



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:36 PM UTC

PDB ID : 3LSK / pdb_00003lsk
Title : Pyranose 2-oxidase T169S acetate complex
Authors : Tan, T.C.; Spadiut, O.; Divne, C.
Deposited on : 2010-02-12
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

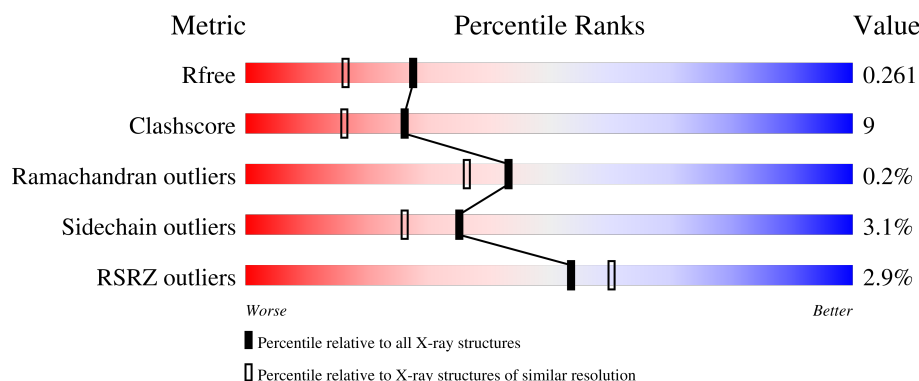
1 Overall quality at a glance

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	2% 74% 16% • 8%
1	B	623	2% 73% 17% • 8%
1	C	623	4% 69% 21% • 8%
1	D	623	3% 73% 17% • 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ACT	A	901	-	-	X	-
3	ACT	B	901	-	-	X	-
3	ACT	C	901	-	-	X	-
3	ACT	D	901	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20361 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
			4541	2867	777	872	25			
1	B	576	Total	C	N	O	S	0	0	0
			4541	2867	777	872	25			
1	C	575	Total	C	N	O	S	0	0	0
			4532	2862	776	870	24			
1	D	574	Total	C	N	O	S	0	0	0
			4525	2858	775	868	24			

There are 4 discrepancies between the modelled and reference sequences:

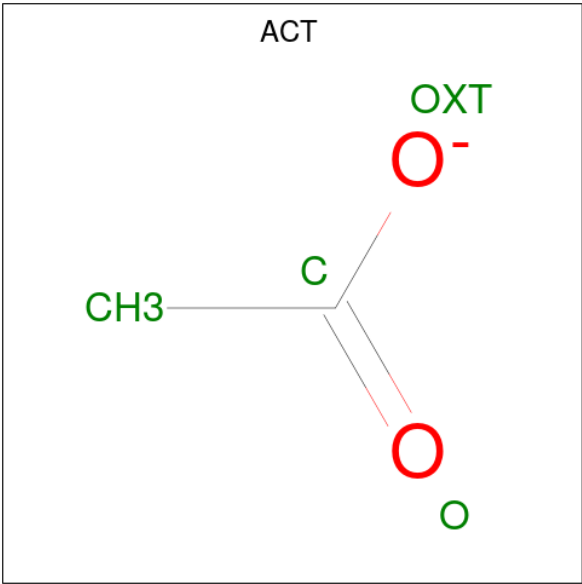
Chain	Residue	Modelled	Actual	Comment	Reference
A	169	SER	THR	engineered mutation	UNP Q7ZA32
B	169	SER	THR	engineered mutation	UNP Q7ZA32
C	169	SER	THR	engineered mutation	UNP Q7ZA32
D	169	SER	THR	engineered mutation	UNP Q7ZA32

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



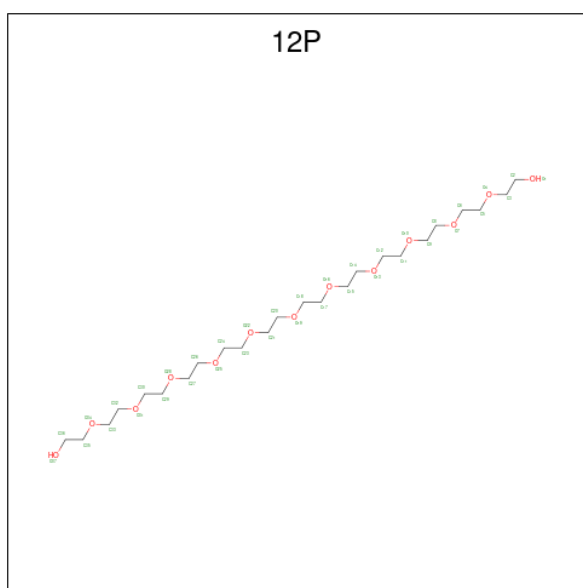
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0

- Molecule 4 is DODECAETHYLENE GLYCOL (CCD ID: 12P) (formula: $C_{24}H_{50}O_{13}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 16 11 5	0	0
4	A	1	Total C O 16 11 5	0	0
4	B	1	Total C O 16 10 6	0	0
4	C	1	Total C O 14 10 4	0	0
4	D	1	Total C O 12 8 4	0	0
4	D	1	Total C O 11 7 4	0	0

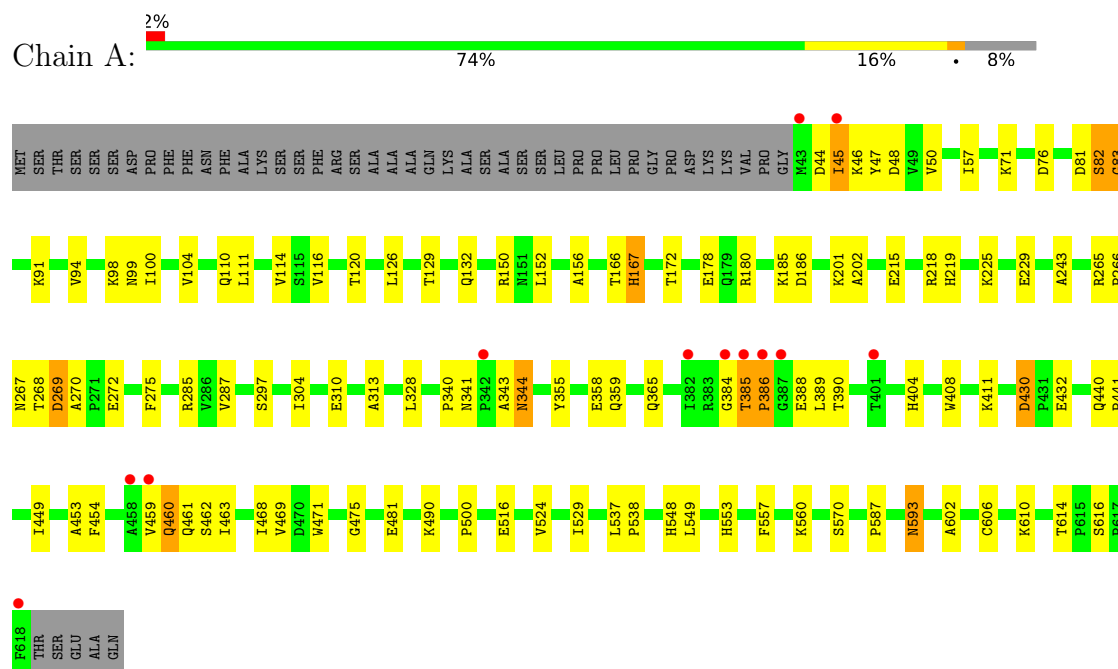
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	518	Total 518	O 518	0	0
5	B	534	Total 534	O 534	0	0
5	C	457	Total 457	O 457	0	0
5	D	400	Total 400	O 400	0	0

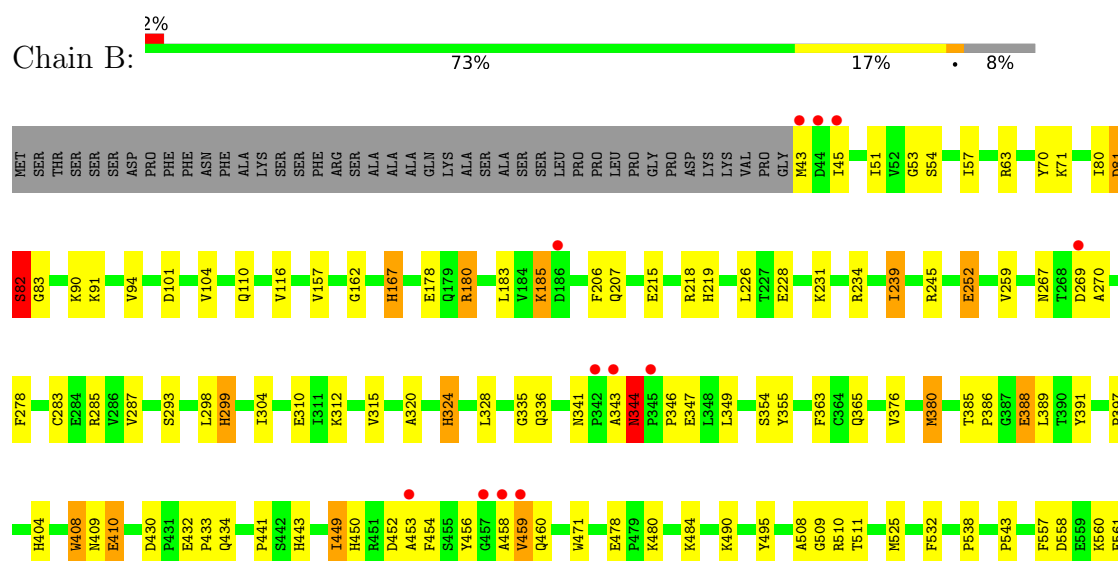
3 Residue-property plots [i](#)

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

• Molecule 1: Pyranose 2-oxidase

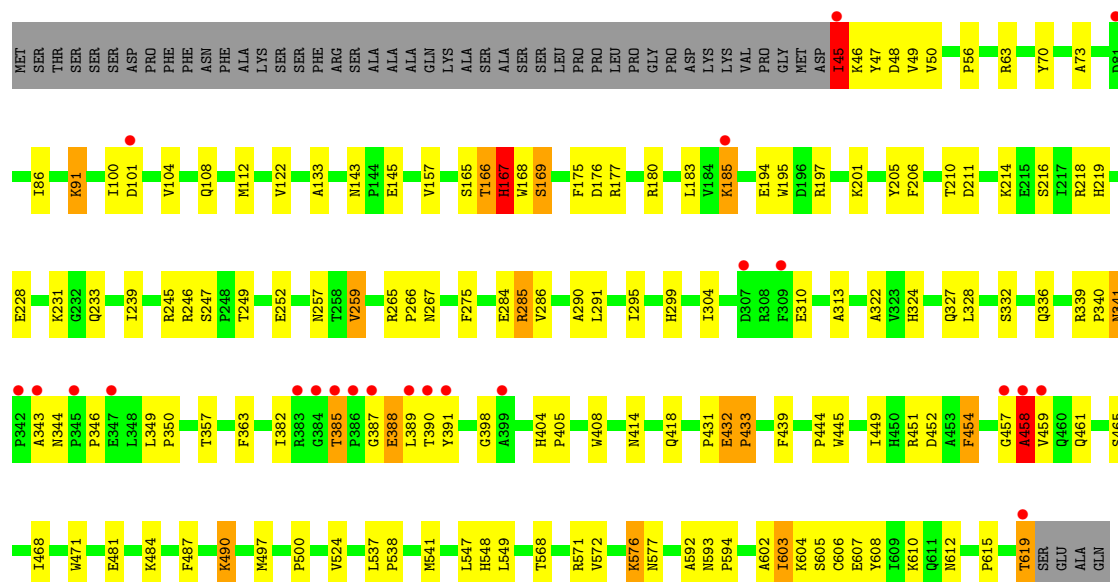


• Molecule 1: Pyranose 2-oxidase

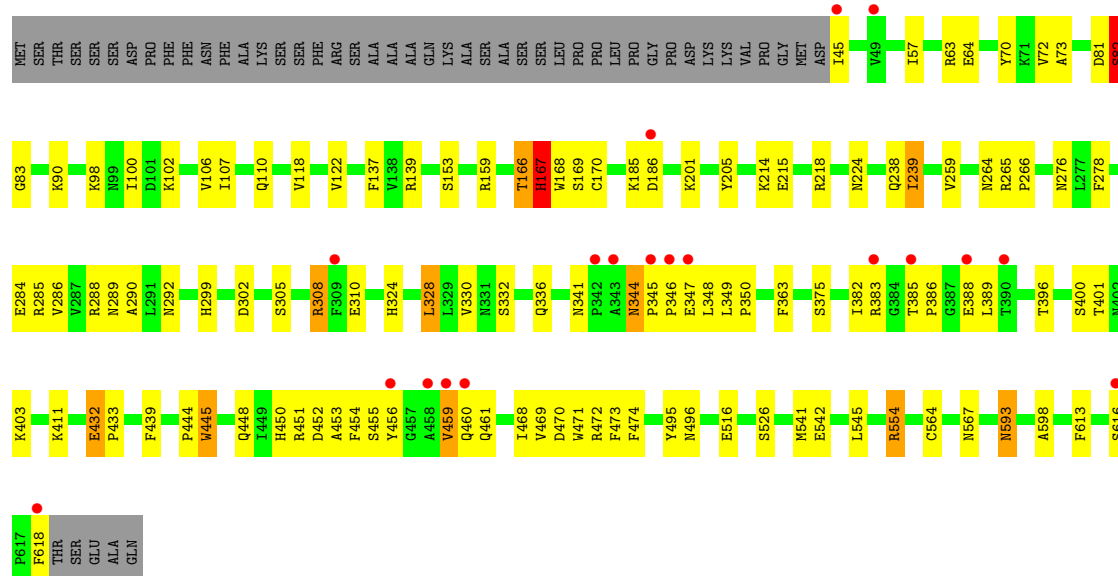
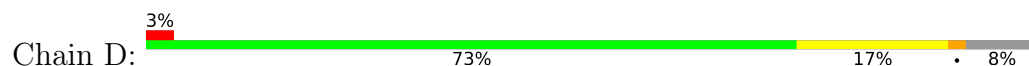




