Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 02:10 PM EDT

PDB ID	:	2IGO
Title	:	Crystal structure of pyranose 2-oxidase H167A mutant with 2-fluoro-2-deoxy-D-glucose
Authors	:	Divne, C.
Deposited on	:	2006-09-22
Resolution	:	1.95 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 following versions of software and data (see references ⓘ) were used in the production of this report:

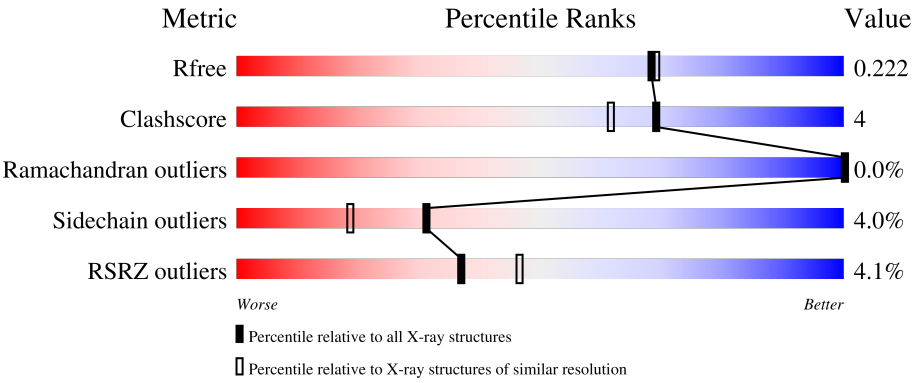
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 <=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	4% 80% 12% • 7%
1	B	623	3% 82% 9% • 7%
1	C	623	4% 82% 10% • 7%
1	D	623	3% 80% 11% • 7%
1	E	623	4% 82% 9% • 7%

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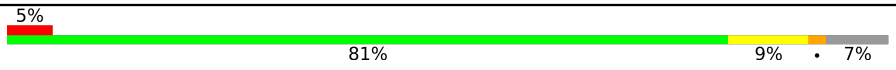
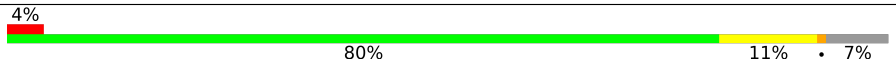
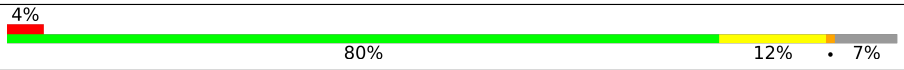
Mol	Chain	Length	Quality of chain
1	F	623	
1	G	623	
1	H	623	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 38602 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.

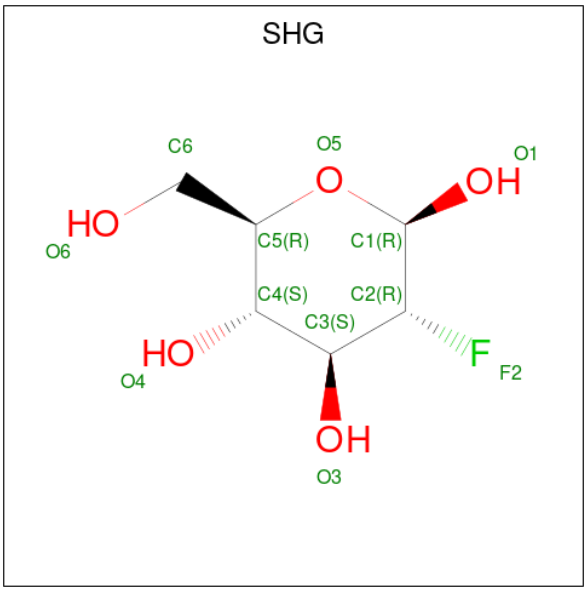
- Molecule 1 is a protein called Pyranose oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	577	Total	C	N	O	S	0	0	0
			4544	2869	776	874	25			
1	B	577	Total	C	N	O	S	0	0	0
			4544	2869	776	874	25			
1	D	577	Total	C	N	O	S	0	0	0
			4544	2869	776	874	25			
1	C	577	Total	C	N	O	S	0	0	0
			4544	2869	776	874	25			
1	E	577	Total	C	N	O	S	0	0	0
			4544	2869	776	874	25			
1	F	577	Total	C	N	O	S	0	0	0
			4544	2869	776	874	25			
1	H	577	Total	C	N	O	S	0	0	0
			4544	2869	776	874	25			
1	G	577	Total	C	N	O	S	0	0	0
			4544	2869	776	874	25			

There are 8 discrepancies between the modelled and reference sequences:

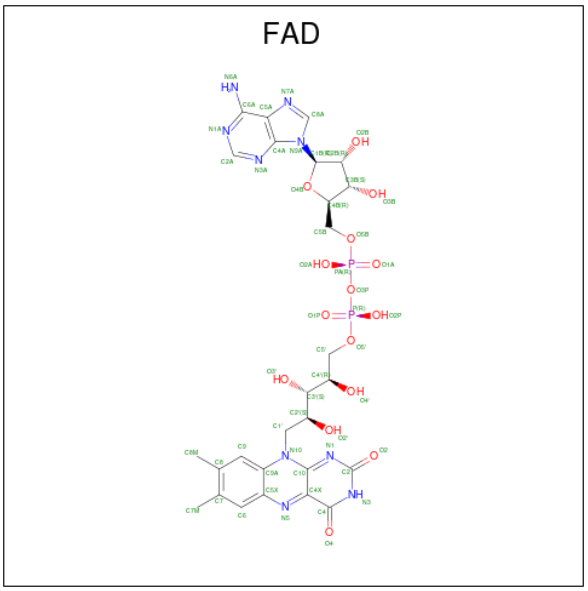
Chain	Residue	Modelled	Actual	Comment	Reference
A	167	ALA	HIS	engineered mutation	UNP Q7ZA32
B	167	ALA	HIS	engineered mutation	UNP Q7ZA32
C	167	ALA	HIS	engineered mutation	UNP Q7ZA32
D	167	ALA	HIS	engineered mutation	UNP Q7ZA32
E	167	ALA	HIS	engineered mutation	UNP Q7ZA32
F	167	ALA	HIS	engineered mutation	UNP Q7ZA32
G	167	ALA	HIS	engineered mutation	UNP Q7ZA32
H	167	ALA	HIS	engineered mutation	UNP Q7ZA32

- Molecule 2 is 2-deoxy-2-fluoro-beta-D-glucopyranose (three-letter code: SHG) (formula: $C_6H_{11}FO_5$).



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

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	244	Total	O	0	0
			244	244		
4	B	251	Total	O	0	0
			251	251		
4	D	222	Total	O	0	0
			222	222		
4	C	199	Total	O	0	0
			199	199		

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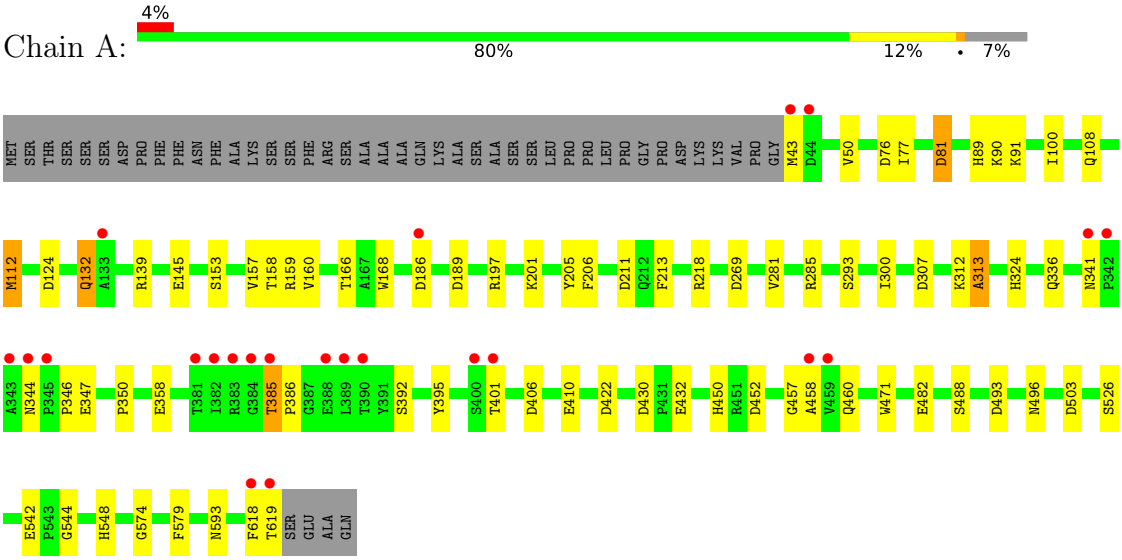
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	195	Total O 195 195	0	0
4	F	192	Total O 192 192	0	0
4	H	217	Total O 217 217	0	0
4	G	210	Total O 210 210	0	0

