	0.46
1:G:343:ALA:O	1:G:347:VAL:HG13	2.16	0.46
1:A:65:MET:HG3	1:A:81:TYR:CD2	2.51	0.45
1:A:297:THR:HB	1:A:298:PRO:HD2	1.98	0.45
1:B:12:GLY:HA3	2:B:1353:FAD:H52A	1.97	0.45
1:E:61:PRO:HG3	1:E:337:THR:HG23	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:318:TRP:CD2	1:G:347:VAL:HG12	2.52	0.45
1:F:61:PRO:HG3	1:F:337:THR:HG23	1.98	0.45
1:C:297:THR:HB	1:C:298:PRO:HD2	1.99	0.45
1:E:21:PHE:HB2	1:E:344:VAL:HG21	1.99	0.45
1:G:61:PRO:HG3	1:G:337:THR:HG23	1.98	0.45
1:B:284:ARG:HG2	1:B:284:ARG:NH1	2.27	0.45
1:C:343:ALA:O	1:C:347:VAL:HG13	2.16	0.45
1:G:117:ARG:HH11	1:G:117:ARG:CG	2.22	0.45
1:F:115:ASP:HB3	3:F:1357:SO4:O2	2.17	0.45
1:H:322:TYR:H	1:H:326:ASN:HD22	1.65	0.45
1:H:159:ALA:HB3	1:H:160:PRO:HD3	1.98	0.45
1:D:297:THR:HB	1:D:298:PRO:HD2	1.99	0.45
1:D:318:TRP:CD2	1:D:347:VAL:HG12	2.52	0.45
1:G:256:PRO:HG3	1:G:264:MET:SD	2.57	0.45
1:H:61:PRO:HG3	1:H:337:THR:HG23	1.98	0.45
1:A:21:PHE:HB2	1:A:344:VAL:HG21	1.99	0.45
1:A:267:ALA:CB	1:D:350:TYR:OH	2.65	0.45
1:C:61:PRO:HG3	1:C:337:THR:HG23	1.97	0.45
1:D:117:ARG:HH11	1:D:117:ARG:CG	2.21	0.45
1:A:256:PRO:HG3	1:A:264:MET:SD	2.57	0.44
1:D:21:PHE:HB2	1:D:344:VAL:HG21	2.00	0.44
1:H:65:MET:HG3	1:H:81:TYR:CD2	2.52	0.44
1:F:256:PRO:HG3	1:F:264:MET:SD	2.57	0.44
1:G:65:MET:HG3	1:G:81:TYR:CD2	2.53	0.44
1:C:284:ARG:HG2	1:C:284:ARG:NH1	2.32	0.44
1:G:322:TYR:H	1:G:326:ASN:HD22	1.64	0.44
2:G:1353:FAD:H9	2:G:1353:FAD:H1'1	1.84	0.44
1:A:319:LEU:HB2	1:A:326:ASN:HD21	1.81	0.44
1:D:322:TYR:H	1:D:326:ASN:HD22	1.65	0.44
1:F:318:TRP:CD2	1:F:347:VAL:HG12	2.53	0.44
1:G:21:PHE:HB2	1:G:344:VAL:HG21	2.00	0.44
1:B:192:THR:HG22	1:B:252:ALA:HB1	1.99	0.44
1:C:159:ALA:HB3	1:C:160:PRO:HD3	1.99	0.44
1:D:195:GLU:HA	1:D:196:PRO:HD3	1.91	0.44
1:B:21:PHE:HB2	1:B:344:VAL:HG21	2.00	0.44
1:E:117:ARG:HH11	1:E:117:ARG:CG	2.24	0.44
1:H:192:THR:HG22	1:H:252:ALA:HB1	1.99	0.44
1:D:98:ARG:NH1	3:D:1354:SO4:O3	2.51	0.43
1:G:259:PHE:CE2	1:G:264:MET:HE2	2.53	0.43
1:C:192:THR:HG22	1:C:252:ALA:HB1	2.00	0.43
1:E:256:PRO:HG3	1:E:264:MET:SD	2.59	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:193:ARG:HH11	1:G:193:ARG:HB2	1.83	0.43
1:A:141:GLY:O	1:A:144:SER:OG	2.28	0.43
1:B:256:PRO:HG3	1:B:264:MET:SD	2.59	0.43
2:B:1353:FAD:N1	2:B:1353:FAD:O2'	2.46	0.43
2:D:1353:FAD:H51A	4:D:2002:HOH:O	2.18	0.43
1:H:21:PHE:HB2	1:H:344:VAL:HG21	1.99	0.43
1:C:21:PHE:HB2	1:C:344:VAL:HG21	2.00	0.43
1:E:65:MET:HG3	1:E:81:TYR:CD2	2.54	0.43
1:G:100:GLN:HG3	1:G:114:ARG:HA	2.01	0.43
1:E:192:THR:HG22	1:E:252:ALA:HB1	2.00	0.43
1:A:349:ALA:O	1:A:350:TYR:C	2.62	0.42
1:B:61:PRO:HG3	1:B:337:THR:HG23	2.00	0.42
1:D:192:THR:HG22	1:D:252:ALA:HB1	2.01	0.42
1:D:256:PRO:HG3	1:D:264:MET:SD	2.60	0.42
2:H:1353:FAD:N1	2:H:1353:FAD:O2'	2.49	0.42
1:A:192:THR:HG22	1:A:252:ALA:HB1	2.00	0.42
2:H:1353:FAD:H2'	2:H:1353:FAD:H5'2	1.87	0.42
1:B:65:MET:HE1	1:B:73:PRO:HG3	2.00	0.42
1:C:318:TRP:CD2	1:C:347:VAL:HG12	2.55	0.42
1:G:159:ALA:HB3	1:G:160:PRO:HD3	2.02	0.42
1:H:256:PRO:HG3	1:H:264:MET:SD	2.59	0.42
1:B:322:TYR:H	1:B:326:ASN:HD22	1.66	0.42
1:C:100:GLN:HG3	1:C:114:ARG:HA	2.01	0.42
1:B:100:GLN:HG3	1:B:114:ARG:HA	2.02	0.42
1:H:192:THR:OG1	3:H:1357:SO4:O3	2.36	0.42
1:A:142:LEU:C	1:A:144:SER:H	2.28	0.42
1:G:65:MET:HE1	1:G:73:PRO:HG3	2.01	0.42
1:C:65:MET:HG3	1:C:81:TYR:CD2	2.54	0.42
1:C:256:PRO:HG3	1:C:264:MET:SD	2.60	0.42
1:F:98:ARG:HD2	3:F:1354:SO4:O3	2.20	0.42
1:H:117:ARG:HH11	1:H:117:ARG:CG	2.23	0.41
1:G:142:LEU:C	1:G:144:SER:H	2.28	0.41
1:B:318:TRP:CD2	1:B:347:VAL:HG12	2.56	0.41
1:G:284:ARG:HG2	1:G:284:ARG:NH1	2.31	0.41
1:A:65:MET:HE1	1:A:73:PRO:HG3	2.01	0.41
1:G:13:GLN:OE1	2:G:1353:FAD:H4'	2.20	0.41
1:G:192:THR:HG22	1:G:252:ALA:HB1	2.02	0.41
1:G:193:ARG:NH1	3:G:1356:SO4:O4	2.53	0.41
1:H:65:MET:HE1	1:H:73:PRO:HG3	2.02	0.41
1:C:117:ARG:HH11	1:C:117:ARG:CG	2.25	0.41
1:E:52:PHE:CD1	1:E:52:PHE:C	2.99	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:100:GLN:HG3	1:E:114:ARG:HA	2.03	0.41
2:B:1353:FAD:H9	2:B:1353:FAD:H1'1	1.74	0.41
1:C:138:GLU:O	1:C:139:TYR:O	2.39	0.41
1:E:259:PHE:CE2	1:E:264:MET:HE2	2.55	0.40
1:F:65:MET:HG3	1:F:81:TYR:CD2	2.56	0.40
1:C:65:MET:HE1	1:C:73:PRO:HG3	2.02	0.40
1:D:245:ARG:HG2	1:D:245:ARG:NH1	2.36	0.40
1:G:305:ASP:OD1	1:G:305:ASP:C	2.63	0.40
1:H:52:PHE:CD1	1:H:52:PHE:C	2.99	0.40
1:H:259:PHE:CE2	1:H:264:MET:HE2	2.56	0.40
1:A:100:GLN:HG3	1:A:114:ARG:HA	2.03	0.40
1:D:65:MET:HE1	1:D:73:PRO:HG3	2.02	0.40
1:E:318:TRP:CD2	1:E:347:VAL:HG12	2.57	0.40
1:F:100:GLN:HG3	1:F:114:ARG:HA	2.04	0.40
2:G:1353:FAD:N1	2:G:1353:FAD:O2'	2.51	0.40
1:G:195:GLU:HA	1:G:196:PRO:HD3	1.97	0.40
1:H:100:GLN:HG3	1:H:114:ARG:HA	2.04	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	317/357 (89%)	296 (93%)	18 (6%)	3 (1%)	14	30
1	B	326/357 (91%)	309 (95%)	16 (5%)	1 (0%)	36	58
1	C	326/357 (91%)	310 (95%)	15 (5%)	1 (0%)	36	58
1	D	329/357 (92%)	316 (96%)	12 (4%)	1 (0%)	36	58
1	E	326/357 (91%)	311 (95%)	14 (4%)	1 (0%)	36	58
1	F	326/357 (91%)	311 (95%)	14 (4%)	1 (0%)	36	58
1	G	326/357 (91%)	312 (96%)	13 (4%)	1 (0%)	36	58

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	327/357 (92%)	312 (95%)	14 (4%)	1 (0%)	36	58
All	All	2603/2856 (91%)	2477 (95%)	116 (4%)	10 (0%)	30	51

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	139	TYR
1	A	350	TYR
1	B	139	TYR
1	C	139	TYR
1	D	139	TYR
1	E	139	TYR
1	F	139	TYR
1	G	139	TYR
1	H	139	TYR
1	A	194	THR

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	193/272 (71%)	184 (95%)	9 (5%)	23	48
1	B	225/272 (83%)	212 (94%)	13 (6%)	18	39
1	C	244/272 (90%)	227 (93%)	17 (7%)	14	31
1	D	246/272 (90%)	224 (91%)	22 (9%)	9	20
1	E	238/272 (88%)	223 (94%)	15 (6%)	16	36
1	F	235/272 (86%)	220 (94%)	15 (6%)	16	35
1	G	237/272 (87%)	220 (93%)	17 (7%)	13	30
1	H	247/272 (91%)	230 (93%)	17 (7%)	14	32
All	All	1865/2176 (86%)	1740 (93%)	125 (7%)	15	33

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

Mol	Chain	Res	Type
1	A	51	LEU
1	A	52	PHE
1	A	103	SER
1	A	117	ARG
1	A	188	THR
1	A	203	VAL
1	A	242	LEU
1	A	253	VAL
1	A	270	THR
1	B	51	LEU
1	B	52	PHE
1	B	87	GLN
1	B	103	SER
1	B	117	ARG
1	B	188	THR
1	B	203	VAL
1	B	211	ARG
1	B	242	LEU
1	B	253	VAL
1	B	270	THR
1	B	284	ARG
1	B	302	VAL
1	C	51	LEU
1	C	52	PHE
1	C	87	GLN
1	C	103	SER
1	C	117	ARG
1	C	188	THR
1	C	193	ARG
1	C	203	VAL
1	C	211	ARG
1	C	242	LEU
1	C	253	VAL
1	C	270	THR
1	C	284	ARG
1	C	291	LYS
1	C	302	VAL
1	C	345	ARG
1	C	347	VAL
1	D	24	ARG
1	D	51	LEU
1	D	52	PHE
1	D	87	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	103	SER
1	D	117	ARG
1	D	187	GLU
1	D	188	THR
1	D	203	VAL
1	D	211	ARG
1	D	213	THR
1	D	235	ILE
1	D	242	LEU
1	D	243	ASP
1	D	253	VAL
1	D	270	THR
1	D	284	ARG
1	D	291	LYS
1	D	299	GLN
1	D	302	VAL
1	D	345	ARG
1	D	347	VAL
1	E	51	LEU
1	E	52	PHE
1	E	87	GLN
1	E	103	SER
1	E	117	ARG
1	E	188	THR
1	E	203	VAL
1	E	211	ARG
1	E	242	LEU
1	E	253	VAL
1	E	270	THR
1	E	302	VAL
1	E	334	ILE
1	E	345	ARG
1	E	347	VAL
1	F	51	LEU
1	F	52	PHE
1	F	87	GLN
1	F	103	SER
1	F	117	ARG
1	F	188	THR
1	F	203	VAL
1	F	211	ARG
1	F	235	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	242	LEU
1	F	253	VAL
1	F	270	THR
1	F	284	ARG
1	F	302	VAL
1	F	347	VAL
1	G	51	LEU
1	G	52	PHE
1	G	69	GLN
1	G	87	GLN
1	G	103	SER
1	G	117	ARG
1	G	188	THR
1	G	193	ARG
1	G	203	VAL
1	G	211	ARG
1	G	242	LEU
1	G	253	VAL
1	G	270	THR
1	G	284	ARG
1	G	291	LYS
1	G	302	VAL
1	G	347	VAL
1	H	51	LEU
1	H	52	PHE
1	H	69	GLN
1	H	87	GLN
1	H	103	SER
1	H	117	ARG
1	H	122	ARG
1	H	188	THR
1	H	203	VAL
1	H	211	ARG
1	H	242	LEU
1	H	253	VAL
1	H	270	THR
1	H	284	ARG
1	H	302	VAL
1	H	345	ARG
1	H	347	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	HIS
1	A	149	GLN
1	A	326	ASN
1	B	104	HIS
1	B	118	GLN
1	B	149	GLN
1	B	154	HIS
1	B	326	ASN
1	C	104	HIS
1	C	149	GLN
1	C	326	ASN
1	D	104	HIS
1	D	118	GLN
1	D	149	GLN
1	D	299	GLN
1	D	326	ASN
1	E	104	HIS
1	E	149	GLN
1	E	154	HIS
1	E	326	ASN
1	F	47	HIS
1	F	69	GLN
1	F	87	GLN
1	F	104	HIS
1	F	149	GLN
1	F	326	ASN
1	G	47	HIS
1	G	104	HIS
1	G	149	GLN
1	G	326	ASN
1	H	87	GLN
1	H	104	HIS
1	H	149	GLN
1	H	154	HIS
1	H	299	GLN
1	H	326	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