• Molecule 1: Pyranose 2-oxidase



• Molecule 1: Pyranose 2-oxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	100.26Å 102.45Å 136.72Å 90.00° 91.13° 90.00°	Depositor
Resolution (Å)	30.00 – 1.95 30.00 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.8 (30.00-1.95) 98.7 (30.00-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.196 , 0.256 0.207 , 0.261	Depositor DCC
R_{free} test set	2008 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å ²)	13.3	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 42.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.059 for -k,-h,-l 0.048 for k,h,-l 0.039 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	20361	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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: ACT, 12P, 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	1.49	32/4657 (0.7%)	1.28	28/6331 (0.4%)
1	B	1.47	20/4657 (0.4%)	1.30	27/6331 (0.4%)
1	C	1.31	11/4648 (0.2%)	1.27	24/6320 (0.4%)
1	D	1.22	10/4641 (0.2%)	1.21	22/6310 (0.3%)
All	All	1.38	73/18603 (0.4%)	1.27	101/25292 (0.4%)

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	C	0	3
1	D	0	2
All	All	0	6

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	166	THR	C-N	20.20	1.64	1.33
1	C	322	ALA	CA-CB	-9.28	1.37	1.53
1	C	133	ALA	CA-CB	-8.06	1.40	1.53
1	A	167	HIS	C-N	7.99	1.43	1.33
1	D	598	ALA	CA-CB	-7.86	1.41	1.53
1	D	166	THR	C-N	7.36	1.48	1.34
1	B	449	ILE	C-O	-7.36	1.15	1.24
1	A	82	SER	N-CA	7.19	1.55	1.46
1	D	57	ILE	CA-CB	-6.89	1.46	1.54
1	B	450	HIS	C-O	-6.80	1.17	1.24
1	B	495	TYR	N-CA	6.74	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	586	ILE	CA-C	-6.52	1.46	1.53
1	A	172	THR	CA-CB	6.48	1.61	1.53
1	D	118	VAL	CA-CB	6.43	1.61	1.54
1	A	463	ILE	CA-C	6.34	1.60	1.52
1	A	94	VAL	CA-CB	-6.33	1.47	1.54
1	A	156	ALA	CA-CB	-6.02	1.43	1.53
1	B	609	ILE	CA-CB	6.00	1.62	1.54
1	A	111	LEU	C-O	-5.99	1.17	1.23
1	D	474	PHE	N-CA	5.90	1.53	1.46
1	A	99	ASN	CA-CB	5.88	1.57	1.53
1	A	219	HIS	C-O	5.86	1.30	1.24
1	C	349	LEU	C-O	-5.84	1.21	1.23
1	B	299	HIS	CA-C	-5.79	1.45	1.52
1	A	602	ALA	C-O	-5.77	1.17	1.24
1	C	603	ILE	CA-CB	5.75	1.60	1.54
1	A	469	VAL	CA-CB	5.75	1.63	1.54
1	B	82	SER	N-CA	5.67	1.53	1.46
1	A	490	LYS	C-O	-5.64	1.18	1.24
1	B	51	ILE	CA-CB	5.64	1.61	1.54
1	A	83	GLY	C-O	-5.62	1.18	1.24
1	D	122	VAL	CA-CB	5.61	1.60	1.54
1	A	152	LEU	CA-C	-5.60	1.46	1.53
1	B	510	ARG	N-CA	-5.60	1.39	1.46
1	A	453	ALA	CA-C	5.54	1.59	1.52
1	B	320	ALA	CA-CB	-5.53	1.45	1.53
1	A	390	THR	CA-CB	5.53	1.60	1.53
1	A	275	PHE	C-O	5.49	1.30	1.23
1	B	53	GLY	N-CA	5.47	1.53	1.45
1	D	445	TRP	C-O	5.47	1.30	1.23
1	B	376	VAL	C-O	5.46	1.30	1.24
1	A	57	ILE	CA-CB	-5.46	1.47	1.54
1	D	330	VAL	CA-CB	-5.42	1.47	1.54
1	A	76	ASP	N-CA	-5.41	1.39	1.46
1	D	349	LEU	N-CA	5.40	1.50	1.46
1	D	469	VAL	C-O	5.37	1.29	1.24
1	B	245	ARG	C-O	-5.37	1.17	1.24
1	B	453	ALA	CA-CB	5.34	1.61	1.53
1	A	553	HIS	CA-CB	5.32	1.57	1.53
1	B	94	VAL	CA-C	-5.28	1.46	1.52
1	C	433	PRO	C-O	5.27	1.29	1.23
1	A	386	PRO	CA-C	-5.25	1.46	1.52
1	A	120	THR	CA-C	-5.24	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	349	LEU	C-O	5.23	1.26	1.23
1	B	57	ILE	CA-CB	-5.21	1.47	1.54
1	C	454	PHE	N-CA	5.20	1.52	1.45
1	B	315	VAL	CA-CB	-5.17	1.48	1.54
1	A	524	VAL	N-CA	-5.14	1.40	1.46
1	A	243	ALA	CA-CB	-5.13	1.44	1.53
1	A	587	PRO	C-O	5.13	1.30	1.24
1	B	410	GLU	C-O	5.13	1.30	1.24
1	C	122	VAL	CA-CB	5.12	1.60	1.54
1	C	524	VAL	CA-C	-5.12	1.46	1.52
1	C	594	PRO	N-CA	-5.09	1.43	1.47
1	A	500	PRO	C-O	5.08	1.29	1.23
1	C	275	PHE	CA-C	5.06	1.58	1.52
1	B	206	PHE	CE1-CZ	-5.05	1.23	1.38
1	A	529	ILE	CA-CB	-5.05	1.48	1.54
1	A	129	THR	N-CA	5.04	1.52	1.46
1	C	239	ILE	CA-C	5.04	1.58	1.52
1	A	385	THR	CA-C	5.02	1.57	1.52
1	A	202	ALA	CA-C	5.01	1.59	1.52
1	A	549	LEU	C-O	5.01	1.30	1.23

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	167	HIS	O-C-N	-10.79	109.10	121.84
1	D	344	ASN	CA-C-N	10.37	127.12	119.66
1	D	344	ASN	C-N-CA	10.37	127.12	119.66
1	B	167	HIS	O-C-N	-8.54	113.04	122.10
1	C	167	HIS	CA-C-N	8.20	134.72	120.87
1	C	167	HIS	C-N-CA	8.20	134.72	120.87
1	A	82	SER	N-CA-C	8.17	128.21	110.80
1	C	247	SER	CA-C-N	8.03	127.69	119.82
1	C	247	SER	C-N-CA	8.03	127.69	119.82
1	B	324	HIS	N-CA-C	7.74	122.49	112.89
1	C	166	THR	CA-C-N	-7.62	108.26	121.52
1	C	166	THR	C-N-CA	-7.62	108.26	121.52
1	D	239	ILE	CA-C-N	-7.36	112.17	119.90
1	D	239	ILE	C-N-CA	-7.36	112.17	119.90
1	B	349	LEU	CA-C-N	-7.28	112.14	119.56
1	B	349	LEU	C-N-CA	-7.28	112.14	119.56
1	B	80	ILE	CA-C-N	-7.16	113.92	122.44
1	B	80	ILE	C-N-CA	-7.16	113.92	122.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	270	ALA	CA-C-N	7.03	126.66	119.56
1	B	270	ALA	C-N-CA	7.03	126.66	119.56
1	C	48	ASP	N-CA-C	-6.85	103.05	111.40
1	B	82	SER	N-CA-C	6.81	125.31	110.80
1	A	116	VAL	CA-C-N	-6.74	113.85	120.52
1	A	116	VAL	C-N-CA	-6.74	113.85	120.52
1	C	328	LEU	N-CA-C	-6.66	103.95	111.14
1	C	143	ASN	CA-C-N	6.65	126.28	119.56
1	C	143	ASN	C-N-CA	6.65	126.28	119.56
1	A	304	ILE	CB-CA-C	-6.61	103.38	112.04
1	D	396	THR	CA-C-N	-6.60	113.18	119.85
1	D	396	THR	C-N-CA	-6.60	113.18	119.85
1	C	45	ILE	CB-CA-C	-6.56	98.48	111.60
1	A	385	THR	CA-C-N	6.54	126.51	119.78
1	A	385	THR	C-N-CA	6.54	126.51	119.78
1	B	614	THR	CA-C-N	-6.53	113.25	119.85
1	B	614	THR	C-N-CA	-6.53	113.25	119.85
1	D	167	HIS	CA-C-O	-6.46	111.74	118.65
1	D	278	PHE	CA-C-N	-6.33	114.25	120.52
1	D	278	PHE	C-N-CA	-6.33	114.25	120.52
1	B	508	ALA	N-CA-C	-6.32	102.64	110.41
1	C	458	ALA	N-CA-C	6.23	124.07	110.80
1	D	459	VAL	N-CA-C	6.22	118.10	109.45
1	B	509	GLY	N-CA-C	-6.21	103.81	111.45
1	A	344	ASN	CA-C-N	-6.15	114.05	120.38
1	A	344	ASN	C-N-CA	-6.15	114.05	120.38
1	C	167	HIS	O-C-N	-6.12	114.11	121.64
1	C	49	VAL	N-CA-C	6.09	117.54	108.46
1	D	593	ASN	CA-C-N	6.08	125.79	119.64
1	D	593	ASN	C-N-CA	6.08	125.79	119.64
1	D	82	SER	N-CA-C	6.02	123.63	110.80
1	A	570	SER	N-CA-C	-5.98	105.93	113.23
1	B	180	ARG	CA-C-N	-5.92	113.59	119.92
1	B	180	ARG	C-N-CA	-5.92	113.59	119.92
1	A	114	VAL	N-CA-C	5.86	116.04	110.53
1	C	572	VAL	N-CA-C	5.81	116.51	108.84
1	D	166	THR	O-C-N	-5.81	113.80	122.39
1	C	295	ILE	N-CA-C	5.74	116.84	108.58
1	A	616	SER	CA-C-N	5.72	125.66	119.76
1	A	616	SER	C-N-CA	5.72	125.66	119.76
1	D	616	SER	CA-C-N	-5.68	114.11	119.85
1	D	616	SER	C-N-CA	-5.68	114.11	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	554	ARG	N-CA-C	5.62	117.95	110.53
1	A	430	ASP	CA-C-N	-5.62	113.91	119.92
1	A	430	ASP	C-N-CA	-5.62	113.91	119.92
1	A	186	ASP	CB-CA-C	-5.57	103.67	111.80
1	B	344	ASN	CA-C-N	5.54	123.65	119.66
1	B	344	ASN	C-N-CA	5.54	123.65	119.66
1	C	218	ARG	N-CA-C	5.52	116.98	111.07
1	C	143	ASN	CB-CA-C	-5.51	105.48	110.44
1	B	404	HIS	CA-C-N	-5.51	114.92	120.21
1	B	404	HIS	C-N-CA	-5.51	114.92	120.21
1	A	270	ALA	CA-C-N	5.50	125.59	119.87
1	A	270	ALA	C-N-CA	5.50	125.59	119.87
1	D	106	VAL	CB-CA-C	-5.48	103.67	112.16
1	D	345	PRO	CA-C-N	5.47	125.23	119.76
1	D	345	PRO	C-N-CA	5.47	125.23	119.76
1	A	404	HIS	CA-C-N	5.46	125.44	120.03
1	A	404	HIS	C-N-CA	5.46	125.44	120.03
1	B	239	ILE	N-CA-C	-5.45	103.02	108.96
1	C	100	ILE	N-CA-C	5.44	116.17	110.62
1	C	259	VAL	N-CA-C	5.35	115.55	110.42
1	B	226	LEU	N-CA-C	-5.29	105.59	111.36
1	B	81	ASP	O-C-N	5.28	127.83	121.76
1	A	614	THR	CA-C-N	-5.26	114.36	119.78
1	A	614	THR	C-N-CA	-5.26	114.36	119.78
1	A	180	ARG	CA-C-N	-5.24	115.18	120.31
1	A	180	ARG	C-N-CA	-5.24	115.18	120.31
1	B	525	MET	CB-CA-C	-5.24	101.95	110.85
1	D	224	ASN	N-CA-C	-5.23	105.25	111.69
1	C	389	LEU	N-CA-C	-5.21	106.87	113.18
1	A	82	SER	CB-CA-C	-5.21	100.05	110.42
1	A	48	ASP	N-CA-C	-5.21	105.05	111.40
1	B	116	VAL	N-CA-C	5.18	113.15	107.60
1	C	577	ASN	N-CA-C	5.16	118.68	111.56
1	C	497	MET	CA-C-N	5.14	125.38	119.83
1	C	497	MET	C-N-CA	5.14	125.38	119.83
1	B	593	ASN	CA-C-N	5.13	124.82	119.64
1	B	593	ASN	C-N-CA	5.13	124.82	119.64
1	A	529	ILE	CB-CA-C	-5.12	106.55	111.06
1	B	380	MET	CG-SD-CE	-5.11	89.66	100.90
1	A	358	GLU	N-CA-C	-5.06	101.04	108.99
1	A	46	LYS	N-CA-C	5.05	117.63	108.69

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	449	ILE	Peptide
1	C	166	THR	Mainchain
1	C	167	HIS	Mainchain
1	C	457	GLY	Peptide
1	D	166	THR	Mainchain
1	D	167	HIS	Mainchain

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	4541	0	4386	60	0
1	B	4541	0	4386	79	0
1	C	4532	0	4380	103	0
1	D	4525	0	4373	99	0
2	A	53	0	27	1	0
2	B	53	0	26	0	0
2	C	53	0	29	14	0
2	D	53	0	26	1	0
3	A	4	0	3	3	0
3	B	4	0	3	2	0
3	C	4	0	3	2	0
3	D	4	0	3	2	0
4	A	32	0	36	0	0
4	B	16	0	21	0	0
4	C	14	0	16	1	0
4	D	23	0	26	9	0
5	A	518	0	0	10	0
5	B	534	0	0	21	0
5	C	457	0	0	13	0
5	D	400	0	0	19	0
All	All	20361	0	17744	339	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 9.