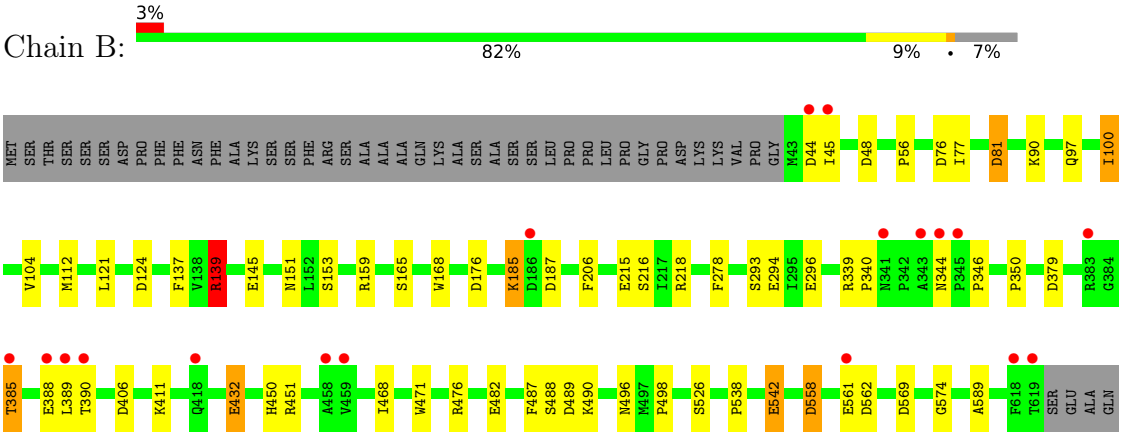
3 Residue-property plots

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

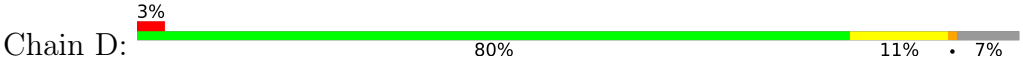
• Molecule 1: Pyranose oxidase

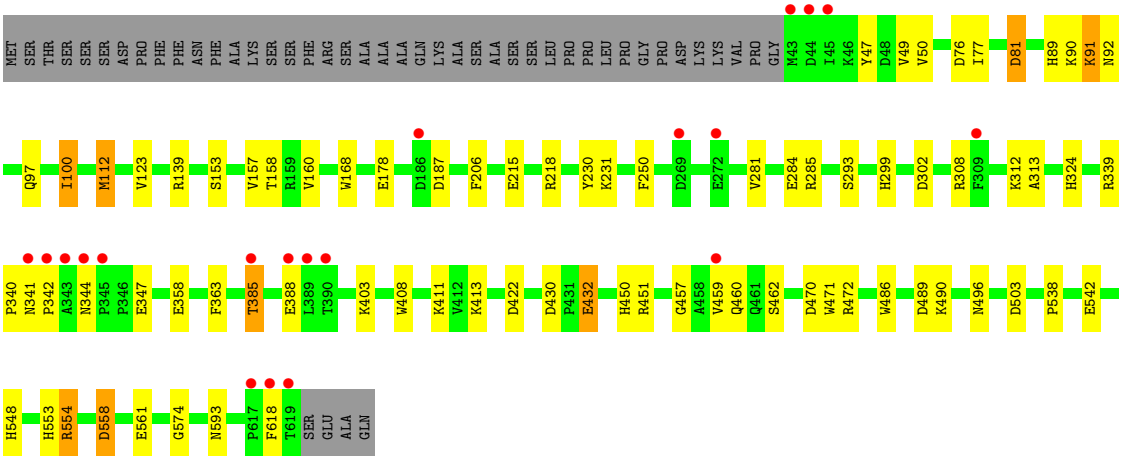


• Molecule 1: Pyranose oxidase

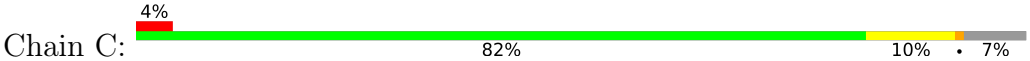


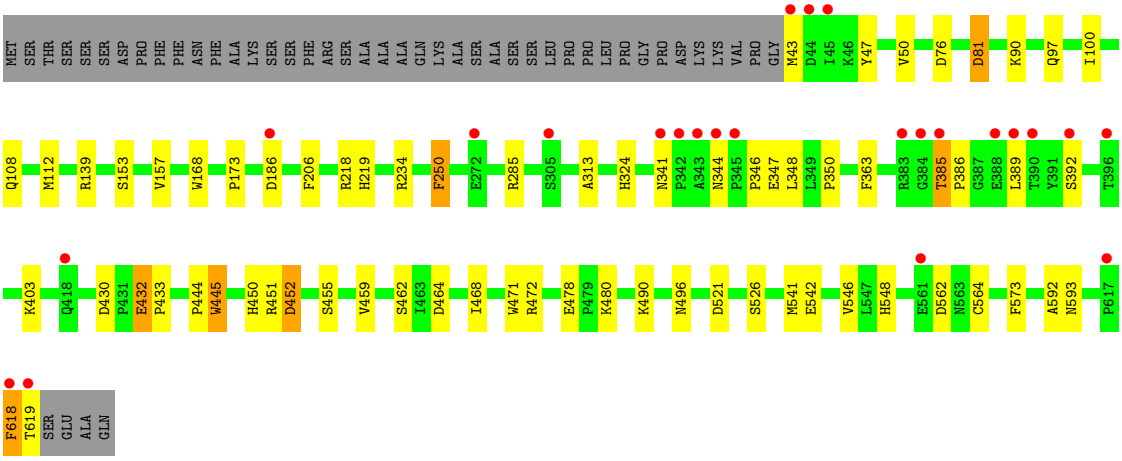
• Molecule 1: Pyranose oxidase



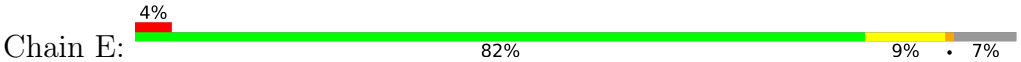


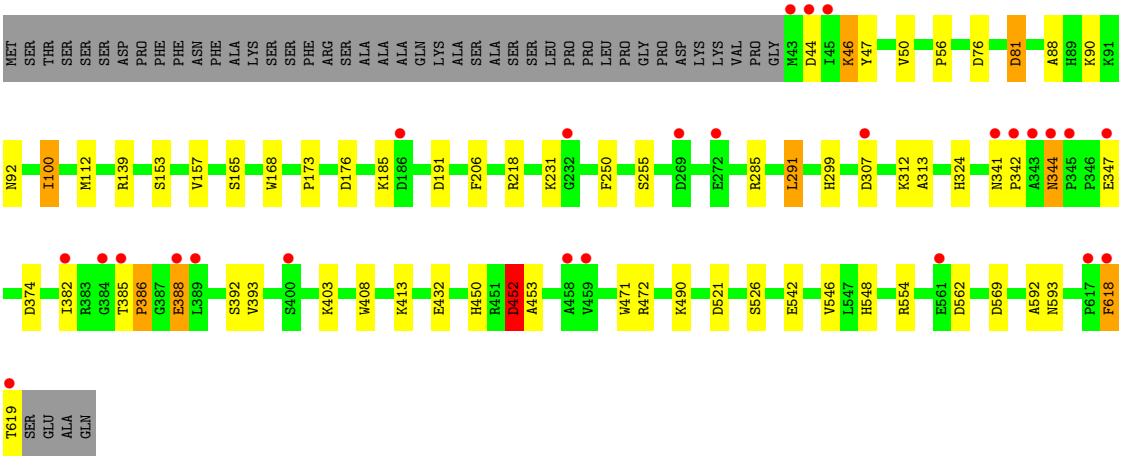
• Molecule 1: Pyranose oxidase





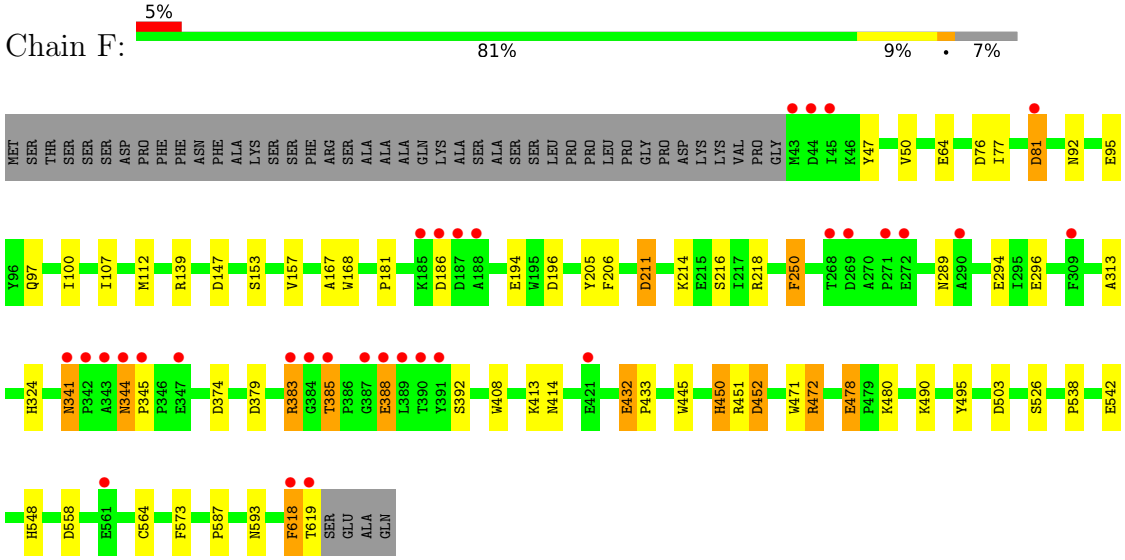
• Molecule 1: Pyranose oxidase





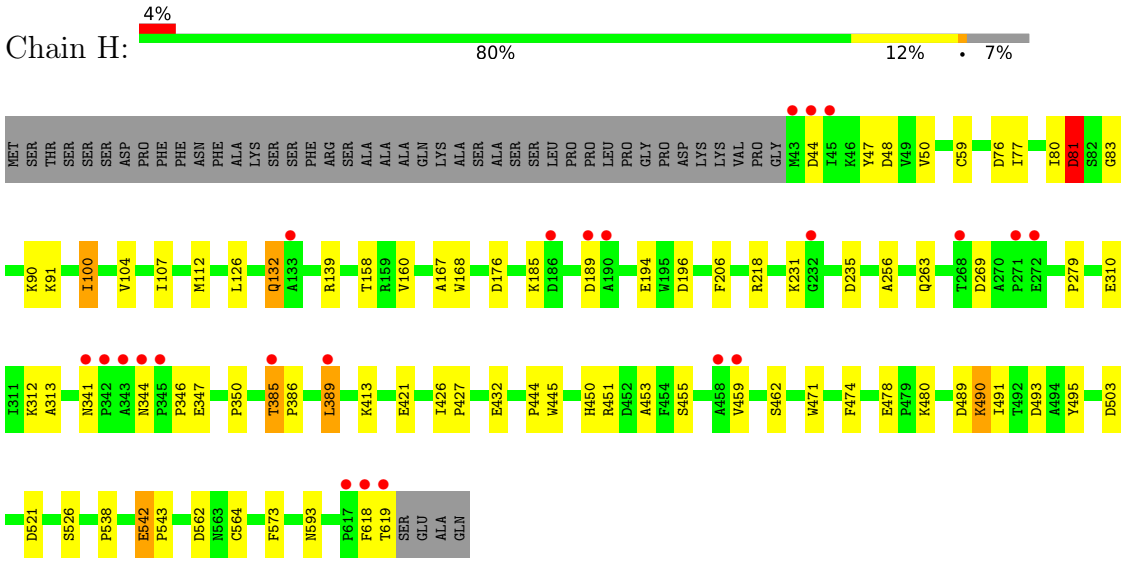
• Molecule 1: Pyranose oxidase

Chain F:



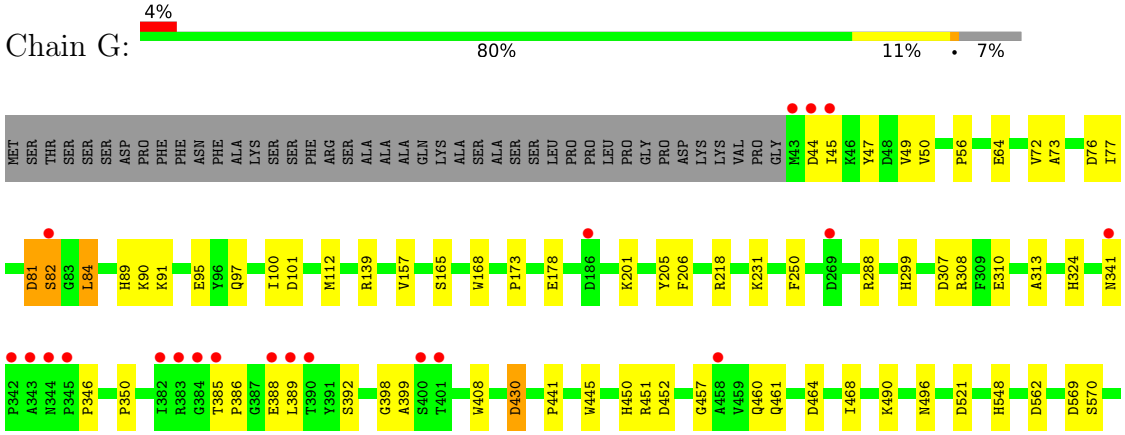
• Molecule 1: Pyranose oxidase

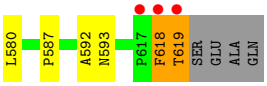
Chain H:



• Molecule 1: Pyranose oxidase

Chain G:




L580
P587
A592
N593
P617
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	168.59Å 103.08Å 169.04Å 90.00° 106.30° 90.00°	Depositor
Resolution (Å)	38.90 – 1.95 38.99 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (38.90-1.95) 99.9 (38.99-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	3.86 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.184 , 0.221 0.188 , 0.222	Depositor DCC
R_{free} test set	4042 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å^2)	21.2	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 41.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.019 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	38602	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.84% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	1.14	7/4659 (0.2%)	1.08	20/6335 (0.3%)
1	B	1.10	4/4659 (0.1%)	1.08	19/6335 (0.3%)
1	C	1.04	3/4659 (0.1%)	1.04	13/6335 (0.2%)
1	D	1.08	5/4659 (0.1%)	1.05	19/6335 (0.3%)
1	E	1.04	1/4659 (0.0%)	1.04	20/6335 (0.3%)
1	F	1.03	3/4659 (0.1%)	1.07	18/6335 (0.3%)
1	G	1.05	0/4659	1.06	18/6335 (0.3%)
1	H	1.07	3/4659 (0.1%)	1.05	23/6335 (0.4%)
All	All	1.07	26/37272 (0.1%)	1.06	150/50680 (0.3%)

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	B	0	1
1	D	0	1
All	All	0	2

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	291	LEU	CG-CD1	7.79	1.80	1.51
1	C	541	MET	CG-SD	6.66	1.98	1.81
1	A	482	GLU	CD-OE1	6.66	1.32	1.25
1	A	313	ALA	CA-CB	6.29	1.65	1.52
1	A	112	MET	CB-CG	5.91	1.70	1.51
1	D	486	TRP	CB-CG	5.88	1.60	1.50
1	C	108	GLN	CG-CD	5.70	1.64	1.51
1	D	358	GLU	CD-OE2	5.63	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	230	TYR	CD1-CE1	5.54	1.47	1.39
1	F	478	GLU	CD-OE1	5.48	1.31	1.25
1	F	250	PHE	CE2-CZ	5.46	1.47	1.37
1	A	108	GLN	CG-CD	5.34	1.63	1.51
1	B	278	PHE	CE2-CZ	5.32	1.47	1.37
1	A	579	PHE	CD2-CE2	5.24	1.49	1.39
1	H	104	VAL	CB-CG2	-5.24	1.41	1.52
1	A	81	ASP	CB-CG	-5.23	1.40	1.51
1	H	196	ASP	CB-CG	5.19	1.62	1.51
1	F	139	ARG	CD-NE	-5.18	1.37	1.46
1	B	482	GLU	CD-OE2	5.17	1.31	1.25
1	D	49	VAL	CB-CG1	5.14	1.63	1.52
1	A	213	PHE	CE1-CZ	5.14	1.47	1.37
1	H	474	PHE	CD1-CE1	5.14	1.49	1.39
1	C	250	PHE	CE2-CZ	5.14	1.47	1.37
1	B	542	GLU	CG-CD	5.13	1.59	1.51
1	D	281	VAL	CB-CG2	5.09	1.63	1.52
1	B	482	GLU	CG-CD	5.07	1.59	1.51

