



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2023 – 08:17 PM EDT

PDB ID : 3BG6
Title : Pyranose 2-oxidase from *Trametes multicolor*, E542K mutant
Authors : Tan, T.C.; Divne, C.
Deposited on : 2007-11-26
Resolution : 1.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

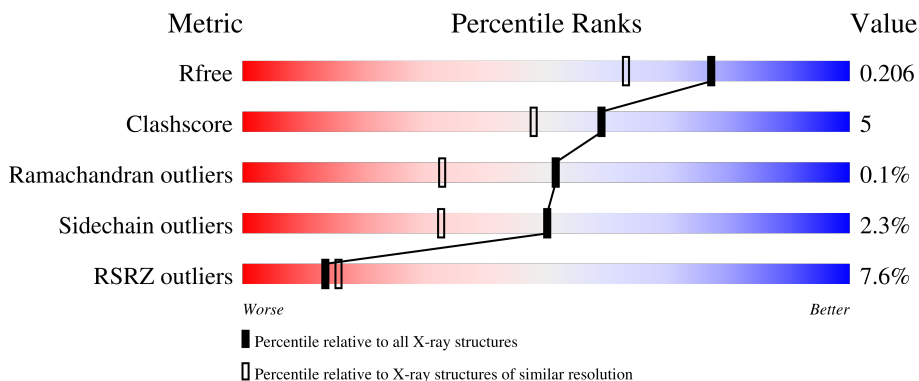
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



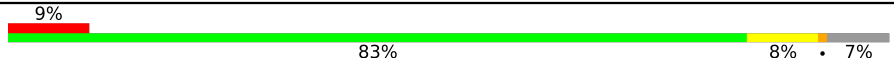
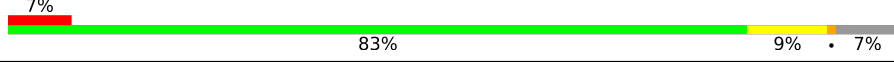

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	623	 7% 83% 8% • 7%
1	B	623	 5% 85% 7% • 7%
1	C	623	 8% 84% 7% • 7%
1	D	623	 6% 82% 10% • 7%
1	E	623	 9% 84% 8% • 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	623	 9% 83% 8% • 7%
1	G	623	 7% 83% 9% • 7%
1	H	623	 6% 83% 9% • 7%

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 39362 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.

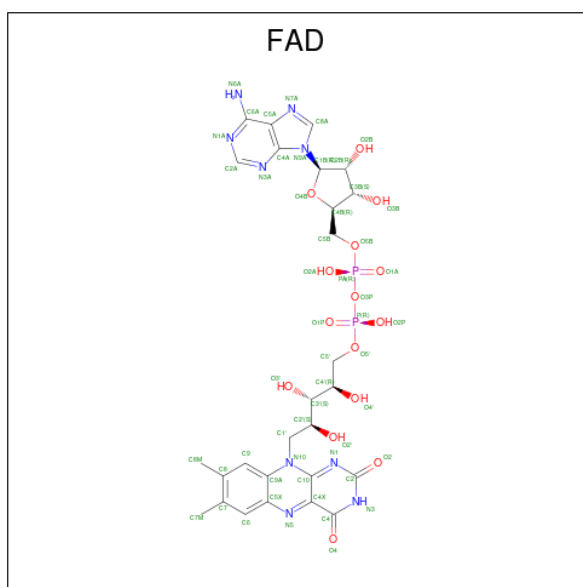
- Molecule 1 is a protein called Pyranose oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	577	4549	2873	779	872	25	0	0	0
1	B	577	4549	2873	779	872	25	0	0	0
1	C	577	4549	2873	779	872	25	0	0	0
1	D	577	4549	2873	779	872	25	0	0	0
1	E	577	4549	2873	779	872	25	0	0	0
1	F	577	4549	2873	779	872	25	0	0	0
1	G	577	4549	2873	779	872	25	0	0	0
1	H	577	4549	2873	779	872	25	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	542	LYS	GLU	engineered mutation	UNP Q7ZA32
B	542	LYS	GLU	engineered mutation	UNP Q7ZA32
C	542	LYS	GLU	engineered mutation	UNP Q7ZA32
D	542	LYS	GLU	engineered mutation	UNP Q7ZA32
E	542	LYS	GLU	engineered mutation	UNP Q7ZA32
F	542	LYS	GLU	engineered mutation	UNP Q7ZA32
G	542	LYS	GLU	engineered mutation	UNP Q7ZA32
H	542	LYS	GLU	engineered mutation	UNP Q7ZA32

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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		
2	G	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	H	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	359	Total	O	0	0
			359	359		
3	B	373	Total	O	0	0
			373	373		
3	C	267	Total	O	0	0
			267	267		
3	D	314	Total	O	0	0
			314	314		

Continued on next page...

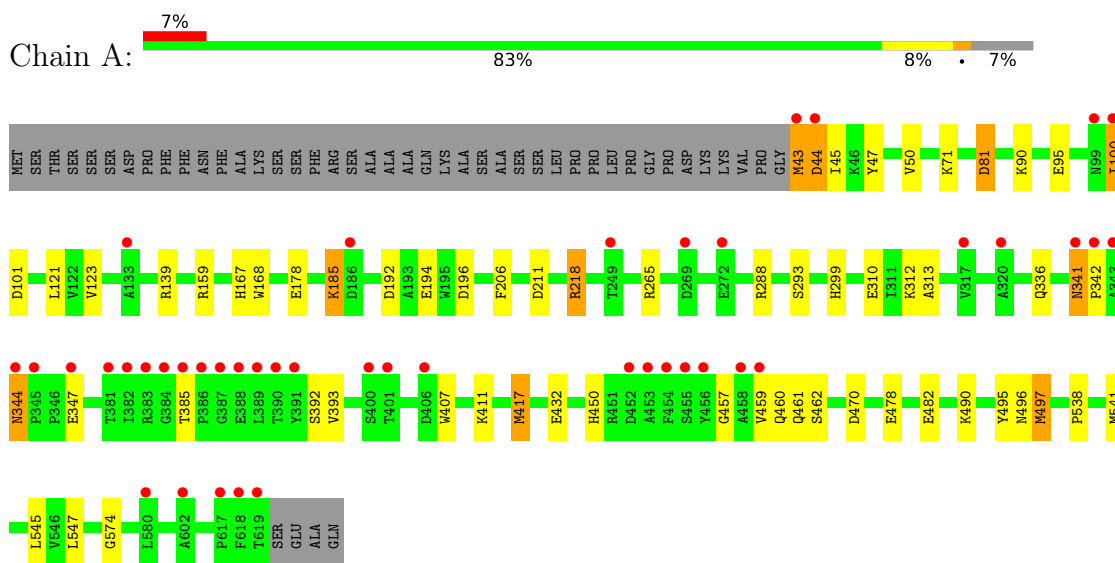
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	301	Total 301	O 301	0	0
3	F	262	Total 262	O 262	0	0
3	G	315	Total 315	O 315	0	0
3	H	355	Total 355	O 355	0	0

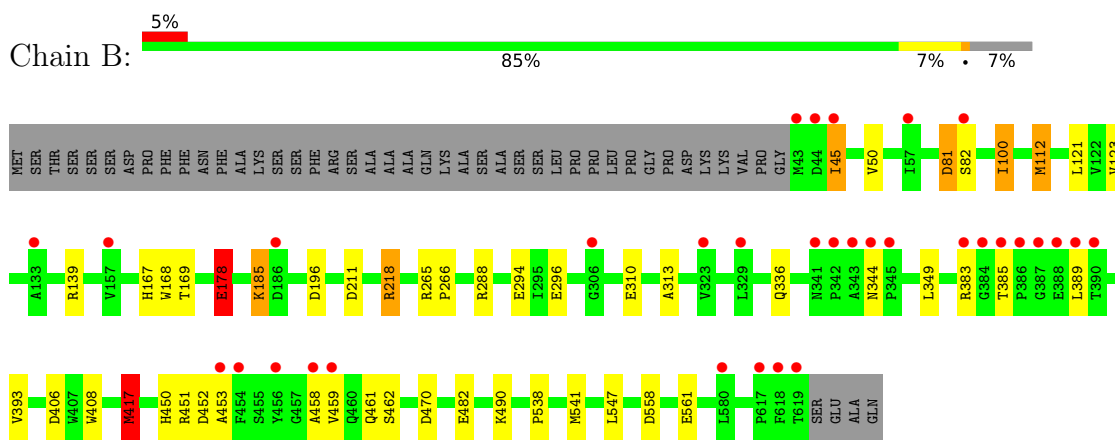
3 Residue-property plots i

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

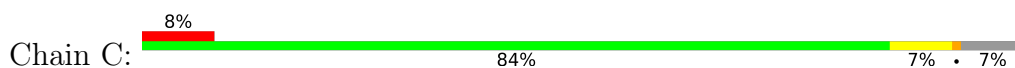
- Molecule 1: Pyranose oxidase

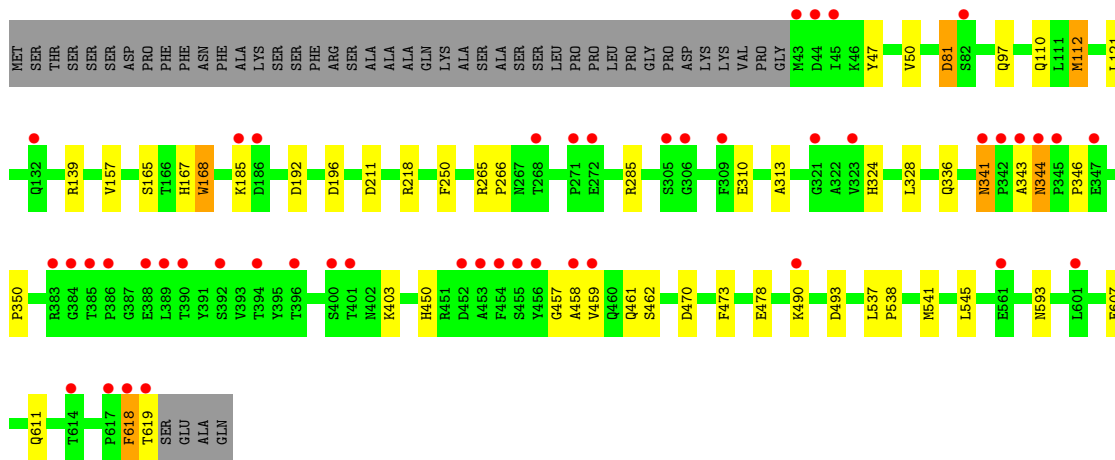


- Molecule 1: Pyranose oxidase

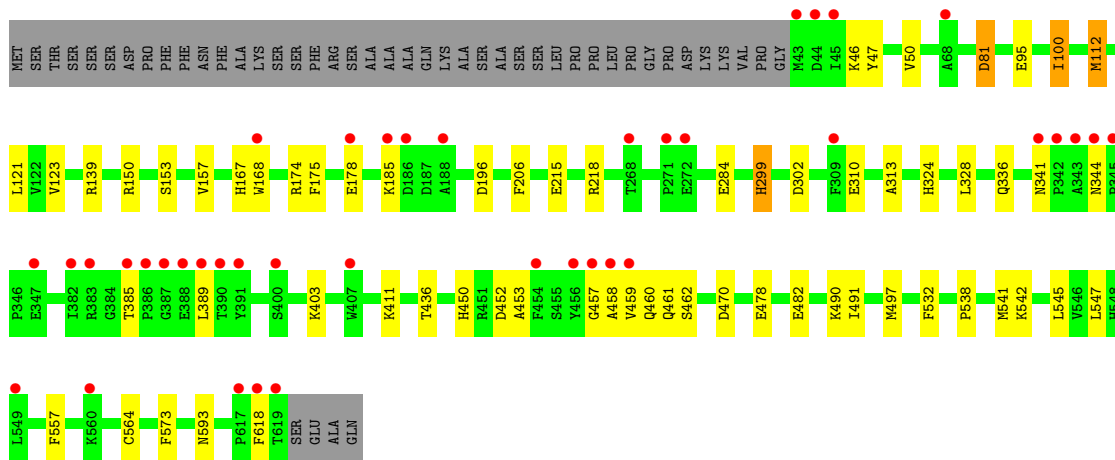
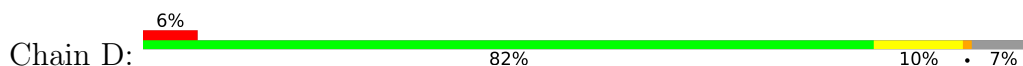


- Molecule 1: Pyranose oxidase

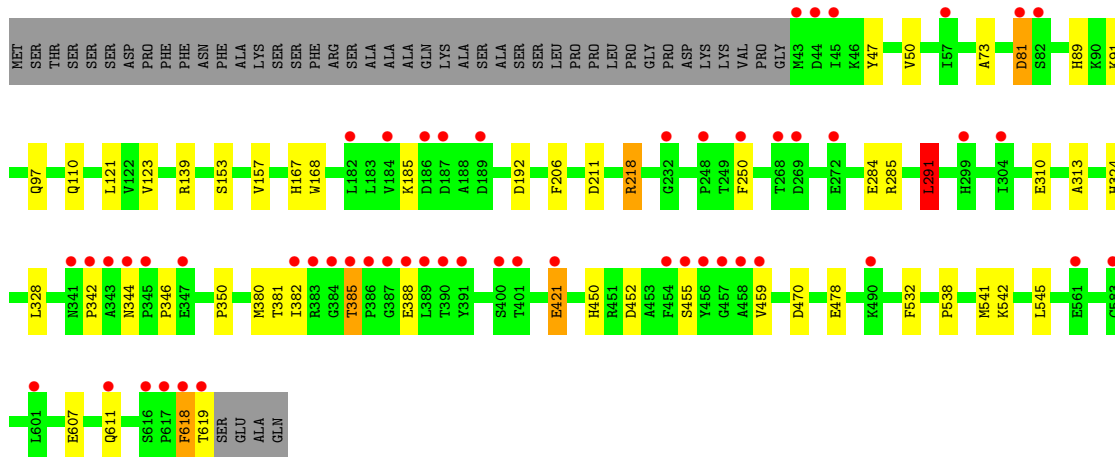
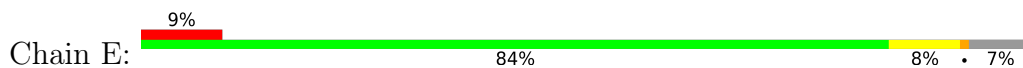




• Molecule 1: Pyranose oxidase



• Molecule 1: Pyranose oxidase



L547	
A592	
F617	●
F618	●
T619	●
SER	
GLU	
ALA	
GLN	

4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	168.86Å 103.75Å 169.33Å 90.00° 106.31° 90.00°	Depositor
Resolution (Å)	40.00 – 1.70 39.18 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.3 (40.00-1.70) 98.3 (39.18-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 1.70Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.166 , 0.198 0.177 , 0.206	Depositor DCC
R_{free} test set	6061 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å ²)	17.8	Xtrriage
Anisotropy	0.134	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.014 for l,-k,h	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	39362	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section:
FAD

