



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:46 AM UTC

PDB ID : 2IGO / pdb_00002igo
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 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

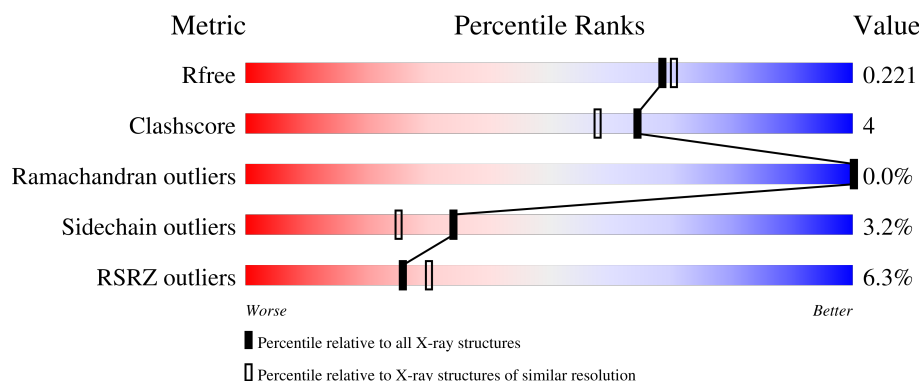
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

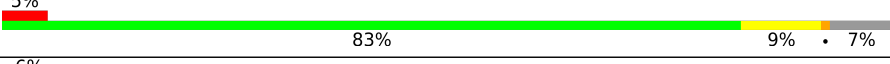
The reported resolution of this entry is 1.95 Å.

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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	623	 7% 82% 10% • 7%
1	B	623	 5% 83% 9% • 7%
1	C	623	 6% 82% 10% • 7%
1	D	623	 4% 81% 11% • 7%
1	E	623	 5% 83% 9% • 7%

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Mol	Chain	Length	Quality of chain
1	F	623	7% 83% 9% 7%
1	G	623	7% 81% 11% 7%
1	H	623	5% 81% 11% 7%

2 Entry composition

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.

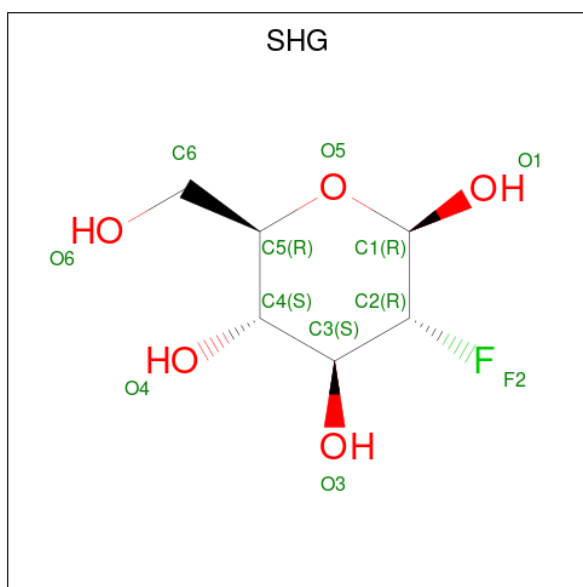
- Molecule 1 is a protein called Pyranose oxidase.

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:

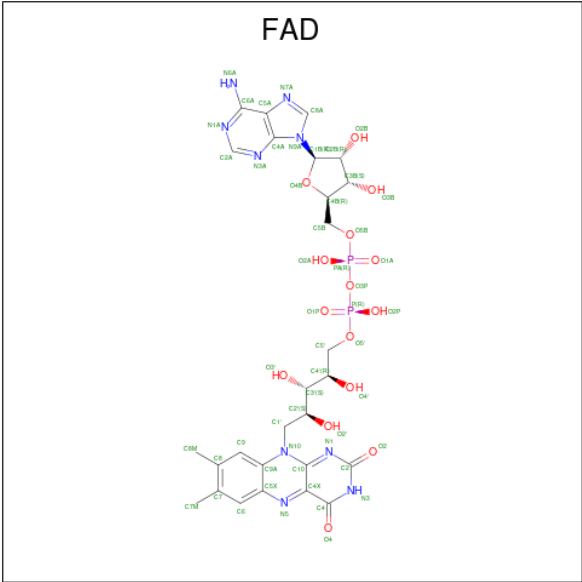
Chain	Residue	Modelled	Actual	Comment	Reference
A	167	ALA	HIS	engineered mutation	UNP Q7ZA32
B	167	ALA	HIS	engineered mutation	UNP Q7ZA32
C	167	ALA	HIS	engineered mutation	UNP Q7ZA32
D	167	ALA	HIS	engineered mutation	UNP Q7ZA32
E	167	ALA	HIS	engineered mutation	UNP Q7ZA32
F	167	ALA	HIS	engineered mutation	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 (CCD ID: SHG) (formula: C₆H₁₁FO₅).



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

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: 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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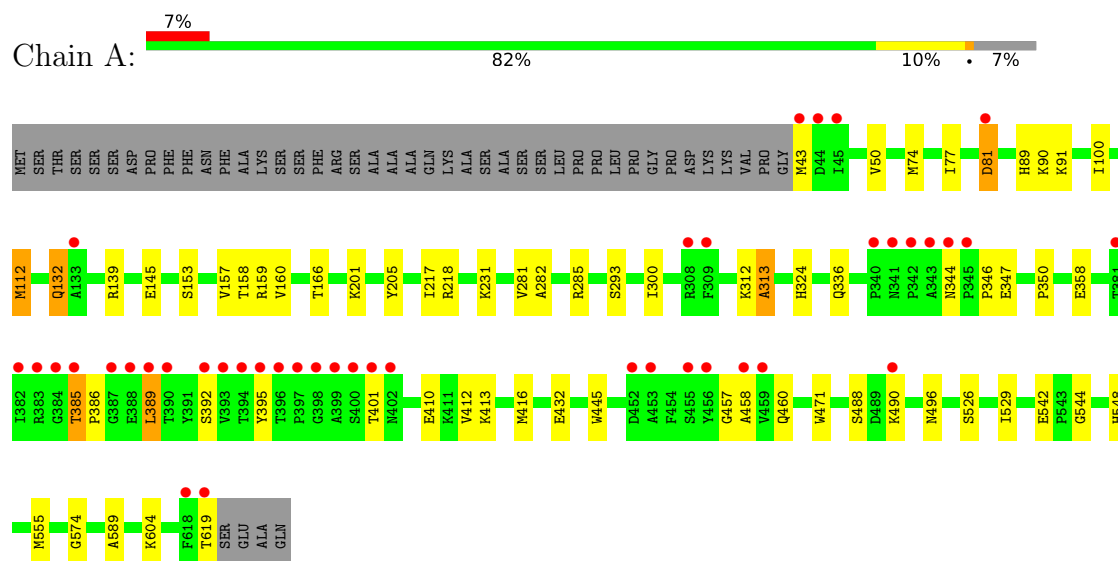
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	195	Total 195	O 195	0	0
4	F	192	Total 192	O 192	0	0
4	H	217	Total 217	O 217	0	0
4	G	210	Total 210	O 210	0	0

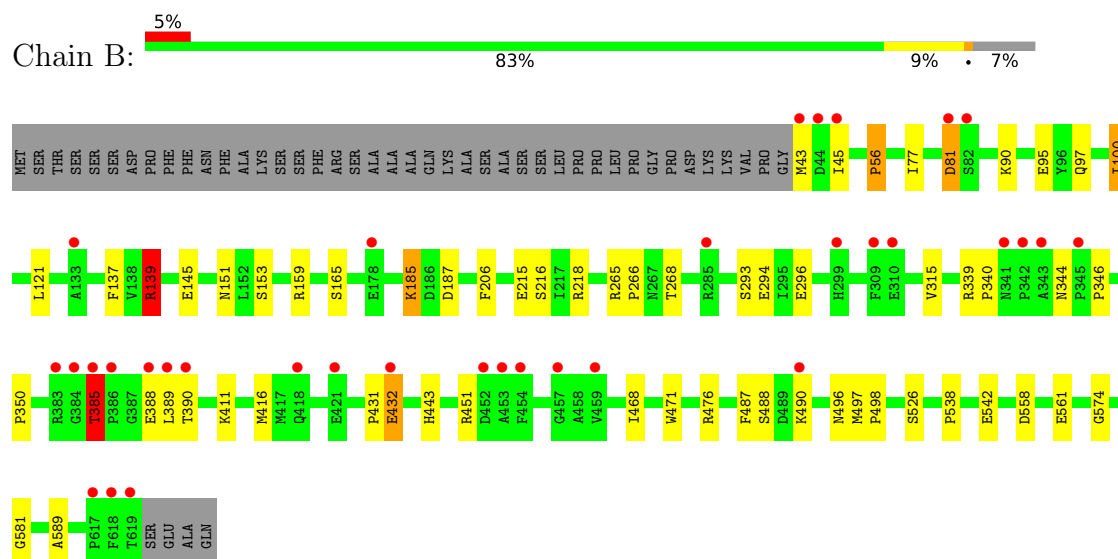
3 Residue-property plots [i](#)

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

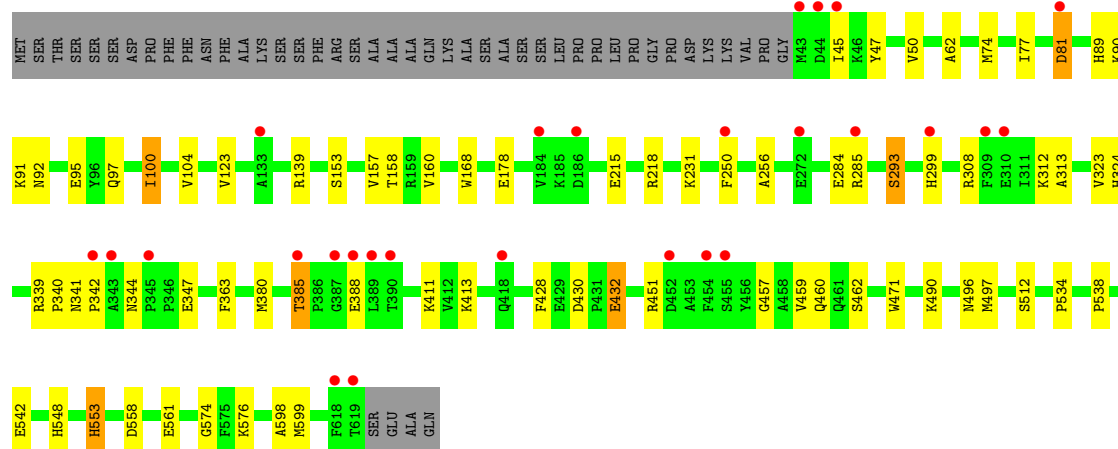
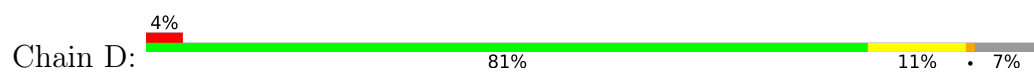
• Molecule 1: Pyranose oxidase



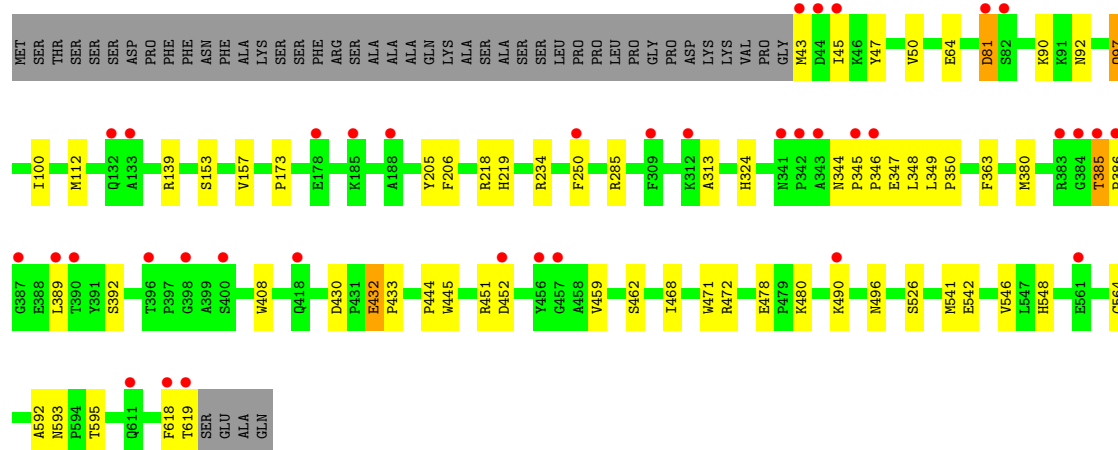
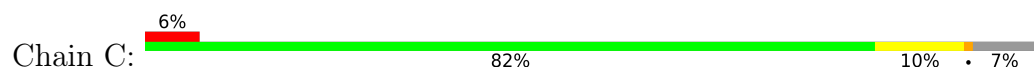
• Molecule 1: Pyranose oxidase



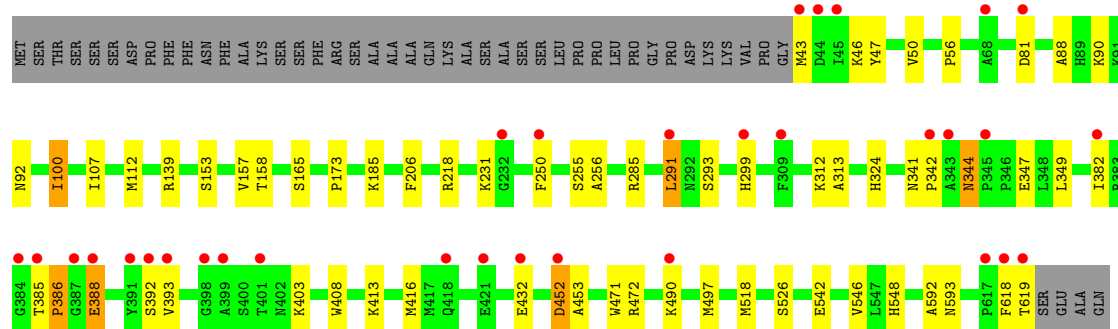
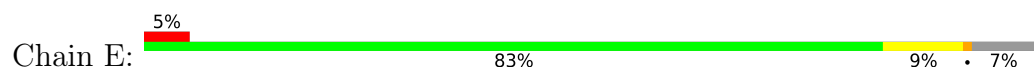
• Molecule 1: Pyranose oxidase