All (339) 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:167:HIS:HE2	2:C:801:FAD:C8M	1.00	1.58
1:C:167:HIS:NE2	2:C:801:FAD:HM82	1.04	1.35
1:B:312:LYS:HG3	5:B:2396:HOH:O	1.41	1.19
1:A:385:THR:O	1:A:388:GLU:HG2	1.38	1.18
1:C:299:HIS:CE1	1:C:310:GLU:HG2	1.78	1.17
1:B:101:ASP:O	1:B:104:VAL:HG12	1.47	1.15
1:D:385:THR:HG23	1:D:388:GLU:HG3	1.29	1.14
1:B:389:LEU:HB2	5:B:2263:HOH:O	1.50	1.09
1:C:458:ALA:HA	5:C:2694:HOH:O	1.56	1.06
1:D:214:LYS:HD2	5:D:2117:HOH:O	1.69	0.93
1:C:167:HIS:CD2	2:C:801:FAD:HM82	2.04	0.91
1:C:167:HIS:HE2	2:C:801:FAD:HM81	1.36	0.89
1:A:459:VAL:HA	5:A:2120:HOH:O	1.73	0.87
1:D:382:ILE:HD13	5:D:2710:HOH:O	1.75	0.86
1:B:558:ASP:OD2	1:B:561:GLU:HG3	1.76	0.86
1:D:382:ILE:CD1	5:D:2710:HOH:O	2.24	0.85
1:D:110:GLN:HE21	1:D:167:HIS:HD1	1.20	0.85
1:D:385:THR:HG23	1:D:388:GLU:CG	2.06	0.84
1:C:388:GLU:N	1:C:388:GLU:OE1	2.10	0.83
1:D:385:THR:CG2	1:D:388:GLU:HG3	2.08	0.82
1:B:365:GLN:OE1	1:B:458:ALA:HB2	1.79	0.82
1:A:110:GLN:HE21	1:A:167:HIS:HD1	1.25	0.81
1:B:207:GLN:HG3	5:B:2725:HOH:O	1.80	0.81
1:B:478:GLU:HG3	1:B:511:THR:OG1	1.80	0.80
1:D:308:ARG:HG3	1:D:308:ARG:HH11	1.46	0.80
1:A:385:THR:HB	1:A:386:PRO:HD2	1.63	0.80
1:A:385:THR:H	1:A:388:GLU:CD	1.91	0.79
1:B:459:VAL:HG12	1:B:459:VAL:O	1.81	0.79
1:B:178:GLU:OE2	1:B:441:PRO:HG3	1.81	0.78
1:C:167:HIS:CE1	2:C:801:FAD:HM82	2.12	0.78
1:C:341:ASN:ND2	1:C:343:ALA:H	1.82	0.77
1:D:308:ARG:HH11	1:D:308:ARG:CG	1.98	0.76
1:B:267:ASN:HB2	5:B:2679:HOH:O	1.85	0.75
1:D:288:ARG:NH1	4:D:907:12P:H121	2.01	0.75
1:C:167:HIS:HE2	2:C:801:FAD:C8	1.98	0.74
1:A:45:ILE:H	1:A:45:ILE:HD12	1.53	0.73
1:C:50:VAL:HG13	1:C:313:ALA:HB2	1.71	0.73
1:A:225:LYS:HE3	1:A:229:GLU:OE2	1.89	0.72
1:B:110:GLN:HE21	1:B:167:HIS:HD1	1.35	0.72
1:C:341:ASN:C	1:C:341:ASN:HD22	1.98	0.71
1:D:411:LYS:HE2	5:D:2736:HOH:O	1.88	0.71
1:D:545:LEU:HD12	5:D:2399:HOH:O	1.88	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:LYS:HD3	5:A:2648:HOH:O	1.91	0.71
1:A:83:GLY:N	1:B:81:ASP:O	2.23	0.70
1:C:216:SER:HB3	1:C:219:HIS:HB3	1.74	0.70
1:C:341:ASN:HD22	1:C:343:ALA:H	1.40	0.69
1:B:101:ASP:O	1:B:104:VAL:CG1	2.35	0.69
1:B:310:GLU:O	1:B:310:GLU:HG3	1.93	0.69
1:D:456:TYR:HB3	5:D:2705:HOH:O	1.93	0.68
1:A:365:GLN:HE22	1:A:459:VAL:HG22	1.59	0.68
5:C:2195:HOH:O	1:D:461:GLN:HG2	1.96	0.66
1:D:81:ASP:OD2	1:D:90:LYS:NZ	2.28	0.65
1:B:185:LYS:HD3	1:B:557:PHE:CD2	2.30	0.65
1:C:432:GLU:HB2	1:C:433:PRO:HD2	1.79	0.65
1:D:288:ARG:O	4:D:907:12P:H152	1.96	0.65
1:D:448:GLN:HE22	3:D:901:ACT:CH3	2.09	0.65
1:B:344:ASN:N	1:B:344:ASN:ND2	2.44	0.65
1:A:81:ASP:N	1:A:81:ASP:OD1	2.24	0.64
1:B:397:PRO:HD3	5:B:2573:HOH:O	1.97	0.64
1:C:228:GLU:HA	1:C:231:LYS:HE2	1.80	0.64
1:B:456:TYR:CD1	1:B:456:TYR:N	2.66	0.63
1:A:126:LEU:HD12	1:A:132:GLN:HG3	1.80	0.63
1:D:137:PHE:CE2	1:D:139:ARG:HG3	2.34	0.63
1:B:490:LYS:HG3	5:B:1609:HOH:O	1.99	0.62
1:C:465:SER:HA	1:C:468:ILE:HD12	1.80	0.62
1:D:299:HIS:ND1	1:D:310:GLU:OE2	2.29	0.62
1:C:194:GLU:OE2	1:C:604:LYS:NZ	2.33	0.61
1:A:269:ASP:OD1	1:A:269:ASP:N	2.33	0.61
1:D:452:ASP:HB3	1:D:454:PHE:CE1	2.35	0.61
1:D:459:VAL:HG12	1:D:461:GLN:NE2	2.16	0.61
1:D:81:ASP:O	1:D:83:GLY:N	2.33	0.60
1:D:452:ASP:HB3	1:D:454:PHE:HE1	1.65	0.60
1:B:185:LYS:HD3	1:B:557:PHE:CE2	2.36	0.60
1:A:343:ALA:C	1:A:344:ASN:HD22	2.07	0.60
1:C:449:ILE:HD13	1:C:471:TRP:CZ3	2.36	0.60
1:B:91:LYS:NZ	1:B:452:ASP:OD1	2.34	0.60
1:B:459:VAL:O	1:B:459:VAL:CG1	2.49	0.60
1:D:290:ALA:HB3	5:D:2315:HOH:O	2.00	0.60
1:A:185:LYS:HE3	1:A:557:PHE:CD2	2.37	0.59
1:C:547:LEU:CD1	2:C:801:FAD:HM83	2.32	0.59
1:B:343:ALA:C	1:B:344:ASN:HD22	2.11	0.59
1:B:71:LYS:HE3	5:B:2295:HOH:O	2.02	0.59
2:A:801:FAD:O4	3:A:901:ACT:H2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ILE:HD12	1:A:45:ILE:N	2.17	0.58
1:B:344:ASN:N	1:B:344:ASN:HD22	2.01	0.58
1:B:82:SER:CB	5:B:1614:HOH:O	2.50	0.58
1:B:81:ASP:OD1	1:B:81:ASP:N	2.32	0.58
1:C:619:THR:O	1:C:619:THR:CG2	2.52	0.58
1:A:44:ASP:OD2	1:A:71:LYS:NZ	2.34	0.57
1:C:336:GLN:NE2	1:C:344:ASN:O	2.38	0.57
1:C:284:GLU:C	1:C:285:ARG:HG2	2.29	0.57
1:C:167:HIS:NE2	2:C:801:FAD:C8	2.64	0.57
1:B:234:ARG:HD3	1:B:443:HIS:CE1	2.40	0.57
1:D:299:HIS:HD1	1:D:310:GLU:CD	2.13	0.57
1:D:444:PRO:HD2	1:D:445:TRP:CZ3	2.40	0.57
1:C:47:TYR:CD2	1:C:73:ALA:HB2	2.41	0.56
1:D:459:VAL:HG12	1:D:461:GLN:HE22	1.70	0.56
1:A:81:ASP:O	1:B:81:ASP:O	2.23	0.56
1:D:288:ARG:HH12	4:D:907:12P:C12	2.18	0.56
1:D:328:LEU:CD1	1:D:328:LEU:C	2.78	0.56
1:B:269:ASP:HB2	5:B:2322:HOH:O	2.05	0.56
1:B:354:SER:O	1:B:355:TYR:HB2	2.04	0.56
1:C:461:GLN:HE21	1:C:461:GLN:HA	1.71	0.56
1:A:440:GLN:HB3	1:A:441:PRO:HD2	1.87	0.56
1:C:619:THR:O	1:C:619:THR:HG22	2.06	0.56
1:B:341:ASN:ND2	1:B:343:ALA:H	2.03	0.55
1:C:346:PRO:HG2	1:C:350:PRO:HA	1.88	0.55
1:D:288:ARG:HH12	4:D:907:12P:H121	1.71	0.55
1:C:214:LYS:HG3	5:C:1393:HOH:O	2.07	0.55
1:C:157:VAL:HG21	1:C:324:HIS:HE1	1.71	0.55
1:D:567:ASN:HB2	5:D:2758:HOH:O	2.05	0.55
1:D:185:LYS:O	1:D:186:ASP:C	2.48	0.54
1:D:453:ALA:C	1:D:454:PHE:CD1	2.85	0.54
1:C:387:GLY:C	1:C:388:GLU:OE1	2.50	0.54
1:D:545:LEU:CD1	5:D:2399:HOH:O	2.52	0.54
1:C:175:PHE:CE1	1:C:592:ALA:HB3	2.42	0.54
1:D:328:LEU:C	1:D:328:LEU:HD12	2.32	0.54
1:C:414:ASN:HB3	1:C:418:GLN:HE22	1.72	0.54
1:C:245:ARG:HG2	5:C:2461:HOH:O	2.08	0.54
1:A:218:ARG:HG3	1:A:430:ASP:OD2	2.08	0.54
1:D:265:ARG:HB3	1:D:266:PRO:HA	1.89	0.54
1:D:153:SER:OG	1:D:542:GLU:HG3	2.07	0.53
1:B:543:PRO:HG3	5:D:1751:HOH:O	2.08	0.53
1:B:43:MET:HG2	1:B:278:PHE:CE1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:265:ARG:HB3	1:C:266:PRO:HA	1.91	0.53
1:B:335:GLY:O	1:B:346:PRO:HB3	2.08	0.53
1:B:82:SER:HB2	5:B:1614:HOH:O	2.06	0.53
1:D:450:HIS:O	1:D:470:ASP:HB2	2.08	0.53
1:A:440:GLN:HB3	1:A:441:PRO:CD	2.38	0.52
1:A:267:ASN:OD1	1:A:267:ASN:C	2.52	0.52
1:A:606:CYS:O	1:A:610:LYS:HG3	2.10	0.52
1:A:516:GLU:HB3	5:A:2035:HOH:O	2.09	0.52
1:C:228:GLU:HG3	1:C:231:LYS:NZ	2.24	0.52
1:D:432:GLU:CB	1:D:433:PRO:HD2	2.40	0.52
1:C:165:SER:HA	1:C:168:TRP:CD1	2.44	0.52
1:C:197:ARG:NH1	1:C:197:ARG:HG2	2.23	0.52
1:C:216:SER:OG	1:C:431:PRO:O	2.20	0.52
1:D:82:SER:HB2	5:D:2176:HOH:O	2.10	0.52
1:D:290:ALA:HB2	5:D:2440:HOH:O	2.09	0.52
1:A:341:ASN:HD21	1:A:343:ALA:HB3	1.75	0.51
1:A:344:ASN:HD22	1:A:344:ASN:N	2.09	0.51
1:D:299:HIS:NE2	1:D:308:ARG:HD3	2.26	0.51
1:D:618:PHE:C	1:D:618:PHE:CD2	2.88	0.51
1:A:91:LYS:HD2	1:A:100:ILE:HD11	1.93	0.51
1:C:547:LEU:HD12	2:C:801:FAD:HM83	1.93	0.51
1:D:218:ARG:HD2	5:D:1518:HOH:O	2.11	0.51
1:B:63:ARG:HD2	1:B:259:VAL:O	2.11	0.51
1:C:47:TYR:CE2	1:C:73:ALA:HB2	2.47	0.50
1:C:169:SER:OG	2:C:801:FAD:N5	2.44	0.50
1:B:408:TRP:CD1	1:B:408:TRP:C	2.89	0.50
1:C:341:ASN:HD21	1:C:343:ALA:HB3	1.75	0.50
1:D:451:ARG:HD3	1:D:468:ILE:O	2.12	0.50
1:D:292:ASN:OD1	4:D:907:12P:H121	2.11	0.50
1:A:215:GLU:O	1:A:411:LYS:NZ	2.45	0.50
1:D:159:ARG:HA	2:D:801:FAD:O2B	2.12	0.50
1:A:365:GLN:HE22	1:A:459:VAL:CG2	2.24	0.50
1:D:168:TRP:HD1	1:D:168:TRP:H	1.59	0.50
1:D:336:GLN:NE2	1:D:344:ASN:O	2.45	0.50
1:D:385:THR:O	1:D:386:PRO:C	2.54	0.50
1:C:145:GLU:OE2	1:C:490:LYS:NZ	2.40	0.49
1:A:218:ARG:HD2	5:A:1538:HOH:O	2.10	0.49
1:A:328:LEU:C	1:A:328:LEU:HD23	2.37	0.49
1:A:384:GLY:N	5:A:2691:HOH:O	2.45	0.49
1:D:618:PHE:C	1:D:618:PHE:HD2	2.20	0.49
1:B:218:ARG:HG3	1:B:430:ASP:OD2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:ASP:CB	5:B:2322:HOH:O	2.60	0.49
1:C:324:HIS:HD2	1:C:327:GLN:OE1	1.96	0.49
1:D:168:TRP:H	1:D:168:TRP:CD1	2.30	0.49
1:D:288:ARG:NH1	4:D:907:12P:C12	2.72	0.49
1:B:341:ASN:C	1:B:341:ASN:HD22	2.20	0.49
1:C:541:MET:HE3	5:C:1385:HOH:O	2.12	0.49
1:D:432:GLU:HB2	1:D:433:PRO:HD2	1.95	0.49