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	1.09	11/4665 (0.2%)	1.03	18/6342 (0.3%)
1	B	1.11	7/4665 (0.2%)	1.05	17/6342 (0.3%)
1	C	0.91	2/4665 (0.0%)	0.94	13/6342 (0.2%)
1	D	0.97	6/4665 (0.1%)	0.96	13/6342 (0.2%)
1	E	0.98	5/4665 (0.1%)	0.96	10/6342 (0.2%)
1	F	0.96	5/4665 (0.1%)	0.99	10/6342 (0.2%)
1	G	1.01	6/4665 (0.1%)	0.96	11/6342 (0.2%)
1	H	1.07	11/4665 (0.2%)	1.03	18/6342 (0.3%)
All	All	1.01	53/37320 (0.1%)	0.99	110/50736 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
All	All	0	2

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	291	LEU	CG-CD1	12.75	1.99	1.51
1	A	194	GLU	CG-CD	-8.00	1.40	1.51
1	H	478	GLU	CD-OE1	7.85	1.34	1.25
1	B	482	GLU	CD-OE1	7.83	1.34	1.25
1	E	478	GLU	CD-OE1	7.68	1.34	1.25
1	A	478	GLU	CD-OE1	7.51	1.33	1.25
1	H	81	ASP	CB-CG	-7.37	1.36	1.51
1	F	371	GLU	CG-CD	7.14	1.62	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	310	GLU	CB-CG	-7.14	1.38	1.52
1	B	482	GLU	CG-CD	7.08	1.62	1.51
1	D	112	MET	CB-CG	6.89	1.73	1.51
1	D	482	GLU	CG-CD	6.77	1.62	1.51
1	C	478	GLU	CD-OE1	6.74	1.33	1.25
1	B	310	GLU	CB-CG	-6.72	1.39	1.52
1	B	112	MET	CB-CG	6.66	1.72	1.51
1	A	482	GLU	CD-OE1	6.54	1.32	1.25
1	H	421	GLU	CB-CG	6.51	1.64	1.52
1	C	310	GLU	CG-CD	6.45	1.61	1.51
1	H	421	GLU	CD-OE1	-6.43	1.18	1.25
1	A	482	GLU	CG-CD	6.38	1.61	1.51
1	H	95	GLU	CB-CG	-6.27	1.40	1.52
1	H	160	VAL	CB-CG1	6.24	1.66	1.52
1	F	112	MET	CB-CG	6.23	1.71	1.51
1	A	81	ASP	CB-CG	-6.20	1.38	1.51
1	E	310	GLU	CG-CD	6.11	1.61	1.51
1	B	139	ARG	CD-NE	-6.05	1.36	1.46
1	F	478	GLU	CD-OE1	6.03	1.32	1.25
1	D	478	GLU	CD-OE1	6.00	1.32	1.25
1	G	91	LYS	CE-NZ	5.98	1.64	1.49
1	B	178	GLU	CB-CG	-5.97	1.40	1.52
1	H	478	GLU	CG-CD	5.86	1.60	1.51
1	D	139	ARG	CD-NE	-5.83	1.36	1.46
1	F	72	VAL	CB-CG2	5.76	1.65	1.52
1	D	482	GLU	CD-OE1	5.73	1.31	1.25
1	G	478	GLU	CD-OE2	5.69	1.31	1.25
1	H	482	GLU	CG-CD	5.63	1.60	1.51
1	A	196	ASP	CB-CG	5.62	1.63	1.51
1	A	139	ARG	CD-NE	-5.61	1.36	1.46
1	F	139	ARG	CD-NE	-5.50	1.37	1.46
1	A	178	GLU	CG-CD	5.46	1.60	1.51
1	D	482	GLU	CD-OE2	5.46	1.31	1.25
1	H	139	ARG	CD-NE	-5.43	1.37	1.46
1	A	95	GLU	CB-CG	-5.41	1.41	1.52
1	H	482	GLU	CD-OE1	5.29	1.31	1.25
1	A	478	GLU	CG-CD	5.28	1.59	1.51
1	E	478	GLU	CG-CD	5.25	1.59	1.51
1	G	122	VAL	CB-CG2	5.18	1.63	1.52
1	H	104	VAL	CB-CG2	-5.14	1.42	1.52
1	G	139	ARG	CD-NE	-5.12	1.37	1.46
1	B	82	SER	N-CA	5.11	1.56	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	81	ASP	CB-CG	-5.07	1.41	1.51
1	G	482	GLU	CG-CD	5.05	1.59	1.51
1	A	432	GLU	CD-OE2	5.03	1.31	1.25

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	139	ARG	NE-CZ-NH2	-23.75	108.43	120.30
1	B	139	ARG	NE-CZ-NH2	-19.64	110.48	120.30
1	E	139	ARG	NE-CZ-NH1	18.29	129.44	120.30
1	F	139	ARG	NE-CZ-NH1	18.25	129.43	120.30
1	D	139	ARG	NE-CZ-NH2	-18.23	111.18	120.30
1	H	139	ARG	NE-CZ-NH2	-17.91	111.34	120.30
1	A	139	ARG	NE-CZ-NH2	-17.80	111.40	120.30
1	E	139	ARG	NE-CZ-NH2	-17.80	111.40	120.30
1	C	139	ARG	NE-CZ-NH2	-17.64	111.48	120.30
1	G	139	ARG	NE-CZ-NH1	17.16	128.88	120.30
1	B	139	ARG	NE-CZ-NH1	16.29	128.45	120.30
1	C	139	ARG	NE-CZ-NH1	16.28	128.44	120.30
1	G	139	ARG	NE-CZ-NH2	-15.21	112.69	120.30
1	H	139	ARG	NE-CZ-NH1	14.75	127.67	120.30
1	A	139	ARG	NE-CZ-NH1	14.18	127.39	120.30
1	D	139	ARG	NE-CZ-NH1	13.37	126.99	120.30
1	F	218	ARG	NE-CZ-NH1	12.72	126.66	120.30
1	H	81	ASP	CB-CG-OD1	-11.80	107.68	118.30
1	H	211	ASP	CB-CG-OD1	11.18	128.36	118.30
1	E	81	ASP	CB-CG-OD1	-10.82	108.56	118.30
1	A	81	ASP	CB-CG-OD1	-10.68	108.69	118.30
1	B	218	ARG	NE-CZ-NH1	10.30	125.45	120.30
1	B	81	ASP	CB-CG-OD1	-10.10	109.22	118.30
1	C	81	ASP	CB-CG-OD1	-9.84	109.45	118.30
1	A	211	ASP	CB-CG-OD1	9.62	126.96	118.30
1	E	218	ARG	NE-CZ-NH1	9.33	124.97	120.30
1	F	81	ASP	CB-CG-OD1	-9.25	109.98	118.30
1	C	81	ASP	CB-CG-OD2	9.01	126.41	118.30
1	B	417	MET	CG-SD-CE	-8.69	86.30	100.20
1	A	218	ARG	NE-CZ-NH1	8.41	124.51	120.30
1	G	196	ASP	CB-CG-OD1	7.97	125.47	118.30
1	B	211	ASP	CB-CG-OD1	7.93	125.44	118.30
1	C	211	ASP	CB-CG-OD1	7.92	125.42	118.30
1	A	196	ASP	CB-CG-OD1	7.34	124.91	118.30
1	B	451	ARG	NE-CZ-NH1	7.30	123.95	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	470	ASP	CB-CG-OD1	7.25	124.83	118.30
1	G	211	ASP	CB-CG-OD1	7.17	124.75	118.30
1	A	159	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	B	470	ASP	CB-CG-OD2	-6.96	112.03	118.30
1	E	211	ASP	CB-CG-OD1	6.89	124.50	118.30
1	A	417	MET	CG-SD-CE	-6.86	89.22	100.20
1	D	81	ASP	CB-CG-OD1	-6.85	112.13	118.30
1	H	112	MET	CG-SD-CE	6.76	111.01	100.20
1	H	211	ASP	CB-CG-OD2	-6.67	112.30	118.30
1	G	218	ARG	NE-CZ-NH1	6.55	123.57	120.30
1	D	470	ASP	CB-CG-OD1	6.51	124.16	118.30
1	H	218	ARG	NE-CZ-NH1	6.51	123.55	120.30
1	F	314	ASP	CB-CG-OD1	6.45	124.11	118.30
1	B	81	ASP	CB-CG-OD2	6.43	124.09	118.30
1	H	473	PHE	CB-CG-CD2	-6.43	116.30	120.80
1	B	196	ASP	CB-CG-OD1	6.42	124.08	118.30
1	D	196	ASP	CB-CG-OD1	6.37	124.03	118.30
1	C	470	ASP	CB-CG-OD2	-6.37	112.57	118.30
1	C	192	ASP	CB-CG-OD1	6.26	123.94	118.30
1	A	288	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	E	81	ASP	CB-CG-OD2	6.22	123.90	118.30
1	H	192	ASP	CB-CG-OD1	6.21	123.89	118.30
1	B	218	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	H	139	ARG	CA-CB-CG	6.07	126.75	113.40
1	A	497	MET	CG-SD-CE	6.06	109.89	100.20
1	H	192	ASP	CB-CG-OD2	-6.06	112.85	118.30
1	H	470	ASP	CB-CG-OD1	6.05	123.75	118.30
1	F	139	ARG	CD-NE-CZ	6.04	132.06	123.60
1	B	470	ASP	CB-CG-OD1	6.02	123.72	118.30
1	D	218	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	G	288	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	C	139	ARG	CD-NE-CZ	5.82	131.75	123.60
1	B	349	LEU	CB-CG-CD2	5.80	120.85	111.00
1	B	406	ASP	CB-CG-OD1	5.77	123.49	118.30
1	B	139	ARG	CD-NE-CZ	5.75	131.65	123.60
1	B	288	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	D	139	ARG	CD-NE-CZ	5.68	131.55	123.60
1	A	265	ARG	NE-CZ-NH2	-5.61	117.49	120.30
1	H	175	PHE	CB-CG-CD1	5.60	124.72	120.80
1	F	261	ASP	CB-CG-OD1	5.57	123.31	118.30
1	H	196	ASP	CB-CG-OD1	5.56	123.30	118.30
1	E	192	ASP	CB-CG-OD1	5.54	123.28	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	470	ASP	CB-CG-OD1	5.50	123.25	118.30
1	A	495	TYR	CD1-CE1-CZ	-5.50	114.85	119.80
1	G	470	ASP	CB-CG-OD2	-5.45	113.40	118.30
1	F	470	ASP	CB-CG-OD1	5.44	123.20	118.30
1	E	291	LEU	CB-CG-CD1	5.41	120.20	111.00
1	A	81	ASP	CB-CG-OD2	5.37	123.14	118.30
1	E	470	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	A	470	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	H	411	LYS	CD-CE-NZ	-5.29	99.53	111.70
1	G	265	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	F	81	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	211	ASP	CB-CG-OD2	-5.25	113.57	118.30
1	B	383	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	G	150	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	C	473	PHE	CB-CG-CD2	-5.23	117.14	120.80
1	D	81	ASP	CB-CG-OD2	5.22	123.00	118.30
1	F	472	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	G	234	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	H	175	PHE	CB-CG-CD2	-5.19	117.17	120.80
1	H	473	PHE	CB-CG-CD1	5.18	124.43	120.80
1	D	389	LEU	CA-CB-CG	5.17	127.19	115.30
1	G	473	PHE	CB-CG-CD2	-5.15	117.20	120.80
1	A	139	ARG	CD-NE-CZ	5.10	130.74	123.60
1	D	175	PHE	CB-CG-CD2	-5.10	117.23	120.80
1	D	302	ASP	CB-CG-OD1	5.09	122.89	118.30
1	C	211	ASP	CB-CG-OD2	-5.07	113.74	118.30
1	D	174	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	D	150	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	H	497	MET	CG-SD-CE	5.02	108.24	100.20
1	C	493	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	A	192	ASP	CB-CG-OD1	5.02	122.82	118.30
1	E	291	LEU	CB-CG-CD2	-5.01	102.49	111.00
1	C	196	ASP	CB-CG-OD1	5.00	122.80	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	43	MET	Peptide
1	D	436	THR	Peptide

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	4549	0	4402	46	0
1	B	4549	0	4402	43	0
1	C	4549	0	4402	42	0
1	D	4549	0	4402	46	0
1	E	4549	0	4402	49	0
1	F	4549	0	4402	42	0
1	G	4549	0	4402	46	0
1	H	4549	0	4402	43	0
2	A	53	0	30	11	0
2	B	53	0	31	12	0
2	C	53	0	29	4	0
2	D	53	0	31	10	0
2	E	53	0	30	5	0
2	F	53	0	29	8	0
2	G	53	0	31	13	0
2	H	53	0	30	5	0
3	A	359	0	0	5	0
3	B	373	0	0	6	0
3	C	267	0	0	3	0
3	D	314	0	0	2	0
3	E	301	0	0	2	0
3	F	262	0	0	5	0
3	G	315	0	0	6	0
3	H	355	0	0	4	0
All	All	39362	0	35457	330	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 5.

