



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:14 AM UTC

PDB ID : 4MIH / pdb_00004mih
Title : Pyranose 2-oxidase from Phanerochaete chrysosporium, recombinant H158A mutant
Authors : Hassan, N.; Tan, T.C.; Spadiut, O.; Pisanelli, I.; Fusco, L.; Haltrich, D.; Peterbauer, C.; Divne, C.
Deposited on : 2013-08-31
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

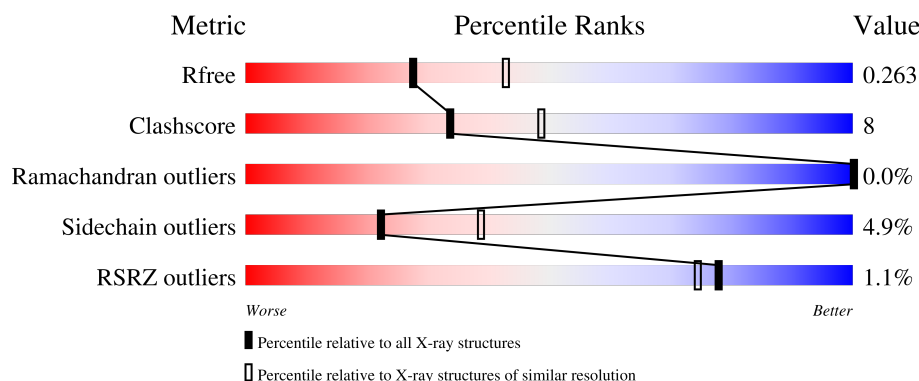
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	621	 75% 16% • 7%
1	B	621	 74% 18% • 7%
1	C	621	 68% 23% • 7%
1	D	621	 72% 20% • 7%

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Mol	Chain	Length	Quality of chain
1	E	621	% 77%14%7%
1	F	621	% 76%15%7%
1	G	621	% 69%22%7%
1	H	621	% 70%23%7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 37799 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 2-oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	576	Total	C	N	O	S	0	0	0
			4548	2895	782	844	27			
1	B	578	Total	C	N	O	S	0	0	0
			4568	2906	787	848	27			
1	C	578	Total	C	N	O	S	0	0	0
			4568	2906	787	848	27			
1	D	578	Total	C	N	O	S	0	0	0
			4568	2906	787	848	27			
1	E	576	Total	C	N	O	S	0	0	0
			4548	2895	782	844	27			
1	F	578	Total	C	N	O	S	0	0	0
			4568	2906	787	848	27			
1	G	578	Total	C	N	O	S	0	0	0
			4568	2906	787	848	27			
1	H	578	Total	C	N	O	S	0	0	0
			4568	2906	787	848	27			

There are 16 discrepancies between the modelled and reference sequences:

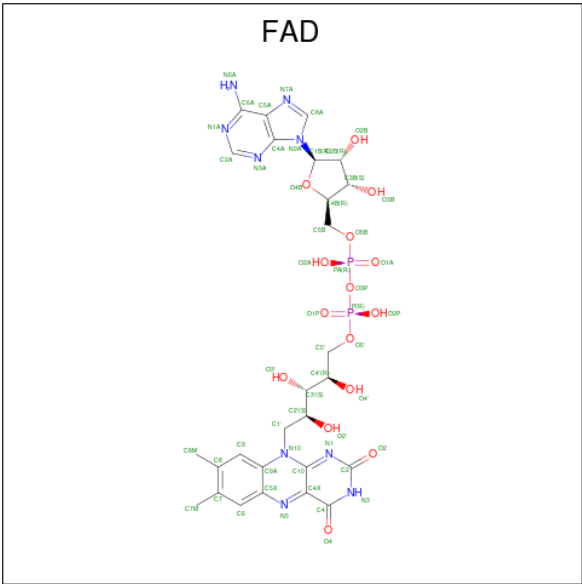
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q6QWR1
A	158	ALA	HIS	engineered mutation	UNP Q6QWR1
B	0	SER	-	expression tag	UNP Q6QWR1
B	158	ALA	HIS	engineered mutation	UNP Q6QWR1
C	0	SER	-	expression tag	UNP Q6QWR1
C	158	ALA	HIS	engineered mutation	UNP Q6QWR1
D	0	SER	-	expression tag	UNP Q6QWR1
D	158	ALA	HIS	engineered mutation	UNP Q6QWR1
E	0	SER	-	expression tag	UNP Q6QWR1
E	158	ALA	HIS	engineered mutation	UNP Q6QWR1
F	0	SER	-	expression tag	UNP Q6QWR1
F	158	ALA	HIS	engineered mutation	UNP Q6QWR1
G	0	SER	-	expression tag	UNP Q6QWR1

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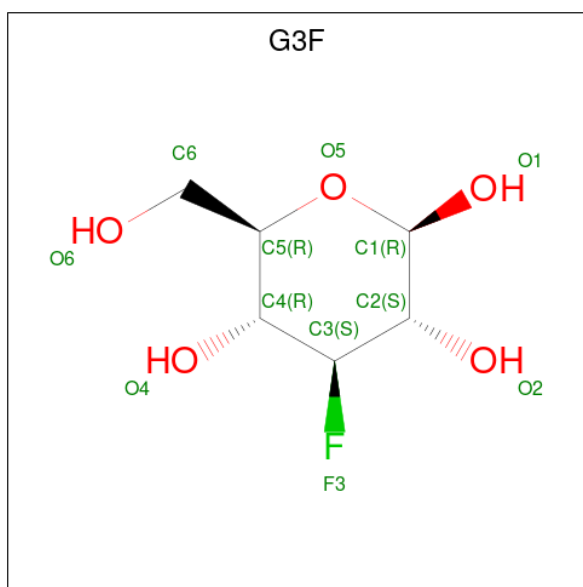
Chain	Residue	Modelled	Actual	Comment	Reference
G	158	ALA	HIS	engineered mutation	UNP Q6QWR1
H	0	SER	-	expression tag	UNP Q6QWR1
H	158	ALA	HIS	engineered mutation	UNP Q6QWR1

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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 3-deoxy-3-fluoro-beta-D-glucopyranose (CCD ID: G3F) (formula: C₆H₁₁FO₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	F	O	0	0
			12	6	1	5		
3	B	1	Total	C	F	O	0	0
			12	6	1	5		
3	C	1	Total	C	F	O	0	0
			12	6	1	5		
3	D	1	Total	C	F	O	0	0
			12	6	1	5		
3	E	1	Total	C	F	O	0	0
			12	6	1	5		
3	F	1	Total	C	F	O	0	0
			12	6	1	5		
3	G	1	Total	C	F	O	0	0
			12	6	1	5		
3	H	1	Total	C	F	O	0	0
			12	6	1	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	133	Total	O	0	0
			133	133		
4	B	109	Total	O	0	0
			109	109		
4	C	77	Total	O	0	0
			77	77		
4	D	59	Total	O	0	0
			59	59		

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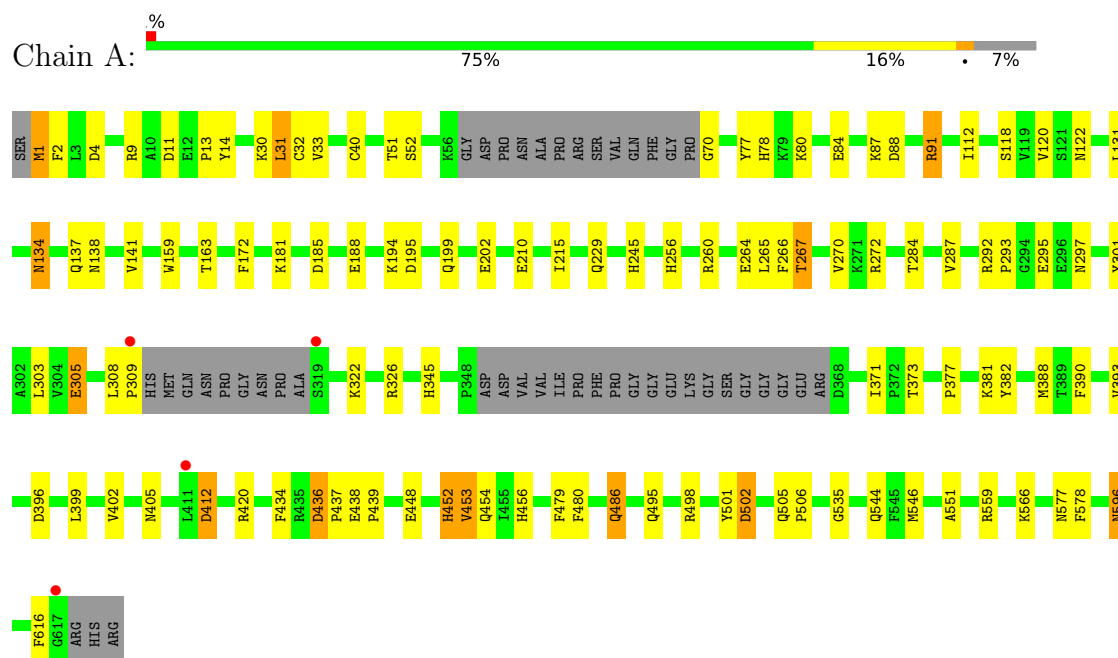
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	129	Total 129	O 129	0	0
4	F	94	Total 94	O 94	0	0
4	G	90	Total 90	O 90	0	0
4	H	84	Total 84	O 84	0	0

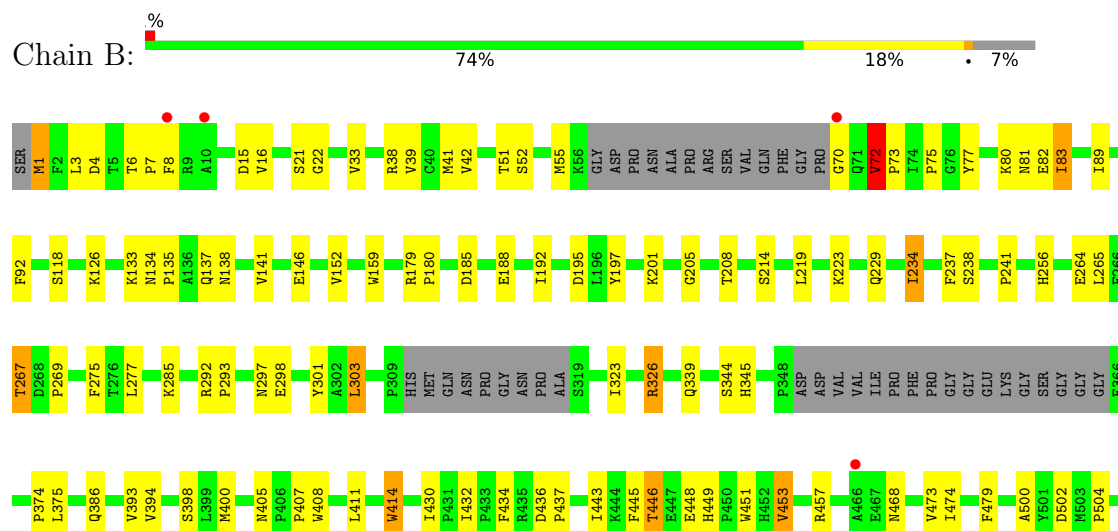
3 Residue-property plots [i](#)

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.