41 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	D	1359	-	4,4,4	0.42	0	6,6,6	0.86	0
3	SO4	D	1358	-	4,4,4	0.46	0	6,6,6	0.22	0
2	FAD	E	1353	-	58,58,58	1.87	15 (25%)	85,89,89	2.12	25 (29%)
2	FAD	C	1353	-	58,58,58	2.20	10 (17%)	85,89,89	2.19	29 (34%)
3	SO4	B	1354	-	4,4,4	0.45	0	6,6,6	0.70	0
3	SO4	H	1355	-	4,4,4	0.51	0	6,6,6	0.37	0
3	SO4	C	1358	-	4,4,4	0.50	0	6,6,6	0.47	0
3	SO4	B	1356	-	4,4,4	0.59	0	6,6,6	0.61	0
3	SO4	F	1355	-	4,4,4	0.49	0	6,6,6	0.64	0
3	SO4	B	1355	-	4,4,4	0.59	0	6,6,6	0.32	0
3	SO4	C	1356	-	4,4,4	0.45	0	6,6,6	0.25	0
3	SO4	H	1354	-	4,4,4	0.62	0	6,6,6	0.56	0
3	SO4	G	1355	-	4,4,4	0.48	0	6,6,6	0.34	0
3	SO4	D	1354	-	4,4,4	0.58	0	6,6,6	0.46	0
3	SO4	H	1356	-	4,4,4	0.50	0	6,6,6	0.27	0
3	SO4	G	1354	-	4,4,4	0.38	0	6,6,6	0.19	0
3	SO4	D	1356	-	4,4,4	0.56	0	6,6,6	0.15	0
3	SO4	E	1355	-	4,4,4	0.59	0	6,6,6	0.70	0
3	SO4	D	1355	-	4,4,4	0.59	0	6,6,6	0.34	0
3	SO4	G	1356	-	4,4,4	0.64	0	6,6,6	0.61	0
2	FAD	H	1353	-	58,58,58	1.74	13 (22%)	85,89,89	2.30	29 (34%)
2	FAD	D	1353	-	58,58,58	1.84	14 (24%)	85,89,89	2.12	31 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	A	1355	-	4,4,4	0.53	0	6,6,6	0.17	0
3	SO4	C	1357	-	4,4,4	0.54	0	6,6,6	0.42	0
3	SO4	F	1357	-	4,4,4	0.59	0	6,6,6	0.46	0
3	SO4	B	1357	-	4,4,4	0.47	0	6,6,6	0.30	0
3	SO4	G	1357	-	4,4,4	0.57	0	6,6,6	0.38	0
3	SO4	E	1354	-	4,4,4	0.66	0	6,6,6	0.41	0
3	SO4	A	1356	-	4,4,4	0.59	0	6,6,6	0.52	0
2	FAD	B	1353	-	58,58,58	1.77	10 (17%)	85,89,89	2.23	30 (35%)
3	SO4	E	1356	-	4,4,4	0.68	0	6,6,6	0.94	0
3	SO4	C	1354	-	4,4,4	0.41	0	6,6,6	0.48	0
3	SO4	C	1355	-	4,4,4	0.52	0	6,6,6	0.43	0
3	SO4	F	1354	-	4,4,4	0.46	0	6,6,6	0.77	0
2	FAD	A	1353	-	58,58,58	1.96	12 (20%)	85,89,89	1.98	23 (27%)
3	SO4	F	1356	-	4,4,4	0.57	0	6,6,6	0.46	0
3	SO4	A	1354	-	4,4,4	0.45	0	6,6,6	0.79	0
3	SO4	H	1357	-	4,4,4	0.45	0	6,6,6	0.94	0
3	SO4	D	1357	-	4,4,4	0.65	0	6,6,6	0.24	0
2	FAD	F	1353	-	58,58,58	1.59	10 (17%)	85,89,89	2.29	28 (32%)
2	FAD	G	1353	-	58,58,58	1.87	12 (20%)	85,89,89	2.02	26 (30%)

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	G	1353	-	-	6/34/50/50	0/6/6/6
2	FAD	E	1353	-	-	12/34/50/50	0/6/6/6
2	FAD	A	1353	-	-	17/34/50/50	0/6/6/6
2	FAD	C	1353	-	-	6/34/50/50	0/6/6/6
2	FAD	H	1353	-	-	9/34/50/50	0/6/6/6
2	FAD	D	1353	-	-	3/34/50/50	0/6/6/6
2	FAD	F	1353	-	-	13/34/50/50	0/6/6/6
2	FAD	B	1353	-	-	9/34/50/50	0/6/6/6

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1353	FAD	PA-O3P	7.70	1.67	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1353	FAD	C9A-C5X	7.59	1.53	1.41
2	C	1353	FAD	P-O3P	6.58	1.66	1.59
2	G	1353	FAD	C9A-C5X	6.52	1.51	1.41
2	C	1353	FAD	C5A-C4A	6.10	1.50	1.39
2	C	1353	FAD	C9A-C5X	5.87	1.50	1.41
2	D	1353	FAD	C9A-C5X	5.84	1.50	1.41
2	B	1353	FAD	C9A-C5X	5.73	1.50	1.41
2	H	1353	FAD	C9A-C5X	5.56	1.50	1.41
2	B	1353	FAD	C5A-C4A	5.33	1.48	1.39
2	A	1353	FAD	C5A-C4A	5.16	1.48	1.39
2	F	1353	FAD	C5A-C4A	4.85	1.47	1.39
2	G	1353	FAD	C8-C7	4.79	1.52	1.40
2	G	1353	FAD	C5A-N7A	-4.73	1.30	1.39
2	F	1353	FAD	C9A-C5X	4.72	1.48	1.41
2	D	1353	FAD	C5A-C4A	4.63	1.47	1.39
2	A	1353	FAD	P-O3P	4.61	1.64	1.59
2	E	1353	FAD	C5A-N7A	-4.53	1.30	1.39
2	E	1353	FAD	C5A-C4A	4.36	1.46	1.39
2	E	1353	FAD	C9A-C5X	4.35	1.48	1.41
2	H	1353	FAD	C5A-C4A	4.31	1.46	1.39
2	D	1353	FAD	P-O3P	4.29	1.64	1.59
2	F	1353	FAD	C8A-N7A	4.28	1.39	1.31
2	C	1353	FAD	C8A-N7A	4.14	1.39	1.31
2	B	1353	FAD	C1'-C2'	-4.14	1.46	1.52
2	A	1353	FAD	C8-C7	4.06	1.50	1.40
2	A	1353	FAD	PA-O3P	3.98	1.63	1.59
2	G	1353	FAD	P-O3P	3.82	1.63	1.59
2	C	1353	FAD	C8-C7	3.81	1.50	1.40
2	D	1353	FAD	C5X-N5	-3.73	1.32	1.39
2	B	1353	FAD	O4-C4	3.73	1.30	1.23
2	B	1353	FAD	C8-C7	3.71	1.49	1.40
2	G	1353	FAD	C5A-C4A	3.64	1.45	1.39
2	H	1353	FAD	O4-C4	3.61	1.30	1.23
2	F	1353	FAD	C5A-N7A	-3.54	1.32	1.39
2	D	1353	FAD	PA-O3P	3.48	1.63	1.59
2	E	1353	FAD	C8-C7	3.46	1.49	1.40
2	E	1353	FAD	O4-C4	3.42	1.30	1.23
2	D	1353	FAD	C5A-N7A	-3.42	1.32	1.39
2	C	1353	FAD	C5A-N7A	-3.38	1.32	1.39
2	D	1353	FAD	C8-C7	3.37	1.49	1.40
2	H	1353	FAD	C4'-C3'	-3.35	1.47	1.53
2	G	1353	FAD	C1'-C2'	-3.32	1.48	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1353	FAD	C5A-N7A	-3.28	1.33	1.39
2	E	1353	FAD	PA-O3P	3.25	1.63	1.59
2	E	1353	FAD	C1'-C2'	-3.24	1.48	1.52
2	A	1353	FAD	C8A-N7A	3.23	1.37	1.31
2	E	1353	FAD	C8A-N7A	3.23	1.37	1.31
2	H	1353	FAD	C5A-N7A	-3.19	1.33	1.39
2	H	1353	FAD	C8-C7	3.18	1.48	1.40
2	F	1353	FAD	O4-C4	3.14	1.29	1.23
2	G	1353	FAD	C4A-N9A	-3.09	1.31	1.37
2	E	1353	FAD	C4-N3	-3.02	1.33	1.38
2	G	1353	FAD	C4X-N5	2.98	1.37	1.30
2	D	1353	FAD	C1'-C2'	-2.88	1.48	1.52
2	H	1353	FAD	P-O3P	2.86	1.62	1.59
2	H	1353	FAD	C1'-C2'	-2.85	1.48	1.52
2	D	1353	FAD	C2-N3	-2.81	1.32	1.39
2	D	1353	FAD	O4-C4	2.79	1.28	1.23
2	D	1353	FAD	O5B-C5B	-2.78	1.34	1.44
2	A	1353	FAD	C10-N10	2.75	1.43	1.37
2	E	1353	FAD	C5X-N5	-2.71	1.34	1.39
2	B	1353	FAD	C4A-N9A	-2.66	1.32	1.37
2	C	1353	FAD	C5X-N5	-2.66	1.34	1.39
2	E	1353	FAD	O4B-C1B	2.65	1.48	1.42
2	H	1353	FAD	C4-N3	-2.65	1.33	1.38
2	B	1353	FAD	C8A-N7A	2.63	1.36	1.31
2	G	1353	FAD	C4-N3	-2.63	1.33	1.38
2	D	1353	FAD	C8A-N7A	2.63	1.36	1.31
2	B	1353	FAD	O5B-C5B	-2.63	1.34	1.44
2	E	1353	FAD	C4'-C3'	-2.58	1.48	1.53
2	H	1353	FAD	O4B-C4B	-2.56	1.39	1.45
2	B	1353	FAD	C4'-C3'	-2.54	1.49	1.53
2	F	1353	FAD	C8-C7	2.52	1.47	1.40
2	F	1353	FAD	O4B-C1B	2.51	1.47	1.42
2	E	1353	FAD	P-O3P	2.39	1.62	1.59
2	E	1353	FAD	PA-O2A	-2.38	1.44	1.55
2	H	1353	FAD	C5X-N5	-2.34	1.35	1.39
2	C	1353	FAD	O4-C4	2.29	1.27	1.23
2	A	1353	FAD	C4X-N5	2.28	1.35	1.30
2	G	1353	FAD	C2-N3	-2.23	1.34	1.39
2	H	1353	FAD	PA-O3P	2.21	1.61	1.59
2	G	1353	FAD	C5X-N5	-2.20	1.35	1.39
2	G	1353	FAD	C5'-C4'	2.19	1.54	1.51
2	F	1353	FAD	C4X-N5	2.18	1.35	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1353	FAD	P-O3P	2.18	1.61	1.59
2	C	1353	FAD	C4-N3	-2.18	1.34	1.38
2	B	1353	FAD	C5A-N7A	-2.15	1.35	1.39
2	E	1353	FAD	C4A-N3A	2.11	1.38	1.34
2	A	1353	FAD	C2-N3	-2.11	1.34	1.39
2	F	1353	FAD	C5X-N5	-2.10	1.35	1.39
2	D	1353	FAD	C4'-C3'	-2.09	1.49	1.53
2	H	1353	FAD	C1'-N10	-2.06	1.42	1.47
2	D	1353	FAD	C10-N10	2.02	1.41	1.37
2	A	1353	FAD	C4A-N9A	-2.01	1.33	1.37
2	A	1353	FAD	C2'-C3'	2.00	1.56	1.53