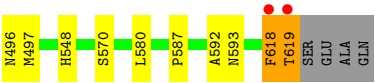
• Molecule 1: Pyranose oxidase



• Molecule 1: Pyranose oxidase



• Molecule 1: Pyranose oxidase



4 Data and refinement statistics

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 38.90 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (38.90-1.95) 99.8 (38.90-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.86 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.184 , 0.221 0.188 , 0.221	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)	0.37 , 32.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

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: SHG, FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.32	13/4659 (0.3%)	1.19	5/6335 (0.1%)
1	B	1.28	7/4659 (0.2%)	1.18	9/6335 (0.1%)
1	C	1.22	4/4659 (0.1%)	1.17	10/6335 (0.2%)
1	D	1.25	11/4659 (0.2%)	1.16	10/6335 (0.2%)
1	E	1.21	7/4659 (0.2%)	1.15	8/6335 (0.1%)
1	F	1.21	5/4659 (0.1%)	1.14	10/6335 (0.2%)
1	G	1.26	13/4659 (0.3%)	1.17	13/6335 (0.2%)
1	H	1.25	6/4659 (0.1%)	1.17	14/6335 (0.2%)
All	All	1.25	66/37272 (0.2%)	1.17	79/50680 (0.2%)

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

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

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	81	ASP	CA-C	11.83	1.66	1.53
1	G	380	MET	SD-CE	-9.03	1.56	1.79
1	H	74	MET	SD-CE	-8.77	1.57	1.79
1	B	416	MET	SD-CE	8.65	2.01	1.79
1	E	291	LEU	CG-CD1	8.52	1.80	1.52
1	G	349	LEU	CA-C	-7.82	1.47	1.53
1	G	497	MET	SD-CE	7.58	1.98	1.79
1	E	497	MET	SD-CE	7.45	1.98	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	81	ASP	CA-C	7.10	1.62	1.52
1	C	541	MET	CG-SD	7.09	1.98	1.80
1	B	497	MET	SD-CE	6.97	1.97	1.79
1	F	81	ASP	CA-C	6.76	1.61	1.52
1	A	313	ALA	CA-CB	6.72	1.65	1.53
1	G	82	SER	C-O	6.50	1.31	1.24
1	H	497	MET	SD-CE	6.42	1.95	1.79
1	G	295	ILE	CA-CB	6.38	1.62	1.54
1	C	234	ARG	CA-C	-6.34	1.45	1.52
1	A	282	ALA	CA-CB	-6.33	1.44	1.53
1	D	553	HIS	CA-CB	6.32	1.57	1.53
1	C	81	ASP	CA-C	6.28	1.61	1.52
1	B	581	GLY	CA-C	6.23	1.57	1.52
1	D	497	MET	SD-CE	6.23	1.95	1.79
1	F	45	ILE	CA-CB	6.22	1.61	1.54
1	F	139	ARG	CD-NE	-6.15	1.37	1.46
1	F	139	ARG	CA-C	6.02	1.59	1.52
1	F	416	MET	SD-CE	6.00	1.94	1.79
1	A	112	MET	CB-CG	5.94	1.70	1.52
1	G	385	THR	CA-CB	5.78	1.62	1.53
1	D	74	MET	SD-CE	5.74	1.93	1.79
1	A	416	MET	SD-CE	5.72	1.93	1.79
1	G	45	ILE	CA-CB	5.72	1.61	1.54
1	H	599	MET	SD-CE	-5.70	1.65	1.79
1	D	599	MET	SD-CE	5.65	1.93	1.79
1	A	217	ILE	CA-CB	5.59	1.60	1.54
1	B	385	THR	CA-CB	5.58	1.62	1.54
1	H	508	ALA	CA-CB	5.56	1.62	1.53
1	G	417	MET	SD-CE	5.51	1.93	1.79
1	H	555	MET	SD-CE	5.50	1.93	1.79
1	B	56	PRO	C-O	5.48	1.30	1.24
1	G	319	THR	C-O	5.45	1.29	1.23
1	D	62	ALA	CA-CB	5.44	1.61	1.53
1	D	380	MET	SD-CE	-5.41	1.66	1.79
1	E	158	THR	C-O	5.41	1.30	1.24
1	E	349	LEU	CA-CB	5.37	1.56	1.52
1	A	555	MET	SD-CE	5.36	1.93	1.79
1	D	139	ARG	CD-NE	-5.35	1.38	1.46
1	B	315	VAL	N-CA	5.33	1.52	1.46
1	A	529	ILE	CA-C	5.31	1.58	1.52
1	A	139	ARG	CD-NE	-5.29	1.38	1.46
1	A	604	LYS	C-O	5.28	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	81	ASP	CA-C	5.28	1.59	1.52
1	A	81	ASP	CA-C	5.26	1.59	1.52
1	A	445	TRP	CA-C	-5.25	1.46	1.52
1	E	416	MET	SD-CE	5.24	1.92	1.79
1	D	323	VAL	CA-CB	5.22	1.61	1.54
1	G	320	ALA	CA-CB	5.21	1.61	1.53
1	D	598	ALA	CA-CB	5.18	1.61	1.53
1	D	256	ALA	CA-C	5.10	1.59	1.52
1	C	380	MET	SD-CE	-5.08	1.66	1.79
1	E	518	MET	CA-C	5.07	1.59	1.52
1	A	589	ALA	CA-CB	5.07	1.60	1.53
1	G	158	THR	C-O	5.06	1.30	1.24
1	E	107	ILE	CA-CB	-5.06	1.48	1.54
1	G	313	ALA	CA-CB	5.05	1.62	1.53
1	H	328	LEU	CA-C	5.04	1.59	1.52
1	A	74	MET	SD-CE	5.01	1.92	1.79

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	139	ARG	NE-CZ-NH2	-12.12	108.29	119.20
1	D	139	ARG	NE-CZ-NH2	-10.41	109.83	119.20
1	B	139	ARG	NE-CZ-NH2	-10.08	110.12	119.20
1	E	139	ARG	NE-CZ-NH2	-9.40	110.74	119.20
1	G	139	ARG	NE-CZ-NH2	-9.27	110.86	119.20
1	C	139	ARG	NE-CZ-NH2	-8.64	111.42	119.20
1	F	139	ARG	CD-NE-CZ	8.29	136.01	124.40
1	E	139	ARG	CG-CD-NE	-8.18	94.01	112.00
1	A	139	ARG	NE-CZ-NH2	-8.17	111.85	119.20
1	B	139	ARG	CG-CD-NE	-8.15	94.08	112.00
1	D	97	GLN	CA-CB-CG	-7.76	98.58	114.10
1	F	139	ARG	CG-CD-NE	-7.42	95.67	112.00
1	F	97	GLN	CA-CB-CG	-7.33	99.44	114.10
1	B	97	GLN	CA-CB-CG	-7.17	99.76	114.10
1	G	431	PRO	CA-C-N	6.99	130.11	120.39
1	G	431	PRO	C-N-CA	6.99	130.11	120.39
1	H	139	ARG	NE-CZ-NH2	-6.97	112.93	119.20
1	C	139	ARG	CD-NE-CZ	6.88	134.03	124.40
1	A	139	ARG	CG-CD-NE	-6.69	97.28	112.00
1	G	139	ARG	NE-CZ-NH1	6.61	128.11	121.50
1	C	139	ARG	NE-CZ-NH1	6.60	128.10	121.50
1	G	385	THR	CB-CA-C	6.50	117.67	108.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	139	ARG	CD-NE-CZ	6.42	133.39	124.40
1	F	139	ARG	NE-CZ-NH1	6.39	127.89	121.50
1	D	139	ARG	CG-CD-NE	-6.19	98.38	112.00
1	G	44	ASP	CA-C-N	-6.18	111.58	121.35
1	G	44	ASP	C-N-CA	-6.18	111.58	121.35
1	C	139	ARG	CG-CD-NE	-6.08	98.62	112.00
1	C	595	THR	N-CA-C	6.07	117.56	111.07
1	E	291	LEU	CB-CG-CD2	-6.06	92.51	110.70
1	G	46	LYS	N-CA-C	6.02	118.94	108.76
1	C	349	LEU	O-C-N	5.99	124.28	121.53
1	G	139	ARG	CG-CD-NE	-5.96	98.89	112.00
1	D	139	ARG	NE-CZ-NH1	5.86	127.36	121.50
1	D	139	ARG	CD-NE-CZ	5.79	132.51	124.40
1	D	104	VAL	CB-CA-C	-5.75	103.25	112.16
1	A	412	VAL	N-CA-C	-5.74	104.92	110.72
1	F	296	GLU	N-CA-C	5.68	118.68	111.69
1	H	139	ARG	CA-CB-CG	5.68	125.46	114.10
1	B	81	ASP	CB-CG-OD2	5.65	131.39	118.40
1	A	139	ARG	CD-NE-CZ	5.64	132.29	124.40
1	D	293	SER	N-CA-C	-5.62	106.25	114.39
1	D	168	TRP	N-CA-C	5.59	117.28	110.41
1	E	139	ARG	NE-CZ-NH1	5.55	127.05	121.50
1	B	431	PRO	CA-C-N	5.53	129.09	120.68
1	B	431	PRO	C-N-CA	5.53	129.09	120.68
1	G	372	LEU	N-CA-C	5.53	117.31	111.28
1	B	443	HIS	O-C-N	5.48	125.19	121.19
1	G	100	ILE	N-CA-C	5.48	116.21	110.62
1	A	389	LEU	N-CA-C	5.46	117.93	111.33
1	C	97	GLN	N-CA-C	-5.46	105.88	112.54
1	H	529	ILE	N-CA-C	-5.43	107.50	111.90
1	C	564	CYS	N-CA-C	5.42	116.51	108.86
1	F	408	TRP	N-CA-C	-5.42	104.79	111.40
1	D	512	SER	N-CA-C	5.40	116.98	111.14
1	E	293	SER	N-CA-C	-5.40	106.43	114.64
1	B	139	ARG	NE-CZ-NH1	5.40	126.90	121.50
1	H	426	ILE	N-CA-C	5.37	113.25	108.63
1	F	44	ASP	N-CA-C	-5.37	103.40	110.43
1	E	349	LEU	CB-CA-C	-5.35	106.35	111.00
1	H	279	PRO	N-CD-CG	-5.30	95.25	103.20
1	H	581	GLY	CA-C-O	-5.28	116.98	121.57
1	G	139	ARG	CD-NE-CZ	5.26	131.77	124.40
1	H	168	TRP	N-CA-C	5.23	116.84	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	97	GLN	CB-CG-CD	5.21	121.46	112.60
1	H	97	GLN	CA-CB-CG	-5.15	103.80	114.10
1	D	428	PHE	N-CA-C	5.14	117.55	111.33
1	G	323	VAL	CB-CA-C	-5.14	105.31	112.04
1	E	291	LEU	CD1-CG-CD2	5.13	122.09	110.80
1	E	291	LEU	CA-CB-CG	-5.12	98.38	116.30
1	F	139	ARG	CA-CB-CG	5.11	124.31	114.10
1	H	91	LYS	CB-CA-C	5.08	119.16	110.01
1	H	139	ARG	NE-CZ-NH1	5.05	126.55	121.50
1	C	345	PRO	O-C-N	5.04	123.52	121.15
1	H	183	LEU	N-CA-C	-5.03	107.69	113.88
1	H	554	ARG	N-CA-C	5.02	117.16	110.53
1	H	594	PRO	N-CA-C	5.01	121.04	114.27
1	C	92	ASN	CB-CA-C	-5.01	105.06	111.22
1	H	470	ASP	CB-CA-C	-5.01	100.94	109.51

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	29	0
1	B	4544	0	4393	34	0
1	C	4544	0	4393	38	0
1	D	4544	0	4393	34	0
1	E	4544	0	4393	39	0
1	F	4544	0	4393	35	0
1	G	4544	0	4393	42	0
1	H	4544	0	4393	29	0
2	A	12	0	11	4	0
2	B	12	0	11	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	280	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 (280) 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:G:81:ASP:C	4:G:2497:HOH:O	2.15	0.88
1:C:97:GLN:HG3	1:C:250:PHE:CE2	2.10	0.87
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:548:HIS:NE2	2:E:805:SHG:O3	2.29	0.66
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
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:G:81:ASP:C	1:G:81:ASP:OD1	2.42	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: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:G:618:PHE:C	1:G:618:PHE:HD1	2.10	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:C:548:HIS:CE1	2:C:804:SHG:HO3	2.20	0.58
1:B:100:ILE:HD13	1:B:100:ILE:O	2.04	0.58
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:81:ASP:OD1	1:B:81:ASP:C	2.45	0.57
1:G:64:GLU:OE2	1:G:205:TYR:OH	2.18	0.56
1:B:346:PRO:HG2	1:B:350:PRO:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:ILE:HD13	1:D:100:ILE:C	2.30	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:G:618:PHE:C	1:G:618:PHE:CD1	2.82	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: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
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:D:95:GLU:HG3	1:C:112:MET:HE2	1.88	0.54
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:B:100:ILE:HD13	1:B:100:ILE:C	2.32	0.54
1:G:97:GLN:HG3	1:G:250:PHE:CE2	2.43	0.54
1:F:92:ASN:O	1:F:250:PHE:HZ	1.91	0.54
1:A:112:MET:HE2	1:B:95:GLU:HG3	1.89	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:E:342:PRO:C	1:E:344:ASN:H	2.18	0.52
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:618:PHE:CD1	1:F:618:PHE:C	2.89	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: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:81:ASP:O	1:E:81:ASP:CG	2.55	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
1:C:81:ASP:OD1	1:C:81:ASP:C	2.52	0.49
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:F:341:ASN:C	1:F:341:ASN:HD22	2.23	0.47
1:H:59:CYS:SG	1:H:256:ALA:HB1	2.55	0.47
1:D:123:VAL:HG22	1:C:459:VAL:CG1	2.44	0.47
1:F:81:ASP:C	1:F:81:ASP:OD1	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:421:GLU:H	1:H:421:GLU:CD	2.23	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
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:E:618:PHE:CD1	1:E:618:PHE:C	2.94	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:C:618:PHE:HD1	1:C:618:PHE:C	2.25	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:C:618:PHE:C	1:C:618:PHE:CD1	2.95	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:D:81:ASP:C	1:D:81:ASP:OD1	2.59	0.44
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:G:398:GLY:O	1:G:399:ALA:C	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:265:ARG:HA	1:B:266:PRO:C	2.43	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:E:165:SER:HG	1:E:256:ALA:H	1.65	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:81:ASP:O	1:C:81:ASP:CG	2.61	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:A:542:GLU:HB2	4:A:2369:HOH:O	2.18	0.43
1:F:433:PRO:C	1:F:434:GLN:HG2	2.44	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:E:341:ASN:C	1:E:341:ASN:HD22	2.26	0.43
1:A:90:LYS:HG3	1:A:166:THR:HB	2.00	0.43
1:C:64:GLU:OE2	1:C:205:TYR:OH	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:478:GLU:CD	1:C:480:LYS:HE2	2.44	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: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:C:408:TRP:CD1	1:C:408:TRP:C	2.98	0.42
1:B:81:ASP:O	1:B:81:ASP:CG	2.63	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:342:PRO:C	1:E:344:ASN:N	2.79	0.41
1:F:478:GLU:HG2	1:F:480:LYS:HE2	2.03	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:H:542:GLU:HA	1:H:543:PRO:HD3	1.95	0.40
1:D:92:ASN:O	1:D:250:PHE:HZ	2.03	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
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%)	43	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 ⓘ