All (150) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	139	ARG	NE-CZ-NH2	-24.01	108.29	120.30
1	D	139	ARG	NE-CZ-NH2	-20.93	109.83	120.30
1	B	139	ARG	NE-CZ-NH2	-20.35	110.12	120.30
1	E	139	ARG	NE-CZ-NH2	-19.12	110.74	120.30
1	G	139	ARG	NE-CZ-NH2	-18.89	110.86	120.30
1	C	139	ARG	NE-CZ-NH2	-17.76	111.42	120.30
1	A	139	ARG	NE-CZ-NH2	-16.90	111.85	120.30
1	G	139	ARG	NE-CZ-NH1	15.63	128.11	120.30
1	C	139	ARG	NE-CZ-NH1	15.60	128.10	120.30
1	F	139	ARG	NE-CZ-NH1	15.18	127.89	120.30
1	H	139	ARG	NE-CZ-NH2	-14.74	112.93	120.30
1	B	81	ASP	CB-CG-OD2	14.54	131.39	118.30
1	D	139	ARG	NE-CZ-NH1	14.11	127.36	120.30
1	E	139	ARG	NE-CZ-NH1	13.50	127.05	120.30
1	B	139	ARG	NE-CZ-NH1	13.20	126.90	120.30
1	G	81	ASP	CB-CG-OD2	12.71	129.74	118.30
1	H	139	ARG	NE-CZ-NH1	12.49	126.55	120.30
1	C	81	ASP	CB-CG-OD2	12.07	129.16	118.30
1	E	291	LEU	CB-CG-CD2	-10.88	92.51	111.00
1	G	81	ASP	CB-CG-OD1	-10.68	108.69	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	81	ASP	CB-CG-OD1	-10.48	108.86	118.30
1	A	139	ARG	NE-CZ-NH1	10.42	125.51	120.30
1	E	81	ASP	CB-CG-OD2	9.67	127.00	118.30
1	F	81	ASP	CB-CG-OD2	9.62	126.96	118.30
1	C	81	ASP	CB-CG-OD1	-9.15	110.06	118.30
1	F	558	ASP	CB-CG-OD2	9.05	126.44	118.30
1	G	76	ASP	CB-CG-OD2	9.04	126.44	118.30
1	F	139	ARG	CD-NE-CZ	8.87	136.01	123.60
1	F	76	ASP	CB-CG-OD2	8.83	126.25	118.30
1	B	76	ASP	CB-CG-OD2	8.62	126.06	118.30
1	E	139	ARG	CG-CD-NE	-8.47	94.01	111.80
1	B	139	ARG	CG-CD-NE	-8.44	94.08	111.80
1	F	472	ARG	NE-CZ-NH1	8.41	124.50	120.30
1	E	76	ASP	CB-CG-OD2	8.36	125.82	118.30
1	G	521	ASP	CB-CG-OD2	8.32	125.79	118.30
1	H	562	ASP	CB-CG-OD2	8.28	125.75	118.30
1	D	81	ASP	CB-CG-OD2	8.24	125.71	118.30
1	D	76	ASP	CB-CG-OD2	8.21	125.69	118.30
1	A	76	ASP	CB-CG-OD2	8.14	125.62	118.30
1	B	558	ASP	CB-CG-OD2	7.85	125.36	118.30
1	E	81	ASP	CB-CG-OD1	-7.85	111.24	118.30
1	C	562	ASP	CB-CG-OD2	7.69	125.22	118.30
1	F	139	ARG	CG-CD-NE	-7.68	95.67	111.80
1	H	493	ASP	CB-CG-OD1	7.68	125.21	118.30
1	H	81	ASP	CB-CG-OD1	-7.66	111.41	118.30
1	E	176	ASP	CB-CG-OD2	7.65	125.18	118.30
1	A	493	ASP	CB-CG-OD1	7.59	125.13	118.30
1	C	139	ARG	CD-NE-CZ	7.45	134.03	123.60
1	E	291	LEU	CA-CB-CG	-7.36	98.38	115.30
1	E	452	ASP	CB-CG-OD2	7.25	124.82	118.30
1	H	81	ASP	CB-CG-OD2	7.18	124.76	118.30
1	G	562	ASP	CB-CG-OD2	7.04	124.63	118.30
1	G	430	ASP	CB-CG-OD2	7.03	124.63	118.30
1	B	139	ARG	CD-NE-CZ	6.99	133.39	123.60
1	A	139	ARG	CG-CD-NE	-6.91	97.28	111.80
1	F	374	ASP	CB-CG-OD2	6.90	124.51	118.30
1	D	470	ASP	CB-CG-OD1	6.84	124.45	118.30
1	D	503	ASP	CB-CG-OD2	6.82	124.44	118.30
1	H	389	LEU	CB-CG-CD2	-6.81	99.43	111.00
1	H	503	ASP	CB-CG-OD2	6.74	124.37	118.30
1	D	97	GLN	CA-CB-CG	-6.74	98.58	113.40
1	F	472	ARG	NE-CZ-NH2	-6.69	116.96	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	430	ASP	CB-CG-OD2	6.63	124.27	118.30
1	F	196	ASP	CB-CG-OD1	6.56	124.20	118.30
1	G	569	ASP	CB-CG-OD2	6.55	124.20	118.30
1	C	76	ASP	CB-CG-OD2	6.50	124.15	118.30
1	E	44	ASP	CB-CG-OD2	6.49	124.14	118.30
1	D	187	ASP	CB-CG-OD2	6.48	124.14	118.30
1	H	521	ASP	CB-CG-OD2	6.46	124.11	118.30
1	D	139	ARG	CG-CD-NE	-6.39	98.38	111.80
1	G	452	ASP	CB-CG-OD2	6.39	124.05	118.30
1	D	139	ARG	CD-NE-CZ	6.36	132.51	123.60
1	B	124	ASP	CB-CG-OD2	6.36	124.02	118.30
1	F	97	GLN	CA-CB-CG	-6.35	99.44	113.40
1	C	139	ARG	CG-CD-NE	-6.28	98.62	111.80
1	A	211	ASP	CB-CG-OD1	6.26	123.93	118.30
1	A	189	ASP	CB-CG-OD2	6.22	123.90	118.30
1	A	139	ARG	CD-NE-CZ	6.21	132.29	123.60
1	A	81	ASP	CB-CG-OD1	-6.20	112.72	118.30
1	B	97	GLN	CA-CB-CG	-6.20	99.76	113.40
1	D	558	ASP	CB-CG-OD2	6.19	123.87	118.30
1	E	569	ASP	CB-CG-OD2	6.18	123.87	118.30
1	H	389	LEU	CA-CB-CG	6.18	129.52	115.30
1	F	211	ASP	CB-CG-OD2	6.17	123.85	118.30
1	G	139	ARG	CG-CD-NE	-6.14	98.89	111.80
1	H	76	ASP	CB-CG-OD2	6.13	123.82	118.30
1	B	489	ASP	CB-CG-OD1	6.13	123.81	118.30
1	D	472	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	G	44	ASP	CB-CG-OD2	6.04	123.74	118.30
1	H	269	ASP	CB-CG-OD2	6.04	123.73	118.30
1	E	554	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	G	288	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	A	452	ASP	CB-CG-OD2	5.99	123.69	118.30
1	A	81	ASP	CB-CG-OD2	5.98	123.68	118.30
1	A	124	ASP	CB-CG-OD2	5.97	123.68	118.30
1	B	379	ASP	CB-CG-OD2	5.93	123.63	118.30
1	H	235	ASP	CB-CG-OD2	5.88	123.59	118.30
1	G	288	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	B	406	ASP	CB-CG-OD1	5.86	123.58	118.30
1	G	139	ARG	CD-NE-CZ	5.83	131.77	123.60
1	F	503	ASP	CB-CG-OD2	5.79	123.51	118.30
1	B	176	ASP	CB-CG-OD2	5.76	123.49	118.30
1	E	374	ASP	CB-CG-OD2	5.75	123.48	118.30
1	A	197	ARG	NE-CZ-NH1	-5.75	117.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	196	ASP	CB-CG-OD2	5.75	123.48	118.30
1	H	489	ASP	CB-CG-OD2	5.73	123.45	118.30
1	A	406	ASP	CB-CG-OD1	5.71	123.44	118.30
1	A	422	ASP	CB-CG-OD2	5.67	123.40	118.30
1	H	176	ASP	CB-CG-OD2	5.67	123.40	118.30
1	F	81	ASP	CB-CG-OD1	-5.65	113.22	118.30
1	C	186	ASP	CB-CG-OD2	5.64	123.38	118.30
1	E	291	LEU	CB-CG-CD1	5.60	120.53	111.00
1	D	472	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	503	ASP	CB-CG-OD2	5.58	123.32	118.30
1	A	186	ASP	CB-CG-OD2	5.57	123.31	118.30
1	E	307	ASP	CB-CG-OD2	5.55	123.30	118.30
1	B	562	ASP	CB-CG-OD2	5.54	123.29	118.30
1	G	464	ASP	CB-CG-OD2	5.53	123.27	118.30
1	A	307	ASP	CB-CG-OD2	5.51	123.26	118.30
1	H	48	ASP	CB-CG-OD2	5.49	123.24	118.30
1	H	139	ARG	CA-CB-CG	5.48	125.46	113.40
1	E	521	ASP	CB-CG-OD2	5.46	123.21	118.30
1	F	147	ASP	CB-CG-OD1	5.45	123.20	118.30
1	B	44	ASP	CB-CG-OD2	5.45	123.20	118.30
1	B	48	ASP	CB-CG-OD2	5.42	123.18	118.30
1	G	101	ASP	CB-CG-OD2	5.41	123.17	118.30
1	C	464	ASP	CB-CG-OD2	5.36	123.12	118.30
1	D	554	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	C	452	ASP	CB-CG-OD2	5.35	123.11	118.30
1	B	104	VAL	CG1-CB-CG2	-5.34	102.36	110.90
1	D	422	ASP	CB-CG-OD2	5.32	123.08	118.30
1	A	269	ASP	CB-CG-OD2	5.31	123.08	118.30
1	H	279	PRO	N-CD-CG	-5.30	95.25	103.20
1	H	189	ASP	CB-CG-OD2	5.29	123.06	118.30
1	H	104	VAL	CG1-CB-CG2	-5.26	102.48	110.90
1	H	139	ARG	CD-NE-CZ	5.24	130.94	123.60
1	H	44	ASP	CB-CG-OD2	5.23	123.01	118.30
1	E	191	ASP	CB-CG-OD2	5.21	122.99	118.30
1	F	379	ASP	CB-CG-OD2	5.20	122.98	118.30
1	C	521	ASP	CB-CG-OD2	5.19	122.97	118.30
1	G	307	ASP	CB-CG-OD2	5.19	122.97	118.30
1	E	554	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	F	186	ASP	CB-CG-OD2	5.17	122.95	118.30
1	D	112	MET	CG-SD-CE	5.15	108.44	100.20
1	C	234	ARG	NE-CZ-NH1	-5.11	117.74	120.30
1	D	489	ASP	CB-CG-OD1	5.10	122.89	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	302	ASP	CB-CG-OD2	5.07	122.86	118.30
1	B	569	ASP	CB-CG-OD2	5.07	122.86	118.30
1	D	81	ASP	CB-CG-OD1	-5.01	113.79	118.30
1	E	562	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	151	ASN	Peptide
1	D	553	HIS	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	4544	0	4393	28	0
1	B	4544	0	4393	31	0
1	C	4544	0	4393	33	0
1	D	4544	0	4393	32	0
1	E	4544	0	4393	36	0
1	F	4544	0	4393	35	0
1	G	4544	0	4393	42	0
1	H	4544	0	4393	30	0
2	A	12	0	11	4	0
2	B	12	0	11	1	0
2	C	12	0	11	5	0
2	D	12	0	11	3	0
2	E	12	0	11	4	0
2	F	12	0	10	2	0
2	G	12	0	11	4	0
2	H	12	0	11	0	0
3	A	53	0	31	4	0
3	B	53	0	31	4	0
3	C	53	0	31	1	0
3	D	53	0	31	2	0
3	E	53	0	31	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	53	0	31	0	0
3	G	53	0	31	2	0
3	H	53	0	31	0	0
4	A	244	0	0	3	0
4	B	251	0	0	1	0
4	C	199	0	0	2	0
4	D	222	0	0	1	0
4	E	195	0	0	2	0
4	F	192	0	0	1	0
4	G	210	0	0	6	0
4	H	217	0	0	3	0
All	All	38602	0	35479	269	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (269) 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:E:291:LEU:CD1	1:E:291:LEU:CG	1.80	1.56
1:G:81:ASP:HA	4:G:2497:HOH:O	1.42	1.16
1:C:432:GLU:HG3	4:C:2381:HOH:O	1.48	1.12
1:G:81:ASP:CA	4:G:2497:HOH:O	2.04	0.98
1:E:291:LEU:CD1	1:E:291:LEU:HG	2.01	0.88
1:C:97:GLN:HG3	1:C:250:PHE:CE2	2.10	0.87
1:G:81:ASP:C	4:G:2497:HOH:O	2.15	0.84
1:G:82:SER:N	4:G:2497:HOH:O	2.10	0.83
1:H:312:LYS:HE3	4:H:1958:HOH:O	1.84	0.77
1:C:97:GLN:HG3	1:C:250:PHE:CD2	2.19	0.77
1:G:385:THR:O	1:G:388:GLU:HG2	1.86	0.75
1:D:385:THR:OG1	1:D:388:GLU:OE1	2.07	0.72
1:H:81:ASP:O	1:H:90:LYS:HE2	1.91	0.70
1:F:157:VAL:HG21	1:F:324:HIS:HE1	1.58	0.69
1:F:548:HIS:NE2	2:F:806:SHG:O3	2.25	0.69
1:G:385:THR:HG22	1:G:386:PRO:HD2	1.75	0.69
1:D:548:HIS:CE1	2:D:803:SHG:HO3	2.10	0.69
1:F:385:THR:O	1:F:388:GLU:HG3	1.93	0.69
1:F:538:PRO:HG2	1:H:538:PRO:HG2	1.77	0.67
1:E:56:PRO:HD3	1:E:165:SER:HB3	1.76	0.67
1:C:548:HIS:NE2	2:C:804:SHG:O3	2.27	0.65
1:C:50:VAL:HG13	1:C:313:ALA:HB2	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:385:THR:HB	1:G:388:GLU:OE2	1.97	0.65
1:H:126:LEU:HD12	1:H:132:GLN:HG3	1.78	0.64
1:E:81:ASP:O	1:E:90:LYS:HE2	1.97	0.63
1:A:132:GLN:HG2	4:A:1684:HOH:O	1.98	0.63
1:F:64:GLU:OE2	1:F:205:TYR:OH	2.15	0.62
1:H:490:LYS:HD2	1:H:491:ILE:HD13	1.80	0.62
1:A:77:ILE:HG22	3:A:701:FAD:C4A	2.29	0.62
1:G:201:LYS:HE2	1:G:205:TYR:OH	1.99	0.61
1:E:548:HIS:NE2	2:E:805:SHG:O3	2.29	0.61
1:C:546:VAL:HA	2:C:804:SHG:H6A	1.83	0.60
1:E:291:LEU:HD12	1:E:291:LEU:H	1.65	0.60
1:F:413:LYS:NZ	1:F:414:ASN:OD1	2.34	0.60
1:H:478:GLU:HG2	1:H:480:LYS:HE2	1.82	0.60
1:F:50:VAL:HG13	1:F:313:ALA:HB2	1.83	0.60
1:B:77:ILE:HG22	3:B:702:FAD:C4A	2.33	0.59
1:C:218:ARG:HD2	4:C:1541:HOH:O	2.02	0.59
1:B:385:THR:N	1:B:388:GLU:OE1	2.34	0.59
1:D:548:HIS:CE1	2:D:803:SHG:O3	2.56	0.58
1:E:618:PHE:HD1	1:E:619:THR:N	2.01	0.58
1:B:153:SER:OG	1:B:542:GLU:HG3	2.03	0.58
1:C:47:TYR:O	1:C:313:ALA:HA	2.03	0.58
1:B:100:ILE:HD13	1:B:100:ILE:O	2.04	0.58
1:G:81:ASP:C	1:G:81:ASP:OD1	2.42	0.57
1:A:50:VAL:HG13	1:A:313:ALA:HB2	1.86	0.57
1:D:89:HIS:CE1	1:D:91:LYS:HE2	2.40	0.57
1:B:346:PRO:HG2	1:B:350:PRO:HA	1.87	0.56
1:C:452:ASP:OD1	1:C:472:ARG:NH1	2.38	0.56
1:G:81:ASP:O	1:G:90:LYS:HE2	2.05	0.56
1:A:336:GLN:NE2	1:A:344:ASN:O	2.38	0.56
1:A:218:ARG:HD2	4:A:1630:HOH:O	2.06	0.56
1:C:548:HIS:CE1	2:C:804:SHG:HO3	2.22	0.56
1:F:181:PRO:HG3	1:F:587:PRO:HD2	1.86	0.56
1:E:50:VAL:HG13	1:E:313:ALA:HB2	1.87	0.56
1:G:56:PRO:HD3	1:G:165:SER:HB3	1.89	0.55
1:C:548:HIS:CE1	2:C:804:SHG:O3	2.59	0.55
1:H:346:PRO:HG2	1:H:350:PRO:HA	1.89	0.55
2:D:803:SHG:H3	3:D:703:FAD:N5	2.22	0.55
1:G:618:PHE:C	1:G:618:PHE:HD1	2.10	0.55
2:A:801:SHG:H3	3:A:701:FAD:N5	2.21	0.54
1:B:538:PRO:HG2	1:D:538:PRO:HG2	1.89	0.54
1:G:64:GLU:OE2	1:G:205:TYR:OH	2.18	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:47:TYR:O	1:G:313:ALA:HA	2.08	0.54
1:E:153:SER:OG	1:E:542:GLU:HG3	2.07	0.54
1:G:97:GLN:HG3	1:G:250:PHE:CE2	2.43	0.54
1:C:564:CYS:HG	1:C:573:PHE:HE2	1.55	0.54
1:F:92:ASN:O	1:F:250:PHE:HZ	1.91	0.54
1:B:81:ASP:OD1	1:B:81:ASP:C	2.45	0.54
1:F:153:SER:OG	1:F:542:GLU:HG2	2.08	0.53
1:G:346:PRO:HG2	1:G:350:PRO:HA	1.90	0.53
1:G:49:VAL:HB	1:G:72:VAL:HG22	1.90	0.52
1:D:50:VAL:HG13	1:D:313:ALA:HB2	1.90	0.52
1:D:81:ASP:O	1:D:90:LYS:HE2	2.10	0.52
1:E:452:ASP:OD1	1:E:472:ARG:NH1	2.42	0.52
1:G:548:HIS:CE1	2:G:808:SHG:HO3	2.26	0.52
1:D:153:SER:OG	1:D:542:GLU:HG3	2.09	0.52
1:E:291:LEU:CD1	1:E:291:LEU:H	2.23	0.52
1:E:548:HIS:CE1	2:E:805:SHG:O3	2.63	0.52
1:D:100:ILE:HD13	1:D:100:ILE:C	2.30	0.52
1:G:618:PHE:C	1:G:618:PHE:CD1	2.82	0.51
1:G:618:PHE:HD1	1:G:619:THR:N	2.08	0.51
1:G:50:VAL:HG13	1:G:313:ALA:HB2	1.93	0.51
1:G:218:ARG:HD2	4:G:1593:HOH:O	2.10	0.51
1:B:137:PHE:CE2	1:B:139:ARG:HG2	2.46	0.51
1:A:81:ASP:O	1:A:90:LYS:HE2	2.12	0.50
1:D:77:ILE:HG22	3:D:703:FAD:C4A	2.40	0.50
1:C:157:VAL:HG21	1:C:324:HIS:HE1	1.76	0.50
1:E:157:VAL:HG21	1:E:324:HIS:HE1	1.76	0.50
1:G:157:VAL:HG21	1:G:324:HIS:HE1	1.76	0.50
1:B:153:SER:OG	1:B:542:GLU:CG	2.58	0.50
1:B:159:ARG:HA	3:B:702:FAD:O2B	2.10	0.50
2:C:804:SHG:H3	3:C:704:FAD:N5	2.26	0.50
1:D:157:VAL:HG21	1:D:324:HIS:HE1	1.77	0.49
1:B:100:ILE:HD13	1:B:100:ILE:C	2.32	0.49
1:F:289:ASN:HB3	1:F:296:GLU:OE2	2.12	0.49
1:G:548:HIS:NE2	2:G:808:SHG:O3	2.38	0.49
1:E:618:PHE:HD1	1:E:619:THR:H	1.60	0.49
1:E:291:LEU:HD13	4:E:2441:HOH:O	2.13	0.49
1:G:84:LEU:N	1:G:84:LEU:HD23	2.28	0.49
1:C:173:PRO:HG2	1:C:592:ALA:HB1	1.93	0.49
1:E:385:THR:O	1:E:388:GLU:HG2	2.12	0.49
1:H:312:LYS:CE	4:H:1958:HOH:O	2.54	0.49
1:A:457:GLY:H	1:A:460:GLN:HE21	1.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:126:LEU:CD1	1:H:132:GLN:HG3	2.42	0.49
1:H:218:ARG:HD2	4:H:1173:HOH:O	2.13	0.49
1:E:471:TRP:CH2	1:E:526:SER:HA	2.47	0.48
1:F:47:TYR:O	1:F:313:ALA:HA	2.14	0.48
1:F:218:ARG:HD2	4:F:2063:HOH:O	2.12	0.48
1:H:432:GLU:HB3	1:H:451:ARG:HB2	1.96	0.48
1:F:452:ASP:N	1:F:452:ASP:OD1	2.47	0.48
1:C:153:SER:OG	1:C:542:GLU:HG3	2.13	0.48
1:F:548:HIS:CE1	2:F:806:SHG:O3	2.66	0.48
1:B:432:GLU:H	1:B:432:GLU:HG2	1.39	0.47
1:D:457:GLY:H	1:D:460:GLN:HE21	1.62	0.47
1:E:47:TYR:O	1:E:313:ALA:HA	2.14	0.47
1:A:157:VAL:HG21	1:A:324:HIS:HE1	1.79	0.47
1:B:81:ASP:O	1:B:90:LYS:HE2	2.14	0.47
1:B:218:ARG:HD2	4:B:948:HOH:O	2.15	0.47
1:H:59:CYS:SG	1:H:256:ALA:HB1	2.55	0.47
1:E:342:PRO:C	1:E:344:ASN:H	2.18	0.47
1:D:123:VAL:HG22	1:C:459:VAL:CG1	2.44	0.47
1:G:457:GLY:O	1:G:461:GLN:HG3	2.15	0.47
1:B:56:PRO:HD3	1:B:165:SER:HB3	1.97	0.46
1:D:158:THR:HG22	1:D:160:VAL:HG22	1.96	0.46
1:D:284:GLU:HB2	1:D:299:HIS:HD2	1.80	0.46
1:A:158:THR:HG22	1:A:160:VAL:HG22	1.96	0.46
1:C:432:GLU:H	1:C:432:GLU:HG2	1.45	0.46
1:D:218:ARG:HG3	1:D:430:ASP:OD2	2.16	0.46
1:F:92:ASN:O	1:F:250:PHE:CZ	2.68	0.46
2:E:805:SHG:H3	3:E:705:FAD:N5	2.31	0.46
1:A:77:ILE:CG2	3:A:701:FAD:C4A	2.93	0.46
1:F:344:ASN:N	1:F:345:PRO:CD	2.78	0.46
1:G:299:HIS:CE1	1:G:308:ARG:HB3	2.51	0.46
1:A:159:ARG:HA	3:A:701:FAD:O2B	2.16	0.46
1:B:487:PHE:HB3	1:B:498:PRO:HB2	1.98	0.46
1:H:471:TRP:CH2	1:H:526:SER:HA	2.51	0.46
1:F:618:PHE:CD1	1:F:618:PHE:C	2.89	0.46
1:B:451:ARG:HD3	1:B:468:ILE:O	2.16	0.45
1:G:178:GLU:OE1	1:G:441:PRO:HG3	2.16	0.45
1:A:548:HIS:CE1	2:A:801:SHG:HO3	2.32	0.45
1:B:294:GLU:OE1	1:B:296:GLU:OE2	2.35	0.45
1:H:490:LYS:HD2	1:H:491:ILE:CD1	2.45	0.45
1:G:173:PRO:HG2	1:G:592:ALA:HB1	1.98	0.45
1:B:471:TRP:CH2	1:B:526:SER:HA	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:293:SER:HA	1:D:574:GLY:O	2.17	0.45
1:H:80:ILE:O	1:H:81:ASP:HB3	2.15	0.45
1:B:45:ILE:H	1:B:45:ILE:HG13	1.65	0.45
1:E:619:THR:HG23	1:E:619:THR:O	2.17	0.45
1:H:459:VAL:O	1:H:462:SER:HB3	2.16	0.45
1:C:478:GLU:OE2	1:C:480:LYS:HE2	2.15	0.45
1:E:218:ARG:HD2	4:E:1659:HOH:O	2.16	0.45
1:H:77:ILE:HD11	1:H:495:TYR:CD2	2.52	0.45
1:D:100:ILE:HD13	1:D:100:ILE:O	2.17	0.45
1:E:385:THR:HG22	1:E:386:PRO:HD2	1.99	0.45
2:G:808:SHG:H3	3:G:708:FAD:N5	2.32	0.45
1:E:291:LEU:HD12	1:E:291:LEU:N	2.32	0.45
1:C:451:ARG:HD3	1:C:468:ILE:O	2.17	0.44
1:E:546:VAL:HA	2:E:805:SHG:H6	1.98	0.44
1:H:50:VAL:HG13	1:H:313:ALA:HB2	1.98	0.44
1:H:107:ILE:HG12	1:H:167:ALA:HB1	1.98	0.44
1:F:77:ILE:HD11	1:F:495:TYR:CD2	2.52	0.44
1:F:432:GLU:HB3	1:F:451:ARG:HB2	1.99	0.44
1:A:548:HIS:CE1	2:A:801:SHG:O3	2.70	0.44
1:E:81:ASP:O	1:E:81:ASP:CG	2.55	0.44
1:H:100:ILE:HD13	1:H:453:ALA:HA	1.99	0.44
1:F:471:TRP:CH2	1:F:526:SER:HA	2.52	0.44
1:G:77:ILE:HG22	3:G:708:FAD:C4A	2.48	0.44
1:B:185:LYS:HB2	1:B:185:LYS:HE3	1.59	0.44
1:F:432:GLU:H	1:F:432:GLU:HG2	1.50	0.44
1:F:618:PHE:HD1	1:F:619:THR:N	2.16	0.44
1:C:81:ASP:OD1	1:C:81:ASP:C	2.52	0.44
1:C:471:TRP:CH2	1:C:526:SER:HA	2.52	0.44
1:E:285:ARG:HG3	1:E:299:HIS:HB3	2.00	0.44
1:H:444:PRO:HD2	1:H:445:TRP:CZ3	2.52	0.44
1:G:89:HIS:CE1	1:G:91:LYS:HB2	2.52	0.44
1:A:358:GLU:HG2	1:A:544:GLY:HA2	1.99	0.44
1:E:291:LEU:CD1	1:E:291:LEU:N	2.81	0.44
1:H:158:THR:HG22	1:H:160:VAL:HG22	2.00	0.44
1:F:452:ASP:OD1	1:F:472:ARG:NH1	2.51	0.44
1:A:548:HIS:NE2	2:A:801:SHG:O3	2.41	0.43
1:D:432:GLU:H	1:D:432:GLU:HG2	1.31	0.43
1:C:459:VAL:O	1:C:462:SER:HB3	2.18	0.43
1:G:385:THR:CG2	1:G:386:PRO:HD2	2.45	0.43
1:A:293:SER:HA	1:A:574:GLY:O	2.18	0.43
1:F:564:CYS:HG	1:F:573:PHE:HE2	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:GLU:HB2	4:A:2369:HOH:O	2.18	0.43
1:B:339:ARG:HA	1:B:340:PRO:HD3	1.93	0.43
1:C:219:HIS:HA	1:C:433:PRO:HA	2.01	0.43
1:C:346:PRO:HG2	1:C:350:PRO:HA	2.01	0.43
1:F:107:ILE:HG12	1:F:167:ALA:HB1	1.99	0.43
1:A:471:TRP:CH2	1:A:526:SER:HA	2.54	0.43
1:B:558:ASP:OD2	1:B:561:GLU:HG3	2.18	0.43
1:E:46:LYS:HD3	1:E:312:LYS:HG2	2.00	0.43
1:G:385:THR:O	1:G:388:GLU:CG	2.62	0.43
1:A:90:LYS:HG3	1:A:166:THR:HB	2.00	0.43
1:D:47:TYR:O	1:D:313:ALA:HA	2.18	0.43
1:D:432:GLU:HB3	1:D:451:ARG:HB2	2.01	0.43
1:E:382:ILE:HG12	1:E:393:VAL:HG22	2.01	0.43
1:E:92:ASN:O	1:E:250:PHE:HZ	2.01	0.42
2:B:802:SHG:H3	3:B:702:FAD:N5	2.33	0.42
1:D:558:ASP:HB3	1:D:561:GLU:HB2	2.01	0.42
1:A:89:HIS:ND1	1:A:91:LYS:HB3	2.34	0.42
1:C:363:PHE:HA	1:C:471:TRP:O	2.20	0.42
1:F:341:ASN:C	1:F:341:ASN:HD22	2.23	0.42
1:G:89:HIS:ND1	1:G:91:LYS:HB2	2.34	0.42
1:B:81:ASP:OD1	1:B:81:ASP:O	2.38	0.42
1:D:215:GLU:O	1:D:411:LYS:NZ	2.53	0.42
1:E:452:ASP:OD1	1:E:452:ASP:N	2.53	0.42
1:F:289:ASN:ND2	1:F:294:GLU:HB3	2.35	0.42
1:B:77:ILE:CG2	3:B:702:FAD:C4A	2.97	0.42
1:G:451:ARG:HD3	1:G:468:ILE:O	2.19	0.42
1:B:476:ARG:HB2	1:B:589:ALA:HB1	2.01	0.42
1:D:299:HIS:CE1	1:D:308:ARG:HB3	2.55	0.42
1:F:81:ASP:C	1:F:81:ASP:OD1	2.56	0.42
1:G:299:HIS:HB2	1:G:310:GLU:OE1	2.20	0.42
1:B:215:GLU:O	1:B:411:LYS:NZ	2.53	0.42
1:D:341:ASN:HA	1:D:342:PRO:HD3	1.92	0.42
1:C:385:THR:HA	1:C:386:PRO:HD3	1.97	0.42
1:C:432:GLU:HB3	1:C:451:ARG:HB2	2.01	0.42
1:F:211:ASP:O	1:F:214:LYS:HG2	2.19	0.42
1:H:426:ILE:HA	1:H:427:PRO:HD3	1.88	0.42
1:A:346:PRO:HG2	1:A:350:PRO:HA	2.01	0.41
1:D:312:LYS:HG3	1:D:313:ALA:N	2.35	0.41
1:C:157:VAL:HG21	1:C:324:HIS:CE1	2.55	0.41
1:C:218:ARG:HG3	1:C:430:ASP:OD2	2.20	0.41
1:C:444:PRO:HD2	1:C:445:TRP:CZ3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:383:ARG:HB3	1:F:392:SER:HB3	2.03	0.41
1:G:548:HIS:CE1	2:G:808:SHG:O3	2.74	0.41
1:E:618:PHE:CD1	1:E:619:THR:N	2.86	0.41
1:F:157:VAL:HG21	1:F:324:HIS:CE1	2.47	0.41
1:H:564:CYS:HG	1:H:573:PHE:HE2	1.65	0.41
1:G:218:ARG:HG3	1:G:430:ASP:OD2	2.20	0.41
1:H:83:GLY:N	4:G:2497:HOH:O	2.53	0.41
1:A:395:TYR:OH	1:A:410:GLU:HB2	2.21	0.41
1:E:173:PRO:HG2	1:E:592:ALA:HB1	2.02	0.41
1:F:194:GLU:OE1	1:F:194:GLU:HA	2.19	0.41
1:F:433:PRO:O	1:F:450:HIS:HA	2.20	0.41
1:H:263:GLN:HE21	1:H:263:GLN:HB3	1.68	0.41
1:G:47:TYR:CE2	1:G:73:ALA:HB2	2.55	0.41
1:G:457:GLY:H	1:G:460:GLN:HE21	1.68	0.41
1:A:201:LYS:HE2	1:A:205:TYR:OH	2.21	0.41
1:B:137:PHE:O	1:B:139:ARG:HG3	2.20	0.41
1:F:478:GLU:HG2	1:F:480:LYS:HE2	2.03	0.41
1:H:421:GLU:H	1:H:421:GLU:CD	2.23	0.41
1:G:570:SER:HB3	1:G:580:LEU:O	2.20	0.41
1:A:145:GLU:HG3	1:A:488:SER:HB2	2.03	0.41
1:A:153:SER:OG	1:A:542:GLU:CG	2.69	0.41
1:A:281:VAL:CG1	1:A:300:ILE:HB	2.51	0.41
1:A:385:THR:HA	1:A:386:PRO:HD3	1.99	0.41
1:B:145:GLU:HG3	1:B:488:SER:HB2	2.03	0.41
1:H:385:THR:HA	1:H:386:PRO:HD3	1.96	0.41
1:D:339:ARG:HA	1:D:340:PRO:HD3	1.92	0.41
1:H:47:TYR:O	1:H:313:ALA:HA	2.21	0.41
1:A:458:ALA:O	1:B:121:LEU:HD12	2.20	0.40
1:D:157:VAL:HG21	1:D:324:HIS:CE1	2.57	0.40
1:D:218:ARG:HD2	4:D:1005:HOH:O	2.19	0.40
1:D:363:PHE:HA	1:D:471:TRP:O	2.21	0.40
1:C:618:PHE:HD1	1:C:618:PHE:C	2.25	0.40
1:H:542:GLU:HA	1:H:543:PRO:HD3	1.95	0.40
1:E:618:PHE:CD1	1:E:618:PHE:C	2.94	0.40
1:D:92:ASN:O	1:D:250:PHE:HZ	2.03	0.40
1:G:398:GLY:O	1:G:399:ALA:C	2.60	0.40
1:B:293:SER:HA	1:B:574:GLY:O	2.21	0.40
1:E:88:ALA:HA	1:E:255:SER:OG	2.21	0.40
1:D:459:VAL:O	1:D:462:SER:HB3	2.21	0.40
1:C:81:ASP:O	1:C:90:LYS:HE2	2.22	0.40
1:C:347:GLU:HG2	1:C:348:LEU:HG	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:100:ILE:HD13	1:E:453:ALA:HA	2.03	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%)	558 (97%)	17 (3%)	0	100	100
1	B	575/623 (92%)	563 (98%)	11 (2%)	1 (0%)	47	38
1	C	575/623 (92%)	554 (96%)	21 (4%)	0	100	100
1	D	575/623 (92%)	561 (98%)	14 (2%)	0	100	100
1	E	575/623 (92%)	558 (97%)	17 (3%)	0	100	100
1	F	575/623 (92%)	559 (97%)	16 (3%)	0	100	100
1	G	575/623 (92%)	558 (97%)	17 (3%)	0	100	100
1	H	575/623 (92%)	559 (97%)	16 (3%)	0	100	100
All	All	4600/4984 (92%)	4470 (97%)	129 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	187	ASP