All (330) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:HIS:HE2	2:D:801:FAD:C8M	0.96	1.56
1:B:167:HIS:HE2	2:B:801:FAD:C8M	0.92	1.55
1:G:167:HIS:HE2	2:G:801:FAD:C8M	0.90	1.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:HIS:HE2	2:A:801:FAD:C8M	0.89	1.51
1:F:167:HIS:HE2	2:F:801:FAD:C8M	0.88	1.51
1:E:291:LEU:CD1	1:E:291:LEU:CG	1.99	1.40
1:B:167:HIS:NE2	2:B:801:FAD:HM82	1.05	1.36
1:G:167:HIS:NE2	2:G:801:FAD:HM82	0.96	1.28
1:D:167:HIS:NE2	2:D:801:FAD:HM82	0.94	1.27
1:A:167:HIS:NE2	2:A:801:FAD:HM82	0.92	1.25
1:F:167:HIS:NE2	2:F:801:FAD:HM82	0.89	1.20
1:F:132:GLN:HG2	3:F:922:HOH:O	1.50	1.09
1:F:167:HIS:CD2	2:F:801:FAD:HM82	1.90	1.06
1:G:167:HIS:CE1	2:G:801:FAD:HM82	1.93	1.03
1:D:167:HIS:CD2	2:D:801:FAD:HM82	1.97	0.99
1:A:167:HIS:CD2	2:A:801:FAD:HM82	1.98	0.98
1:B:167:HIS:HE2	2:B:801:FAD:HM81	1.26	0.98
1:A:167:HIS:CE1	2:A:801:FAD:HM82	1.99	0.96
1:G:167:HIS:HE2	2:G:801:FAD:C8	1.79	0.96
1:D:167:HIS:CE1	2:D:801:FAD:HM82	2.01	0.95
1:F:167:HIS:HE2	2:F:801:FAD:HM81	1.31	0.95
1:D:100:ILE:HD13	1:D:100:ILE:O	1.67	0.94
1:B:167:HIS:HE2	2:B:801:FAD:C8	1.84	0.91
1:F:167:HIS:CE1	2:F:801:FAD:HM82	2.04	0.91
1:B:167:HIS:CD2	2:B:801:FAD:HM82	2.05	0.91
1:B:45:ILE:HD12	1:B:45:ILE:H	1.35	0.89
1:D:167:HIS:HE2	2:D:801:FAD:HM81	1.36	0.89
1:G:481:GLU:HG2	3:G:970:HOH:O	1.73	0.89
1:E:167:HIS:NE2	2:E:801:FAD:HM81	1.86	0.88
1:G:167:HIS:CD2	2:G:801:FAD:HM82	2.08	0.87
1:B:167:HIS:CE1	2:B:801:FAD:HM82	2.08	0.87
1:H:110:GLN:HE21	1:H:167:HIS:HD1	1.24	0.86
1:A:167:HIS:HE2	2:A:801:FAD:HM81	1.34	0.84
1:G:490:LYS:HD3	1:G:491:ILE:HD13	1.61	0.82
1:A:167:HIS:HE2	2:A:801:FAD:C8	1.88	0.82
1:B:178:GLU:HG3	3:B:1035:HOH:O	1.80	0.81
1:E:110:GLN:HE21	1:E:167:HIS:HD1	1.27	0.81
1:E:97:GLN:HG3	1:E:250:PHE:CE2	2.16	0.80
1:C:110:GLN:HE21	1:C:167:HIS:HD1	1.27	0.80
1:C:285:ARG:HA	1:C:328:LEU:HD11	1.63	0.79
1:F:97:GLN:HG3	1:F:250:PHE:CE2	2.17	0.79
1:G:167:HIS:HE2	2:G:801:FAD:HM81	1.37	0.79
1:C:97:GLN:HG3	1:C:250:PHE:CD2	2.18	0.79
1:E:459:VAL:HG22	1:F:121:LEU:HD13	1.65	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:VAL:HG22	1:B:121:LEU:HD13	1.66	0.77
1:E:541:MET:CE	1:E:545:LEU:HD23	2.16	0.76
1:F:132:GLN:CG	3:F:922:HOH:O	2.18	0.75
1:A:81:ASP:C	1:A:81:ASP:OD1	2.22	0.74
1:B:393:VAL:HB	1:B:417:MET:HG2	1.69	0.74
1:B:81:ASP:OD1	1:B:81:ASP:C	2.21	0.74
1:D:167:HIS:HE2	2:D:801:FAD:C8	1.94	0.74
1:C:167:HIS:CD2	2:C:801:FAD:C8M	2.69	0.73
1:E:97:GLN:HG3	1:E:250:PHE:CD2	2.23	0.73
1:C:167:HIS:CE1	2:C:801:FAD:C8M	2.70	0.72
1:E:167:HIS:CE1	2:E:801:FAD:C8M	2.69	0.72
1:E:167:HIS:CD2	2:E:801:FAD:C8M	2.69	0.71
1:H:167:HIS:CD2	2:H:801:FAD:C8M	2.71	0.71
1:A:167:HIS:CE1	2:A:801:FAD:C8M	2.69	0.71
1:C:97:GLN:HG3	1:C:250:PHE:CE2	2.26	0.71
1:F:538:PRO:HG2	1:H:538:PRO:HG2	1.73	0.70
1:C:541:MET:HE3	3:C:929:HOH:O	1.91	0.70
1:H:167:HIS:CE1	2:H:801:FAD:C8M	2.69	0.69
1:C:541:MET:CE	3:C:929:HOH:O	2.40	0.69
1:H:619:THR:O	1:H:619:THR:HG23	1.93	0.69
1:F:541:MET:HE3	3:F:925:HOH:O	1.91	0.69
1:B:541:MET:CE	3:B:964:HOH:O	2.40	0.68
1:H:167:HIS:NE2	2:H:801:FAD:HM81	1.99	0.67
1:A:336:GLN:NE2	1:A:344:ASN:O	2.27	0.67
1:E:541:MET:HE2	1:E:545:LEU:HD23	1.76	0.67
1:C:285:ARG:HA	1:C:328:LEU:CD1	2.24	0.67
1:G:167:HIS:CE1	2:G:801:FAD:C8M	2.65	0.66
1:B:541:MET:HE3	3:B:964:HOH:O	1.95	0.66
1:H:417:MET:HE3	1:H:417:MET:HA	1.78	0.66
1:B:167:HIS:NE2	2:B:801:FAD:C8	2.52	0.66
1:C:459:VAL:HG12	1:D:123:VAL:HG22	1.77	0.66
1:G:132:GLN:HG2	3:G:891:HOH:O	1.96	0.66
1:E:291:LEU:CD1	1:E:291:LEU:HG	2.19	0.66
1:B:167:HIS:CE1	2:B:801:FAD:C8M	2.73	0.65
1:D:458:ALA:HA	1:D:461:GLN:HE21	1.61	0.65
1:H:417:MET:CE	1:H:420:GLN:NE2	2.60	0.64
1:C:341:ASN:HD21	1:C:343:ALA:HB3	1.62	0.64
1:C:607:GLU:O	1:C:611:GLN:NE2	2.31	0.64
1:H:417:MET:HA	1:H:417:MET:CE	2.27	0.64
1:A:541:MET:CE	1:A:545:LEU:HD23	2.27	0.63
1:G:97:GLN:HG3	1:G:250:PHE:CE2	2.32	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:167:HIS:NE2	2:G:801:FAD:C8	2.49	0.63
1:E:291:LEU:HD12	1:E:291:LEU:H	1.63	0.63
1:D:497:MET:HE1	3:D:1202:HOH:O	1.99	0.62
1:E:167:HIS:NE2	2:E:801:FAD:C8	2.57	0.62
1:D:541:MET:HE2	1:D:545:LEU:HD23	1.83	0.61
1:C:541:MET:HE2	1:C:545:LEU:HD23	1.81	0.61
1:F:541:MET:CE	3:F:925:HOH:O	2.47	0.61
1:E:421:GLU:CD	1:E:421:GLU:H	2.04	0.61
1:F:459:VAL:O	1:F:462:SER:HB3	2.00	0.61
1:C:81:ASP:OD1	1:C:81:ASP:C	2.37	0.61
1:C:50:VAL:HG13	1:C:313:ALA:HB2	1.81	0.61
1:E:291:LEU:CD1	1:E:291:LEU:H	2.14	0.60
1:A:167:HIS:NE2	2:A:801:FAD:HM81	2.02	0.60
1:D:497:MET:CE	3:D:1202:HOH:O	2.48	0.60
1:F:417:MET:HE3	1:F:417:MET:O	2.01	0.60
1:G:100:ILE:HD13	1:G:100:ILE:C	2.22	0.60
1:G:459:VAL:HG22	1:H:121:LEU:HD13	1.82	0.60
1:C:167:HIS:NE2	2:C:801:FAD:HM81	2.02	0.60
1:E:81:ASP:OD1	1:E:81:ASP:C	2.37	0.60
1:E:291:LEU:HD13	3:E:1365:HOH:O	2.01	0.60
1:B:417:MET:HE3	1:B:417:MET:HA	1.82	0.60
1:A:299:HIS:CD2	1:A:310:GLU:HG2	2.37	0.60
1:E:381:THR:C	1:E:382:ILE:HD12	2.23	0.59
1:H:132:GLN:HG2	3:H:1000:HOH:O	2.02	0.59
1:A:167:HIS:NE2	2:A:801:FAD:C8	2.57	0.59
1:A:393:VAL:H	1:A:417:MET:HE2	1.66	0.59
1:A:299:HIS:NE2	1:A:310:GLU:HG2	2.17	0.59
1:D:100:ILE:HD13	1:D:100:ILE:C	2.23	0.59
1:G:167:HIS:NE2	2:G:801:FAD:HM81	2.04	0.59
1:C:541:MET:CE	1:C:545:LEU:HD23	2.33	0.58
1:C:619:THR:O	1:C:619:THR:HG23	2.03	0.58
1:E:541:MET:HE3	1:E:545:LEU:HD23	1.85	0.58
1:B:538:PRO:HG2	1:D:538:PRO:HG2	1.85	0.58
1:G:132:GLN:CG	3:G:891:HOH:O	2.50	0.58
1:C:457:GLY:O	1:C:461:GLN:HG3	2.03	0.57
1:H:167:HIS:NE2	2:H:801:FAD:C8	2.61	0.57
1:C:121:LEU:HD13	1:D:459:VAL:CG2	2.33	0.57
1:F:81:ASP:C	1:F:81:ASP:OD1	2.41	0.57
1:G:459:VAL:HG12	1:H:123:VAL:HG22	1.87	0.57
1:A:459:VAL:HG12	1:B:123:VAL:HG22	1.86	0.57
1:H:417:MET:CE	1:H:420:GLN:HE21	2.18	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:VAL:HG13	1:A:313:ALA:HB2	1.86	0.57
1:F:167:HIS:CE1	2:F:801:FAD:C8M	2.75	0.56
1:E:382:ILE:HD12	1:E:382:ILE:N	2.20	0.56
1:D:167:HIS:CE1	2:D:801:FAD:C8M	2.76	0.56
1:D:541:MET:CE	1:D:545:LEU:HD23	2.35	0.56
1:C:285:ARG:CA	1:C:328:LEU:HD11	2.34	0.56
1:A:392:SER:HA	1:A:417:MET:HE1	1.88	0.56
1:F:167:HIS:NE2	2:F:801:FAD:HM81	2.02	0.56
1:A:541:MET:HE3	1:A:545:LEU:HD23	1.89	0.55
1:C:121:LEU:HD13	1:D:459:VAL:HG22	1.87	0.55
1:F:541:MET:HE3	1:F:545:LEU:HD23	1.89	0.55
1:D:50:VAL:HG13	1:D:313:ALA:HB2	1.88	0.55
1:F:459:VAL:O	1:F:462:SER:CB	2.55	0.54
1:C:121:LEU:HD12	1:D:458:ALA:O	2.06	0.54
1:F:541:MET:CE	1:F:545:LEU:HD23	2.36	0.54
1:C:167:HIS:NE2	2:C:801:FAD:C8	2.64	0.54
1:A:185:LYS:HG2	3:A:1080:HOH:O	2.08	0.53
1:A:45:ILE:C	1:A:45:ILE:HD12	2.28	0.53
1:G:459:VAL:O	1:G:462:SER:HB2	2.08	0.53
1:C:157:VAL:HG21	1:C:324:HIS:HE1	1.74	0.53
1:D:46:LYS:HE3	1:D:47:TYR:O	2.09	0.53
1:E:123:VAL:HG22	1:F:459:VAL:HG12	1.91	0.53
1:F:167:HIS:NE2	2:F:801:FAD:C8	2.66	0.53
1:D:457:GLY:O	1:D:461:GLN:HG3	2.09	0.52
1:E:47:TYR:O	1:E:313:ALA:HA	2.09	0.52
1:D:157:VAL:HG21	1:D:324:HIS:HE1	1.74	0.52
1:B:50:VAL:HG13	1:B:313:ALA:HB2	1.92	0.52
1:B:167:HIS:NE2	2:B:801:FAD:HM81	1.97	0.52
1:E:89:HIS:CE1	1:E:91:LYS:HG2	2.44	0.52
1:G:82:SER:O	1:H:81:ASP:HA	2.10	0.52
1:G:459:VAL:O	1:G:462:SER:CB	2.57	0.52
1:A:459:VAL:O	1:A:462:SER:CB	2.58	0.52
1:C:459:VAL:O	1:C:462:SER:CB	2.59	0.51
1:G:50:VAL:HG13	1:G:313:ALA:HB2	1.93	0.51
1:B:547:LEU:HD12	2:B:801:FAD:HM83	1.92	0.51
1:E:157:VAL:HG21	1:E:324:HIS:HE1	1.75	0.51
1:E:607:GLU:O	1:E:611:GLN:HG3	2.11	0.51
1:E:618:PHE:HD1	1:E:619:THR:N	2.10	0.50
1:E:346:PRO:HG2	1:E:350:PRO:HA	1.94	0.50
1:H:417:MET:CE	1:H:417:MET:CA	2.89	0.50
1:B:336:GLN:NE2	1:B:344:ASN:O	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:LEU:HD12	1:B:458:ALA:O	2.12	0.49
1:A:538:PRO:HG2	1:C:538:PRO:HG2	1.94	0.49
1:A:541:MET:HE3	3:A:1067:HOH:O	2.12	0.49
1:C:346:PRO:HG2	1:C:350:PRO:HA	1.93	0.49
1:F:478:GLU:CD	1:F:480:LYS:HE2	2.32	0.49
1:G:336:GLN:NE2	1:G:344:ASN:O	2.45	0.49
1:E:618:PHE:HD1	1:E:618:PHE:C	2.15	0.49
1:E:452:ASP:OD1	1:E:452:ASP:N	2.46	0.49
1:A:541:MET:HE2	1:A:545:LEU:HD23	1.92	0.49
1:C:218:ARG:HD2	3:C:911:HOH:O	2.11	0.49
1:H:284:GLU:C	1:H:328:LEU:CD1	2.81	0.49
1:H:452:ASP:O	1:H:453:ALA:C	2.51	0.49
1:H:619:THR:O	1:H:619:THR:CG2	2.61	0.49
1:H:50:VAL:HG13	1:H:313:ALA:HB2	1.95	0.49
1:F:47:TYR:O	1:F:313:ALA:HA	2.13	0.49
1:B:100:ILE:HD13	1:B:100:ILE:C	2.33	0.49
1:B:459:VAL:O	1:B:462:SER:CB	2.60	0.49
1:D:167:HIS:NE2	2:D:801:FAD:C8	2.65	0.49
1:B:547:LEU:CD1	2:B:801:FAD:HM83	2.43	0.49
1:C:459:VAL:CG1	1:D:123:VAL:HG22	2.43	0.49
1:H:459:VAL:O	1:H:462:SER:CB	2.61	0.48
1:D:490:LYS:HD3	1:D:491:ILE:HD13	1.95	0.48
1:G:541:MET:HE2	1:G:545:LEU:HD23	1.95	0.48
1:A:457:GLY:H	1:A:460:GLN:HE21	1.60	0.48
1:G:457:GLY:O	1:G:461:GLN:HG3	2.13	0.48
1:B:417:MET:HB3	1:B:417:MET:HE2	1.68	0.48
1:D:167:HIS:NE2	2:D:801:FAD:HM81	2.10	0.48
1:E:618:PHE:C	1:E:618:PHE:CD1	2.87	0.47
1:E:50:VAL:HG13	1:E:313:ALA:HB2	1.96	0.47
1:F:417:MET:HE3	1:F:417:MET:CA	2.44	0.47
1:E:385:THR:O	1:E:388:GLU:HB3	2.15	0.47
1:G:547:LEU:CD1	2:G:801:FAD:HM83	2.44	0.47
1:H:81:ASP:O	1:H:90:LYS:HE2	2.14	0.47
1:A:547:LEU:HD12	2:A:801:FAD:HM83	1.97	0.47
1:F:121:LEU:CD2	1:G:121:LEU:CD2	2.93	0.47
1:E:385:THR:O	1:E:388:GLU:CB	2.63	0.47
1:H:341:ASN:C	1:H:341:ASN:HD22	2.18	0.47
1:B:452:ASP:O	1:B:453:ALA:C	2.54	0.47
1:H:542:LYS:CE	3:H:1138:HOH:O	2.62	0.47
3:G:1107:HOH:O	1:H:112:MET:HB3	2.16	0.46
1:D:81:ASP:C	1:D:81:ASP:OD1	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:MET:HE3	1:D:95:GLU:HG3	1.96	0.46
1:C:618:PHE:HD1	1:C:618:PHE:C	2.18	0.46
1:D:153:SER:OG	1:D:542:LYS:CG	2.64	0.46
1:D:547:LEU:HD12	2:D:801:FAD:HM83	1.98	0.46
1:F:50:VAL:HG12	1:F:73:ALA:HB3	1.98	0.46
1:F:218:ARG:HG3	1:F:430:ASP:OD2	2.16	0.46
1:A:123:VAL:HG22	1:B:459:VAL:HG12	1.98	0.46
1:A:497:MET:CE	3:A:1109:HOH:O	2.65	0.45
1:C:47:TYR:O	1:C:313:ALA:HA	2.15	0.45
1:E:218:ARG:HD2	3:E:1194:HOH:O	2.16	0.45
1:F:324:HIS:HD2	1:F:327:GLN:OE1	1.99	0.45
1:G:341:ASN:HD21	1:G:343:ALA:HB3	1.80	0.45
1:E:541:MET:HE3	1:E:545:LEU:CD2	2.45	0.45
1:H:346:PRO:HG2	1:H:350:PRO:HA	1.98	0.45
1:B:81:ASP:OD1	1:B:81:ASP:O	2.33	0.45
1:B:169:THR:HG22	1:B:169:THR:O	2.17	0.45
1:C:336:GLN:NE2	1:C:344:ASN:O	2.49	0.45
1:A:497:MET:HE2	3:A:1109:HOH:O	2.17	0.45
1:C:618:PHE:C	1:C:618:PHE:CD1	2.89	0.45
1:G:547:LEU:HD12	2:G:801:FAD:HM83	1.99	0.45
1:A:459:VAL:O	1:A:462:SER:HB3	2.16	0.45
1:E:47:TYR:CD2	1:E:73:ALA:HB2	2.52	0.45
1:H:417:MET:HE1	1:H:420:GLN:NE2	2.30	0.45
1:A:393:VAL:H	1:A:417:MET:CE	2.29	0.45
1:B:294:GLU:OE1	1:B:296:GLU:OE2	2.35	0.45
1:C:343:ALA:C	1:C:344:ASN:HD22	2.20	0.45
1:F:121:LEU:HD21	1:G:121:LEU:CD2	2.47	0.45
1:H:459:VAL:O	1:H:462:SER:HB3	2.17	0.45
1:A:100:ILE:HG23	1:A:101:ASP:N	2.32	0.45
1:B:167:HIS:CD2	2:B:801:FAD:C8	3.00	0.45
1:C:537:LEU:HB3	1:C:538:PRO:HD2	1.98	0.45
1:E:342:PRO:C	1:E:344:ASN:H	2.20	0.45
1:G:363:PHE:HA	1:G:471:TRP:O	2.17	0.45
1:D:100:ILE:CD1	1:D:453:ALA:HA	2.47	0.44
1:G:541:MET:CE	1:G:545:LEU:HD23	2.48	0.44
1:B:265:ARG:HA	1:B:266:PRO:C	2.38	0.44
1:H:542:LYS:HE2	3:H:1138:HOH:O	2.17	0.44
1:F:610:LYS:NZ	3:F:976:HOH:O	2.48	0.44
1:G:312:LYS:HE3	3:G:941:HOH:O	2.17	0.44
1:G:47:TYR:O	1:G:313:ALA:HA	2.17	0.44
1:H:126:LEU:HD12	1:H:132:GLN:HG3	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:541:MET:HE3	3:H:962:HOH:O	2.18	0.44
1:A:541:MET:HE3	1:A:545:LEU:CD2	2.47	0.44
1:C:458:ALA:O	1:D:121:LEU:HD12	2.17	0.44
1:F:97:GLN:HG3	1:F:250:PHE:CD2	2.53	0.44
1:F:121:LEU:CD2	1:G:121:LEU:HD21	2.48	0.44
1:E:291:LEU:HD12	1:E:291:LEU:N	2.29	0.43
1:B:185:LYS:CB	1:B:185:LYS:NZ	2.81	0.43
1:H:81:ASP:OD1	1:H:81:ASP:C	2.51	0.43
1:D:47:TYR:O	1:D:313:ALA:HA	2.18	0.43
1:B:100:ILE:HD13	1:B:100:ILE:O	2.18	0.43
1:B:218:ARG:HD2	3:B:838:HOH:O	2.18	0.43
1:F:564:CYS:HG	1:F:573:PHE:HE2	1.66	0.43
1:G:104:VAL:HG22	1:G:453:ALA:HB1	2.00	0.43
1:B:45:ILE:H	1:B:45:ILE:CD1	2.07	0.43
1:E:167:HIS:CD2	2:E:801:FAD:C8	3.01	0.43
1:F:336:GLN:HB2	1:F:346:PRO:HG3	2.00	0.43
1:A:44:ASP:OD2	1:A:71:LYS:NZ	2.41	0.43
1:A:47:TYR:O	1:A:313:ALA:HA	2.19	0.43
1:G:167:HIS:CD2	2:G:801:FAD:C8	3.02	0.43
1:E:284:GLU:C	1:E:328:LEU:CD1	2.87	0.43
1:A:293:SER:HA	1:A:574:GLY:O	2.19	0.43
1:H:173:PRO:HG2	1:H:592:ALA:HB1	2.00	0.43
1:E:153:SER:OG	1:E:542:LYS:HG2	2.19	0.42
1:H:45:ILE:C	1:H:45:ILE:HD12	2.39	0.42
1:D:541:MET:CE	1:D:545:LEU:CD2	2.97	0.42
1:G:167:HIS:CD2	1:G:167:HIS:C	2.93	0.42
1:A:341:ASN:HA	1:A:342:PRO:HD2	1.89	0.42
1:E:380:MET:CB	1:E:382:ILE:HD11	2.49	0.42
1:G:537:LEU:HB3	1:G:538:PRO:HD2	2.00	0.42
1:H:541:MET:CE	1:H:545:LEU:HD23	2.49	0.42
1:A:218:ARG:HD2	3:A:906:HOH:O	2.19	0.42
1:B:541:MET:HE1	3:B:964:HOH:O	2.11	0.42
1:D:284:GLU:C	1:D:328:LEU:CD1	2.87	0.42
1:G:201:LYS:HE2	1:G:205:TYR:OH	2.20	0.42
1:G:459:VAL:CG1	1:H:123:VAL:HG22	2.48	0.42
1:D:336:GLN:NE2	1:D:344:ASN:O	2.53	0.42
1:F:417:MET:HE3	1:F:417:MET:C	2.39	0.42
1:B:121:LEU:CD2	1:C:121:LEU:CD2	2.98	0.42
1:C:459:VAL:O	1:C:462:SER:HB3	2.20	0.42
1:D:185:LYS:HE3	1:D:557:PHE:CD2	2.55	0.42
1:D:299:HIS:CE1	1:D:310:GLU:HG3	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:478:GLU:CD	1:H:480:LYS:HE2	2.39	0.42
1:F:293:SER:HA	1:F:574:GLY:O	2.20	0.42
1:A:81:ASP:O	1:A:90:LYS:HE2	2.20	0.41
1:D:284:GLU:O	1:D:328:LEU:CD1	2.68	0.41
1:D:564:CYS:HG	1:D:573:PHE:HE2	1.68	0.41
1:A:547:LEU:CD1	2:A:801:FAD:HM83	2.51	0.41
1:D:215:GLU:O	1:D:411:LYS:NZ	2.53	0.41
1:G:393:VAL:O	1:G:413:LYS:HE2	2.20	0.41
1:F:383:ARG:O	1:F:391:TYR:HA	2.20	0.41
1:G:97:GLN:HG3	1:G:250:PHE:CD2	2.56	0.41
1:A:341:ASN:C	1:A:341:ASN:HD22	2.24	0.41
1:E:121:LEU:HD12	1:F:458:ALA:O	2.21	0.41
1:E:285:ARG:HA	1:E:328:LEU:CD1	2.51	0.41
1:H:336:GLN:OE1	1:H:340:PRO:HA	2.21	0.41
1:H:459:VAL:CG1	1:H:460:GLN:N	2.83	0.41
1:E:121:LEU:CD2	1:H:121:LEU:HD21	2.51	0.41
1:E:291:LEU:CD1	1:E:291:LEU:N	2.83	0.41
1:F:157:VAL:HG21	1:F:324:HIS:HE1	1.85	0.41
1:F:181:PRO:HG3	1:F:587:PRO:HD2	2.03	0.41
1:G:481:GLU:CG	3:G:970:HOH:O	2.48	0.41
1:H:417:MET:O	1:H:417:MET:HE2	2.21	0.41
1:B:558:ASP:OD2	1:B:561:GLU:HG3	2.21	0.41
1:C:165:SER:HA	1:C:168:TRP:CD1	2.56	0.41
1:C:265:ARG:HA	1:C:266:PRO:C	2.41	0.41
1:G:104:VAL:HG21	1:G:454:PHE:C	2.41	0.41
1:G:478:GLU:CD	1:G:480:LYS:HE2	2.40	0.41
1:H:547:LEU:HD12	2:H:801:FAD:HM83	2.02	0.41
1:A:167:HIS:CD2	1:A:167:HIS:C	2.95	0.40
1:D:284:GLU:O	1:D:328:LEU:HD12	2.22	0.40
1:H:180:ARG:HA	1:H:181:PRO:HD3	1.84	0.40
1:E:532:PHE:CZ	1:E:538:PRO:HG3	2.57	0.40
1:A:407:TRP:O	1:A:411:LYS:HG3	2.20	0.40
1:B:459:VAL:O	1:B:462:SER:HB2	2.20	0.40
1:E:167:HIS:CD2	1:E:167:HIS:C	2.95	0.40
1:E:459:VAL:HG12	1:F:123:VAL:HG22	2.02	0.40
1:D:452:ASP:OD1	1:D:452:ASP:N	2.54	0.40
1:D:460:GLN:C	1:D:462:SER:H	2.22	0.40
1:B:121:LEU:HD23	3:B:1050:HOH:O	2.20	0.40
1:D:532:PHE:CZ	1:D:538:PRO:HG3	2.57	0.40
1:G:159:ARG:HA	2:G:801:FAD:O2B	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	575/623 (92%)	557 (97%)	17 (3%)	1 (0%)	47	30
1	B	575/623 (92%)	555 (96%)	18 (3%)	2 (0%)	41	24
1	C	575/623 (92%)	561 (98%)	14 (2%)	0	100	100
1	D	575/623 (92%)	560 (97%)	15 (3%)	0	100	100
1	E	575/623 (92%)	558 (97%)	17 (3%)	0	100	100
1	F	575/623 (92%)	562 (98%)	13 (2%)	0	100	100
1	G	575/623 (92%)	558 (97%)	15 (3%)	2 (0%)	41	24
1	H	575/623 (92%)	557 (97%)	18 (3%)	0	100	100
All	All	4600/4984 (92%)	4468 (97%)	127 (3%)	5 (0%)	51	33