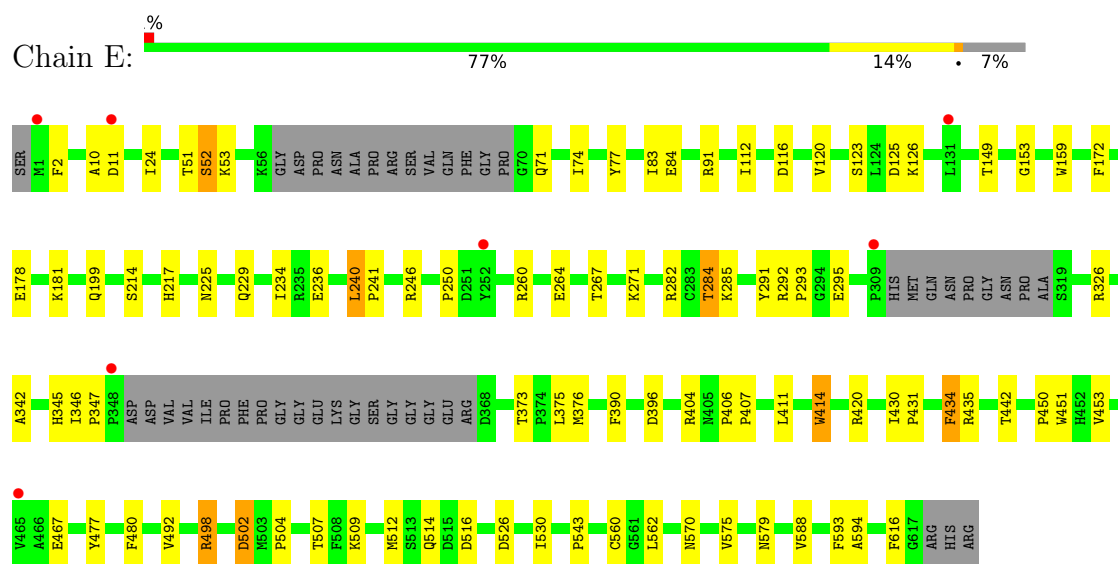
• Molecule 1: Pyranose 2-oxidase



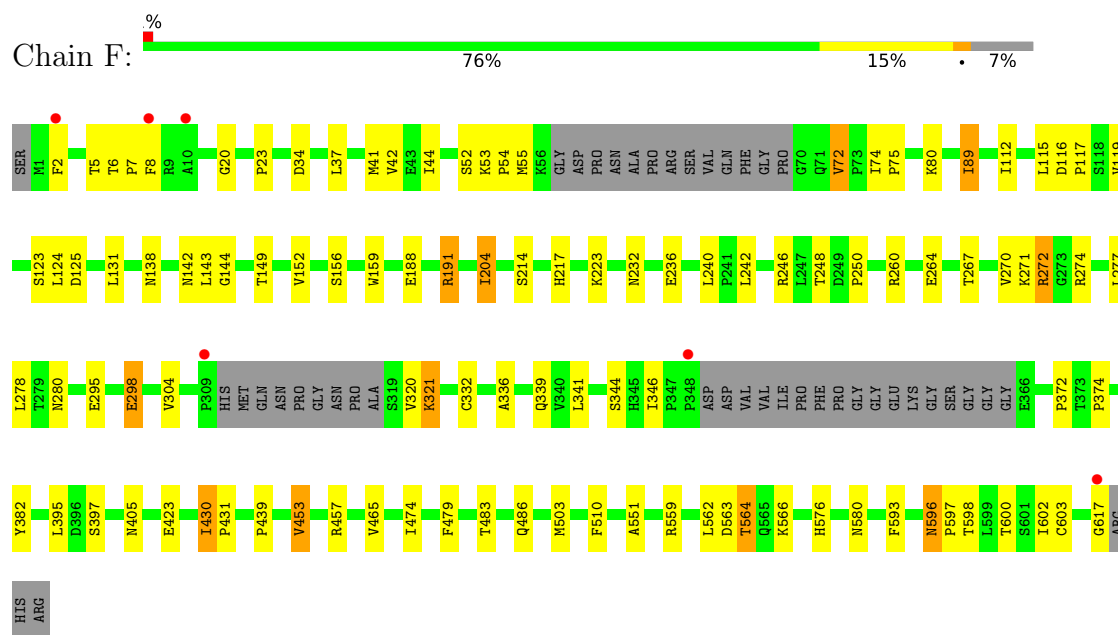
• Molecule 1: Pyranose 2-oxidase



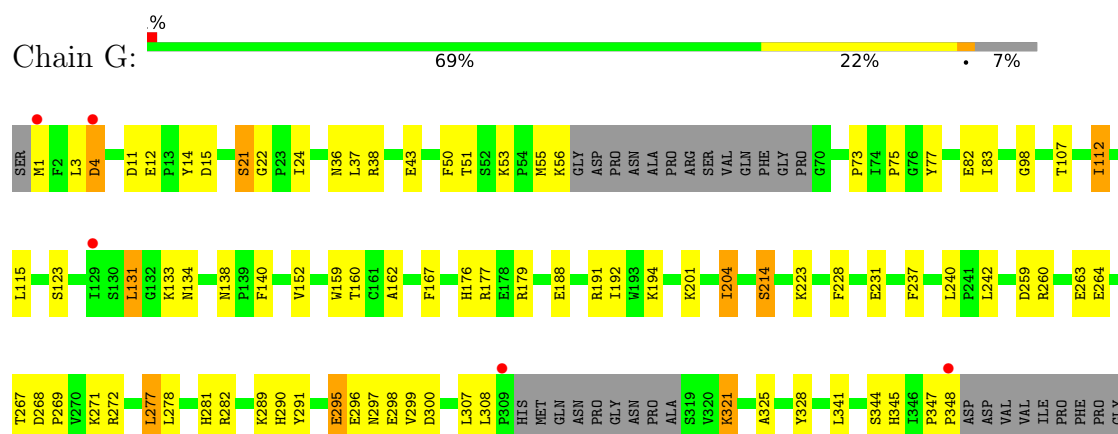


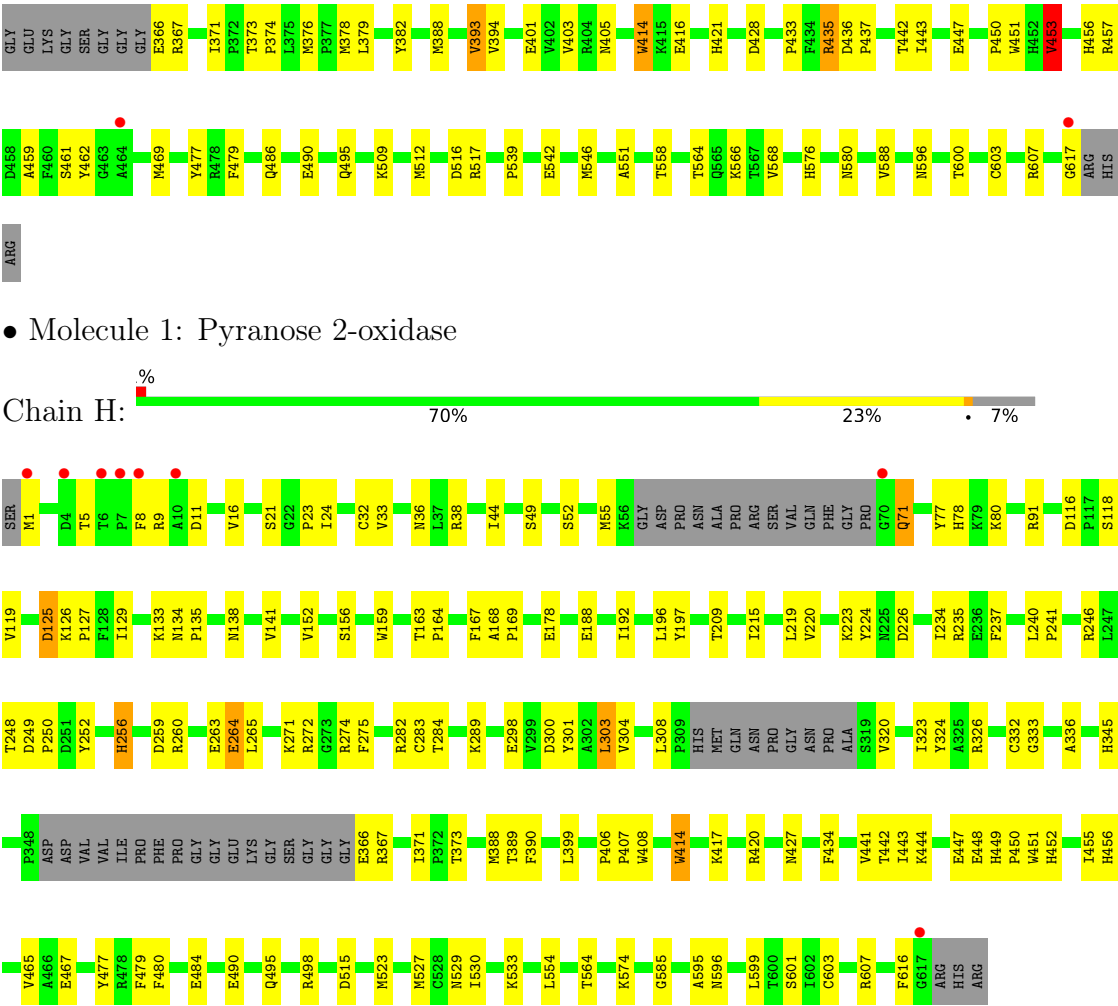


• Molecule 1: Pyranose 2-oxidase

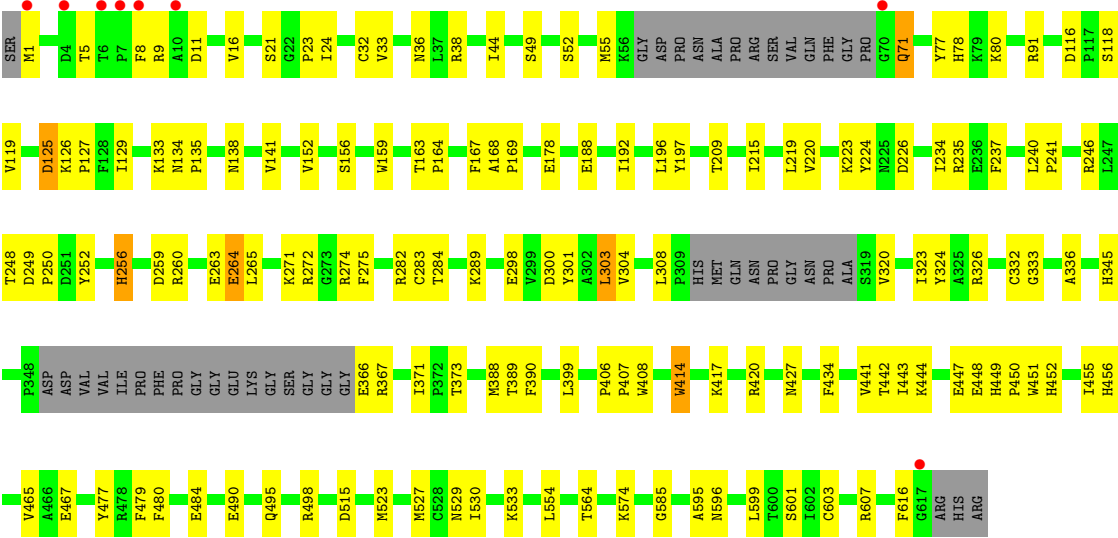


• Molecule 1: Pyranose 2-oxidase





• Molecule 1: Pyranose 2-oxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	110.10Å 167.10Å 168.47Å 90.00° 93.98° 90.00°	Depositor
Resolution (Å)	48.56 – 2.40 48.56 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.4 (48.56-2.40) 98.4 (48.56-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.205 , 0.265 0.206 , 0.263	Depositor DCC
R_{free} test set	1500 reflections (0.63%)	wwPDB-VP
Wilson B-factor (Å ²)	44.5	Xtriage
Anisotropy	0.503	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	37799	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: G3F, 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	0.73	7/4670 (0.1%)	0.96	9/6356 (0.1%)
1	B	0.64	3/4690 (0.1%)	0.94	8/6382 (0.1%)
1	C	0.65	4/4690 (0.1%)	0.97	21/6382 (0.3%)
1	D	0.59	1/4690 (0.0%)	0.95	17/6382 (0.3%)
1	E	0.58	1/4670 (0.0%)	0.92	8/6356 (0.1%)
1	F	0.53	1/4690 (0.0%)	0.88	8/6382 (0.1%)
1	G	0.60	4/4690 (0.1%)	0.91	14/6382 (0.2%)
1	H	0.58	7/4690 (0.1%)	0.87	6/6382 (0.1%)
All	All	0.61	28/37480 (0.1%)	0.93	91/51004 (0.2%)

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	256	HIS	C-N	-7.66	1.23	1.33
1	G	456	HIS	CD2-NE2	-6.87	1.30	1.37
1	H	456	HIS	CG-ND1	-6.61	1.30	1.38
1	H	256	HIS	CG-ND1	-6.46	1.31	1.38
1	A	452	HIS	CD2-NE2	-6.32	1.30	1.37
1	H	456	HIS	CD2-NE2	-6.23	1.31	1.37
1	A	454	GLN	C-O	-6.11	1.16	1.24
1	A	452	HIS	CG-ND1	-6.08	1.31	1.38
1	H	456	HIS	C-O	-5.90	1.18	1.24
1	H	256	HIS	CD2-NE2	-5.87	1.31	1.37
1	D	333	GLY	C-O	-5.80	1.16	1.23
1	H	127	PRO	C-O	-5.65	1.17	1.23
1	C	256	HIS	CD2-NE2	-5.64	1.31	1.37
1	G	459	ALA	C-O	-5.51	1.17	1.24
1	B	126	LYS	C-O	-5.48	1.18	1.24
1	H	264	GLU	C-O	-5.39	1.17	1.24
1	A	9	ARG	C-O	-5.35	1.17	1.24
1	B	446	THR	C-O	-5.34	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	81	ASN	C-O	-5.33	1.17	1.24
1	A	453	VAL	C-O	-5.30	1.18	1.24
1	C	560	CYS	C-O	-5.28	1.18	1.24
1	A	31	LEU	C-O	-5.24	1.18	1.24
1	E	560	CYS	C-O	-5.22	1.17	1.24
1	A	32	CYS	N-CA	-5.21	1.40	1.46
1	F	563	ASP	C-O	-5.12	1.17	1.23
1	G	457	ARG	C-O	-5.12	1.18	1.24
1	G	456	HIS	CG-ND1	-5.02	1.32	1.38
1	C	256	HIS	CG-ND1	-5.01	1.32	1.38

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	453	VAL	N-CA-C	8.79	120.48	108.17
1	D	427	ASN	N-CA-C	8.53	121.52	111.71
1	C	48	ASP	N-CA-C	8.45	120.57	111.36
1	G	596	ASN	CA-C-N	7.92	127.59	119.19
1	G	596	ASN	C-N-CA	7.92	127.59	119.19
1	E	562	LEU	N-CA-C	7.64	119.69	111.36
1	D	333	GLY	N-CA-C	-7.49	103.24	112.68
1	D	376	MET	CA-C-N	7.13	127.12	119.28
1	D	376	MET	C-N-CA	7.13	127.12	119.28
1	C	434	PHE	N-CA-C	6.99	120.70	111.75
1	A	134	ASN	CA-C-N	6.99	126.62	119.56
1	A	134	ASN	C-N-CA	6.99	126.62	119.56
1	C	126	LYS	CA-C-N	6.89	127.34	120.52
1	C	126	LYS	C-N-CA	6.89	127.34	120.52
1	C	256	HIS	O-C-N	-6.73	115.41	122.94
1	G	138	ASN	CA-C-N	6.44	126.36	119.28
1	G	138	ASN	C-N-CA	6.44	126.36	119.28
1	E	10	ALA	N-CA-C	-6.33	105.13	112.92
1	H	449	HIS	CA-C-N	6.31	127.72	119.84
1	H	449	HIS	C-N-CA	6.31	127.72	119.84
1	C	540	GLY	N-CA-C	-6.22	106.53	114.37
1	G	436	ASP	CA-C-N	6.19	126.15	119.78
1	G	436	ASP	C-N-CA	6.19	126.15	119.78
1	C	86	GLN	N-CA-C	-6.14	106.77	114.56
1	C	53	LYS	CA-C-N	6.12	127.49	119.84
1	C	53	LYS	C-N-CA	6.12	127.49	119.84
1	C	292	ARG	CA-C-N	6.12	126.32	119.90
1	C	292	ARG	C-N-CA	6.12	126.32	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	406	PRO	CA-C-N	6.11	127.23	120.45
1	D	406	PRO	C-N-CA	6.11	127.23	120.45
1	F	562	LEU	N-CA-C	6.06	117.69	111.14
1	D	367	ARG	N-CA-C	-6.02	105.20	112.54
1	F	430	ILE	CA-C-N	6.01	127.12	120.45
1	F	430	ILE	C-N-CA	6.01	127.12	120.45
1	A	434	PHE	N-CA-C	5.80	119.17	111.75
1	A	91	ARG	N-CA-C	5.75	119.56	112.54
1	F	346	ILE	CA-C-N	-5.74	115.52	119.66
1	F	346	ILE	C-N-CA	-5.74	115.52	119.66
1	C	453	VAL	N-CA-C	5.72	116.11	108.11
1	B	159	TRP	N-CA-C	5.57	117.72	110.53
1	H	443	ILE	CB-CA-C	-5.57	104.58	111.32
1	B	92	PHE	N-CA-C	5.55	118.10	111.71
1	D	449	HIS	CA-C-N	5.55	126.77	119.84
1	D	449	HIS	C-N-CA	5.55	126.77	119.84
1	D	268	ASP	CA-C-N	5.53	125.89	119.47
1	D	268	ASP	C-N-CA	5.53	125.89	119.47
1	H	490	GLU	N-CA-C	5.51	117.77	109.23
1	E	116	ASP	CA-C-N	5.48	125.15	119.56
1	E	116	ASP	C-N-CA	5.48	125.15	119.56
1	A	163	THR	CA-C-N	-5.36	115.06	120.85
1	A	163	THR	C-N-CA	-5.36	115.06	120.85
1	B	275	PHE	N-CA-C	5.36	117.13	108.34
1	G	134	ASN	CA-C-N	5.33	125.14	119.28
1	G	134	ASN	C-N-CA	5.33	125.14	119.28
1	D	614	ALA	N-CA-C	-5.30	107.11	113.21
1	D	138	ASN	CA-C-N	5.29	125.61	119.47
1	D	138	ASN	C-N-CA	5.29	125.61	119.47
1	F	138	ASN	CA-C-N	5.29	124.92	119.05
1	F	138	ASN	C-N-CA	5.29	124.92	119.05
1	E	153	GLY	N-CA-C	-5.29	108.05	114.92
1	B	134	ASN	CA-C-N	5.27	124.98	119.82
1	B	134	ASN	C-N-CA	5.27	124.98	119.82
1	B	386	GLN	N-CA-C	5.26	117.20	109.42
1	D	334	ALA	N-CA-C	5.25	117.74	111.71
1	G	36	ASN	N-CA-C	5.24	118.98	112.58
1	D	386	GLN	N-CA-C	5.23	117.20	109.62
1	C	406	PRO	CA-C-N	5.22	127.21	120.89
1	C	406	PRO	C-N-CA	5.22	127.21	120.89
1	C	299	VAL	N-CA-C	-5.19	102.90	109.80
1	G	376	MET	CA-C-N	5.15	124.76	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	376	MET	C-N-CA	5.15	124.76	119.05
1	E	240	LEU	CA-C-N	5.14	125.30	119.90
1	E	240	LEU	C-N-CA	5.14	125.30	119.90
1	G	321	LYS	N-CA-C	5.12	117.40	108.76
1	B	434	PHE	N-CA-C	5.09	116.83	111.28
1	D	432	ILE	N-CA-C	5.09	113.94	108.95
1	C	368	ASP	N-CA-C	-5.08	106.76	113.17
1	C	172	PHE	N-CA-C	-5.06	107.14	113.72
1	C	376	MET	CA-C-N	5.05	126.16	119.84
1	C	376	MET	C-N-CA	5.05	126.16	119.84
1	H	134	ASN	CA-C-N	5.05	124.66	119.56
1	H	134	ASN	C-N-CA	5.05	124.66	119.56
1	G	83	ILE	N-CA-C	5.04	115.81	110.72
1	B	72	VAL	N-CA-C	5.03	113.41	107.77
1	C	174	ALA	CA-C-N	5.03	126.13	119.84
1	C	174	ALA	C-N-CA	5.03	126.13	119.84
1	F	72	VAL	N-CA-C	5.03	113.98	108.05
1	E	434	PHE	N-CA-C	5.02	116.75	111.28
1	A	436	ASP	CA-C-N	5.02	125.29	119.92
1	A	436	ASP	C-N-CA	5.02	125.29	119.92
1	G	453	VAL	N-CA-C	5.00	115.17	108.17

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	4548	0	4440	68	0
1	B	4568	0	4459	62	0
1	C	4568	0	4459	99	0
1	D	4568	0	4459	86	0
1	E	4548	0	4440	50	0
1	F	4568	0	4459	60	0
1	G	4568	0	4459	84	0
1	H	4568	0	4459	74	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	53	0	31	3	0
2	B	53	0	31	2	0
2	C	53	0	31	2	0
2	D	53	0	31	3	0
2	E	53	0	31	2	0
2	F	53	0	31	3	0
2	G	53	0	31	3	0
2	H	53	0	31	3	0
3	A	12	0	11	2	0
3	B	12	0	11	0	0
3	C	12	0	11	1	0
3	D	12	0	11	0	0
3	E	12	0	11	1	0
3	F	12	0	11	2	0
3	G	12	0	11	0	0
3	H	12	0	11	1	0
4	A	133	0	0	1	0
4	B	109	0	0	1	0
4	C	77	0	0	2	0
4	D	59	0	0	2	0
4	E	129	0	0	3	0
4	F	94	0	0	1	0
4	G	90	0	0	5	0
4	H	84	0	0	1	0
All	All	37799	0	35970	564	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 8.