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	504/541 (93%)	485 (96%)	19 (4%)	33	21
1	B	504/541 (93%)	489 (97%)	15 (3%)	41	30
1	C	504/541 (93%)	483 (96%)	21 (4%)	30	17
1	D	504/541 (93%)	483 (96%)	21 (4%)	30	17
1	E	504/541 (93%)	482 (96%)	22 (4%)	28	15
1	F	504/541 (93%)	485 (96%)	19 (4%)	33	21
1	G	504/541 (93%)	483 (96%)	21 (4%)	30	17
1	H	504/541 (93%)	480 (95%)	24 (5%)	25	12
All	All	4032/4328 (93%)	3870 (96%)	162 (4%)	31	19

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	MET
1	A	100	ILE
1	A	112	MET
1	A	132	GLN
1	A	168	TRP
1	A	206	PHE
1	A	285	ARG
1	A	312	LYS
1	A	341	ASN
1	A	347	GLU
1	A	385	THR
1	A	392	SER
1	A	401	THR
1	A	432	GLU
1	A	450	HIS
1	A	496	ASN
1	A	593	ASN
1	A	618	PHE
1	A	619	THR
1	B	100	ILE
1	B	112	MET
1	B	139	ARG
1	B	168	TRP
1	B	185	LYS
1	B	206	PHE

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Mol	Chain	Res	Type
1	B	216	SER
1	B	344	ASN
1	B	385	THR
1	B	389	LEU
1	B	390	THR
1	B	432	GLU
1	B	450	HIS
1	B	490	LYS
1	B	496	ASN
1	D	91	LYS
1	D	100	ILE
1	D	112	MET
1	D	168	TRP
1	D	178	GLU
1	D	206	PHE
1	D	231	LYS
1	D	285	ARG
1	D	344	ASN
1	D	347	GLU
1	D	385	THR
1	D	403	LYS
1	D	408	TRP
1	D	413	LYS
1	D	432	GLU
1	D	450	HIS
1	D	490	LYS
1	D	496	ASN
1	D	554	ARG
1	D	593	ASN
1	D	618	PHE
1	C	43	MET
1	C	100	ILE
1	C	112	MET
1	C	168	TRP
1	C	206	PHE
1	C	285	ARG
1	C	341	ASN
1	C	344	ASN
1	C	385	THR
1	C	389	LEU
1	C	392	SER
1	C	403	LYS

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Mol	Chain	Res	Type
1	C	432	GLU
1	C	445	TRP
1	C	450	HIS
1	C	455	SER
1	C	490	LYS
1	C	496	ASN
1	C	593	ASN
1	C	618	PHE
1	C	619	THR
1	E	46	LYS
1	E	100	ILE
1	E	112	MET
1	E	168	TRP
1	E	185	LYS
1	E	206	PHE
1	E	231	LYS
1	E	341	ASN
1	E	344	ASN
1	E	347	GLU
1	E	386	PRO
1	E	388	GLU
1	E	392	SER
1	E	403	LYS
1	E	408	TRP
1	E	413	LYS
1	E	432	GLU
1	E	450	HIS
1	E	452	ASP
1	E	490	LYS
1	E	593	ASN
1	E	618	PHE
1	F	95	GLU
1	F	100	ILE
1	F	112	MET
1	F	168	TRP
1	F	206	PHE
1	F	216	SER
1	F	341	ASN
1	F	344	ASN
1	F	383	ARG
1	F	385	THR
1	F	388	GLU

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Mol	Chain	Res	Type
1	F	408	TRP
1	F	432	GLU
1	F	445	TRP
1	F	450	HIS
1	F	452	ASP
1	F	490	LYS
1	F	593	ASN
1	F	618	PHE
1	H	81	ASP
1	H	91	LYS
1	H	100	ILE
1	H	112	MET
1	H	132	GLN
1	H	168	TRP
1	H	185	LYS
1	H	194	GLU
1	H	206	PHE
1	H	231	LYS
1	H	310	GLU
1	H	341	ASN
1	H	344	ASN
1	H	347	GLU
1	H	385	THR
1	H	389	LEU
1	H	413	LYS
1	H	450	HIS
1	H	455	SER
1	H	490	LYS
1	H	542	GLU
1	H	593	ASN
1	H	618	PHE
1	H	619	THR
1	G	45	ILE
1	G	82	SER
1	G	84	LEU
1	G	95	GLU
1	G	100	ILE
1	G	112	MET
1	G	168	TRP
1	G	206	PHE
1	G	231	LYS
1	G	341	ASN

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Mol	Chain	Res	Type
1	G	389	LEU
1	G	392	SER
1	G	408	TRP
1	G	445	TRP
1	G	450	HIS
1	G	490	LYS
1	G	496	ASN
1	G	587	PRO
1	G	593	ASN
1	G	618	PHE
1	G	619	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	341	ASN
1	A	460	GLN
1	B	341	ASN
1	B	460	GLN
1	D	299	HIS
1	D	324	HIS
1	D	341	ASN
1	D	460	GLN
1	C	341	ASN
1	E	263	GLN
1	E	341	ASN
1	E	460	GLN
1	F	341	ASN
1	F	460	GLN
1	H	263	GLN
1	H	341	ASN
1	H	460	GLN
1	G	263	GLN
1	G	299	HIS
1	G	460	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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	$\#\|Z\| > 2$
3	FAD	A	701	-	51,58,58	1.83	10 (19%)	60,89,89	2.32	11 (18%)
3	FAD	G	708	-	51,58,58	1.69	7 (13%)	60,89,89	2.01	9 (15%)
2	SHG	G	808	-	12,12,12	0.91	0	16,17,17	4.80	9 (56%)
3	FAD	C	704	-	51,58,58	1.71	11 (21%)	60,89,89	2.06	9 (15%)
2	SHG	E	805	-	12,12,12	0.89	0	16,17,17	4.93	8 (50%)
3	FAD	E	705	-	51,58,58	1.45	7 (13%)	60,89,89	2.44	10 (16%)
2	SHG	H	807	-	12,12,12	0.55	0	16,17,17	4.55	13 (81%)
3	FAD	B	702	-	51,58,58	1.61	7 (13%)	60,89,89	2.20	10 (16%)
3	FAD	D	703	-	51,58,58	1.50	6 (11%)	60,89,89	1.83	9 (15%)
3	FAD	F	706	-	51,58,58	1.40	7 (13%)	60,89,89	2.20	14 (23%)
2	SHG	D	803	-	12,12,12	1.48	2 (16%)	16,17,17	4.33	9 (56%)
3	FAD	H	707	-	51,58,58	1.51	6 (11%)	60,89,89	2.07	10 (16%)
2	SHG	C	804	-	12,12,12	0.72	0	16,17,17	5.09	11 (68%)
2	SHG	B	802	-	12,12,12	0.95	1 (8%)	16,17,17	4.45	10 (62%)
2	SHG	F	806	-	12,12,12	0.74	0	16,17,17	4.41	8 (50%)
2	SHG	A	801	-	12,12,12	0.75	0	16,17,17	4.63	10 (62%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FAD	A	701	-	-	1/30/50/50	0/6/6/6
3	FAD	G	708	-	-	1/30/50/50	0/6/6/6
2	SHG	G	808	-	-	0/2/22/22	0/1/1/1
3	FAD	C	704	-	-	1/30/50/50	0/6/6/6
2	SHG	E	805	-	-	1/2/22/22	0/1/1/1
3	FAD	E	705	-	-	1/30/50/50	0/6/6/6
2	SHG	H	807	-	-	0/2/22/22	0/1/1/1
3	FAD	B	702	-	-	2/30/50/50	0/6/6/6
3	FAD	D	703	-	-	2/30/50/50	0/6/6/6
3	FAD	F	706	-	-	1/30/50/50	0/6/6/6
2	SHG	D	803	-	-	0/2/22/22	0/1/1/1
3	FAD	H	707	-	-	2/30/50/50	0/6/6/6
2	SHG	C	804	-	-	1/2/22/22	0/1/1/1
2	SHG	B	802	-	-	1/2/22/22	0/1/1/1
2	SHG	F	806	-	-	0/2/22/22	0/1/1/1
2	SHG	A	801	-	-	0/2/22/22	0/1/1/1

