



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:35 PM UTC

PDB ID : 3LSH / pdb_00003lsh
Title : Pyranose 2-oxidase T169A, monoclinic
Authors : Divne, C.; Tan, T.C.; Spadiut, O.
Deposited on : 2010-02-12
Resolution : 1.90 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

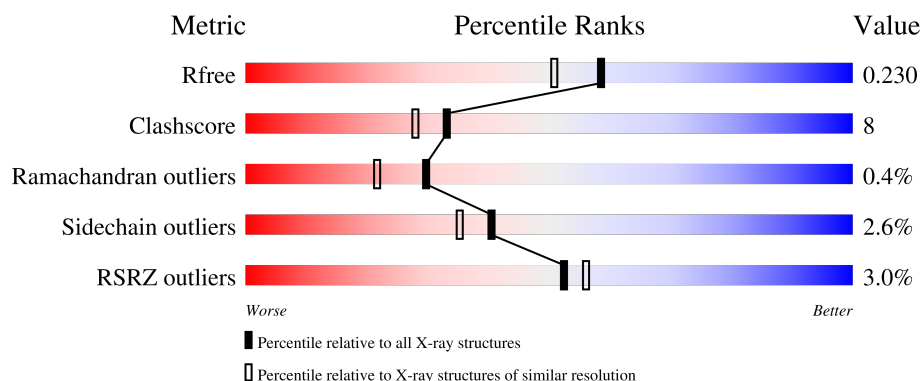
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

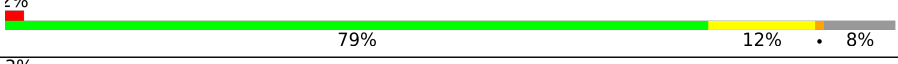
The reported resolution of this entry is 1.90 Å.

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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	
1	B	623	
1	C	623	
1	D	623	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20177 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

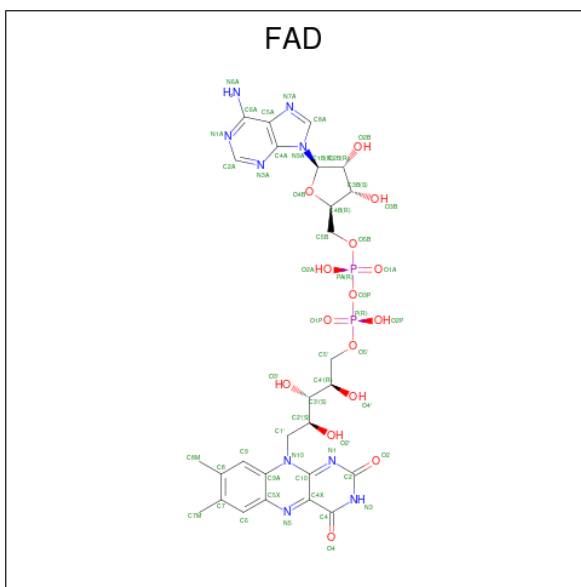
- Molecule 1 is a protein called Pyranose 2-oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	576	Total	C	N	O	S	0	0	0
			4540	2867	777	871	25			
1	B	576	Total	C	N	O	S	0	0	0
			4540	2867	777	871	25			
1	C	575	Total	C	N	O	S	0	0	0
			4531	2862	776	869	24			
1	D	574	Total	C	N	O	S	0	0	0
			4524	2858	775	867	24			

There are 4 discrepancies between the modelled and reference sequences:

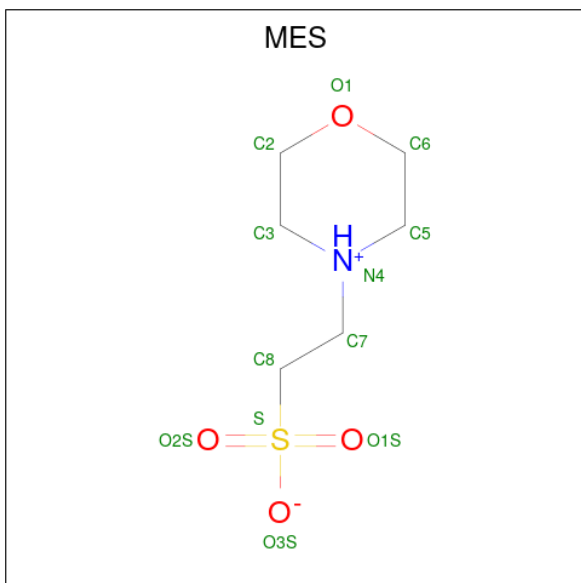
Chain	Residue	Modelled	Actual	Comment	Reference
A	169	ALA	THR	engineered mutation	UNP Q7ZA32
B	169	ALA	THR	engineered mutation	UNP Q7ZA32
C	169	ALA	THR	engineered mutation	UNP Q7ZA32
D	169	ALA	THR	engineered mutation	UNP Q7ZA32

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



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

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $\text{C}_6\text{H}_{13}\text{NO}_4\text{S}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

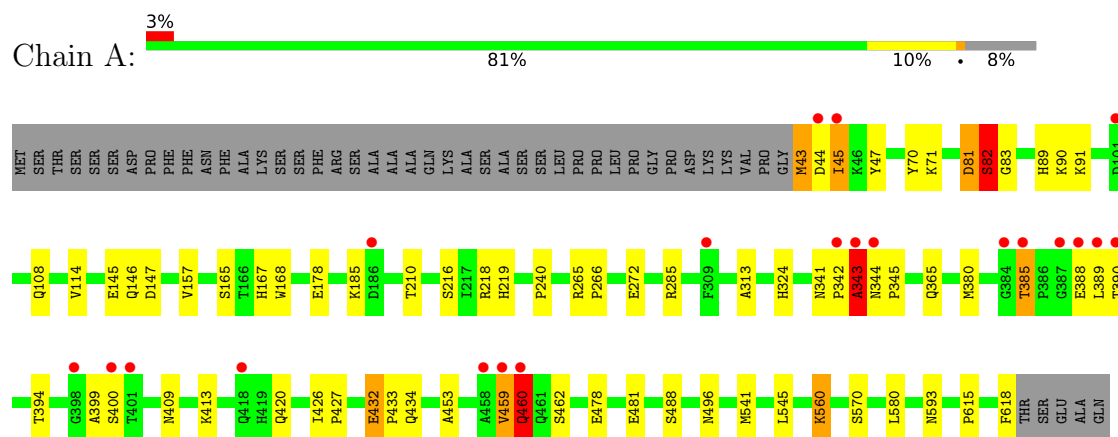
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	450	Total	O	0	0
			450	450		
4	B	554	Total	O	0	0
			554	554		
4	C	472	Total	O	0	0
			472	472		
4	D	342	Total	O	0	0
			342	342		

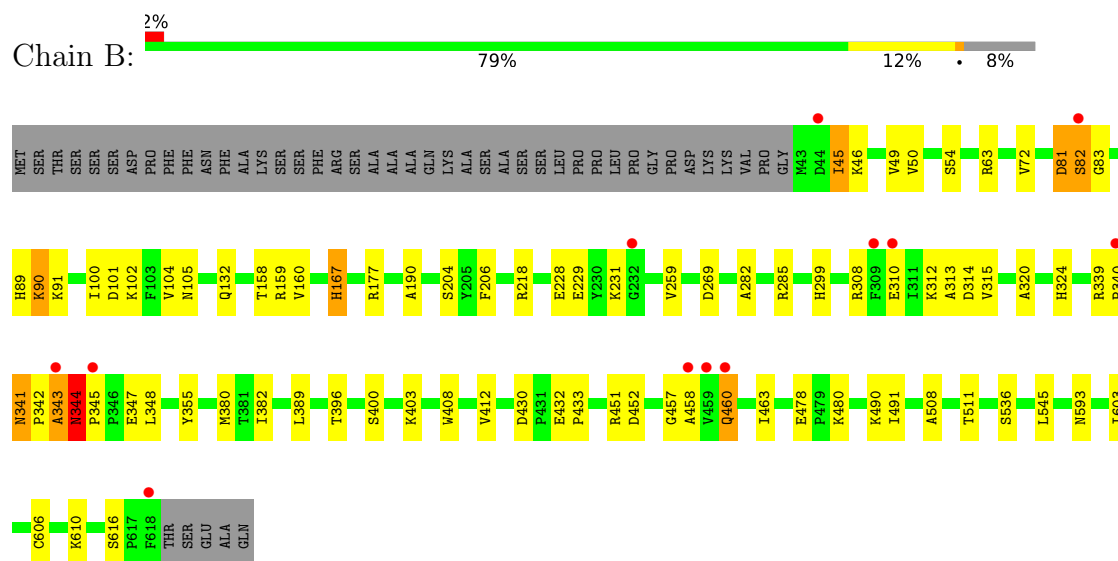
3 Residue-property plots [i](#)