All (564) 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:55:MET:HE1	1:D:272:ARG:HH11	1.15	1.08
1:C:16:VAL:HG13	1:C:39:VAL:HG13	1.33	1.06
1:D:55:MET:HE1	1:D:272:ARG:NH1	1.71	1.05
1:A:405:ASN:OD1	1:A:405:ASN:O	1.90	0.89
1:E:264:GLU:HA	1:E:267:THR:HG22	1.60	0.84
1:D:4:ASP:O	1:D:5:THR:HG22	1.77	0.83
1:A:371:ILE:HA	1:A:495:GLN:HE21	1.42	0.83
1:D:385:GLU:HG3	1:D:386:GLN:H	1.42	0.81
1:D:4:ASP:O	1:D:5:THR:CG2	2.29	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:MET:CE	1:D:272:ARG:NH1	2.46	0.78
1:C:112:ILE:HD11	1:D:468:ASN:HB2	1.67	0.76
1:B:229:GLN:HA	1:B:234:ILE:HD13	1.68	0.76
1:H:24:ILE:HG13	1:H:585:GLY:HA2	1.69	0.73
1:A:292:ARG:NE	1:A:295:GLU:OE1	2.21	0.72
1:H:326:ARG:NH2	1:H:616:PHE:O	2.21	0.72
1:G:378:MET:HE3	1:G:566:LYS:HA	1.72	0.72
1:D:401:GLU:OE1	1:D:401:GLU:HA	1.89	0.72
1:A:87:LYS:NZ	1:B:500:ALA:O	2.25	0.70
1:D:1:MET:HE3	1:D:3:LEU:HD23	1.74	0.70
1:G:490:GLU:OE1	1:G:509:LYS:NZ	2.24	0.70
1:G:289:LYS:HD3	1:G:290:HIS:HD2	1.58	0.68
1:D:4:ASP:C	1:D:5:THR:CG2	2.69	0.65
1:D:4:ASP:C	1:D:5:THR:HG23	2.23	0.64
1:F:270:VAL:HG12	1:F:274:ARG:HH22	1.63	0.64
1:G:21:SER:HB3	1:G:43:GLU:HB2	1.78	0.64
1:D:385:GLU:HG3	1:D:386:GLN:N	2.13	0.64
1:F:42:VAL:HG12	1:F:278:LEU:HD12	1.80	0.64
1:D:16:VAL:HB	1:D:39:VAL:HG22	1.80	0.64
1:G:192:ILE:HD13	1:G:607:ARG:HH12	1.64	0.63
1:F:37:LEU:HD21	1:F:617:GLY:HA2	1.80	0.63
1:C:268:ASP:HB3	1:C:271:LYS:HB2	1.80	0.63
1:A:544:GLN:HG3	1:A:546:MET:HE2	1.79	0.63
1:C:48:ASP:OD1	1:C:48:ASP:N	2.30	0.63
1:E:199:GLN:NE2	4:E:950:HOH:O	2.31	0.62
1:D:570:ASN:HD21	1:D:574:LYS:HB3	1.64	0.62
1:G:290:HIS:CE1	1:G:295:GLU:HG2	2.34	0.62
1:C:289:LYS:HE3	1:C:290:HIS:HD2	1.64	0.62
1:A:51:THR:HB	1:A:77:TYR:CD1	2.35	0.62
1:H:36:ASN:HA	1:H:274:ARG:HE	1.64	0.62
1:H:215:ILE:HD11	1:H:417:LYS:HD2	1.81	0.62
1:H:52:SER:HB3	1:H:71:GLN:HE21	1.64	0.61
1:A:501:TYR:CE2	1:B:83:ILE:HD11	2.35	0.61
1:C:214:SER:HB3	1:C:217:HIS:HB3	1.82	0.61
1:G:341:LEU:O	1:G:344:SER:HB2	1.99	0.61
1:A:266:PHE:O	1:A:272:ARG:NH1	2.33	0.61
1:D:97:LYS:NZ	4:D:955:HOH:O	2.33	0.61
1:E:2:PHE:H	1:F:52:SER:HB2	1.65	0.61
1:F:23:PRO:HG3	1:F:156:SER:HB3	1.83	0.60
1:B:15:ASP:HA	1:B:326:ARG:HG3	1.83	0.60
1:G:188:GLU:OE2	1:G:191:ARG:NH1	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:612:ILE:O	1:C:616:PHE:HB2	2.01	0.60
1:D:385:GLU:CG	1:D:386:GLN:H	2.12	0.60
1:B:301:TYR:HE1	1:B:303:LEU:HD12	1.67	0.60
1:C:271:LYS:HA	1:C:274:ARG:HH21	1.66	0.60
1:H:78:HIS:CE1	1:H:80:LYS:HB2	2.37	0.60
1:F:217:HIS:HA	1:F:439:PRO:HB3	1.84	0.59
1:C:596:ASN:OD1	1:C:596:ASN:N	2.26	0.59
1:F:332:CYS:O	1:F:336:ALA:HB3	2.02	0.59
1:D:42:VAL:HG12	1:D:278:LEU:HB2	1.84	0.59
1:H:21:SER:OG	1:H:152:VAL:HA	2.03	0.59
1:B:33:VAL:HG23	1:B:39:VAL:HG21	1.83	0.58
1:C:98:GLY:O	1:D:91:ARG:NH1	2.36	0.58
1:D:246:ARG:NH1	1:D:250:PRO:O	2.36	0.58
1:G:345:HIS:CD2	1:G:373:THR:HA	2.38	0.58
1:C:16:VAL:HG12	1:C:39:VAL:HG22	1.85	0.58
1:B:408:TRP:HB2	1:B:411:LEU:HD11	1.86	0.58
1:A:78:HIS:CE1	1:A:80:LYS:HB2	2.39	0.58
1:C:16:VAL:CG1	1:C:39:VAL:HG22	2.33	0.58
1:D:167:PHE:CE2	1:D:447:GLU:HG2	2.39	0.57
1:A:501:TYR:HE2	1:B:83:ILE:HD11	1.68	0.57
1:G:176:HIS:ND1	1:G:447:GLU:OE2	2.25	0.57
1:B:297:ASN:OD1	1:B:298:GLU:N	2.38	0.57
1:B:339:GLN:NE2	1:B:504:PRO:O	2.28	0.57
1:D:386:GLN:HB3	1:D:481:GLY:O	2.04	0.57
1:E:411:LEU:HB3	1:E:414:TRP:HB3	1.86	0.57
1:A:390:PHE:HB3	1:A:546:MET:HE3	1.85	0.57
1:C:21:SER:OG	1:C:152:VAL:HA	2.04	0.57
1:D:146:GLU:OE2	1:D:385:GLU:OE1	2.23	0.57
1:D:385:GLU:CG	1:D:386:GLN:N	2.68	0.57
1:C:109:ASN:ND2	1:C:127:PRO:HB3	2.20	0.56
1:G:55:MET:HE3	1:G:269:PRO:HG3	1.87	0.56
1:B:55:MET:HE3	1:B:269:PRO:HG3	1.86	0.56
1:D:43:GLU:OE2	2:D:801:FAD:O2B	2.23	0.56
1:D:24:ILE:HG21	1:D:585:GLY:N	2.21	0.55
1:G:388:MET:HE2	1:G:551:ALA:HB2	1.88	0.55
1:H:219:LEU:HD21	1:H:399:LEU:HD13	1.87	0.55
1:H:371:ILE:HG12	1:H:495:GLN:HG2	1.88	0.55
1:F:55:MET:HE1	1:F:272:ARG:HD2	1.87	0.55
1:D:182:LEU:HD22	1:D:571:THR:HB	1.86	0.55
1:C:42:VAL:HG12	1:C:278:LEU:HB2	1.89	0.55
1:B:41:MET:HG2	1:B:277:LEU:HD13	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:PRO:HB2	1:B:152:VAL:HG11	1.89	0.55
1:D:75:PRO:HB2	1:D:152:VAL:HG11	1.89	0.55
1:E:345:HIS:NE2	1:E:375:LEU:HB2	2.21	0.55
1:C:159:TRP:HA	2:C:801:FAD:C6	2.37	0.55
1:D:376:MET:HE2	1:D:575:VAL:HG11	1.88	0.55
1:D:308:LEU:O	1:D:308:LEU:HD12	2.07	0.54
1:A:70:GLY:N	1:B:4:ASP:OD2	2.40	0.54
1:B:33:VAL:HG23	1:B:39:VAL:CG2	2.38	0.54
1:D:332:CYS:O	1:D:336:ALA:HB3	2.07	0.54
1:E:292:ARG:NE	1:E:295:GLU:OE1	2.36	0.54
1:G:98:GLY:O	1:H:91:ARG:NH1	2.41	0.54
1:F:264:GLU:HA	1:F:267:THR:HG22	1.88	0.54
1:C:116:ASP:HB3	1:C:119:VAL:HG13	1.89	0.54
1:F:483:THR:HG21	1:F:510:PHE:HZ	1.73	0.54
1:A:112:ILE:HD11	1:B:468:ASN:HB2	1.90	0.54
1:E:543:PRO:O	1:G:542:GLU:HG2	2.08	0.54
1:G:345:HIS:HD2	1:G:374:PRO:HD2	1.73	0.54
1:D:558:THR:O	1:D:588:VAL:HA	2.07	0.53
1:C:16:VAL:CG1	1:C:39:VAL:HG13	2.24	0.53
1:G:56:LYS:HB2	1:G:269:PRO:HD3	1.90	0.53
1:A:4:ASP:OD1	1:B:70:GLY:N	2.41	0.53
1:E:264:GLU:OE1	1:E:271:LYS:NZ	2.40	0.53
1:C:264:GLU:HA	1:C:267:THR:HG22	1.89	0.53
1:D:99:ALA:HB1	1:D:149:THR:HG23	1.89	0.53
1:H:125:ASP:OD1	1:H:125:ASP:N	2.40	0.53
1:H:138:ASN:HB3	1:H:141:VAL:HG22	1.88	0.53
1:F:75:PRO:HB2	1:F:152:VAL:HG11	1.89	0.53
1:F:382:TYR:HA	1:F:486:GLN:O	2.07	0.53
1:D:188:GLU:O	1:D:192:ILE:HG13	2.08	0.53
1:F:54:PRO:O	1:F:267:THR:OG1	2.26	0.53
1:C:16:VAL:HG13	1:C:39:VAL:CG1	2.24	0.53
1:G:37:LEU:HD21	1:G:617:GLY:HA2	1.91	0.53
1:C:55:MET:HE3	1:C:269:PRO:HD3	1.89	0.53
1:E:225:ASN:O	1:E:229:GLN:HG2	2.09	0.53
1:F:159:TRP:HA	2:F:801:FAD:C6	2.39	0.53
1:C:245:HIS:CE1	1:C:254:GLU:HG2	2.44	0.52
1:G:112:ILE:HB	1:G:115:LEU:HG	1.91	0.52
1:H:407:PRO:HD2	1:H:408:TRP:CE3	2.44	0.52
1:A:210:GLU:HG3	1:A:245:HIS:HA	1.91	0.52
1:C:562:LEU:HD21	1:C:571:THR:HG21	1.90	0.52
1:G:188:GLU:O	1:G:192:ILE:HG13	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:8:PHE:CE2	1:F:321:LYS:HE2	2.45	0.52
1:F:34:ASP:OD1	1:F:271:LYS:NZ	2.30	0.52
1:G:296:GLU:HG3	1:G:297:ASN:N	2.24	0.52
1:C:52:SER:OG	1:D:2:PHE:N	2.41	0.52
1:D:166:PHE:HB3	1:D:178:GLU:HB3	1.91	0.52
1:H:441:VAL:HB	1:H:455:ILE:HB	1.91	0.52
1:G:394:VAL:HG21	1:G:469:MET:HE3	1.92	0.52
1:E:492:VAL:HG23	1:E:507:THR:HB	1.92	0.52
1:G:177:ARG:NE	1:G:179:ARG:O	2.39	0.52
1:E:342:ALA:O	1:E:345:HIS:HB2	2.10	0.52
1:F:8:PHE:HE2	1:F:321:LYS:HE2	1.74	0.52
1:C:265:LEU:HA	1:C:271:LYS:HB3	1.91	0.52
1:F:457:ARG:HD3	1:F:474:ILE:O	2.09	0.52
1:G:228:PHE:HA	1:G:231:GLU:HG2	1.92	0.52
1:H:196:LEU:HD11	1:H:607:ARG:HD3	1.91	0.52
1:G:73:PRO:HB3	1:H:1:MET:SD	2.49	0.52
1:C:28:PHE:HA	1:C:609:SER:OG	2.10	0.51
1:D:613:ILE:C	1:D:615:LYS:H	2.19	0.51
1:E:172:PHE:CZ	1:E:181:LYS:HD3	2.45	0.51
2:E:801:FAD:N5	3:E:802:G3F:H2	2.25	0.51
1:F:188:GLU:OE1	1:F:191:ARG:NE	2.35	0.51
1:G:201:LYS:HE2	4:G:926:HOH:O	2.10	0.51
1:H:163:THR:HB	1:H:599:LEU:HB2	1.92	0.51
2:C:801:FAD:N5	3:C:802:G3F:H2	2.25	0.51
1:E:84:GLU:OE2	1:E:91:ARG:NH1	2.44	0.51
1:A:297:ASN:N	1:A:577:ASN:O	2.42	0.51
1:B:345:HIS:NE2	1:B:375:LEU:HB2	2.25	0.51
1:A:551:ALA:O	3:A:802:G3F:O1	2.26	0.51
1:E:498:ARG:HG2	1:E:502:ASP:HA	1.92	0.51
1:A:412:ASP:N	1:A:412:ASP:OD1	2.41	0.51
1:B:345:HIS:CD2	1:B:374:PRO:HD2	2.45	0.51
1:D:116:ASP:O	1:D:119:VAL:HG22	2.11	0.51
1:H:220:VAL:HG12	1:H:441:VAL:HG21	1.93	0.51
1:H:448:GLU:OE1	1:H:448:GLU:N	2.44	0.51
1:A:33:VAL:HG11	1:A:265:LEU:HD22	1.92	0.50
1:A:438:GLU:OE2	1:A:438:GLU:N	2.36	0.50
1:C:287:VAL:HB	1:C:301:TYR:CE2	2.46	0.50
1:B:414:TRP:CD1	1:B:414:TRP:C	2.89	0.50
1:A:559:ARG:NH1	1:A:566:LYS:O	2.44	0.50
1:C:53:LYS:HG2	1:C:263:GLU:CD	2.36	0.50
1:E:420:ARG:HG2	4:E:903:HOH:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:MET:SD	1:C:272:ARG:NH2	2.85	0.50
1:C:138:ASN:HB3	1:C:141:VAL:HG22	1.93	0.50
1:D:44:ILE:HB	2:D:801:FAD:C2A	2.42	0.50
1:G:600:THR:O	1:G:603:CYS:HB2	2.11	0.50
1:A:256:HIS:HB3	1:A:260:ARG:HD3	1.93	0.50
1:G:268:ASP:OD2	1:G:271:LYS:HG3	2.12	0.50
1:B:3:LEU:HD12	1:B:277:LEU:HG	1.94	0.50
1:F:5:THR:HG21	1:F:277:LEU:HB3	1.93	0.50
1:C:112:ILE:HD11	1:D:468:ASN:CB	2.37	0.50
1:C:282:ARG:NE	1:C:284:THR:OG1	2.34	0.50
1:A:11:ASP:O	1:A:13:PRO:HD3	2.12	0.49
1:B:80:LYS:HD2	1:B:89:ILE:HD11	1.93	0.49
1:F:339:GLN:HG2	1:F:503:MET:HE3	1.94	0.49
1:C:327:SER:HB3	1:C:616:PHE:CE2	2.47	0.49
1:D:492:VAL:HG23	1:D:507:THR:HB	1.94	0.49
1:E:512:MET:HG2	4:E:902:HOH:O	2.11	0.49
1:E:480:PHE:O	1:E:594:ALA:HB1	2.12	0.49
1:D:283:CYS:HA	1:D:304:VAL:HG22	1.94	0.49
1:E:376:MET:HE2	1:E:575:VAL:HG11	1.94	0.49
1:G:414:TRP:CD1	1:G:414:TRP:C	2.91	0.49
1:H:49:SER:OG	1:H:77:TYR:O	2.30	0.49
1:D:4:ASP:O	1:D:5:THR:HG23	2.13	0.49
1:F:564:THR:HG23	1:F:576:HIS:CE1	2.48	0.49
1:G:1:MET:HG2	1:G:50:PHE:HZ	1.77	0.49
1:E:240:LEU:HD13	1:E:442:THR:HB	1.94	0.49
1:H:388:MET:HE2	1:H:480:PHE:CE2	2.48	0.49
1:C:291:TYR:CZ	1:C:347:PRO:HB3	2.48	0.49
1:H:345:HIS:CD2	1:H:373:THR:HA	2.47	0.49
1:B:453:VAL:HB	1:B:479:PHE:CE1	2.47	0.49
1:D:291:TYR:CE1	1:D:347:PRO:HB3	2.48	0.49
1:D:412:ASP:OD1	1:D:412:ASP:N	2.46	0.49
1:D:558:THR:O	1:D:558:THR:OG1	2.30	0.49
1:D:210:GLU:HG3	1:D:245:HIS:HA	1.95	0.49
1:D:488:ALA:O	1:D:490:GLU:HG3	2.12	0.48
1:A:596:ASN:OD1	1:A:596:ASN:N	2.41	0.48
1:C:204:ILE:O	1:C:256:HIS:ND1	2.38	0.48
1:D:56:LYS:HG3	1:D:267:THR:HG23	1.95	0.48
1:F:246:ARG:NH1	1:F:250:PRO:O	2.46	0.48
1:G:512:MET:HE3	1:G:516:ASP:HB3	1.95	0.48
1:C:52:SER:CB	1:D:2:PHE:H	2.27	0.48
1:C:414:TRP:CD1	1:C:414:TRP:C	2.92	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:462:TYR:CD2	1:D:546:MET:HE2	2.49	0.48
1:F:272:ARG:HH11	1:F:272:ARG:HB3	1.79	0.48
1:H:223:LYS:HD2	1:H:223:LYS:HA	1.64	0.48
1:G:539:PRO:HA	1:G:542:GLU:OE2	2.14	0.48
1:A:396:ASP:OD1	1:A:535:GLY:HA2	2.14	0.48
1:C:110:ASN:HB2	1:D:468:ASN:OD1	2.13	0.48
1:F:270:VAL:HG12	1:F:274:ARG:NH2	2.29	0.48
1:E:246:ARG:NH1	1:E:250:PRO:O	2.47	0.48
1:E:390:PHE:HA	1:E:477:TYR:O	2.13	0.48
1:G:299:VAL:H	1:G:580:ASN:HD21	1.62	0.48
1:C:112:ILE:HB	1:C:115:LEU:HG	1.95	0.48
1:H:450:PRO:HD2	1:H:451:TRP:CZ3	2.49	0.48
1:C:38:ARG:HA	1:C:274:ARG:HB3	1.95	0.48
1:H:390:PHE:HA	1:H:477:TYR:O	2.14	0.48
1:C:171:ASP:HB3	1:C:174:ALA:HB2	1.95	0.47
1:D:24:ILE:HG22	1:D:331:ALA:HB1	1.96	0.47
1:E:291:TYR:CD2	1:E:347:PRO:HG3	2.49	0.47
1:G:75:PRO:HB2	1:G:152:VAL:HG11	1.96	0.47
1:A:284:THR:OG1	1:A:305:GLU:OE1	2.31	0.47
1:A:264:GLU:HA	1:A:267:THR:HG22	1.96	0.47
1:A:287:VAL:HG21	1:A:301:TYR:CZ	2.48	0.47
2:F:801:FAD:N5	3:F:802:G3F:H2	2.29	0.47
1:G:393:VAL:HG22	1:G:477:TYR:HE1	1.78	0.47
1:D:36:ASN:HA	1:D:274:ARG:CZ	2.45	0.47
1:H:451:TRP:CG	1:H:523:MET:HG3	2.50	0.47
2:H:801:FAD:N5	3:H:802:G3F:H2	2.30	0.47
1:E:404:ARG:HH11	1:E:431:PRO:HG3	1.80	0.47
1:D:330:VAL:CG1	1:D:337:THR:HG23	2.44	0.47
1:E:285:LYS:NZ	1:E:346:ILE:O	2.42	0.47
1:G:371:ILE:HG12	1:G:495:GLN:HG3	1.97	0.47
1:H:116:ASP:O	1:H:119:VAL:HG22	2.14	0.47
1:D:329:VAL:HG22	1:D:582:TYR:HB2	1.97	0.47
1:D:387:PRO:HB3	1:D:512:MET:HE1	1.96	0.47
1:F:217:HIS:HB2	1:F:439:PRO:HA	1.96	0.47
1:G:347:PRO:HA	1:G:348:PRO:HD2	1.80	0.47
1:H:240:LEU:HD13	1:H:442:THR:HB	1.95	0.47
1:H:529:ASN:O	1:H:533:LYS:HG2	2.15	0.47
1:D:89:ILE:HD12	1:D:89:ILE:HA	1.74	0.47
1:E:414:TRP:CD1	1:E:414:TRP:C	2.93	0.47
1:G:53:LYS:HG3	1:G:263:GLU:OE2	2.15	0.47
1:G:453:VAL:HB	1:G:479:PHE:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:411:LEU:O	1:C:415:LYS:HG3	2.14	0.47
1:D:55:MET:HE1	1:D:272:ARG:HD2	1.97	0.47
1:H:164:PRO:HG2	1:H:595:ALA:HB1	1.96	0.47
1:A:382:TYR:OH	1:A:566:LYS:HD2	2.15	0.47
1:B:208:THR:HG22	1:B:241:PRO:HA	1.97	0.47
1:E:450:PRO:HD2	1:E:451:TRP:CZ3	2.50	0.47
1:F:112:ILE:HB	1:F:115:LEU:HG	1.97	0.47
1:G:297:ASN:OD1	1:G:298:GLU:N	2.48	0.47
1:H:38:ARG:HA	1:H:274:ARG:HB2	1.97	0.47
1:C:33:VAL:HG11	1:C:265:LEU:HD22	1.97	0.46
1:G:240:LEU:HD13	1:G:442:THR:HB	1.96	0.46
1:G:291:TYR:CZ	1:G:347:PRO:HB3	2.49	0.46
1:H:33:VAL:HG21	1:H:265:LEU:HD21	1.96	0.46
1:D:372:PRO:C	1:D:374:PRO:HD3	2.39	0.46
1:D:55:MET:SD	1:D:72:VAL:HG21	2.55	0.46
1:F:44:ILE:O	1:F:280:ASN:HA	2.15	0.46
1:G:435:ARG:NH1	4:G:985:HOH:O	2.49	0.46
1:G:462:TYR:CD2	1:G:546:MET:HE2	2.51	0.46
1:A:120:VAL:HG21	1:B:400:MET:HE3	1.97	0.46
1:C:116:ASP:O	1:C:119:VAL:HG22	2.15	0.46
1:C:188:GLU:O	1:C:192:ILE:HG13	2.15	0.46
1:A:498:ARG:HG2	1:A:502:ASP:C	2.40	0.46
1:C:91:ARG:HH11	1:C:91:ARG:HG2	1.80	0.46
1:E:326:ARG:NH2	1:E:616:PHE:O	2.49	0.46
1:G:3:LEU:HD12	1:G:277:LEU:HB3	1.98	0.46
1:A:131:LEU:HD23	1:A:131:LEU:HA	1.74	0.46
1:A:172:PHE:O	1:A:181:LYS:NZ	2.45	0.46
1:G:15:ASP:OD2	1:G:38:ARG:N	2.47	0.46
1:G:167:PHE:CE2	1:G:447:GLU:HG2	2.51	0.46
1:A:439:PRO:O	1:A:456:HIS:HA	2.16	0.46
1:B:8:PHE:CZ	1:B:323:ILE:HG12	2.51	0.46
1:C:377:PRO:HB2	1:C:378:MET:HE2	1.98	0.46
1:C:406:PRO:HA	1:C:407:PRO:HD3	1.86	0.46