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%)	488 (97%)	16 (3%)	34	25
1	B	504/541 (93%)	490 (97%)	14 (3%)	38	30
1	C	504/541 (93%)	490 (97%)	14 (3%)	38	30
1	D	504/541 (93%)	490 (97%)	14 (3%)	38	30
1	E	504/541 (93%)	486 (96%)	18 (4%)	31	21
1	F	504/541 (93%)	488 (97%)	16 (3%)	34	25
1	G	504/541 (93%)	487 (97%)	17 (3%)	32	23
1	H	504/541 (93%)	482 (96%)	22 (4%)	25	15
All	All	4032/4328 (93%)	3901 (97%)	131 (3%)	34	25

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	MET

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Mol	Chain	Res	Type
1	A	100	ILE
1	A	132	GLN
1	A	231	LYS
1	A	285	ARG
1	A	312	LYS
1	A	347	GLU
1	A	385	THR
1	A	389	LEU
1	A	392	SER
1	A	401	THR
1	A	413	LYS
1	A	432	GLU
1	A	490	LYS
1	A	496	ASN
1	A	619	THR
1	B	43	MET
1	B	100	ILE
1	B	139	ARG
1	B	185	LYS
1	B	206	PHE
1	B	216	SER
1	B	268	THR
1	B	344	ASN
1	B	385	THR
1	B	389	LEU
1	B	390	THR
1	B	432	GLU
1	B	490	LYS
1	B	496	ASN
1	D	45	ILE
1	D	100	ILE
1	D	178	GLU
1	D	231	LYS
1	D	285	ARG
1	D	344	ASN
1	D	347	GLU
1	D	385	THR
1	D	413	LYS
1	D	432	GLU
1	D	490	LYS
1	D	496	ASN
1	D	534	PRO

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Mol	Chain	Res	Type
1	D	576	LYS
1	C	43	MET
1	C	45	ILE
1	C	100	ILE
1	C	206	PHE
1	C	285	ARG
1	C	344	ASN
1	C	385	THR
1	C	389	LEU
1	C	392	SER
1	C	432	GLU
1	C	490	LYS
1	C	496	ASN
1	C	593	ASN
1	C	619	THR
1	E	43	MET
1	E	100	ILE
1	E	112	MET
1	E	185	LYS
1	E	206	PHE
1	E	231	LYS
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	452	ASP
1	E	490	LYS
1	E	593	ASN
1	F	95	GLU
1	F	100	ILE
1	F	132	GLN
1	F	206	PHE
1	F	216	SER
1	F	310	GLU
1	F	344	ASN
1	F	383	ARG
1	F	385	THR

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Mol	Chain	Res	Type
1	F	388	GLU
1	F	408	TRP
1	F	413	LYS
1	F	432	GLU
1	F	452	ASP
1	F	490	LYS
1	F	593	ASN
1	H	81	ASP
1	H	91	LYS
1	H	100	ILE
1	H	132	GLN
1	H	185	LYS
1	H	194	GLU
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	401	THR
1	H	413	LYS
1	H	432	GLU
1	H	455	SER
1	H	490	LYS
1	H	496	ASN
1	H	542	GLU
1	H	593	ASN
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	206	PHE
1	G	341	ASN
1	G	382	ILE
1	G	389	LEU
1	G	392	SER
1	G	408	TRP
1	G	490	LYS
1	G	496	ASN

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Mol	Chain	Res	Type
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 (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	GLN
1	A	257	ASN
1	A	263	GLN
1	A	276	ASN
1	A	341	ASN
1	A	419	HIS
1	A	460	GLN
1	B	132	GLN
1	B	257	ASN
1	B	263	GLN
1	B	276	ASN
1	B	460	GLN
1	D	233	GLN
1	D	257	ASN
1	D	263	GLN
1	D	299	HIS
1	D	324	HIS
1	D	341	ASN
1	D	419	HIS
1	D	460	GLN
1	C	105	ASN
1	C	257	ASN
1	C	263	GLN
1	C	276	ASN
1	C	341	ASN
1	C	419	HIS
1	C	461	GLN
1	E	105	ASN
1	E	233	GLN
1	E	263	GLN
1	E	299	HIS
1	E	336	GLN
1	E	341	ASN
1	E	419	HIS

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Mol	Chain	Res	Type
1	E	460	GLN
1	E	499	GLN
1	F	341	ASN
1	F	460	GLN
1	H	105	ASN
1	H	108	GLN
1	H	257	ASN
1	H	263	GLN
1	H	276	ASN
1	H	301	HIS
1	H	341	ASN
1	H	419	HIS
1	H	440	GLN
1	H	460	GLN
1	G	105	ASN
1	G	108	GLN
1	G	132	GLN
1	G	257	ASN
1	G	263	GLN
1	G	276	ASN
1	G	299	HIS
1	G	344	ASN
1	G	419	HIS
1	G	440	GLN
1	G	460	GLN
1	G	461	GLN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	SHG	F	806	-	12,12,12	0.77	0	16,17,17	4.46	8 (50%)
2	SHG	H	807	-	12,12,12	0.57	0	16,17,17	4.58	13 (81%)
2	SHG	C	804	-	12,12,12	0.75	0	16,17,17	5.15	11 (68%)
3	FAD	D	703	-	58,58,58	1.39	8 (13%)	85,89,89	1.84	21 (24%)
2	SHG	G	808	-	12,12,12	0.91	0	16,17,17	4.88	9 (56%)
3	FAD	C	704	-	58,58,58	1.62	12 (20%)	85,89,89	1.60	15 (17%)
3	FAD	B	702	-	58,58,58	1.40	9 (15%)	85,89,89	1.77	17 (20%)
3	FAD	A	701	-	58,58,58	1.57	8 (13%)	85,89,89	1.68	19 (22%)
2	SHG	A	801	-	12,12,12	0.74	0	16,17,17	4.67	10 (62%)
3	FAD	E	705	-	58,58,58	1.40	7 (12%)	85,89,89	1.57	12 (14%)
3	FAD	F	706	-	58,58,58	1.19	7 (12%)	85,89,89	1.76	20 (23%)
3	FAD	G	708	-	58,58,58	1.35	6 (10%)	85,89,89	1.68	16 (18%)
2	SHG	E	805	-	12,12,12	0.89	0	16,17,17	4.99	8 (50%)
2	SHG	B	802	-	12,12,12	0.94	0	16,17,17	4.46	10 (62%)
2	SHG	D	803	-	12,12,12	1.46	2 (16%)	16,17,17	4.35	8 (50%)
3	FAD	H	707	-	58,58,58	1.21	6 (10%)	85,89,89	1.75	19 (22%)

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	SHG	F	806	-	-	0/2/22/22	0/1/1/1
2	SHG	H	807	-	-	0/2/22/22	0/1/1/1
2	SHG	C	804	-	-	1/2/22/22	0/1/1/1
3	FAD	D	703	-	-	1/34/50/50	0/6/6/6
2	SHG	G	808	-	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FAD	C	704	-	-	0/34/50/50	0/6/6/6
3	FAD	B	702	-	-	1/34/50/50	0/6/6/6
3	FAD	A	701	-	-	1/34/50/50	0/6/6/6
2	SHG	A	801	-	-	0/2/22/22	0/1/1/1
3	FAD	E	705	-	-	0/34/50/50	0/6/6/6
3	FAD	F	706	-	-	1/34/50/50	0/6/6/6
3	FAD	G	708	-	-	0/34/50/50	0/6/6/6
2	SHG	E	805	-	-	1/2/22/22	0/1/1/1
2	SHG	B	802	-	-	1/2/22/22	0/1/1/1
2	SHG	D	803	-	-	0/2/22/22	0/1/1/1
3	FAD	H	707	-	-	0/34/50/50	0/6/6/6

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	FAD	P-O3P	5.73	1.65	1.59
3	E	705	FAD	P-O3P	5.22	1.65	1.59
3	C	704	FAD	C4X-N5	4.71	1.40	1.30
3	C	704	FAD	P-O3P	4.68	1.64	1.59
3	D	703	FAD	P-O3P	4.65	1.64	1.59
3	G	708	FAD	C10-N1	4.32	1.42	1.33
3	A	701	FAD	C10-N1	4.08	1.41	1.33
3	E	705	FAD	PA-O3P	3.99	1.63	1.59
3	G	708	FAD	C5'-C4'	3.86	1.57	1.51
3	A	701	FAD	C4X-N5	3.84	1.39	1.30
3	B	702	FAD	PA-O3P	3.78	1.63	1.59
3	D	703	FAD	C4X-N5	3.61	1.38	1.30
3	A	701	FAD	C2A-N1A	3.51	1.40	1.33
2	D	803	SHG	C2-C1	3.43	1.56	1.52
3	C	704	FAD	C5'-C4'	3.43	1.56	1.51
3	G	708	FAD	P-O3P	3.37	1.63	1.59
3	B	702	FAD	C4X-N5	3.30	1.37	1.30
3	E	705	FAD	C10-N1	3.29	1.39	1.33
3	F	706	FAD	C4X-N5	3.28	1.37	1.30
3	E	705	FAD	C4X-N5	3.27	1.37	1.30
3	C	704	FAD	C10-N1	3.25	1.39	1.33
3	G	708	FAD	C4X-N5	3.24	1.37	1.30
3	D	703	FAD	PA-O3P	3.24	1.63	1.59
3	A	701	FAD	C5'-C4'	3.07	1.56	1.51
3	H	707	FAD	C10-N1	3.05	1.39	1.33
3	B	702	FAD	C2A-N1A	3.04	1.39	1.33
3	H	707	FAD	C4X-N5	3.02	1.37	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	FAD	C10-N1	2.96	1.39	1.33
3	C	704	FAD	C2A-N1A	2.91	1.39	1.33
3	D	703	FAD	C2A-N1A	2.87	1.39	1.33
2	D	803	SHG	C2-C3	-2.68	1.50	1.52
3	B	702	FAD	C5A-N7A	-2.63	1.34	1.39
3	C	704	FAD	C5A-N7A	-2.59	1.34	1.39
3	F	706	FAD	C5A-N7A	-2.55	1.34	1.39
3	F	706	FAD	C1'-C2'	2.50	1.56	1.52
3	B	702	FAD	C2A-N3A	2.46	1.38	1.33
3	H	707	FAD	C5A-N7A	-2.45	1.34	1.39
3	F	706	FAD	C10-N1	2.43	1.38	1.33
3	H	707	FAD	C2A-N1A	2.42	1.38	1.33
3	C	704	FAD	C1'-C2'	2.39	1.56	1.52
3	C	704	FAD	C9-C8	2.38	1.42	1.39
3	D	703	FAD	C2A-N3A	2.37	1.38	1.33
3	E	705	FAD	C5A-N7A	-2.35	1.34	1.39
3	F	706	FAD	C2A-N1A	2.34	1.38	1.33
3	B	702	FAD	P-O3P	2.33	1.62	1.59
3	H	707	FAD	C6-C7	2.31	1.42	1.39
3	G	708	FAD	C2A-N1A	2.31	1.38	1.33
3	G	708	FAD	C5A-N7A	-2.31	1.34	1.39
3	C	704	FAD	P-O1P	-2.30	1.42	1.50
3	D	703	FAD	C5A-N7A	-2.26	1.35	1.39
3	A	701	FAD	O4-C4	2.24	1.27	1.23
3	D	703	FAD	C4X-C10	-2.23	1.37	1.44
3	C	704	FAD	C2A-N3A	2.19	1.37	1.33
3	C	704	FAD	C8M-C8	2.18	1.55	1.51
3	B	702	FAD	C8A-N7A	2.17	1.35	1.31
3	E	705	FAD	C2A-N3A	2.16	1.37	1.33
3	D	703	FAD	C10-N1	2.14	1.37	1.33
3	A	701	FAD	C5A-N7A	-2.13	1.35	1.39
3	F	706	FAD	O4B-C4B	-2.13	1.40	1.45
3	E	705	FAD	C2A-N1A	2.12	1.37	1.33
3	C	704	FAD	PA-O1A	-2.08	1.43	1.50
3	H	707	FAD	C2A-N3A	2.07	1.37	1.33
3	F	706	FAD	C2A-N3A	2.07	1.37	1.33
3	B	702	FAD	C6-C7	-2.06	1.36	1.39
3	A	701	FAD	C9-C8	2.00	1.42	1.39