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

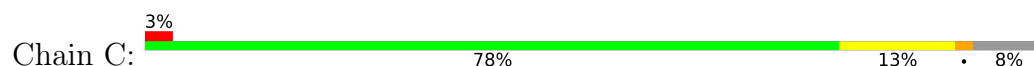
- Molecule 1: Pyranose 2-oxidase

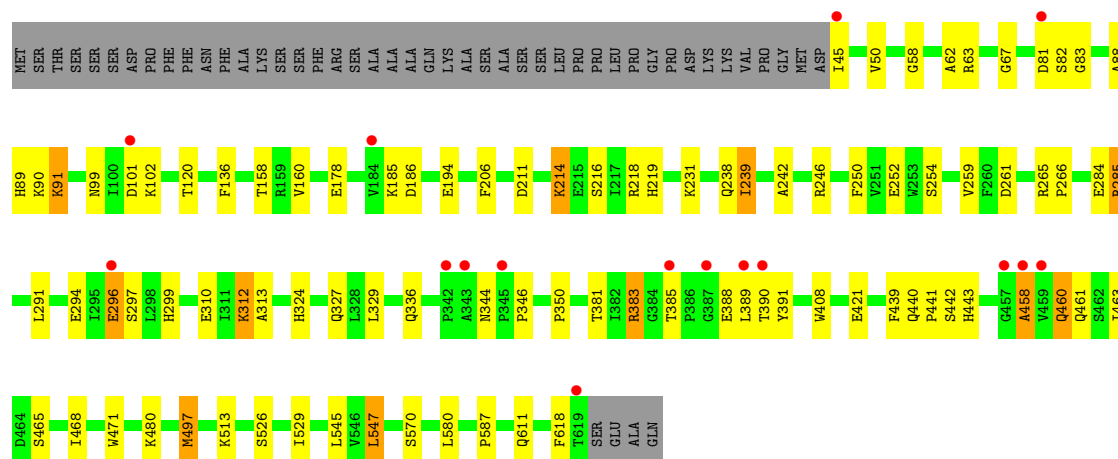


- Molecule 1: Pyranose 2-oxidase

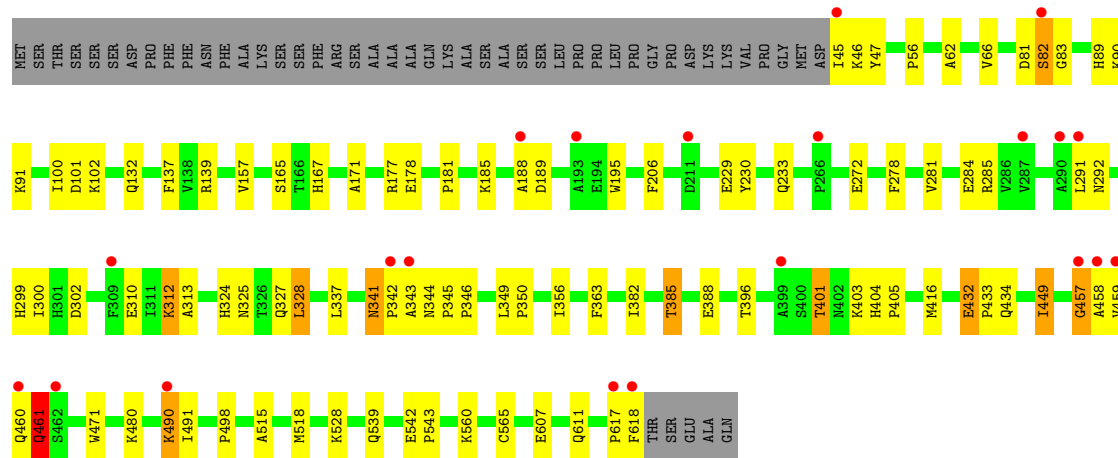
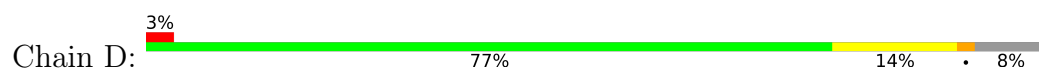


- Molecule 1: Pyranose 2-oxidase





• Molecule 1: Pyranose 2-oxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	100.40Å 102.73Å 137.82Å 90.00° 91.02° 90.00°	Depositor
Resolution (Å)	28.50 – 1.90 28.50 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.8 (28.50-1.90) 98.8 (28.50-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.35 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.195 , 0.246 (Not available) , 0.230	Depositor DCC
R_{free} test set	3217 reflections (1.46%)	wwPDB-VP
Wilson B-factor (Å ²)	21.2	Xtriage
Anisotropy	0.405	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.011 for -k,-h,-l 0.008 for k,h,-l 0.015 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20177	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MES, 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	1.30	5/4656 (0.1%)	1.18	15/6330 (0.2%)
1	B	1.41	15/4656 (0.3%)	1.21	13/6330 (0.2%)
1	C	1.26	8/4647 (0.2%)	1.15	7/6319 (0.1%)
1	D	1.13	3/4640 (0.1%)	1.16	14/6309 (0.2%)
All	All	1.28	31/18599 (0.2%)	1.18	49/25288 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	D	0	1
All	All	0	3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	81	ASP	CA-C	10.78	1.61	1.52
1	B	282	ALA	CA-CB	-9.10	1.41	1.53
1	B	82	SER	N-CA	8.49	1.57	1.46
1	A	81	ASP	CA-C	7.28	1.58	1.52
1	A	453	ALA	CA-CB	-7.17	1.43	1.53
1	D	449	ILE	CA-C	-7.04	1.47	1.53
1	C	62	ALA	C-O	6.90	1.32	1.24
1	C	88	ALA	CA-CB	6.32	1.63	1.53
1	B	603	ILE	CA-C	6.16	1.60	1.52
1	B	72	VAL	CA-CB	-6.02	1.47	1.54
1	B	72	VAL	N-CA	5.92	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	114	VAL	CA-CB	5.88	1.62	1.54
1	D	539	GLN	C-O	-5.85	1.16	1.23
1	B	46	LYS	N-CA	5.84	1.53	1.46
1	C	587	PRO	N-CA	-5.72	1.42	1.47
1	C	296	GLU	CG-CD	5.61	1.66	1.52
1	B	491	ILE	CA-CB	5.57	1.61	1.54
1	B	54	SER	C-O	5.56	1.31	1.23
1	B	320	ALA	CA-CB	-5.53	1.44	1.53
1	B	90	LYS	CA-C	-5.51	1.45	1.52
1	C	529	ILE	CA-CB	-5.41	1.48	1.54
1	C	250	PHE	CA-C	5.37	1.58	1.52
1	B	190	ALA	CA-CB	-5.27	1.45	1.53
1	B	536	SER	C-O	-5.19	1.18	1.23
1	B	177	ARG	C-O	-5.14	1.18	1.24
1	D	171	ALA	CA-CB	-5.05	1.45	1.53
1	A	460	GLN	CA-C	-5.04	1.46	1.53
1	C	329	LEU	CA-C	5.04	1.59	1.52
1	B	229	GLU	C-O	-5.03	1.17	1.24
1	A	82	SER	N-CA	5.02	1.52	1.46
1	C	312	LYS	CA-C	5.01	1.58	1.52

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	344	ASN	CA-C-N	10.52	131.21	120.38
1	B	344	ASN	C-N-CA	10.52	131.21	120.38
1	D	396	THR	CA-C-N	-9.20	110.93	120.03
1	D	396	THR	C-N-CA	-9.20	110.93	120.03
1	D	278	PHE	CA-C-N	-7.77	112.83	120.52
1	D	278	PHE	C-N-CA	-7.77	112.83	120.52
1	D	404	HIS	CA-C-N	-7.57	113.03	120.52
1	D	404	HIS	C-N-CA	-7.57	113.03	120.52
1	B	81	ASP	CB-CA-C	7.51	123.80	112.31
1	A	345	PRO	CA-C-N	-7.45	112.66	120.03
1	A	345	PRO	C-N-CA	-7.45	112.66	120.03
1	A	82	SER	N-CA-C	7.28	126.31	110.80
1	B	508	ALA	N-CA-C	-7.27	101.46	110.41
1	B	82	SER	N-CA-C	7.13	125.98	110.80
1	A	147	ASP	CA-C-N	-7.12	112.35	120.04
1	A	147	ASP	C-N-CA	-7.12	112.35	120.04
1	D	457	GLY	N-CA-C	-6.87	102.97	112.18
1	A	82	SER	CB-CA-C	-6.60	97.29	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	616	SER	CA-C-N	-6.50	112.97	119.99
1	B	616	SER	C-N-CA	-6.50	112.97	119.99
1	A	343	ALA	CA-C-N	-6.31	116.50	122.37
1	A	343	ALA	C-N-CA	-6.31	116.50	122.37
1	D	461	GLN	N-CA-C	-6.19	104.11	113.89
1	A	478	GLU	CA-C-N	-6.18	113.15	120.13
1	A	478	GLU	C-N-CA	-6.18	113.15	120.13
1	D	396	THR	CB-CA-C	-6.11	104.10	110.33
1	D	82	SER	N-CA-C	5.98	123.55	110.80
1	A	82	SER	CA-CB-OG	5.90	122.90	111.10
1	B	324	HIS	N-CA-C	5.89	119.73	112.54
1	D	341	ASN	CA-C-N	5.82	125.30	119.24
1	D	341	ASN	C-N-CA	5.82	125.30	119.24
1	C	297	SER	N-CA-C	5.53	116.54	108.14
1	A	81	ASP	CB-CA-C	5.48	120.69	112.31
1	D	82	SER	CB-CA-C	-5.47	99.53	110.42
1	C	547	LEU	CB-CA-C	-5.45	104.16	111.89
1	A	146	GLN	N-CA-C	5.43	117.56	109.25
1	B	396	THR	CA-C-N	-5.37	114.03	119.83
1	B	396	THR	C-N-CA	-5.37	114.03	119.83
1	C	239	ILE	N-CA-C	-5.36	103.70	108.95
1	C	67	GLY	N-CA-C	-5.34	107.16	113.99
1	A	459	VAL	CA-C-N	-5.32	113.66	122.39
1	A	459	VAL	C-N-CA	-5.32	113.66	122.39
1	B	167	HIS	N-CA-C	5.28	121.53	113.19
1	C	58	GLY	N-CA-C	-5.24	106.44	112.73
1	B	45	ILE	CB-CA-C	5.24	117.69	111.20
1	B	204	SER	N-CA-CB	5.22	117.79	110.12
1	D	325	ASN	N-CA-C	-5.22	105.51	111.14
1	C	497	MET	CA-C-N	5.06	125.35	119.93
1	C	497	MET	C-N-CA	5.06	125.35	119.93