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	708	FAD	C10-N1	6.79	1.42	1.33
3	A	701	FAD	C10-N1	6.40	1.41	1.33
3	C	704	FAD	C4X-N5	5.31	1.40	1.33
3	E	705	FAD	C10-N1	5.15	1.39	1.33
3	C	704	FAD	C10-N1	5.09	1.39	1.33
3	H	707	FAD	C10-N1	4.77	1.39	1.33
3	B	702	FAD	C10-N1	4.64	1.39	1.33
3	G	708	FAD	C1'-N10	4.01	1.52	1.48
3	A	701	FAD	C4X-N5	4.00	1.39	1.33
3	B	702	FAD	C2A-N3A	3.86	1.38	1.32
3	B	702	FAD	C1'-N10	3.81	1.52	1.48
3	F	706	FAD	C10-N1	3.79	1.38	1.33
3	D	703	FAD	C2A-N3A	3.75	1.38	1.32
3	H	707	FAD	C1'-N10	3.74	1.52	1.48
3	D	703	FAD	C5X-N5	3.73	1.41	1.35
3	G	708	FAD	C5'-C4'	3.72	1.57	1.51
3	D	703	FAD	C4-N3	3.68	1.39	1.33
3	D	703	FAD	C4X-N5	3.65	1.38	1.33
2	D	803	SHG	C2-C1	3.62	1.56	1.52
3	C	704	FAD	C2A-N3A	3.56	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	705	FAD	C2A-N3A	3.52	1.37	1.32
3	B	702	FAD	C4-N3	3.45	1.39	1.33
3	H	707	FAD	C2A-N3A	3.42	1.37	1.32
3	F	706	FAD	C2A-N3A	3.42	1.37	1.32
3	A	701	FAD	C2A-N1A	3.37	1.40	1.33
3	A	701	FAD	C1'-N10	3.35	1.51	1.48
3	D	703	FAD	C10-N1	3.33	1.37	1.33
3	E	705	FAD	C1'-N10	3.32	1.51	1.48
3	C	704	FAD	C5'-C4'	3.31	1.56	1.51
3	G	708	FAD	C2A-N3A	3.21	1.37	1.32
3	A	701	FAD	C2A-N3A	3.19	1.37	1.32
3	B	702	FAD	C4X-N5	3.17	1.37	1.33
3	A	701	FAD	C5X-N5	3.17	1.40	1.35
3	F	706	FAD	C4X-N5	3.15	1.37	1.33
3	E	705	FAD	C4-N3	3.14	1.38	1.33
3	E	705	FAD	C4X-N5	3.13	1.37	1.33
3	G	708	FAD	C4X-N5	3.10	1.37	1.33
3	A	701	FAD	C9A-N10	3.06	1.42	1.38
3	F	706	FAD	C9A-N10	3.02	1.42	1.38
3	A	701	FAD	C5'-C4'	2.96	1.56	1.51
3	B	702	FAD	C2A-N1A	2.92	1.39	1.33
3	C	704	FAD	C2A-N1A	2.79	1.39	1.33
3	H	707	FAD	C4X-N5	2.76	1.37	1.33
3	D	703	FAD	C2A-N1A	2.75	1.39	1.33
2	D	803	SHG	C2-C3	-2.72	1.50	1.52
3	A	701	FAD	C4X-C10	2.64	1.41	1.38
3	A	701	FAD	C4-N3	2.62	1.37	1.33
3	C	704	FAD	C5X-N5	2.57	1.39	1.35
3	E	705	FAD	C5X-N5	2.50	1.39	1.35
3	G	708	FAD	C4-N3	2.49	1.37	1.33
3	C	704	FAD	C4-N3	2.48	1.37	1.33
3	F	706	FAD	C4-N3	2.44	1.37	1.33
3	B	702	FAD	C4X-C10	2.34	1.41	1.38
3	H	707	FAD	C2A-N1A	2.33	1.38	1.33
3	C	704	FAD	P-O1P	-2.27	1.42	1.50
3	F	706	FAD	C2A-N1A	2.25	1.38	1.33
3	G	708	FAD	C2A-N1A	2.22	1.38	1.33
3	F	706	FAD	O4B-C4B	-2.12	1.40	1.45
2	B	802	SHG	O3-C3	-2.07	1.38	1.43
3	C	704	FAD	PA-O1A	-2.05	1.43	1.50
3	E	705	FAD	C2A-N1A	2.04	1.37	1.33
3	H	707	FAD	C4-N3	2.04	1.36	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	704	FAD	C8M-C8	2.03	1.55	1.51
3	C	704	FAD	C9-C8	2.03	1.42	1.37

All (160) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	804	SHG	F2-C2-C3	13.78	121.08	108.85
2	G	808	SHG	F2-C2-C3	13.54	120.87	108.85
3	A	701	FAD	C4-N3-C2	12.29	125.51	115.14
3	E	705	FAD	C4-N3-C2	11.64	124.97	115.14
2	E	805	SHG	F2-C2-C3	11.23	118.82	108.85
2	A	801	SHG	F2-C2-C3	11.05	118.66	108.85
2	B	802	SHG	F2-C2-C1	10.69	119.58	107.77
2	F	806	SHG	F2-C2-C3	10.26	117.96	108.85
2	C	804	SHG	O5-C1-C2	10.15	122.89	109.80
3	C	704	FAD	C4-N3-C2	10.07	123.65	115.14
3	G	708	FAD	C4-N3-C2	9.51	123.17	115.14
2	F	806	SHG	O5-C1-C2	9.50	122.05	109.80
3	E	705	FAD	C1'-N10-C9A	9.04	125.41	118.29
2	H	807	SHG	F2-C2-C3	8.96	116.80	108.85
2	E	805	SHG	F2-C2-C1	8.89	117.60	107.77
2	E	805	SHG	O5-C1-C2	8.79	121.14	109.80
2	D	803	SHG	F2-C2-C1	8.75	117.44	107.77
2	H	807	SHG	O5-C1-C2	8.69	121.00	109.80
2	H	807	SHG	F2-C2-C1	8.61	117.29	107.77
2	G	808	SHG	O5-C1-C2	8.44	120.68	109.80
3	B	702	FAD	C4-N3-C2	8.40	122.23	115.14
3	F	706	FAD	C4-N3-C2	8.40	122.23	115.14
2	A	801	SHG	F2-C2-C1	7.65	116.23	107.77
2	B	802	SHG	F2-C2-C3	7.63	115.62	108.85
2	A	801	SHG	O5-C1-C2	7.44	119.40	109.80
2	D	803	SHG	O5-C1-C2	7.27	119.18	109.80
2	D	803	SHG	F2-C2-C3	7.20	115.24	108.85
3	F	706	FAD	C1'-N10-C9A	7.09	123.87	118.29
2	B	802	SHG	O5-C1-C2	6.93	118.73	109.80
3	H	707	FAD	C4-N3-C2	6.84	120.92	115.14
3	H	707	FAD	C1'-N10-C9A	6.78	123.63	118.29
3	B	702	FAD	C1'-N10-C9A	6.41	123.33	118.29
3	A	701	FAD	N3A-C2A-N1A	-6.36	118.73	128.68
2	H	807	SHG	O5-C5-C4	6.31	121.15	109.69
2	D	803	SHG	O5-C5-C4	6.24	121.02	109.69
2	B	802	SHG	O5-C5-C4	6.18	120.91	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	703	FAD	C4-N3-C2	6.15	120.33	115.14
3	H	707	FAD	N3A-C2A-N1A	-6.08	119.18	128.68
2	F	806	SHG	F2-C2-C1	6.06	114.46	107.77
3	E	705	FAD	N3A-C2A-N1A	-5.95	119.37	128.68
3	G	708	FAD	N3A-C2A-N1A	-5.93	119.41	128.68
2	G	808	SHG	O5-C5-C4	5.79	120.21	109.69
3	D	703	FAD	N3A-C2A-N1A	-5.78	119.64	128.68
3	C	704	FAD	N3A-C2A-N1A	-5.72	119.74	128.68
3	F	706	FAD	N3A-C2A-N1A	-5.70	119.77	128.68
3	B	702	FAD	N3A-C2A-N1A	-5.61	119.91	128.68
2	E	805	SHG	O5-C5-C4	5.58	119.82	109.69
2	F	806	SHG	O5-C5-C4	5.38	119.46	109.69
3	D	703	FAD	C1'-N10-C9A	5.36	122.51	118.29
2	C	804	SHG	F2-C2-C1	5.23	113.55	107.77
3	E	705	FAD	C4X-C4-N3	-5.03	116.55	123.43
2	D	803	SHG	C1-C2-C3	5.01	118.23	110.75
2	C	804	SHG	O5-C5-C4	4.92	118.62	109.69
3	B	702	FAD	C4X-N5-C5X	4.91	121.68	116.77
3	A	701	FAD	C4X-C4-N3	-4.90	116.73	123.43
2	A	801	SHG	O5-C5-C4	4.90	118.59	109.69
3	B	702	FAD	C10-C4X-N5	-4.86	117.90	121.26
2	E	805	SHG	O3-C3-C2	4.76	119.13	109.68
3	H	707	FAD	C5'-C4'-C3'	-4.71	103.11	112.20
3	H	707	FAD	C4X-N5-C5X	4.63	121.40	116.77
3	F	706	FAD	C4X-N5-C5X	4.62	121.39	116.77
2	A	801	SHG	C1-O5-C5	4.61	122.37	113.66
2	C	804	SHG	C3-C4-C5	4.57	118.40	110.24
3	C	704	FAD	C1'-N10-C9A	4.56	121.88	118.29
3	G	708	FAD	C4X-C4-N3	-4.48	117.30	123.43
3	C	704	FAD	C4X-C4-N3	-4.27	117.59	123.43
3	G	708	FAD	C4X-N5-C5X	4.24	121.00	116.77
2	D	803	SHG	C3-C4-C5	4.11	117.58	110.24
3	B	702	FAD	C4X-C4-N3	-4.07	117.87	123.43
2	G	808	SHG	C1-O5-C5	3.92	121.06	113.66
2	A	801	SHG	C3-C4-C5	3.85	117.11	110.24
2	B	802	SHG	C1-O5-C5	3.83	120.90	113.66
3	G	708	FAD	C5'-C4'-C3'	-3.74	104.97	112.20
2	E	805	SHG	C3-C4-C5	3.73	116.89	110.24
3	D	703	FAD	O4'-C4'-C3'	3.72	118.13	109.10
2	F	806	SHG	O3-C3-C2	3.70	117.02	109.68
3	H	707	FAD	C4X-C4-N3	-3.60	118.50	123.43
3	A	701	FAD	C4X-N5-C5X	3.57	120.34	116.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	808	SHG	O3-C3-C4	3.51	118.46	110.35
2	G	808	SHG	F2-C2-C1	3.51	111.64	107.77
2	A	801	SHG	C1-C2-C3	3.51	115.99	110.75
2	F	806	SHG	C1-O5-C5	3.50	120.27	113.66
2	D	803	SHG	C1-O5-C5	3.49	120.25	113.66
3	F	706	FAD	C4X-C4-N3	-3.49	118.66	123.43
2	D	803	SHG	O3-C3-C2	3.44	116.50	109.68
2	C	804	SHG	C1-O5-C5	3.38	120.05	113.66
3	F	706	FAD	C5X-C9A-N10	3.37	120.16	117.72
2	G	808	SHG	C1-C2-C3	3.37	115.78	110.75
2	E	805	SHG	C1-O5-C5	3.36	120.00	113.66
2	G	808	SHG	O3-C3-C2	3.33	116.28	109.68
2	E	805	SHG	O5-C5-C6	3.32	114.68	106.44
2	H	807	SHG	C1-C2-C3	3.31	115.70	110.75
3	B	702	FAD	C4-C4X-N5	3.31	122.38	118.60
3	D	703	FAD	C4X-C4-N3	-3.12	119.17	123.43
3	E	705	FAD	C1'-N10-C10	-3.11	115.63	118.41
3	D	703	FAD	P-O3P-PA	-3.09	122.24	132.83
3	C	704	FAD	C4X-N5-C5X	3.06	119.83	116.77
2	G	808	SHG	C3-C4-C5	3.03	115.64	110.24
3	H	707	FAD	C5X-C9A-N10	3.00	119.89	117.72
2	B	802	SHG	O3-C3-C4	2.99	117.25	110.35
2	C	804	SHG	O3-C3-C4	2.98	117.23	110.35
2	F	806	SHG	O5-C5-C6	2.95	113.78	106.44
3	E	705	FAD	C5'-C4'-C3'	-2.93	106.55	112.20
2	A	801	SHG	O3-C3-C2	2.93	115.49	109.68
2	A	801	SHG	O4-C4-C5	2.92	116.55	109.30
2	H	807	SHG	C3-C4-C5	2.89	115.39	110.24
3	F	706	FAD	C10-C4X-N5	-2.86	119.28	121.26
3	C	704	FAD	C5X-C9A-N10	2.85	119.78	117.72
2	C	804	SHG	C1-C2-C3	2.85	115.01	110.75
2	B	802	SHG	C1-C2-C3	2.83	114.97	110.75
3	A	701	FAD	C5'-C4'-C3'	-2.82	106.76	112.20
3	A	701	FAD	C5X-C9A-N10	2.79	119.74	117.72
3	F	706	FAD	C4-C4X-N5	2.70	121.68	118.60
3	F	706	FAD	C9A-N10-C10	-2.67	118.41	121.91
2	H	807	SHG	O5-C5-C6	2.65	113.03	106.44
3	A	701	FAD	O3'-C3'-C4'	-2.63	102.45	108.81
3	A	701	FAD	C6-C5X-N5	2.62	121.93	119.05
2	H	807	SHG	O3-C3-C4	2.61	116.39	110.35
2	H	807	SHG	O4-C4-C5	2.59	115.74	109.30
2	C	804	SHG	C6-C5-C4	2.59	119.08	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	704	FAD	P-O3P-PA	-2.57	123.99	132.83
3	F	706	FAD	C6-C5X-C9A	2.55	122.39	119.05
2	B	802	SHG	O3-C3-C2	2.53	114.70	109.68
3	F	706	FAD	C8M-C8-C9	-2.48	114.41	120.34
2	F	806	SHG	C3-C4-C5	2.44	114.60	110.24
2	A	801	SHG	O5-C5-C6	2.44	112.50	106.44
3	G	708	FAD	P-O3P-PA	-2.44	124.47	132.83
3	E	705	FAD	C5X-C9A-N10	2.42	119.47	117.72
2	H	807	SHG	O3-C3-C2	2.41	114.45	109.68
3	D	703	FAD	C4X-N5-C5X	2.40	119.17	116.77
3	G	708	FAD	O4'-C4'-C3'	2.39	114.92	109.10
2	H	807	SHG	C1-O5-C5	2.35	118.09	113.66
3	F	706	FAD	C5'-C4'-C3'	-2.34	107.69	112.20
3	C	704	FAD	O2A-PA-O1A	2.31	123.64	112.24
3	D	703	FAD	C10-C4X-N5	-2.31	119.66	121.26
3	F	706	FAD	C7-C6-C5X	-2.31	117.95	121.22
3	E	705	FAD	O2P-P-O1P	2.29	123.54	112.24
3	A	701	FAD	C9A-C5X-N5	-2.28	118.79	122.36
3	G	708	FAD	C1'-N10-C9A	2.28	120.08	118.29
3	D	703	FAD	O5'-P-O1P	-2.26	100.25	109.07
3	E	705	FAD	C9A-N10-C10	-2.25	118.96	121.91
2	B	802	SHG	C3-C4-C5	2.24	114.23	110.24
3	H	707	FAD	C9A-C5X-N5	-2.22	118.89	122.36
2	H	807	SHG	O1-C1-O5	2.20	116.98	110.38
3	H	707	FAD	O3'-C3'-C2'	-2.18	103.56	108.81
3	C	704	FAD	C5'-C4'-C3'	-2.17	108.00	112.20
3	B	702	FAD	C1'-N10-C10	-2.16	116.47	118.41
3	E	705	FAD	O2'-C2'-C1'	2.16	114.80	109.59
2	B	802	SHG	O1-C1-C2	2.16	118.58	109.36
3	H	707	FAD	C1'-N10-C10	-2.16	116.48	118.41
3	A	701	FAD	C4-C4X-C10	-2.15	118.53	119.95
2	C	804	SHG	O6-C6-C5	-2.14	103.96	111.29
3	G	708	FAD	O4B-C1B-C2B	-2.14	103.81	106.93
2	C	804	SHG	O3-C3-C2	2.13	113.91	109.68
2	H	807	SHG	O6-C6-C5	-2.10	104.08	111.29
3	F	706	FAD	O4'-C4'-C3'	2.09	114.19	109.10
3	A	701	FAD	P-O3P-PA	-2.09	125.66	132.83
3	B	702	FAD	O4B-C1B-C2B	-2.06	103.91	106.93
3	B	702	FAD	P-O3P-PA	-2.03	125.86	132.83
2	D	803	SHG	O3-C3-C4	2.01	114.99	110.35

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	805	SHG	O5-C5-C6-O6
3	B	702	FAD	PA-O3P-P-O5'
3	D	703	FAD	PA-O3P-P-O5'
3	H	707	FAD	C5'-O5'-P-O3P
2	B	802	SHG	C4-C5-C6-O6
2	C	804	SHG	C4-C5-C6-O6
3	A	701	FAD	O4B-C4B-C5B-O5B
3	F	706	FAD	O4B-C4B-C5B-O5B
3	C	704	FAD	O4B-C4B-C5B-O5B
3	E	705	FAD	O4B-C4B-C5B-O5B
3	H	707	FAD	O4B-C4B-C5B-O5B
3	G	708	FAD	O4B-C4B-C5B-O5B
3	B	702	FAD	O4B-C4B-C5B-O5B
3	D	703	FAD	O4B-C4B-C5B-O5B

There are no ring outliers.