All (216) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	804	SHG	F2-C2-C3	14.17	121.08	108.81
2	G	808	SHG	F2-C2-C3	13.92	120.87	108.81
2	E	805	SHG	F2-C2-C3	11.55	118.82	108.81
2	A	801	SHG	F2-C2-C3	11.37	118.66	108.81
2	F	806	SHG	F2-C2-C3	10.56	117.96	108.81
2	B	802	SHG	F2-C2-C1	10.50	119.58	107.81
2	C	804	SHG	O5-C1-C2	10.18	122.89	109.75
2	F	806	SHG	O5-C1-C2	9.53	122.05	109.75
2	H	807	SHG	F2-C2-C3	9.23	116.80	108.81
2	E	805	SHG	O5-C1-C2	8.82	121.14	109.75
2	E	805	SHG	F2-C2-C1	8.73	117.60	107.81
2	H	807	SHG	O5-C1-C2	8.72	121.00	109.75
2	D	803	SHG	F2-C2-C1	8.59	117.44	107.81
2	G	808	SHG	O5-C1-C2	8.47	120.68	109.75
2	H	807	SHG	F2-C2-C1	8.46	117.29	107.81
2	B	802	SHG	F2-C2-C3	7.86	115.62	108.81
2	A	801	SHG	F2-C2-C1	7.51	116.23	107.81
2	A	801	SHG	O5-C1-C2	7.48	119.40	109.75
2	D	803	SHG	F2-C2-C3	7.42	115.24	108.81
2	D	803	SHG	O5-C1-C2	7.30	119.18	109.75
2	B	802	SHG	O5-C1-C2	6.96	118.73	109.75
3	A	701	FAD	N3A-C2A-N1A	-6.51	118.73	128.58
2	H	807	SHG	O5-C5-C4	6.35	121.15	109.70
2	D	803	SHG	O5-C5-C4	6.28	121.02	109.70
2	B	802	SHG	O5-C5-C4	6.22	120.91	109.70
3	H	707	FAD	N3A-C2A-N1A	-6.21	119.18	128.58
3	E	705	FAD	N3A-C2A-N1A	-6.08	119.37	128.58
3	G	708	FAD	N3A-C2A-N1A	-6.06	119.41	128.58
2	F	806	SHG	F2-C2-C1	5.94	114.46	107.81
3	D	703	FAD	N3A-C2A-N1A	-5.91	119.64	128.58
3	C	704	FAD	N3A-C2A-N1A	-5.84	119.74	128.58
2	G	808	SHG	O5-C5-C4	5.83	120.21	109.70
3	F	706	FAD	N3A-C2A-N1A	-5.82	119.77	128.58
3	B	702	FAD	N3A-C2A-N1A	-5.73	119.91	128.58
2	E	805	SHG	O5-C5-C4	5.62	119.82	109.70
2	F	806	SHG	O5-C5-C4	5.42	119.46	109.70
2	E	805	SHG	O3-C3-C2	5.14	119.13	109.63
2	C	804	SHG	F2-C2-C1	5.12	113.55	107.81
2	D	803	SHG	C1-C2-C3	5.06	118.23	110.69
2	C	804	SHG	O5-C5-C4	4.95	118.62	109.70
2	A	801	SHG	O5-C5-C4	4.93	118.59	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	707	FAD	C5'-C4'-C3'	-4.83	103.11	112.22
2	A	801	SHG	C1-O5-C5	4.50	122.37	113.65
2	C	804	SHG	C3-C4-C5	4.50	118.40	110.23
3	D	703	FAD	O2A-PA-O3P	4.48	119.39	107.27
3	G	708	FAD	C5A-C4A-N3A	-4.44	120.61	126.72
3	E	705	FAD	C5A-C4A-N3A	-4.40	120.65	126.72
3	D	703	FAD	O3P-PA-O1A	-4.39	97.51	110.70
3	B	702	FAD	C5A-C4A-N3A	-4.32	120.77	126.72
3	F	706	FAD	C5A-C4A-N3A	-4.27	120.84	126.72
3	D	703	FAD	C5A-C4A-N3A	-4.14	121.01	126.72
3	H	707	FAD	C5A-C4A-N3A	-4.07	121.11	126.72
2	D	803	SHG	C3-C4-C5	4.05	117.58	110.23
3	C	704	FAD	C5A-C4A-N3A	-4.03	121.16	126.72
3	F	706	FAD	O2A-PA-O3P	4.02	118.13	107.27
2	F	806	SHG	O3-C3-C2	4.00	117.02	109.63
3	H	707	FAD	N9A-C8A-N7A	-3.99	108.28	113.94
3	D	703	FAD	C4X-C10-N10	3.98	122.18	116.48
3	D	703	FAD	N9A-C8A-N7A	-3.96	108.31	113.94
3	G	708	FAD	C5'-C4'-C3'	-3.84	104.97	112.22
3	E	705	FAD	N9A-C8A-N7A	-3.84	108.49	113.94
2	G	808	SHG	C1-O5-C5	3.83	121.06	113.65
3	D	703	FAD	O4'-C4'-C3'	3.80	118.13	109.25
3	F	706	FAD	N9A-C8A-N7A	-3.79	108.55	113.94
2	A	801	SHG	C3-C4-C5	3.79	117.11	110.23
3	A	701	FAD	N9A-C8A-N7A	-3.75	108.61	113.94
2	B	802	SHG	C1-O5-C5	3.74	120.90	113.65
2	D	803	SHG	O3-C3-C2	3.71	116.50	109.63
3	B	702	FAD	C4X-C10-N10	3.71	121.80	116.48
3	C	704	FAD	O3P-PA-O1A	-3.71	99.54	110.70
3	B	702	FAD	O2P-P-O3P	-3.68	97.33	107.27
2	E	805	SHG	C3-C4-C5	3.67	116.89	110.23
3	C	704	FAD	O2A-PA-O3P	3.67	117.19	107.27
3	G	708	FAD	N9A-C8A-N7A	-3.67	108.74	113.94
3	B	702	FAD	O3P-PA-O1A	-3.65	99.73	110.70
2	G	808	SHG	O3-C3-C2	3.60	116.28	109.63
3	G	708	FAD	C2A-N3A-C4A	3.56	120.53	111.83
2	A	801	SHG	C1-C2-C3	3.56	115.99	110.69
3	A	701	FAD	O2A-PA-O3P	3.52	116.79	107.27
3	F	706	FAD	O3P-PA-O1A	-3.51	100.14	110.70
3	E	705	FAD	C2A-N3A-C4A	3.49	120.37	111.83
3	A	701	FAD	C9A-C5X-N5	-3.45	118.79	122.45
2	G	808	SHG	O3-C3-C4	3.43	118.46	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	707	FAD	C2A-N3A-C4A	3.43	120.20	111.83
2	F	806	SHG	C1-O5-C5	3.42	120.27	113.65
2	G	808	SHG	F2-C2-C1	3.42	111.64	107.81
2	G	808	SHG	C1-C2-C3	3.42	115.78	110.69
3	F	706	FAD	C2A-N3A-C4A	3.42	120.17	111.83
3	B	702	FAD	N9A-C8A-N7A	-3.41	109.09	113.94
3	G	708	FAD	C5A-N7A-C8A	3.41	108.81	103.45
2	D	803	SHG	C1-O5-C5	3.41	120.25	113.65
3	B	702	FAD	C10-C4X-N5	-3.38	117.90	124.81
3	E	705	FAD	C5A-N7A-C8A	3.38	108.76	103.45
3	H	707	FAD	C9A-C5X-N5	-3.36	118.89	122.45
2	H	807	SHG	C1-C2-C3	3.36	115.70	110.69
3	D	703	FAD	C5A-N7A-C8A	3.34	108.70	103.45
2	E	805	SHG	O5-C5-C6	3.32	114.68	106.44
3	D	703	FAD	C2A-N3A-C4A	3.32	119.94	111.83
2	C	804	SHG	C1-O5-C5	3.30	120.05	113.65
3	B	702	FAD	C5A-N7A-C8A	3.28	108.61	103.45
2	E	805	SHG	C1-O5-C5	3.28	120.00	113.65
3	A	701	FAD	O3P-PA-O1A	-3.27	100.86	110.70
3	C	704	FAD	N9A-C8A-N7A	-3.26	109.31	113.94
3	F	706	FAD	C5A-N7A-C8A	3.26	108.57	103.45
3	B	702	FAD	C2A-N3A-C4A	3.25	119.77	111.83
3	A	701	FAD	C2A-N3A-C4A	3.24	119.75	111.83
3	H	707	FAD	C5A-N7A-C8A	3.23	108.52	103.45
3	C	704	FAD	C2A-N3A-C4A	3.22	119.69	111.83
3	F	706	FAD	C4X-C10-N10	3.20	121.06	116.48
2	A	801	SHG	O3-C3-C2	3.17	115.49	109.63
3	A	701	FAD	C5A-C4A-N3A	-3.17	122.35	126.72
3	E	705	FAD	C4X-C10-N10	3.11	120.93	116.48
3	B	702	FAD	O2A-PA-O3P	3.03	115.47	107.27
3	B	702	FAD	C4-C4X-N5	3.02	122.38	118.21
3	E	705	FAD	C5'-C4'-C3'	-3.01	106.55	112.22
3	D	703	FAD	C4-N3-C2	-2.99	120.33	125.64
2	G	808	SHG	C3-C4-C5	2.98	115.64	110.23
3	G	708	FAD	O2A-PA-O3P	2.97	115.30	107.27
2	F	806	SHG	O5-C5-C6	2.96	113.78	106.44
3	C	704	FAD	C5A-N7A-C8A	2.95	108.08	103.45
2	A	801	SHG	O4-C4-C5	2.93	116.55	109.32
3	F	706	FAD	C8M-C8-C9	-2.93	114.41	119.57
2	B	802	SHG	O3-C3-C4	2.92	117.25	110.38
2	C	804	SHG	O3-C3-C4	2.91	117.23	110.38
2	C	804	SHG	C1-C2-C3	2.90	115.01	110.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	FAD	C5'-C4'-C3'	-2.89	106.76	112.22
3	D	703	FAD	N3A-C4A-N9A	2.88	132.06	127.17
2	B	802	SHG	C1-C2-C3	2.87	114.97	110.69
3	A	701	FAD	O3'-C3'-C4'	-2.85	102.45	108.93
2	H	807	SHG	C3-C4-C5	2.84	115.39	110.23
3	E	705	FAD	N3A-C4A-N9A	2.83	131.98	127.17
3	G	708	FAD	O3P-PA-O1A	-2.81	102.25	110.70
3	G	708	FAD	O4B-C1B-N9A	2.80	113.46	108.09
3	C	704	FAD	C9A-C5X-N5	-2.79	119.50	122.45
3	H	707	FAD	N3A-C4A-N9A	2.78	131.90	127.17
3	A	701	FAD	C5A-N7A-C8A	2.78	107.81	103.45
3	F	706	FAD	N3A-C4A-N9A	2.75	131.84	127.17
2	B	802	SHG	O3-C3-C2	2.74	114.70	109.63
3	G	708	FAD	C9A-C5X-N5	-2.74	119.54	122.45
3	F	706	FAD	C10-C4X-N5	-2.71	119.28	124.81
3	F	706	FAD	C9A-C5X-N5	-2.69	119.60	122.45
3	E	705	FAD	O3P-PA-O1A	-2.68	102.65	110.70
3	H	707	FAD	C4-N3-C2	-2.66	120.92	125.64
2	H	807	SHG	O5-C5-C6	2.66	113.03	106.44
3	G	708	FAD	C4A-C5A-N7A	-2.66	107.55	110.58
3	G	708	FAD	N3A-C4A-N9A	2.65	131.68	127.17
2	H	807	SHG	O3-C3-C2	2.61	114.45	109.63
2	H	807	SHG	O4-C4-C5	2.60	115.74	109.32
3	B	702	FAD	N3A-C4A-N9A	2.57	131.54	127.17
3	D	703	FAD	O2P-P-O3P	-2.56	100.34	107.27
3	C	704	FAD	C4X-C10-N10	2.56	120.14	116.48
2	H	807	SHG	O3-C3-C4	2.55	116.39	110.38
3	D	703	FAD	C10-C4X-N5	-2.52	119.66	124.81
3	F	706	FAD	C4-C4X-N5	2.51	121.68	118.21
3	B	702	FAD	C4A-C5A-N7A	-2.51	107.71	110.58
3	A	701	FAD	N3A-C4A-N9A	2.47	131.37	127.17
2	C	804	SHG	C6-C5-C4	2.47	119.08	113.02
3	E	705	FAD	C1'-N10-C9A	2.46	125.41	120.63
3	H	707	FAD	C4'-C3'-C2'	-2.45	109.49	113.57
2	A	801	SHG	O5-C5-C6	2.45	112.50	106.44
3	F	706	FAD	C6-C5X-C9A	2.44	122.39	119.05
3	C	704	FAD	N3A-C4A-N9A	2.43	131.31	127.17
3	F	706	FAD	C5X-C9A-N10	2.42	120.16	117.97
3	G	708	FAD	O4'-C4'-C3'	2.42	114.92	109.25
2	F	806	SHG	C3-C4-C5	2.41	114.60	110.23
3	C	704	FAD	O2A-PA-O1A	2.41	123.64	112.44
3	A	701	FAD	O4B-C1B-N9A	2.40	112.71	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	706	FAD	C5'-C4'-C3'	-2.40	107.69	112.22
3	E	705	FAD	O2P-P-O1P	2.39	123.54	112.44
3	H	707	FAD	O3'-C3'-C2'	-2.37	103.56	108.93
3	H	707	FAD	C4X-C10-N10	2.34	119.83	116.48
3	B	702	FAD	C6A-C5A-C4A	2.33	120.36	117.18
3	D	703	FAD	C4X-C4-N3	2.32	119.17	113.25
3	H	707	FAD	C9A-C9-C8	2.32	123.89	119.22
2	C	804	SHG	O3-C3-C2	2.31	113.91	109.63
3	E	705	FAD	C4A-C5A-N7A	-2.30	107.95	110.58
3	A	701	FAD	C4A-N9A-C8A	2.30	108.15	105.74
2	H	807	SHG	C1-O5-C5	2.29	118.09	113.65
3	D	703	FAD	C9A-C5X-N5	-2.28	120.04	122.45
3	F	706	FAD	C4A-C5A-N7A	-2.25	108.01	110.58
3	H	707	FAD	C10-C4X-N5	-2.24	120.24	124.81
2	B	802	SHG	O1-C1-C2	2.23	118.58	109.33
3	C	704	FAD	C5'-C4'-C3'	-2.23	108.00	112.22
3	B	702	FAD	C5X-N5-C4X	2.22	121.68	118.09
2	H	807	SHG	O1-C1-O5	2.21	116.98	110.41
3	G	708	FAD	C10-C4X-N5	-2.21	120.30	124.81
2	B	802	SHG	C3-C4-C5	2.21	114.23	110.23
3	D	703	FAD	O5'-P-O1P	-2.19	100.25	108.94
3	A	701	FAD	C8M-C8-C9	-2.18	115.72	119.57
3	G	708	FAD	O4-C4-C4X	-2.18	120.78	126.53
3	D	703	FAD	C10-N1-C2	2.17	121.55	116.85
3	B	702	FAD	O4B-C1B-N9A	2.17	112.25	108.09
2	C	804	SHG	O6-C6-C5	-2.17	103.96	111.33
3	D	703	FAD	O4-C4-C4X	-2.15	120.85	126.53
3	D	703	FAD	C4A-C5A-N7A	-2.14	108.14	110.58
2	H	807	SHG	O6-C6-C5	-2.13	104.08	111.33
3	H	707	FAD	C5X-C9A-N10	2.13	119.89	117.97
3	F	706	FAD	C4X-C4-N3	2.12	118.66	113.25
3	F	706	FAD	O4'-C4'-C3'	2.11	114.19	109.25
3	A	701	FAD	C6-C5X-N5	2.10	121.93	118.44
3	D	703	FAD	O3P-P-O1P	2.09	117.00	110.70
3	D	703	FAD	C4A-N9A-C8A	2.07	107.92	105.74
3	A	701	FAD	O2P-P-O3P	-2.07	101.69	107.27
3	A	701	FAD	C10-C4X-N5	-2.06	120.59	124.81
3	H	707	FAD	C4X-C4-N3	2.06	118.50	113.25
3	A	701	FAD	C4X-C10-N10	2.06	119.43	116.48
3	H	707	FAD	C5X-N5-C4X	2.05	121.40	118.09
3	F	706	FAD	C5X-N5-C4X	2.04	121.39	118.09
3	C	704	FAD	C10-C4X-N5	-2.04	120.65	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	702	FAD	O3'-C3'-C2'	-2.03	104.31	108.93
3	G	708	FAD	C4-C4X-C10	2.03	120.41	116.93
3	C	704	FAD	C4A-C5A-N7A	-2.02	108.27	110.58
3	A	701	FAD	O3'-C3'-C2'	-2.01	104.36	108.93
3	H	707	FAD	C4A-N9A-C8A	2.01	107.84	105.74
3	C	704	FAD	C5X-C9A-N10	2.01	119.78	117.97
3	H	707	FAD	O2A-PA-O1A	2.01	121.78	112.44

There are no chirality outliers.