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	460	GLN	Peptide
1	C	458	ALA	Peptide
1	D	458	ALA	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4540	0	4386	71	0
1	B	4540	0	4386	58	0
1	C	4531	0	4380	71	0
1	D	4524	0	4373	83	0
2	A	53	0	30	2	0
2	B	53	0	29	2	0
2	C	53	0	29	2	0
2	D	53	0	28	4	0
3	C	12	0	12	1	0
4	A	450	0	0	15	0
4	B	554	0	0	12	0
4	C	472	0	0	18	0
4	D	342	0	0	14	0
All	All	20177	0	17653	282	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (282) 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:C:383:ARG:HB3	1:C:383:ARG:NH1	1.29	1.41
1:C:383:ARG:HH11	1:C:383:ARG:CB	1.45	1.28
1:C:285:ARG:HD3	4:C:2746:HOH:O	1.30	1.23
1:B:458:ALA:HB2	4:B:2756:HOH:O	1.33	1.22
1:C:383:ARG:NH1	1:C:383:ARG:CB	2.03	1.16
1:C:299:HIS:CE1	1:C:310:GLU:HG2	1.84	1.13
1:B:460:GLN:HB3	4:B:2630:HOH:O	1.54	1.07
1:D:299:HIS:NE2	1:D:310:GLU:CG	2.21	1.03
1:D:285:ARG:HA	1:D:328:LEU:CD1	1.88	1.03
1:B:343:ALA:O	1:B:344:ASN:ND2	1.91	1.02
1:B:101:ASP:O	1:B:104:VAL:HG12	1.60	0.97
1:D:299:HIS:CD2	1:D:310:GLU:CG	2.52	0.93
1:D:299:HIS:CD2	1:D:310:GLU:HG2	2.04	0.93
1:D:299:HIS:NE2	1:D:310:GLU:HG3	1.88	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:560:LYS:NZ	1:A:560:LYS:HB3	1.89	0.87
1:B:308:ARG:HG3	1:B:308:ARG:HH11	1.38	0.87
1:D:299:HIS:HE2	1:D:310:GLU:CD	1.85	0.84
1:D:457:GLY:HA2	4:D:2302:HOH:O	1.78	0.84
1:C:285:ARG:HH12	1:C:299:HIS:HD2	1.21	0.84
1:D:285:ARG:HA	1:D:328:LEU:HD11	1.59	0.82
1:A:459:VAL:HG12	1:A:460:GLN:N	1.94	0.82
1:B:132:GLN:HG2	4:B:2633:HOH:O	1.78	0.82
1:C:211:ASP:O	1:C:214:LYS:HD3	1.80	0.82
1:D:299:HIS:CD2	1:D:310:GLU:HG3	2.15	0.81
1:A:459:VAL:O	1:A:460:GLN:HG2	1.82	0.79
1:A:560:LYS:HB3	1:A:560:LYS:HZ2	1.45	0.79
1:C:385:THR:HG23	1:C:388:GLU:OE2	1.82	0.78
1:D:299:HIS:HE2	1:D:310:GLU:CG	1.92	0.78
1:A:344:ASN:C	1:A:344:ASN:HD22	1.92	0.77
1:B:308:ARG:HG3	1:B:308:ARG:NH1	2.00	0.77
1:A:459:VAL:CG1	1:A:460:GLN:N	2.48	0.76
1:C:285:ARG:HH12	1:C:299:HIS:CD2	2.03	0.76
1:D:461:GLN:HG3	4:D:2627:HOH:O	1.87	0.74
1:C:299:HIS:HE1	1:C:310:GLU:HG2	1.53	0.73
1:C:443:HIS:HB3	4:C:2237:HOH:O	1.89	0.73
1:A:560:LYS:NZ	1:A:560:LYS:CB	2.52	0.71
1:C:299:HIS:CE1	1:C:310:GLU:CG	2.70	0.71
1:D:490:LYS:HE3	1:D:491:ILE:CD1	2.21	0.71
1:A:365:GLN:HE22	1:A:459:VAL:CG2	2.03	0.70
1:B:342:PRO:O	1:B:344:ASN:N	2.21	0.70
1:D:457:GLY:CA	4:D:2302:HOH:O	2.35	0.70
1:A:618:PHE:HD1	1:A:618:PHE:C	2.00	0.70
1:B:341:ASN:C	1:B:341:ASN:HD22	2.00	0.70
1:A:343:ALA:C	4:A:2620:HOH:O	2.36	0.69
1:D:490:LYS:HE3	1:D:491:ILE:HD13	1.75	0.69
1:A:459:VAL:CG1	1:A:460:GLN:H	2.05	0.69
1:A:481:GLU:HG2	4:A:2559:HOH:O	1.92	0.68
1:C:460:GLN:O	1:C:460:GLN:HG3	1.93	0.68
1:C:285:ARG:NH1	1:C:299:HIS:HD2	1.91	0.67
1:D:285:ARG:NE	4:D:2772:HOH:O	2.25	0.67
1:B:132:GLN:CG	4:B:2633:HOH:O	2.40	0.67
1:C:185:LYS:NZ	4:C:2610:HOH:O	2.27	0.67
1:A:45:ILE:N	1:A:45:ILE:HD12	2.10	0.66
1:B:310:GLU:OE1	1:B:312:LYS:NZ	2.28	0.66
1:A:157:VAL:HG21	1:A:324:HIS:HE1	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:HIS:CG	4:C:2768:HOH:O	2.47	0.65
1:B:452:ASP:HA	4:B:2765:HOH:O	1.97	0.65
1:A:167:HIS:CD2	2:A:801:FAD:HM82	2.31	0.65
1:A:541:MET:HE1	4:A:2585:HOH:O	1.96	0.65
1:A:618:PHE:C	1:A:618:PHE:CD1	2.73	0.65
1:A:344:ASN:C	1:A:344:ASN:ND2	2.53	0.64
1:D:349:LEU:HD22	1:D:565:CYS:HA	1.80	0.64
1:A:481:GLU:CG	4:A:2559:HOH:O	2.44	0.63
1:C:383:ARG:CB	1:C:383:ARG:CZ	2.73	0.63
1:C:383:ARG:NH1	1:C:383:ARG:HB2	2.07	0.63
1:A:342:PRO:C	1:A:344:ASN:H	2.07	0.62
1:D:299:HIS:NE2	1:D:310:GLU:CD	2.55	0.62
1:B:460:GLN:OE1	1:B:463:ILE:N	2.23	0.62
1:A:185:LYS:HD2	4:A:2187:HOH:O	1.99	0.62
1:B:308:ARG:NH1	4:B:2448:HOH:O	2.33	0.62
1:A:432:GLU:H	1:A:432:GLU:CD	2.06	0.61
1:D:81:ASP:O	1:D:83:GLY:N	2.32	0.61
1:B:389:LEU:HG	4:B:2647:HOH:O	2.00	0.61
1:C:383:ARG:O	1:C:391:TYR:HA	2.01	0.61
1:D:81:ASP:OD2	1:D:90:LYS:NZ	2.24	0.60
1:A:560:LYS:HZ2	1:A:560:LYS:CB	2.13	0.60
1:B:457:GLY:HA2	4:B:2433:HOH:O	2.01	0.60
1:A:459:VAL:C	1:A:460:GLN:CG	2.75	0.60
1:D:299:HIS:NE2	1:D:310:GLU:HG2	2.07	0.60
1:D:449:ILE:HG12	1:D:471:TRP:CZ3	2.37	0.60
1:C:442:SER:C	4:C:2237:HOH:O	2.45	0.59
1:C:285:ARG:NH1	1:C:299:HIS:CD2	2.67	0.59
1:D:432:GLU:CB	1:D:433:PRO:HD2	2.33	0.59
1:A:394:THR:HA	1:A:413:LYS:HD2	1.85	0.58
1:B:478:GLU:HG3	1:B:511:THR:OG1	2.03	0.58
1:D:382:ILE:CD1	4:D:2488:HOH:O	2.51	0.58
1:C:461:GLN:HE21	1:C:461:GLN:HA	1.68	0.58
1:A:481:GLU:CD	4:A:2559:HOH:O	2.47	0.57
1:B:101:ASP:O	1:B:104:VAL:CG1	2.44	0.57
1:D:291:LEU:O	1:D:292:ASN:HB2	2.04	0.57
1:D:432:GLU:HB2	1:D:433:PRO:HD2	1.86	0.57
1:B:81:ASP:OD1	1:B:81:ASP:N	2.34	0.57
1:B:308:ARG:NH1	1:B:308:ARG:CG	2.65	0.56
1:C:299:HIS:ND1	1:C:310:GLU:HG2	2.18	0.56
1:D:132:GLN:CG	4:D:2213:HOH:O	2.53	0.56
1:A:70:TYR:CZ	1:A:615:PRO:HD3	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:363:PHE:HA	1:D:471:TRP:O	2.06	0.56
1:B:343:ALA:O	1:B:344:ASN:CG	2.49	0.56
1:B:342:PRO:C	1:B:344:ASN:H	2.11	0.56
1:A:89:HIS:CE1	1:A:91:LYS:HB2	2.40	0.55
1:A:218:ARG:HD2	4:A:1614:HOH:O	2.05	0.55
1:A:45:ILE:HG22	1:A:45:ILE:O	2.05	0.55
1:A:342:PRO:C	1:A:344:ASN:N	2.65	0.55
1:D:302:ASP:OD1	1:D:302:ASP:C	2.49	0.55
1:B:308:ARG:HH11	1:B:308:ARG:CG	2.06	0.54
1:C:246:ARG:NH2	1:C:252:GLU:OE1	2.31	0.54
1:C:547:LEU:CD1	2:C:801:FAD:HM83	2.37	0.54
1:A:216:SER:HB3	1:A:219:HIS:HB3	1.88	0.54
1:A:178:GLU:O	1:A:178:GLU:HG3	2.07	0.54
1:A:341:ASN:HD21	1:A:343:ALA:HB3	1.73	0.54
1:B:89:HIS:CE1	1:B:91:LYS:HE3	2.43	0.54
1:D:382:ILE:HD11	1:D:416:MET:HE1	1.89	0.54
1:C:296:GLU:OE1	1:C:312:LYS:NZ	2.41	0.54
1:B:343:ALA:C	1:B:344:ASN:HD22	2.16	0.54
1:B:339:ARG:O	1:B:340:PRO:C	2.50	0.53
1:D:284:GLU:O	1:D:285:ARG:HB3	2.08	0.53
1:C:383:ARG:HB3	1:C:383:ARG:HH11	0.53	0.53
1:C:216:SER:HB3	1:C:219:HIS:HB3	1.90	0.53
1:C:294:GLU:HB2	4:C:2800:HOH:O	2.08	0.53
1:C:421:GLU:OE1	1:C:421:GLU:N	2.37	0.53
1:A:185:LYS:CE	4:A:2160:HOH:O	2.55	0.53
1:D:480:LYS:HD2	4:D:2568:HOH:O	2.07	0.53
1:D:346:PRO:HG2	1:D:350:PRO:HA	1.89	0.53
1:A:81:ASP:OD2	1:A:90:LYS:NZ	2.42	0.53
1:B:91:LYS:HD3	1:B:100:ILE:HD11	1.91	0.53
1:A:45:ILE:HD12	1:A:45:ILE:H	1.74	0.52
1:C:460:GLN:OE1	1:C:463:ILE:N	2.28	0.52
1:C:284:GLU:C	1:C:285:ARG:HG2	2.33	0.52
1:A:185:LYS:CD	4:A:2187:HOH:O	2.56	0.52
1:D:56:PRO:HG3	1:D:165:SER:HB3	1.92	0.51
1:D:285:ARG:HA	1:D:328:LEU:HD12	1.85	0.51
1:A:459:VAL:O	1:A:460:GLN:CG	2.57	0.51
1:D:607:GLU:O	1:D:611:GLN:HG3	2.10	0.51
1:D:47:TYR:O	1:D:313:ALA:HA	2.11	0.51
1:D:167:HIS:CD2	2:D:801:FAD:HM82	2.44	0.51
1:D:167:HIS:HD2	2:D:801:FAD:HM82	1.74	0.51
1:D:449:ILE:HG12	1:D:471:TRP:CE3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:SER:HB2	4:A:2548:HOH:O	2.11	0.51