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	389	LEU
1	G	453	ALA
1	A	44	ASP
1	B	461	GLN
1	G	45	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	505/542 (93%)	491 (97%)	14 (3%)	43	25

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	505/542 (93%)	494 (98%)	11 (2%)	52	34
1	C	505/542 (93%)	495 (98%)	10 (2%)	55	38
1	D	505/542 (93%)	493 (98%)	12 (2%)	49	31
1	E	505/542 (93%)	496 (98%)	9 (2%)	59	43
1	F	505/542 (93%)	489 (97%)	16 (3%)	39	20
1	G	505/542 (93%)	495 (98%)	10 (2%)	55	38
1	H	505/542 (93%)	493 (98%)	12 (2%)	49	31
All	All	4040/4336 (93%)	3946 (98%)	94 (2%)	50	33

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	MET
1	A	100	ILE
1	A	168	TRP
1	A	185	LYS
1	A	206	PHE
1	A	312	LYS
1	A	341	ASN
1	A	344	ASN
1	A	347	GLU
1	A	385	THR
1	A	450	HIS
1	A	461	GLN
1	A	490	LYS
1	A	496	ASN
1	B	45	ILE
1	B	100	ILE
1	B	112	MET
1	B	168	TRP
1	B	178	GLU
1	B	185	LYS
1	B	385	THR
1	B	408	TRP
1	B	417	MET
1	B	450	HIS
1	B	490	LYS
1	C	112	MET
1	C	168	TRP
1	C	185	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	341	ASN
1	C	344	ASN
1	C	403	LYS
1	C	450	HIS
1	C	490	LYS
1	C	593	ASN
1	C	618	PHE
1	D	100	ILE
1	D	112	MET
1	D	168	TRP
1	D	178	GLU
1	D	206	PHE
1	D	299	HIS
1	D	341	ASN
1	D	385	THR
1	D	403	LYS
1	D	450	HIS
1	D	593	ASN
1	D	618	PHE
1	E	168	TRP
1	E	185	LYS
1	E	206	PHE
1	E	291	LEU
1	E	385	THR
1	E	421	GLU
1	E	450	HIS
1	E	455	SER
1	E	618	PHE
1	F	100	ILE
1	F	112	MET
1	F	132	GLN
1	F	168	TRP
1	F	206	PHE
1	F	272	GLU
1	F	328	LEU
1	F	341	ASN
1	F	385	THR
1	F	408	TRP
1	F	417	MET
1	F	450	HIS
1	F	461	GLN
1	F	576	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	593	ASN
1	F	618	PHE
1	G	45	ILE
1	G	100	ILE
1	G	168	TRP
1	G	385	THR
1	G	408	TRP
1	G	450	HIS
1	G	496	ASN
1	G	593	ASN
1	G	618	PHE
1	G	619	THR
1	H	100	ILE
1	H	132	GLN
1	H	168	TRP
1	H	185	LYS
1	H	206	PHE
1	H	341	ASN
1	H	400	SER
1	H	413	LYS
1	H	417	MET
1	H	450	HIS
1	H	459	VAL
1	H	618	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	341	ASN
1	A	344	ASN
1	A	460	GLN
1	A	461	GLN
1	B	341	ASN
1	B	460	GLN
1	C	341	ASN
1	C	344	ASN
1	C	611	GLN
1	D	299	HIS
1	D	324	HIS
1	D	341	ASN
1	D	460	GLN
1	D	461	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	341	ASN
1	E	460	GLN
1	E	461	GLN
1	E	611	GLN
1	F	324	HIS
1	F	341	ASN
1	F	460	GLN
1	F	461	GLN
1	G	263	GLN
1	G	324	HIS
1	G	341	ASN
1	G	460	GLN
1	H	263	GLN
1	H	341	ASN
1	H	460	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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
2	FAD	C	801	1	53,58,58	1.48	10 (18%)	68,89,89	1.82	18 (26%)
2	FAD	A	801	1	53,58,58	1.49	11 (20%)	68,89,89	1.68	15 (22%)
2	FAD	D	801	1	53,58,58	1.26	5 (9%)	68,89,89	1.90	21 (30%)
2	FAD	E	801	1	53,58,58	1.48	11 (20%)	68,89,89	1.67	12 (17%)
2	FAD	F	801	1	53,58,58	1.38	8 (15%)	68,89,89	1.75	16 (23%)
2	FAD	G	801	1	53,58,58	1.43	9 (16%)	68,89,89	1.69	14 (20%)
2	FAD	H	801	1	53,58,58	1.36	5 (9%)	68,89,89	1.54	14 (20%)
2	FAD	B	801	1	53,58,58	1.66	9 (16%)	68,89,89	2.08	18 (26%)