1:D:450:PRO:HD2	1:D:451:TRP:CZ3	2.50	0.46
1:D:574:LYS:HB2	1:D:582:TYR:CE2	2.51	0.46
1:E:430:ILE:HA	1:E:431:PRO:HD3	1.76	0.46
1:C:72:VAL:HG11	1:C:266:PHE:O	2.16	0.45
2:A:801:FAD:N5	3:A:802:G3F:H2	2.32	0.45
1:B:6:THR:HA	1:B:7:PRO:HD3	1.83	0.45
1:D:291:TYR:CZ	1:D:347:PRO:HB3	2.50	0.45
1:D:373:THR:HG21	1:D:379:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:ASP:OD2	1:A:199:GLN:NE2	2.46	0.45
1:A:287:VAL:HG21	1:A:301:TYR:CE1	2.52	0.45
1:C:593:PHE:CE1	1:C:597:PRO:HB3	2.52	0.45
1:F:596:ASN:OD1	1:F:596:ASN:N	2.49	0.45
1:G:21:SER:OG	1:G:152:VAL:HA	2.17	0.45
1:H:8:PHE:CZ	1:H:323:ILE:HG12	2.51	0.45
1:A:134:ASN:ND2	1:A:137:GLN:HB2	2.32	0.45
1:D:345:HIS:CD2	1:D:373:THR:HA	2.51	0.45
1:H:167:PHE:CE2	1:H:447:GLU:HG2	2.51	0.45
1:H:452:HIS:HB3	1:H:480:PHE:HB2	1.98	0.45
1:C:51:THR:HB	1:C:77:TYR:CD1	2.51	0.45
1:E:52:SER:O	1:E:53:LYS:HD3	2.16	0.45
1:H:125:ASP:O	1:H:126:LYS:HG2	2.17	0.45
1:H:389:THR:OG1	1:H:479:PHE:HB2	2.17	0.45
1:A:185:ASP:OD2	1:A:188:GLU:N	2.50	0.45
1:A:194:LYS:HB2	1:A:194:LYS:HE3	1.76	0.45
1:H:192:ILE:HG21	1:H:607:ARG:HD2	1.99	0.45
1:B:72:VAL:HA	1:B:73:PRO:HD2	1.89	0.45
1:E:159:TRP:HA	2:E:801:FAD:C6	2.46	0.45
1:F:453:VAL:HB	1:F:479:PHE:CE1	2.51	0.45
1:H:196:LEU:HD13	1:H:603:CYS:HB3	1.99	0.45
1:H:495:GLN:O	1:H:498:ARG:NH1	2.49	0.45
1:B:192:ILE:HD13	1:B:607:ARG:HH12	1.82	0.45
1:C:299:VAL:HB	1:C:580:ASN:HD21	1.82	0.45
1:H:133:LYS:O	1:H:135:PRO:HD3	2.16	0.45
1:C:270:VAL:HG12	1:C:274:ARG:NH2	2.32	0.45
1:D:1:MET:HG2	1:D:50:PHE:CZ	2.52	0.45
1:A:138:ASN:HB3	1:A:141:VAL:HG22	1.98	0.45
1:C:73:PRO:HB3	1:D:1:MET:HE1	1.99	0.45
1:D:600:THR:O	1:D:603:CYS:HB2	2.17	0.45
1:E:512:MET:HE3	1:E:516:ASP:HB3	1.99	0.45
1:F:551:ALA:O	3:F:802:G3F:O1	2.33	0.45
1:H:414:TRP:CD1	1:H:414:TRP:C	2.95	0.45
1:B:407:PRO:HD2	1:B:408:TRP:CE3	2.52	0.44
1:F:42:VAL:HG11	1:F:304:VAL:HG11	1.99	0.44
1:H:283:CYS:HA	1:H:304:VAL:HG22	1.98	0.44
1:H:574:LYS:HE2	1:H:574:LYS:HB3	1.88	0.44
1:A:436:ASP:HA	1:A:437:PRO:HD3	1.77	0.44
1:C:31:LEU:HD11	1:C:606:ILE:HG12	1.98	0.44
1:F:430:ILE:HA	1:F:431:PRO:HD3	1.72	0.44
1:F:600:THR:O	1:F:603:CYS:HB2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:PHE:C	1:A:2:PHE:CD2	2.95	0.44
1:A:122:ASN:OD1	1:A:122:ASN:N	2.50	0.44
1:A:377:PRO:O	1:A:381:LYS:HE2	2.17	0.44
2:B:801:FAD:H1'1	2:B:801:FAD:H9	1.69	0.44
1:C:246:ARG:NH1	1:C:250:PRO:O	2.48	0.44
1:G:263:GLU:O	1:G:267:THR:HG22	2.18	0.44
1:H:259:ASP:OD1	1:H:260:ARG:N	2.51	0.44
1:H:284:THR:HB	1:H:303:LEU:HD23	1.99	0.44
1:A:301:TYR:CE1	1:A:322:LYS:HE3	2.52	0.44
1:C:301:TYR:H	1:C:301:TYR:HD2	1.64	0.44
1:D:55:MET:CE	1:D:272:ARG:HD2	2.48	0.44
1:B:133:LYS:O	1:B:135:PRO:HD3	2.18	0.44
1:C:224:TYR:CZ	1:C:534:ILE:HG12	2.53	0.44
1:E:52:SER:HB3	1:E:71:GLN:HE21	1.83	0.44
1:G:55:MET:HE1	1:G:272:ARG:HD2	1.99	0.44
1:G:107:THR:HG22	1:G:133:LYS:HB2	1.98	0.44
1:G:450:PRO:HD2	1:G:451:TRP:CZ3	2.53	0.44
1:H:78:HIS:ND1	1:H:80:LYS:HB2	2.33	0.44
1:A:159:TRP:HA	2:A:801:FAD:C6	2.47	0.44
1:G:382:TYR:HA	1:G:486:GLN:O	2.18	0.44
1:A:303:LEU:HD12	1:A:303:LEU:HA	1.72	0.44
1:C:373:THR:HG21	1:C:379:LEU:HD23	1.99	0.44
1:C:421:HIS:ND1	1:C:433:PRO:HA	2.33	0.44
1:D:325:ALA:N	1:D:328:TYR:OH	2.36	0.44
1:E:240:LEU:HA	1:E:241:PRO:HD3	1.75	0.44
1:H:301:TYR:HB3	1:H:324:TYR:CE2	2.53	0.44
1:A:202:GLU:O	1:A:260:ARG:NH2	2.51	0.43
1:B:445:PHE:CD1	1:B:445:PHE:C	2.96	0.43
1:C:301:TYR:CD2	1:C:301:TYR:N	2.85	0.43
1:A:1:MET:SD	1:A:2:PHE:N	2.91	0.43
1:B:22:GLY:HA3	2:B:801:FAD:O1P	2.18	0.43
1:G:214:SER:HB2	1:G:437:PRO:HB2	2.00	0.43
1:C:432:ILE:HA	1:C:433:PRO:HD3	1.80	0.43
1:C:533:LYS:NZ	4:C:908:HOH:O	2.50	0.43
1:D:225:ASN:O	1:D:229:GLN:HG2	2.19	0.43
1:G:11:ASP:OD2	1:G:12:GLU:HG3	2.18	0.43
1:G:564:THR:HG23	1:G:576:HIS:CE1	2.53	0.43
1:A:292:ARG:HA	1:A:293:PRO:HD3	1.87	0.43
1:C:14:TYR:HB2	1:C:325:ALA:HB2	2.01	0.43
1:C:166:PHE:CZ	1:C:597:PRO:HA	2.54	0.43
1:C:430:ILE:HA	1:C:431:PRO:HD2	1.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:345:HIS:HD2	1:D:374:PRO:HD2	1.83	0.43
1:G:282:ARG:HB2	1:G:307:LEU:HD11	2.01	0.43
1:G:291:TYR:CE1	1:G:347:PRO:HB3	2.54	0.43
1:G:442:THR:OG1	1:G:443:ILE:N	2.51	0.43
1:H:246:ARG:NH1	1:H:250:PRO:O	2.51	0.43
1:A:84:GLU:HG2	4:A:933:HOH:O	2.19	0.43
1:B:51:THR:HB	1:B:77:TYR:CD1	2.53	0.43
1:B:394:VAL:HA	1:B:473:VAL:O	2.19	0.43
1:B:560:CYS:HB3	1:B:570:ASN:O	2.18	0.43
1:C:24:ILE:HG22	1:C:331:ALA:HB1	1.99	0.43
1:E:52:SER:HB2	1:F:2:PHE:H	1.84	0.43
1:E:282:ARG:NE	1:E:284:THR:OG1	2.51	0.43
1:F:80:LYS:HD2	1:F:89:ILE:HD11	2.01	0.43
1:F:341:LEU:O	1:F:344:SER:HB2	2.17	0.43
1:G:237:PHE:CE2	1:G:443:ILE:HD11	2.53	0.43
1:H:447:GLU:O	1:H:450:PRO:HG3	2.18	0.43
1:A:505:GLN:OE1	1:A:506:PRO:HD2	2.19	0.43
1:H:23:PRO:HD3	1:H:156:SER:HB3	2.01	0.43
1:B:205:GLY:HA3	1:B:256:HIS:ND1	2.34	0.43
1:C:345:HIS:HD2	1:C:374:PRO:HD2	1.84	0.43
1:C:596:ASN:HA	1:C:597:PRO:HD3	1.92	0.43
1:E:84:GLU:HG3	4:F:925:HOH:O	2.19	0.43
1:F:6:THR:HA	1:F:7:PRO:HD3	1.88	0.43
2:G:801:FAD:O4'	2:G:801:FAD:O2'	2.35	0.43
1:H:249:ASP:HB3	1:H:252:TYR:HD1	1.84	0.43
1:A:14:TYR:CE2	1:A:40:CYS:HB2	2.54	0.43
1:C:26:ALA:HB2	1:C:258:THR:HG23	1.99	0.43
1:C:55:MET:HG3	1:C:267:THR:O	2.18	0.43
1:D:385:GLU:OE2	1:D:553:HIS:N	2.51	0.43
1:F:123:SER:HA	1:G:140:PHE:CD2	2.53	0.43
1:G:568:VAL:HA	4:G:933:HOH:O	2.18	0.43
1:C:134:ASN:HA	1:C:135:PRO:HD3	1.85	0.43
1:C:240:LEU:HA	1:C:241:PRO:HD3	1.93	0.43
1:C:287:VAL:HG11	1:C:301:TYR:HE2	1.84	0.43
1:F:143:LEU:HD23	1:F:143:LEU:HA	1.86	0.43
1:G:4:ASP:O	1:G:272:ARG:NH2	2.52	0.43
1:H:264:GLU:OE1	1:H:271:LYS:HE2	2.19	0.43
1:A:11:ASP:OD2	1:E:570:ASN:HB2	2.18	0.43
1:C:326:ARG:NH2	1:C:616:PHE:HD1	2.17	0.43
1:C:347:PRO:HA	1:C:348:PRO:HD3	1.89	0.43
1:D:330:VAL:HG11	1:D:337:THR:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:292:ARG:HA	1:E:293:PRO:HD2	1.82	0.43
1:B:138:ASN:HB3	1:B:141:VAL:HG22	2.00	0.42
1:B:443:ILE:HD12	1:B:453:VAL:HG21	2.00	0.42
1:D:182:LEU:HD23	1:D:182:LEU:HA	1.71	0.42
1:E:396:ASP:HA	1:F:119:VAL:HA	2.01	0.42
1:G:204:ILE:HD12	1:G:204:ILE:HA	1.77	0.42
1:B:21:SER:OG	1:B:152:VAL:HA	2.19	0.42
1:H:224:TYR:HB3	1:H:237:PHE:CD1	2.54	0.42
1:H:289:LYS:HD3	1:H:298:GLU:HB2	2.01	0.42
1:H:399:LEU:HD23	1:H:399:LEU:HA	1.80	0.42
1:A:390:PHE:HB3	1:A:546:MET:CE	2.47	0.42
1:B:446:THR:HB	1:B:448:GLU:HG2	2.00	0.42
1:C:416:GLU:O	1:C:420:ARG:HG3	2.18	0.42
1:D:204:ILE:HD12	1:D:204:ILE:HA	1.74	0.42
1:H:5:THR:HB	1:H:275:PHE:O	2.19	0.42
1:A:297:ASN:O	1:A:578:PHE:HA	2.19	0.42
1:B:449:HIS:O	1:B:451:TRP:N	2.47	0.42
1:G:228:PHE:CD2	1:G:231:GLU:HG3	2.54	0.42
1:H:159:TRP:HA	2:H:801:FAD:C6	2.48	0.42
1:A:308:LEU:HA	1:A:309:PRO:HD2	1.79	0.42
1:F:240:LEU:HD23	1:F:242:LEU:HD21	2.00	0.42
1:F:298:GLU:HG2	1:F:580:ASN:CG	2.44	0.42
1:F:321:LYS:HD3	1:F:321:LYS:HA	1.66	0.42
1:G:379:LEU:HD11	1:G:558:THR:HG22	2.01	0.42
1:A:88:ASP:OD2	1:A:91:ARG:HG3	2.20	0.42
1:A:326:ARG:NH2	1:A:616:PHE:HB3	2.35	0.42
1:C:50:PHE:HA	1:C:74:ILE:O	2.20	0.42
1:E:120:VAL:HG23	1:F:395:LEU:O	2.19	0.42
1:H:16:VAL:HG21	1:H:32:CYS:SG	2.60	0.42
1:A:452:HIS:HB3	1:A:480:PHE:HB2	2.00	0.42
2:A:801:FAD:HM71	2:A:801:FAD:HM83	1.81	0.42
1:B:237:PHE:CE2	1:B:443:ILE:HD11	2.55	0.42
1:B:264:GLU:HA	1:B:267:THR:HG22	2.02	0.42
1:B:285:LYS:HB2	1:B:344:SER:HA	2.02	0.42
1:D:43:GLU:O	1:D:280:ASN:N	2.52	0.42
1:G:159:TRP:HA	2:G:801:FAD:C6	2.50	0.42
1:H:332:CYS:O	1:H:336:ALA:HB3	2.19	0.42
1:H:444:LYS:HE3	1:H:444:LYS:HB2	1.85	0.42
1:A:345:HIS:CD2	1:A:373:THR:HA	2.55	0.42
1:A:448:GLU:OE1	1:A:448:GLU:N	2.53	0.42
1:B:197:TYR:O	1:B:201:LYS:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:457:ARG:HD3	1:B:474:ILE:O	2.20	0.42
1:C:448:GLU:N	1:C:448:GLU:OE2	2.53	0.42
1:E:120:VAL:HA	1:F:397:SER:HB3	2.02	0.42
1:F:124:LEU:HD12	1:F:124:LEU:HA	1.62	0.42
1:F:559:ARG:NH1	1:F:566:LYS:O	2.52	0.42
1:G:328:TYR:N	1:G:580:ASN:O	2.52	0.42
1:H:55:MET:HE1	1:H:272:ARG:NH1	2.33	0.42
2:H:801:FAD:HM71	2:H:801:FAD:HM83	1.81	0.42
1:B:179:ARG:HA	1:B:180:PRO:HD3	1.82	0.42
1:B:185:ASP:HB3	1:B:188:GLU:HB3	2.01	0.42
1:C:223:LYS:HD2	1:C:223:LYS:HA	1.90	0.42
1:F:204:ILE:HD12	1:F:204:ILE:HA	1.66	0.42
1:H:406:PRO:HA	1:H:407:PRO:HD3	1.94	0.42
1:B:512:MET:HG2	1:B:516:ASP:HB3	2.02	0.42
1:D:162:ALA:HA	1:D:242:LEU:HD23	2.01	0.42
1:D:436:ASP:HA	1:D:437:PRO:HD3	1.89	0.42
1:D:560:CYS:SG	1:D:588:VAL:HB	2.60	0.42
1:H:240:LEU:HD12	1:H:241:PRO:HD2	2.01	0.42
1:C:299:VAL:HB	1:C:580:ASN:ND2	2.35	0.41
1:D:1:MET:CE	1:D:3:LEU:HD23	2.47	0.41
1:D:382:TYR:HB2	1:D:559:ARG:HD2	2.02	0.41
1:F:142:ASN:ND2	1:F:144:GLY:HA2	2.35	0.41
1:G:131:LEU:HG	1:H:434:PHE:CD1	2.55	0.41
1:F:336:ALA:HA	1:F:339:GLN:HB3	2.02	0.41
1:G:403:VAL:HA	1:G:414:TRP:HZ2	1.83	0.41
1:H:44:ILE:HD12	1:H:282:ARG:HG3	2.02	0.41
1:A:388:MET:HA	1:A:479:PHE:O	2.20	0.41
1:B:430:ILE:HD13	1:B:473:VAL:HG13	2.01	0.41
1:C:8:PHE:HA	1:C:14:TYR:OH	2.20	0.41
1:C:200:ALA:HA	1:C:203:ILE:HD12	2.02	0.41
1:D:486:GLN:N	4:D:949:HOH:O	2.47	0.41
1:F:117:PRO:O	1:G:517:ARG:NH1	2.52	0.41
1:B:345:HIS:HD2	1:B:374:PRO:HD2	1.84	0.41
1:E:178:GLU:HG2	1:E:593:PHE:HA	2.03	0.41
1:F:116:ASP:O	1:F:119:VAL:HG22	2.20	0.41
1:F:116:ASP:HA	1:F:117:PRO:HD3	1.95	0.41
2:F:801:FAD:H9	2:F:801:FAD:H1'1	1.85	0.41
1:G:428:ASP:HB2	1:H:129:ILE:HD12	2.01	0.41
1:A:301:TYR:CZ	1:A:322:LYS:HE3	2.55	0.41
1:A:399:LEU:O	1:A:402:VAL:HB	2.20	0.41
1:E:526:ASP:O	1:E:530:ILE:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:234:ILE:O	1:H:235:ARG:HD2	2.20	0.41
1:H:256:HIS:HB3	1:H:260:ARG:HD3	2.02	0.41
1:B:292:ARG:HA	1:B:293:PRO:HD3	1.75	0.41
1:C:282:ARG:HB2	1:C:307:LEU:HD11	2.02	0.41
1:C:327:SER:HA	1:C:580:ASN:HB2	2.02	0.41
1:F:372:PRO:C	1:F:374:PRO:HD3	2.46	0.41
1:F:598:THR:O	1:F:602:ILE:HG13	2.21	0.41
1:G:22:GLY:HA3	2:G:801:FAD:O1P	2.20	0.41
1:C:3:LEU:HD13	1:C:277:LEU:HG	2.03	0.41
1:C:48:ASP:HB2	1:C:79:LYS:HE2	2.03	0.41
1:B:146:GLU:OE1	1:B:552:LEU:HA	2.21	0.41
1:C:47:ALA:HB1	1:C:50:PHE:CZ	2.55	0.41
1:E:123:SER:OG	1:E:126:LYS:HB2	2.21	0.41
1:G:421:HIS:ND1	1:G:433:PRO:HA	2.35	0.41
1:A:52:SER:HB2	1:B:1:MET:HA	2.03	0.41
1:B:118:SER:HB2	1:C:521:ARG:NH2	2.36	0.41
1:B:219:LEU:O	1:B:223:LYS:HB2	2.20	0.41
1:C:26:ALA:CB	1:C:258:THR:HG23	2.51	0.41
1:C:203:ILE:HA	4:C:937:HOH:O	2.21	0.41
1:C:204:ILE:HD12	1:C:204:ILE:HA	1.96	0.41
1:C:278:LEU:O	1:C:281:HIS:HB2	2.21	0.41
1:C:372:PRO:C	1:C:374:PRO:HD3	2.46	0.41
1:C:600:THR:O	1:C:603:CYS:HB2	2.21	0.41
1:D:319:SER:O	1:D:319:SER:OG	2.33	0.41
1:D:414:TRP:CD1	1:D:414:TRP:C	2.99	0.41
2:D:801:FAD:HM71	2:D:801:FAD:HM83	1.92	0.41
1:G:82:GLU:HA	4:G:921:HOH:O	2.21	0.41
1:B:430:ILE:HG22	1:B:432:ILE:H	1.85	0.41
1:C:52:SER:HB3	1:C:71:GLN:OE1	2.20	0.41
1:D:391:CYS:SG	1:D:527:MET:HE3	2.61	0.41
1:E:214:SER:HB3	1:E:217:HIS:HB3	2.03	0.41
1:E:406:PRO:HG3	1:E:414:TRP:CE2	2.56	0.41
1:E:434:PHE:CD1	1:F:131:LEU:HG	2.55	0.41
1:H:527:MET:HE2	1:H:527:MET:HB3	1.99	0.41
1:B:137:GLN:NE2	4:B:926:HOH:O	2.54	0.40
1:C:6:THR:HA	1:C:7:PRO:HD3	1.80	0.40
1:E:498:ARG:HH21	1:E:504:PRO:HB3	1.85	0.40
1:F:20:GLY:O	1:F:41:MET:HE2	2.20	0.40
1:H:417:LYS:HG2	1:H:420:ARG:NH2	2.36	0.40
1:H:417:LYS:HG2	1:H:420:ARG:HH21	1.86	0.40
1:A:215:ILE:N	1:A:436:ASP:OD1	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:TYR:HA	1:A:486:GLN:O	2.21	0.40
1:B:558:THR:O	1:B:588:VAL:HA	2.21	0.40
1:B:570:ASN:ND2	1:B:574:LYS:HB3	2.36	0.40
1:C:301:TYR:HD2	1:C:301:TYR:N	2.19	0.40
1:F:593:PHE:CE1	1:F:597:PRO:HB3	2.56	0.40
1:G:4:ASP:OD2	1:G:4:ASP:N	2.50	0.40
1:H:333:GLY:HA2	4:H:952:HOH:O	2.21	0.40
1:E:51:THR:HB	1:E:77:TYR:CD1	2.56	0.40
1:F:298:GLU:HG2	1:F:580:ASN:ND2	2.36	0.40
1:G:14:TYR:O	1:G:325:ALA:HA	2.21	0.40
1:G:51:THR:HB	1:G:77:TYR:CD1	2.57	0.40
1:G:264:GLU:HA	1:G:267:THR:HG22	2.02	0.40
1:G:290:HIS:HE1	1:G:295:GLU:HG2	1.80	0.40
1:B:436:ASP:HA	1:B:437:PRO:HD3	1.82	0.40
1:G:162:ALA:HA	1:G:242:LEU:HD23	2.03	0.40
1:G:223:LYS:HD2	1:G:223:LYS:HA	1.90	0.40
1:G:558:THR:O	1:G:558:THR:OG1	2.38	0.40
1:C:345:HIS:CD2	1:C:373:THR:HA	2.57	0.40
1:E:345:HIS:CD2	1:E:373:THR:HA	2.57	0.40
1:G:278:LEU:HB3	1:G:281:HIS:CD2	2.57	0.40
1:G:461:SER:HB2	4:G:987:HOH:O	2.22	0.40
1:H:168:ALA:HA	1:H:169:PRO:HD2	1.96	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	568/621 (92%)	548 (96%)	20 (4%)	0	100	100
1	B	570/621 (92%)	547 (96%)	23 (4%)	0	100	100
1	C	570/621 (92%)	539 (95%)	31 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	570/621 (92%)	530 (93%)	39 (7%)	1 (0%)	43	58
1	E	568/621 (92%)	545 (96%)	22 (4%)	1 (0%)	43	58
1	F	570/621 (92%)	552 (97%)	18 (3%)	0	100	100
1	G	570/621 (92%)	546 (96%)	24 (4%)	0	100	100
1	H	570/621 (92%)	545 (96%)	25 (4%)	0	100	100
All	All	4556/4968 (92%)	4352 (96%)	202 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	407	PRO
1	D	597	PRO