1:B:336:GLN:HG2	5:B:2181:HOH:O	2.12	0.49
1:D:439:PHE:CD1	1:D:439:PHE:C	2.92	0.48
1:C:388:GLU:N	1:C:388:GLU:CD	2.71	0.48
1:C:461:GLN:HA	1:C:461:GLN:NE2	2.29	0.48
1:A:548:HIS:NE2	3:A:901:ACT:O	2.46	0.48
1:C:444:PRO:HD2	1:C:445:TRP:CZ3	2.49	0.48
1:D:169:SER:O	1:D:170:CYS:HB2	2.13	0.48
1:D:284:GLU:O	1:D:285:ARG:HB3	2.14	0.48
1:B:433:PRO:C	1:B:434:GLN:HG2	2.39	0.48
1:C:183:LEU:HD12	1:C:195:TRP:CE2	2.47	0.48
1:C:414:ASN:HB3	1:C:418:GLN:NE2	2.28	0.48
1:A:297:SER:OG	1:A:310:GLU:OE1	2.27	0.48
1:D:185:LYS:HD2	1:D:186:ASP:OD2	2.13	0.48
1:D:459:VAL:CG1	1:D:460:GLN:N	2.76	0.48
1:B:454:PHE:CE2	3:B:901:ACT:H1	2.49	0.48
1:C:197:ARG:HG2	1:C:197:ARG:HH11	1.77	0.48
1:D:81:ASP:N	1:D:81:ASP:OD1	2.47	0.48
1:D:167:HIS:CD2	1:D:167:HIS:C	2.92	0.47
1:B:484:LYS:HB3	5:B:2003:HOH:O	2.14	0.47
1:D:265:ARG:HA	1:D:266:PRO:C	2.39	0.47
1:C:341:ASN:ND2	1:C:341:ASN:C	2.68	0.47
1:A:50:VAL:HG13	1:A:313:ALA:HB2	1.97	0.47
1:B:336:GLN:NE2	1:B:344:ASN:O	2.47	0.47
1:D:324:HIS:CE1	5:D:2193:HOH:O	2.67	0.47
1:C:56:PRO:HD3	1:C:165:SER:HB3	1.97	0.47
1:A:44:ASP:HB2	1:A:47:TYR:CZ	2.50	0.47
1:A:341:ASN:C	1:A:341:ASN:HD22	2.23	0.46
1:B:328:LEU:HD23	1:B:328:LEU:C	2.39	0.46
1:B:267:ASN:CB	5:B:2679:HOH:O	2.54	0.46
1:B:269:ASP:HA	5:B:2322:HOH:O	2.15	0.46
1:D:341:ASN:C	1:D:341:ASN:ND2	2.71	0.46
1:A:449:ILE:HG12	1:A:471:TRP:CE3	2.50	0.46
1:C:104:VAL:HG13	1:C:454:PHE:O	2.15	0.46
1:C:571:ARG:NH2	5:C:2535:HOH:O	2.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:516:GLU:HB3	5:D:2049:HOH:O	2.15	0.46
1:A:132:GLN:OE1	5:A:1776:HOH:O	2.20	0.46
1:C:246:ARG:NH2	1:C:252:GLU:OE1	2.43	0.46
1:C:185:LYS:HA	1:C:185:LYS:HD3	1.70	0.46
1:C:490:LYS:HG2	5:C:2430:HOH:O	2.15	0.46
1:C:608:TYR:CE2	1:C:612:ASN:ND2	2.84	0.46
1:C:357:THR:O	1:C:549:LEU:HD12	2.16	0.46
1:D:100:ILE:O	1:D:100:ILE:HG13	2.15	0.46
1:D:336:GLN:HG3	5:D:2042:HOH:O	2.15	0.46
1:B:219:HIS:HB2	1:B:433:PRO:HA	1.97	0.46
1:D:411:LYS:CE	5:D:2736:HOH:O	2.56	0.46
1:D:459:VAL:CG1	1:D:461:GLN:NE2	2.78	0.46
1:C:233:GLN:NE2	5:C:2213:HOH:O	2.49	0.45
1:D:308:ARG:CG	1:D:308:ARG:NH1	2.63	0.45
1:B:304:ILE:HG12	5:B:2217:HOH:O	2.17	0.45
1:D:375:SER:HA	5:D:2094:HOH:O	2.17	0.45
1:C:167:HIS:CE1	2:C:801:FAD:C8M	2.85	0.45
1:A:459:VAL:HG22	5:A:2120:HOH:O	2.17	0.45
1:B:283:CYS:HB3	1:B:298:LEU:HD11	1.98	0.45
1:C:398:GLY:HA3	5:C:2523:HOH:O	2.17	0.45
1:C:267:ASN:OD1	1:C:267:ASN:C	2.59	0.45
1:B:432:GLU:HB2	1:B:433:PRO:HD2	1.97	0.45
1:D:98:LYS:HG2	5:D:2364:HOH:O	2.17	0.45
1:D:448:GLN:HE22	3:D:901:ACT:H3	1.82	0.45
1:B:532:PHE:CE1	1:B:538:PRO:HG3	2.51	0.45
1:B:157:VAL:HG21	1:B:324:HIS:HE1	1.82	0.44
1:D:455:SER:OG	1:D:545:LEU:HD11	2.17	0.44
1:C:454:PHE:CE2	3:C:901:ACT:H1	2.52	0.44
1:C:461:GLN:HE21	1:C:461:GLN:CA	2.28	0.44
1:A:81:ASP:O	1:B:83:GLY:N	2.50	0.44
1:B:70:TYR:HA	1:B:615:PRO:HB3	1.99	0.44
1:B:410:GLU:OE2	5:B:2343:HOH:O	2.21	0.44
1:A:225:LYS:CE	1:A:229:GLU:OE2	2.63	0.44
1:C:290:ALA:HA	4:C:905:12P:H122	1.99	0.44
1:D:64:GLU:OE2	1:D:205:TYR:OH	2.35	0.44
1:A:285:ARG:NH1	1:A:287:VAL:HG22	2.32	0.44
1:D:289:ASN:O	4:D:907:12P:H141	2.18	0.44
1:A:150:ARG:NH1	5:A:1483:HOH:O	2.42	0.44
1:D:302:ASP:OD2	1:D:305:SER:OG	2.22	0.44
1:A:537:LEU:HB3	1:A:538:PRO:HD2	1.99	0.44
1:A:593:ASN:ND2	3:A:901:ACT:H3	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:404:HIS:HB3	1:C:405:PRO:HD2	1.99	0.44
1:C:432:GLU:HB2	1:C:451:ARG:HB2	1.99	0.44
1:C:568:THR:O	1:C:604:LYS:HD3	2.17	0.44
1:C:606:CYS:O	1:C:610:LYS:HG3	2.18	0.44
1:C:265:ARG:HA	1:C:266:PRO:C	2.43	0.44
1:C:339:ARG:HA	1:C:340:PRO:HD3	1.90	0.44
1:B:452:ASP:HB3	1:B:454:PHE:CE1	2.52	0.43
1:C:91:LYS:NZ	1:C:452:ASP:OD1	2.51	0.43
1:C:481:GLU:OE2	1:C:484:LYS:NZ	2.48	0.43
1:A:460:GLN:H	1:A:460:GLN:HG3	1.47	0.43
1:B:478:GLU:HG3	1:B:478:GLU:H	1.64	0.43
1:C:104:VAL:O	1:C:108:GLN:HG3	2.17	0.43
1:D:346:PRO:HG2	1:D:350:PRO:HA	2.00	0.43
1:D:363:PHE:HA	1:D:471:TRP:O	2.18	0.43
1:D:541:MET:O	1:D:542:GLU:C	2.60	0.43
1:B:180:ARG:NH1	5:B:2571:HOH:O	2.32	0.43
1:D:288:ARG:O	4:D:907:12P:C15	2.65	0.43
1:B:183:LEU:HA	1:B:183:LEU:HD23	1.78	0.43
1:C:86:ILE:O	1:C:257:ASN:HB2	2.18	0.43
1:D:70:TYR:OH	1:D:613:PHE:O	2.31	0.43
1:D:185:LYS:HG2	1:D:186:ASP:N	2.33	0.43
1:D:389:LEU:HD12	1:D:389:LEU:HA	1.17	0.43
1:A:328:LEU:HD23	1:A:328:LEU:O	2.19	0.43
1:B:385:THR:HB	1:B:388:GLU:HG3	2.00	0.43
1:C:70:TYR:HA	1:C:615:PRO:HB3	2.01	0.43
1:D:328:LEU:CD1	1:D:328:LEU:O	2.66	0.43
1:D:459:VAL:CG1	1:D:461:GLN:HE22	2.32	0.43
1:B:252:GLU:OE2	5:B:1817:HOH:O	2.21	0.43
1:A:104:VAL:HG13	1:A:454:PHE:O	2.19	0.42
1:B:354:SER:O	1:B:355:TYR:CB	2.66	0.42
1:C:63:ARG:HD2	1:C:259:VAL:O	2.19	0.42
1:B:239:ILE:HG21	1:B:239:ILE:HD13	1.85	0.42
1:C:167:HIS:NE2	2:C:801:FAD:HM81	2.11	0.42
1:A:267:ASN:O	1:A:268:THR:C	2.61	0.42
1:A:460:GLN:O	1:A:461:GLN:NE2	2.52	0.42
1:C:390:THR:O	1:C:391:TYR:C	2.60	0.42
1:D:238:GLN:HG2	1:D:239:ILE:N	2.34	0.42
1:C:363:PHE:HA	1:C:471:TRP:O	2.20	0.42
1:C:602:ALA:O	1:C:605:SER:HB3	2.19	0.42
1:D:286:VAL:O	1:D:332:SER:HB3	2.19	0.42
1:C:291:LEU:HG	5:C:2216:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:SER:O	1:B:576:LYS:NZ	2.52	0.42
1:B:363:PHE:HA	1:B:471:TRP:O	2.20	0.42
1:C:228:GLU:HG3	1:C:231:LYS:HZ3	1.85	0.42
1:C:341:ASN:HD21	1:C:343:ALA:CB	2.32	0.42
1:D:554:ARG:O	1:D:564:CYS:HB2	2.20	0.42
1:B:341:ASN:ND2	1:B:341:ASN:C	2.77	0.42
1:C:45:ILE:N	5:C:2639:HOH:O	2.52	0.42
1:B:167:HIS:CD2	1:B:167:HIS:C	2.97	0.42
1:B:386:PRO:HG3	1:B:391:TYR:CE1	2.54	0.42
1:C:537:LEU:HB3	1:C:538:PRO:HD2	2.02	0.42
1:D:285:ARG:HA	1:D:328:LEU:HD13	2.02	0.41
1:A:355:TYR:CZ	1:A:481:GLU:HB2	2.54	0.41
1:B:267:ASN:CA	5:B:2679:HOH:O	2.67	0.41
1:B:454:PHE:CZ	3:B:901:ACT:H1	2.55	0.41
1:C:385:THR:O	1:C:391:TYR:HB2	2.20	0.41
1:C:548:HIS:NE2	3:C:901:ACT:O	2.53	0.41
2:C:801:FAD:H8A	5:C:1581:HOH:O	2.20	0.41
1:D:63:ARG:HD2	1:D:259:VAL:O	2.20	0.41
1:D:264:ASN:OD1	1:D:276:ASN:HA	2.20	0.41
1:A:408:TRP:CD1	1:A:408:TRP:C	2.97	0.41
1:C:167:HIS:CD2	2:C:801:FAD:C8M	2.85	0.41
1:A:215:GLU:OE2	5:A:2805:HOH:O	2.21	0.41
1:D:347:GLU:OE1	4:D:907:12P:H82	2.20	0.41
1:C:201:LYS:HE2	1:C:205:TYR:OH	2.21	0.41
1:B:82:SER:HB2	5:B:1650:HOH:O	2.19	0.41
1:B:380:MET:HE1	1:B:409:ASN:HB3	2.01	0.41
1:A:265:ARG:HA	1:A:266:PRO:C	2.45	0.41
1:C:112:MET:HE3	1:D:102:LYS:HG3	2.02	0.41
1:C:216:SER:HB3	1:C:219:HIS:CB	2.46	0.41
1:C:439:PHE:CE2	1:C:444:PRO:C	2.99	0.41
1:C:603:ILE:O	1:C:607:GLU:HG3	2.20	0.41
1:A:385:THR:CB	1:A:386:PRO:HD2	2.39	0.41
1:B:54:SER:O	1:B:162:GLY:HA2	2.21	0.41
1:B:355:TYR:HA	1:B:480:LYS:O	2.21	0.41
1:C:210:THR:HG23	5:C:2860:HOH:O	2.19	0.41
1:C:286:VAL:O	1:C:332:SER:HB3	2.21	0.41
1:C:487:PHE:CE1	1:C:500:PRO:HB3	2.56	0.41
1:D:72:VAL:HG12	1:D:73:ALA:N	2.36	0.41
1:D:107:ILE:HG12	1:D:167:HIS:HB2	2.03	0.41
1:D:472:ARG:C	1:D:473:PHE:HD1	2.28	0.41
1:A:359:GLN:HG2	1:A:475:GLY:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:ASN:HD21	1:B:343:ALA:HB3	1.86	0.41
1:D:471:TRP:CH2	1:D:526:SER:HA	2.56	0.41
1:C:176:ASP:O	1:C:177:ARG:C	2.64	0.40
1:B:287:VAL:CG2	1:B:299:HIS:CD2	3.04	0.40
1:A:385:THR:OG1	1:A:388:GLU:OE1	2.28	0.40
1:C:180:ARG:HD2	1:C:195:TRP:CD2	2.57	0.40
1:C:576:LYS:HD2	1:C:576:LYS:HA	1.72	0.40
1:D:495:TYR:O	1:D:496:ASN:HB2	2.20	0.40
1:A:98:LYS:C	5:A:2407:HOH:O	2.64	0.40
1:A:459:VAL:CG1	1:A:460:GLN:N	2.84	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%)	551 (96%)	22 (4%)	1 (0%)	43	36
1	B	574/623 (92%)	553 (96%)	20 (4%)	1 (0%)	43	36
1	C	573/623 (92%)	545 (95%)	26 (4%)	2 (0%)	36	28
1	D	572/623 (92%)	546 (96%)	25 (4%)	1 (0%)	43	36
All	All	2293/2492 (92%)	2195 (96%)	93 (4%)	5 (0%)	43	36