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	C	801	1	-	3/30/50/50	0/6/6/6
2	FAD	A	801	1	-	3/30/50/50	0/6/6/6
2	FAD	D	801	1	-	4/30/50/50	0/6/6/6
2	FAD	E	801	1	-	1/30/50/50	0/6/6/6
2	FAD	F	801	1	-	3/30/50/50	0/6/6/6
2	FAD	G	801	1	-	2/30/50/50	0/6/6/6
2	FAD	H	801	1	-	2/30/50/50	0/6/6/6
2	FAD	B	801	1	-	2/30/50/50	0/6/6/6

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	FAD	C4X-N5	4.85	1.40	1.30
2	B	801	FAD	C8A-N7A	-4.08	1.27	1.34
2	A	801	FAD	C4X-N5	3.76	1.38	1.30
2	B	801	FAD	O4B-C4B	-3.75	1.36	1.45
2	G	801	FAD	O4B-C1B	3.71	1.46	1.41
2	C	801	FAD	C4X-N5	3.59	1.37	1.30
2	E	801	FAD	O4B-C4B	-3.50	1.37	1.45
2	F	801	FAD	C6-C5X	3.44	1.45	1.40
2	H	801	FAD	C10-N1	3.40	1.40	1.33
2	B	801	FAD	C10-N1	3.32	1.40	1.33
2	B	801	FAD	C6-C5X	3.31	1.45	1.40
2	H	801	FAD	C2B-C1B	-3.28	1.48	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	FAD	C2B-C3B	-3.19	1.44	1.53
2	F	801	FAD	O3B-C3B	-3.15	1.35	1.43
2	G	801	FAD	C2B-C3B	-3.13	1.44	1.53
2	B	801	FAD	C2-N3	-3.10	1.31	1.39
2	E	801	FAD	C4X-N5	3.03	1.36	1.30
2	E	801	FAD	C5X-N5	-3.00	1.33	1.39
2	E	801	FAD	C2B-C3B	-2.98	1.45	1.53
2	D	801	FAD	C2B-C3B	-2.97	1.45	1.53
2	G	801	FAD	C6-C7	2.89	1.43	1.39
2	D	801	FAD	C4X-N5	2.88	1.36	1.30
2	A	801	FAD	O3B-C3B	-2.87	1.36	1.43
2	E	801	FAD	C6-C5X	2.84	1.44	1.40
2	C	801	FAD	C6-C5X	2.82	1.44	1.40
2	A	801	FAD	O4B-C4B	-2.76	1.38	1.45
2	D	801	FAD	C2A-N3A	2.74	1.36	1.32
2	E	801	FAD	C2-N3	-2.74	1.32	1.39
2	D	801	FAD	O4B-C4B	-2.74	1.38	1.45
2	A	801	FAD	C5'-C4'	2.71	1.55	1.51
2	F	801	FAD	C2B-C1B	-2.71	1.49	1.53
2	B	801	FAD	O4B-C1B	2.68	1.44	1.41
2	G	801	FAD	C2A-N3A	2.65	1.36	1.32
2	F	801	FAD	C2B-C3B	-2.63	1.46	1.53
2	C	801	FAD	O2B-C2B	-2.63	1.36	1.43
2	B	801	FAD	C2A-N1A	2.63	1.38	1.33
2	F	801	FAD	C4X-N5	2.62	1.35	1.30
2	A	801	FAD	O2B-C2B	-2.59	1.36	1.43
2	G	801	FAD	C4X-N5	2.58	1.35	1.30
2	A	801	FAD	C4-N3	-2.57	1.34	1.38
2	E	801	FAD	C10-N1	2.56	1.38	1.33
2	E	801	FAD	O2B-C2B	-2.55	1.37	1.43
2	H	801	FAD	C4X-N5	2.52	1.35	1.30
2	C	801	FAD	C2A-N1A	2.49	1.38	1.33
2	H	801	FAD	C2A-N1A	2.47	1.38	1.33
2	C	801	FAD	C2B-C3B	-2.47	1.46	1.53
2	B	801	FAD	C2B-C3B	-2.46	1.46	1.53
2	A	801	FAD	C2B-C1B	-2.46	1.50	1.53
2	A	801	FAD	C6-C5X	2.45	1.43	1.40
2	C	801	FAD	C5'-C4'	2.44	1.55	1.51
2	F	801	FAD	C10-N1	2.42	1.38	1.33
2	C	801	FAD	C10-N1	2.37	1.38	1.33
2	D	801	FAD	C10-N1	2.36	1.38	1.33
2	G	801	FAD	O4B-C4B	-2.35	1.39	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	801	FAD	C2A-N1A	2.33	1.38	1.33
2	A	801	FAD	O4B-C1B	2.31	1.44	1.41
2	A	801	FAD	C2-N1	-2.29	1.31	1.36
2	C	801	FAD	C4X-C10	-2.29	1.37	1.44
2	F	801	FAD	C5'-C4'	2.23	1.54	1.51
2	C	801	FAD	O4B-C1B	2.19	1.44	1.41
2	F	801	FAD	C2-N3	-2.18	1.33	1.39
2	G	801	FAD	C10-N1	2.16	1.37	1.33
2	E	801	FAD	C4X-C10	-2.13	1.37	1.44
2	C	801	FAD	C4-N3	2.12	1.42	1.38
2	E	801	FAD	O3B-C3B	-2.11	1.38	1.43
2	G	801	FAD	O2B-C2B	-2.04	1.38	1.43
2	G	801	FAD	PA-O1A	-2.04	1.43	1.50
2	H	801	FAD	C9-C8	2.00	1.42	1.39

All (128) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	FAD	N3A-C2A-N1A	-6.57	118.41	128.68
2	A	801	FAD	N3A-C2A-N1A	-5.65	119.85	128.68
2	B	801	FAD	C4-C4X-N5	5.28	125.75	118.23
2	C	801	FAD	N3A-C2A-N1A	-5.20	120.55	128.68
2	D	801	FAD	O3B-C3B-C4B	4.85	125.08	111.05
2	D	801	FAD	N3A-C2A-N1A	-4.73	121.29	128.68
2	E	801	FAD	C5A-C6A-N6A	4.71	127.51	120.35
2	C	801	FAD	C3B-C2B-C1B	4.69	108.04	100.98
2	G	801	FAD	N3A-C2A-N1A	-4.65	121.41	128.68
2	C	801	FAD	C5A-C6A-N6A	4.44	127.11	120.35
2	B	801	FAD	C5A-C6A-N6A	4.42	127.07	120.35
2	C	801	FAD	O3B-C3B-C4B	4.40	123.77	111.05
2	B	801	FAD	O3B-C3B-C4B	4.13	123.00	111.05
2	D	801	FAD	O4-C4-C4X	-4.13	115.65	126.60
2	F	801	FAD	C5A-C6A-N6A	4.05	126.50	120.35
2	B	801	FAD	O4-C4-C4X	-4.04	115.87	126.60
2	G	801	FAD	C5A-C6A-N6A	4.03	126.48	120.35
2	E	801	FAD	O4B-C4B-C3B	3.95	112.94	105.11
2	G	801	FAD	C4-C4X-N5	3.92	123.82	118.23
2	E	801	FAD	O3B-C3B-C4B	3.84	122.16	111.05
2	F	801	FAD	O3B-C3B-C4B	3.77	121.94	111.05
2	F	801	FAD	C4-C4X-N5	3.74	123.55	118.23
2	H	801	FAD	N3A-C2A-N1A	-3.70	122.89	128.68
2	F	801	FAD	N3A-C2A-N1A	-3.69	122.91	128.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	FAD	C8M-C8-C9	-3.67	112.71	119.49
2	H	801	FAD	O2B-C2B-C3B	3.66	123.68	111.82
2	F	801	FAD	O4-C4-C4X	-3.65	116.91	126.60
2	F	801	FAD	O2B-C2B-C3B	3.65	123.63	111.82
2	B	801	FAD	C10-C4X-N5	-3.61	117.20	124.86
2	B	801	FAD	C2A-N1A-C6A	3.59	124.89	118.75
2	C	801	FAD	O2-C2-N1	-3.54	115.96	121.83
2	F	801	FAD	C9A-C5X-N5	-3.52	118.60	122.43
2	B	801	FAD	O2B-C2B-C3B	3.50	123.14	111.82
2	H	801	FAD	O3B-C3B-C4B	3.46	121.07	111.05
2	A	801	FAD	C4-N3-C2	3.43	131.98	125.64
2	D	801	FAD	C3B-C2B-C1B	3.43	106.14	100.98
2	G	801	FAD	O3B-C3B-C4B	3.33	120.67	111.05
2	G	801	FAD	O2B-C2B-C3B	3.32	122.56	111.82
2	G	801	FAD	C2B-C3B-C4B	3.30	109.05	102.64
2	F	801	FAD	C2B-C3B-C4B	3.30	109.05	102.64
2	B	801	FAD	C10-N1-C2	3.21	123.32	116.90
2	E	801	FAD	C3B-C2B-C1B	3.17	105.75	100.98
2	E	801	FAD	N3A-C2A-N1A	-3.15	123.76	128.68
2	C	801	FAD	O4'-C4'-C3'	3.14	116.74	109.10
2	G	801	FAD	O4'-C4'-C3'	3.09	116.61	109.10
2	E	801	FAD	C10-N1-C2	3.08	123.06	116.90
2	A	801	FAD	C5A-C6A-N6A	3.08	125.03	120.35
2	A	801	FAD	O2B-C2B-C3B	3.07	121.76	111.82
2	A	801	FAD	C10-N1-C2	3.06	123.03	116.90
2	D	801	FAD	O4B-C4B-C3B	3.04	111.13	105.11
2	D	801	FAD	O2B-C2B-C3B	2.98	121.45	111.82
2	G	801	FAD	C2A-N1A-C6A	2.95	123.80	118.75
2	B	801	FAD	O4-C4-N3	2.94	125.76	120.12
2	F	801	FAD	O4B-C4B-C5B	2.85	118.76	109.37
2	A	801	FAD	N3-C2-N1	-2.85	113.78	119.38
2	D	801	FAD	O4B-C4B-C5B	2.85	118.76	109.37
2	H	801	FAD	C5A-C6A-N6A	2.84	124.67	120.35
2	F	801	FAD	C2A-N1A-C6A	2.79	123.53	118.75
2	G	801	FAD	C5A-C6A-N1A	-2.79	114.03	120.35
2	D	801	FAD	O4'-C4'-C3'	2.73	115.74	109.10
2	B	801	FAD	C7M-C7-C6	-2.71	114.47	119.49
2	B	801	FAD	C4X-C10-N10	2.70	120.42	116.48
2	A	801	FAD	C2A-N1A-C6A	2.70	123.36	118.75
2	D	801	FAD	C4-C4X-N5	2.69	122.06	118.23
2	E	801	FAD	O2B-C2B-C3B	2.66	120.44	111.82
2	D	801	FAD	C5A-C6A-N6A	2.66	124.39	120.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	FAD	O2A-PA-O1A	2.65	125.34	112.24
2	D	801	FAD	C4A-C5A-N7A	-2.63	106.66	109.40
2	A	801	FAD	O3B-C3B-C4B	2.62	118.62	111.05
2	H	801	FAD	O4B-C1B-C2B	2.61	110.75	106.93
2	E	801	FAD	O2B-C2B-C1B	2.60	120.46	110.85
2	E	801	FAD	C7M-C7-C6	-2.57	114.74	119.49
2	H	801	FAD	O4'-C4'-C3'	2.57	115.35	109.10
2	H	801	FAD	C2B-C3B-C4B	2.56	107.62	102.64
2	D	801	FAD	O4-C4-N3	2.55	125.00	120.12
2	D	801	FAD	C2A-N1A-C6A	2.53	123.09	118.75
2	E	801	FAD	O2A-PA-O1A	2.50	124.62	112.24
2	A	801	FAD	O2'-C2'-C3'	2.50	115.17	109.10
2	H	801	FAD	C9-C8-C7	2.49	123.24	119.67
2	A	801	FAD	O4'-C4'-C3'	2.48	115.12	109.10
2	H	801	FAD	O2-C2-N1	-2.46	117.74	121.83
2	E	801	FAD	O4'-C4'-C5'	2.44	115.41	109.92
2	C	801	FAD	O2B-C2B-C1B	2.40	119.73	110.85
2	C	801	FAD	C9A-C5X-N5	-2.40	119.82	122.43
2	H	801	FAD	O2'-C2'-C3'	2.40	114.94	109.10
2	G	801	FAD	O4-C4-C4X	-2.38	120.29	126.60
2	B	801	FAD	C4X-C10-N1	-2.37	119.23	124.73
2	C	801	FAD	C6-C5X-C9A	2.36	122.28	118.94
2	B	801	FAD	O4B-C4B-C3B	2.35	109.76	105.11
2	F	801	FAD	C6-C7-C8	-2.34	116.32	119.67
2	D	801	FAD	C4-N3-C2	-2.33	121.33	125.64
2	B	801	FAD	C7M-C7-C8	2.32	125.50	120.74
2	F	801	FAD	O2A-PA-O1A	2.32	123.71	112.24
2	H	801	FAD	O4B-C4B-C5B	2.32	117.00	109.37
2	G	801	FAD	C6-C5X-C9A	2.31	122.21	118.94
2	D	801	FAD	C4X-C10-N10	2.31	119.86	116.48
2	E	801	FAD	O2-C2-N3	2.31	123.13	118.65
2	D	801	FAD	C1'-N10-C9A	2.29	124.33	120.51
2	B	801	FAD	O2A-PA-O1A	2.29	123.58	112.24
2	C	801	FAD	O4B-C1B-C2B	-2.29	103.58	106.93
2	D	801	FAD	C4X-C4-N3	2.28	118.98	113.19
2	F	801	FAD	C5X-C9A-N10	2.27	120.30	117.95
2	H	801	FAD	C8M-C8-C9	-2.26	115.30	119.49
2	A	801	FAD	C9A-C9-C8	2.25	123.84	119.30
2	A	801	FAD	C2B-C3B-C4B	2.25	107.02	102.64
2	G	801	FAD	C5'-C4'-C3'	-2.23	107.89	112.20
2	F	801	FAD	C5A-C6A-N1A	-2.21	115.35	120.35
2	G	801	FAD	C8M-C8-C9	-2.19	115.45	119.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	FAD	C9-C8-C7	2.18	122.80	119.67
2	C	801	FAD	C4-C4X-C10	2.18	120.46	116.79
2	F	801	FAD	O4B-C1B-C2B	2.17	110.10	106.93
2	C	801	FAD	C5'-C4'-C3'	-2.17	108.01	112.20
2	F	801	FAD	O2P-P-O1P	2.17	122.96	112.24
2	H	801	FAD	C6-C7-C8	-2.17	116.56	119.67
2	D	801	FAD	C7M-C7-C6	-2.16	115.50	119.49
2	C	801	FAD	O2B-C2B-C3B	2.13	118.72	111.82
2	C	801	FAD	O2P-P-O1P	2.13	122.78	112.24
2	A	801	FAD	O4-C4-N3	2.13	124.20	120.12
2	A	801	FAD	C5X-C9A-N10	2.12	120.15	117.95
2	G	801	FAD	O4B-C4B-C5B	2.10	116.27	109.37
2	B	801	FAD	C5A-C6A-N1A	-2.08	115.63	120.35
2	A	801	FAD	O2-C2-N3	2.08	122.70	118.65
2	B	801	FAD	C3B-C2B-C1B	2.06	104.09	100.98
2	C	801	FAD	O5'-C5'-C4'	-2.06	103.87	109.36
2	C	801	FAD	O4-C4-N3	-2.03	116.23	120.12
2	H	801	FAD	C6-C5X-C9A	2.01	121.79	118.94
2	C	801	FAD	C4A-C5A-N7A	-2.01	107.31	109.40
2	D	801	FAD	C10-N1-C2	2.00	120.91	116.90

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	FAD	PA-O3P-P-O5'
2	D	801	FAD	PA-O3P-P-O5'
2	F	801	FAD	PA-O3P-P-O5'
2	B	801	FAD	PA-O3P-P-O5'
2	C	801	FAD	PA-O3P-P-O5'
2	G	801	FAD	PA-O3P-P-O5'
2	H	801	FAD	PA-O3P-P-O5'
2	D	801	FAD	P-O3P-PA-O1A
2	A	801	FAD	P-O3P-PA-O2A
2	C	801	FAD	P-O3P-PA-O2A
2	F	801	FAD	P-O3P-PA-O2A
2	F	801	FAD	O4B-C4B-C5B-O5B
2	A	801	FAD	O4B-C4B-C5B-O5B
2	D	801	FAD	P-O3P-PA-O2A
2	B	801	FAD	O4B-C4B-C5B-O5B
2	C	801	FAD	O4B-C4B-C5B-O5B
2	D	801	FAD	O4B-C4B-C5B-O5B

Continued on next page...