All (221) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1353	FAD	C5A-C4A-N3A	-7.85	115.91	126.72
2	F	1353	FAD	C5A-C4A-N3A	-7.60	116.25	126.72
2	B	1353	FAD	C5A-C4A-N3A	-6.41	117.90	126.72
2	C	1353	FAD	C5A-C4A-N3A	-6.39	117.92	126.72
2	G	1353	FAD	C5A-C4A-N3A	-6.36	117.96	126.72
2	H	1353	FAD	C5A-C4A-N3A	-6.29	118.05	126.72
2	A	1353	FAD	C5A-C4A-N3A	-6.19	118.20	126.72
2	C	1353	FAD	O2-C2-N1	-5.92	111.96	121.80
2	F	1353	FAD	O3P-P-O1P	-5.85	93.11	110.70
2	E	1353	FAD	N3A-C4A-N9A	5.74	136.93	127.17
2	F	1353	FAD	N3A-C4A-N9A	5.73	136.91	127.17
2	H	1353	FAD	N3A-C4A-N9A	5.71	136.88	127.17
2	B	1353	FAD	O2'-C2'-C3'	5.70	122.58	109.25
2	G	1353	FAD	O2'-C2'-C3'	5.66	122.49	109.25
2	G	1353	FAD	N3A-C4A-N9A	5.30	136.17	127.17
2	H	1353	FAD	O4B-C1B-N9A	4.96	117.61	108.09
2	B	1353	FAD	O2-C2-N1	-4.95	113.58	121.80
2	B	1353	FAD	N3A-C4A-N9A	4.94	135.56	127.17
2	A	1353	FAD	N3A-C4A-N9A	4.91	135.51	127.17
2	C	1353	FAD	N3A-C4A-N9A	4.77	135.28	127.17
2	C	1353	FAD	C4X-C10-N10	4.74	123.27	116.48
2	F	1353	FAD	O2-C2-N1	-4.69	114.01	121.80
2	F	1353	FAD	O4B-C1B-N9A	4.52	116.77	108.09
2	D	1353	FAD	N3A-C2A-N1A	-4.51	121.75	128.58
2	A	1353	FAD	C4X-C10-N10	4.42	122.81	116.48
2	D	1353	FAD	O4-C4-C4X	-4.41	114.88	126.53
2	C	1353	FAD	O4B-C4B-C5B	4.41	123.47	109.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1353	FAD	O2-C2-N1	-4.38	114.52	121.80
2	D	1353	FAD	C5A-C4A-N3A	-4.38	120.69	126.72
2	E	1353	FAD	O2'-C2'-C3'	4.37	119.47	109.25
2	E	1353	FAD	C2A-N3A-C4A	4.27	122.27	111.83
2	C	1353	FAD	O4B-C1B-N9A	4.27	116.30	108.09
2	E	1353	FAD	O4B-C1B-N9A	4.27	116.29	108.09
2	B	1353	FAD	O4B-C1B-N9A	4.24	116.24	108.09
2	B	1353	FAD	C2A-N3A-C4A	4.24	122.18	111.83
2	A	1353	FAD	C4X-C10-N1	-4.14	114.44	124.59
2	D	1353	FAD	N3A-C4A-N9A	4.05	134.06	127.17
2	H	1353	FAD	C4-N3-C2	-4.04	118.47	125.64
2	C	1353	FAD	O2'-C2'-C3'	4.03	118.69	109.25
2	E	1353	FAD	C4A-C5A-N7A	-4.03	105.98	110.58
2	G	1353	FAD	O4B-C1B-N9A	4.01	115.78	108.09
2	B	1353	FAD	O5B-PA-O1A	3.96	124.62	108.94
2	H	1353	FAD	C2A-N3A-C4A	3.94	121.45	111.83
2	A	1353	FAD	C10-N1-C2	3.93	125.36	116.85
2	D	1353	FAD	O4B-C4B-C5B	3.92	121.90	109.33
2	F	1353	FAD	C2A-N3A-C4A	3.92	121.40	111.83
2	D	1353	FAD	C9A-N10-C10	-3.92	114.78	120.75
2	F	1353	FAD	C4B-O4B-C1B	-3.92	100.82	109.47
2	H	1353	FAD	C4B-O4B-C1B	-3.91	100.83	109.47
2	H	1353	FAD	C5X-N5-C4X	3.89	124.39	118.09
2	H	1353	FAD	N3A-C2A-N1A	-3.88	122.71	128.58
2	D	1353	FAD	C5A-N7A-C8A	3.87	109.53	103.45
2	D	1353	FAD	C5X-C9A-N10	3.84	121.44	117.97
2	F	1353	FAD	O4-C4-C4X	-3.83	116.41	126.53
2	A	1353	FAD	N3A-C2A-N1A	-3.81	122.81	128.58
2	E	1353	FAD	C5A-N7A-C8A	3.81	109.44	103.45
2	G	1353	FAD	N3A-C2A-N1A	-3.80	122.84	128.58
2	B	1353	FAD	N3A-C2A-N1A	-3.78	122.87	128.58
2	A	1353	FAD	C4-N3-C2	-3.76	118.97	125.64
2	D	1353	FAD	N9A-C8A-N7A	-3.74	108.63	113.94
2	E	1353	FAD	N3A-C2A-N1A	-3.74	122.93	128.58
2	C	1353	FAD	C9A-N10-C10	-3.73	115.06	120.75
2	H	1353	FAD	C4X-C10-N10	3.72	121.81	116.48
2	E	1353	FAD	C4B-O4B-C1B	-3.72	101.25	109.47
2	H	1353	FAD	C4X-C10-N1	-3.70	115.51	124.59
2	A	1353	FAD	O2-C2-N1	-3.65	115.73	121.80
2	F	1353	FAD	O5B-PA-O1A	3.64	123.35	108.94
2	G	1353	FAD	O3'-C3'-C2'	-3.61	100.73	108.93
2	F	1353	FAD	O4-C4-N3	3.61	126.90	120.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1353	FAD	O4-C4-N3	3.61	126.90	120.11
2	C	1353	FAD	C2A-N3A-C4A	3.58	120.58	111.83
2	H	1353	FAD	N3-C2-N1	3.58	127.11	119.50
2	G	1353	FAD	C2'-C1'-N10	3.58	127.11	110.20
2	B	1353	FAD	C4B-O4B-C1B	-3.58	101.57	109.47
2	H	1353	FAD	C4A-N9A-C8A	3.54	109.46	105.74
2	C	1353	FAD	C4A-C5A-N7A	-3.54	106.53	110.58
2	A	1353	FAD	C2A-N3A-C4A	3.53	120.46	111.83
2	D	1353	FAD	C4A-N9A-C8A	3.53	109.44	105.74
2	D	1353	FAD	O5B-PA-O1A	3.52	122.89	108.94
2	G	1353	FAD	C2A-N3A-C4A	3.52	120.43	111.83
2	H	1353	FAD	O5B-PA-O1A	3.50	122.81	108.94
2	G	1353	FAD	O2P-P-O3P	3.48	116.67	107.27
2	B	1353	FAD	C2'-C1'-N10	3.45	126.49	110.20
2	D	1353	FAD	O4B-C1B-N9A	3.45	114.71	108.09
2	B	1353	FAD	O4-C4-N3	3.43	126.56	120.11
2	G	1353	FAD	O5B-PA-O1A	3.43	122.51	108.94
2	H	1353	FAD	C5A-N7A-C8A	3.41	108.81	103.45
2	C	1353	FAD	C4'-C3'-C2'	3.37	119.18	113.57
2	C	1353	FAD	N3A-C2A-N1A	-3.36	123.50	128.58
2	C	1353	FAD	C2'-C1'-N10	3.35	126.06	110.20
2	F	1353	FAD	C4A-C5A-N7A	-3.34	106.77	110.58
2	B	1353	FAD	N3-C2-N1	3.32	126.56	119.50
2	A	1353	FAD	O2'-C2'-C3'	3.31	117.00	109.25
2	F	1353	FAD	C5A-N7A-C8A	3.31	108.65	103.45
2	F	1353	FAD	O2P-P-O3P	3.29	116.17	107.27
2	H	1353	FAD	O2'-C2'-C3'	3.28	116.92	109.25
2	D	1353	FAD	C2A-N1A-C6A	3.24	124.06	118.73
2	H	1353	FAD	C9A-C5X-N5	-3.24	119.02	122.45
2	H	1353	FAD	N9A-C8A-N7A	-3.21	109.38	113.94
2	B	1353	FAD	O3'-C3'-C4'	-3.21	101.64	108.93
2	D	1353	FAD	O2-C2-N1	-3.21	116.47	121.80
2	F	1353	FAD	C2'-C1'-N10	3.20	125.32	110.20
2	A	1353	FAD	O4-C4-C4X	-3.19	118.12	126.53
2	C	1353	FAD	C4-N3-C2	-3.15	120.04	125.64
2	D	1353	FAD	C2A-N3A-C4A	3.11	119.42	111.83
2	C	1353	FAD	C4X-C10-N1	-3.11	116.97	124.59
2	A	1353	FAD	C9A-N10-C10	-3.06	116.08	120.75
2	C	1353	FAD	C4B-O4B-C1B	-3.05	102.73	109.47
2	F	1353	FAD	C4'-C3'-C2'	-3.05	108.50	113.57
2	F	1353	FAD	O4B-C4B-C5B	3.01	118.98	109.33
2	C	1353	FAD	N3-C2-N1	3.00	125.87	119.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1353	FAD	C4A-C5A-N7A	-2.99	107.16	110.58
2	C	1353	FAD	C5A-N7A-C8A	2.98	108.13	103.45
2	A	1353	FAD	C4A-C5A-N7A	-2.97	107.19	110.58
2	F	1353	FAD	O2A-PA-O5B	-2.97	94.11	107.57
2	B	1353	FAD	O3P-P-O1P	-2.95	101.83	110.70
2	D	1353	FAD	C2'-C1'-N10	2.95	124.12	110.20
2	B	1353	FAD	C4A-C5A-N7A	-2.94	107.22	110.58
2	F	1353	FAD	O4B-C1B-C2B	-2.94	100.33	106.62
2	G	1353	FAD	C4'-C3'-C2'	2.94	118.46	113.57
2	B	1353	FAD	O4-C4-C4X	-2.94	118.78	126.53
2	A	1353	FAD	O5B-C5B-C4B	2.91	118.89	108.99
2	H	1353	FAD	C4A-C5A-N7A	-2.90	107.27	110.58
2	D	1353	FAD	C1'-N10-C9A	2.89	126.25	120.63
2	H	1353	FAD	C10-C4X-N5	-2.88	118.92	124.81
2	C	1353	FAD	O4B-C1B-C2B	-2.88	100.45	106.62
2	G	1353	FAD	C4-N3-C2	-2.87	120.55	125.64
2	B	1353	FAD	C1'-C2'-C3'	-2.83	101.98	109.66
2	B	1353	FAD	O4B-C4B-C5B	2.82	118.36	109.33
2	H	1353	FAD	O4B-C1B-C2B	-2.82	100.59	106.62
2	B	1353	FAD	C2B-C1B-N9A	-2.81	106.32	113.30
2	G	1353	FAD	C4-C4X-N5	2.81	122.09	118.21
2	B	1353	FAD	C4X-C10-N10	2.80	120.49	116.48
2	E	1353	FAD	C4X-C10-N1	-2.80	117.73	124.59
2	B	1353	FAD	O3P-PA-O1A	-2.78	102.34	110.70
2	A	1353	FAD	C2'-C1'-N10	2.77	123.31	110.20
2	E	1353	FAD	N9A-C8A-N7A	-2.77	110.00	113.94
2	D	1353	FAD	C1'-C2'-C3'	-2.75	102.21	109.66
2	G	1353	FAD	C4X-C4-N3	2.74	120.23	113.25
2	E	1353	FAD	C9A-C5X-N5	-2.73	119.55	122.45
2	B	1353	FAD	C4X-C10-N1	-2.73	117.89	124.59
2	E	1353	FAD	O2-C2-N1	-2.73	117.27	121.80
2	H	1353	FAD	O2B-C2B-C3B	2.72	120.54	111.82
2	F	1353	FAD	N9A-C8A-N7A	-2.72	110.08	113.94
2	F	1353	FAD	O3'-C3'-C4'	2.71	115.08	108.93
2	E	1353	FAD	C5X-N5-C4X	2.70	122.46	118.09
2	F	1353	FAD	O2'-C2'-C3'	2.68	115.53	109.25
2	D	1353	FAD	O3B-C3B-C4B	-2.67	103.42	111.08
2	G	1353	FAD	O4-C4-C4X	-2.65	119.54	126.53
2	D	1353	FAD	O4'-C4'-C3'	-2.61	103.15	109.25
2	E	1353	FAD	C5X-C9A-N10	2.59	120.31	117.97
2	F	1353	FAD	N3A-C2A-N1A	-2.57	124.69	128.58
2	B	1353	FAD	C5'-C4'-C3'	-2.55	107.41	112.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1353	FAD	O2P-P-O3P	2.54	114.15	107.27
2	B	1353	FAD	O2P-P-O3P	2.54	114.14	107.27
2	D	1353	FAD	C4X-C10-N1	-2.53	118.38	124.59
2	A	1353	FAD	C4X-C4-N3	2.53	119.69	113.25
2	D	1353	FAD	C4B-O4B-C1B	-2.52	103.91	109.47
2	C	1353	FAD	C4-C4X-N5	2.50	121.67	118.21
2	H	1353	FAD	O2A-PA-O5B	-2.49	96.29	107.57
2	G	1353	FAD	C4X-C10-N1	-2.47	118.55	124.59
2	D	1353	FAD	O2'-C2'-C3'	2.46	115.02	109.25
2	B	1353	FAD	C4A-N9A-C8A	2.44	108.31	105.74
2	H	1353	FAD	O5B-C5B-C4B	2.44	117.31	108.99
2	A	1353	FAD	O2A-PA-O3P	-2.41	100.76	107.27
2	G	1353	FAD	O2A-PA-O3P	2.39	113.74	107.27
2	D	1353	FAD	C4-N3-C2	-2.38	121.41	125.64
2	A	1353	FAD	C4A-N9A-C8A	2.38	108.24	105.74
2	G	1353	FAD	O3P-P-O1P	-2.38	103.55	110.70
2	E	1353	FAD	O4B-C1B-C2B	-2.38	101.53	106.62
2	A	1353	FAD	O5B-PA-O1A	-2.37	99.54	108.94
2	H	1353	FAD	C2'-C1'-N10	2.36	121.36	110.20
2	E	1353	FAD	C4X-C10-N10	2.35	119.85	116.48
2	H	1353	FAD	C9A-N10-C10	-2.35	117.17	120.75
2	G	1353	FAD	C5A-C6A-N6A	-2.35	117.47	123.29
2	B	1353	FAD	C6A-C5A-N7A	2.35	136.61	132.09
2	F	1353	FAD	C5A-C6A-N6A	-2.33	117.51	123.29
2	H	1353	FAD	C4-C4X-C10	2.33	120.92	116.93
2	E	1353	FAD	O4'-C4'-C5'	-2.32	104.86	109.99
2	C	1353	FAD	C10-C4X-N5	-2.32	120.08	124.81
2	B	1353	FAD	C4-N3-C2	-2.30	121.56	125.64
2	E	1353	FAD	C10-C4X-N5	-2.29	120.13	124.81
2	C	1353	FAD	O3'-C3'-C4'	-2.29	103.73	108.93
2	C	1353	FAD	C10-N1-C2	2.28	121.78	116.85
2	G	1353	FAD	C4B-O4B-C1B	-2.27	104.46	109.47
2	H	1353	FAD	O2B-C2B-C1B	-2.26	102.31	110.10
2	C	1353	FAD	O4-C4-C4X	-2.25	120.58	126.53
2	E	1353	FAD	C2'-C1'-N10	2.25	120.83	110.20
2	G	1353	FAD	O4B-C1B-C2B	-2.24	101.83	106.62
2	C	1353	FAD	O5B-PA-O1A	2.24	117.80	108.94
2	D	1353	FAD	C6A-C5A-N7A	2.23	136.38	132.09
2	E	1353	FAD	O2A-PA-O1A	2.22	122.79	112.44
2	A	1353	FAD	C5A-N7A-C8A	2.21	106.92	103.45
2	E	1353	FAD	N3-C2-N1	2.18	124.14	119.50
2	F	1353	FAD	C4X-C10-N10	2.18	119.60	116.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1353	FAD	O5'-P-O1P	2.18	117.57	108.94
2	D	1353	FAD	C4X-C10-N10	2.16	119.58	116.48
2	C	1353	FAD	N9A-C8A-N7A	-2.15	110.89	113.94
2	G	1353	FAD	O2-C2-N1	-2.14	118.24	121.80
2	A	1353	FAD	C4-C4X-N5	2.13	121.15	118.21
2	G	1353	FAD	C10-N1-C2	2.13	121.46	116.85
2	A	1353	FAD	N6A-C6A-N1A	2.12	123.09	118.38
2	G	1353	FAD	N6A-C6A-N1A	2.12	123.09	118.38
2	C	1353	FAD	C5X-C9A-N10	2.10	119.87	117.97
2	F	1353	FAD	C4-N3-C2	-2.10	121.92	125.64
2	F	1353	FAD	N3-C2-N1	2.09	123.94	119.50
2	C	1353	FAD	C2A-N1A-C6A	2.09	122.16	118.73
2	B	1353	FAD	O4B-C4B-C3B	2.08	109.29	105.15
2	F	1353	FAD	C1'-N10-C9A	2.08	124.67	120.63
2	D	1353	FAD	N3-C2-N1	2.07	123.90	119.50
2	A	1353	FAD	C3B-C2B-C1B	2.06	105.36	101.46
2	B	1353	FAD	O2A-PA-O1A	2.06	122.02	112.44
2	G	1353	FAD	C4X-C10-N10	2.05	119.42	116.48
2	C	1353	FAD	O2P-P-O3P	2.04	112.78	107.27
2	E	1353	FAD	C5A-C6A-N6A	-2.03	118.26	123.29
2	H	1353	FAD	C2B-C1B-N9A	-2.01	108.30	113.30
2	G	1353	FAD	C9A-C5X-N5	-2.01	120.32	122.45
2	B	1353	FAD	C9A-N10-C10	-2.01	117.69	120.75
2	E	1353	FAD	C9A-N10-C10	-2.01	117.69	120.75
2	D	1353	FAD	C4A-N9A-C1B	-2.00	121.95	126.63
2	D	1353	FAD	C9A-C9-C8	2.00	123.24	119.22