All (7) 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'
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

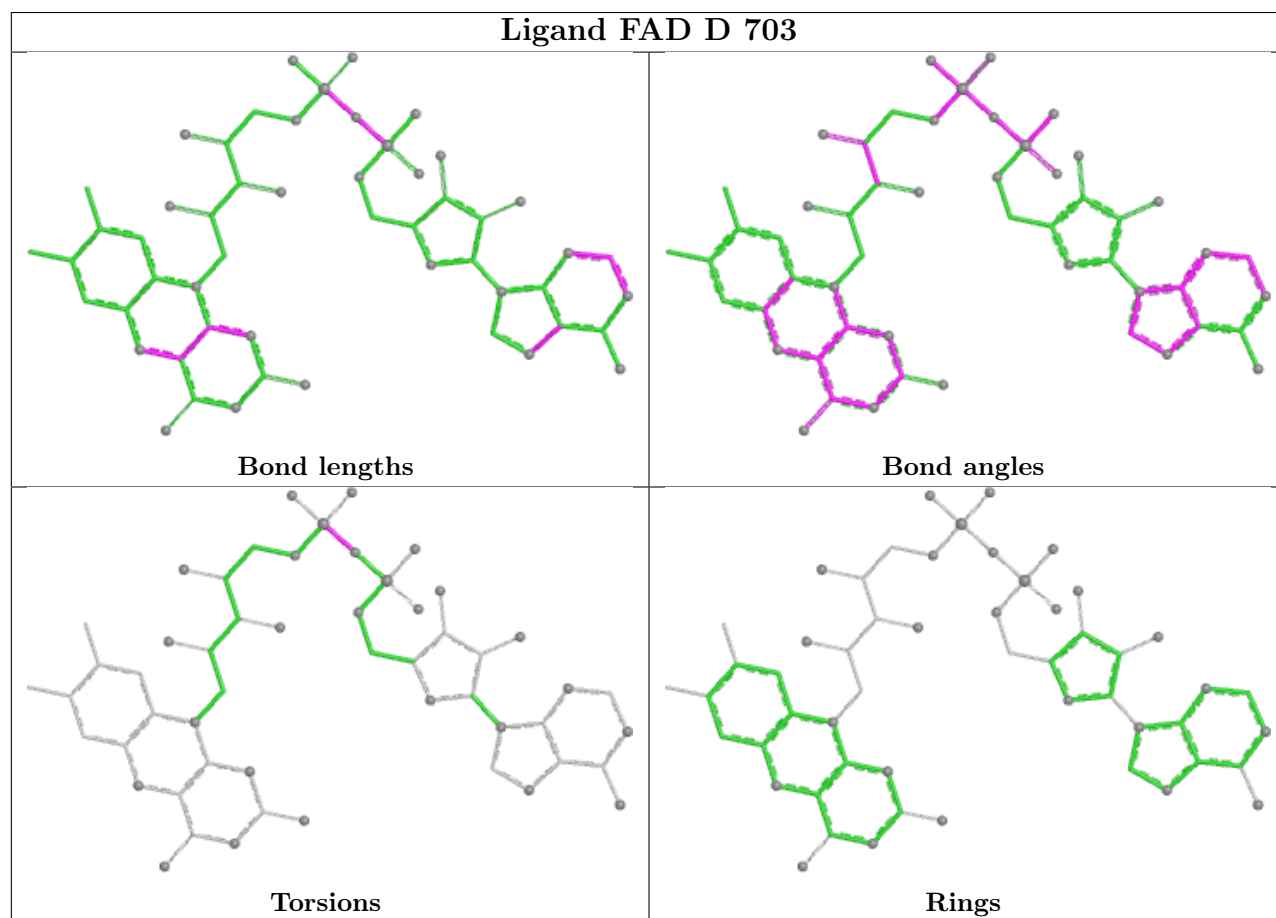
There are no ring outliers.

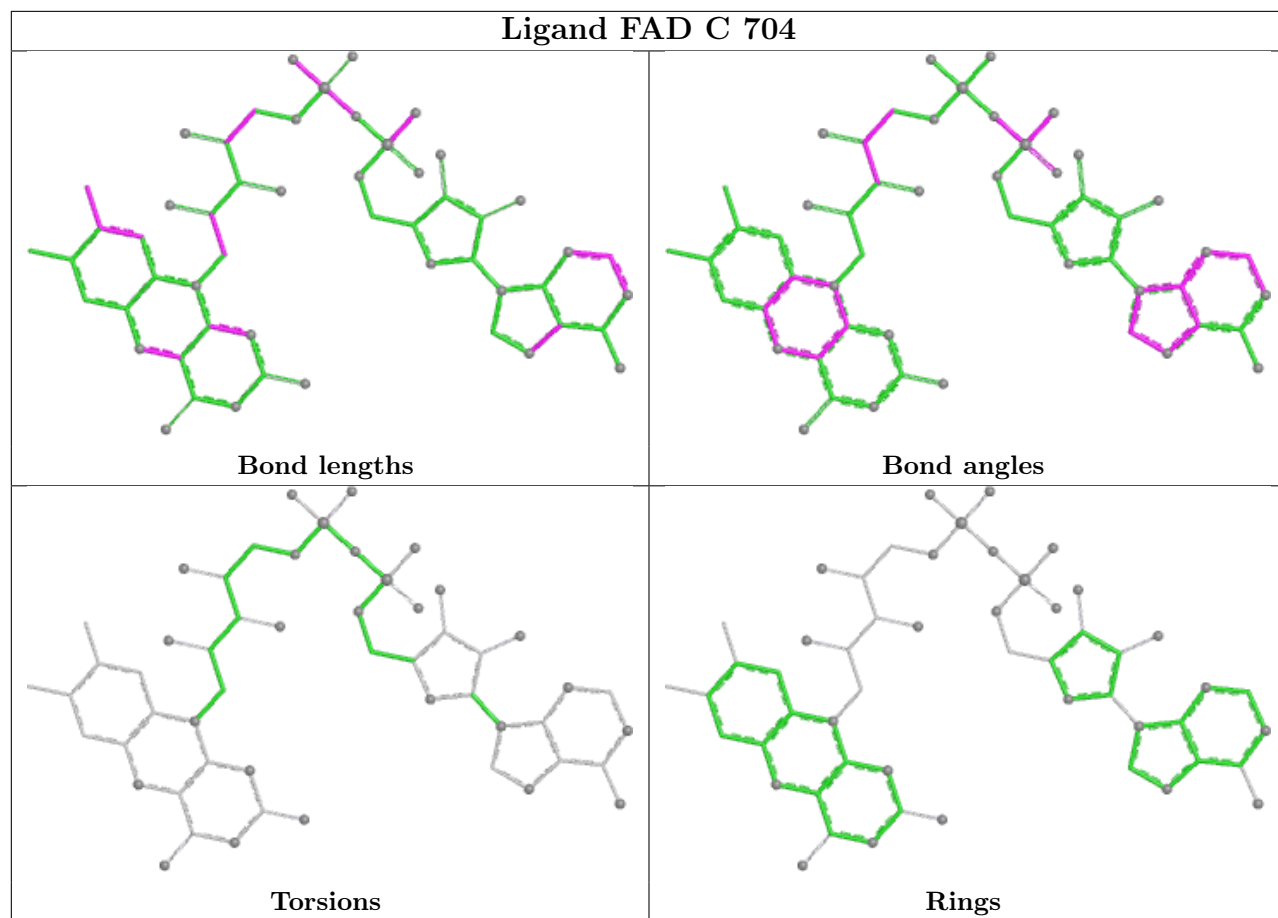
13 monomers are involved in 31 short contacts:

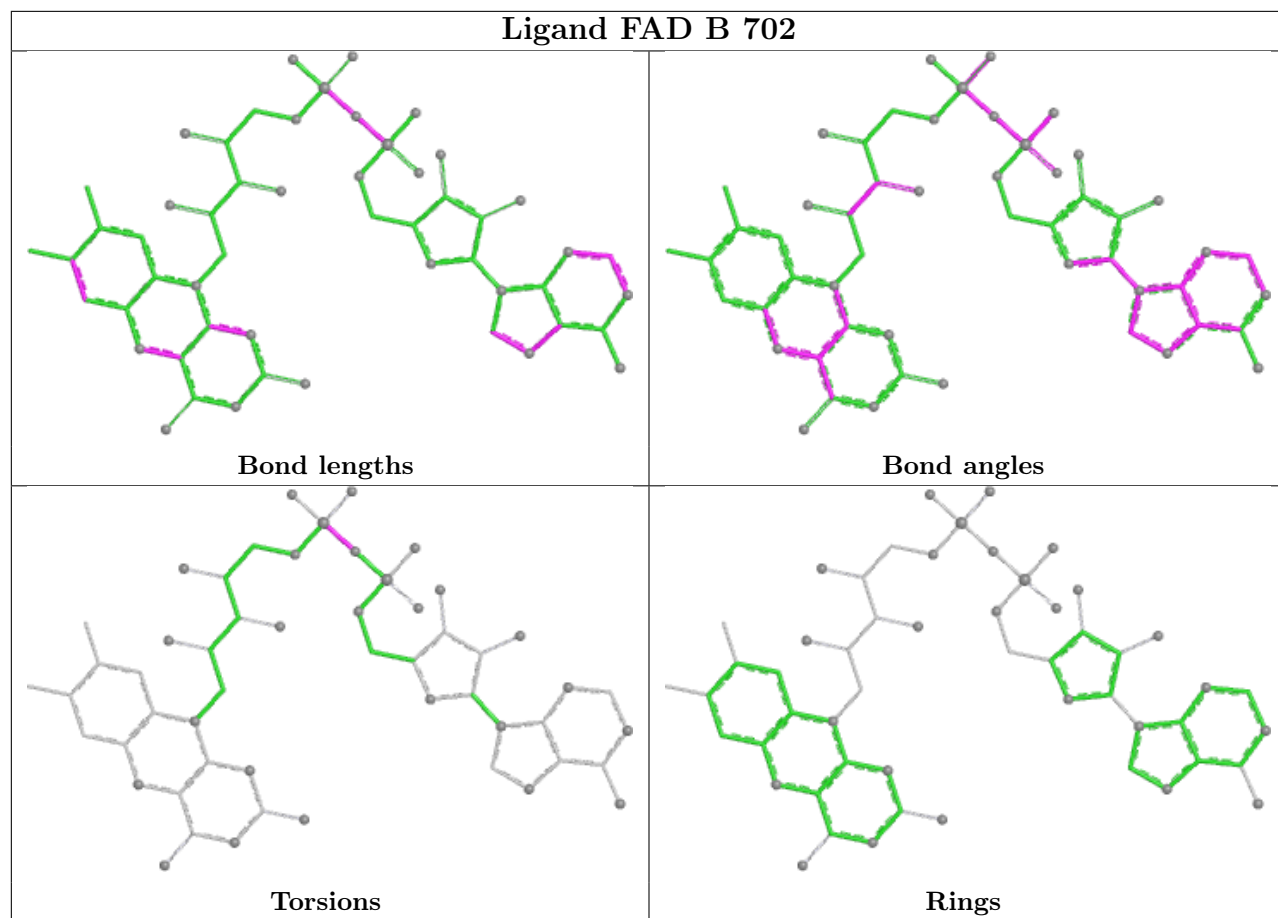
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	806	SHG	2	0
2	C	804	SHG	5	0
3	D	703	FAD	2	0
2	G	808	SHG	4	0
3	C	704	FAD	1	0
3	B	702	FAD	4	0
3	A	701	FAD	4	0
2	A	801	SHG	4	0
3	E	705	FAD	1	0
3	G	708	FAD	2	0
2	E	805	SHG	4	0
2	B	802	SHG	1	0
2	D	803	SHG	3	0