Continued from previous page...

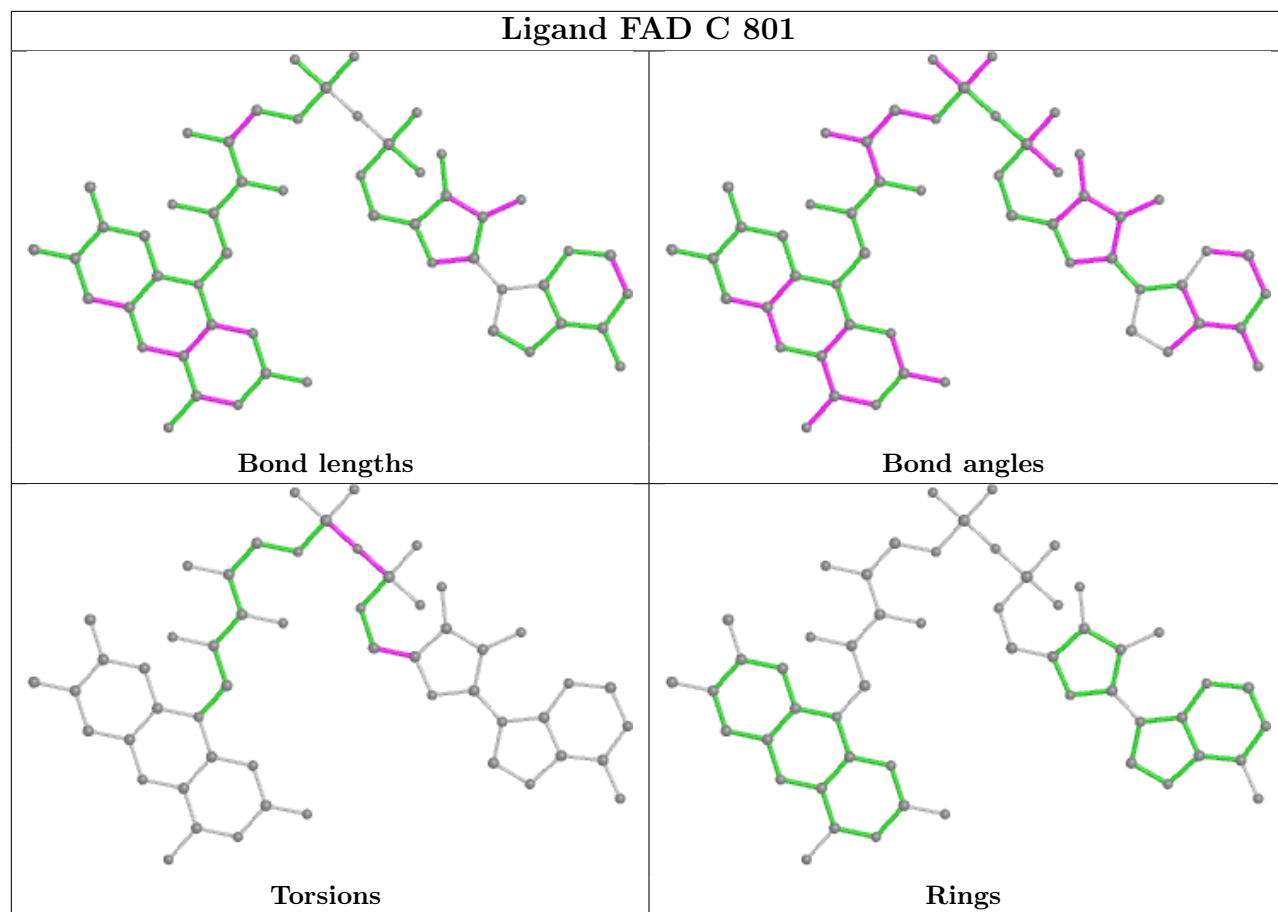
Mol	Chain	Res	Type	Atoms
2	E	801	FAD	O4B-C4B-C5B-O5B
2	G	801	FAD	O4B-C4B-C5B-O5B
2	H	801	FAD	O4B-C4B-C5B-O5B

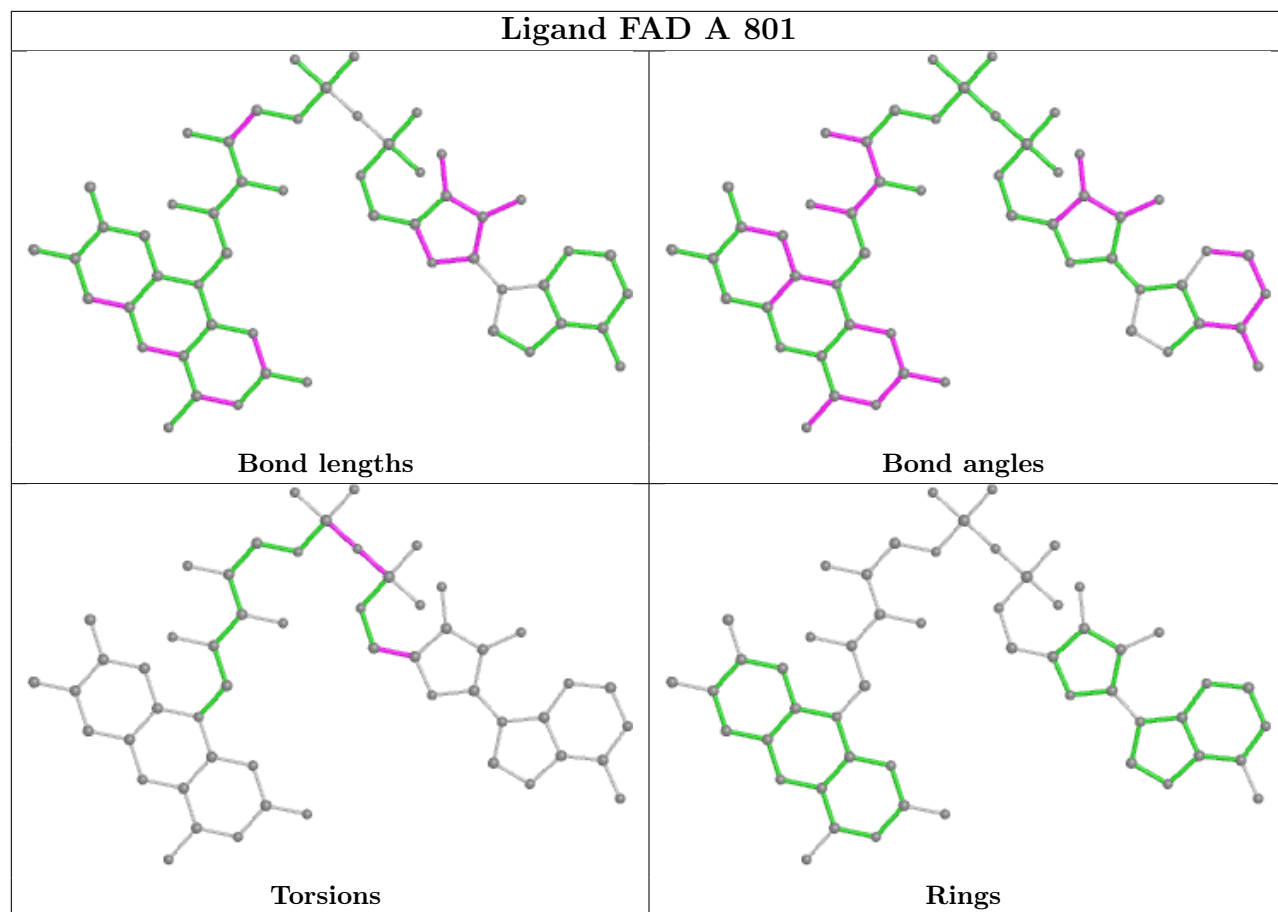
There are no ring outliers.

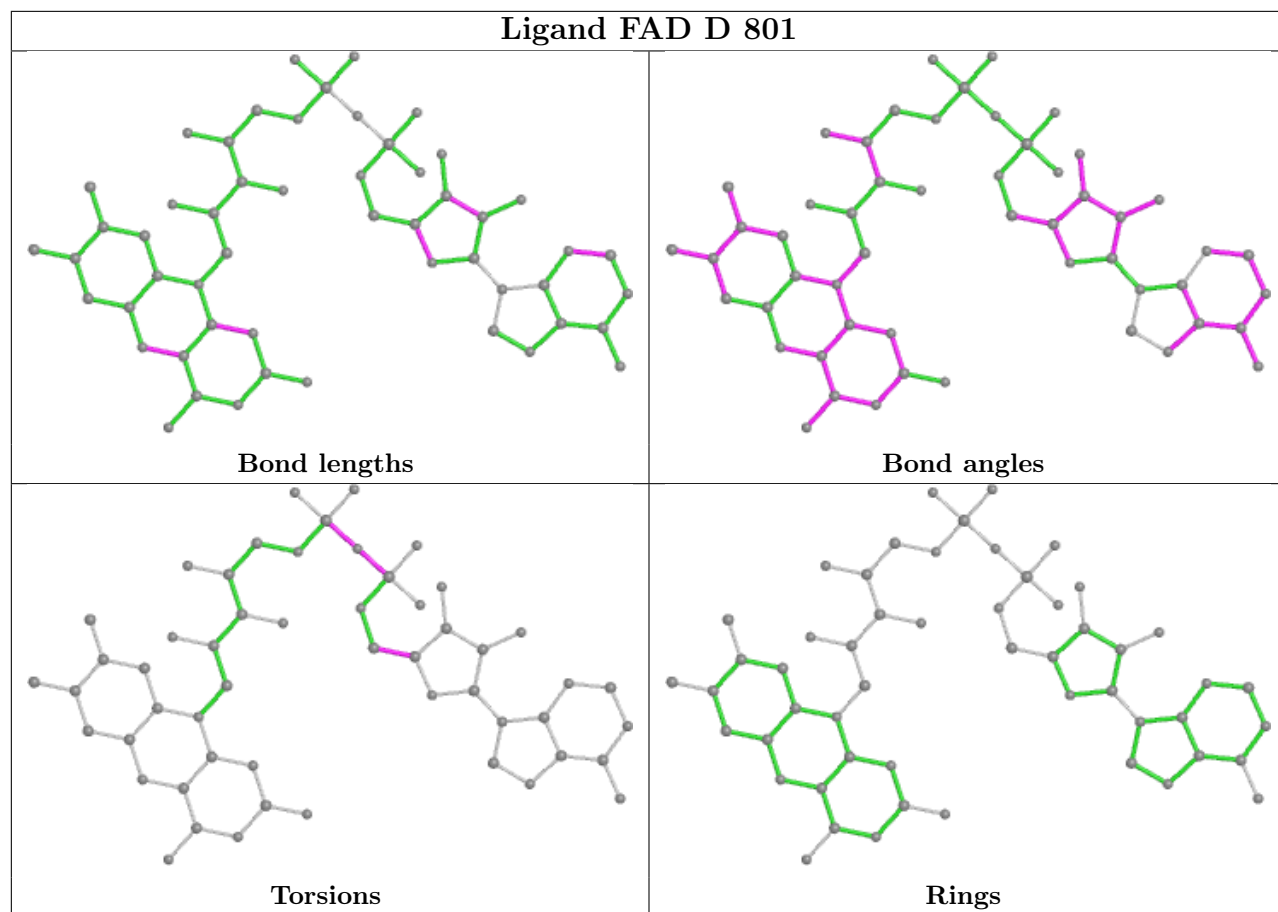
8 monomers are involved in 68 short contacts:

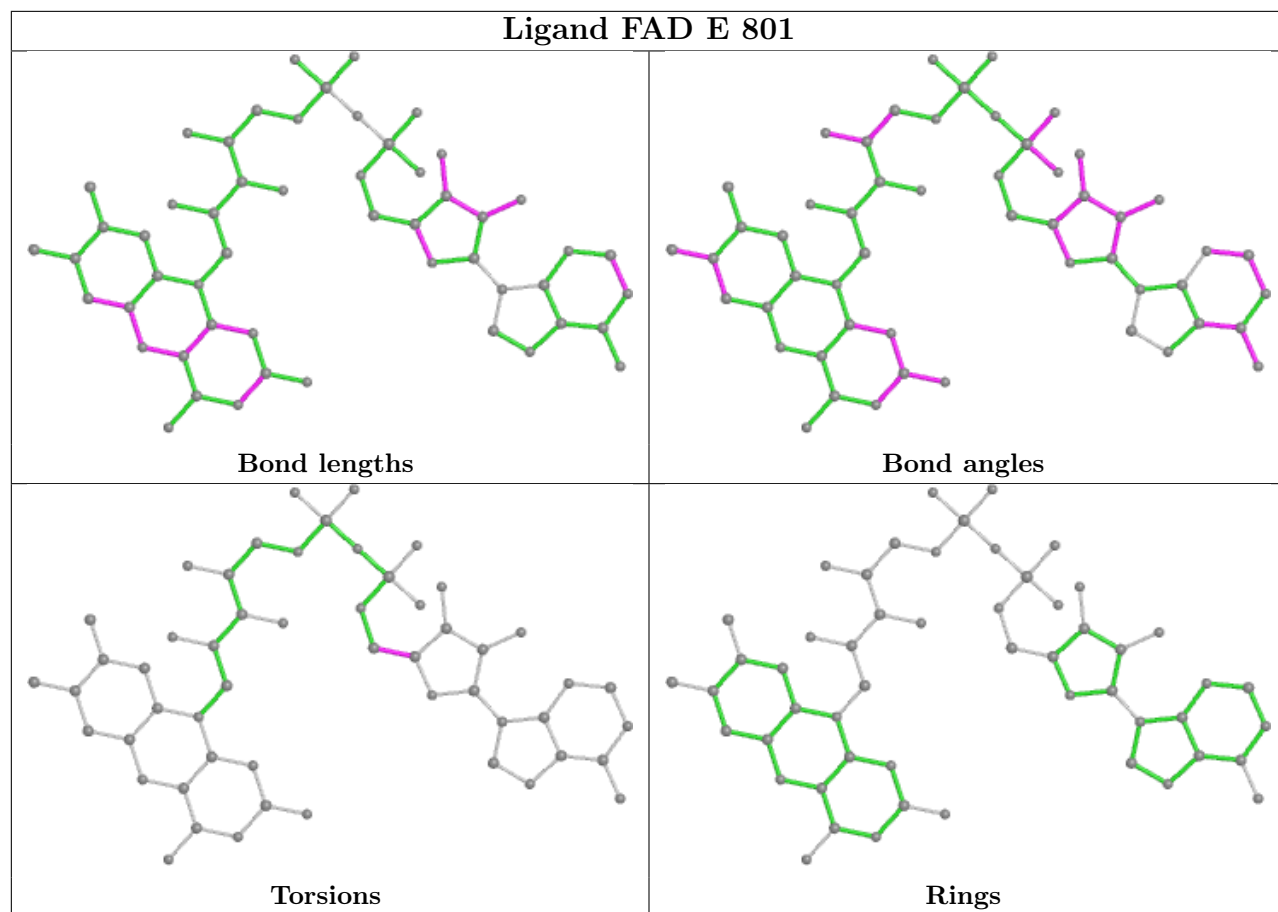
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	801	FAD	4	0
2	A	801	FAD	11	0
2	D	801	FAD	10	0
2	E	801	FAD	5	0
2	F	801	FAD	8	0
2	G	801	FAD	13	0
2	H	801	FAD	5	0
2	B	801	FAD	12	0

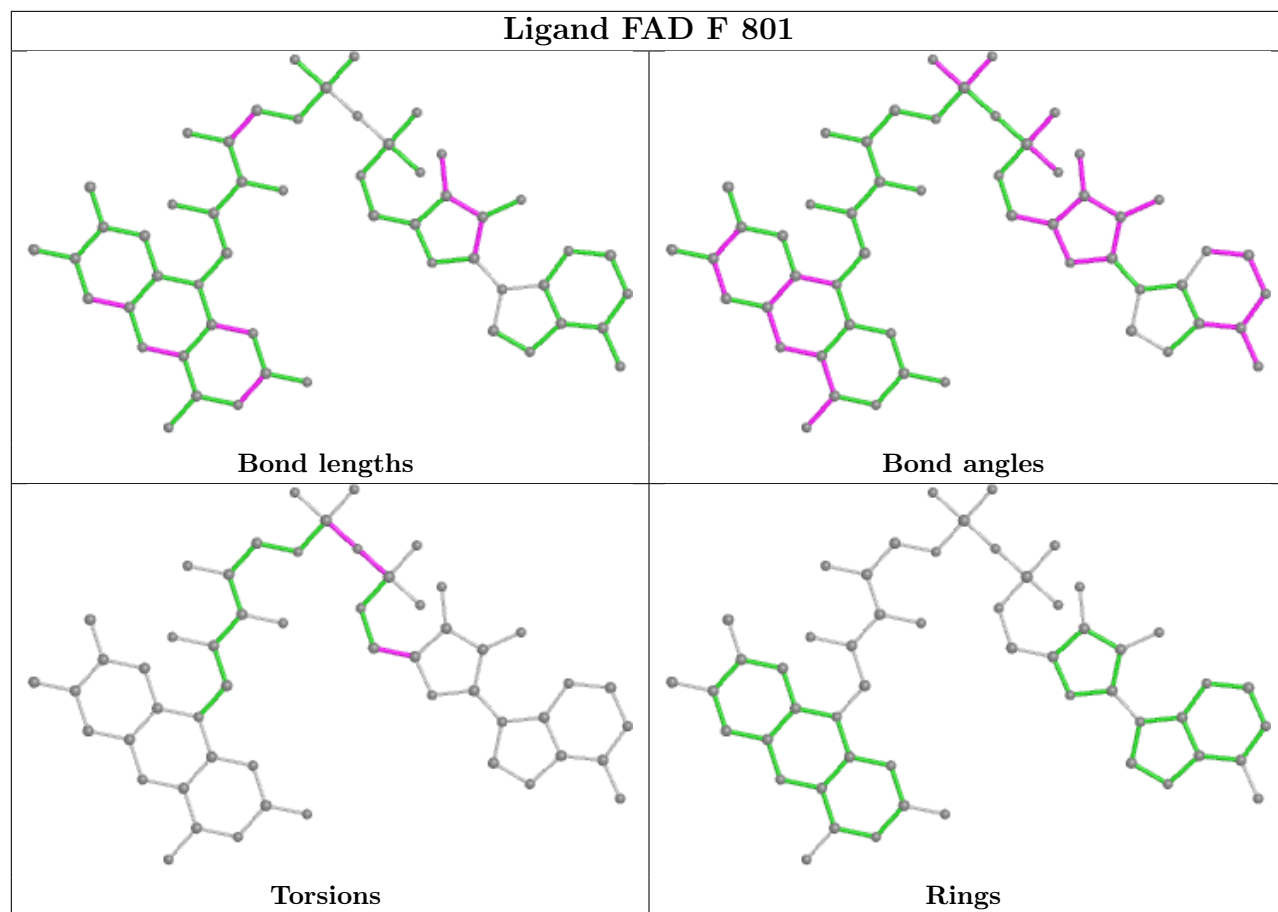
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