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	495/529 (94%)	480 (97%)	15 (3%)	36	58
1	B	497/529 (94%)	473 (95%)	24 (5%)	23	40
1	C	497/529 (94%)	467 (94%)	30 (6%)	17	31
1	D	497/529 (94%)	474 (95%)	23 (5%)	24	41
1	E	495/529 (94%)	473 (96%)	22 (4%)	25	43
1	F	497/529 (94%)	472 (95%)	25 (5%)	22	38
1	G	497/529 (94%)	470 (95%)	27 (5%)	20	35
1	H	497/529 (94%)	468 (94%)	29 (6%)	18	32
All	All	3972/4232 (94%)	3777 (95%)	195 (5%)	22	39

All (195) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET

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Mol	Chain	Res	Type
1	A	30	LYS
1	A	31	LEU
1	A	118	SER
1	A	229	GLN
1	A	267	THR
1	A	270	VAL
1	A	305	GLU
1	A	393	VAL
1	A	412	ASP
1	A	420	ARG
1	A	453	VAL
1	A	486	GLN
1	A	502	ASP
1	A	596	ASN
1	B	1	MET
1	B	16	VAL
1	B	38	ARG
1	B	42	VAL
1	B	52	SER
1	B	72	VAL
1	B	82	GLU
1	B	83	ILE
1	B	195	ASP
1	B	214	SER
1	B	234	ILE
1	B	238	SER
1	B	265	LEU
1	B	267	THR
1	B	303	LEU
1	B	326	ARG
1	B	393	VAL
1	B	398	SER
1	B	405	ASN
1	B	414	TRP
1	B	453	VAL
1	B	502	ASP
1	B	590	GLU
1	B	596	ASN
1	C	6	THR
1	C	48	ASP
1	C	49	SER
1	C	74	ILE

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Mol	Chain	Res	Type
1	C	101	SER
1	C	125	ASP
1	C	131	LEU
1	C	157	THR
1	C	160	THR
1	C	184	THR
1	C	227	ILE
1	C	232	ASN
1	C	254	GLU
1	C	260	ARG
1	C	295	GLU
1	C	301	TYR
1	C	414	TRP
1	C	447	GLU
1	C	453	VAL
1	C	456	HIS
1	C	467	GLU
1	C	509	LYS
1	C	514	GLN
1	C	515	ASP
1	C	568	VAL
1	C	579	ASN
1	C	591	THR
1	C	596	ASN
1	C	609	SER
1	C	615	LYS
1	D	49	SER
1	D	89	ILE
1	D	156	SER
1	D	160	THR
1	D	204	ILE
1	D	214	SER
1	D	229	GLN
1	D	231	GLU
1	D	238	SER
1	D	258	THR
1	D	267	THR
1	D	276	THR
1	D	303	LEU
1	D	305	GLU
1	D	414	TRP
1	D	453	VAL

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Mol	Chain	Res	Type
1	D	498	ARG
1	D	514	GLN
1	D	559	ARG
1	D	577	ASN
1	D	579	ASN
1	D	596	ASN
1	D	615	LYS
1	E	11	ASP
1	E	24	ILE
1	E	52	SER
1	E	74	ILE
1	E	83	ILE
1	E	112	ILE
1	E	125	ASP
1	E	149	THR
1	E	234	ILE
1	E	236	GLU
1	E	260	ARG
1	E	284	THR
1	E	414	TRP
1	E	435	ARG
1	E	453	VAL
1	E	467	GLU
1	E	498	ARG
1	E	502	ASP
1	E	509	LYS
1	E	514	GLN
1	E	579	ASN
1	E	588	VAL
1	F	53	LYS
1	F	72	VAL
1	F	74	ILE
1	F	89	ILE
1	F	125	ASP
1	F	149	THR
1	F	191	ARG
1	F	204	ILE
1	F	214	SER
1	F	223	LYS
1	F	232	ASN
1	F	236	GLU
1	F	248	THR

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Mol	Chain	Res	Type
1	F	260	ARG
1	F	272	ARG
1	F	295	GLU
1	F	298	GLU
1	F	320	VAL
1	F	321	LYS
1	F	405	ASN
1	F	423	GLU
1	F	453	VAL
1	F	465	VAL
1	F	564	THR
1	F	596	ASN
1	G	4	ASP
1	G	21	SER
1	G	24	ILE
1	G	112	ILE
1	G	123	SER
1	G	131	LEU
1	G	160	THR
1	G	194	LYS
1	G	204	ILE
1	G	214	SER
1	G	259	ASP
1	G	260	ARG
1	G	277	LEU
1	G	295	GLU
1	G	300	ASP
1	G	308	LEU
1	G	321	LYS
1	G	366	GLU
1	G	367	ARG
1	G	393	VAL
1	G	401	GLU
1	G	405	ASN
1	G	414	TRP
1	G	416	GLU
1	G	435	ARG
1	G	453	VAL
1	G	588	VAL
1	H	9	ARG
1	H	11	ASP
1	H	71	GLN

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Mol	Chain	Res	Type
1	H	118	SER
1	H	125	ASP
1	H	178	GLU
1	H	188	GLU
1	H	197	TYR
1	H	209	THR
1	H	226	ASP
1	H	248	THR
1	H	263	GLU
1	H	300	ASP
1	H	303	LEU
1	H	308	LEU
1	H	320	VAL
1	H	366	GLU
1	H	367	ARG
1	H	414	TRP
1	H	427	ASN
1	H	465	VAL
1	H	467	GLU
1	H	484	GLU
1	H	515	ASP
1	H	530	ILE
1	H	554	LEU
1	H	564	THR
1	H	596	ASN
1	H	601	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	111	HIS
1	A	392	GLN
1	A	405	ASN
1	A	468	ASN
1	A	486	GLN
1	A	495	GLN
1	A	505	GLN
1	A	565	GLN
1	B	94	ASN
1	B	110	ASN
1	B	213	HIS

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Mol	Chain	Res	Type
1	B	405	ASN
1	B	452	HIS
1	B	496	HIS
1	B	529	ASN
1	C	110	ASN
1	C	111	HIS
1	C	345	HIS
1	C	529	ASN
1	D	280	ASN
1	D	392	GLN
1	D	572	HIS
1	D	586	ASN
1	E	71	GLN
1	E	94	ASN
1	E	494	GLN
1	E	496	HIS
1	E	579	ASN
1	F	71	GLN
1	F	94	ASN
1	F	142	ASN
1	F	405	ASN
1	F	427	ASN
1	F	449	HIS
1	F	544	GLN
1	G	94	ASN
1	G	110	ASN
1	G	213	HIS
1	G	345	HIS
1	G	392	GLN
1	G	456	HIS
1	G	576	HIS
1	H	94	ASN
1	H	280	ASN
1	H	405	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 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	H	801	-	58,58,58	1.15	7 (12%)	85,89,89	1.53	14 (16%)
2	FAD	C	801	-	58,58,58	1.14	7 (12%)	85,89,89	1.65	18 (21%)
2	FAD	G	801	-	58,58,58	1.16	6 (10%)	85,89,89	1.51	15 (17%)
3	G3F	G	802	-	12,12,12	2.19	6 (50%)	17,17,17	1.33	1 (5%)
2	FAD	E	801	-	58,58,58	1.05	5 (8%)	85,89,89	1.58	13 (15%)
3	G3F	C	802	-	12,12,12	1.94	5 (41%)	17,17,17	1.48	2 (11%)
3	G3F	F	802	-	12,12,12	1.89	4 (33%)	17,17,17	1.21	2 (11%)
2	FAD	B	801	-	58,58,58	1.18	7 (12%)	85,89,89	1.65	17 (20%)
3	G3F	A	802	-	12,12,12	2.49	7 (58%)	17,17,17	1.62	3 (17%)
3	G3F	B	802	-	12,12,12	2.17	4 (33%)	17,17,17	1.63	3 (17%)
3	G3F	H	802	-	12,12,12	1.96	4 (33%)	17,17,17	0.90	1 (5%)
2	FAD	A	801	-	58,58,58	1.14	9 (15%)	85,89,89	1.60	18 (21%)
2	FAD	F	801	-	58,58,58	1.14	5 (8%)	85,89,89	1.73	20 (23%)
3	G3F	D	802	-	12,12,12	1.99	4 (33%)	17,17,17	1.81	3 (17%)
2	FAD	D	801	-	58,58,58	1.06	3 (5%)	85,89,89	1.57	17 (20%)
3	G3F	E	802	-	12,12,12	2.09	6 (50%)	17,17,17	1.38	2 (11%)

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	H	801	-	-	1/34/50/50	0/6/6/6
2	FAD	C	801	-	-	2/34/50/50	0/6/6/6
2	FAD	G	801	-	-	0/34/50/50	0/6/6/6
3	G3F	G	802	-	-	0/2/22/22	0/1/1/1
2	FAD	E	801	-	-	1/34/50/50	0/6/6/6
3	G3F	C	802	-	-	0/2/22/22	0/1/1/1
3	G3F	F	802	-	-	0/2/22/22	0/1/1/1
2	FAD	B	801	-	-	0/34/50/50	0/6/6/6
3	G3F	A	802	-	-	0/2/22/22	0/1/1/1
3	G3F	B	802	-	-	0/2/22/22	0/1/1/1
3	G3F	H	802	-	-	0/2/22/22	0/1/1/1
2	FAD	A	801	-	-	2/34/50/50	0/6/6/6
2	FAD	F	801	-	-	3/34/50/50	0/6/6/6
3	G3F	D	802	-	-	0/2/22/22	0/1/1/1
2	FAD	D	801	-	-	3/34/50/50	0/6/6/6
3	G3F	E	802	-	-	0/2/22/22	0/1/1/1

All (89) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	G3F	C3-C2	-4.62	1.48	1.52
2	B	801	FAD	C4X-N5	4.29	1.40	1.30
3	B	802	G3F	C3-C2	-4.01	1.48	1.52
3	A	802	G3F	F3-C3	-3.97	1.32	1.40
3	E	802	G3F	F3-C3	-3.78	1.32	1.40
3	G	802	G3F	F3-C3	-3.69	1.33	1.40
3	D	802	G3F	F3-C3	-3.67	1.33	1.40
3	F	802	G3F	F3-C3	-3.63	1.33	1.40
3	C	802	G3F	F3-C3	-3.59	1.33	1.40
3	H	802	G3F	F3-C3	-3.53	1.33	1.40
3	B	802	G3F	F3-C3	-3.41	1.33	1.40
2	G	801	FAD	C4X-N5	3.39	1.38	1.30
2	F	801	FAD	C4X-N5	3.35	1.38	1.30
3	G	802	G3F	C3-C2	-3.34	1.49	1.52
2	H	801	FAD	C4X-N5	3.33	1.38	1.30
2	D	801	FAD	C4X-N5	3.32	1.37	1.30
2	E	801	FAD	C4X-N5	3.20	1.37	1.30
3	A	802	G3F	C3-C4	-3.13	1.49	1.52
2	C	801	FAD	C4X-N5	3.11	1.37	1.30
3	F	802	G3F	O5-C5	-3.03	1.37	1.44
3	B	802	G3F	O5-C5	-3.00	1.37	1.44
2	A	801	FAD	C4X-N5	2.95	1.37	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	802	G3F	O5-C5	-2.93	1.37	1.44
3	A	802	G3F	O5-C5	-2.85	1.37	1.44
2	G	801	FAD	P-O3P	2.85	1.62	1.59
3	G	802	G3F	O5-C5	-2.83	1.37	1.44
2	H	801	FAD	C2A-N1A	2.80	1.38	1.33
2	C	801	FAD	PA-O3P	2.79	1.62	1.59
2	F	801	FAD	C2A-N3A	2.77	1.38	1.33
2	C	801	FAD	C2A-N1A	2.76	1.38	1.33
3	D	802	G3F	O5-C5	-2.74	1.37	1.44
3	G	802	G3F	C3-C4	-2.73	1.50	1.52
3	C	802	G3F	O5-C5	-2.73	1.37	1.44
2	D	801	FAD	C2A-N1A	2.67	1.38	1.33
3	H	802	G3F	O5-C5	-2.67	1.37	1.44
3	H	802	G3F	C3-C2	-2.66	1.50	1.52
2	B	801	FAD	C2A-N3A	2.63	1.38	1.33
2	A	801	FAD	C2A-N1A	2.63	1.38	1.33
2	B	801	FAD	C5A-N7A	-2.62	1.34	1.39
2	G	801	FAD	C10-N1	2.59	1.38	1.33
3	E	802	G3F	C3-C2	-2.55	1.50	1.52
3	C	802	G3F	C3-C2	-2.51	1.50	1.52
2	G	801	FAD	C2A-N3A	2.44	1.38	1.33
2	B	801	FAD	C2A-N1A	2.44	1.38	1.33
2	F	801	FAD	C2A-N1A	2.43	1.38	1.33
2	B	801	FAD	C8A-N7A	2.43	1.36	1.31
2	D	801	FAD	C2A-N3A	2.43	1.38	1.33
3	D	802	G3F	C3-C4	-2.42	1.50	1.52
2	H	801	FAD	C8A-N7A	2.41	1.36	1.31
2	H	801	FAD	P-O3P	2.40	1.62	1.59
2	H	801	FAD	C2A-N3A	2.38	1.38	1.33
2	G	801	FAD	C2A-N1A	2.35	1.38	1.33
2	H	801	FAD	C10-N1	2.33	1.37	1.33
3	D	802	G3F	O4-C4	-2.33	1.37	1.43
3	A	802	G3F	O5-C1	-2.33	1.37	1.42
2	B	801	FAD	C10-N1	2.31	1.37	1.33
3	H	802	G3F	C3-C4	-2.29	1.50	1.52
3	E	802	G3F	O2-C2	-2.29	1.37	1.43
2	A	801	FAD	C2A-N3A	2.28	1.38	1.33
2	A	801	FAD	C5A-N7A	-2.27	1.34	1.39
2	A	801	FAD	C8A-N7A	2.26	1.36	1.31
2	H	801	FAD	PA-O3P	2.25	1.61	1.59
2	E	801	FAD	C2A-N3A	2.24	1.37	1.33
3	A	802	G3F	O4-C4	-2.24	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	FAD	P-O3P	2.24	1.61	1.59
3	B	802	G3F	O2-C2	-2.21	1.37	1.43
2	C	801	FAD	C2A-N3A	2.20	1.37	1.33
3	E	802	G3F	O5-C1	-2.18	1.37	1.42
2	F	801	FAD	C2'-C3'	-2.18	1.49	1.53
3	A	802	G3F	O2-C2	-2.13	1.37	1.43
2	E	801	FAD	C2A-N1A	2.13	1.37	1.33
3	C	802	G3F	O4-C4	-2.13	1.37	1.43
2	C	801	FAD	C8A-N7A	2.12	1.35	1.31
2	E	801	FAD	C5'-C4'	2.11	1.54	1.51
2	C	801	FAD	C9A-N10	-2.10	1.37	1.41
2	E	801	FAD	C10-N1	2.09	1.37	1.33
2	F	801	FAD	C10-N1	2.06	1.37	1.33
2	A	801	FAD	PA-O3P	2.05	1.61	1.59
2	G	801	FAD	C8A-N7A	2.05	1.35	1.31
3	E	802	G3F	C3-C4	-2.05	1.50	1.52
3	F	802	G3F	O5-C1	-2.05	1.37	1.42
2	A	801	FAD	C10-N1	2.03	1.37	1.33
2	A	801	FAD	C4X-C4	-2.03	1.37	1.44
3	G	802	G3F	O2-C2	-2.03	1.37	1.43
3	C	802	G3F	O2-C2	-2.02	1.37	1.43
2	C	801	FAD	C4X-C10	-2.01	1.38	1.44
3	G	802	G3F	O5-C1	-2.01	1.38	1.42
2	A	801	FAD	P-O3P	2.01	1.61	1.59
3	F	802	G3F	O4-C4	-2.00	1.38	1.43