There are no chirality outliers.

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1353	FAD	C5B-O5B-PA-O1A
2	A	1353	FAD	C5B-O5B-PA-O3P
2	A	1353	FAD	C2'-C1'-N10-C10
2	A	1353	FAD	N10-C1'-C2'-C3'
2	A	1353	FAD	C1'-C2'-C3'-O3'
2	A	1353	FAD	C1'-C2'-C3'-C4'
2	A	1353	FAD	C5'-O5'-P-O1P
2	A	1353	FAD	C5'-O5'-P-O2P
2	A	1353	FAD	C5'-O5'-P-O3P
2	B	1353	FAD	C5B-O5B-PA-O1A
2	B	1353	FAD	C5B-O5B-PA-O3P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	1353	FAD	N10-C1'-C2'-C3'
2	B	1353	FAD	C5'-O5'-P-O1P
2	B	1353	FAD	C5'-O5'-P-O3P
2	C	1353	FAD	C5B-O5B-PA-O1A
2	C	1353	FAD	C5B-O5B-PA-O2A
2	C	1353	FAD	C5B-O5B-PA-O3P
2	D	1353	FAD	C5B-O5B-PA-O1A
2	D	1353	FAD	C5B-O5B-PA-O3P
2	E	1353	FAD	C5B-O5B-PA-O1A
2	E	1353	FAD	C5B-O5B-PA-O3P
2	E	1353	FAD	N10-C1'-C2'-C3'
2	E	1353	FAD	C5'-O5'-P-O1P
2	F	1353	FAD	C5B-O5B-PA-O1A
2	F	1353	FAD	C5B-O5B-PA-O2A
2	F	1353	FAD	C5B-O5B-PA-O3P
2	F	1353	FAD	C5'-O5'-P-O3P
2	G	1353	FAD	C5B-O5B-PA-O1A
2	G	1353	FAD	C5B-O5B-PA-O2A
2	G	1353	FAD	C5B-O5B-PA-O3P
2	H	1353	FAD	C5B-O5B-PA-O1A
2	H	1353	FAD	C5B-O5B-PA-O3P
2	H	1353	FAD	N10-C1'-C2'-C3'
2	H	1353	FAD	C5'-O5'-P-O1P
2	H	1353	FAD	C5'-O5'-P-O3P
2	A	1353	FAD	O2'-C2'-C3'-O3'
2	F	1353	FAD	O3'-C3'-C4'-O4'
2	E	1353	FAD	O4'-C4'-C5'-O5'
2	F	1353	FAD	O4'-C4'-C5'-O5'
2	F	1353	FAD	O3'-C3'-C4'-C5'
2	A	1353	FAD	O4B-C4B-C5B-O5B
2	F	1353	FAD	C3'-C4'-C5'-O5'
2	A	1353	FAD	O2'-C2'-C3'-C4'
2	F	1353	FAD	C2'-C3'-C4'-O4'
2	F	1353	FAD	C2'-C3'-C4'-C5'
2	A	1353	FAD	C3B-C4B-C5B-O5B
2	E	1353	FAD	PA-O3P-P-O1P
2	G	1353	FAD	PA-O3P-P-O1P
2	H	1353	FAD	PA-O3P-P-O1P
2	A	1353	FAD	C5B-O5B-PA-O2A
2	B	1353	FAD	C5B-O5B-PA-O2A
2	C	1353	FAD	C5'-O5'-P-O1P
2	D	1353	FAD	C5B-O5B-PA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	E	1353	FAD	C5B-O5B-PA-O2A
2	E	1353	FAD	C5'-O5'-P-O2P
2	E	1353	FAD	C5'-O5'-P-O3P
2	F	1353	FAD	C5'-O5'-P-O1P
2	G	1353	FAD	C5'-O5'-P-O1P
2	H	1353	FAD	C5B-O5B-PA-O2A
2	A	1353	FAD	C4B-C5B-O5B-PA
2	A	1353	FAD	C4'-C5'-O5'-P
2	B	1353	FAD	PA-O3P-P-O1P
2	F	1353	FAD	C3B-C4B-C5B-O5B
2	A	1353	FAD	C3'-C4'-C5'-O5'
2	E	1353	FAD	C3'-C4'-C5'-O5'
2	F	1353	FAD	O4B-C4B-C5B-O5B
2	G	1353	FAD	PA-O3P-P-O2P
2	H	1353	FAD	PA-O3P-P-O2P
2	B	1353	FAD	O4'-C4'-C5'-O5'
2	C	1353	FAD	O4'-C4'-C5'-O5'
2	H	1353	FAD	O4'-C4'-C5'-O5'
2	C	1353	FAD	C3'-C4'-C5'-O5'
2	B	1353	FAD	PA-O3P-P-O2P
2	E	1353	FAD	PA-O3P-P-O2P
2	E	1353	FAD	O3'-C3'-C4'-C5'

There are no ring outliers.

20 monomers are involved in 32 short contacts:

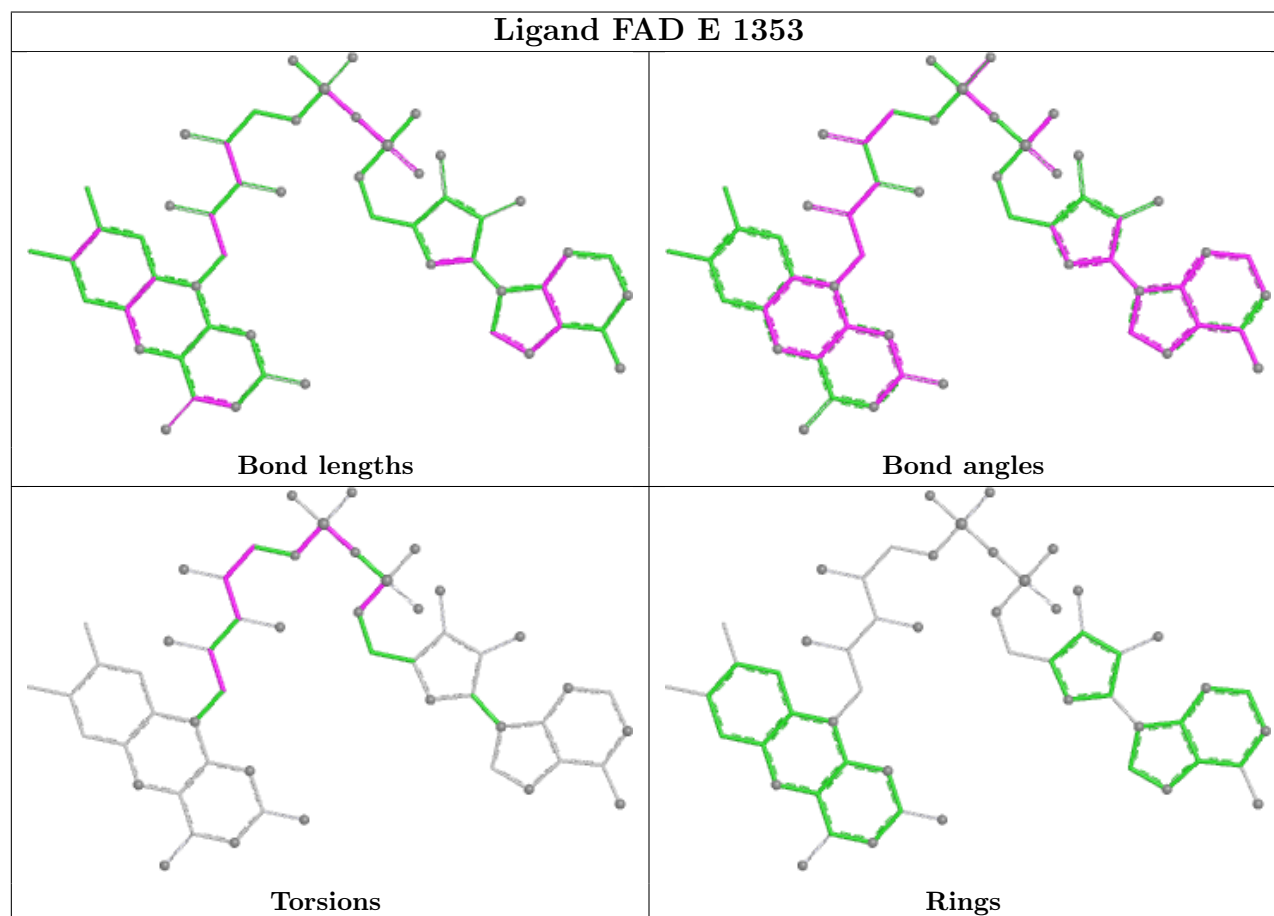
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1358	SO4	1	0
2	E	1353	FAD	2	0
3	B	1354	SO4	1	0
3	C	1356	SO4	1	0
3	D	1354	SO4	1	0
3	G	1354	SO4	1	0
3	D	1355	SO4	1	0
3	G	1356	SO4	1	0
2	H	1353	FAD	2	0
2	D	1353	FAD	1	0
3	F	1357	SO4	2	0
3	B	1357	SO4	1	0
3	E	1354	SO4	1	0
2	B	1353	FAD	4	0
3	E	1356	SO4	1	0