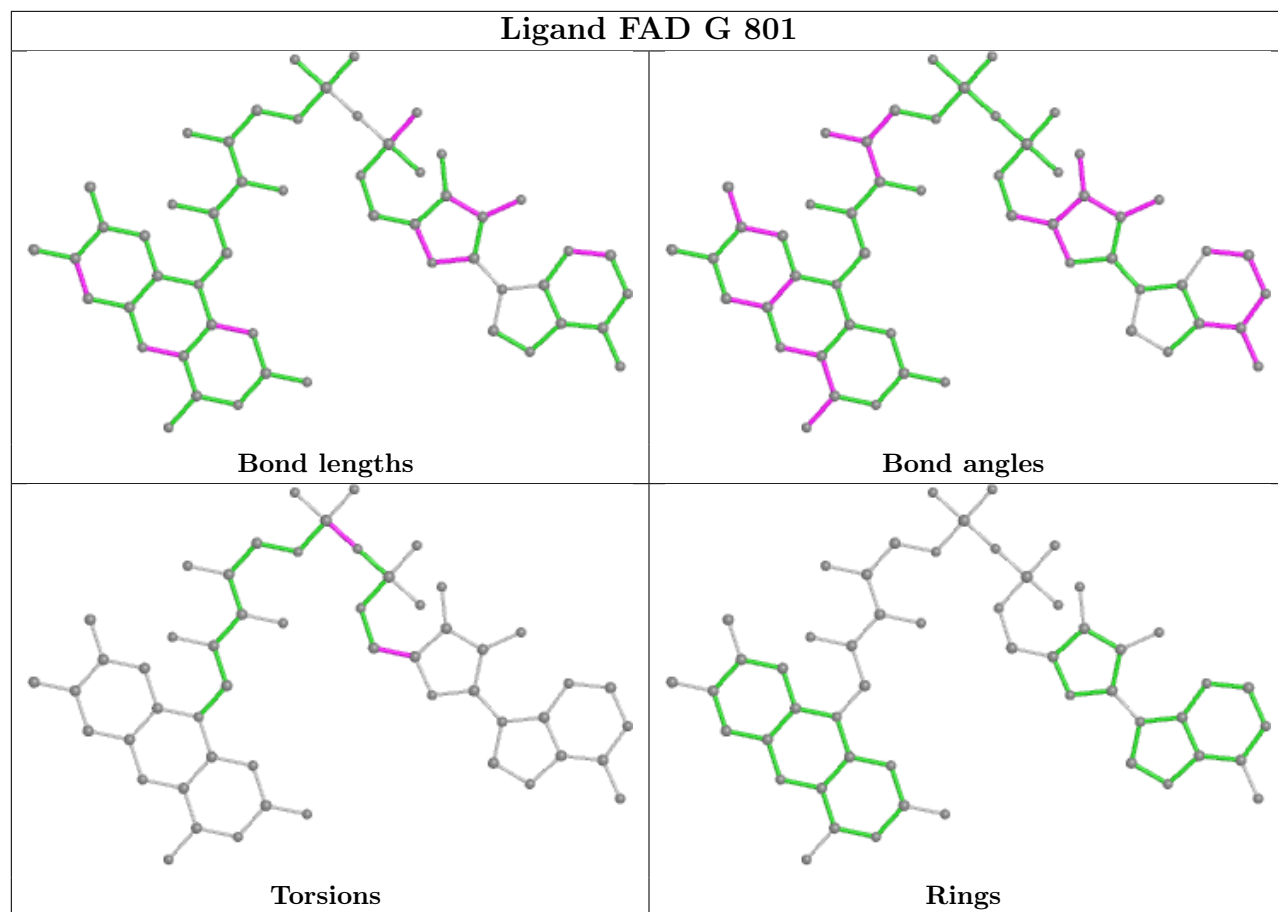


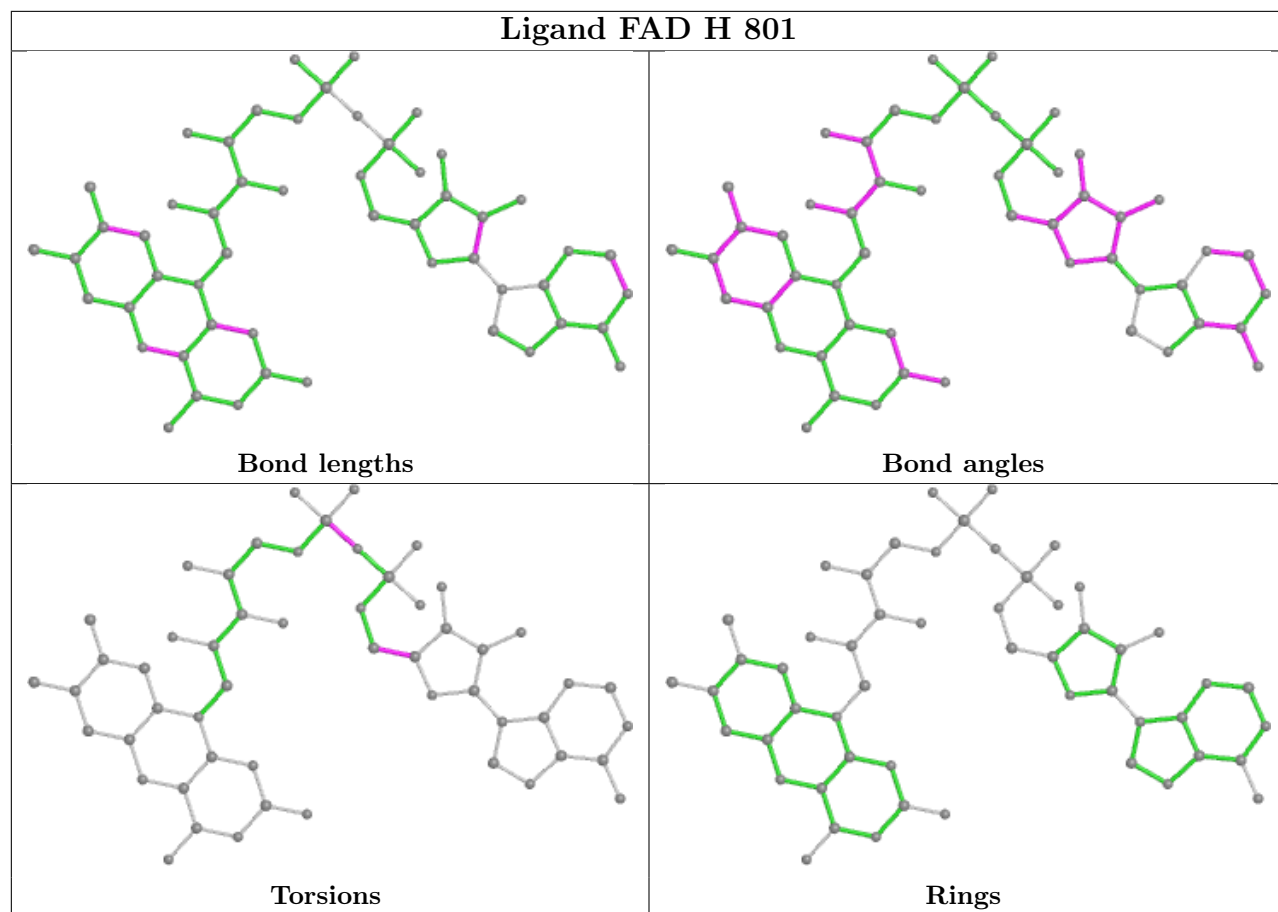


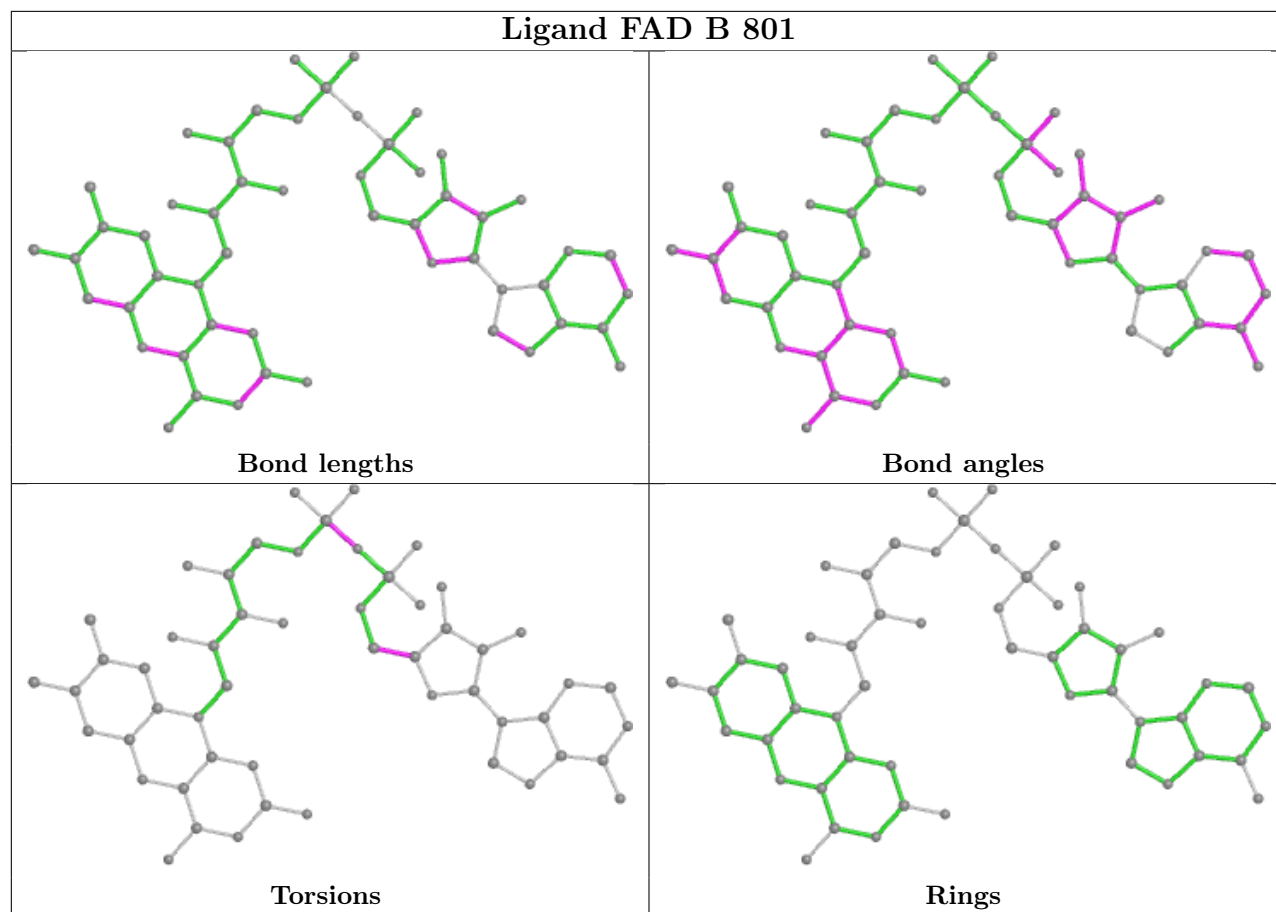












5.7 Other polymers [i](#)

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	577/623 (92%)	0.65	43 (7%) 14 16	15, 21, 40, 56	0
1	B	577/623 (92%)	0.60	33 (5%) 23 26	17, 22, 39, 65	0
1	C	577/623 (92%)	0.75	47 (8%) 12 14	20, 27, 45, 65	0
1	D	577/623 (92%)	0.63	40 (6%) 16 19	19, 25, 41, 62	0
1	E	577/623 (92%)	0.71	53 (9%) 9 10	18, 26, 42, 63	0
1	F	577/623 (92%)	0.78	56 (9%) 7 8	19, 27, 42, 64	0
1	G	577/623 (92%)	0.63	42 (7%) 15 17	18, 24, 42, 59	0
1	H	577/623 (92%)	0.60	38 (6%) 18 20	18, 23, 38, 61	0
All	All	4616/4984 (92%)	0.67	352 (7%) 13 16	15, 25, 42, 65	0

All (352) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	619	THR	15.2
1	E	389	LEU	15.1
1	C	619	THR	14.3
1	A	459	VAL	14.0
1	B	619	THR	12.9
1	D	619	THR	12.7
1	A	619	THR	12.4
1	F	619	THR	11.8
1	A	343	ALA	11.6
1	F	343	ALA	11.0
1	G	619	THR	10.9
1	E	459	VAL	10.9
1	C	389	LEU	10.5
1	G	389	LEU	10.4
1	B	45	ILE	10.4
1	E	619	THR	10.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	43	MET	9.3
1	C	618	PHE	9.2
1	B	43	MET	9.2
1	D	459	VAL	9.2
1	G	343	ALA	9.1
1	G	43	MET	8.8
1	A	389	LEU	8.8
1	F	43	MET	8.7
1	F	459	VAL	8.7
1	B	44	ASP	8.7
1	B	343	ALA	8.7
1	A	43	MET	8.6
1	F	389	LEU	8.5
1	H	45	ILE	8.5
1	C	345	PRO	8.0
1	F	342	PRO	8.0
1	F	344	ASN	7.9
1	C	456	TYR	7.8
1	G	459	VAL	7.7
1	B	459	VAL	7.7
1	H	343	ALA	7.7
1	B	345	PRO	7.6
1	G	458	ALA	7.5
1	C	385	THR	7.5
1	G	345	PRO	7.4
1	A	458	ALA	7.4
1	D	345	PRO	7.4
1	B	456	TYR	7.3
1	G	44	ASP	7.2
1	C	459	VAL	7.1
1	D	343	ALA	7.1
1	E	43	MET	7.1
1	D	618	PHE	7.0
1	D	454	PHE	7.0
1	E	618	PHE	7.0
1	E	44	ASP	7.0
1	H	459	VAL	6.9
1	C	44	ASP	6.8
1	D	458	ALA	6.8
1	F	345	PRO	6.7
1	E	385	THR	6.7
1	F	44	ASP	6.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	45	ILE	6.6
1	C	343	ALA	6.5
1	C	390	THR	6.5
1	E	45	ILE	6.5
1	E	343	ALA	6.4
1	H	344	ASN	6.4
1	A	345	PRO	6.3
1	D	344	ASN	6.3
1	B	389	LEU	6.3
1	F	618	PHE	6.2
1	D	388	GLU	6.2
1	D	43	MET	6.1
1	D	389	LEU	6.1
1	H	342	PRO	6.0
1	G	385	THR	6.0
1	F	385	THR	5.9
1	E	384	GLY	5.9
1	A	388	GLU	5.9
1	E	458	ALA	5.9
1	C	45	ILE	5.9
1	E	390	THR	5.8
1	A	344	ASN	5.8
1	H	453	ALA	5.8
1	B	344	ASN	5.8
1	E	388	GLU	5.8
1	F	458	ALA	5.7
1	G	186	ASP	5.7
1	C	43	MET	5.7
1	E	342	PRO	5.5
1	A	401	THR	5.5
1	E	387	GLY	5.5
1	H	345	PRO	5.4
1	C	344	ASN	5.4
1	A	385	THR	5.4
1	B	618	PHE	5.3
1	H	456	TYR	5.3
1	C	388	GLU	5.2
1	C	342	PRO	5.2
1	C	383	ARG	5.2
1	G	618	PHE	5.2
1	B	385	THR	5.2
1	G	344	ASN	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	454	PHE	5.1
1	H	617	PRO	4.9
1	H	44	ASP	4.9
1	D	385	THR	4.9
1	B	458	ALA	4.8
1	C	458	ALA	4.8
1	C	400	SER	4.8
1	E	344	ASN	4.8
1	F	384	GLY	4.8
1	B	341	ASN	4.8
1	G	45	ILE	4.7
1	G	401	THR	4.7
1	H	458	ALA	4.7
1	F	341	ASN	4.6
1	C	384	GLY	4.6
1	G	400	SER	4.6
1	F	45	ILE	4.6
1	G	455	SER	4.6
1	F	454	PHE	4.5
1	C	401	THR	4.4
1	F	232	GLY	4.4
1	F	387	GLY	4.4
1	C	617	PRO	4.4
1	G	100	ILE	4.3
1	A	390	THR	4.3
1	C	396	THR	4.3
1	B	342	PRO	4.3
1	D	44	ASP	4.2
1	H	618	PHE	4.2
1	A	384	GLY	4.2
1	A	456	TYR	4.2
1	H	389	LEU	4.2
1	D	617	PRO	4.2
1	D	341	ASN	4.1
1	D	342	PRO	4.1
1	C	309	PHE	4.1
1	F	390	THR	4.1
1	A	341	ASN	4.0
1	D	456	TYR	4.0
1	E	383	ARG	4.0
1	B	388	GLU	3.9
1	G	617	PRO	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	341	ASN	3.9
1	E	345	PRO	3.9
1	G	342	PRO	3.9
1	F	456	TYR	3.9
1	A	342	PRO	3.9
1	H	185	LYS	3.8
1	H	454	PHE	3.8
1	B	387	GLY	3.8
1	B	453	ALA	3.8
1	E	341	ASN	3.8
1	D	186	ASP	3.8
1	F	388	GLU	3.8
1	E	617	PRO	3.7
1	B	390	THR	3.7
1	A	618	PHE	3.7
1	G	341	ASN	3.7
1	D	309	PHE	3.7
1	D	390	THR	3.7
1	A	383	ARG	3.6
1	F	347	GLU	3.6
1	G	390	THR	3.6
1	C	268	THR	3.6
1	A	44	ASP	3.5
1	G	384	GLY	3.5
1	H	100	ILE	3.5
1	E	457	GLY	3.5
1	H	341	ASN	3.5
1	F	186	ASP	3.5
1	C	455	SER	3.5
1	H	340	PRO	3.4
1	G	382	ILE	3.4
1	F	383	ARG	3.4
1	E	400	SER	3.4
1	F	382	ILE	3.4
1	F	272	GLU	3.4
1	H	347	GLU	3.4
1	D	457	GLY	3.4
1	G	388	GLU	3.4
1	F	452	ASP	3.3
1	E	347	GLU	3.3
1	A	454	PHE	3.3
1	F	455	SER	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	452	ASP	3.2
1	E	454	PHE	3.2
1	G	454	PHE	3.2
1	E	382	ILE	3.2
1	E	186	ASP	3.2
1	B	82	SER	3.2
1	A	391	TYR	3.2
1	E	269	ASP	3.2
1	F	561	GLU	3.2
1	H	231	LYS	3.1
1	A	386	PRO	3.1
1	F	386	PRO	3.1
1	A	406	ASP	3.1
1	C	271	PRO	3.1
1	E	250	PHE	3.1
1	C	82	SER	3.1
1	D	400	SER	3.1
1	A	186	ASP	3.0
1	D	271	PRO	3.0
1	F	391	TYR	3.0
1	A	99	ASN	3.0
1	F	401	THR	2.9
1	C	186	ASP	2.9
1	E	272	GLU	2.9
1	A	400	SER	2.9
1	C	305	SER	2.9
1	E	391	TYR	2.9
1	D	383	ARG	2.9
1	A	381	THR	2.9
1	H	189	ASP	2.9
1	A	272	GLU	2.9
1	D	382	ILE	2.9
1	A	249	THR	2.9
1	B	186	ASP	2.9
1	H	457	GLY	2.9
1	F	453	ALA	2.9
1	G	185	LYS	2.8
1	G	340	PRO	2.8
1	F	189	ASP	2.8
1	G	399	ALA	2.8
1	E	456	TYR	2.8
1	E	268	THR	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	306	GLY	2.8
1	C	347	GLU	2.7
1	A	382	ILE	2.7
1	E	184	VAL	2.7
1	C	272	GLU	2.7
1	G	309	PHE	2.7
1	D	560	LYS	2.7
1	G	453	ALA	2.7
1	H	57	ILE	2.7
1	D	272	GLU	2.7
1	F	346	PRO	2.7
1	C	392	SER	2.7
1	C	323	VAL	2.6
1	F	546	VAL	2.6
1	H	305	SER	2.6
1	E	187	ASP	2.6
1	G	456	TYR	2.6
1	A	617	PRO	2.6
1	F	394	THR	2.6
1	E	182	LEU	2.6
1	F	490	LYS	2.6
1	H	271	PRO	2.6
1	C	561	GLU	2.5
1	G	187	ASP	2.5
1	C	454	PHE	2.5
1	E	421	GLU	2.5
1	E	616	SER	2.5
1	F	309	PHE	2.5
1	H	232	GLY	2.5
1	F	187	ASP	2.5
1	D	549	LEU	2.5
1	G	188	ALA	2.5
1	E	601	LEU	2.5
1	C	386	PRO	2.5
1	D	386	PRO	2.5
1	E	304	ILE	2.5
1	H	455	SER	2.4
1	H	121	LEU	2.4
1	E	561	GLU	2.4
1	G	396	THR	2.4
1	F	308	ARG	2.4
1	E	248	PRO	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	386	PRO	2.4
1	F	185	LYS	2.4
1	A	100	ILE	2.4
1	F	188	ALA	2.4
1	D	391	TYR	2.4
1	F	617	PRO	2.4
1	E	57	ILE	2.4
1	H	186	ASP	2.4
1	B	386	PRO	2.4
1	B	617	PRO	2.4
1	D	68	ALA	2.4
1	A	347	GLU	2.4
1	B	57	ILE	2.3
1	B	329	LEU	2.3
1	E	490	LYS	2.3
1	D	407	TRP	2.3
1	C	614	THR	2.3
1	H	272	GLU	2.3
1	A	602	ALA	2.3
1	C	490	LYS	2.3
1	F	168	TRP	2.3
1	C	601	LEU	2.3
1	B	383	ARG	2.3
1	D	188	ALA	2.3
1	G	386	PRO	2.3
1	G	347	GLU	2.3
1	E	189	ASP	2.3
1	F	81	ASP	2.3
1	E	455	SER	2.2
1	D	268	THR	2.2
1	F	413	LYS	2.2
1	F	249	THR	2.2
1	C	453	ALA	2.2
1	A	317	VAL	2.2
1	F	299	HIS	2.2
1	B	580	LEU	2.2
1	F	549	LEU	2.2
1	H	461	GLN	2.2
1	E	82	SER	2.2
1	H	299	HIS	2.2
1	H	268	THR	2.2
1	B	133	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	582	GLY	2.2
1	F	586	ILE	2.2
1	D	387	GLY	2.2
1	E	401	THR	2.2
1	A	133	ALA	2.2
1	E	583	CYS	2.2
1	G	387	GLY	2.2
1	F	133	ALA	2.2
1	C	132	GLN	2.1
1	E	611	GLN	2.1
1	H	309	PHE	2.1
1	D	185	LYS	2.1
1	A	580	LEU	2.1
1	B	306	GLY	2.1
1	E	81	ASP	2.1
1	A	455	SER	2.1
1	B	323	VAL	2.1
1	F	580	LEU	2.1
1	A	387	GLY	2.1
1	C	185	LYS	2.1
1	A	269	ASP	2.1
1	F	82	SER	2.1
1	B	157	VAL	2.1
1	E	232	GLY	2.1
1	G	583	CYS	2.1
1	G	57	ILE	2.1
1	G	461	GLN	2.0
1	D	347	GLU	2.0
1	B	384	GLY	2.0
1	A	452	ASP	2.0
1	H	160	VAL	2.0
1	D	168	TRP	2.0
1	F	285	ARG	2.0
1	D	178	GLU	2.0
1	F	268	THR	2.0
1	G	189	ASP	2.0
1	A	320	ALA	2.0
1	A	453	ALA	2.0
1	E	299	HIS	2.0
1	C	394	THR	2.0
1	C	452	ASP	2.0
1	C	321	GLY	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 monosaccharides 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(\AA^2)	Q<0.9
2	FAD	E	801	53/53	0.93	0.12	14,18,21,22	0
2	FAD	C	801	53/53	0.94	0.14	7,16,21,24	0
2	FAD	D	801	53/53	0.94	0.16	14,17,20,20	0
2	FAD	B	801	53/53	0.94	0.17	10,15,17,21	0
2	FAD	F	801	53/53	0.94	0.12	16,19,21,22	0
2	FAD	A	801	53/53	0.95	0.15	12,17,21,23	0
2	FAD	G	801	53/53	0.95	0.12	14,18,20,21	0
2	FAD	H	801	53/53	0.95	0.14	11,15,18,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.