1:D:137:PHE:CE2	1:D:139:ARG:HG3	2.46	0.51
1:D:490:LYS:HE3	1:D:491:ILE:HD11	1.92	0.51
1:D:89:HIS:CE1	1:D:91:LYS:HB2	2.47	0.51
1:D:233:GLN:CD	4:D:2754:HOH:O	2.53	0.51
1:C:458:ALA:HB3	4:C:2203:HOH:O	2.11	0.50
1:C:265:ARG:HB3	1:C:266:PRO:HA	1.93	0.50
1:A:81:ASP:O	1:A:83:GLY:N	2.43	0.50
1:A:385:THR:HG23	1:A:388:GLU:HB3	1.92	0.50
1:B:347:GLU:HB3	1:B:348:LEU:HG	1.93	0.50
1:D:617:PRO:O	1:D:618:PHE:C	2.55	0.50
1:D:401:THR:O	1:D:401:THR:HG23	2.10	0.49
1:A:365:GLN:HE22	1:A:459:VAL:HG22	1.75	0.49
1:D:81:ASP:OD1	1:D:81:ASP:N	2.43	0.49
1:C:385:THR:CG2	1:C:388:GLU:OE2	2.55	0.49
1:D:230:TYR:CZ	1:D:528:LYS:HE3	2.48	0.48
1:A:459:VAL:C	1:A:460:GLN:HG2	2.38	0.48
1:C:513:LYS:NZ	4:C:2361:HOH:O	2.45	0.48
1:B:432:GLU:HB2	1:B:433:PRO:HD2	1.96	0.48
1:B:89:HIS:CE1	1:B:91:LYS:HB3	2.48	0.48
1:A:459:VAL:HG13	1:A:460:GLN:H	1.79	0.48
1:D:344:ASN:O	1:D:345:PRO:C	2.54	0.48
1:C:291:LEU:HA	4:C:2749:HOH:O	2.14	0.48
1:A:432:GLU:CD	1:A:432:GLU:N	2.72	0.48
1:C:618:PHE:CD1	1:C:618:PHE:C	2.92	0.48
1:D:132:GLN:HG2	4:D:2213:HOH:O	2.14	0.48
1:C:443:HIS:CB	4:C:2237:HOH:O	2.56	0.47
1:C:50:VAL:HG13	1:C:313:ALA:HB2	1.96	0.47
1:A:560:LYS:HB3	1:A:560:LYS:HZ3	1.72	0.47
1:A:89:HIS:ND1	1:A:91:LYS:HB2	2.30	0.47
1:B:355:TYR:HA	1:B:480:LYS:O	2.15	0.47
1:B:460:GLN:CB	4:B:2630:HOH:O	2.34	0.47
1:D:157:VAL:HG21	1:D:324:HIS:HE1	1.80	0.47
1:D:385:THR:OG1	1:D:388:GLU:CD	2.58	0.47
1:B:50:VAL:HG13	1:B:313:ALA:HB2	1.97	0.47
1:B:606:CYS:O	1:B:610:LYS:HG3	2.15	0.47
1:C:471:TRP:CH2	1:C:526:SER:HA	2.50	0.46
1:D:324:HIS:HD2	1:D:327:GLN:OE1	1.98	0.46
1:A:570:SER:HB3	1:A:580:LEU:O	2.15	0.46
1:B:63:ARG:HD2	1:B:259:VAL:O	2.16	0.46
1:D:337:LEU:HD21	4:D:2566:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:THR:HG22	1:B:160:VAL:HG22	1.97	0.46
1:C:89:HIS:CE1	1:C:91:LYS:HE2	2.51	0.46
1:C:390:THR:HB	4:C:2802:HOH:O	2.15	0.46
3:C:903:MES:H82	3:C:903:MES:H51	1.63	0.46
1:D:341:ASN:C	1:D:341:ASN:ND2	2.73	0.45
1:D:341:ASN:HD22	1:D:342:PRO:HD2	1.80	0.45
1:D:432:GLU:CB	1:D:433:PRO:CD	2.94	0.45
1:D:177:ARG:HG3	4:D:2751:HOH:O	2.15	0.45
1:B:89:HIS:ND1	1:B:91:LYS:HB3	2.32	0.45
1:C:618:PHE:C	1:C:618:PHE:HD1	2.25	0.45
1:B:104:VAL:HG13	1:B:105:ASN:N	2.31	0.45
1:B:167:HIS:CD2	2:B:801:FAD:HM82	2.51	0.45
1:C:120:THR:HA	1:C:136:PHE:CD1	2.51	0.45
1:A:108:GLN:HG2	4:A:2267:HOH:O	2.16	0.45
1:C:465:SER:HA	1:C:468:ILE:HD12	1.98	0.45
1:D:405:PRO:HG3	4:D:2742:HOH:O	2.16	0.45
1:A:388:GLU:O	1:A:390:THR:N	2.50	0.45
1:B:432:GLU:HB2	1:B:451:ARG:HB2	1.99	0.45
1:D:328:LEU:HD12	1:D:328:LEU:O	2.17	0.45
1:A:593:ASN:HB3	2:A:801:FAD:C2	2.48	0.44
1:A:47:TYR:O	1:A:313:ALA:HA	2.17	0.44
1:C:324:HIS:HD2	1:C:327:GLN:OE1	2.00	0.44
1:C:346:PRO:HG2	1:C:350:PRO:HA	1.99	0.44
1:C:440:GLN:O	1:C:441:PRO:C	2.60	0.44
1:D:342:PRO:C	1:D:344:ASN:H	2.25	0.44
1:A:380:MET:HE1	1:A:409:ASN:HB3	1.99	0.44
1:A:399:ALA:O	1:A:400:SER:C	2.58	0.44
1:B:342:PRO:C	1:B:344:ASN:N	2.68	0.44
1:D:285:ARG:CA	1:D:328:LEU:HD11	2.39	0.44
1:A:44:ASP:OD2	1:A:71:LYS:NZ	2.45	0.44
1:B:218:ARG:HG3	1:B:430:ASP:OD2	2.17	0.44
1:A:83:GLY:N	1:B:81:ASP:O	2.51	0.43
1:D:515:ALA:O	1:D:518:MET:HB3	2.17	0.43
1:C:99:ASN:HB3	1:C:102:LYS:HG2	2.00	0.43
1:C:81:ASP:O	1:D:81:ASP:O	2.37	0.43
1:A:185:LYS:HE2	4:A:2160:HOH:O	2.15	0.43
1:C:381:THR:HG23	4:C:2341:HOH:O	2.18	0.43
1:B:380:MET:HE3	1:B:412:VAL:HB	2.00	0.43
1:B:408:TRP:CD1	1:B:408:TRP:C	2.96	0.43
1:C:158:THR:HG22	1:C:160:VAL:HG22	2.00	0.43
1:D:542:GLU:HA	1:D:543:PRO:HD3	1.89	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:439:PHE:C	1:C:439:PHE:CD1	2.96	0.43
1:B:285:ARG:NH1	1:B:299:HIS:ND1	2.67	0.43
1:B:102:LYS:HA	1:B:102:LYS:HD2	1.78	0.43
1:C:81:ASP:OD2	1:C:90:LYS:NZ	2.51	0.43
1:C:497:MET:HG3	4:C:2391:HOH:O	2.17	0.43
1:D:188:ALA:O	1:D:189:ASP:C	2.61	0.43
1:C:461:GLN:HA	1:C:461:GLN:NE2	2.34	0.43
1:B:81:ASP:O	1:B:83:GLY:N	2.49	0.43
1:C:480:LYS:HD3	1:C:480:LYS:HA	1.74	0.43
1:A:433:PRO:C	1:A:434:GLN:HG2	2.43	0.42
1:C:238:GLN:HG2	1:C:239:ILE:N	2.34	0.42
1:D:299:HIS:HD2	1:D:310:GLU:HG2	1.76	0.42
1:D:101:ASP:HB3	1:D:459:VAL:HG12	2.01	0.42
1:A:145:GLU:HG3	1:A:488:SER:HB2	2.00	0.42
1:D:498:PRO:HA	4:D:2161:HOH:O	2.18	0.42
1:B:159:ARG:HA	2:B:801:FAD:O2B	2.19	0.42
1:D:229:GLU:OE2	4:D:2649:HOH:O	2.20	0.42
1:D:56:PRO:HD2	2:D:801:FAD:O1P	2.19	0.42
1:D:100:ILE:HD12	1:D:100:ILE:HA	1.92	0.42
1:D:272:GLU:OE2	1:D:272:GLU:HA	2.20	0.42
1:B:91:LYS:NZ	1:B:452:ASP:OD1	2.52	0.42
1:D:46:LYS:HD2	1:D:312:LYS:HD2	2.01	0.42
1:D:281:VAL:HG11	1:D:300:ILE:HD12	2.02	0.42
1:A:344:ASN:ND2	1:A:344:ASN:O	2.53	0.42
1:C:194:GLU:OE1	4:C:2154:HOH:O	2.21	0.42
1:D:62:ALA:O	1:D:66:VAL:HB	2.20	0.42
1:D:356:ILE:HD13	1:D:356:ILE:HG21	1.73	0.42
1:A:91:LYS:NZ	4:A:1656:HOH:O	2.53	0.41
1:B:310:GLU:CD	1:B:312:LYS:NZ	2.78	0.41
1:C:547:LEU:HD12	2:C:801:FAD:HM83	2.02	0.41
1:D:433:PRO:C	1:D:434:GLN:HG2	2.44	0.41
1:A:43:MET:HA	4:A:2377:HOH:O	2.19	0.41
1:A:45:ILE:N	1:A:45:ILE:CD1	2.80	0.41
1:B:314:ASP:OD1	4:B:2780:HOH:O	2.21	0.41
1:B:460:GLN:CG	4:B:2630:HOH:O	2.66	0.41
1:D:102:LYS:HD2	1:D:102:LYS:HA	1.82	0.41
2:D:801:FAD:H9	2:D:801:FAD:H1'1	1.82	0.41
1:A:210:THR:HG22	1:A:240:PRO:HA	2.02	0.41
1:B:344:ASN:N	1:B:345:PRO:CD	2.83	0.41
1:A:81:ASP:N	1:A:81:ASP:OD1	2.53	0.41
1:D:285:ARG:CA	1:D:328:LEU:CD1	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:ARG:HA	1:A:266:PRO:C	2.46	0.41
1:A:342:PRO:O	1:A:344:ASN:N	2.53	0.41
1:D:89:HIS:CE1	1:D:91:LYS:HD3	2.55	0.41
1:A:420:GLN:HG3	4:A:2157:HOH:O	2.20	0.41
1:A:426:ILE:HA	1:A:427:PRO:HD3	1.93	0.41
1:C:83:GLY:N	1:D:81:ASP:O	2.53	0.41
1:C:218:ARG:HD2	4:C:1448:HOH:O	2.21	0.41
1:C:242:ALA:HB1	1:C:254:SER:HB2	2.02	0.41
1:C:261:ASP:OD1	1:C:261:ASP:C	2.62	0.41
1:B:228:GLU:OE1	1:B:228:GLU:HA	2.21	0.41
1:B:382:ILE:HD13	4:B:1452:HOH:O	2.21	0.41
1:A:165:SER:HA	1:A:168:TRP:CD1	2.56	0.40
1:B:310:GLU:CD	1:B:312:LYS:HZ1	2.29	0.40
1:C:381:THR:HA	4:C:2341:HOH:O	2.21	0.40
1:B:49:VAL:HG22	1:B:315:VAL:HB	2.03	0.40
1:C:299:HIS:CB	4:C:2768:HOH:O	2.69	0.40
1:C:570:SER:HB3	1:C:580:LEU:O	2.20	0.40
1:C:265:ARG:HA	1:C:266:PRO:C	2.47	0.40
1:C:63:ARG:HD2	1:C:259:VAL:O	2.21	0.40
1:D:181:PRO:HG2	1:D:195:TRP:HZ2	1.86	0.40
1:D:432:GLU:HB2	1:D:433:PRO:CD	2.51	0.40
1:C:299:HIS:CD2	4:C:2768:HOH:O	2.70	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	574/623 (92%)	549 (96%)	22 (4%)	3 (0%)	24	16
1	B	574/623 (92%)	555 (97%)	16 (3%)	3 (0%)	24	16
1	C	573/623 (92%)	554 (97%)	17 (3%)	2 (0%)	36	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	572/623 (92%)	548 (96%)	22 (4%)	2 (0%)	36	29
All	All	2293/2492 (92%)	2206 (96%)	77 (3%)	10 (0%)	30	22