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	801	FAD	N3A-C2A-N1A	-5.84	119.75	128.58
2	C	801	FAD	N3A-C2A-N1A	-5.80	119.80	128.58
2	E	801	FAD	N3A-C2A-N1A	-5.80	119.80	128.58
2	G	801	FAD	N3A-C2A-N1A	-5.80	119.81	128.58
2	F	801	FAD	N3A-C2A-N1A	-5.44	120.35	128.58
2	D	801	FAD	N3A-C2A-N1A	-5.34	120.50	128.58
2	A	801	FAD	N3A-C2A-N1A	-5.29	120.57	128.58
2	B	801	FAD	N3A-C2A-N1A	-5.19	120.73	128.58
2	F	801	FAD	N9A-C8A-N7A	-5.11	106.68	113.94
3	A	802	G3F	F3-C3-C4	5.05	113.19	108.81
2	B	801	FAD	C5A-C4A-N3A	-4.91	119.95	126.72
3	D	802	G3F	C4-C3-C2	-4.78	105.96	111.50
2	E	801	FAD	N9A-C8A-N7A	-4.62	107.39	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	801	FAD	C5A-C4A-N3A	-4.49	120.53	126.72
2	F	801	FAD	C5A-N7A-C8A	4.38	110.33	103.45
2	B	801	FAD	N9A-C8A-N7A	-4.29	107.85	113.94
2	B	801	FAD	C5A-N7A-C8A	4.24	110.11	103.45
2	E	801	FAD	C5A-C4A-N3A	-4.21	120.92	126.72
2	A	801	FAD	C5A-C4A-N3A	-4.18	120.96	126.72
2	D	801	FAD	N9A-C8A-N7A	-4.14	108.06	113.94
2	H	801	FAD	N9A-C8A-N7A	-4.13	108.08	113.94
3	B	802	G3F	F3-C3-C4	4.10	112.37	108.81
2	D	801	FAD	C5A-C4A-N3A	-4.09	121.09	126.72
2	E	801	FAD	C5A-N7A-C8A	4.04	109.80	103.45
2	C	801	FAD	N9A-C8A-N7A	-4.02	108.23	113.94
2	H	801	FAD	C5A-C4A-N3A	-4.01	121.19	126.72
2	G	801	FAD	C5A-C4A-N3A	-3.86	121.40	126.72
3	C	802	G3F	F3-C3-C4	3.81	112.11	108.81
3	G	802	G3F	C4-C3-C2	-3.81	107.08	111.50
2	C	801	FAD	C5A-C4A-N3A	-3.80	121.48	126.72
3	D	802	G3F	F3-C3-C2	3.69	112.01	108.81
2	H	801	FAD	C5A-N7A-C8A	3.61	109.12	103.45
2	G	801	FAD	N9A-C8A-N7A	-3.60	108.82	113.94
3	E	802	G3F	C4-C3-C2	-3.60	107.32	111.50
2	C	801	FAD	C4X-C10-N10	3.60	121.64	116.48
2	A	801	FAD	N9A-C8A-N7A	-3.56	108.89	113.94
2	B	801	FAD	C4A-C5A-N7A	-3.55	106.52	110.58
2	A	801	FAD	C5A-N7A-C8A	3.54	109.02	103.45
2	E	801	FAD	C2A-N3A-C4A	3.50	120.38	111.83
2	C	801	FAD	C5A-N7A-C8A	3.45	108.88	103.45
2	D	801	FAD	C5A-N7A-C8A	3.44	108.86	103.45
2	H	801	FAD	C2A-N3A-C4A	3.42	120.18	111.83
2	B	801	FAD	C2A-N3A-C4A	3.39	120.11	111.83
2	F	801	FAD	C2A-N3A-C4A	3.33	119.97	111.83
2	F	801	FAD	C4X-C10-N10	3.29	121.19	116.48
2	F	801	FAD	C4-N3-C2	-3.26	119.86	125.64
2	G	801	FAD	C2A-N3A-C4A	3.23	119.72	111.83
2	A	801	FAD	C5'-C4'-C3'	-3.22	106.14	112.22
2	F	801	FAD	C4A-N9A-C8A	3.22	109.12	105.74
2	F	801	FAD	C4A-C5A-N7A	-3.20	106.93	110.58
2	E	801	FAD	C4A-C5A-N7A	-3.17	106.96	110.58
2	F	801	FAD	N3A-C4A-N9A	3.16	132.53	127.17
2	A	801	FAD	O4-C4-C4X	-3.14	118.25	126.53
2	C	801	FAD	O2P-P-O3P	3.12	115.70	107.27
2	A	801	FAD	C2A-N3A-C4A	3.09	119.37	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	802	G3F	C4-C3-C2	-3.07	107.94	111.50
3	E	802	G3F	F3-C3-C4	3.06	111.47	108.81
2	G	801	FAD	C4-N3-C2	-3.04	120.25	125.64
2	B	801	FAD	C4X-C10-N10	3.01	120.80	116.48
2	G	801	FAD	C9A-C5X-N5	-2.99	119.28	122.45
2	D	801	FAD	C2A-N3A-C4A	2.98	119.12	111.83
2	C	801	FAD	C2A-N3A-C4A	2.98	119.11	111.83
2	G	801	FAD	C5A-N7A-C8A	2.97	108.12	103.45
2	C	801	FAD	C10-C4X-N5	-2.96	118.76	124.81
2	C	801	FAD	C5A-C6A-N6A	-2.95	115.99	123.29
2	D	801	FAD	N3A-C4A-N9A	2.87	132.05	127.17
3	B	802	G3F	C4-C3-C2	-2.87	108.17	111.50
2	D	801	FAD	C5X-C9A-N10	2.84	120.54	117.97
2	B	801	FAD	C5X-C9A-N10	2.83	120.53	117.97
2	D	801	FAD	C4-N3-C2	-2.83	120.62	125.64
2	D	801	FAD	C4X-C10-N10	2.82	120.51	116.48
2	H	801	FAD	C4A-C5A-N7A	-2.80	107.38	110.58
2	B	801	FAD	C4-N3-C2	-2.80	120.67	125.64
2	B	801	FAD	N3A-C4A-N9A	2.79	131.91	127.17
2	B	801	FAD	C4X-C4-N3	2.78	120.33	113.25
2	B	801	FAD	C4-C4X-N5	2.78	122.04	118.21
2	A	801	FAD	C4X-C10-N10	2.75	120.42	116.48
2	C	801	FAD	C4-C4X-N5	2.74	122.00	118.21
2	H	801	FAD	C4-N3-C2	-2.74	120.77	125.64
2	C	801	FAD	O2A-PA-O3P	2.74	114.68	107.27
2	D	801	FAD	O4-C4-C4X	-2.74	119.30	126.53
2	C	801	FAD	C4-N3-C2	-2.73	120.80	125.64
2	G	801	FAD	C4X-C4-N3	2.73	120.19	113.25
2	H	801	FAD	C4X-C10-N10	2.71	120.37	116.48
2	C	801	FAD	N3A-C4A-N9A	2.71	131.77	127.17
2	B	801	FAD	C9A-C5X-N5	-2.67	119.62	122.45
2	A	801	FAD	C4A-C5A-N7A	-2.65	107.56	110.58
2	E	801	FAD	C4X-C10-N10	2.64	120.26	116.48
2	A	801	FAD	C4-N3-C2	-2.64	120.96	125.64
2	B	801	FAD	C10-C4X-N5	-2.63	119.44	124.81
3	F	802	G3F	O5-C1-C2	-2.63	105.68	110.30
2	F	801	FAD	O2A-PA-O3P	2.62	114.36	107.27
2	D	801	FAD	C9A-C5X-N5	-2.58	119.72	122.45
2	A	801	FAD	O2-C2-N1	-2.57	117.53	121.80
2	G	801	FAD	C10-C4X-N5	-2.56	119.58	124.81
2	F	801	FAD	C5'-C4'-C3'	-2.56	107.39	112.22
2	B	801	FAD	C9-C9A-N10	-2.53	118.45	121.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	FAD	N3A-C4A-N9A	2.53	131.46	127.17
2	F	801	FAD	C5X-C9A-N10	2.52	120.25	117.97
2	D	801	FAD	O2A-PA-O3P	2.50	114.03	107.27
2	D	801	FAD	C4A-N9A-C8A	2.50	108.36	105.74
2	E	801	FAD	N3A-C4A-N9A	2.49	131.41	127.17
2	H	801	FAD	N3A-C4A-N9A	2.46	131.36	127.17
2	C	801	FAD	C4X-C4-N3	2.45	119.50	113.25
3	H	802	G3F	C4-C3-C2	-2.42	108.69	111.50
2	H	801	FAD	C10-C4X-N5	-2.41	119.88	124.81
2	H	801	FAD	C9A-C5X-N5	-2.40	119.91	122.45
2	F	801	FAD	C10-C4X-N5	-2.40	119.91	124.81
2	E	801	FAD	O4B-C1B-N9A	2.39	112.69	108.09
2	E	801	FAD	O4-C4-C4X	-2.39	120.23	126.53
2	D	801	FAD	C4A-C5A-N7A	-2.38	107.86	110.58
2	D	801	FAD	C4X-C4-N3	2.38	119.30	113.25
2	F	801	FAD	C6A-C5A-C4A	2.35	120.39	117.18
2	B	801	FAD	C6A-C5A-C4A	2.34	120.37	117.18
3	F	802	G3F	F3-C3-C4	2.33	110.83	108.81
2	E	801	FAD	C4A-N9A-C8A	2.33	108.19	105.74
2	F	801	FAD	C4X-C4-N3	2.33	119.17	113.25
3	A	802	G3F	C3-C2-C1	-2.31	107.12	110.84
2	H	801	FAD	C4X-C4-N3	2.31	119.13	113.25
2	H	801	FAD	O4-C4-C4X	-2.30	120.47	126.53
2	C	801	FAD	C4A-N9A-C8A	2.29	108.15	105.74
2	A	801	FAD	C4-C4X-C10	2.26	120.81	116.93
2	D	801	FAD	C6A-C5A-C4A	2.25	120.25	117.18
2	G	801	FAD	N3A-C4A-N9A	2.25	130.99	127.17
2	C	801	FAD	C4A-C5A-N7A	-2.25	108.01	110.58
2	A	801	FAD	O2-C2-N3	2.23	122.87	118.58
2	E	801	FAD	C9A-C5X-N5	-2.23	120.09	122.45
2	G	801	FAD	C4X-C10-N10	2.23	119.67	116.48
2	D	801	FAD	O4'-C4'-C3'	2.22	114.44	109.25
2	A	801	FAD	C5X-C9A-N10	2.21	119.96	117.97
2	G	801	FAD	C4X-C10-N1	-2.20	119.20	124.59
2	F	801	FAD	C9A-C5X-N5	-2.17	120.16	122.45
3	D	802	G3F	C6-C5-C4	-2.16	107.71	113.02
2	G	801	FAD	C4A-C5A-N7A	-2.16	108.11	110.58
2	C	801	FAD	C6A-C5A-C4A	2.15	120.12	117.18
2	G	801	FAD	O4B-C1B-N9A	2.14	112.20	108.09
2	F	801	FAD	O4-C4-C4X	-2.14	120.89	126.53
2	H	801	FAD	C4A-N9A-C8A	2.13	107.98	105.74
2	B	801	FAD	C5A-C4A-N9A	2.13	108.14	105.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	802	G3F	F3-C3-C2	-2.13	106.97	108.81
2	A	801	FAD	C10-C4X-N5	-2.12	120.47	124.81
2	A	801	FAD	O4B-C1B-N9A	2.12	112.16	108.09
2	G	801	FAD	C5X-N5-C4X	2.11	121.51	118.09
2	A	801	FAD	C4X-C4-N3	2.09	118.57	113.25
2	F	801	FAD	O2-C2-N1	-2.07	118.35	121.80
2	F	801	FAD	C4'-C3'-C2'	-2.05	110.16	113.57
2	C	801	FAD	O5'-C5'-C4'	-2.04	103.92	109.36
2	E	801	FAD	C4X-C4-N3	2.04	118.44	113.25
3	A	802	G3F	C4-C3-C2	-2.03	109.14	111.50

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	FAD	PA-O3P-P-O5'
2	C	801	FAD	C3'-C4'-C5'-O5'
2	C	801	FAD	O4'-C4'-C5'-O5'
2	F	801	FAD	O4B-C4B-C5B-O5B
2	F	801	FAD	C3B-C4B-C5B-O5B
2	F	801	FAD	PA-O3P-P-O5'
2	H	801	FAD	PA-O3P-P-O5'
2	D	801	FAD	O4B-C4B-C5B-O5B
2	D	801	FAD	C3B-C4B-C5B-O5B
2	D	801	FAD	O4'-C4'-C5'-O5'
2	A	801	FAD	O4B-C4B-C5B-O5B
2	E	801	FAD	O4B-C4B-C5B-O5B

There are no ring outliers.

13 monomers are involved in 23 short contacts:

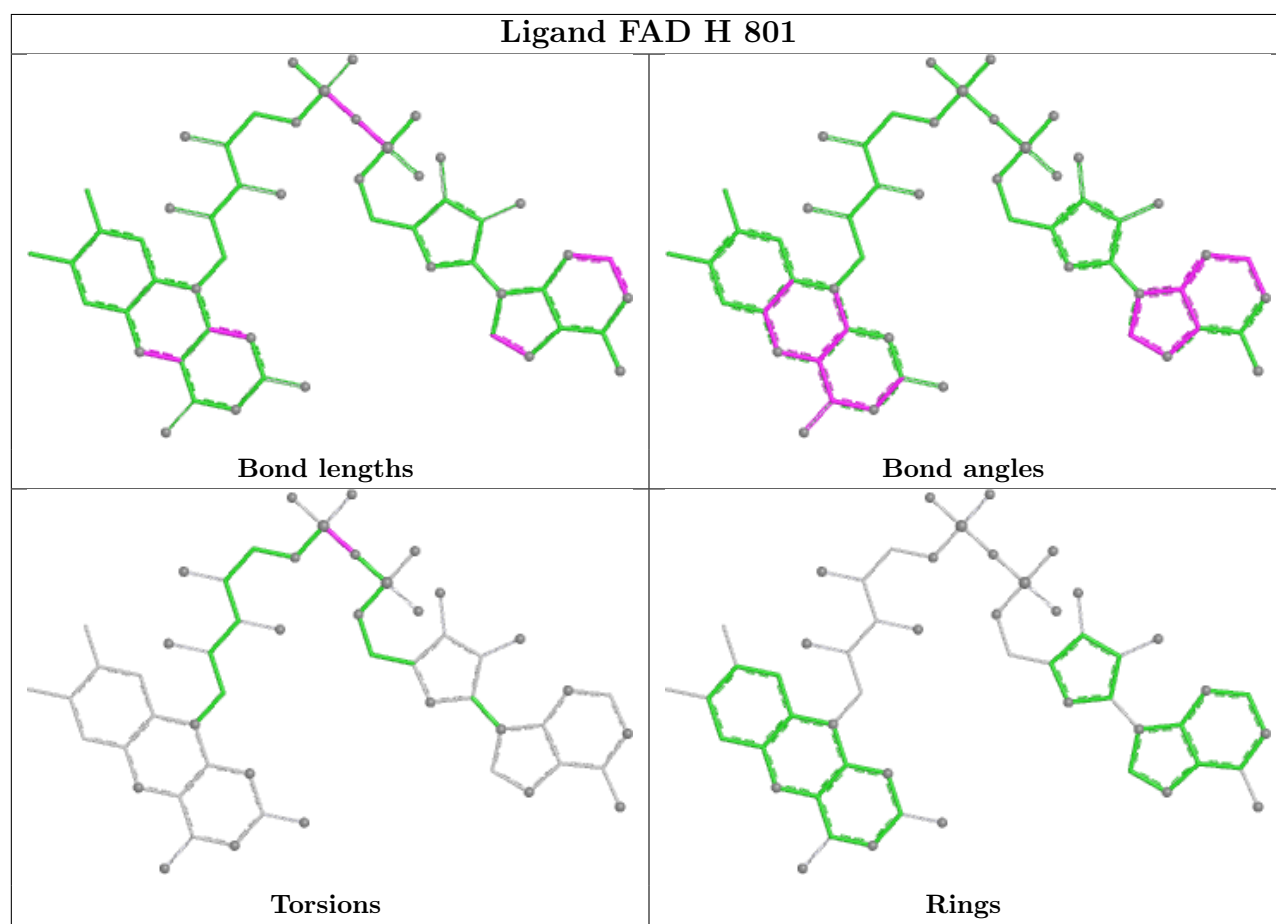
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	801	FAD	3	0
2	C	801	FAD	2	0
2	G	801	FAD	3	0
2	E	801	FAD	2	0
3	C	802	G3F	1	0
3	F	802	G3F	2	0
2	B	801	FAD	2	0
3	A	802	G3F	2	0
3	H	802	G3F	1	0