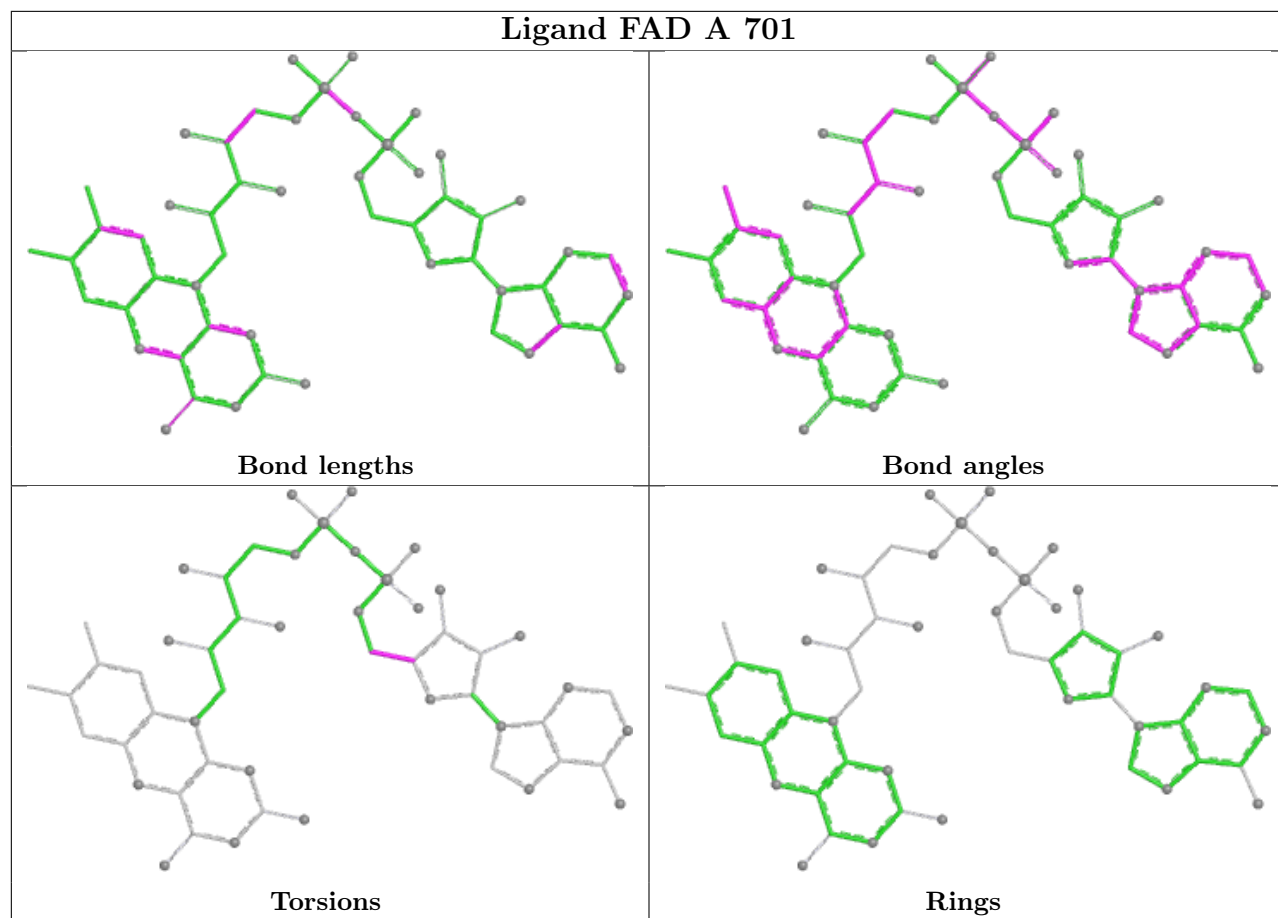
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

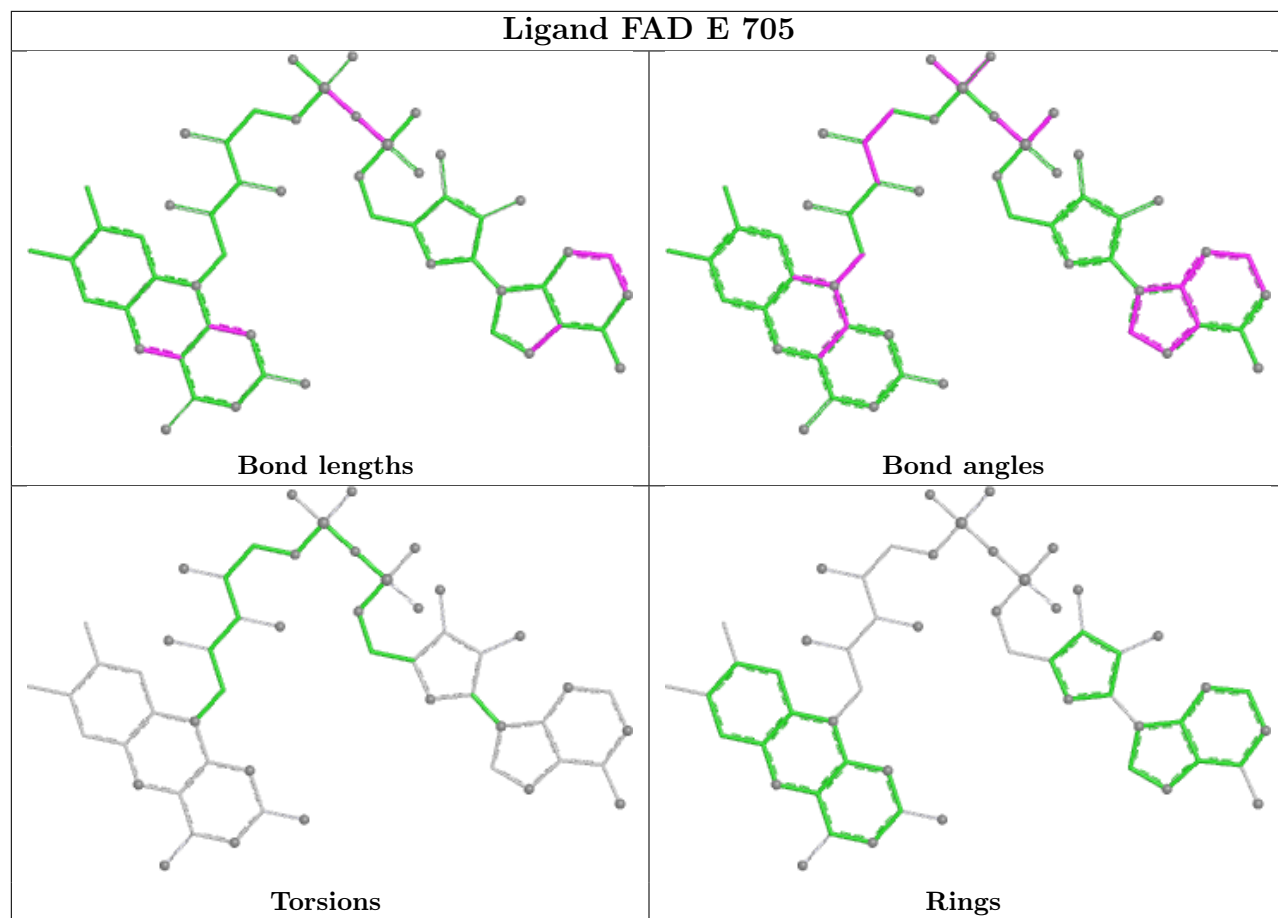
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