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	SER
1	A	389	LEU
1	B	82	SER
1	C	186	ASP
1	D	82	SER
1	B	343	ALA
1	A	343	ALA
1	C	82	SER
1	B	344	ASN
1	D	343	ALA

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	503/541 (93%)	493 (98%)	10 (2%)	48	46
1	B	503/541 (93%)	491 (98%)	12 (2%)	43	38
1	C	502/541 (93%)	486 (97%)	16 (3%)	34	27
1	D	501/541 (93%)	487 (97%)	14 (3%)	38	32
All	All	2009/2164 (93%)	1957 (97%)	52 (3%)	40	35

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	MET
1	A	45	ILE
1	A	272	GLU
1	A	285	ARG

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Mol	Chain	Res	Type
1	A	385	THR
1	A	432	GLU
1	A	462	SER
1	A	496	ASN
1	A	545	LEU
1	A	560	LYS
1	B	45	ILE
1	B	90	LYS
1	B	206	PHE
1	B	231	LYS
1	B	269	ASP
1	B	341	ASN
1	B	400	SER
1	B	403	LYS
1	B	460	GLN
1	B	490	LYS
1	B	545	LEU
1	B	593	ASN
1	C	45	ILE
1	C	91	LYS
1	C	101	ASP
1	C	178	GLU
1	C	206	PHE
1	C	214	LYS
1	C	231	LYS
1	C	285	ARG
1	C	336	GLN
1	C	344	ASN
1	C	383	ARG
1	C	389	LEU
1	C	408	TRP
1	C	460	GLN
1	C	545	LEU
1	C	611	GLN
1	D	45	ILE
1	D	178	GLU
1	D	185	LYS
1	D	206	PHE
1	D	312	LYS
1	D	328	LEU
1	D	385	THR
1	D	401	THR

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Mol	Chain	Res	Type
1	D	403	LYS
1	D	432	GLU
1	D	460	GLN
1	D	461	GLN
1	D	490	LYS
1	D	560	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	GLN
1	A	263	GLN
1	A	341	ASN
1	A	344	ASN
1	A	365	GLN
1	A	419	HIS
1	B	167	HIS
1	B	257	ASN
1	B	263	GLN
1	B	324	HIS
1	B	341	ASN
1	B	344	ASN
1	B	434	GLN
1	B	461	GLN
1	B	539	GLN
1	B	611	GLN
1	C	132	GLN
1	C	238	GLN
1	C	257	ASN
1	C	263	GLN
1	C	299	HIS
1	C	324	HIS
1	C	341	ASN
1	C	419	HIS
1	C	461	GLN
1	D	132	GLN
1	D	167	HIS
1	D	263	GLN
1	D	324	HIS
1	D	341	ASN
1	D	365	GLN
1	D	461	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	FAD	A	801	-	58,58,58	1.45	8 (13%)	85,89,89	2.22	26 (30%)
3	MES	C	903	-	12,12,12	1.78	1 (8%)	15,16,16	5.56	10 (66%)
2	FAD	B	801	-	58,58,58	1.61	9 (15%)	85,89,89	2.07	25 (29%)
2	FAD	C	801	-	58,58,58	1.32	8 (13%)	85,89,89	2.23	28 (32%)
2	FAD	D	801	-	58,58,58	1.36	5 (8%)	85,89,89	2.44	29 (34%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	801	-	-	1/34/50/50	0/6/6/6
3	MES	C	903	-	-	2/6/14/14	0/1/1/1
2	FAD	B	801	-	-	1/34/50/50	0/6/6/6
2	FAD	C	801	-	-	0/34/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	D	801	-	-	0/34/50/50	0/6/6/6

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	FAD	P-O3P	6.53	1.66	1.59
3	C	903	MES	C8-S	-5.68	1.69	1.77
2	D	801	FAD	P-O3P	5.38	1.65	1.59
2	C	801	FAD	PA-O3P	-4.23	1.54	1.59
2	A	801	FAD	O4B-C4B	-3.89	1.36	1.45
2	A	801	FAD	C8A-N7A	3.76	1.38	1.31
2	B	801	FAD	C9A-N10	-3.63	1.34	1.41
2	B	801	FAD	O3B-C3B	-2.95	1.35	1.43
2	B	801	FAD	C5X-N5	-2.92	1.34	1.39
2	B	801	FAD	C8A-N7A	2.91	1.37	1.31
2	A	801	FAD	C5'-C4'	2.90	1.55	1.51
2	B	801	FAD	C5'-C4'	2.90	1.55	1.51
2	D	801	FAD	C8A-N9A	-2.82	1.32	1.37
2	A	801	FAD	C1'-N10	2.77	1.54	1.47
2	C	801	FAD	C5X-N5	-2.73	1.34	1.39
2	A	801	FAD	C8A-N9A	-2.69	1.33	1.37
2	A	801	FAD	O3B-C3B	-2.64	1.36	1.43
2	C	801	FAD	C9A-N10	-2.63	1.36	1.41
2	D	801	FAD	O2B-C2B	-2.56	1.36	1.43
2	D	801	FAD	C5'-C4'	2.54	1.55	1.51
2	A	801	FAD	C4-N3	-2.48	1.34	1.38
2	D	801	FAD	C6-C5X	2.44	1.43	1.40
2	C	801	FAD	C4-N3	-2.37	1.34	1.38
2	C	801	FAD	P-O3P	2.31	1.62	1.59
2	A	801	FAD	P-O3P	2.28	1.62	1.59
2	C	801	FAD	C2A-N3A	2.20	1.37	1.33
2	B	801	FAD	PA-O3P	-2.20	1.57	1.59
2	B	801	FAD	C8A-N9A	-2.16	1.33	1.37
2	C	801	FAD	C3B-C4B	-2.15	1.47	1.53
2	B	801	FAD	C2A-N1A	2.11	1.37	1.33
2	C	801	FAD	O5B-C5B	-2.01	1.37	1.44