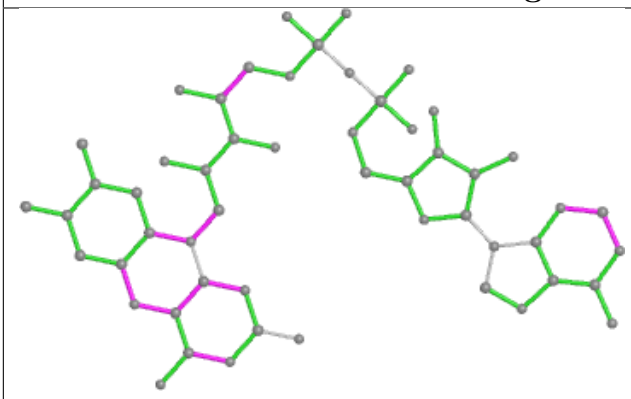
13 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	701	FAD	4	0
3	G	708	FAD	2	0
2	G	808	SHG	4	0
3	C	704	FAD	1	0
2	E	805	SHG	4	0
3	E	705	FAD	1	0
3	B	702	FAD	4	0
3	D	703	FAD	2	0
2	D	803	SHG	3	0
2	C	804	SHG	5	0
2	B	802	SHG	1	0
2	F	806	SHG	2	0
2	A	801	SHG	4	0

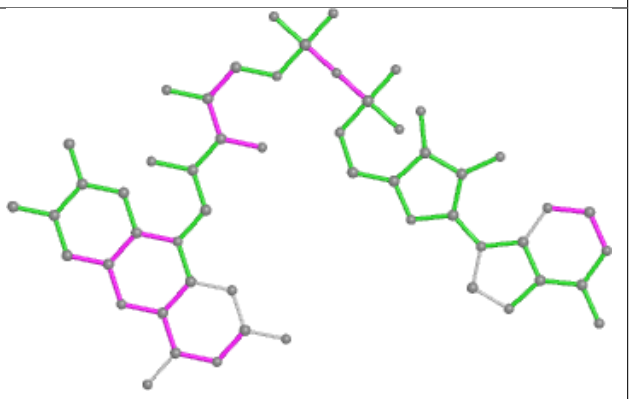
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

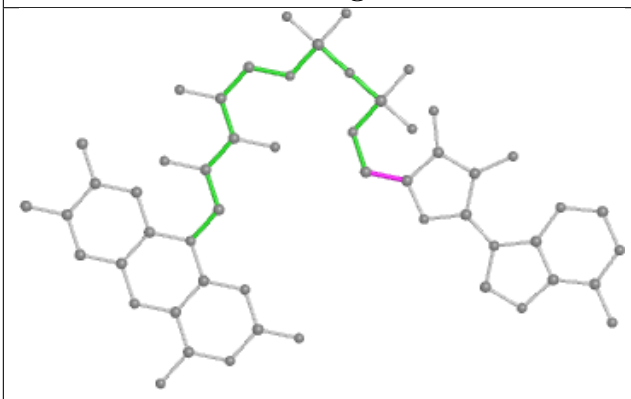
Ligand FAD A 701



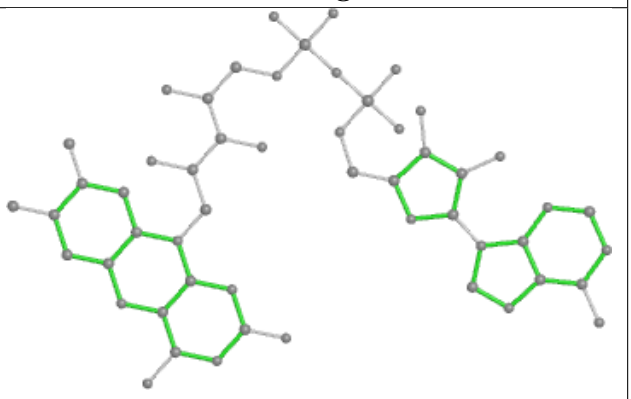
Bond lengths



Bond angles

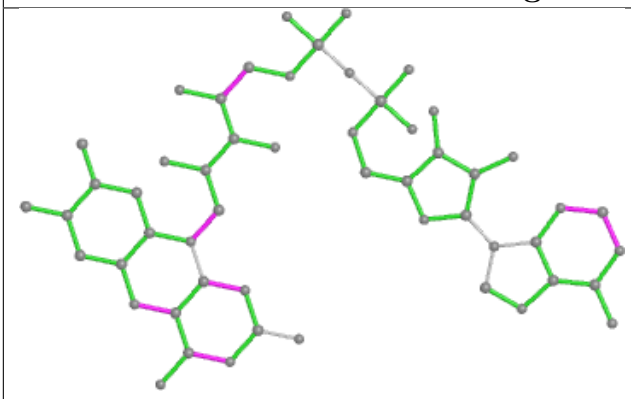


Torsions

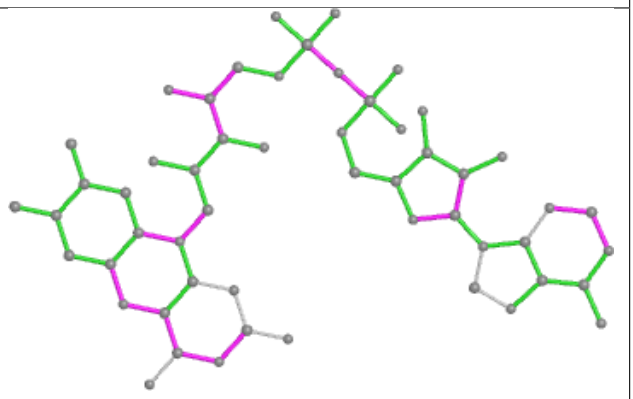


Rings

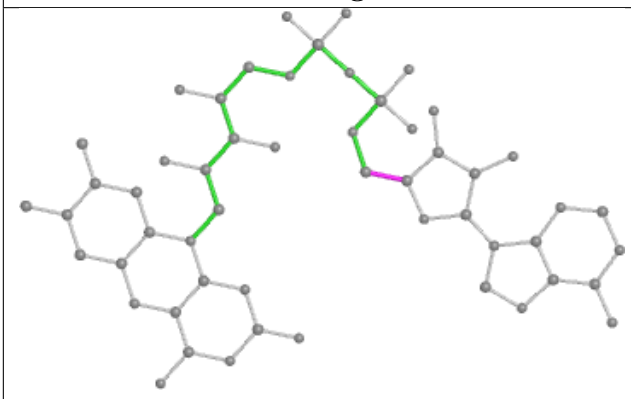
Ligand FAD G 708



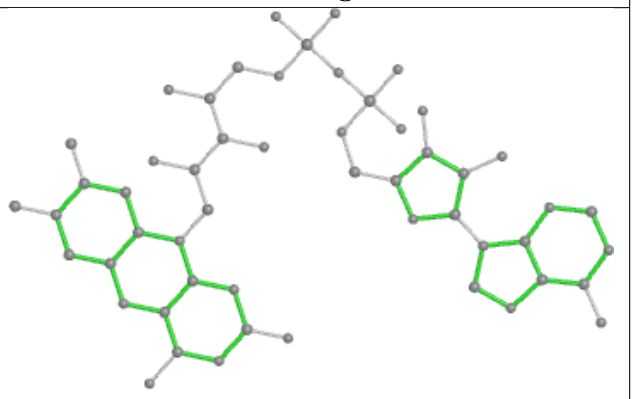
Bond lengths



Bond angles

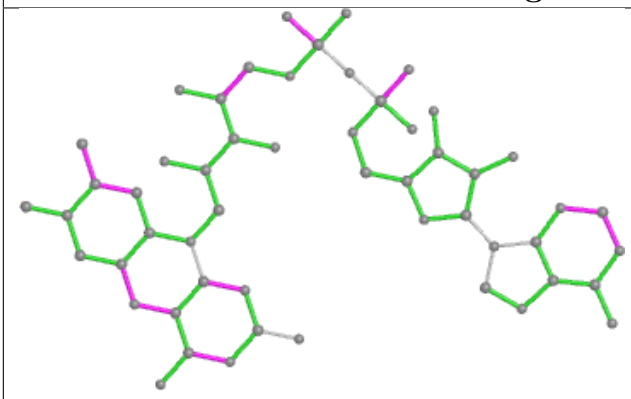


Torsions

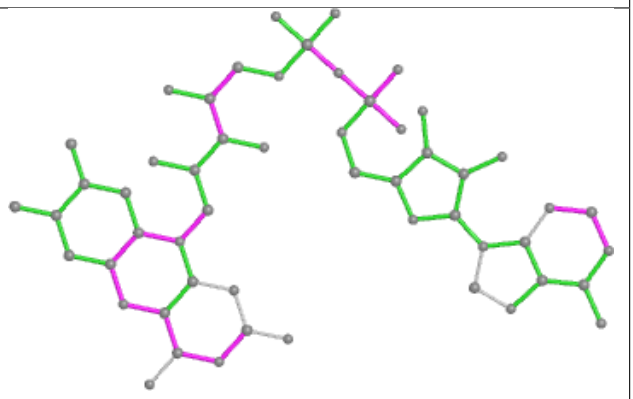


Rings

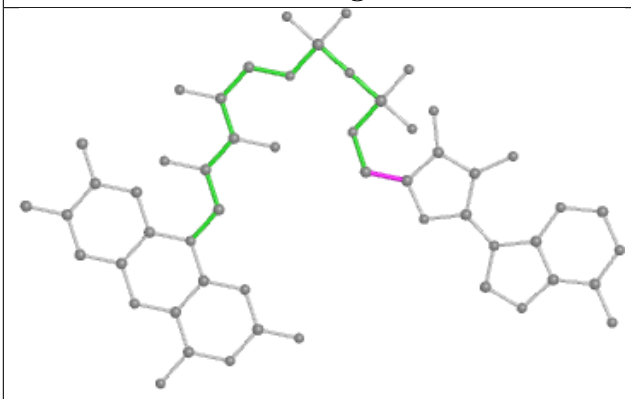
Ligand FAD C 704



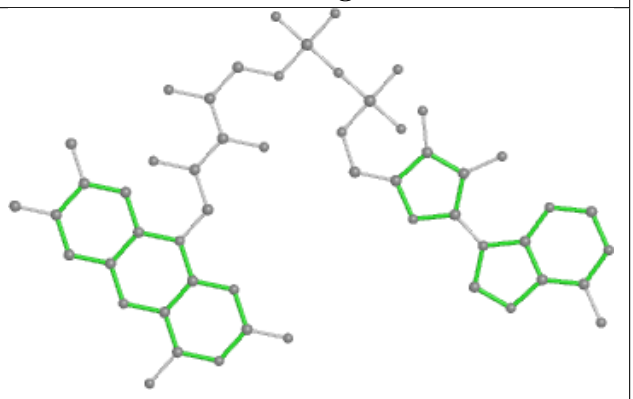
Bond lengths



Bond angles

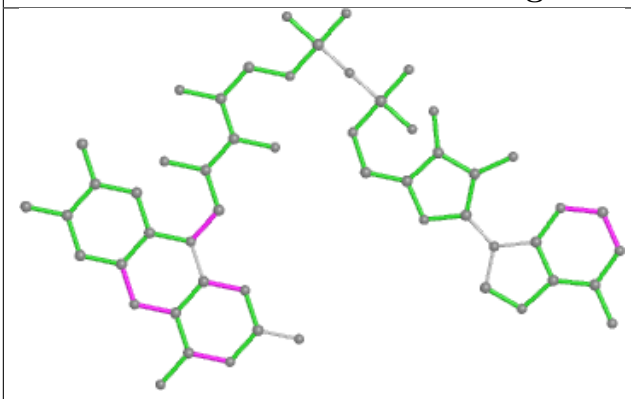


Torsions

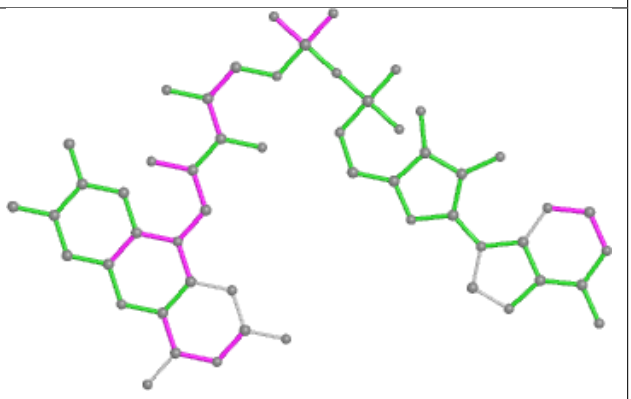


Rings

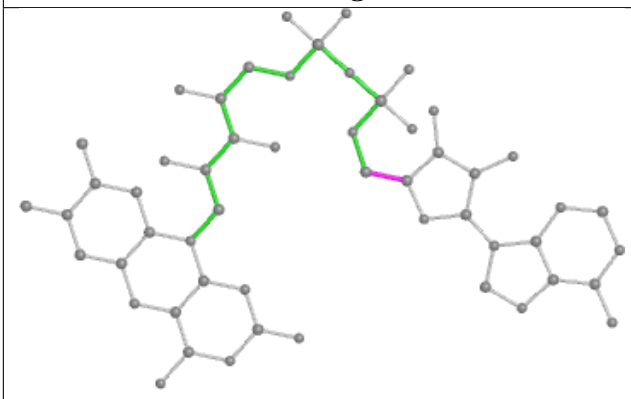
Ligand FAD E 705



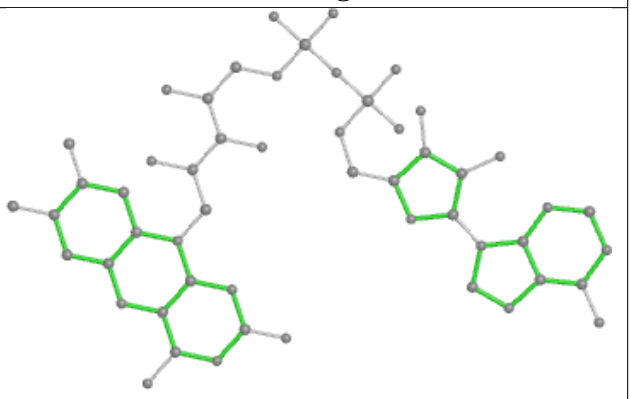
Bond lengths



Bond angles

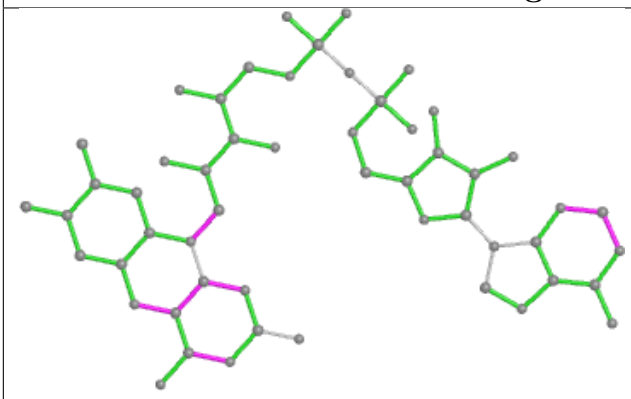


Torsions

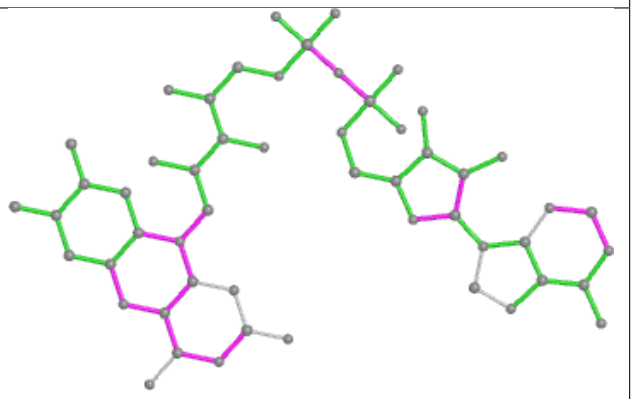


Rings

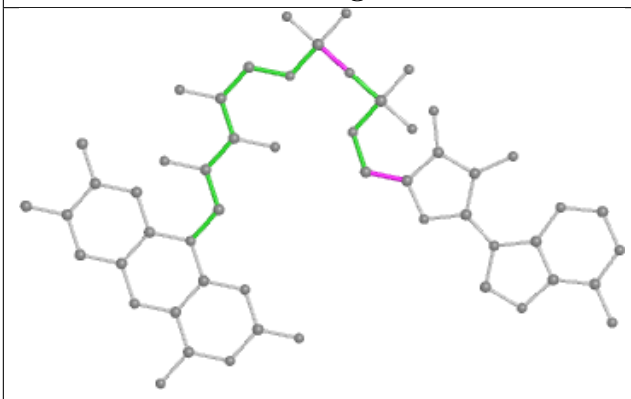
Ligand FAD B 702



Bond lengths



Bond angles



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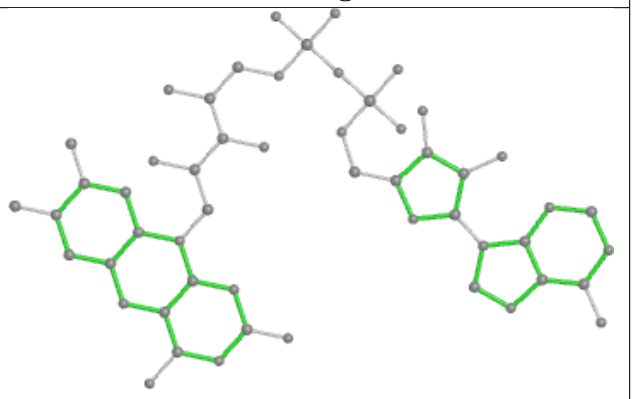
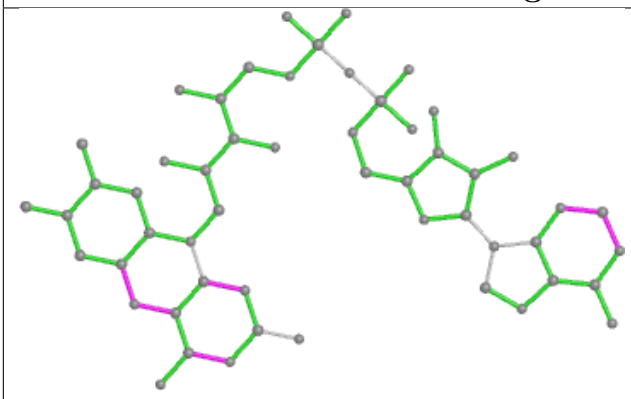
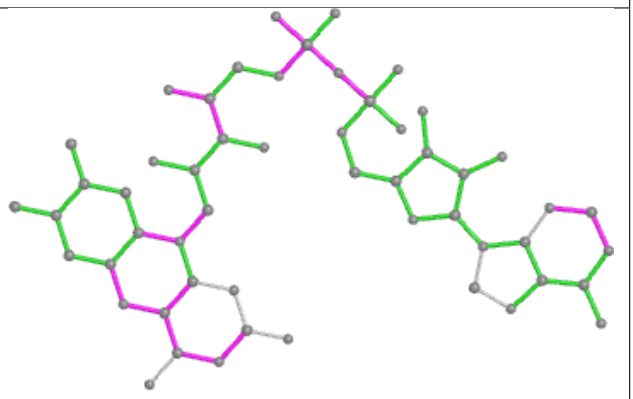