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	SER
1	B	82	SER
1	C	458	ALA
1	C	459	VAL
1	D	82	SER

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	504/542 (93%)	491 (97%)	13 (3%)	40	33
1	B	504/542 (93%)	487 (97%)	17 (3%)	32	23
1	C	503/542 (93%)	482 (96%)	21 (4%)	26	16
1	D	502/542 (93%)	490 (98%)	12 (2%)	43	36
All	All	2013/2168 (93%)	1950 (97%)	63 (3%)	35	26

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ILE
1	A	178	GLU
1	A	201	LYS
1	A	269	ASP
1	A	272	GLU
1	A	340	PRO
1	A	389	LEU
1	A	432	GLU
1	A	460	GLN
1	A	462	SER
1	A	468	ILE
1	A	560	LYS
1	A	593	ASN
1	B	45	ILE
1	B	82	SER
1	B	90	LYS
1	B	185	LYS
1	B	215	GLU
1	B	228	GLU
1	B	231	LYS
1	B	252	GLU
1	B	285	ARG
1	B	344	ASN
1	B	347	GLU

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Mol	Chain	Res	Type
1	B	388	GLU
1	B	408	TRP
1	B	459	VAL
1	B	460	GLN
1	B	560	LYS
1	B	576	LYS
1	C	45	ILE
1	C	46	LYS
1	C	91	LYS
1	C	101	ASP
1	C	169	SER
1	C	185	LYS
1	C	206	PHE
1	C	211	ASP
1	C	249	THR
1	C	285	ARG
1	C	304	ILE
1	C	341	ASN
1	C	382	ILE
1	C	385	THR
1	C	388	GLU
1	C	408	TRP
1	C	432	GLU
1	C	490	LYS
1	C	576	LYS
1	C	593	ASN
1	C	619	THR
1	D	45	ILE
1	D	201	LYS
1	D	215	GLU
1	D	308	ARG
1	D	328	LEU
1	D	348	LEU
1	D	383	ARG
1	D	400	SER
1	D	401	THR
1	D	403	LYS
1	D	432	GLU
1	D	593	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	ASN
1	A	132	GLN
1	A	257	ASN
1	A	263	GLN
1	A	341	ASN
1	A	344	ASN
1	A	365	GLN
1	A	461	GLN
1	B	110	GLN
1	B	263	GLN
1	B	276	ASN
1	B	299	HIS
1	B	324	HIS
1	B	341	ASN
1	B	344	ASN
1	B	419	HIS
1	B	460	GLN
1	B	461	GLN
1	B	496	ASN
1	C	108	GLN
1	C	119	ASN
1	C	132	GLN
1	C	224	ASN
1	C	257	ASN
1	C	299	HIS
1	C	324	HIS
1	C	341	ASN
1	C	418	GLN
1	C	461	GLN
1	C	612	ASN
1	D	110	GLN
1	D	237	GLN
1	D	238	GLN
1	D	257	ASN
1	D	263	GLN
1	D	341	ASN
1	D	418	GLN
1	D	419	HIS
1	D	448	GLN
1	D	461	GLN
1	D	496	ASN
1	D	593	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

14 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	$\# Z > 2$
4	12P	A	904	-	15,15,36	0.72	0	14,14,35	0.43	0
2	FAD	C	801	1	58,58,58	1.61	9 (15%)	85,89,89	2.53	29 (34%)
4	12P	C	905	-	13,13,36	0.78	0	12,12,35	0.32	0
3	ACT	D	901	-	3,3,3	1.00	0	3,3,3	0.59	0
4	12P	D	907	-	10,10,36	0.63	0	9,9,35	0.25	0
4	12P	D	906	-	11,11,36	0.53	0	10,10,35	0.27	0
3	ACT	A	901	-	3,3,3	0.80	0	3,3,3	1.58	1 (33%)
2	FAD	B	801	1	58,58,58	1.65	13 (22%)	85,89,89	2.90	37 (43%)
3	ACT	C	901	-	3,3,3	0.82	0	3,3,3	1.98	2 (66%)
2	FAD	A	801	1	58,58,58	1.42	9 (15%)	85,89,89	2.35	27 (31%)
3	ACT	B	901	-	3,3,3	0.89	0	3,3,3	1.64	1 (33%)
4	12P	B	902	-	15,15,36	0.48	0	14,14,35	0.43	0
4	12P	A	903	-	15,15,36	0.69	0	14,14,35	0.52	0
2	FAD	D	801	1	58,58,58	1.26	7 (12%)	85,89,89	2.54	30 (35%)

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
4	12P	A	904	-	-	2/13/13/34	-
2	FAD	C	801	1	-	1/34/50/50	0/6/6/6
4	12P	C	905	-	-	3/11/11/34	-
4	12P	D	907	-	-	3/8/8/34	-
4	12P	D	906	-	-	1/9/9/34	-
2	FAD	B	801	1	-	1/34/50/50	0/6/6/6
2	FAD	A	801	1	-	3/34/50/50	0/6/6/6
4	12P	A	903	-	-	6/13/13/34	-
4	12P	B	902	-	-	4/13/13/34	-
2	FAD	D	801	1	-	2/34/50/50	0/6/6/6

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	FAD	P-O3P	6.59	1.66	1.59
2	B	801	FAD	PA-O3P	5.81	1.65	1.59
2	B	801	FAD	C2A-N1A	3.91	1.40	1.33
2	A	801	FAD	O4B-C4B	-3.89	1.36	1.45
2	A	801	FAD	C8A-N9A	-3.82	1.31	1.37
2	C	801	FAD	PA-O3P	3.31	1.63	1.59
2	B	801	FAD	PA-O1A	-3.14	1.39	1.50
2	D	801	FAD	C8A-N7A	3.13	1.37	1.31
2	B	801	FAD	C1'-C2'	3.08	1.56	1.52
2	C	801	FAD	C8A-N7A	2.95	1.37	1.31
2	B	801	FAD	C8A-N9A	-2.93	1.32	1.37
2	C	801	FAD	C8A-N9A	-2.85	1.32	1.37
2	C	801	FAD	C5X-N5	-2.74	1.34	1.39
2	C	801	FAD	C9A-N10	-2.74	1.36	1.41
2	A	801	FAD	C4A-N3A	-2.68	1.29	1.34
2	D	801	FAD	O4B-C4B	-2.63	1.39	1.45
2	C	801	FAD	C1'-C2'	2.54	1.56	1.52
2	D	801	FAD	C2A-N1A	2.49	1.38	1.33
2	D	801	FAD	C10-N1	2.36	1.38	1.33
2	C	801	FAD	O4B-C4B	-2.36	1.39	1.45
2	B	801	FAD	C6-C5X	2.30	1.43	1.40
2	B	801	FAD	O4B-C4B	-2.29	1.39	1.45
2	B	801	FAD	O3B-C3B	-2.27	1.37	1.43
2	B	801	FAD	C5X-N5	-2.26	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	801	FAD	C1'-C2'	-2.25	1.49	1.52
2	A	801	FAD	C2B-C3B	-2.23	1.47	1.53
2	A	801	FAD	O2B-C2B	-2.22	1.37	1.43
2	C	801	FAD	C2A-N3A	2.19	1.37	1.33
2	A	801	FAD	C5X-N5	-2.18	1.35	1.39
2	B	801	FAD	C10-N1	2.14	1.37	1.33
2	D	801	FAD	P-O3P	2.14	1.61	1.59
2	D	801	FAD	O4-C4	2.14	1.27	1.23
2	B	801	FAD	C7M-C7	2.10	1.54	1.51
2	A	801	FAD	C7M-C7	2.08	1.54	1.51
2	B	801	FAD	C4A-N3A	2.03	1.38	1.34
2	A	801	FAD	C2B-C1B	-2.02	1.47	1.53
2	B	801	FAD	O4'-C4'	-2.01	1.39	1.43
2	A	801	FAD	O3B-C3B	-2.00	1.38	1.43