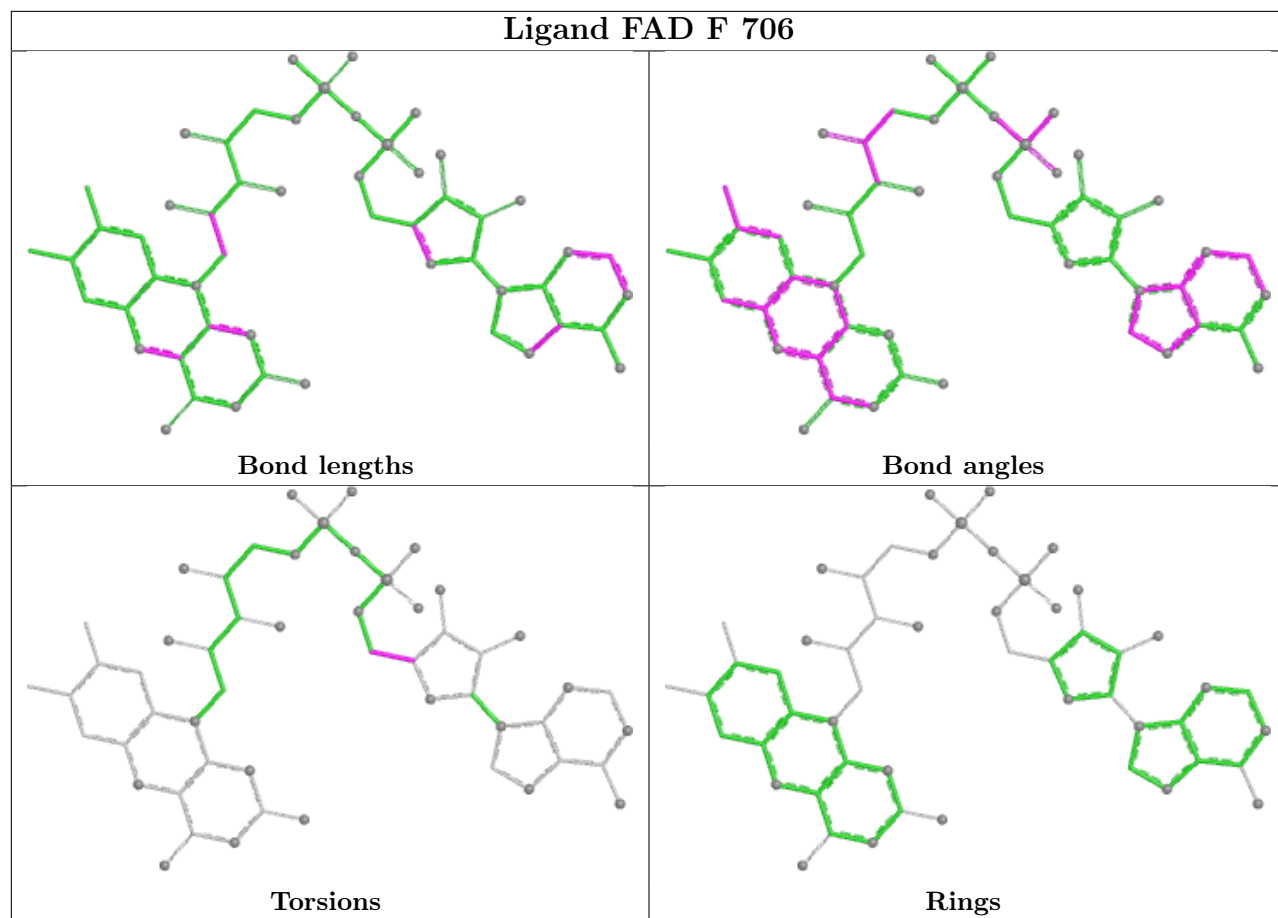


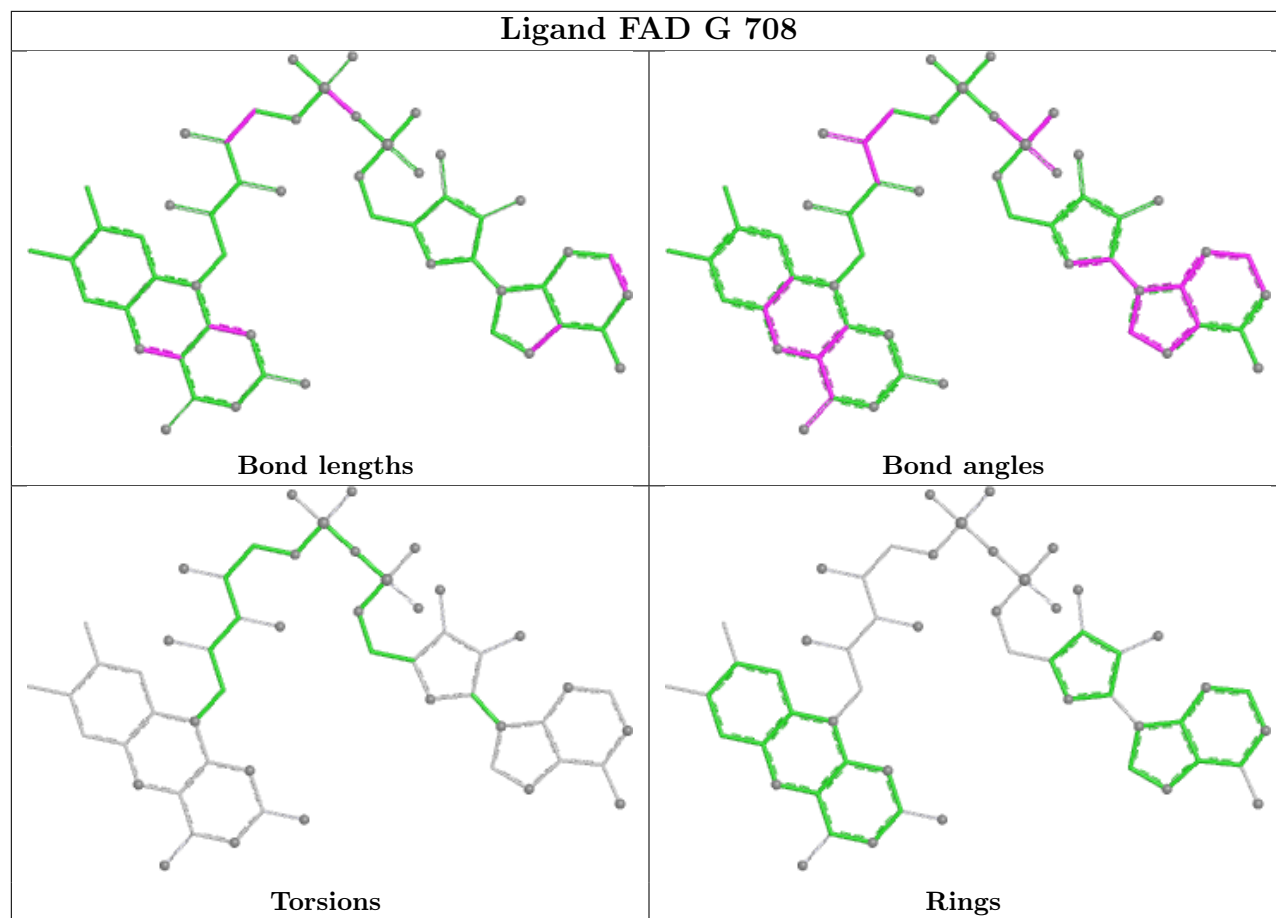


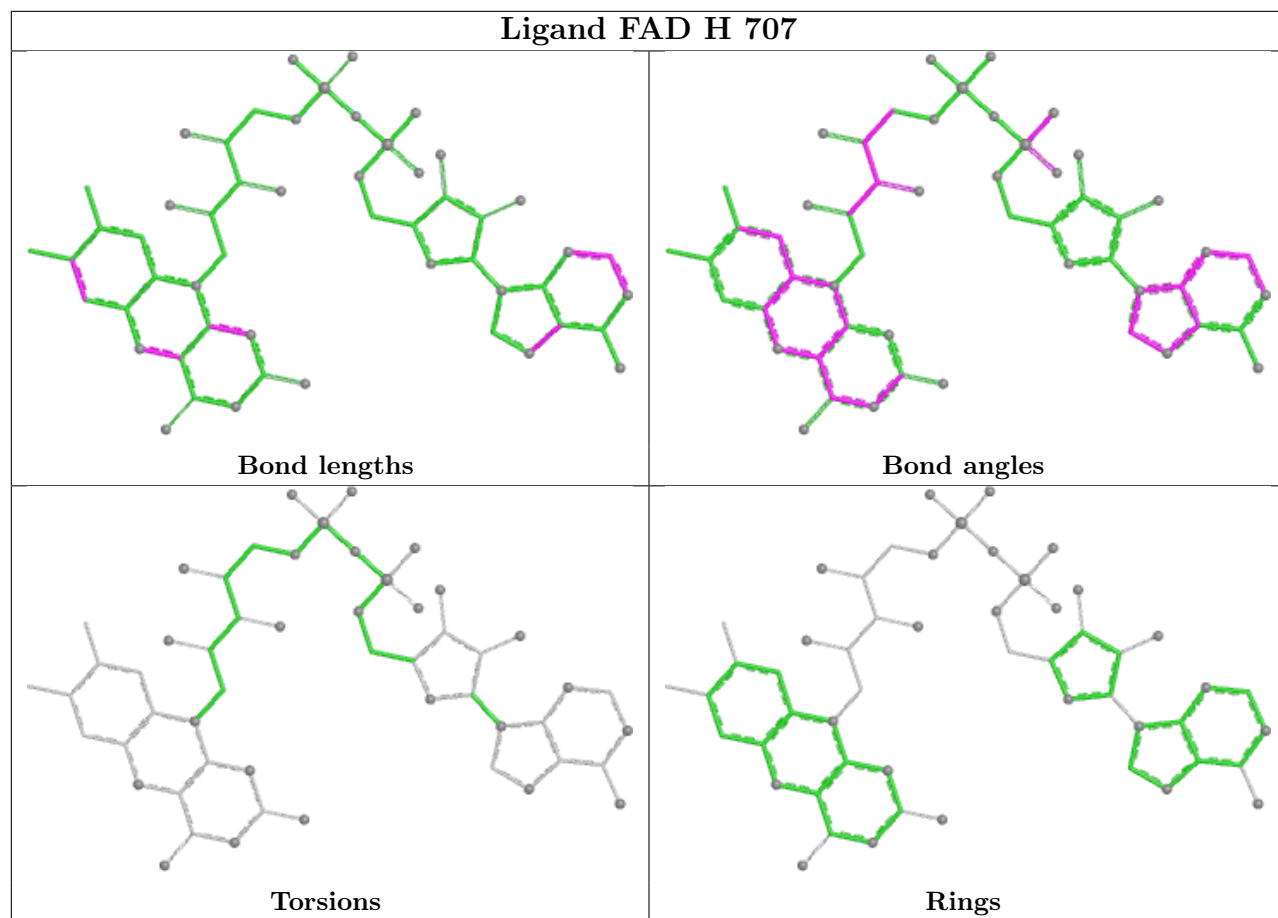












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	577/623 (92%)	0.01	42 (7%)	21	24	16, 22, 44, 69	0
1	B	577/623 (92%)	0.01	34 (5%)	28	32	15, 23, 42, 67	0
1	C	577/623 (92%)	0.26	37 (6%)	25	29	18, 26, 46, 71	0
1	D	577/623 (92%)	0.10	27 (4%)	36	42	16, 25, 45, 72	0
1	E	577/623 (92%)	0.20	32 (5%)	30	36	18, 26, 45, 72	0
1	F	577/623 (92%)	0.29	43 (7%)	20	23	17, 27, 47, 71	0
1	G	577/623 (92%)	0.20	44 (7%)	20	22	18, 25, 48, 67	0
1	H	577/623 (92%)	0.10	31 (5%)	31	37	16, 24, 43, 71	0
All	All	4616/4984 (92%)	0.15	290 (6%)	26	30	15, 25, 45, 72	0

All (290) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	45	ILE	9.0
1	C	619	THR	8.5
1	E	619	THR	7.6
1	C	45	ILE	7.6
1	F	45	ILE	7.5
1	F	389	LEU	7.1
1	F	619	THR	7.0
1	C	389	LEU	6.9
1	F	44	ASP	6.8
1	D	45	ILE	6.8
1	C	44	ASP	6.6
1	H	45	ILE	6.4
1	B	389	LEU	6.4
1	G	389	LEU	6.3
1	D	619	THR	6.1
1	A	389	LEU	5.8

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Mol	Chain	Res	Type	RSRZ
1	H	619	THR	5.7
1	A	619	THR	5.6
1	G	385	THR	5.4
1	B	619	THR	5.3
1	A	390	THR	5.1
1	B	618	PHE	5.0
1	H	44	ASP	4.9
1	C	618	PHE	4.9
1	F	387	GLY	4.8
1	H	618	PHE	4.6
1	G	619	THR	4.6
1	B	385	THR	4.5
1	C	342	PRO	4.4
1	G	618	PHE	4.2
1	F	385	THR	4.2
1	A	401	THR	4.1
1	A	45	ILE	4.0
1	D	618	PHE	4.0
1	G	44	ASP	4.0
1	B	388	GLU	4.0
1	A	133	ALA	4.0
1	E	45	ILE	4.0
1	H	342	PRO	3.9
1	F	43	MET	3.9
1	H	459	VAL	3.9
1	G	81	ASP	3.9
1	C	43	MET	3.8
1	G	82	SER	3.8
1	B	342	PRO	3.8
1	E	44	ASP	3.8
1	D	388	GLU	3.8
1	F	81	ASP	3.8
1	G	390	THR	3.8
1	A	452	ASP	3.7
1	G	388	GLU	3.7
1	F	309	PHE	3.7
1	F	343	ALA	3.7
1	F	250	PHE	3.7
1	C	385	THR	3.6
1	F	342	PRO	3.6
1	D	389	LEU	3.6
1	H	343	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	385	THR	3.6
1	A	399	ALA	3.5
1	B	418	GLN	3.5
1	G	343	ALA	3.5
1	C	452	ASP	3.5
1	C	390	THR	3.5
1	H	345	PRO	3.5
1	E	618	PHE	3.5
1	A	44	ASP	3.4
1	E	452	ASP	3.4
1	G	397	PRO	3.4
1	E	343	ALA	3.4
1	C	188	ALA	3.4
1	H	133	ALA	3.4
1	F	432	GLU	3.3
1	F	184	VAL	3.3
1	A	381	THR	3.3
1	A	345	PRO	3.3
1	D	455	SER	3.3
1	A	394	THR	3.3
1	A	397	PRO	3.3
1	C	343	ALA	3.3
1	G	250	PHE	3.3
1	A	398	GLY	3.3
1	B	45	ILE	3.2
1	G	309	PHE	3.2
1	B	133	ALA	3.1
1	D	385	THR	3.1
1	C	345	PRO	3.1
1	G	43	MET	3.1
1	D	452	ASP	3.1
1	E	432	GLU	3.1
1	C	133	ALA	3.1
1	G	345	PRO	3.1
1	D	387	GLY	3.1
1	B	452	ASP	3.1
1	B	390	THR	3.1
1	H	385	THR	3.1
1	A	382	ILE	3.1
1	E	291	LEU	3.1
1	A	385	THR	3.1
1	A	308	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	383	ARG	3.0
1	H	389	LEU	3.0
1	H	81	ASP	3.0
1	D	343	ALA	3.0
1	C	383	ARG	3.0
1	A	459	VAL	3.0
1	D	81	ASP	3.0
1	C	185	LYS	3.0
1	H	232	GLY	3.0
1	E	342	PRO	3.0
1	A	81	ASP	2.9
1	E	232	GLY	2.9
1	G	100	ILE	2.9
1	G	400	SER	2.9
1	D	44	ASP	2.9
1	H	43	MET	2.9
1	B	341	ASN	2.9
1	B	345	PRO	2.9
1	G	342	PRO	2.9
1	A	453	ALA	2.9
1	H	418	GLN	2.9
1	F	296	GLU	2.9
1	F	384	GLY	2.9
1	F	185	LYS	2.8
1	B	343	ALA	2.8
1	F	190	ALA	2.8
1	F	290	ALA	2.8
1	A	388	GLU	2.8
1	H	452	ASP	2.8
1	F	291	LEU	2.8
1	A	396	THR	2.8
1	F	452	ASP	2.8
1	F	618	PHE	2.8
1	H	309	PHE	2.8
1	E	387	GLY	2.8
1	G	490	LYS	2.8
1	C	250	PHE	2.7
1	A	387	GLY	2.7
1	E	388	GLU	2.7
1	E	345	PRO	2.7
1	H	344	ASN	2.7
1	C	387	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	82	SER	2.7
1	G	432	GLU	2.7
1	G	299	HIS	2.7
1	E	309	PHE	2.7
1	A	400	SER	2.7
1	B	432	GLU	2.7
1	B	490	LYS	2.6
1	D	342	PRO	2.6
1	A	618	PHE	2.6
1	F	617	PRO	2.6
1	A	43	MET	2.6
1	B	44	ASP	2.6
1	B	454	PHE	2.6
1	E	399	ALA	2.6
1	G	453	ALA	2.6
1	B	299	HIS	2.5
1	D	250	PHE	2.5
1	F	132	GLN	2.5
1	G	452	ASP	2.5
1	G	398	GLY	2.5
1	G	133	ALA	2.5
1	D	43	MET	2.5
1	H	189	ASP	2.5
1	E	250	PHE	2.5
1	E	382	ILE	2.5
1	A	455	SER	2.5
1	H	453	ALA	2.5
1	H	458	ALA	2.5
1	D	186	ASP	2.5
1	D	310	GLU	2.5
1	H	432	GLU	2.5
1	B	81	ASP	2.5
1	H	388	GLU	2.4
1	G	418	GLN	2.4
1	B	82	SER	2.4
1	G	312	LYS	2.4
1	G	458	ALA	2.4
1	H	269	ASP	2.4
1	A	341	ASN	2.4
1	H	455	SER	2.4
1	C	490	LYS	2.4
1	A	343	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	383	ARG	2.4
1	A	393	VAL	2.4
1	C	132	GLN	2.4
1	D	309	PHE	2.4
1	E	81	ASP	2.4
1	G	383	ARG	2.4
1	G	399	ALA	2.4
1	F	310	GLU	2.4
1	D	345	PRO	2.4
1	H	346	PRO	2.4
1	F	490	LYS	2.4
1	D	390	THR	2.3
1	F	268	THR	2.3
1	G	310	GLU	2.3
1	A	458	ALA	2.3
1	E	617	PRO	2.3
1	C	457	GLY	2.3
1	E	393	VAL	2.3
1	B	285	ARG	2.3
1	F	388	GLU	2.3
1	C	396	THR	2.3
1	C	341	ASN	2.3
1	G	185	LYS	2.3
1	F	347	GLU	2.3
1	H	611	GLN	2.3
1	A	344	ASN	2.3
1	B	309	PHE	2.3
1	E	68	ALA	2.3
1	A	384	GLY	2.3
1	C	82	SER	2.3
1	H	272	GLU	2.3
1	A	309	PHE	2.2
1	C	309	PHE	2.2
1	H	617	PRO	2.2
1	G	387	GLY	2.2
1	D	299	HIS	2.2
1	B	43	MET	2.2
1	F	390	THR	2.2
1	B	310	GLU	2.2
1	C	400	SER	2.2
1	A	456	TYR	2.2
1	G	344	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	285	ARG	2.2
1	F	308	ARG	2.2
1	B	421	GLU	2.2
1	C	561	GLU	2.2
1	G	396	THR	2.2
1	F	418	GLN	2.2
1	E	384	GLY	2.2
1	A	342	PRO	2.2
1	G	340	PRO	2.2
1	D	133	ALA	2.2
1	F	188	ALA	2.2
1	E	299	HIS	2.2
1	D	184	VAL	2.2
1	C	611	GLN	2.2
1	E	418	GLN	2.2
1	F	84	LEU	2.2
1	F	345	PRO	2.2
1	A	490	LYS	2.2
1	B	383	ARG	2.2
1	E	490	LYS	2.2
1	H	454	PHE	2.1
1	C	418	GLN	2.1
1	F	394	THR	2.1
1	B	384	GLY	2.1
1	E	398	GLY	2.1
1	F	328	LEU	2.1
1	D	272	GLU	2.1
1	C	456	TYR	2.1
1	G	382	ILE	2.1
1	C	81	ASP	2.1
1	G	269	ASP	2.1
1	G	401	THR	2.1
1	B	178	GLU	2.1
1	E	421	GLU	2.1
1	F	228	GLU	2.1
1	B	386	PRO	2.1
1	F	386	PRO	2.1
1	E	391	TYR	2.1
1	F	395	TYR	2.1
1	A	392	SER	2.1
1	E	401	THR	2.1
1	G	394	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	457	GLY	2.1
1	E	43	MET	2.1
1	G	341	ASN	2.1
1	B	617	PRO	2.1
1	B	453	ALA	2.1
1	D	454	PHE	2.0
1	C	312	LYS	2.0
1	A	395	TYR	2.0
1	C	384	GLY	2.0
1	C	398	GLY	2.0
1	H	457	GLY	2.0
1	A	402	ASN	2.0
1	B	459	VAL	2.0
1	C	386	PRO	2.0
1	G	459	VAL	2.0
1	C	178	GLU	2.0
1	E	392	SER	2.0
1	D	418	GLN	2.0
1	F	381	THR	2.0
1	G	132	GLN	2.0
1	A	340	PRO	2.0
1	C	346	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SHG	C	804	12/12	0.87	0.12	29,37,41,41	0