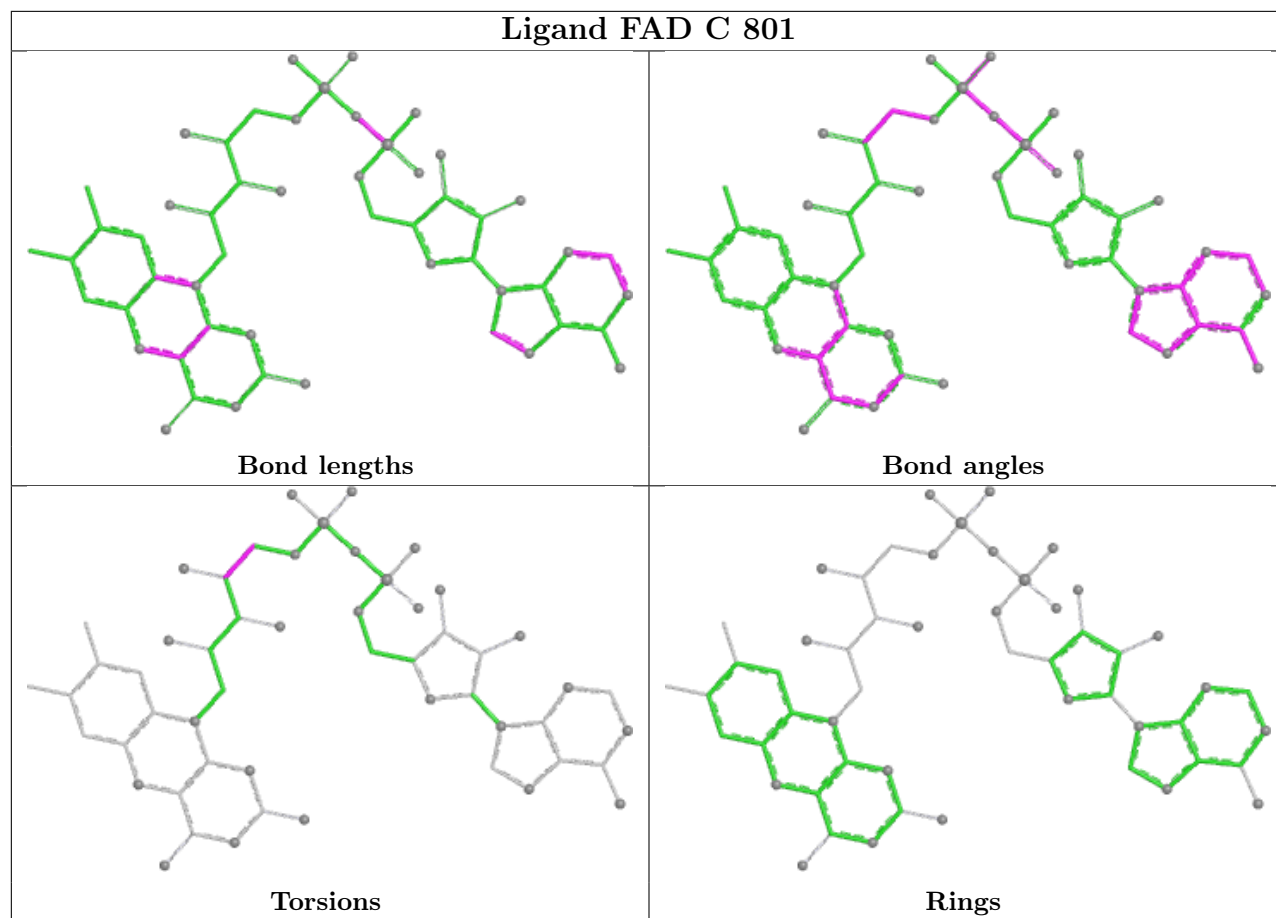
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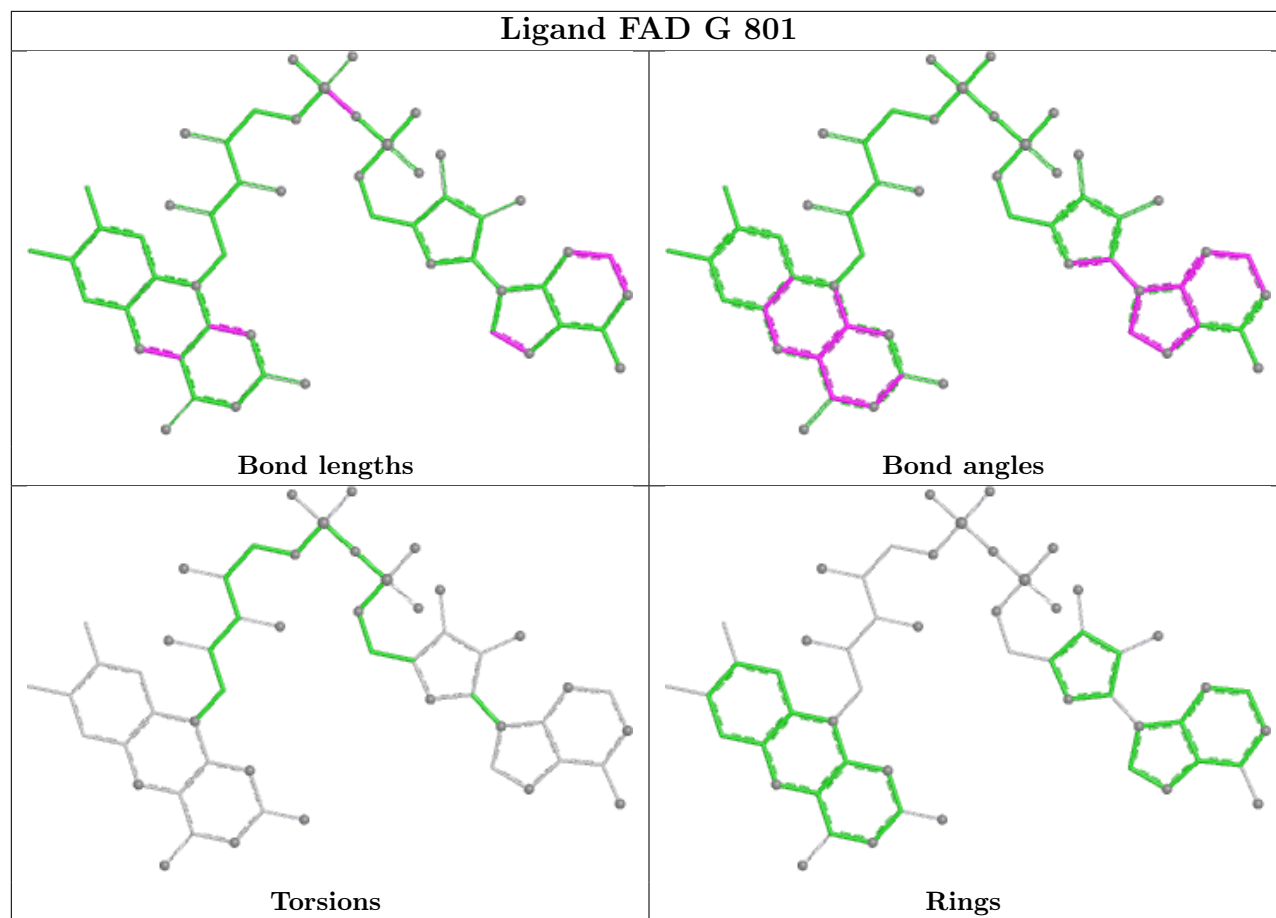
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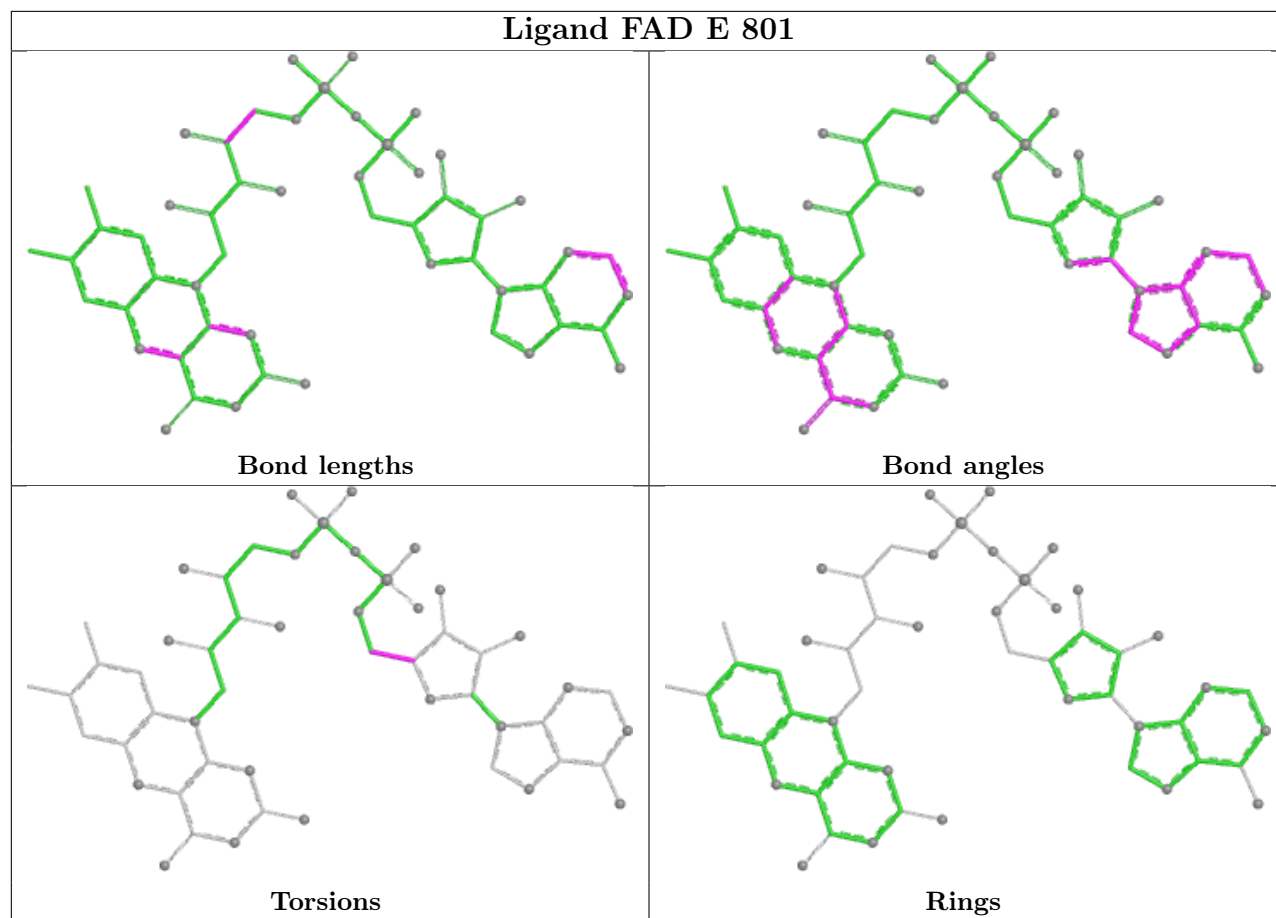
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	FAD	3	0
2	F	801	FAD	3	0
2	D	801	FAD	3	0
3	E	802	G3F	1	0

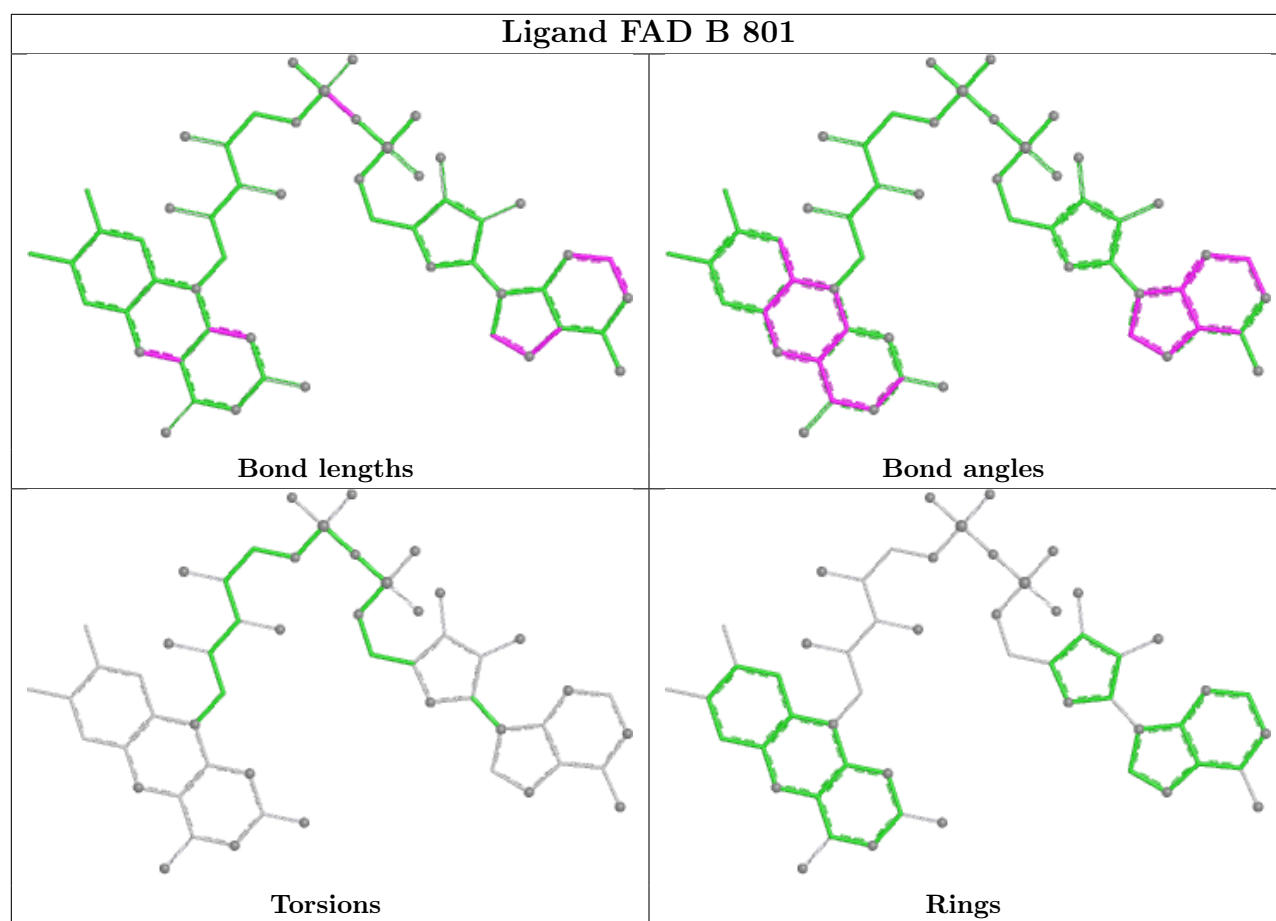
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