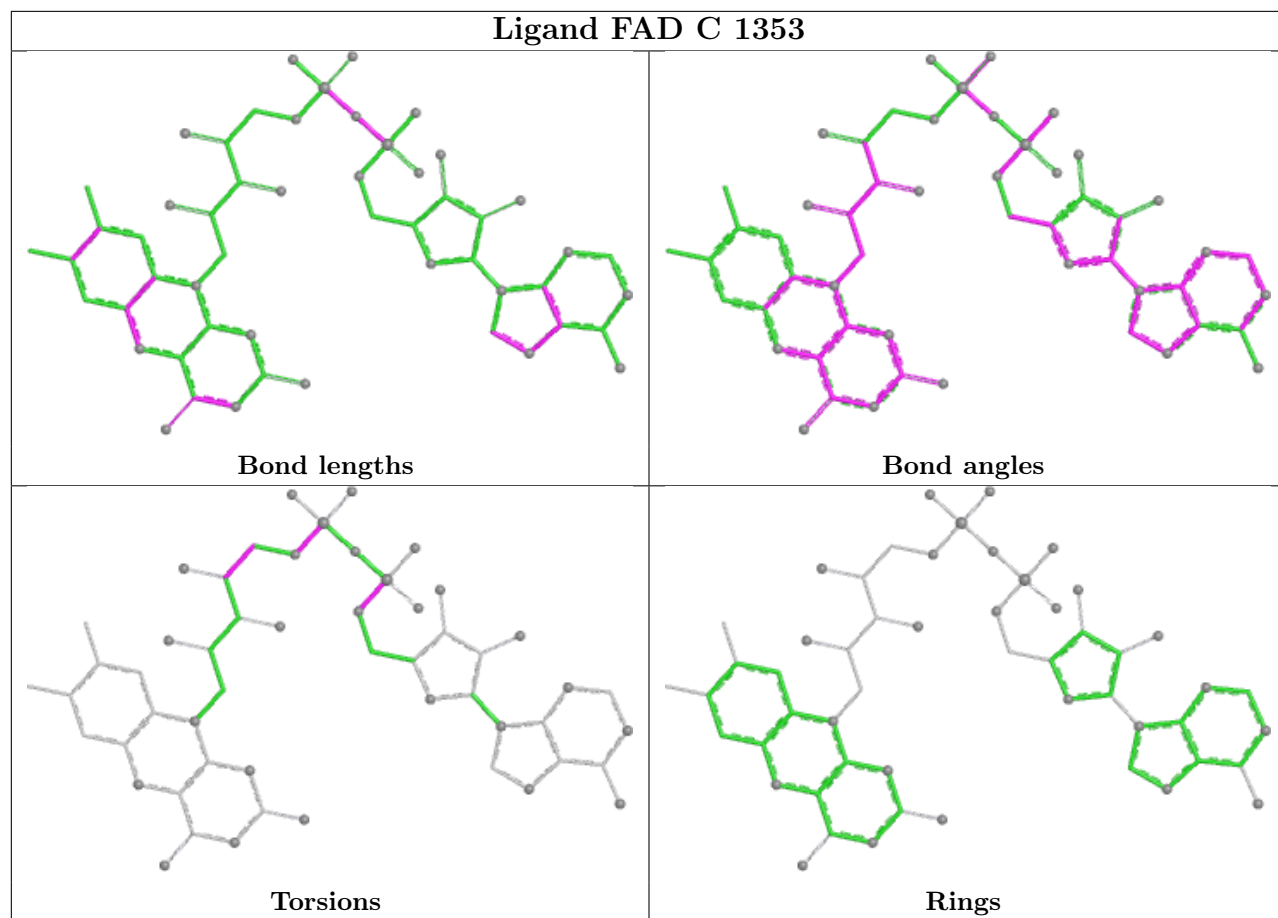
Continued on next page...

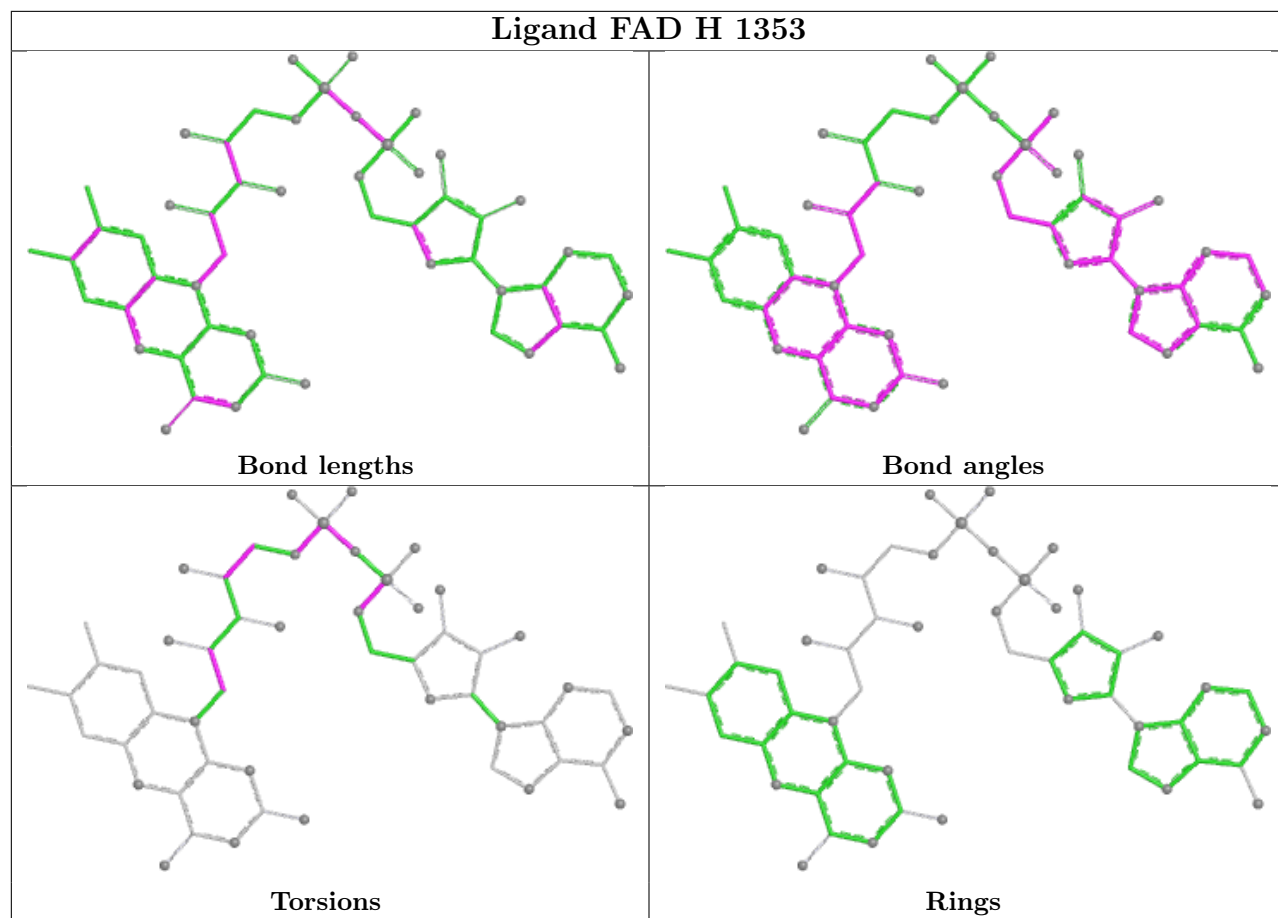
Continued from previous page...

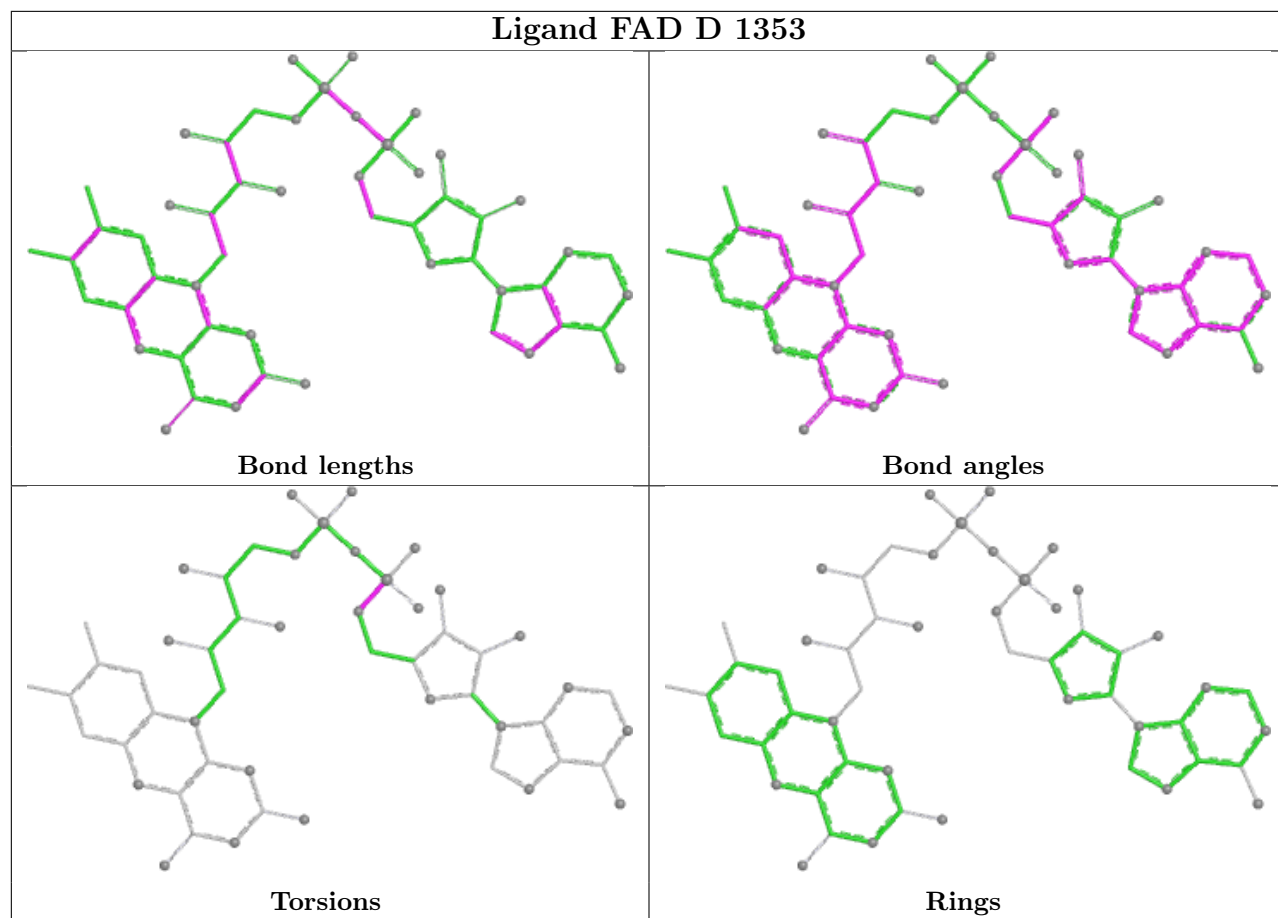
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1354	SO4	1	0
2	A	1353	FAD	4	0
3	A	1354	SO4	1	0
3	H	1357	SO4	1	0
2	G	1353	FAD	4	0

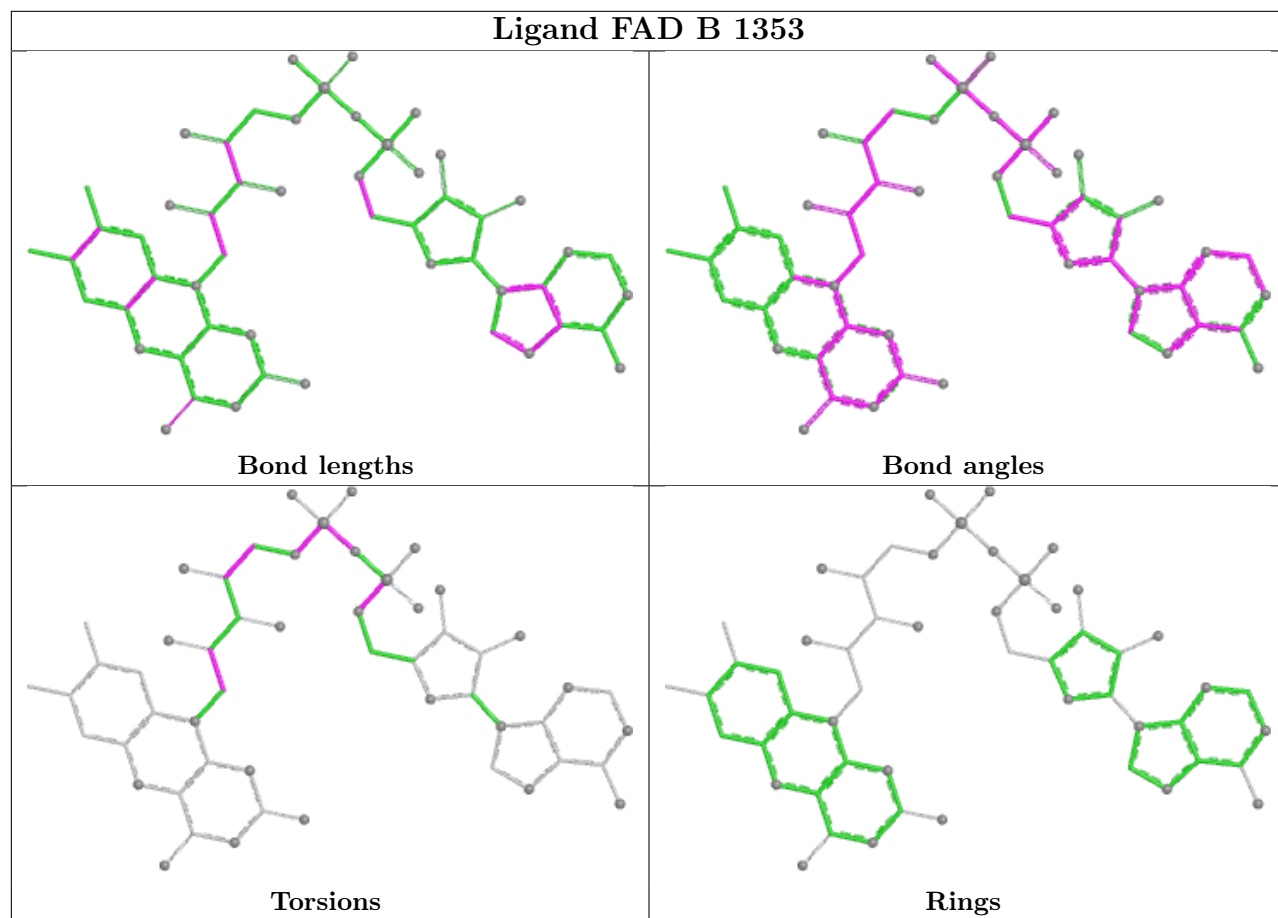
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