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	903	MES	O2S-S-C8	-13.91	85.72	106.73
3	C	903	MES	O1S-S-C8	-10.60	90.72	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	903	MES	O3S-S-C8	-8.12	90.12	106.00
2	D	801	FAD	C4A-N9A-C8A	7.73	113.85	105.74
2	D	801	FAD	O4-C4-C4X	-7.48	106.79	126.53
2	C	801	FAD	C4A-N9A-C8A	7.00	113.09	105.74
2	A	801	FAD	N3-C2-N1	-6.82	105.01	119.50
2	B	801	FAD	C4A-N9A-C8A	6.70	112.77	105.74
2	D	801	FAD	C2B-C1B-N9A	6.65	129.83	113.30
2	D	801	FAD	N3A-C2A-N1A	-6.24	119.13	128.58
2	C	801	FAD	C2B-C1B-N9A	6.12	128.52	113.30
2	C	801	FAD	O4-C4-N3	5.90	131.20	120.11
2	A	801	FAD	C4-C4X-N5	5.71	126.09	118.21
2	B	801	FAD	C2B-C1B-N9A	5.46	126.86	113.30
2	D	801	FAD	N9A-C8A-N7A	-5.35	106.34	113.94
2	C	801	FAD	N3A-C2A-N1A	-5.30	120.57	128.58
2	B	801	FAD	N9A-C8A-N7A	-5.21	106.55	113.94
2	C	801	FAD	N9A-C8A-N7A	-5.20	106.56	113.94
2	A	801	FAD	N3A-C2A-N1A	-5.02	120.99	128.58
2	A	801	FAD	O4-C4-C4X	-5.00	113.34	126.53
2	A	801	FAD	C4A-N9A-C8A	4.89	110.88	105.74
2	A	801	FAD	O4-C4-N3	4.54	128.66	120.11
2	A	801	FAD	O4B-C1B-N9A	4.51	116.76	108.09
2	A	801	FAD	C2B-C1B-N9A	4.51	124.51	113.30
2	D	801	FAD	O4B-C1B-N9A	4.45	116.64	108.09
3	C	903	MES	O3S-S-O1S	4.42	122.45	111.40
2	A	801	FAD	N9A-C8A-N7A	-4.40	107.69	113.94
2	D	801	FAD	O3B-C3B-C4B	4.36	123.61	111.08
3	C	903	MES	C5-N4-C3	4.29	118.08	108.84
2	D	801	FAD	N3A-C4A-N9A	4.19	134.29	127.17
2	C	801	FAD	O2B-C2B-C1B	4.14	124.38	110.10
2	B	801	FAD	N3A-C2A-N1A	-4.10	122.37	128.58
3	C	903	MES	C7-N4-C5	4.07	122.09	111.24
2	B	801	FAD	O4B-C1B-N9A	3.96	115.69	108.09
2	C	801	FAD	O3B-C3B-C4B	3.94	122.39	111.08
2	B	801	FAD	N3A-C4A-N9A	3.93	133.84	127.17
2	C	801	FAD	O4B-C1B-N9A	3.89	115.56	108.09
2	A	801	FAD	O3B-C3B-C4B	3.82	122.05	111.08
2	B	801	FAD	O4-C4-C4X	-3.76	116.60	126.53
2	D	801	FAD	O4-C4-N3	3.74	127.15	120.11
2	B	801	FAD	C1B-N9A-C8A	-3.72	118.83	127.09
2	D	801	FAD	O4B-C4B-C5B	3.69	121.14	109.33
2	A	801	FAD	C10-N1-C2	3.65	124.75	116.85
2	A	801	FAD	C5A-C4A-N3A	-3.58	121.78	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	FAD	O2B-C2B-C3B	3.57	123.25	111.82
2	B	801	FAD	C5A-C4A-N3A	-3.51	121.88	126.72
2	C	801	FAD	C4X-C10-N10	3.38	121.32	116.48
2	A	801	FAD	O2B-C2B-C3B	3.36	122.60	111.82
2	C	801	FAD	O4B-C4B-C5B	3.33	120.01	109.33
2	D	801	FAD	C1B-N9A-C8A	-3.33	119.71	127.09
2	C	801	FAD	N3A-C4A-N9A	3.26	132.72	127.17
3	C	903	MES	C7-N4-C3	3.17	119.68	111.24
2	D	801	FAD	O2P-P-O1P	3.14	127.04	112.44
2	C	801	FAD	C10-C4X-N5	-3.10	118.48	124.81
2	A	801	FAD	N3A-C4A-N9A	3.07	132.39	127.17
3	C	903	MES	O1-C2-C3	3.07	118.39	111.77
2	D	801	FAD	O3P-PA-O1A	-3.07	101.48	110.70
2	C	801	FAD	C4-C4X-C10	3.02	122.11	116.93
2	A	801	FAD	O2B-C2B-C1B	2.99	120.39	110.10
2	B	801	FAD	O4B-C4B-C3B	2.96	111.04	105.15
2	C	801	FAD	C5A-N7A-C8A	2.95	108.09	103.45
2	B	801	FAD	O2B-C2B-C3B	2.93	121.21	111.82
2	B	801	FAD	O4B-C4B-C5B	2.91	118.67	109.33
2	B	801	FAD	C5A-N7A-C8A	2.91	108.03	103.45
2	D	801	FAD	C2A-N3A-C4A	2.89	118.89	111.83
2	D	801	FAD	C4-C4X-N5	2.88	122.19	118.21
2	D	801	FAD	O3B-C3B-C2B	2.87	121.03	111.82
2	D	801	FAD	C5A-N7A-C8A	2.86	107.94	103.45
2	D	801	FAD	C5A-C4A-N3A	-2.84	122.80	126.72
2	D	801	FAD	C5A-C4A-N9A	-2.80	102.76	105.81
2	C	801	FAD	C1B-N9A-C8A	-2.76	120.98	127.09
2	C	801	FAD	C5B-C4B-C3B	2.76	125.13	115.21
2	C	801	FAD	C4-N3-C2	2.71	130.46	125.64
2	C	801	FAD	O2B-C2B-C3B	2.68	120.42	111.82
2	C	801	FAD	C2A-N1A-C6A	2.67	123.11	118.73
2	B	801	FAD	C4X-C10-N10	2.66	120.29	116.48
3	C	903	MES	O3S-S-O2S	2.65	118.02	111.40
2	D	801	FAD	C5B-C4B-C3B	2.59	124.54	115.21
2	B	801	FAD	C5'-C4'-C3'	-2.59	107.33	112.22
2	B	801	FAD	C9A-N10-C10	-2.55	116.87	120.75
2	A	801	FAD	C1B-N9A-C8A	-2.53	121.47	127.09
2	D	801	FAD	C10-C4X-N5	-2.53	119.64	124.81
2	D	801	FAD	C7M-C7-C6	-2.51	115.15	119.57
2	C	801	FAD	O2A-PA-O3P	2.48	113.97	107.27
2	B	801	FAD	O3P-P-O1P	2.47	118.13	110.70
2	D	801	FAD	O2B-C2B-C1B	2.47	118.60	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	FAD	O3P-P-O1P	2.46	118.12	110.70
2	B	801	FAD	C10-N1-C2	2.46	122.17	116.85
2	B	801	FAD	C6-C7-C8	2.44	123.28	119.69
2	A	801	FAD	C4-C4X-C10	-2.43	112.76	116.93
2	D	801	FAD	O2P-P-O3P	-2.42	100.73	107.27
2	A	801	FAD	C4X-C10-N10	2.41	119.94	116.48
2	C	801	FAD	C8M-C8-C9	-2.40	115.35	119.57
2	D	801	FAD	C2A-N1A-C6A	2.39	122.65	118.73
2	C	801	FAD	O4-C4-C4X	-2.38	120.25	126.53
2	D	801	FAD	C4X-C10-N10	2.34	119.83	116.48
2	A	801	FAD	C2A-N3A-C4A	2.32	117.51	111.83
2	C	801	FAD	C5A-C4A-N3A	-2.31	123.54	126.72
2	B	801	FAD	C2A-N3A-C4A	2.30	117.46	111.83
2	A	801	FAD	C6A-C5A-C4A	2.30	120.31	117.18
2	C	801	FAD	C4X-C4-N3	-2.29	107.42	113.25
2	B	801	FAD	C4-C4X-N5	2.29	121.37	118.21
2	A	801	FAD	O2-C2-N3	2.28	122.95	118.58
2	A	801	FAD	C2A-N1A-C6A	2.26	122.45	118.73
2	C	801	FAD	O4B-C4B-C3B	2.22	109.55	105.15
2	C	801	FAD	C2A-N3A-C4A	2.18	117.15	111.83
2	B	801	FAD	C4-N3-C2	-2.17	121.79	125.64
2	A	801	FAD	C5B-C4B-C3B	2.16	123.00	115.21
2	A	801	FAD	C5A-N7A-C8A	2.15	106.82	103.45
2	A	801	FAD	C4X-C10-N1	-2.13	119.37	124.59
2	B	801	FAD	O4'-C4'-C3'	2.12	114.22	109.25
2	B	801	FAD	C1'-N10-C9A	2.12	124.75	120.63
2	D	801	FAD	O2A-PA-O1A	2.11	122.28	112.44
2	D	801	FAD	O4B-C4B-C3B	2.10	109.33	105.15
3	C	903	MES	C6-O1-C2	2.10	116.68	109.88
2	A	801	FAD	C1'-N10-C9A	2.08	124.68	120.63
2	C	801	FAD	C5A-C4A-N9A	-2.06	103.57	105.81
2	B	801	FAD	C5B-C4B-C3B	2.03	122.53	115.21

There are no chirality outliers.

All (4) torsion outliers are listed below:

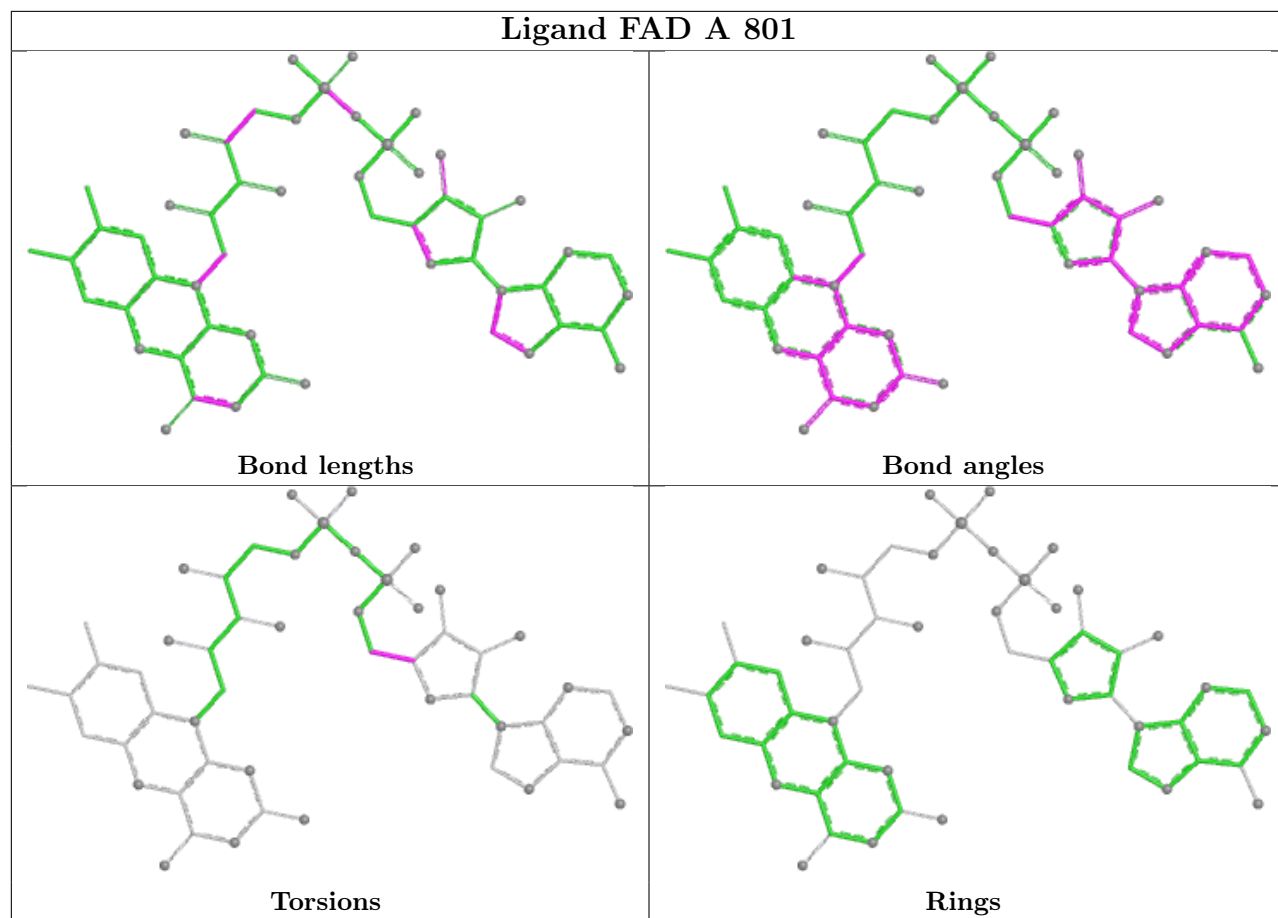
Mol	Chain	Res	Type	Atoms
3	C	903	MES	C8-C7-N4-C5
3	C	903	MES	N4-C7-C8-S
2	B	801	FAD	O4B-C4B-C5B-O5B
2	A	801	FAD	O4B-C4B-C5B-O5B