Rings

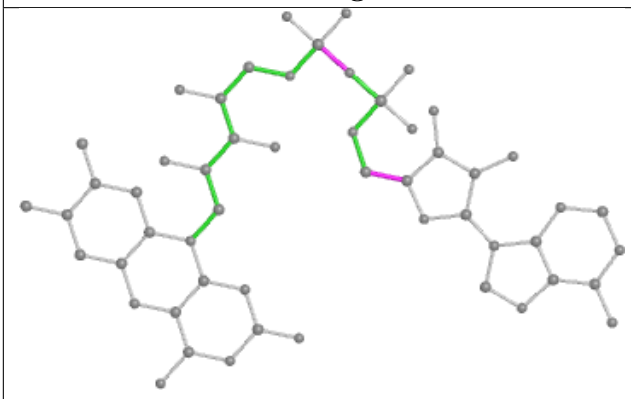
Ligand FAD D 703



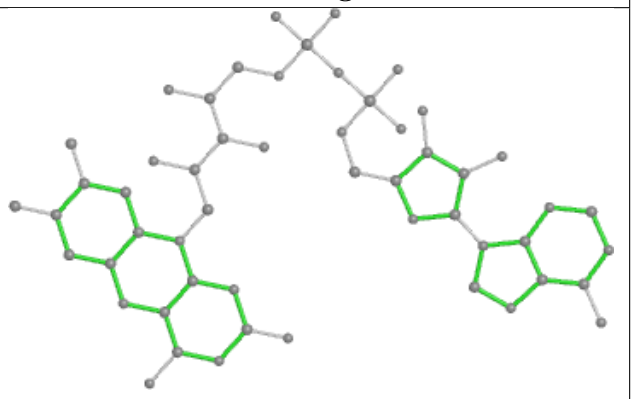
Bond lengths



Bond angles

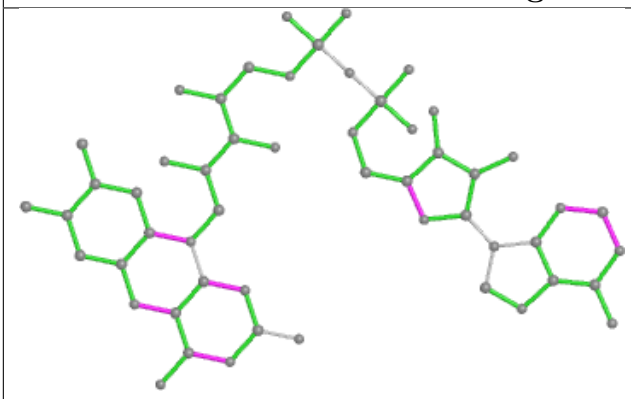


Torsions

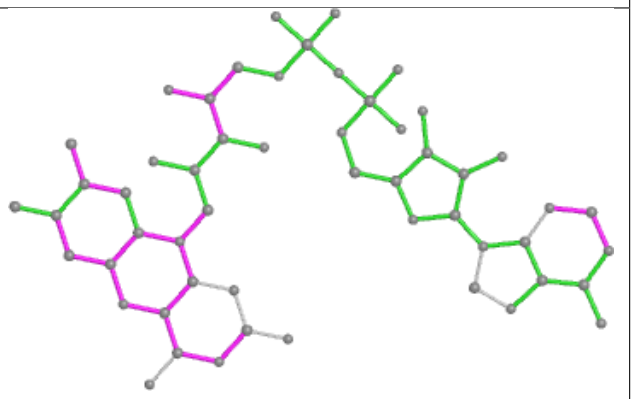


Rings

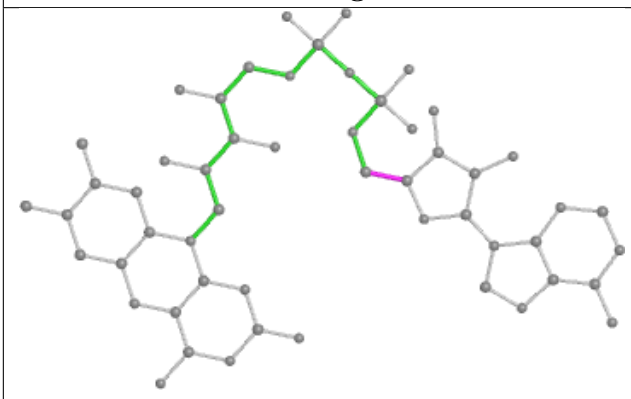
Ligand FAD F 706



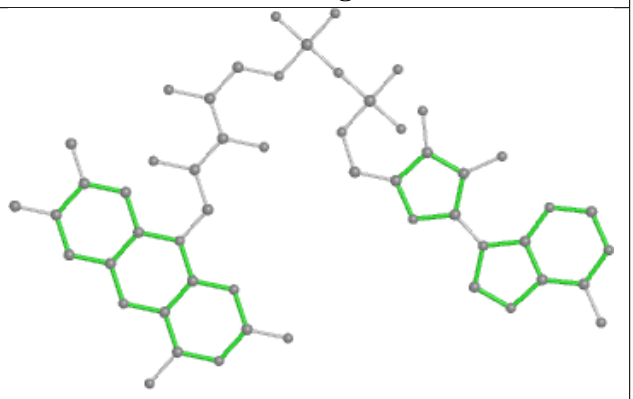
Bond lengths



Bond angles

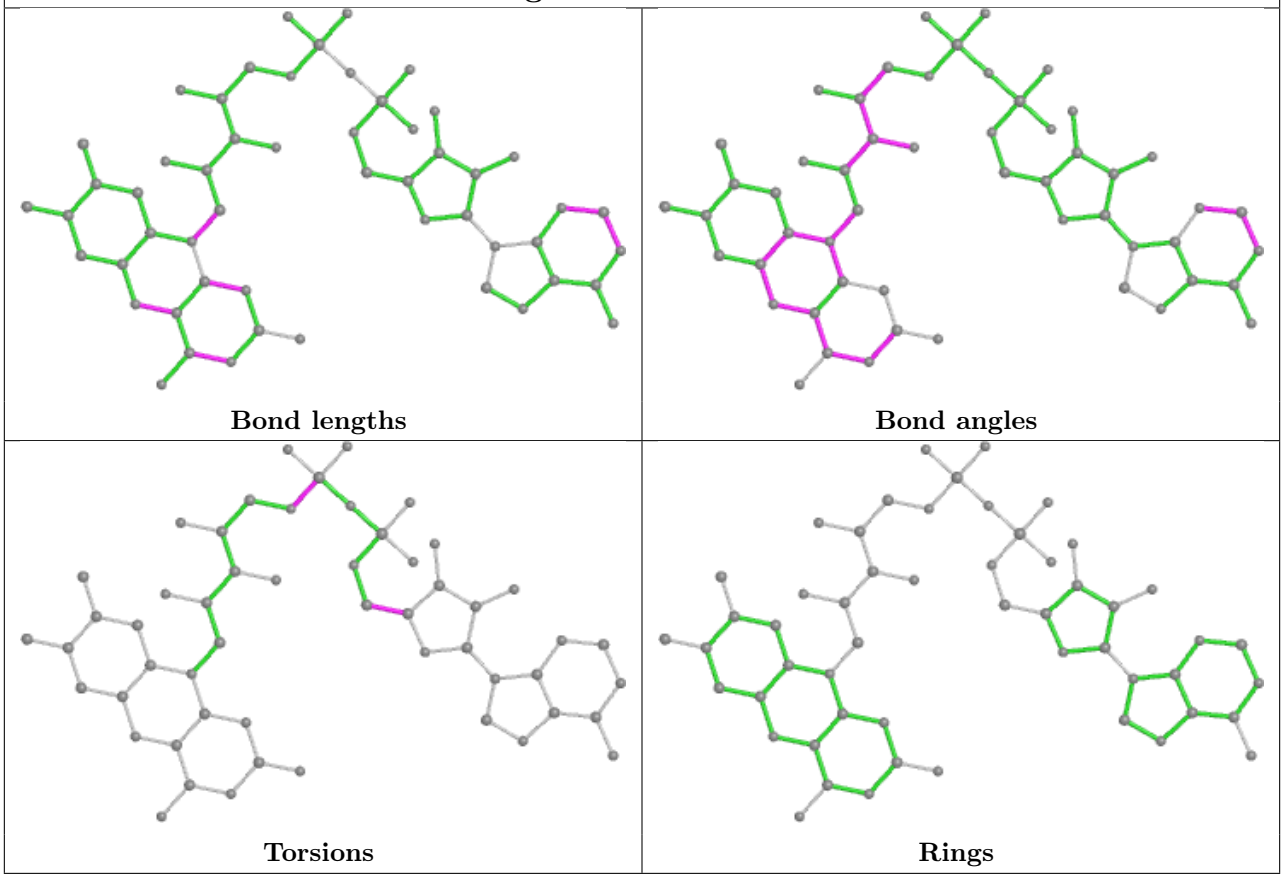


Torsions



Rings

Ligand FAD H 707



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, 95^{th} 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%)	-0.07	23 (3%)	38	48	16, 22, 44, 69	0
1	B	577/623 (92%)	-0.10	18 (3%)	49	58	15, 23, 42, 67	0
1	C	577/623 (92%)	0.03	24 (4%)	36	45	18, 26, 46, 71	0
1	D	577/623 (92%)	-0.05	20 (3%)	44	53	16, 25, 45, 72	0
1	E	577/623 (92%)	-0.00	26 (4%)	33	43	18, 26, 45, 72	0
1	F	577/623 (92%)	0.06	32 (5%)	25	34	17, 27, 47, 71	0
1	G	577/623 (92%)	-0.02	24 (4%)	36	45	18, 25, 48, 67	0
1	H	577/623 (92%)	-0.08	23 (3%)	38	48	16, 24, 43, 71	0
All	All	4616/4984 (92%)	-0.03	190 (4%)	37	46	15, 25, 45, 72	0

All (190) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	619	THR	13.2
1	H	619	THR	12.8
1	E	619	THR	10.9
1	A	619	THR	10.5
1	D	619	THR	9.5
1	G	619	THR	9.0
1	B	619	THR	8.9
1	F	619	THR	8.3
1	F	44	ASP	8.0
1	F	343	ALA	8.0
1	D	45	ILE	7.4
1	G	343	ALA	7.1
1	D	343	ALA	6.7
1	B	343	ALA	6.7
1	C	389	LEU	6.5
1	G	45	ILE	6.3

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Mol	Chain	Res	Type	RSRZ
1	C	44	ASP	6.3
1	B	618	PHE	6.3
1	H	344	ASN	6.2
1	G	389	LEU	6.0
1	F	45	ILE	5.9
1	E	343	ALA	5.9
1	H	343	ALA	5.9
1	G	385	THR	5.9
1	H	45	ILE	5.6
1	C	383	ARG	5.5
1	A	389	LEU	5.4
1	A	343	ALA	5.4
1	F	344	ASN	5.4
1	F	388	GLU	5.3
1	C	618	PHE	5.3
1	A	390	THR	5.2
1	F	342	PRO	5.2
1	A	388	GLU	5.1
1	D	388	GLU	5.1
1	E	618	PHE	5.0
1	C	384	GLY	4.9
1	D	618	PHE	4.8
1	C	45	ILE	4.8
1	F	384	GLY	4.7
1	A	344	ASN	4.7
1	H	345	PRO	4.7
1	A	384	GLY	4.6
1	A	385	THR	4.6
1	D	385	THR	4.5
1	F	389	LEU	4.5
1	C	345	PRO	4.5
1	C	385	THR	4.5
1	F	385	THR	4.5
1	H	44	ASP	4.4
1	C	343	ALA	4.4
1	D	344	ASN	4.3
1	H	43	MET	4.3
1	E	345	PRO	4.3
1	G	344	ASN	4.2
1	E	44	ASP	4.2
1	C	390	THR	4.2
1	G	618	PHE	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	345	PRO	4.0
1	G	342	PRO	4.0
1	C	617	PRO	4.0
1	G	390	THR	4.0
1	A	43	MET	3.9
1	F	345	PRO	3.9
1	F	390	THR	3.9
1	H	618	PHE	3.9
1	E	388	GLU	3.9
1	A	459	VAL	3.9
1	G	186	ASP	3.9
1	C	341	ASN	3.8
1	E	385	THR	3.8
1	G	44	ASP	3.8
1	A	383	ARG	3.8
1	C	388	GLU	3.8
1	A	345	PRO	3.7
1	G	401	THR	3.6
1	E	384	GLY	3.6
1	D	617	PRO	3.6
1	E	342	PRO	3.5
1	C	344	ASN	3.5
1	B	345	PRO	3.5
1	H	459	VAL	3.5
1	H	617	PRO	3.5
1	G	345	PRO	3.5
1	E	344	ASN	3.4
1	B	341	ASN	3.3
1	G	43	MET	3.3
1	B	389	LEU	3.3
1	B	385	THR	3.2
1	F	43	MET	3.2
1	D	186	ASP	3.2
1	F	618	PHE	3.2
1	H	341	ASN	3.2
1	B	186	ASP	3.2
1	B	45	ILE	3.2
1	E	45	ILE	3.2
1	F	186	ASP	3.1
1	A	618	PHE	3.1
1	E	341	ASN	3.1
1	F	383	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	H	458	ALA	3.0
1	A	341	ASN	3.0
1	E	561	GLU	3.0
1	F	341	ASN	3.0
1	B	344	ASN	3.0
1	C	392	SER	3.0
1	D	44	ASP	2.9
1	C	43	MET	2.9
1	H	186	ASP	2.9
1	D	389	LEU	2.9
1	F	272	GLU	2.9
1	C	186	ASP	2.9
1	F	187	ASP	2.9
1	F	347	GLU	2.9
1	D	342	PRO	2.9
1	G	82	SER	2.8
1	D	43	MET	2.8
1	A	400	SER	2.7
1	D	269	ASP	2.7
1	A	381	THR	2.7
1	G	269	ASP	2.7
1	G	458	ALA	2.7
1	A	458	ALA	2.6
1	G	384	GLY	2.6
1	D	272	GLU	2.6
1	A	382	ILE	2.6
1	F	290	ALA	2.6
1	H	232	GLY	2.6
1	B	44	ASP	2.6
1	B	388	GLU	2.6
1	E	269	ASP	2.6
1	H	389	LEU	2.6
1	A	401	THR	2.6
1	C	396	THR	2.6
1	F	81	ASP	2.6
1	F	391	TYR	2.5
1	E	458	ALA	2.5
1	F	188	ALA	2.5
1	G	388	GLU	2.5
1	F	268	THR	2.5
1	H	342	PRO	2.5
1	E	43	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	305	SER	2.5
1	G	617	PRO	2.5
1	B	390	THR	2.5
1	A	342	PRO	2.4
1	D	390	THR	2.4
1	E	347	GLU	2.4
1	E	389	LEU	2.4
1	E	232	GLY	2.4
1	A	133	ALA	2.4
1	H	385	THR	2.4
1	E	307	ASP	2.4
1	D	341	ASN	2.4
1	F	561	GLU	2.4
1	G	400	SER	2.4
1	H	190	ALA	2.4
1	F	387	GLY	2.3
1	E	400	SER	2.3
1	E	459	VAL	2.3
1	E	186	ASP	2.3
1	C	418	GLN	2.3
1	H	133	ALA	2.3
1	C	342	PRO	2.3
1	C	272	GLU	2.3
1	H	268	THR	2.3
1	D	309	PHE	2.3
1	F	421	GLU	2.3
1	F	271	PRO	2.3
1	F	269	ASP	2.3
1	D	459	VAL	2.2
1	A	44	ASP	2.2
1	B	458	ALA	2.2
1	H	189	ASP	2.2
1	F	309	PHE	2.2
1	H	272	GLU	2.2
1	E	617	PRO	2.2
1	E	382	ILE	2.1
1	B	383	ARG	2.1
1	F	185	LYS	2.1
1	G	341	ASN	2.1
1	B	459	VAL	2.1
1	G	383	ARG	2.0
1	A	186	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	561	GLU	2.0
1	H	271	PRO	2.0
1	G	382	ILE	2.0
1	C	561	GLU	2.0
1	E	272	GLU	2.0
1	B	418	GLN	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)

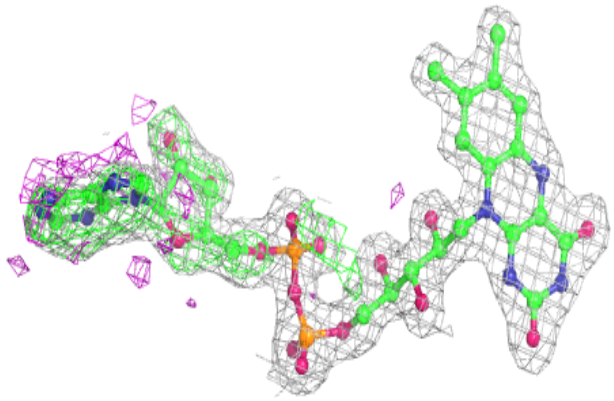
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

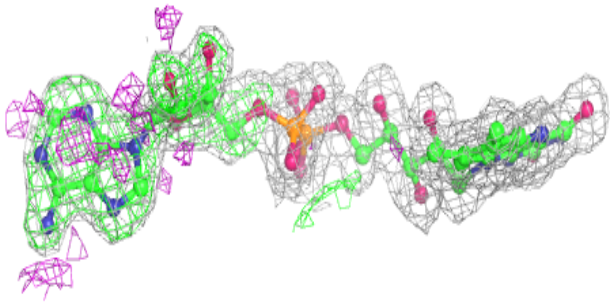
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FAD	C	704	53/53	0.86	0.21	16,23,113,114	0
3	FAD	D	703	53/53	0.88	0.22	16,20,105,106	0
3	FAD	A	701	53/53	0.88	0.21	12,18,94,95	0
3	FAD	G	708	53/53	0.88	0.21	16,21,101,103	0
2	SHG	G	808	12/12	0.89	0.16	27,35,39,42	0
2	SHG	C	804	12/12	0.89	0.12	29,37,41,41	0
3	FAD	E	705	53/53	0.89	0.22	15,21,119,120	0
3	FAD	F	706	53/53	0.89	0.20	16,21,115,116	0
3	FAD	H	707	53/53	0.89	0.22	15,21,119,120	0
3	FAD	B	702	53/53	0.89	0.21	14,19,107,107	0
2	SHG	E	805	12/12	0.91	0.11	31,37,40,41	0
2	SHG	D	803	12/12	0.93	0.12	30,35,40,41	0
2	SHG	A	801	12/12	0.94	0.10	24,35,41,44	0
2	SHG	F	806	12/12	0.94	0.11	31,34,40,42	0
2	SHG	H	807	12/12	0.94	0.10	28,35,38,41	0
2	SHG	B	802	12/12	0.96	0.08	24,29,35,39	0