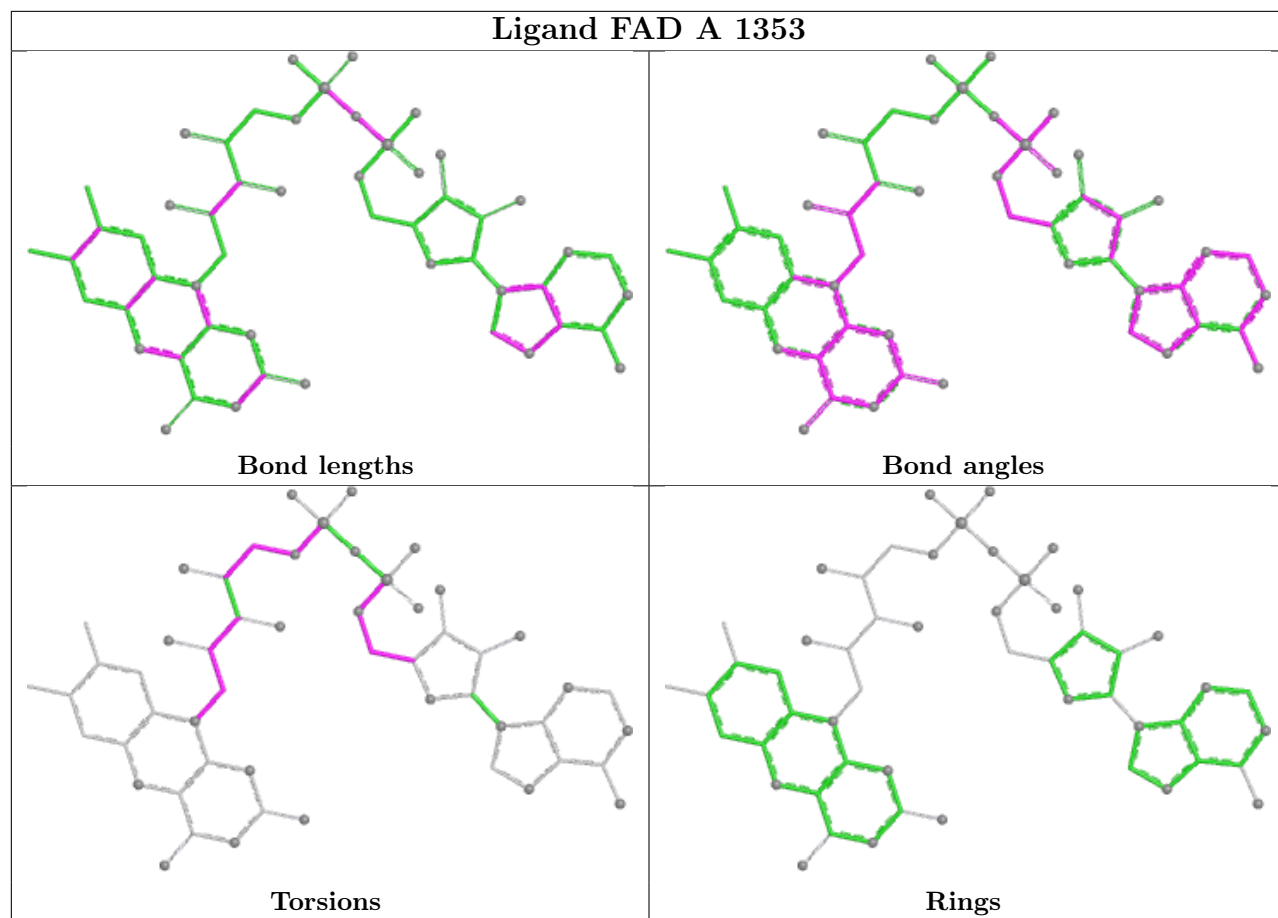


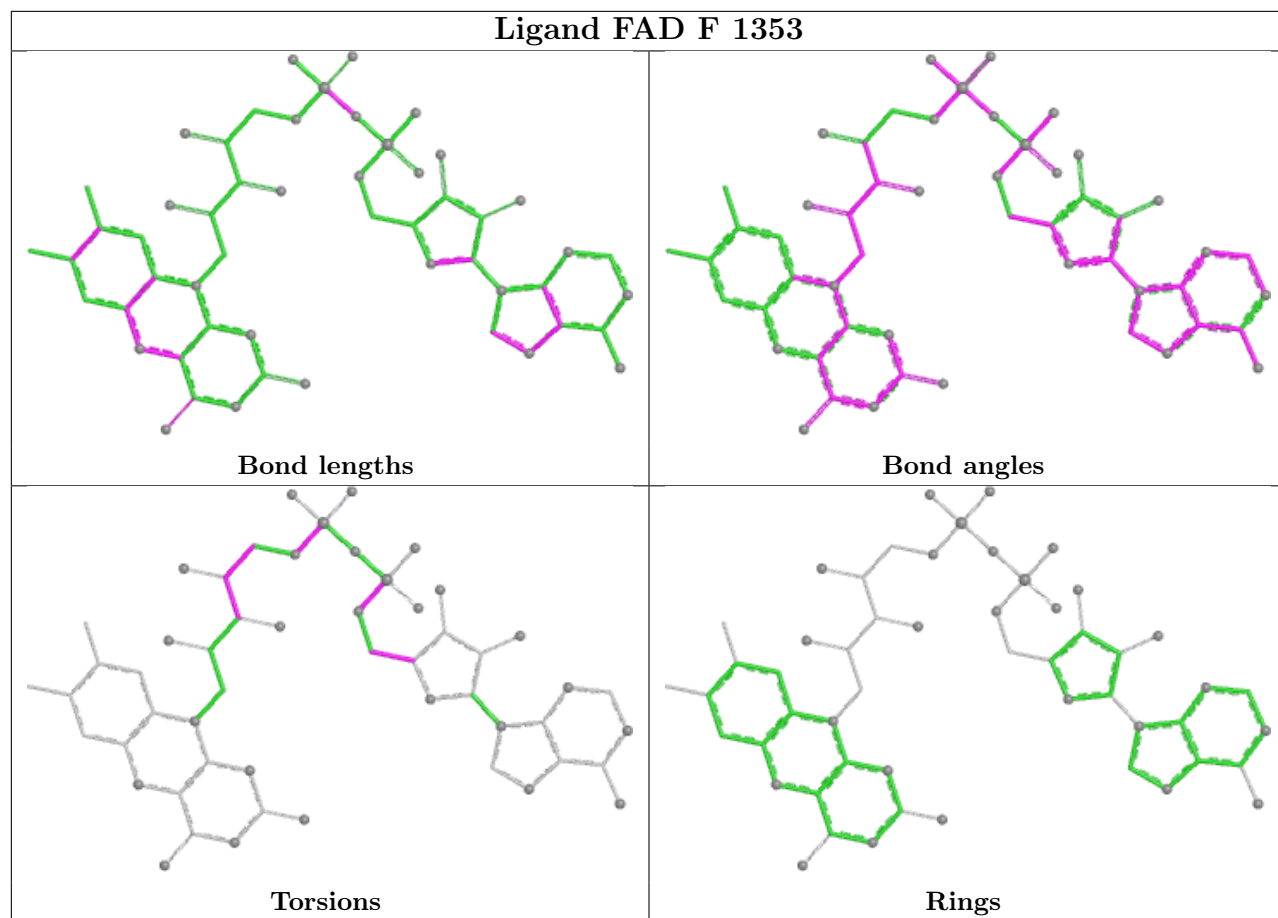


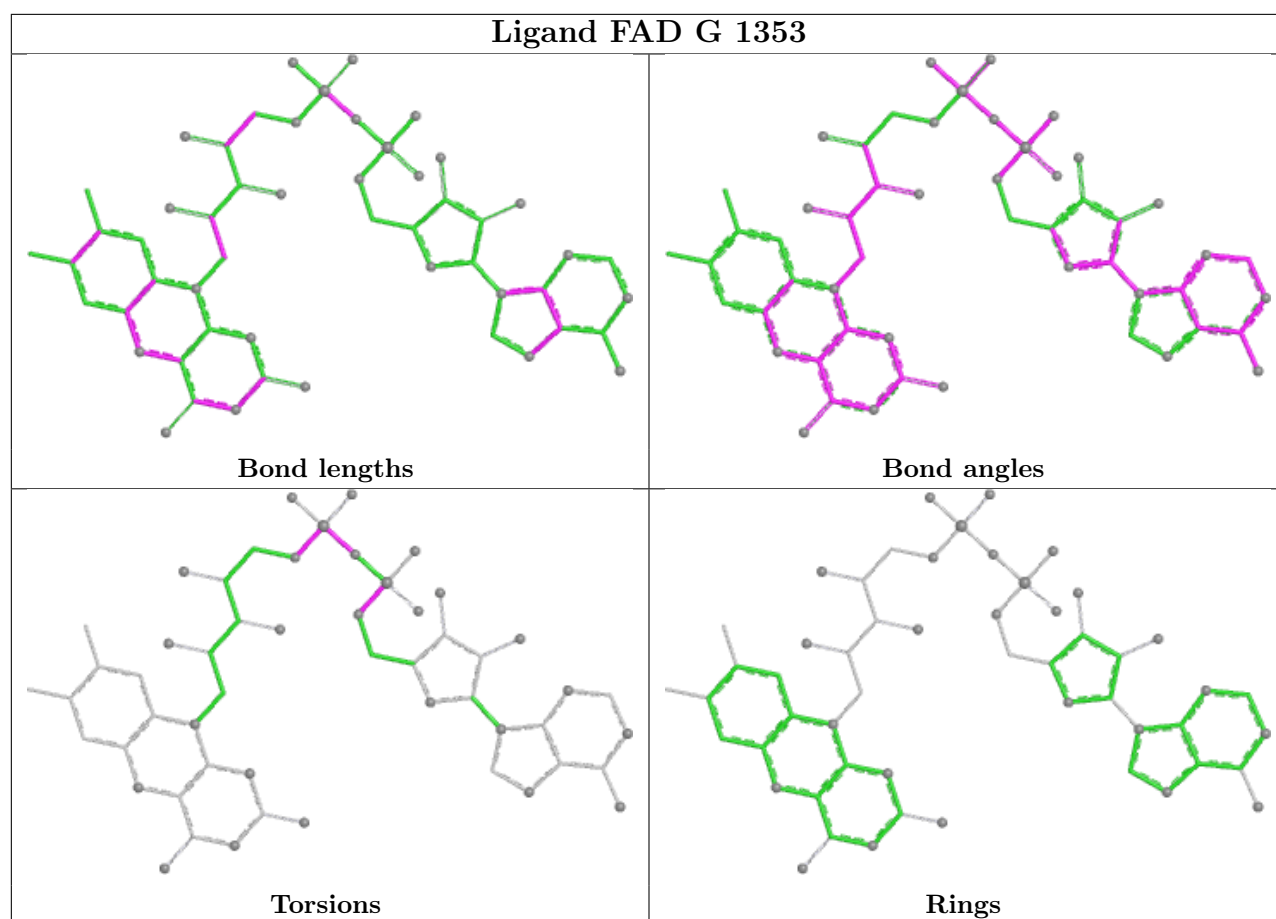












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	327/357 (91%)	2.05	149 (45%) 0 0	40, 79, 111, 127	0
1	B	330/357 (92%)	1.26	67 (20%) 3 2	31, 65, 95, 135	0
1	C	330/357 (92%)	0.27	6 (1%) 67 63	26, 45, 69, 86	0
1	D	333/357 (93%)	0.45	18 (5%) 31 26	25, 46, 74, 94	0
1	E	330/357 (92%)	0.33	16 (4%) 35 30	22, 46, 70, 110	0
1	F	330/357 (92%)	0.63	20 (6%) 27 22	29, 48, 74, 101	0
1	G	330/357 (92%)	0.39	13 (3%) 43 38	24, 46, 77, 108	0
1	H	331/357 (92%)	0.12	9 (2%) 56 50	20, 40, 67, 96	0
All	All	2641/2856 (92%)	0.69	298 (11%) 10 8	20, 49, 90, 135	0