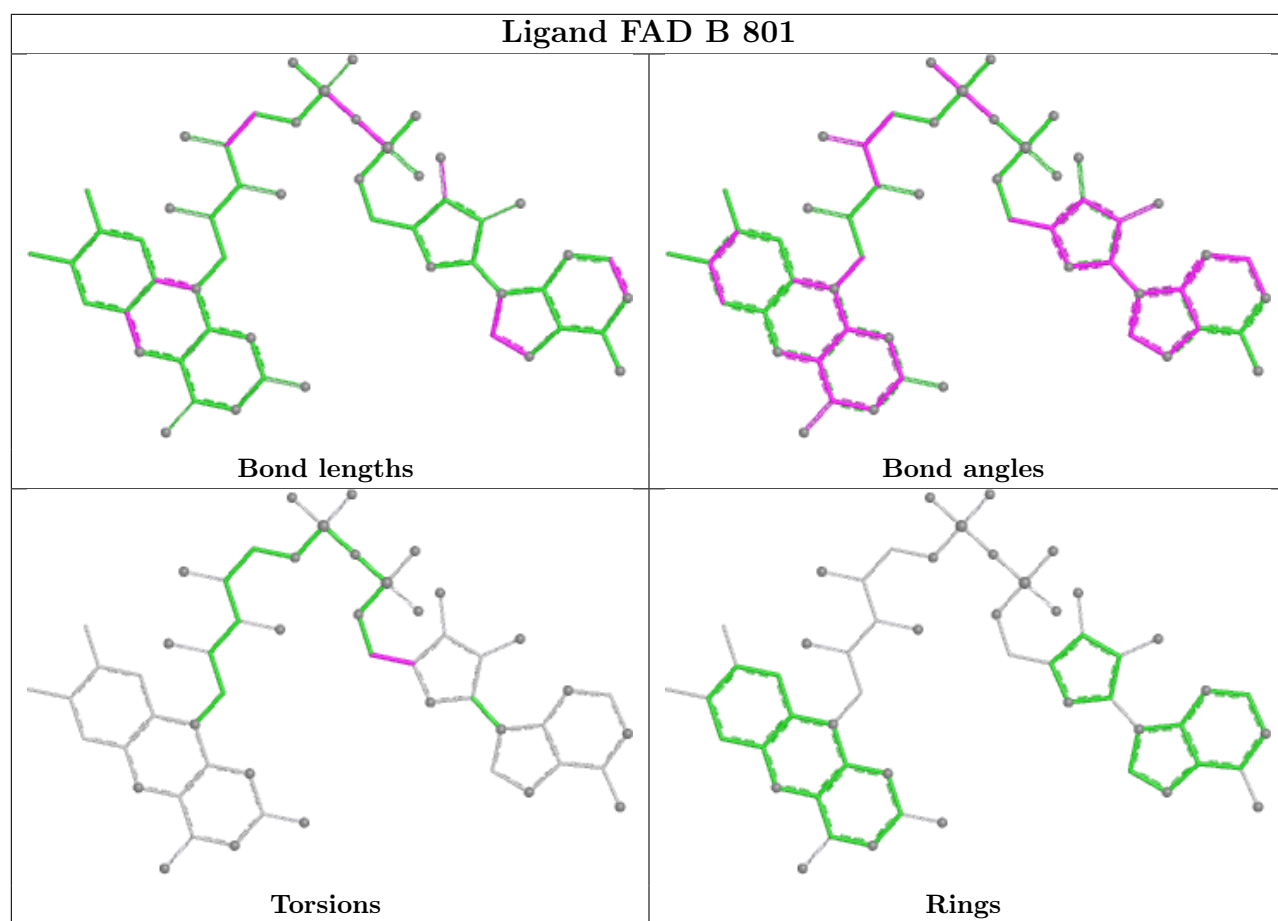
There are no ring outliers.

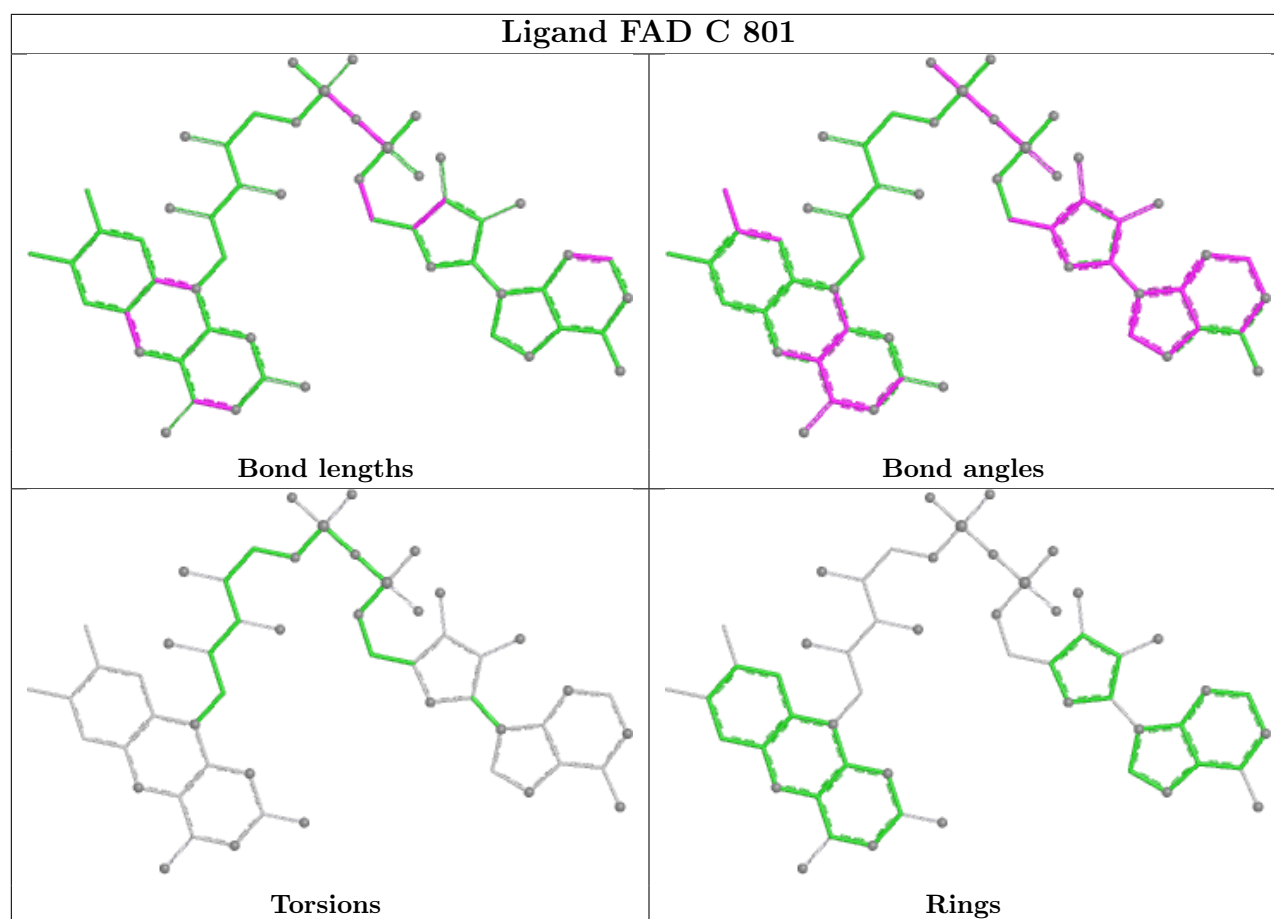
5 monomers are involved in 11 short contacts:

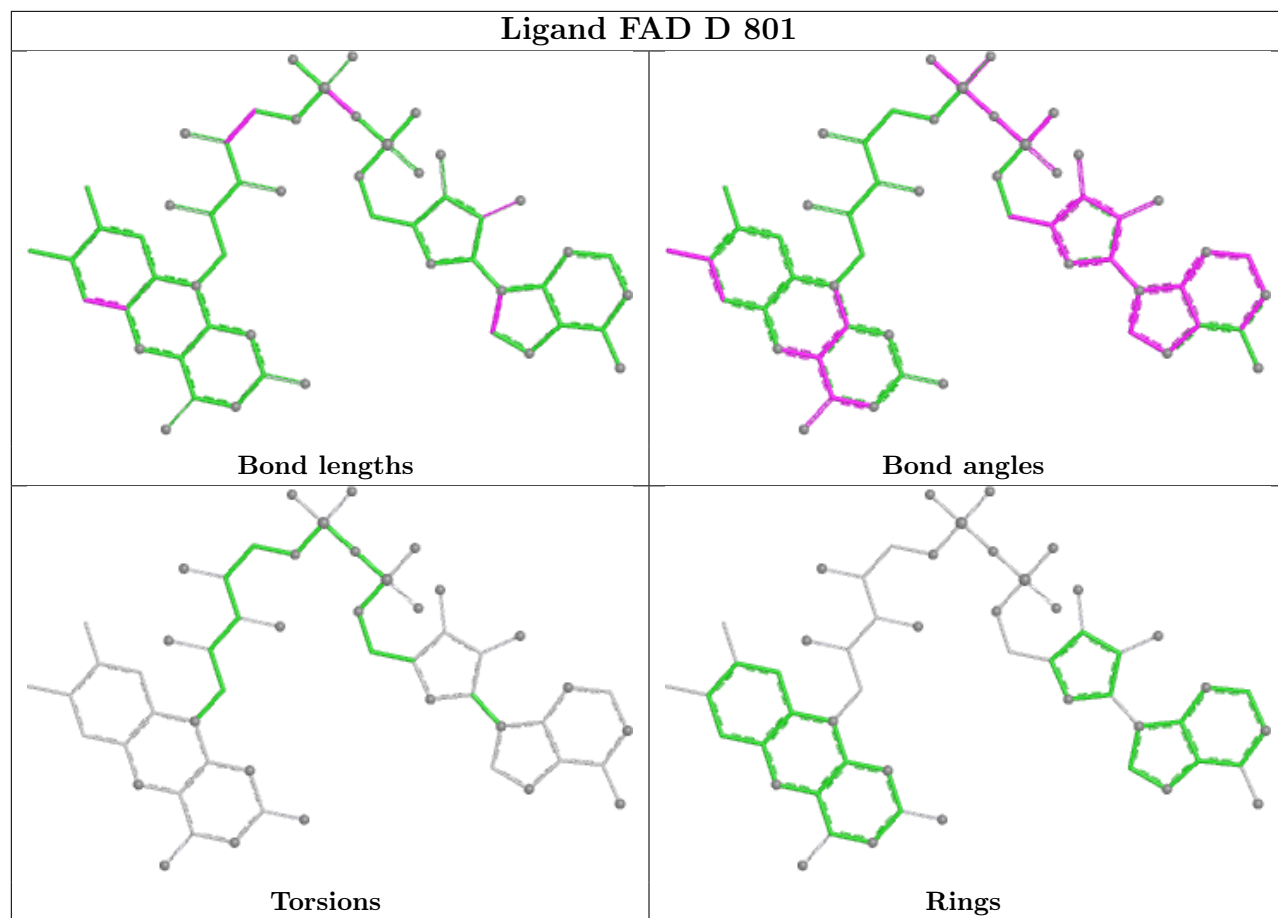
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	FAD	2	0
3	C	903	MES	1	0
2	B	801	FAD	2	0
2	C	801	FAD	2	0
2	D	801	FAD	4	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	576/623 (92%)	-0.03	21 (3%)	46 49	15, 22, 44, 71	0
1	B	576/623 (92%)	-0.11	12 (2%)	63 67	14, 21, 38, 58	0
1	C	575/623 (92%)	0.12	16 (2%)	55 59	17, 27, 48, 72	0
1	D	574/623 (92%)	0.42	21 (3%)	45 48	19, 34, 56, 74	0
All	All	2301/2492 (92%)	0.10	70 (3%)	52 56	14, 26, 49, 74	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	389	LEU	7.0
1	B	459	VAL	6.4
1	A	459	VAL	6.2
1	D	45	ILE	5.6
1	A	400	SER	5.2
1	A	388	GLU	4.9
1	C	459	VAL	4.7
1	D	459	VAL	4.6
1	D	618	PHE	4.3
1	C	45	ILE	4.1
1	B	618	PHE	4.0
1	A	343	ALA	3.9
1	A	458	ALA	3.9
1	C	458	ALA	3.9
1	B	44	ASP	3.7
1	C	619	THR	3.7
1	A	44	ASP	3.6
1	A	344	ASN	3.6
1	A	390	THR	3.4
1	C	457	GLY	3.4
1	A	385	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	291	LEU	3.4
1	D	188	ALA	3.3
1	B	309	PHE	3.3
1	C	390	THR	3.2
1	A	384	GLY	3.2
1	D	458	ALA	3.1
1	D	342	PRO	2.9
1	A	387	GLY	2.9
1	C	343	ALA	2.8
1	D	343	ALA	2.8
1	D	309	PHE	2.8
1	D	211	ASP	2.7
1	A	460	GLN	2.6
1	C	385	THR	2.6
1	D	399	ALA	2.6
1	B	232	GLY	2.5
1	C	184	VAL	2.5
1	B	460	GLN	2.5
1	B	458	ALA	2.5
1	A	342	PRO	2.5
1	C	345	PRO	2.5
1	D	617	PRO	2.5
1	B	310	GLU	2.4
1	C	389	LEU	2.4
1	B	343	ALA	2.4
1	C	101	ASP	2.3
1	C	296	GLU	2.3
1	D	490	LYS	2.3
1	B	82	SER	2.3
1	D	460	GLN	2.3
1	A	401	THR	2.3
1	A	45	ILE	2.2
1	C	81	ASP	2.2
1	A	101	ASP	2.2
1	D	457	GLY	2.2
1	B	345	PRO	2.2
1	C	387	GLY	2.1
1	B	340	PRO	2.1
1	D	266	PRO	2.1
1	D	287	VAL	2.1
1	C	342	PRO	2.1
1	A	418	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	290	ALA	2.1
1	A	186	ASP	2.1
1	D	82	SER	2.0
1	D	462	SER	2.0
1	A	398	GLY	2.0
1	D	193	ALA	2.0
1	A	309	PHE	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](#)

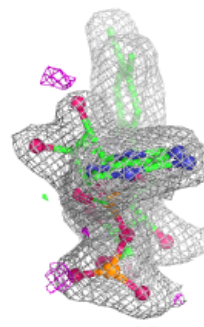
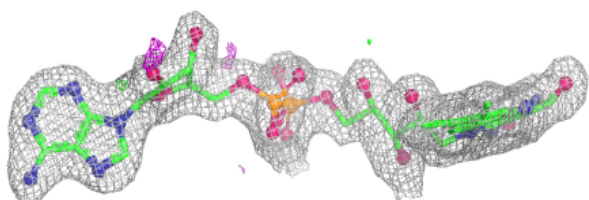
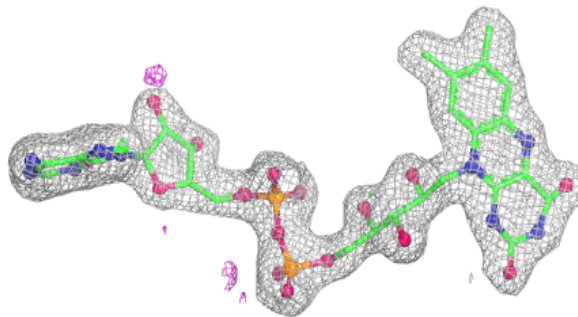
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MES	C	903	12/12	0.91	0.11	40,41,43,47	0
2	FAD	D	801	53/53	0.96	0.06	23,28,32,34	0
2	FAD	C	801	53/53	0.97	0.06	17,22,25,27	0
2	FAD	B	801	53/53	0.98	0.05	12,15,20,21	0
2	FAD	A	801	53/53	0.98	0.05	12,17,21,22	0

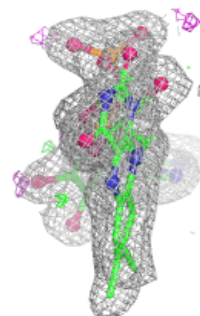
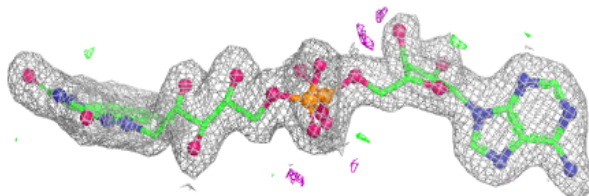
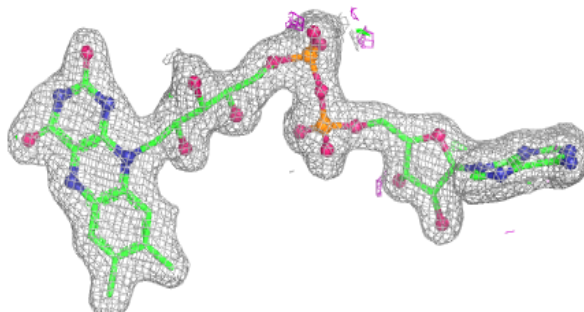
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD D 801:

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

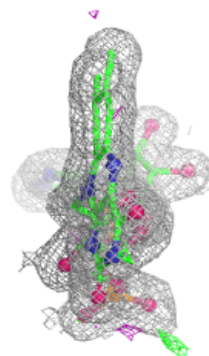
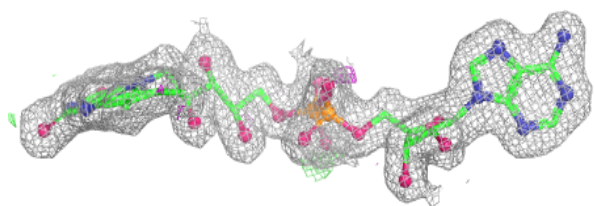
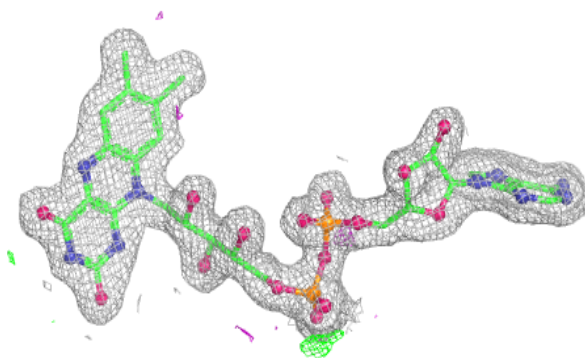
**Electron density around FAD C 801:**

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

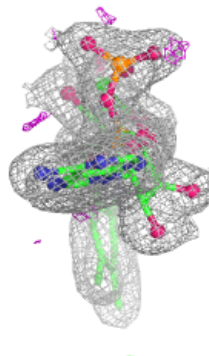
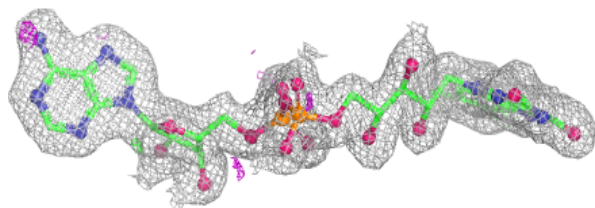
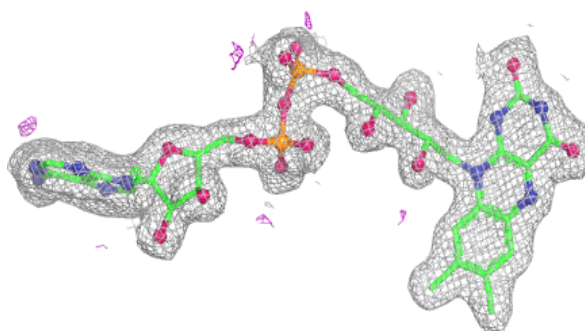


Electron density around FAD B 801:

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

**Electron density around FAD A 801:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.