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	FAD	C4A-N9A-C8A	12.10	118.45	105.74
2	B	801	FAD	N9A-C8A-N7A	-8.97	101.22	113.94
2	C	801	FAD	C4A-N9A-C8A	7.96	114.09	105.74
2	B	801	FAD	N3A-C2A-N1A	-7.05	117.91	128.58
2	D	801	FAD	C4A-N9A-C8A	6.92	113.00	105.74
2	C	801	FAD	O4-C4-C4X	-6.91	108.29	126.53
2	B	801	FAD	C2B-C1B-N9A	6.38	129.15	113.30
2	C	801	FAD	N9A-C8A-N7A	-6.35	104.92	113.94
2	D	801	FAD	N9A-C8A-N7A	-6.22	105.11	113.94
2	D	801	FAD	O3B-C3B-C4B	6.18	128.83	111.08
2	A	801	FAD	O4B-C1B-N9A	6.16	119.91	108.09
2	D	801	FAD	O4-C4-C4X	-6.13	110.36	126.53
2	D	801	FAD	C2B-C1B-N9A	6.00	128.22	113.30
2	A	801	FAD	O3B-C3B-C4B	5.83	127.82	111.08
2	C	801	FAD	O3B-C3B-C4B	5.71	127.47	111.08
2	B	801	FAD	C1B-N9A-C8A	-5.50	114.89	127.09
2	A	801	FAD	N3A-C2A-N1A	-5.29	120.58	128.58
2	D	801	FAD	O4B-C1B-N9A	5.22	118.12	108.09
2	B	801	FAD	C5A-N7A-C8A	5.21	111.64	103.45
2	D	801	FAD	O2B-C2B-C1B	5.10	127.67	110.10
2	C	801	FAD	O2B-C2B-C3B	5.05	127.99	111.82
2	B	801	FAD	N3A-C4A-N9A	5.03	135.73	127.17
2	A	801	FAD	C2B-C1B-N9A	4.95	125.61	113.30
2	A	801	FAD	O2B-C2B-C3B	4.94	127.64	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	FAD	N3A-C2A-N1A	-4.84	121.26	128.58
2	C	801	FAD	C4-C4X-N5	4.81	124.85	118.21
2	A	801	FAD	O4-C4-C4X	-4.80	113.85	126.53
2	C	801	FAD	C2B-C1B-N9A	4.67	124.92	113.30
2	B	801	FAD	C5A-C4A-N9A	-4.53	100.88	105.81
2	A	801	FAD	C5A-C4A-N3A	-4.51	120.51	126.72
2	A	801	FAD	N9A-C8A-N7A	-4.34	107.78	113.94
2	C	801	FAD	N3A-C4A-N9A	4.31	134.50	127.17
2	C	801	FAD	N3A-C2A-N1A	-4.28	122.10	128.58
2	C	801	FAD	C5A-C4A-N3A	-4.19	120.94	126.72
2	B	801	FAD	O2B-C2B-C3B	4.15	125.13	111.82
2	A	801	FAD	C4-N3-C2	-4.12	118.32	125.64
2	A	801	FAD	C4A-C5A-N7A	-4.11	105.88	110.58
2	B	801	FAD	O2B-C2B-C1B	4.03	123.98	110.10
2	A	801	FAD	C5A-N7A-C8A	4.02	109.77	103.45
2	A	801	FAD	C4A-N9A-C8A	4.02	109.95	105.74
2	B	801	FAD	O2-C2-N1	-4.01	115.14	121.80
2	D	801	FAD	C9A-C5X-N5	-3.99	118.22	122.45
2	A	801	FAD	C1B-N9A-C8A	-3.88	118.49	127.09
2	D	801	FAD	C5A-C4A-N3A	-3.84	121.42	126.72
2	C	801	FAD	O2B-C2B-C1B	3.81	123.22	110.10
2	C	801	FAD	O4B-C1B-N9A	3.81	115.40	108.09
2	B	801	FAD	C4-N3-C2	3.76	132.32	125.64
2	B	801	FAD	N3-C2-N1	-3.74	111.56	119.50
2	D	801	FAD	C5A-N7A-C8A	3.73	109.32	103.45
2	A	801	FAD	N3A-C4A-N9A	3.71	133.47	127.17
2	D	801	FAD	N3A-C4A-N9A	3.68	133.43	127.17
2	A	801	FAD	C5B-C4B-C3B	3.64	128.33	115.21
2	D	801	FAD	C4-C4X-N5	3.62	123.21	118.21
2	B	801	FAD	O4-C4-N3	3.60	126.89	120.11
2	D	801	FAD	C4-N3-C2	-3.60	119.25	125.64
2	C	801	FAD	C5A-N7A-C8A	3.50	108.95	103.45
2	B	801	FAD	C5B-C4B-C3B	3.37	127.35	115.21
2	D	801	FAD	C1B-N9A-C8A	-3.35	119.65	127.09
2	C	801	FAD	C1B-N9A-C8A	-3.29	119.80	127.09
2	D	801	FAD	C5B-C4B-C3B	3.29	127.05	115.21
2	C	801	FAD	O4-C4-N3	3.28	126.28	120.11
2	D	801	FAD	O4B-C4B-C5B	3.26	119.78	109.33
2	B	801	FAD	O3B-C3B-C4B	3.22	120.33	111.08
2	B	801	FAD	O4B-C1B-N9A	3.21	114.26	108.09
2	A	801	FAD	C9A-C5X-N5	-3.18	119.08	122.45
2	D	801	FAD	O2A-PA-O3P	3.18	115.86	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	FAD	O2B-C2B-C3B	3.17	121.97	111.82
2	C	801	FAD	C5B-C4B-C3B	3.16	126.59	115.21
2	D	801	FAD	C2A-N3A-C4A	3.13	119.49	111.83
2	B	801	FAD	C9A-N10-C10	-3.13	115.98	120.75
2	A	801	FAD	C2A-N3A-C4A	3.12	119.46	111.83
2	C	801	FAD	O2-C2-N1	-3.11	116.64	121.80
2	D	801	FAD	C4X-C10-N1	-3.10	116.99	124.59
2	D	801	FAD	C5X-N5-C4X	3.10	123.10	118.09
2	D	801	FAD	O3P-PA-O1A	-3.06	101.48	110.70
2	A	801	FAD	C4-C4X-N5	3.04	122.41	118.21
2	C	801	FAD	C2A-N3A-C4A	3.03	119.24	111.83
2	A	801	FAD	C6A-C5A-C4A	2.98	121.25	117.18
2	A	801	FAD	O4-C4-N3	2.96	125.67	120.11
2	C	801	FAD	O5'-P-O1P	-2.92	97.34	108.94
2	D	801	FAD	O4-C4-N3	2.88	125.53	120.11
2	B	801	FAD	O2A-PA-O1A	2.87	125.79	112.44
2	D	801	FAD	C10-C4X-N5	-2.86	118.96	124.81
2	B	801	FAD	C2A-N3A-C4A	2.85	118.78	111.83
2	A	801	FAD	C10-C4X-N5	-2.84	119.02	124.81
2	C	801	FAD	O4'-C4'-C3'	2.83	115.87	109.25
2	D	801	FAD	O2P-P-O5'	2.82	120.36	107.57
2	A	801	FAD	C4X-C4-N3	2.80	120.39	113.25
2	D	801	FAD	C4A-C5A-N7A	-2.78	107.40	110.58
2	B	801	FAD	C4X-C4-N3	-2.77	106.20	113.25
2	C	801	FAD	O4B-C1B-C2B	2.76	112.53	106.62
2	B	801	FAD	O4B-C1B-C2B	2.76	112.52	106.62
2	B	801	FAD	C4-C4X-C10	2.75	121.65	116.93
2	A	801	FAD	O2B-C2B-C1B	2.74	119.56	110.10
2	C	801	FAD	C4A-C5A-N7A	-2.71	107.48	110.58
2	D	801	FAD	O3B-C3B-C2B	2.67	120.38	111.82
2	B	801	FAD	O2P-P-O5'	2.64	119.55	107.57
2	B	801	FAD	C8M-C8-C7	-2.64	115.36	120.76
2	C	801	FAD	C1'-C2'-C3'	2.64	116.81	109.66
2	C	801	FAD	O4B-C4B-C5B	2.60	117.65	109.33
3	C	901	ACT	OXT-C-CH3	2.58	125.87	115.05
2	B	801	FAD	C4A-C5A-N7A	-2.47	107.75	110.58
2	B	801	FAD	C4X-C10-N10	2.47	120.02	116.48
2	C	801	FAD	O3P-PA-O1A	-2.44	103.37	110.70
2	B	801	FAD	C5A-C4A-N3A	-2.42	123.38	126.72
2	B	801	FAD	C10-C4X-N5	-2.41	119.88	124.81
2	B	801	FAD	O2P-P-O3P	-2.41	100.76	107.27
2	C	801	FAD	C4-C4X-C10	-2.40	112.81	116.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	FAD	O3P-PA-O1A	-2.40	103.48	110.70
3	B	901	ACT	OXT-C-O	-2.33	113.37	122.03
2	B	801	FAD	O5'-P-O1P	-2.32	99.76	108.94
2	B	801	FAD	O3P-P-O1P	2.30	117.62	110.70
2	B	801	FAD	C9A-C5X-N5	-2.30	120.02	122.45
2	A	801	FAD	O2-C2-N1	-2.27	118.03	121.80
2	B	801	FAD	C1'-N10-C9A	2.26	125.03	120.63
2	B	801	FAD	C4X-C10-N1	-2.25	119.07	124.59
2	C	801	FAD	C10-C4X-N5	-2.20	120.31	124.81
3	C	901	ACT	OXT-C-O	-2.19	113.91	122.03
2	D	801	FAD	O4'-C4'-C5'	-2.16	105.23	109.99
2	B	801	FAD	C2A-N1A-C6A	2.15	122.26	118.73
2	C	801	FAD	C4-N3-C2	-2.13	121.86	125.64
2	A	801	FAD	C10-N1-C2	2.12	121.43	116.85
2	C	801	FAD	C2B-C3B-C4B	2.09	106.65	102.61
2	A	801	FAD	C3B-C2B-C1B	2.04	105.32	101.46
3	A	901	ACT	OXT-C-CH3	2.04	123.60	115.05
2	D	801	FAD	C2'-C1'-N10	2.03	119.79	110.20
2	A	801	FAD	O4B-C4B-C5B	2.01	115.78	109.33

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	FAD	PA-O3P-P-O5'
2	C	801	FAD	PA-O3P-P-O5'
2	D	801	FAD	PA-O3P-P-O5'
4	D	907	12P	O10-C11-C12-O13
4	B	902	12P	O13-C14-C15-O16
4	A	903	12P	O10-C11-C12-O13
2	D	801	FAD	O4B-C4B-C5B-O5B
4	A	904	12P	O4-C5-C6-O7
4	A	903	12P	C15-C14-O13-C12
4	A	903	12P	C2-C3-O4-C5
4	B	902	12P	O1-C2-C3-O4
4	A	903	12P	O13-C14-C15-O16
4	C	905	12P	C14-C15-O16-C17
4	A	903	12P	O7-C8-C9-O10
2	A	801	FAD	P-O3P-PA-O1A
4	A	903	12P	O4-C5-C6-O7
4	B	902	12P	C15-C14-O13-C12
2	A	801	FAD	P-O3P-PA-O2A

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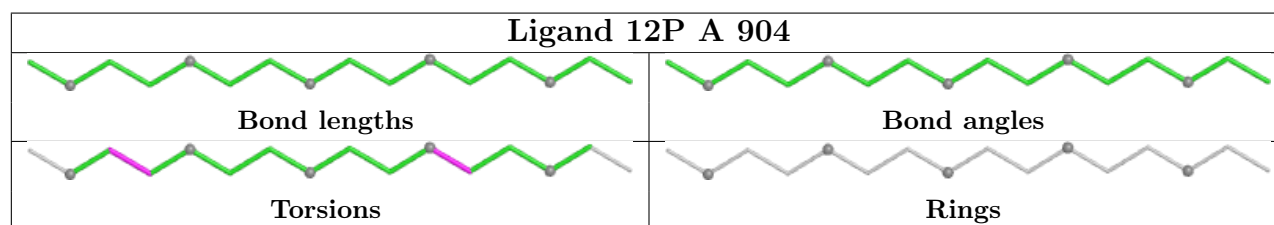
Mol	Chain	Res	Type	Atoms
4	C	905	12P	C18-C17-O16-C15
4	D	906	12P	C9-C8-O7-C6
4	D	907	12P	C8-C9-O10-C11
4	C	905	12P	C8-C9-O10-C11
4	D	907	12P	C15-C14-O13-C12
4	A	904	12P	C15-C14-O13-C12
4	B	902	12P	C2-C3-O4-C5
2	B	801	FAD	O4B-C4B-C5B-O5B

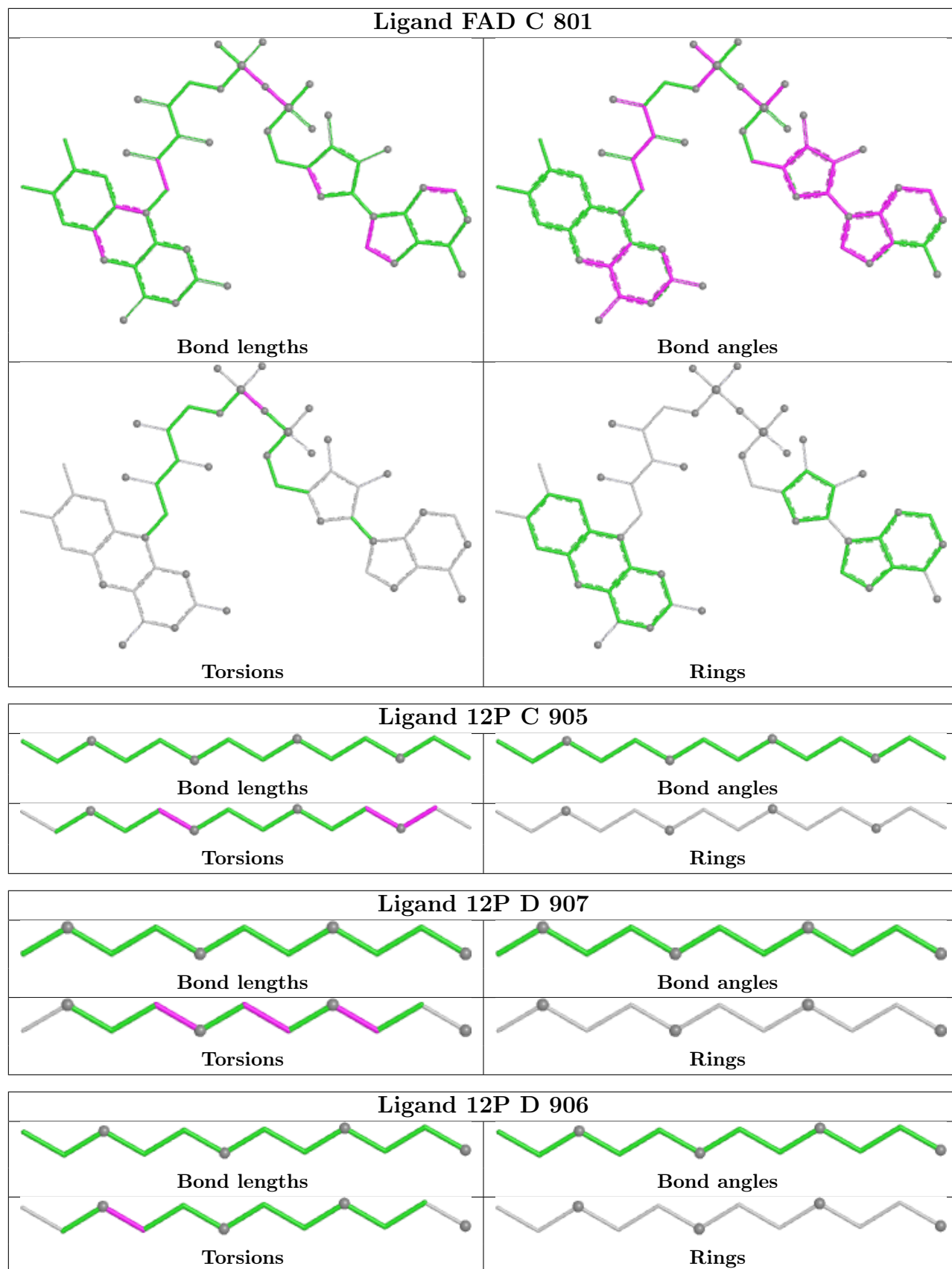
There are no ring outliers.