All (298) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	318	TRP	6.3
1	B	267	ALA	6.2
1	A	251	ALA	5.7
1	A	27	LEU	5.6
1	A	94	LEU	5.6
1	G	351	CYS	5.4
1	A	20	TYR	5.1
1	A	19	GLY	5.1
1	A	123	ALA	5.0
1	B	1	MET	4.9
1	A	7	VAL	4.7
1	G	352	ALA	4.7
1	A	2	ASP	4.6
1	A	29	TYR	4.5
1	A	317	VAL	4.4
1	A	200	ALA	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	1	MET	4.4
1	H	212	ALA	4.3
1	A	12	GLY	4.3
1	A	347	VAL	4.2
1	A	119	TRP	4.2
1	A	36	ALA	4.2
1	B	88	LYS	4.2
1	A	57	TRP	4.1
1	A	321	GLY	4.1
1	A	350	TYR	4.1
1	A	301	GLN	4.1
1	A	121	ALA	4.1
1	D	212	ALA	4.1
1	G	315	PRO	4.1
1	A	325	TRP	4.1
1	F	313	ALA	4.1
1	A	336	VAL	4.0
1	B	89	TYR	4.0
1	A	24	ARG	4.0
1	A	340	ALA	4.0
1	A	17	SER	3.9
1	H	267	ALA	3.9
1	A	60	ILE	3.9
1	A	210	GLU	3.9
1	A	30	VAL	3.9
1	A	344	VAL	3.9
1	A	202	ASP	3.8
1	B	70	GLY	3.8
1	F	312	LEU	3.8
1	A	16	LEU	3.8
1	A	103	SER	3.8
1	E	26	GLY	3.8
1	F	26	GLY	3.8
1	A	21	PHE	3.7
1	B	187	GLU	3.7
1	D	1	MET	3.7
1	B	27	LEU	3.7
1	E	69	GLN	3.7
1	B	148	ILE	3.7
1	E	267	ALA	3.7
1	B	140	GLN	3.7
1	A	185	VAL	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	295	LEU	3.6
1	A	309	LEU	3.6
1	A	89	TYR	3.6
1	A	246	ALA	3.5
1	A	25	SER	3.5
1	A	314	VAL	3.5
1	B	26	GLY	3.5
1	A	179	LEU	3.5
1	A	203	VAL	3.5
1	G	211	ARG	3.5
1	A	108	ARG	3.5
1	A	91	LEU	3.4
1	A	245	ARG	3.4
1	A	352	ALA	3.4
1	A	302	VAL	3.4
1	A	303	GLU	3.4
1	D	86	GLU	3.4
1	A	312	LEU	3.4
1	A	87	GLN	3.4
1	A	8	VAL	3.3
1	A	211	ARG	3.3
1	A	315	PRO	3.3
1	A	316	SER	3.2
1	B	352	ALA	3.2
1	A	299	GLN	3.2
1	A	322	TYR	3.2
1	A	334	ILE	3.2
1	A	247	ARG	3.2
1	A	61	PRO	3.2
1	F	62	GLY	3.2
1	C	352	ALA	3.2
1	A	207	VAL	3.2
1	A	22	LEU	3.2
1	A	300	GLY	3.2
1	B	120	LEU	3.1
1	D	87	GLN	3.1
1	A	83	ALA	3.1
1	F	25	SER	3.1
1	A	23	ARG	3.1
1	A	320	LEU	3.1
1	A	187	GLU	3.1
1	A	97	ILE	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	313	ALA	3.1
1	H	352	ALA	3.1
1	A	293	LEU	3.1
1	F	308	GLY	3.1
1	B	86	GLU	3.0
1	B	87	GLN	3.0
1	A	4	VAL	3.0
1	A	124	VAL	3.0
1	A	63	TRP	2.9
1	A	209	PHE	2.9
1	B	119	TRP	2.9
1	A	351	CYS	2.9
1	D	352	ALA	2.9
1	A	236	VAL	2.9
1	C	271	GLU	2.9
1	A	6	VAL	2.9
1	A	111	VAL	2.9
1	A	79	LEU	2.9
1	B	265	GLN	2.8
1	B	272	ARG	2.8
1	A	46	TRP	2.8
1	A	242	LEU	2.8
1	A	319	LEU	2.8
1	A	333	LEU	2.8
1	A	271	GLU	2.8
1	B	165	ARG	2.8
1	B	5	ASP	2.8
1	A	180	ALA	2.8
1	E	352	ALA	2.8
1	B	24	ARG	2.8
1	E	268	ASP	2.8
1	A	313	ALA	2.8
1	B	60	ILE	2.8
1	A	244	ALA	2.8
1	A	249	VAL	2.8
1	B	182	VAL	2.8
1	A	206	ARG	2.8
1	B	3	SER	2.7
1	B	259	PHE	2.7
1	A	85	TYR	2.7
1	A	65	MET	2.7
1	A	122	ARG	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	138	GLU	2.7
1	A	157	THR	2.7
1	A	184	THR	2.7
1	D	89	TYR	2.7
1	G	1	MET	2.7
1	A	53	SER	2.7
1	E	86	GLU	2.7
1	A	102	VAL	2.7
1	A	176	ALA	2.7
1	E	89	TYR	2.6
1	A	172	GLY	2.6
1	A	304	VAL	2.6
1	F	71	PRO	2.6
1	F	105	PHE	2.6
1	B	234	ASP	2.6
1	E	87	GLN	2.6
1	A	346	GLN	2.6
1	A	115	ASP	2.6
1	B	22	LEU	2.6
1	B	193	ARG	2.6
1	E	138	GLU	2.6
1	A	343	ALA	2.6
1	B	21	PHE	2.6
1	A	72	TYR	2.5
1	B	69	GLN	2.5
1	A	294	ASP	2.5
1	A	86	GLU	2.5
1	A	339	TYR	2.5
1	B	93	VAL	2.5
1	A	93	VAL	2.5
1	B	253	VAL	2.5
1	D	140	GLN	2.5
1	B	94	LEU	2.5
1	D	94	LEU	2.5
1	D	47	HIS	2.5
1	A	328	MET	2.5
1	G	251	ALA	2.5
1	A	348	THR	2.4
1	B	47	HIS	2.4
1	F	299	GLN	2.4
1	B	146	ALA	2.4
1	B	349	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	211	ARG	2.4
1	A	31	ILE	2.4
1	D	88	LYS	2.4
1	B	29	TYR	2.4
1	A	286	ALA	2.4
1	G	210	GLU	2.4
1	H	1	MET	2.4
1	A	239	PRO	2.4
1	A	329	ALA	2.4
1	B	334	ILE	2.4
1	A	173	ASN	2.4
1	B	183	SER	2.4
1	B	243	ASP	2.4
1	A	105	PHE	2.4
1	C	313	ALA	2.4
1	F	235	ILE	2.3
1	A	237	MET	2.3
1	B	71	PRO	2.3
1	A	106	GLY	2.3
1	H	269	GLY	2.3
1	A	296	VAL	2.3
1	A	159	ALA	2.3
1	A	267	ALA	2.3
1	B	291	LYS	2.3
1	B	266	TRP	2.3
1	C	351	CYS	2.3
1	B	36	ALA	2.3
1	G	291	LYS	2.3
1	F	66	PRO	2.3
1	A	82	LEU	2.3
1	A	195	GLU	2.3
1	A	38	PRO	2.3
1	A	64	PRO	2.3
1	F	292	GLY	2.3
1	B	312	LEU	2.3
1	E	313	ALA	2.2
1	B	348	THR	2.2
1	B	195	GLU	2.2
1	F	210	GLU	2.2
1	B	185	VAL	2.2
1	F	94	LEU	2.2
1	F	87	GLN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	37	SER	2.2
1	A	40	GLY	2.2
1	A	307	SER	2.2
1	B	115	ASP	2.2
1	E	115	ASP	2.2
1	D	82	LEU	2.2
1	B	4	VAL	2.2
1	A	127	ALA	2.2
1	A	162	ALA	2.2
1	A	107	GLU	2.2
1	H	299	GLN	2.2
1	B	56	GLY	2.2
1	F	68	SER	2.2
1	G	243	ASP	2.2
1	A	241	VAL	2.2
1	D	63	TRP	2.2
1	B	83	ALA	2.2
1	B	273	ALA	2.2
1	G	313	ALA	2.2
1	D	138	GLU	2.2
1	A	165	ARG	2.2
1	H	211	ARG	2.2
1	A	62	GLY	2.2
1	A	324	ASP	2.2
1	H	93	VAL	2.2
1	A	167	ALA	2.1
1	B	159	ALA	2.1
1	C	251	ALA	2.1
1	A	332	THR	2.1
1	B	85	TYR	2.1
1	F	317	VAL	2.1
1	G	5	ASP	2.1
1	B	307	SER	2.1
1	A	145	PHE	2.1
1	B	257	ALA	2.1
1	A	101	ARG	2.1
1	D	213	THR	2.1
1	A	265	GLN	2.1
1	A	308	GLY	2.1
1	B	166	VAL	2.1
1	F	302	VAL	2.1
1	A	90	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	24	ARG	2.1
1	A	337	THR	2.1
1	B	254	PRO	2.1
1	B	261	PRO	2.1
1	B	164	MET	2.1
1	B	350	TYR	2.1
1	D	62	GLY	2.1
1	B	302	VAL	2.1
1	E	235	ILE	2.1
1	A	183	SER	2.1
1	E	195	GLU	2.1
1	C	347	VAL	2.1
1	A	181	GLU	2.0
1	F	258	ARG	2.0
1	A	92	PRO	2.0
1	B	66	PRO	2.0
1	D	71	PRO	2.0
1	A	199	LEU	2.0
1	A	250	LEU	2.0
1	D	120	LEU	2.0
1	A	104	HIS	2.0
1	A	163	GLY	2.0
1	B	351	CYS	2.0
1	G	6	VAL	2.0
1	B	105	PHE	2.0
1	G	24	ARG	2.0
1	H	338	ARG	2.0
1	B	202	ASP	2.0
1	E	18	ALA	2.0
1	A	170	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	G	1355	5/5	0.36	0.13	132,142,147,158	0
3	SO4	B	1355	5/5	0.50	0.20	112,113,123,131	0
3	SO4	B	1356	5/5	0.58	0.16	87,90,105,107	0
3	SO4	D	1356	5/5	0.63	0.23	145,150,156,159	0
3	SO4	C	1357	5/5	0.64	0.14	90,91,104,108	0
3	SO4	B	1357	5/5	0.65	0.14	132,135,144,151	0
3	SO4	C	1355	5/5	0.66	0.23	98,122,126,127	0
3	SO4	E	1355	5/5	0.67	0.18	93,94,105,111	0
3	SO4	A	1355	5/5	0.72	0.18	137,139,145,159	0
3	SO4	D	1358	5/5	0.73	0.15	137,141,153,154	0
3	SO4	F	1356	5/5	0.76	0.20	76,83,93,111	0
3	SO4	C	1356	5/5	0.76	0.16	106,114,117,127	0
3	SO4	G	1357	5/5	0.77	0.13	66,73,80,83	0
3	SO4	H	1356	5/5	0.78	0.13	123,129,130,138	0
3	SO4	H	1355	5/5	0.82	0.16	105,117,124,131	0
3	SO4	D	1355	5/5	0.83	0.24	86,89,99,100	0
3	SO4	A	1356	5/5	0.85	0.10	57,66,83,83	0
3	SO4	F	1357	5/5	0.85	0.32	83,88,97,113	0
2	FAD	A	1353	53/53	0.89	0.11	33,48,57,59	0
3	SO4	D	1357	5/5	0.89	0.13	58,60,68,69	0
3	SO4	G	1356	5/5	0.91	0.08	54,56,67,75	0
3	SO4	B	1354	5/5	0.92	0.12	48,49,59,63	0
3	SO4	A	1354	5/5	0.93	0.17	50,52,61,62	0
3	SO4	E	1354	5/5	0.94	0.16	36,42,44,45	0
3	SO4	C	1358	5/5	0.94	0.07	59,60,68,70	0
3	SO4	D	1359	5/5	0.94	0.08	50,56,58,64	0
3	SO4	E	1356	5/5	0.95	0.07	42,50,51,55	0
2	FAD	F	1353	53/53	0.95	0.07	23,29,33,43	0
2	FAD	C	1353	53/53	0.96	0.07	23,29,37,38	0
2	FAD	D	1353	53/53	0.96	0.07	22,28,36,44	0
2	FAD	B	1353	53/53	0.96	0.07	25,31,39,44	0
3	SO4	F	1354	5/5	0.96	0.09	33,36,41,45	0
3	SO4	F	1355	5/5	0.96	0.07	46,56,58,68	0
2	FAD	G	1353	53/53	0.96	0.07	24,30,34,39	0
3	SO4	H	1357	5/5	0.96	0.05	42,47,51,54	0
3	SO4	D	1354	5/5	0.97	0.10	36,40,49,50	0
3	SO4	H	1354	5/5	0.97	0.08	34,41,44,45	0

Continued on next page...