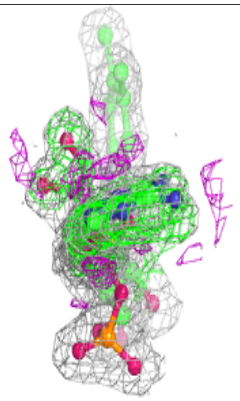
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD C 704:

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

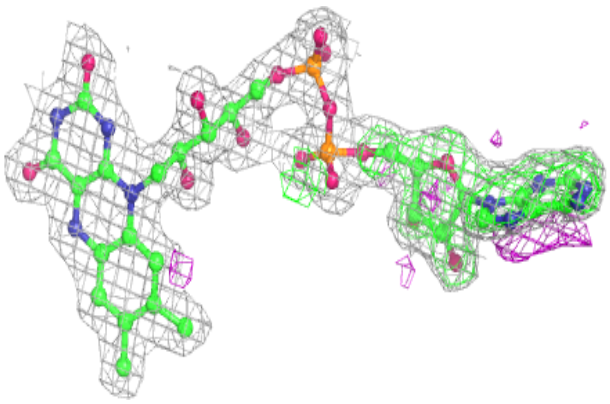


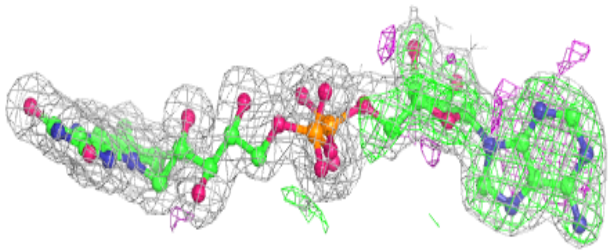


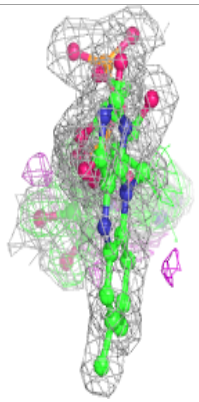


Electron density around FAD D 703:

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

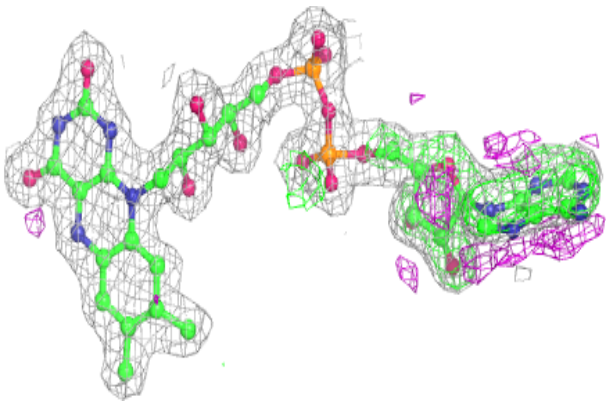


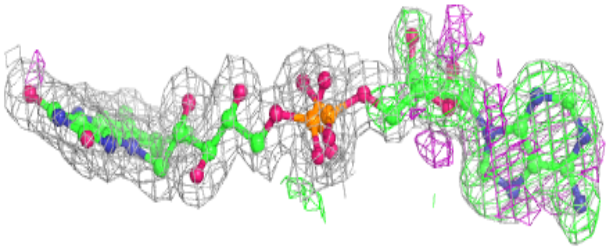


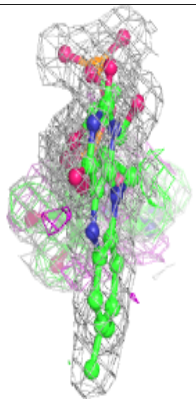


Electron density around FAD A 701:

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

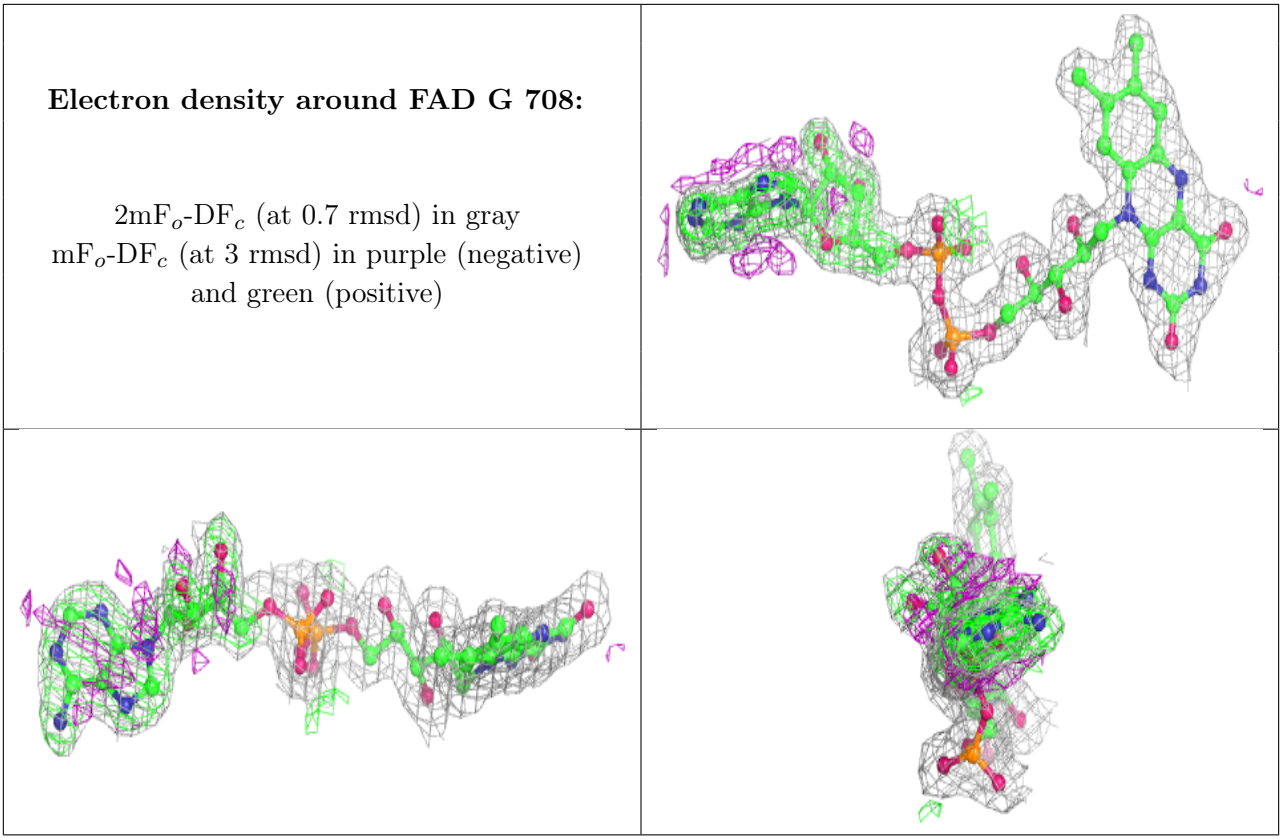






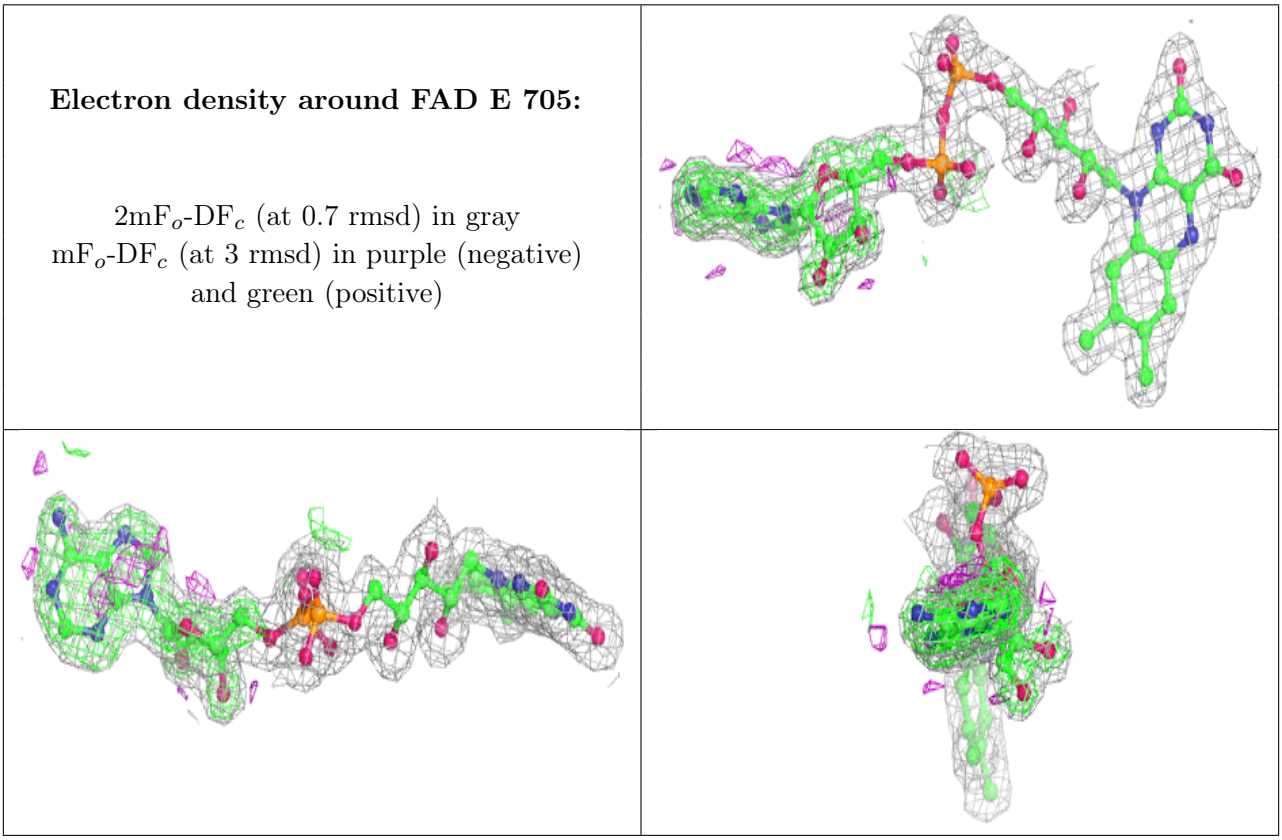
Electron density around FAD G 708:

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



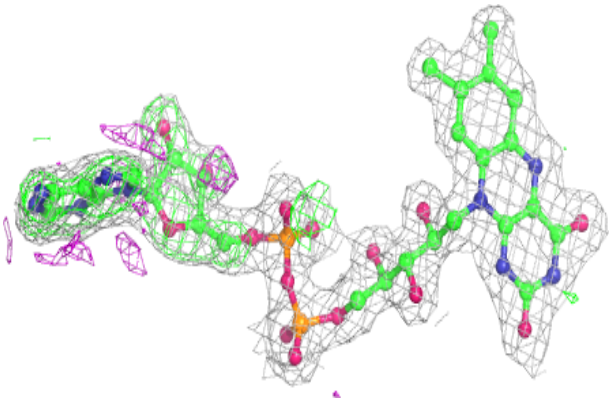
Electron density around FAD E 705:

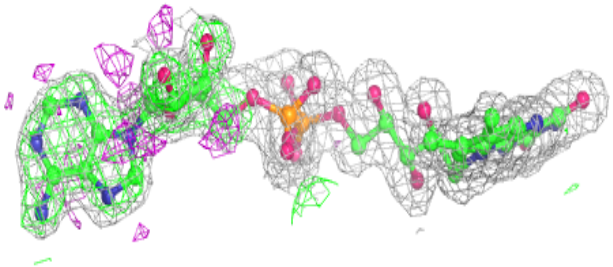
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

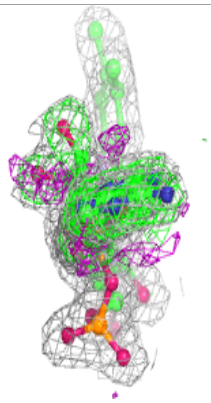


Electron density around FAD F 706:

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

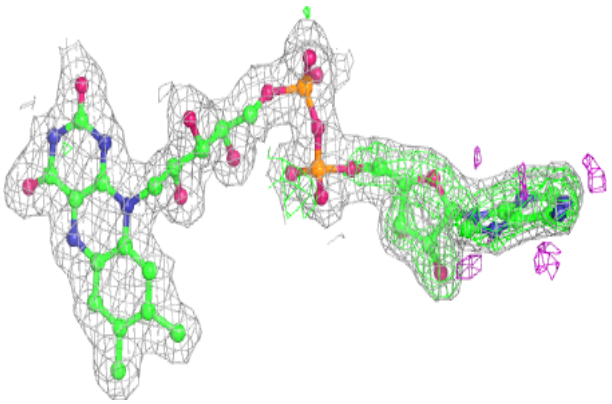


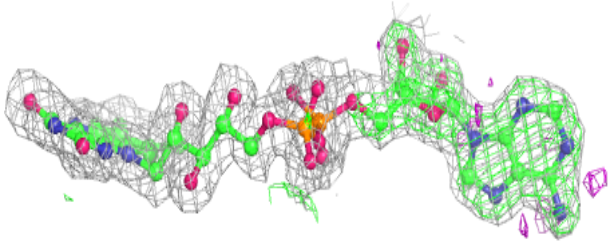


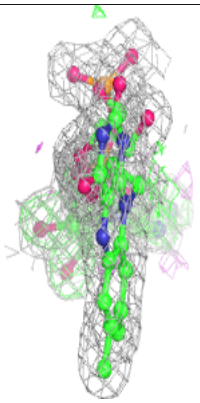


Electron density around FAD H 707:

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

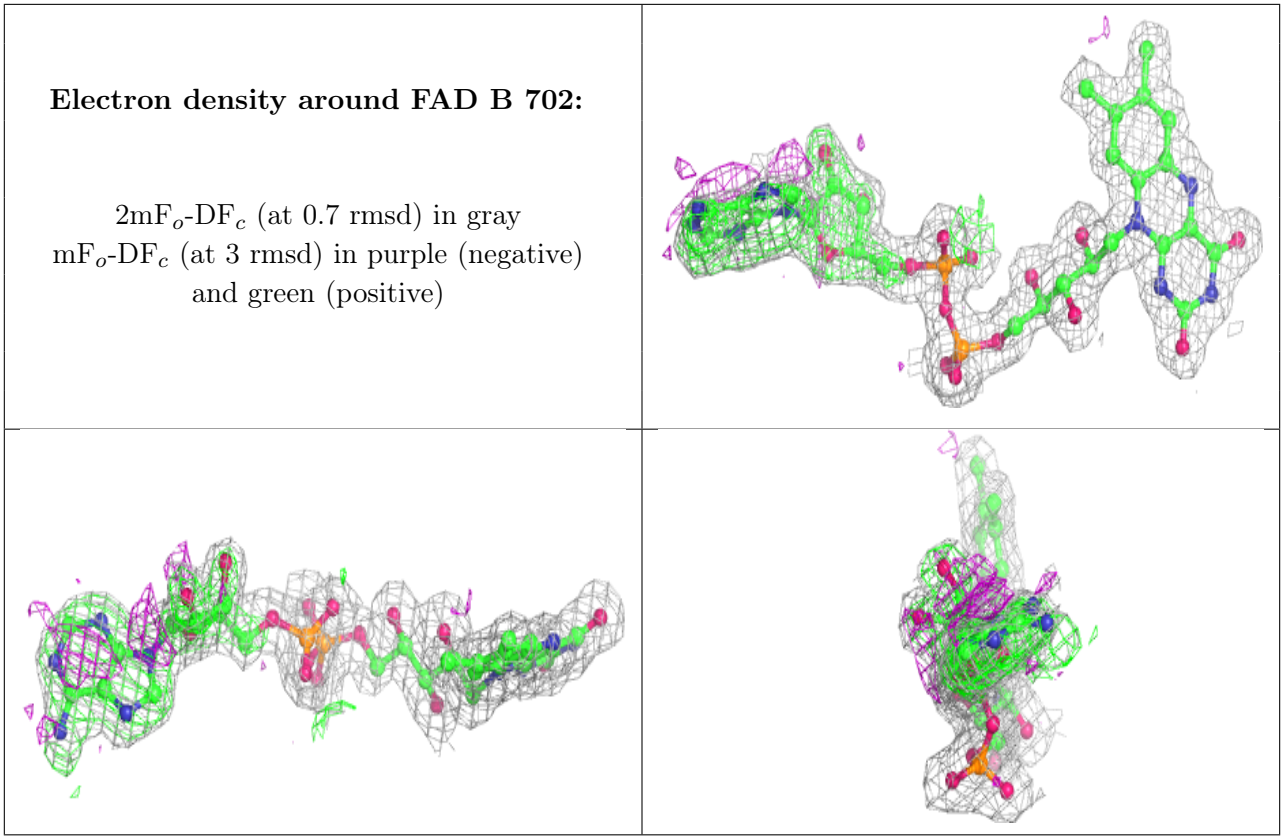






Electron density around FAD B 702:

$2mF_o$-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.