9 monomers are involved in 34 short contacts:

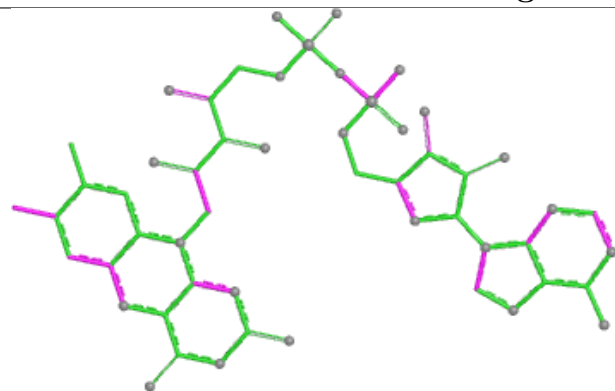
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	801	FAD	14	0
4	C	905	12P	1	0
3	D	901	ACT	2	0
4	D	907	12P	9	0
3	A	901	ACT	3	0
3	C	901	ACT	2	0
2	A	801	FAD	1	0
3	B	901	ACT	2	0
2	D	801	FAD	1	0

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

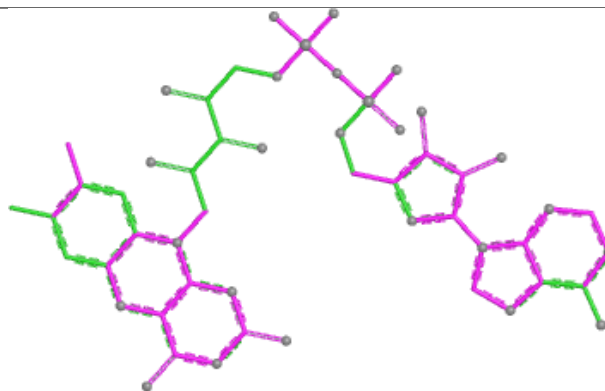




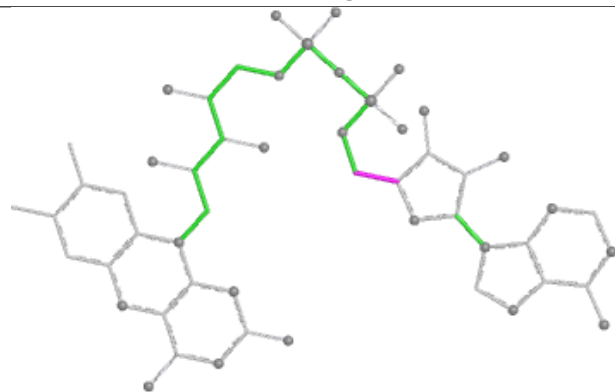
Ligand FAD B 801



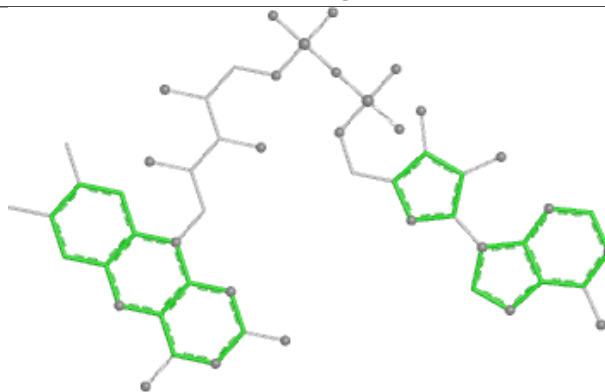
Bond lengths



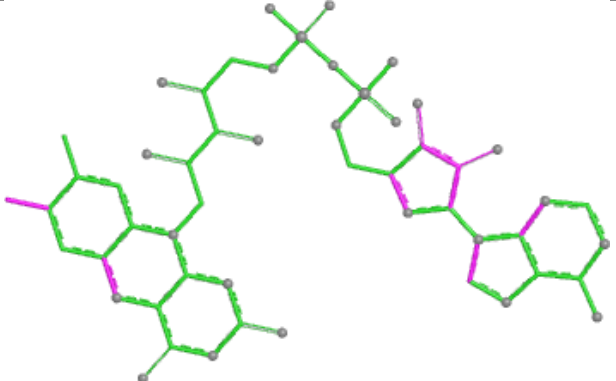
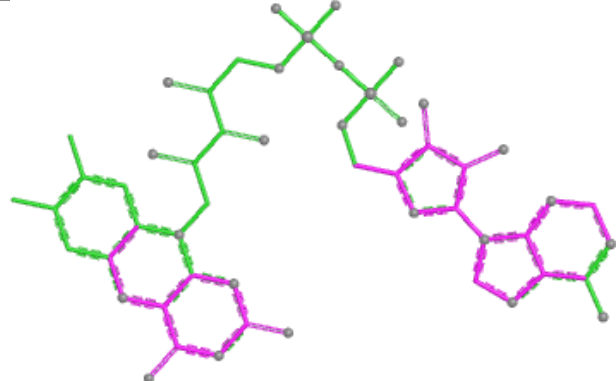
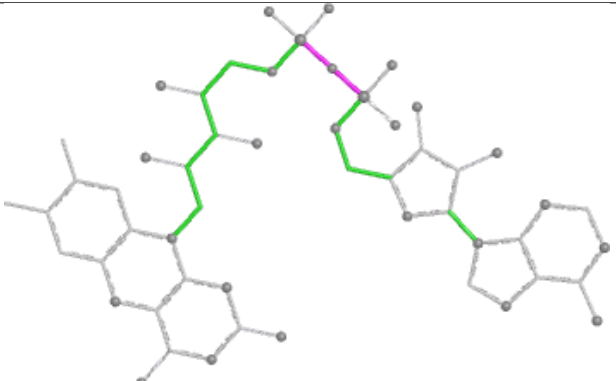
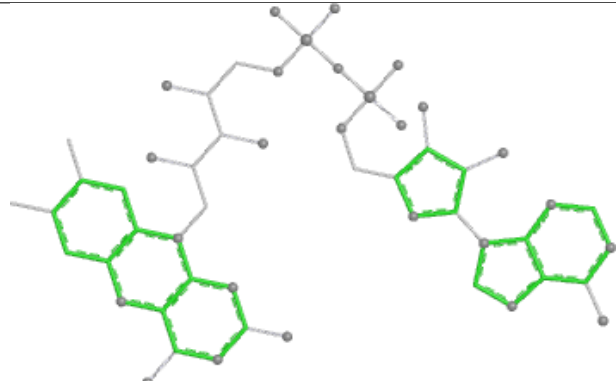
Bond angles



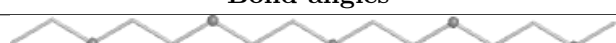
Torsions

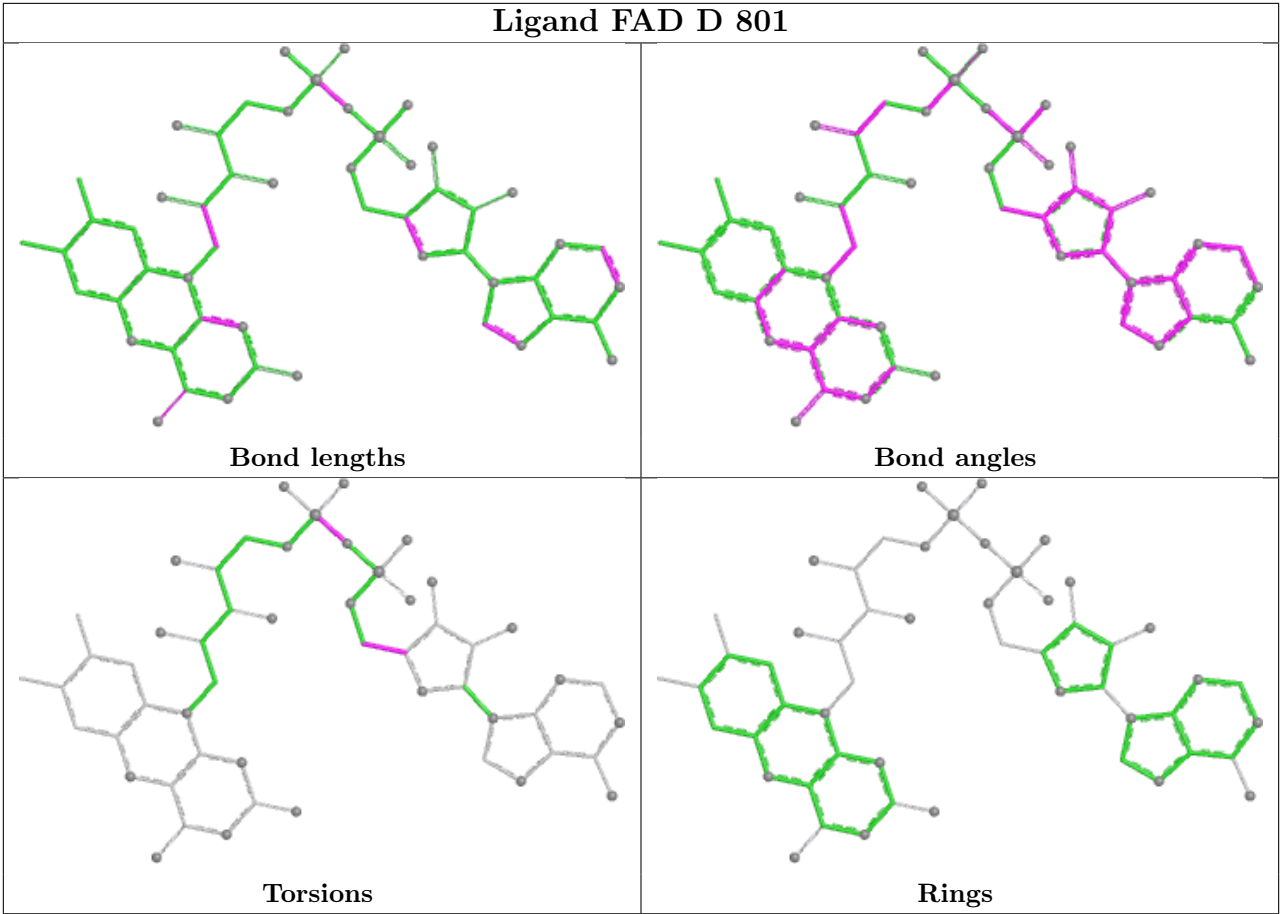


Rings

Ligand FAD A 801	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand 12P B 902	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand 12P A 903	
	
Bond lengths	Bond angles
	
Torsions	Rings



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	166:THR	C	167:HIS	N	1.64

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	12 (2%) 63 70	7, 13, 31, 43	0
1	B	576/623 (92%)	-0.07	13 (2%) 61 68	7, 13, 27, 48	0
1	C	575/623 (92%)	0.21	23 (4%) 42 49	9, 18, 36, 55	0
1	D	574/623 (92%)	0.39	19 (3%) 49 55	10, 22, 41, 51	0
All	All	2301/2492 (92%)	0.13	67 (2%) 53 60	7, 17, 35, 55	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	458	ALA	6.5
1	C	459	VAL	5.9
1	C	458	ALA	5.7
1	D	459	VAL	5.6
1	B	459	VAL	5.3
1	B	458	ALA	4.8
1	B	44	ASP	4.5
1	D	45	ILE	4.3
1	A	459	VAL	4.1
1	D	385	THR	4.0
1	C	45	ILE	3.9
1	C	343	ALA	3.5
1	C	389	LEU	3.4
1	D	309	PHE	3.3
1	B	618	PHE	3.3
1	C	619	THR	3.3
1	B	343	ALA	3.3
1	B	457	GLY	3.2
1	C	387	GLY	3.2
1	B	45	ILE	3.1
1	B	186	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	390	THR	2.9
1	A	458	ALA	2.9
1	B	43	MET	2.9
1	D	618	PHE	2.9
1	A	401	THR	2.8
1	C	383	ARG	2.8
1	A	384	GLY	2.7
1	A	385	THR	2.7
1	D	390	THR	2.7
1	B	345	PRO	2.7
1	C	309	PHE	2.7
1	D	388	GLU	2.6
1	C	385	THR	2.6
1	A	382	ILE	2.6
1	D	346	PRO	2.5
1	D	616	SER	2.5
1	D	383	ARG	2.4
1	D	343	ALA	2.4
1	A	43	MET	2.4
1	C	399	ALA	2.4
1	D	342	PRO	2.4
1	B	342	PRO	2.4
1	A	342	PRO	2.3
1	A	387	GLY	2.3
1	A	45	ILE	2.3
1	C	342	PRO	2.3
1	D	460	GLN	2.3
1	A	618	PHE	2.2
1	C	391	TYR	2.2
1	D	347	GLU	2.2
1	C	101	ASP	2.2
1	C	384	GLY	2.2
1	D	345	PRO	2.2
1	C	81	ASP	2.2
1	C	185	LYS	2.2
1	D	456	TYR	2.1
1	A	386	PRO	2.1
1	C	386	PRO	2.1
1	B	453	ALA	2.1
1	B	269	ASP	2.1
1	C	307	ASP	2.1
1	D	186	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	457	GLY	2.1
1	D	49	VAL	2.1
1	C	347	GLU	2.0
1	C	345	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](#)