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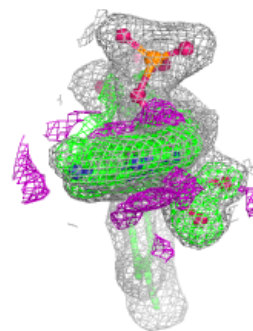
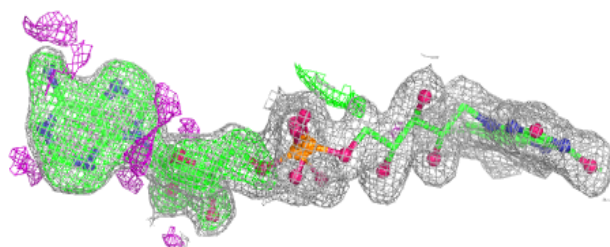
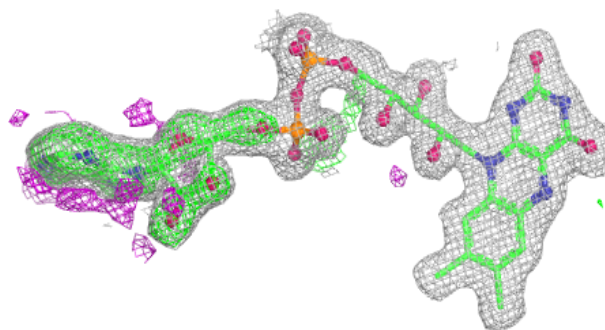
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SHG	G	808	12/12	0.88	0.12	27,35,39,42	0
2	SHG	D	803	12/12	0.90	0.11	30,35,40,41	0
2	SHG	E	805	12/12	0.91	0.09	31,37,40,41	0
2	SHG	A	801	12/12	0.91	0.10	24,35,41,44	0
2	SHG	H	807	12/12	0.92	0.09	28,35,38,41	0
2	SHG	F	806	12/12	0.92	0.10	31,34,40,42	0
3	FAD	C	704	53/53	0.93	0.20	16,23,113,114	0
3	FAD	A	701	53/53	0.94	0.18	12,18,94,95	0
3	FAD	D	703	53/53	0.94	0.19	16,20,105,106	0
2	SHG	B	802	12/12	0.94	0.08	24,29,35,39	0
3	FAD	E	705	53/53	0.94	0.19	15,21,119,120	0
3	FAD	F	706	53/53	0.94	0.20	16,21,115,116	0
3	FAD	H	707	53/53	0.94	0.20	15,21,119,120	0
3	FAD	G	708	53/53	0.94	0.18	16,21,101,103	0
3	FAD	B	702	53/53	0.95	0.19	14,19,107,107	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.

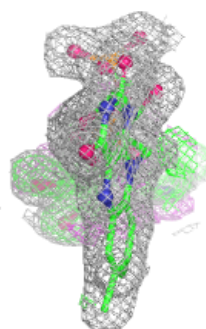
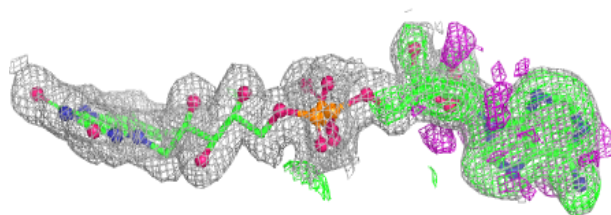
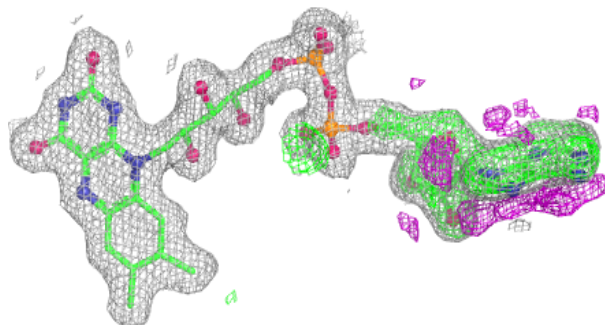
Electron density around FAD C 704:

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

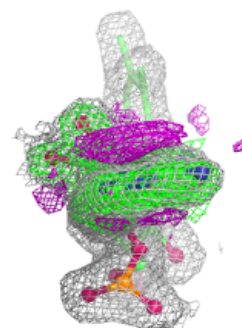
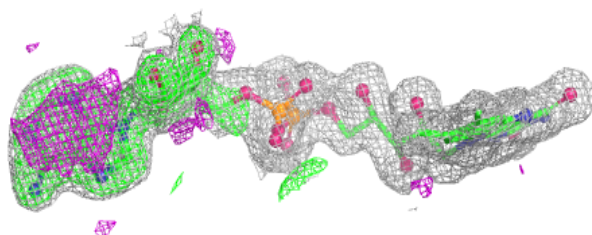
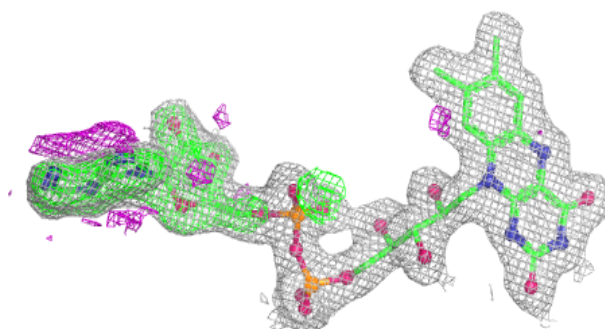


Electron density around FAD A 701:

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

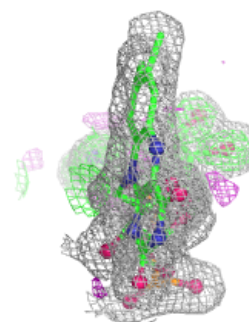
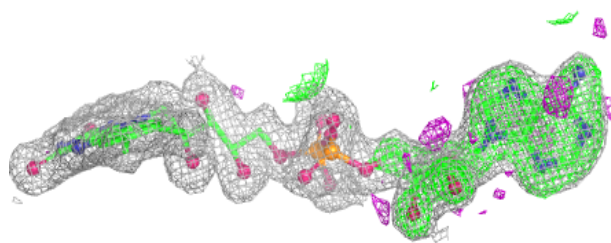
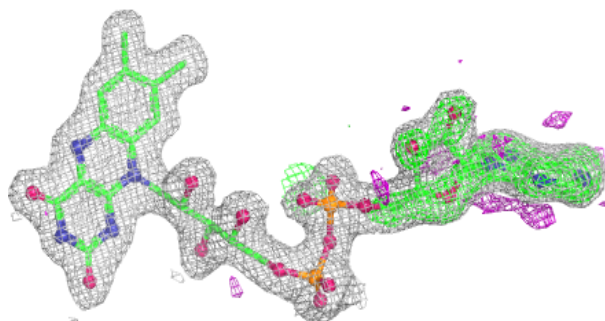
**Electron density around FAD D 703:**

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

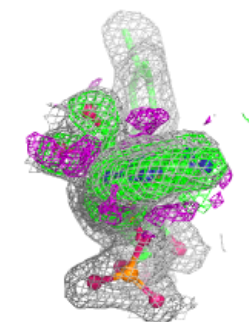
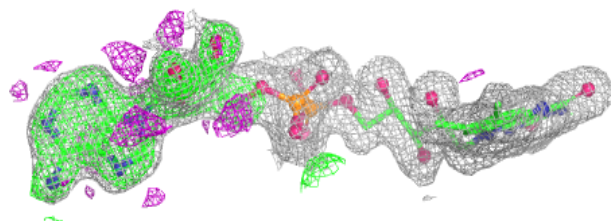
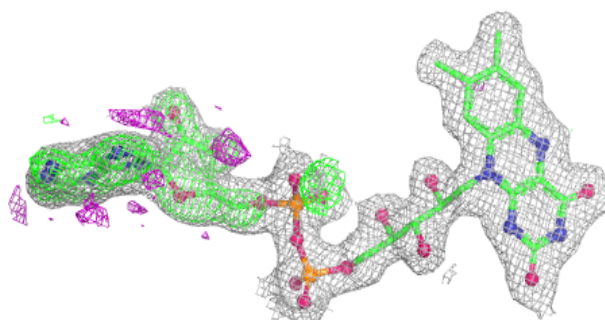


Electron density around FAD E 705:

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

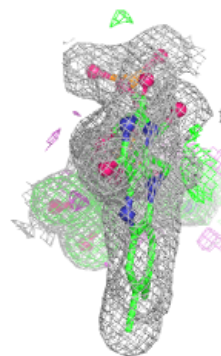
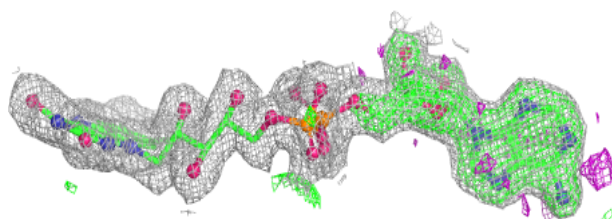
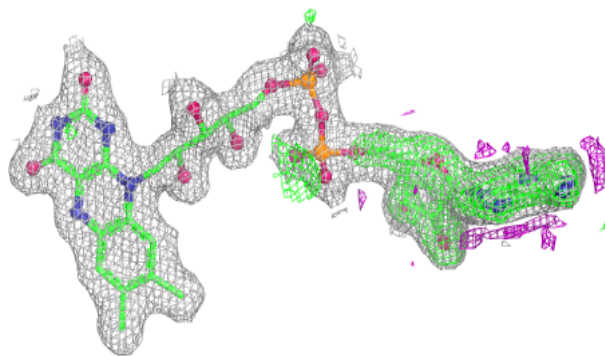
**Electron density around FAD F 706:**

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

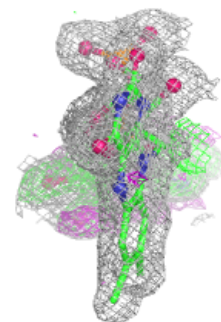
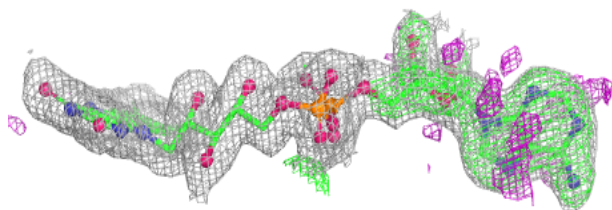
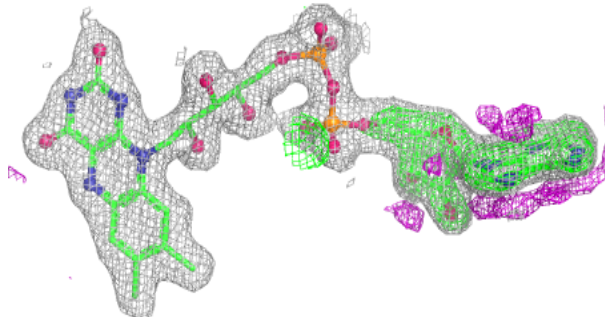


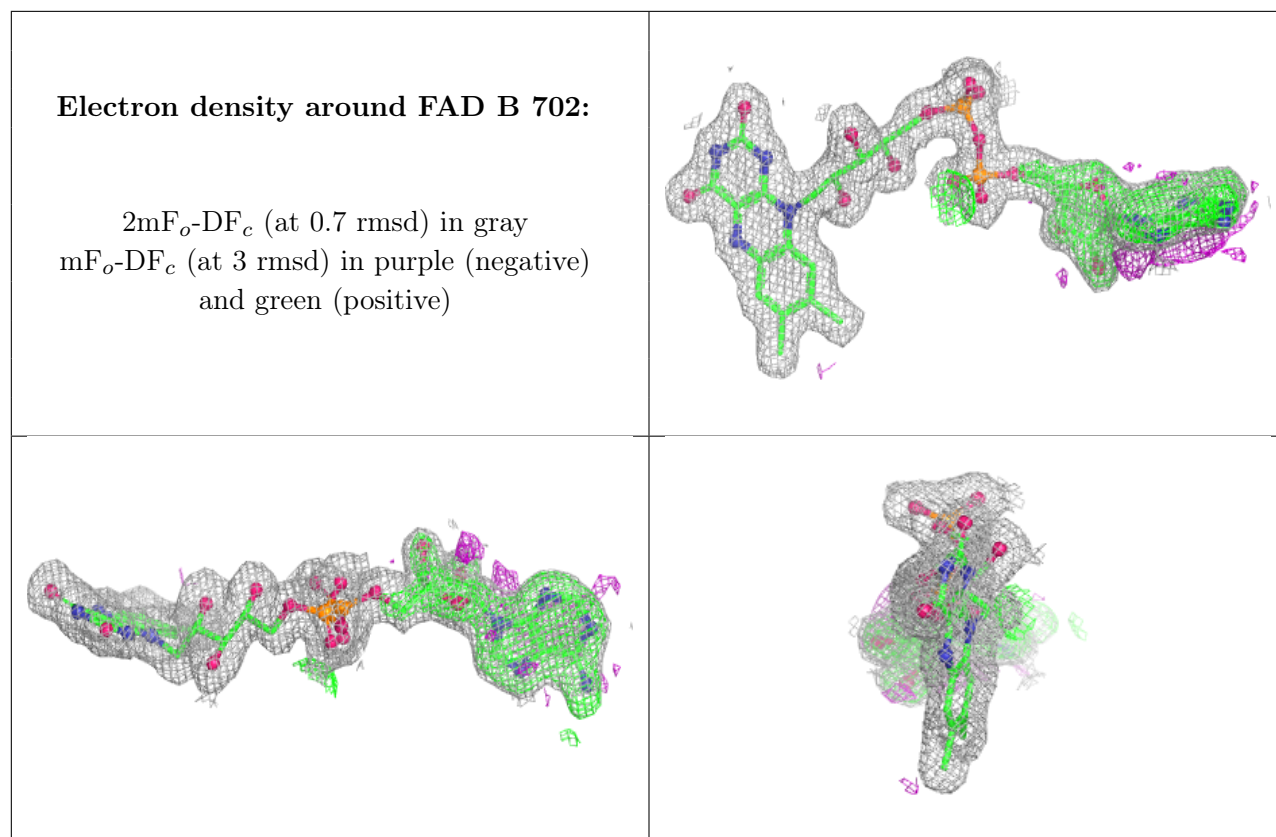
Electron density around FAD H 707:

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

**Electron density around FAD 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.