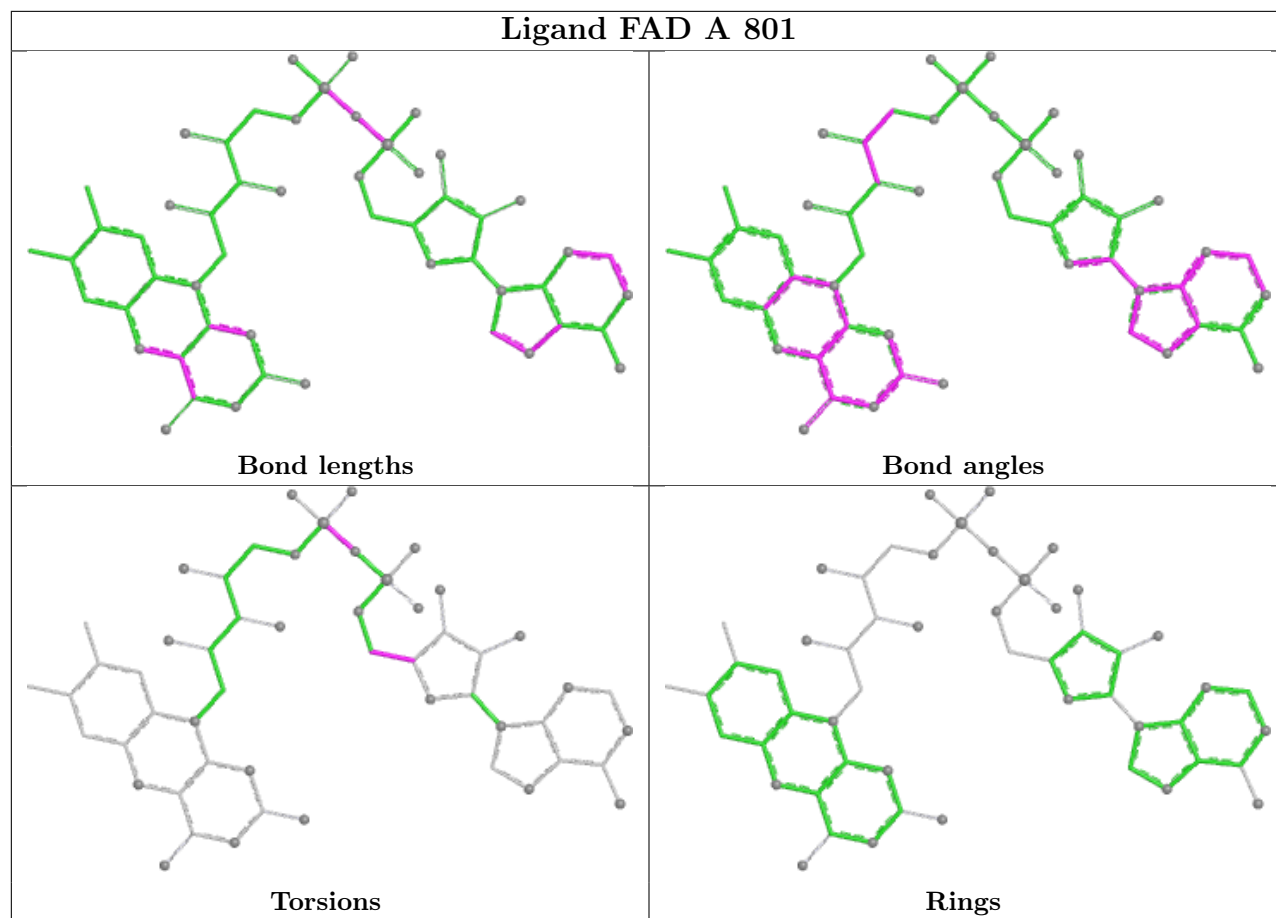


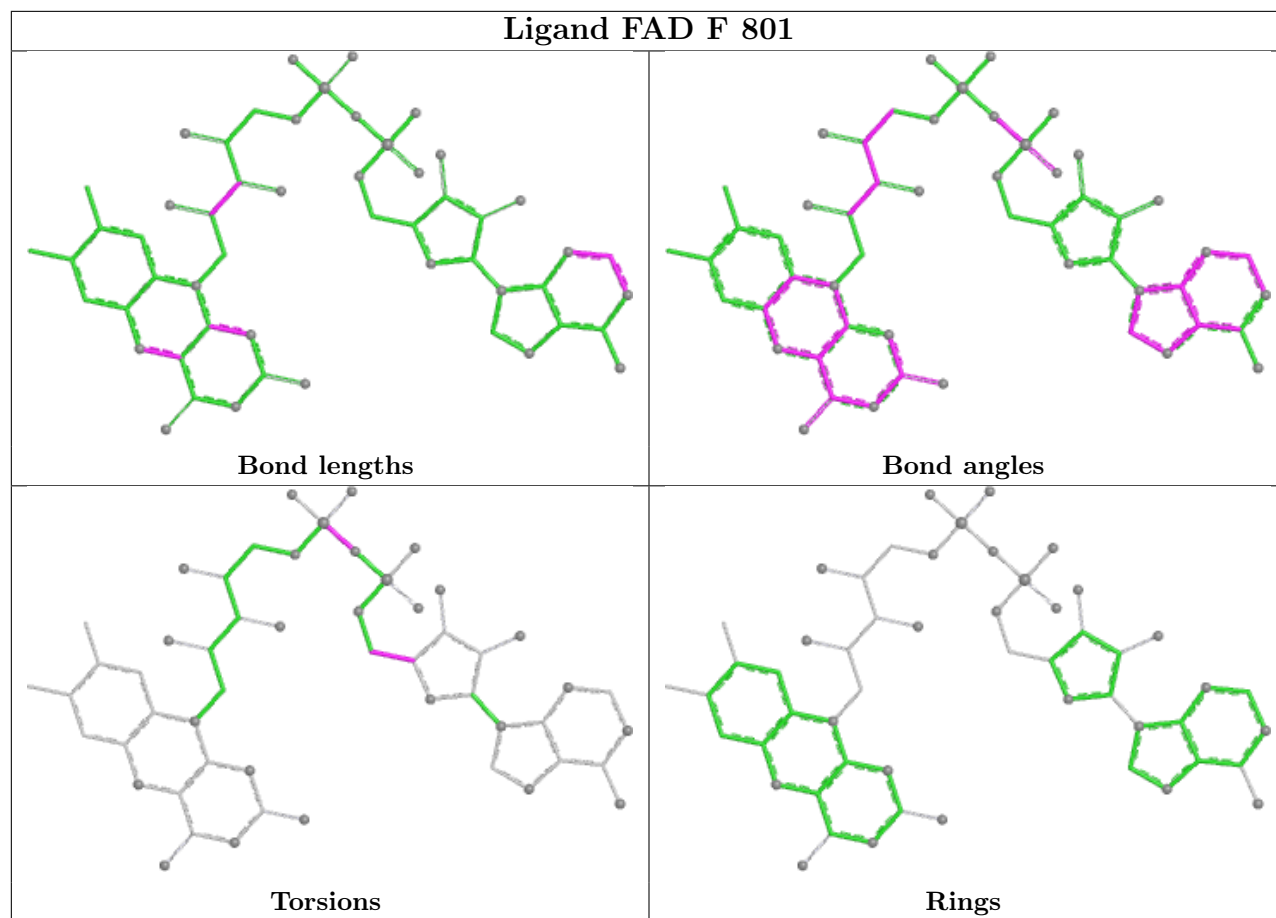


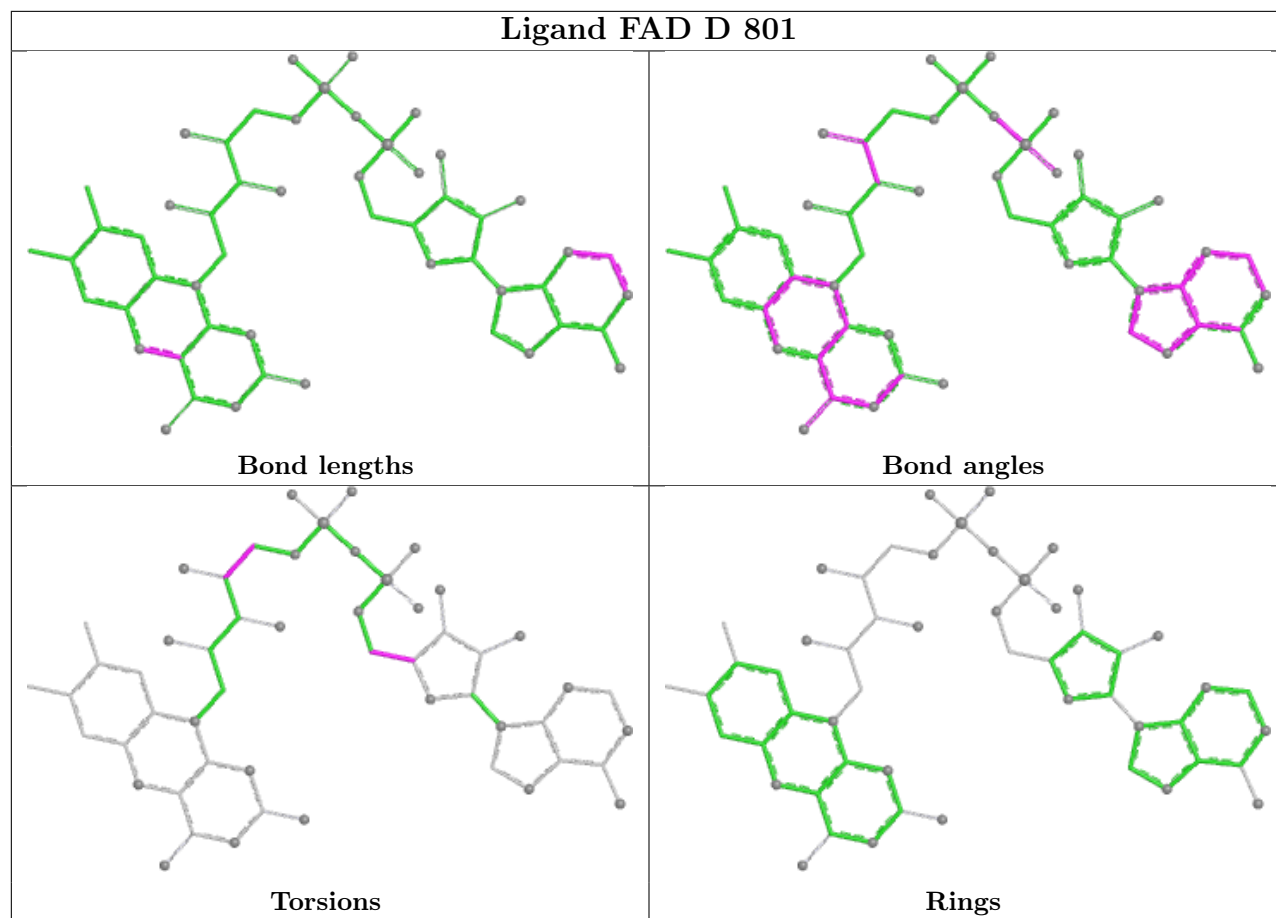












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	576/621 (92%)	-0.43	4 (0%) 84 81	10, 26, 47, 59	0
1	B	578/621 (93%)	-0.35	5 (0%) 81 78	14, 30, 57, 85	0
1	C	578/621 (93%)	0.02	13 (2%) 62 58	14, 43, 73, 113	0
1	D	578/621 (93%)	-0.02	3 (0%) 87 85	18, 42, 68, 98	0
1	E	576/621 (92%)	-0.41	7 (1%) 76 73	12, 26, 52, 94	0
1	F	578/621 (93%)	-0.30	6 (1%) 79 76	19, 33, 57, 86	0
1	G	578/621 (93%)	-0.15	7 (1%) 76 73	15, 38, 66, 97	0
1	H	578/621 (93%)	-0.09	8 (1%) 73 69	15, 41, 69, 96	0
All	All	4620/4968 (92%)	-0.22	53 (1%) 78 74	10, 34, 64, 113	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	348	PRO	4.4
1	C	348	PRO	3.8
1	A	319	SER	3.7
1	H	617	GLY	3.5
1	H	7	PRO	3.5
1	D	617	GLY	3.3
1	C	617	GLY	3.2
1	G	617	GLY	3.2
1	C	13	PRO	3.2
1	C	6	THR	3.2
1	C	466	ALA	3.1
1	H	6	THR	3.0
1	C	7	PRO	2.9
1	C	10	ALA	2.9
1	F	8	PHE	2.9
1	A	617	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	4	ASP	2.9
1	A	309	PRO	2.8
1	C	8	PHE	2.8
1	E	131	LEU	2.7
1	C	70	GLY	2.7
1	F	617	GLY	2.6
1	G	4	ASP	2.6
1	C	2	PHE	2.5
1	B	70	GLY	2.5
1	F	10	ALA	2.5
1	F	309	PRO	2.4
1	H	8	PHE	2.4
1	G	309	PRO	2.4
1	H	70	GLY	2.4
1	F	2	PHE	2.4
1	E	252	TYR	2.4
1	C	1	MET	2.4
1	H	10	ALA	2.4
1	G	129	ILE	2.3
1	B	617	GLY	2.3
1	C	319	SER	2.3
1	H	1	MET	2.2
1	E	1	MET	2.2
1	C	72	VAL	2.1
1	B	10	ALA	2.1
1	A	411	LEU	2.1
1	F	348	PRO	2.1
1	E	465	VAL	2.1
1	B	466	ALA	2.1
1	E	348	PRO	2.1
1	B	8	PHE	2.1
1	E	11	ASP	2.1
1	D	319	SER	2.1
1	G	1	MET	2.1
1	E	309	PRO	2.0
1	G	464	ALA	2.0
1	H	4	ASP	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 ⓘ

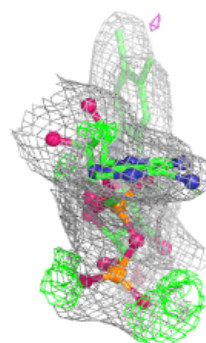
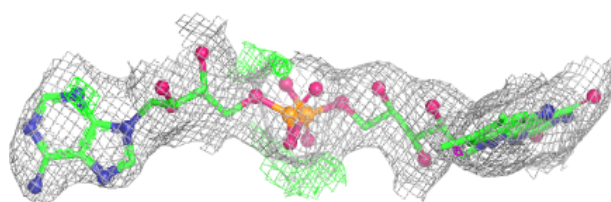
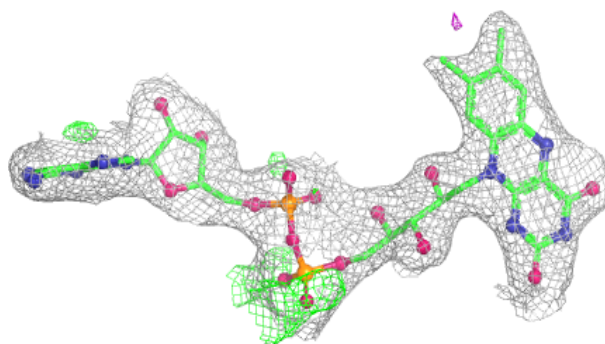
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	G3F	D	802	12/12	0.88	0.07	25,35,43,46	0
3	G3F	G	802	12/12	0.92	0.07	30,33,37,40	0
2	FAD	D	801	53/53	0.93	0.08	17,34,44,61	0
3	G3F	H	802	12/12	0.93	0.07	24,31,33,35	0
3	G3F	F	802	12/12	0.94	0.07	23,35,41,41	0
3	G3F	C	802	12/12	0.94	0.07	24,32,39,40	0
3	G3F	B	802	12/12	0.94	0.07	18,24,27,35	0
2	FAD	C	801	53/53	0.95	0.07	9,23,51,55	0
2	FAD	H	801	53/53	0.95	0.07	15,28,37,44	0
3	G3F	A	802	12/12	0.95	0.06	8,16,22,26	0
2	FAD	G	801	53/53	0.96	0.06	17,29,35,41	0
2	FAD	F	801	53/53	0.96	0.06	5,23,31,45	0
3	G3F	E	802	12/12	0.96	0.06	15,19,24,35	0
2	FAD	E	801	53/53	0.97	0.06	10,17,25,29	0
2	FAD	A	801	53/53	0.97	0.05	2,12,20,23	0
2	FAD	B	801	53/53	0.97	0.06	7,18,29,37	0

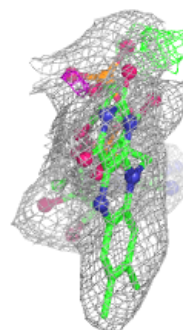
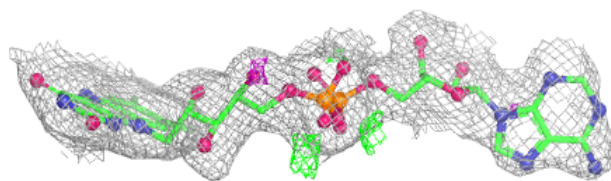
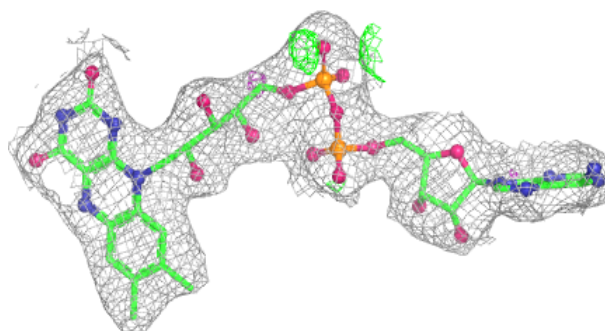
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD D 801:

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

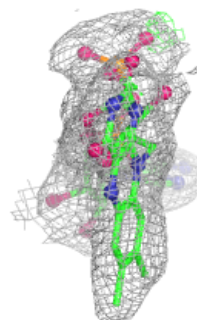
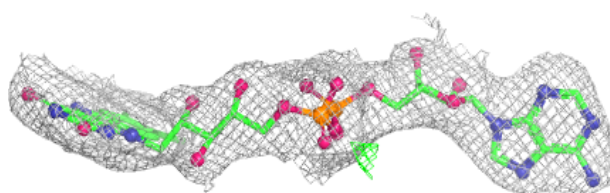
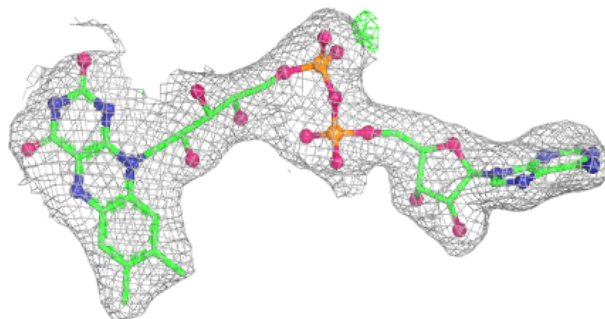
**Electron density around FAD C 801:**

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

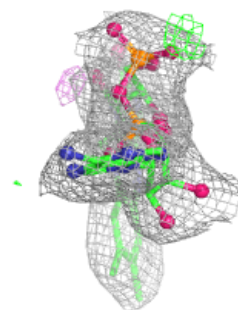
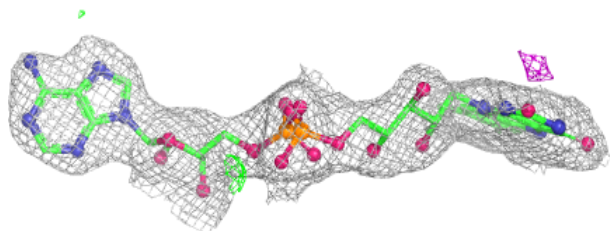
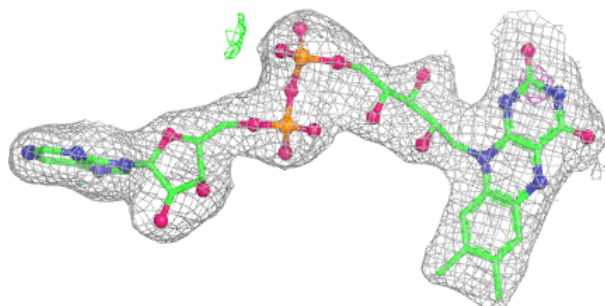


Electron density around FAD H 801:

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

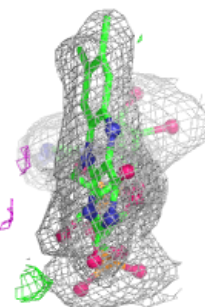
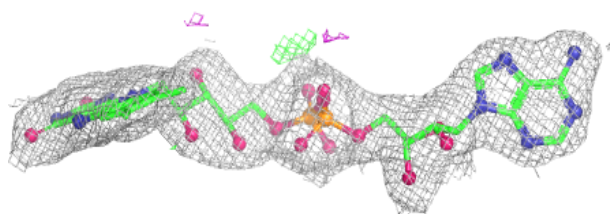
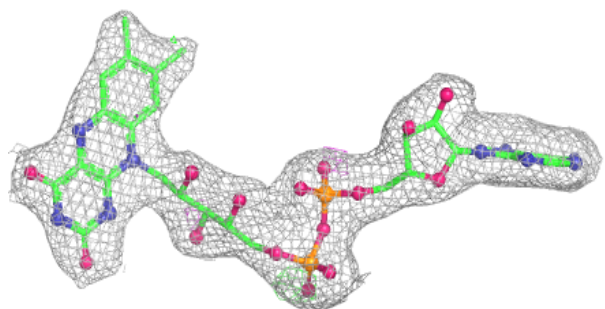
**Electron density around FAD G 801:**

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

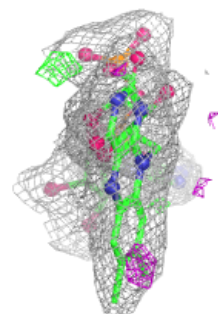
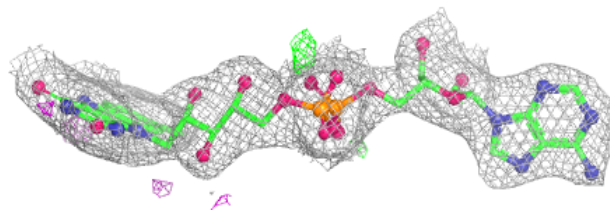
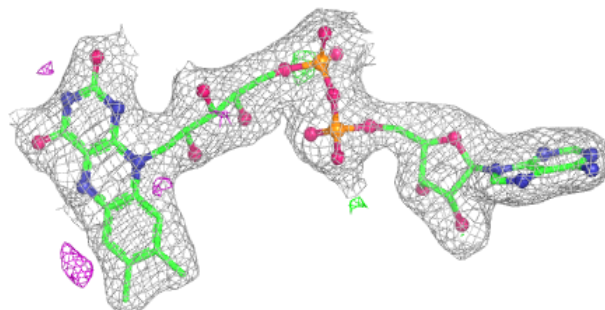


Electron density around FAD F 801:

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

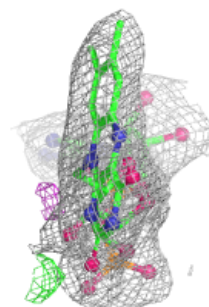
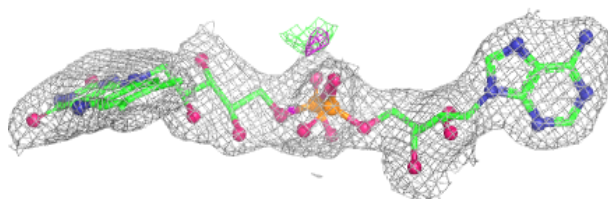
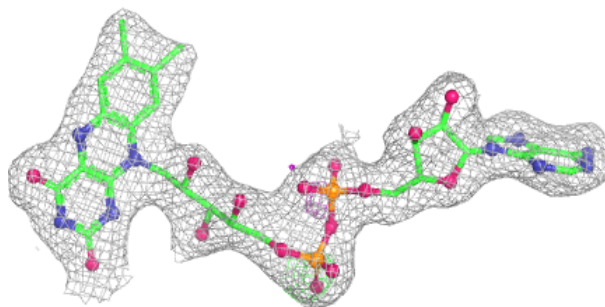
**Electron density around FAD E 801:**

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

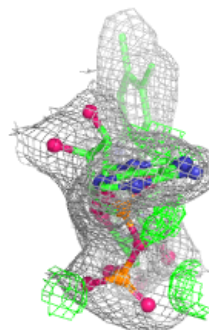
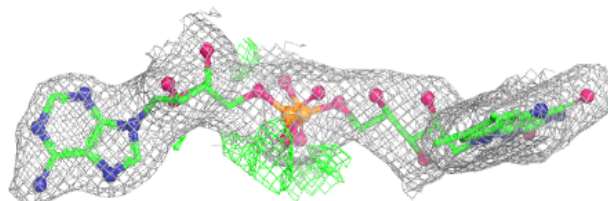
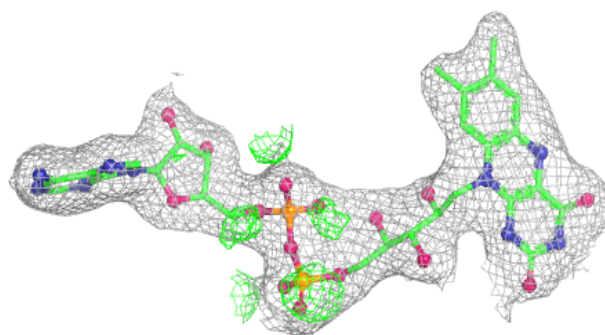


Electron density around FAD A 801:

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

**Electron density around FAD B 801:**

$2mF_o-DF_c$ (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.