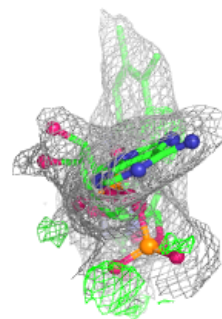
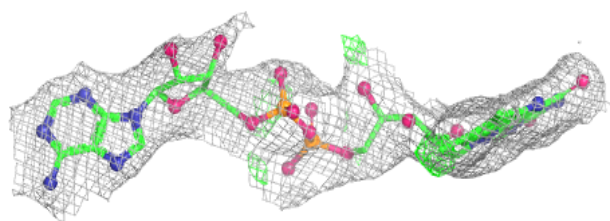
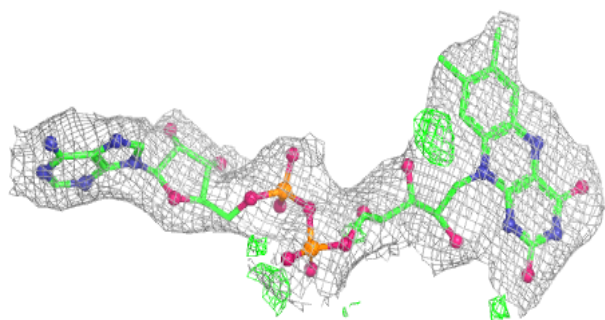
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	G	1354	5/5	0.97	0.11	47,48,52,52	0
2	FAD	H	1353	53/53	0.97	0.06	18,25,30,32	0
2	FAD	E	1353	53/53	0.97	0.06	21,26,33,36	0
3	SO4	C	1354	5/5	0.98	0.13	37,39,40,42	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.

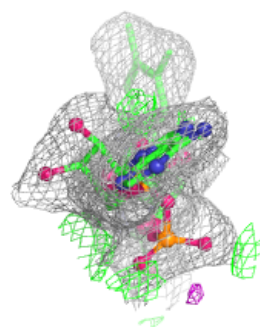
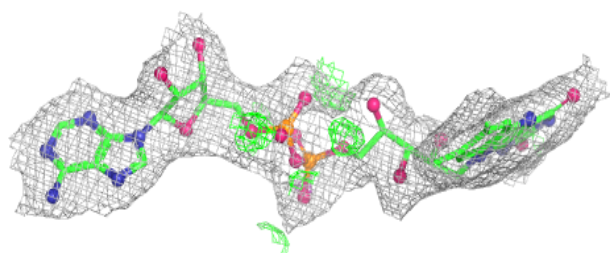
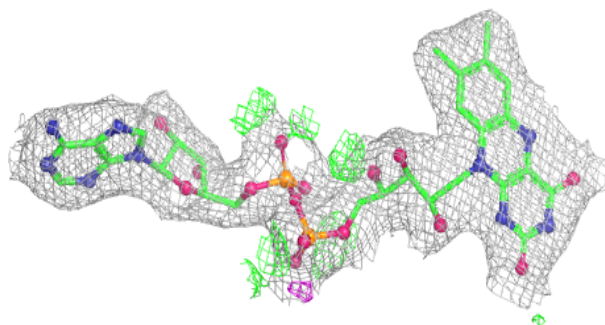
Electron density around FAD A 1353:

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

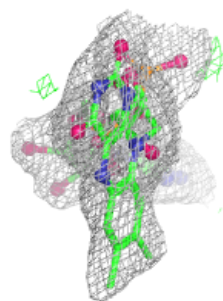
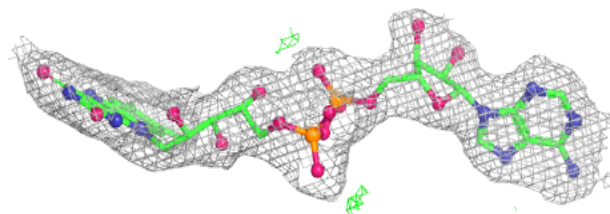
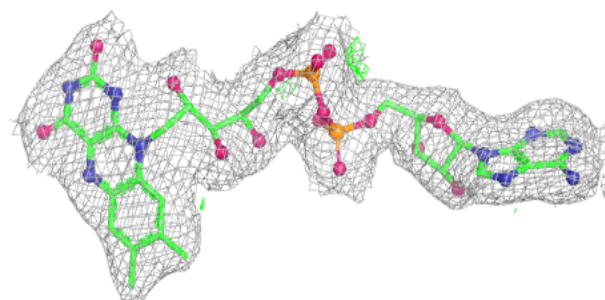


Electron density around FAD F 1353:

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

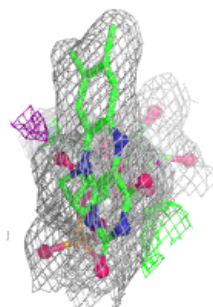
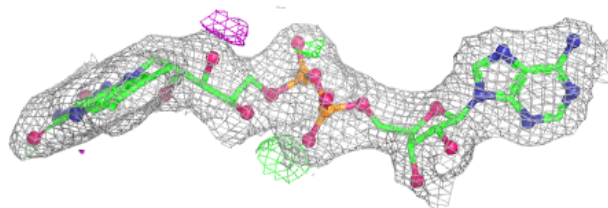
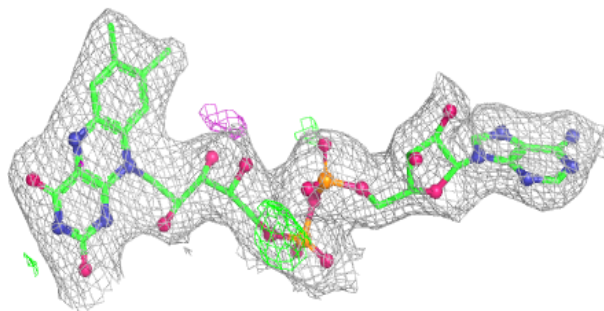
**Electron density around FAD C 1353:**

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

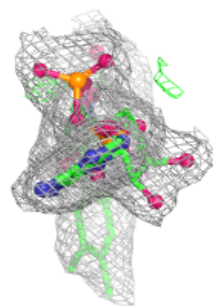
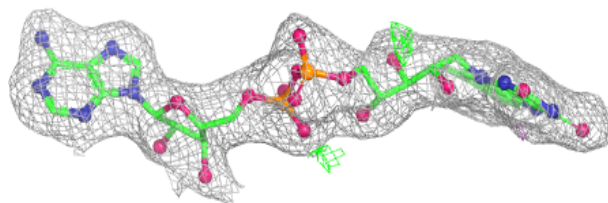
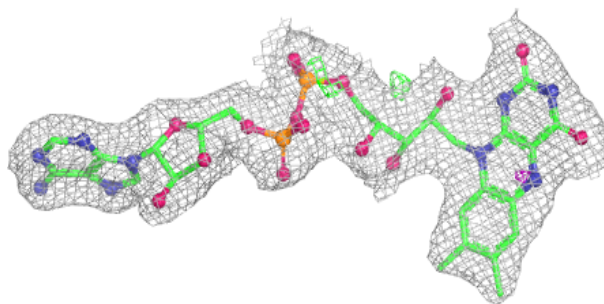


Electron density around FAD D 1353:

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

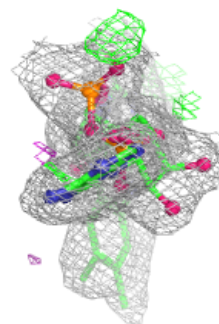
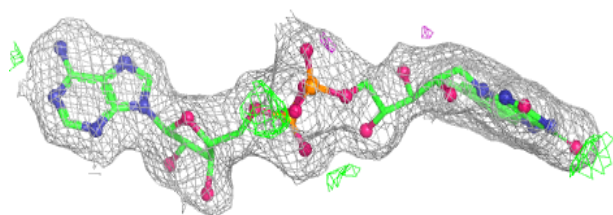
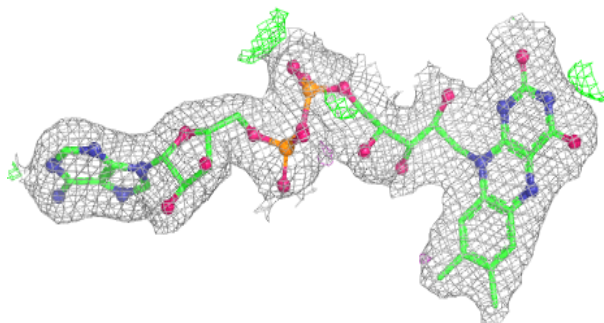
**Electron density around FAD B 1353:**

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

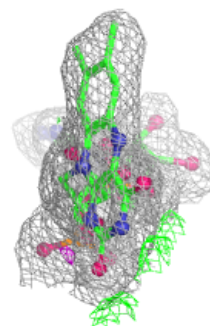
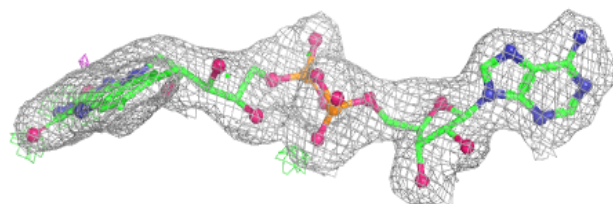
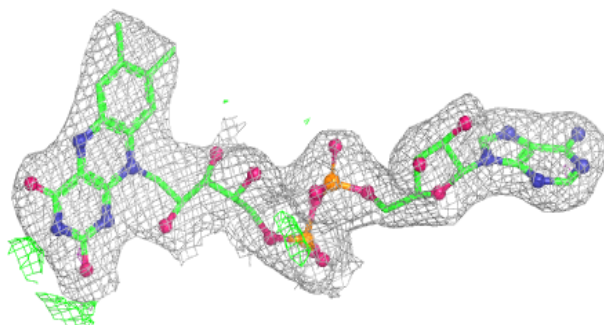


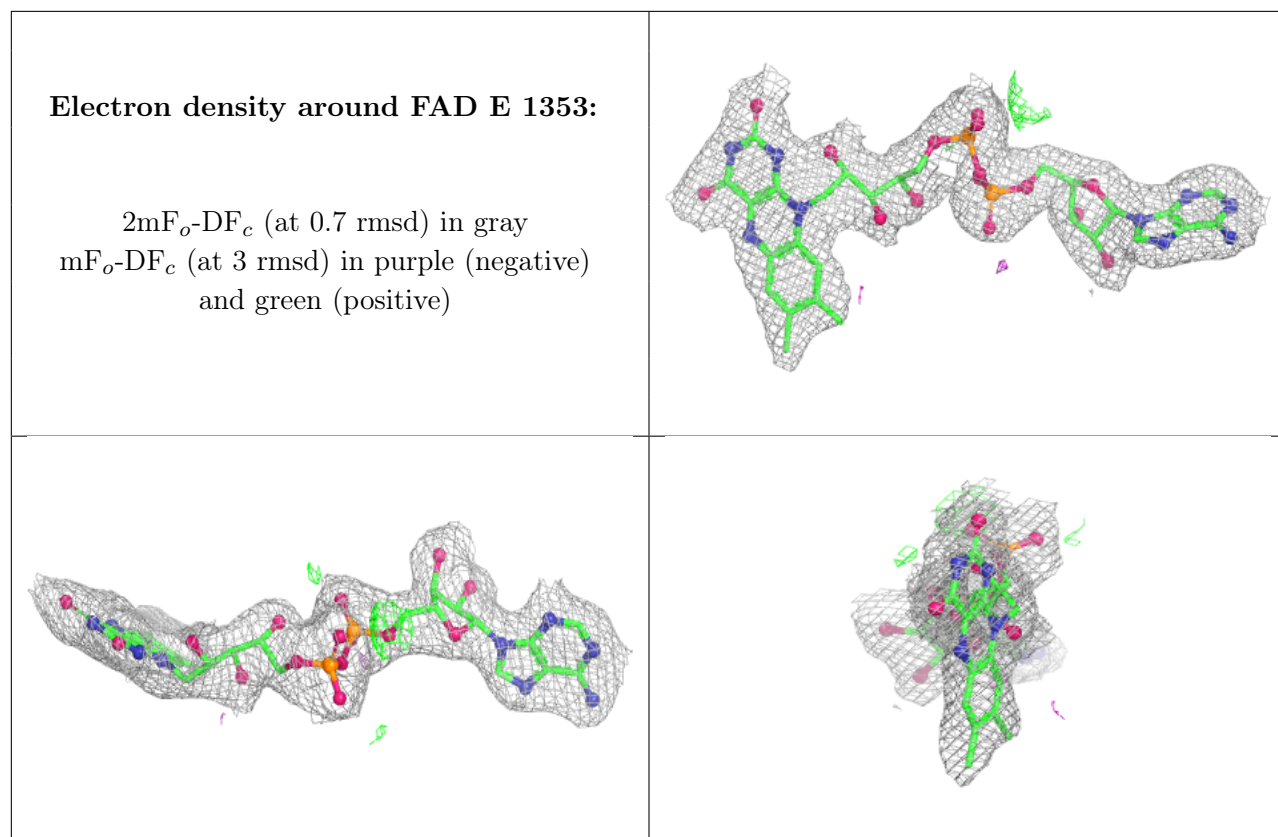
Electron density around FAD G 1353:

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

**Electron density around FAD H 1353:**

$2mF_o-DF_c$ (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.