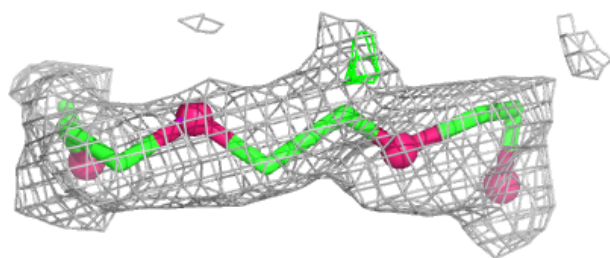
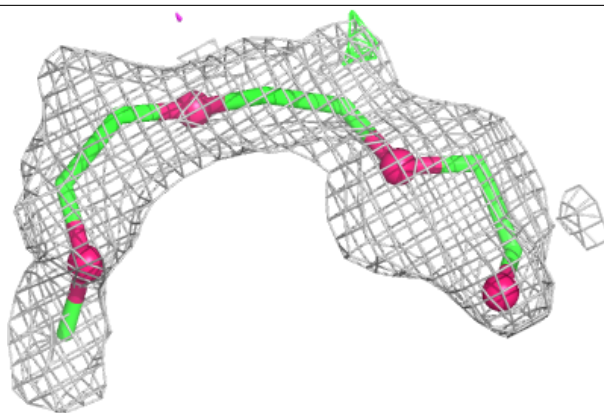
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	12P	D	907	11/37	0.71	0.19	45,47,48,49	0
4	12P	C	905	14/37	0.72	0.19	35,42,44,45	0
4	12P	A	904	16/37	0.83	0.14	23,26,39,40	0
3	ACT	C	901	4/4	0.85	0.14	30,31,31,31	0
4	12P	A	903	16/37	0.86	0.13	21,26,38,38	0
4	12P	D	906	12/37	0.88	0.12	23,27,34,34	0
3	ACT	B	901	4/4	0.89	0.17	27,27,27,29	0
3	ACT	A	901	4/4	0.90	0.12	29,31,32,33	0
4	12P	B	902	16/37	0.91	0.11	22,24,39,42	0
3	ACT	D	901	4/4	0.91	0.10	26,27,28,28	0
2	FAD	D	801	53/53	0.95	0.07	12,16,19,21	0
2	FAD	C	801	53/53	0.97	0.06	7,14,18,19	0
2	FAD	A	801	53/53	0.97	0.06	4,10,13,16	0
2	FAD	B	801	53/53	0.98	0.05	2,9,14,18	0

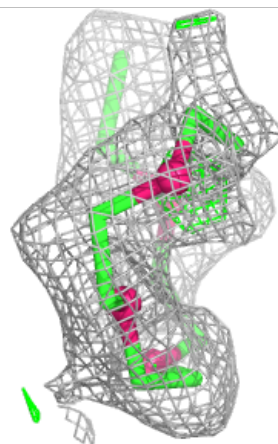
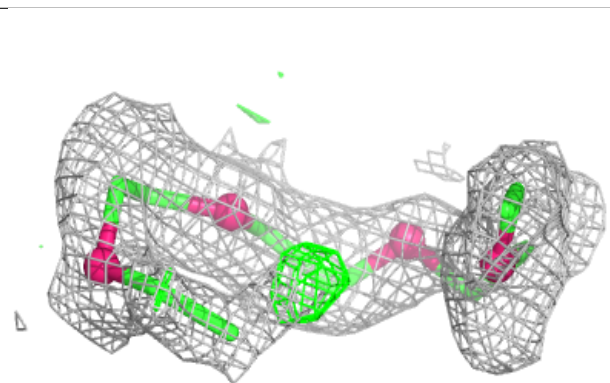
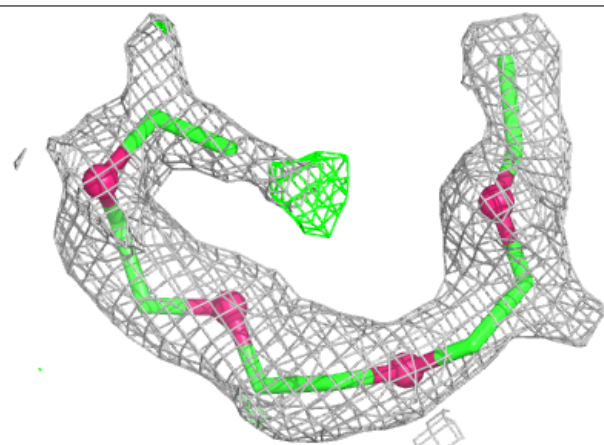
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 12P D 907:

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

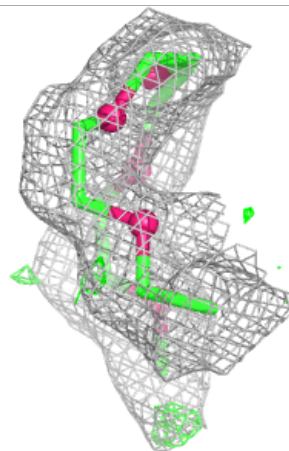
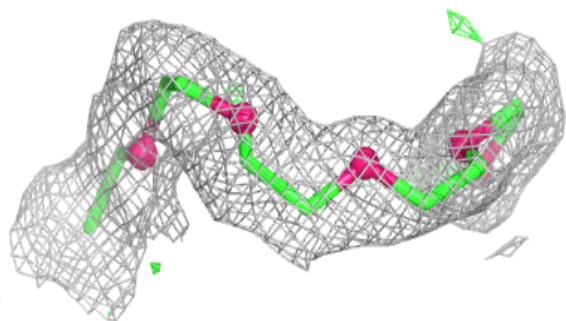
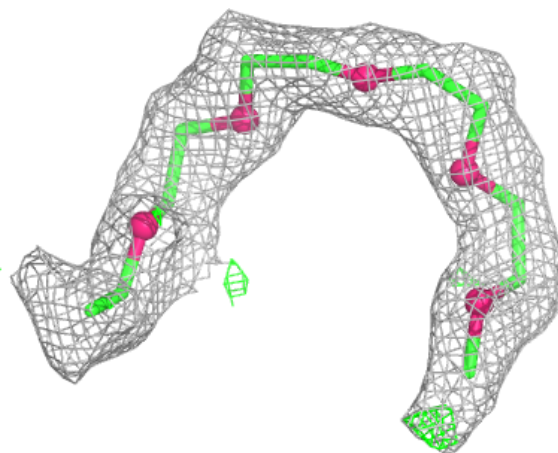
**Electron density around 12P C 905:**

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



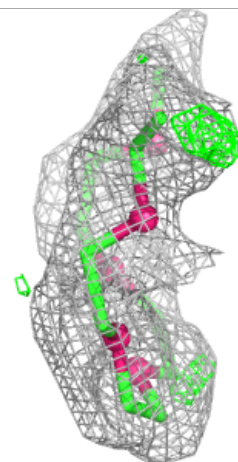
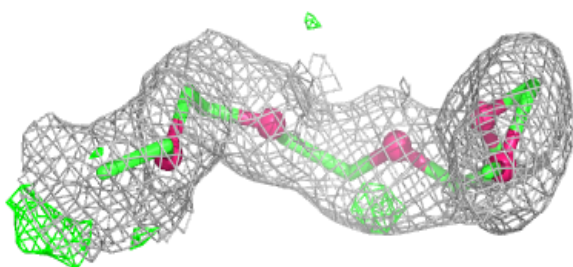
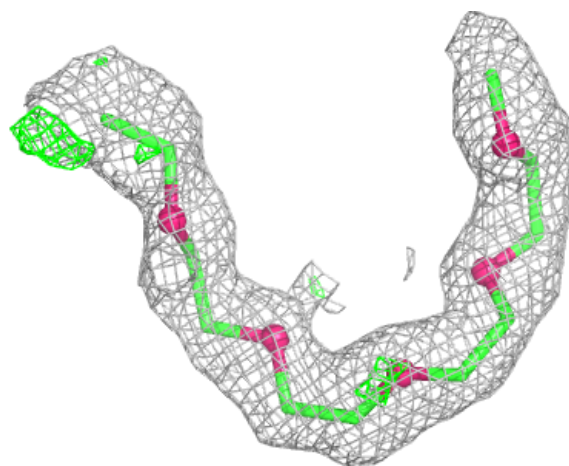
Electron density around 12P A 904:

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



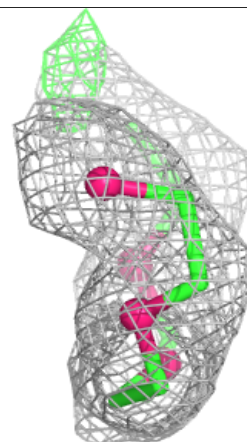
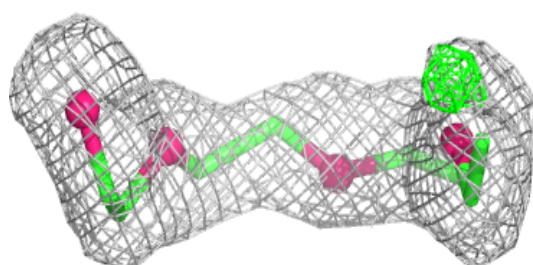
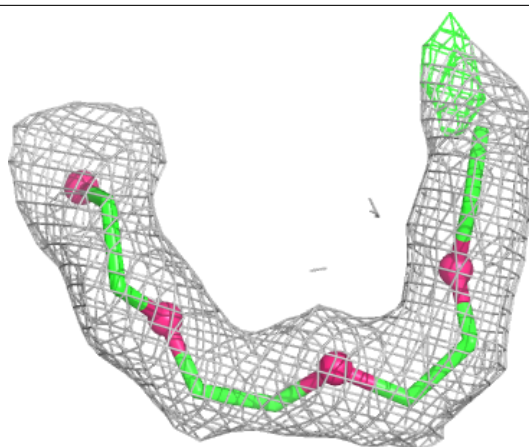
Electron density around 12P A 903:

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



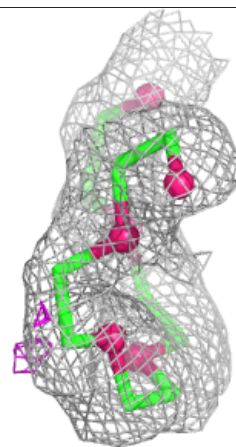
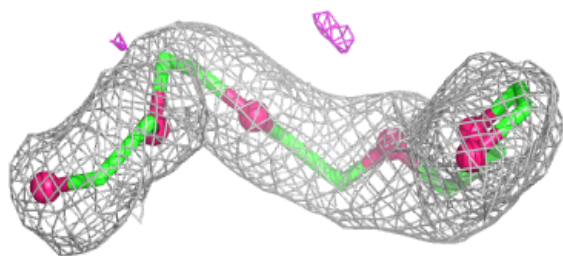
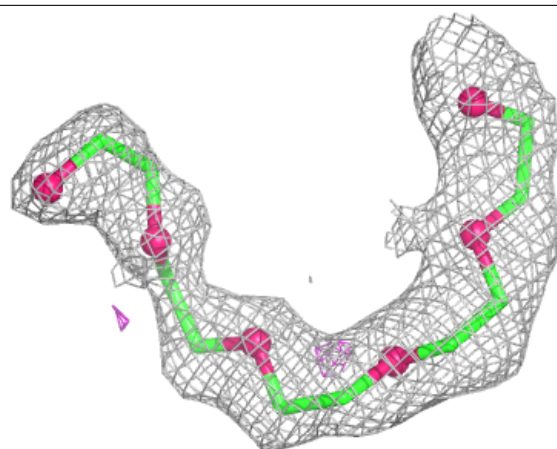
Electron density around 12P D 906:

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

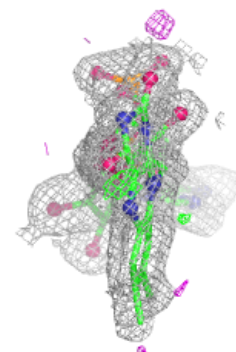
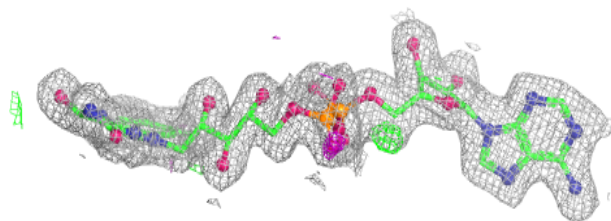
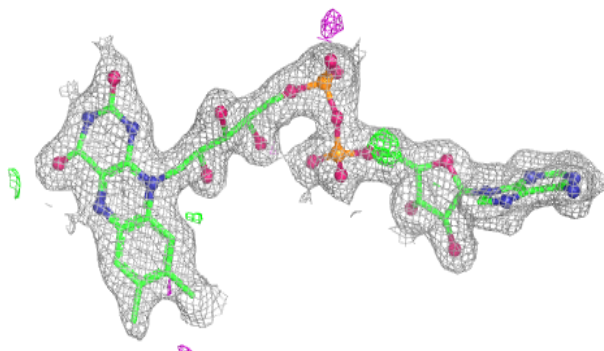


Electron density around 12P B 902:

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

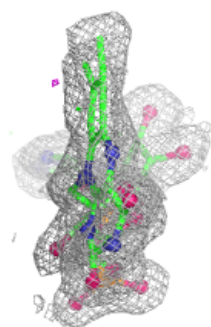
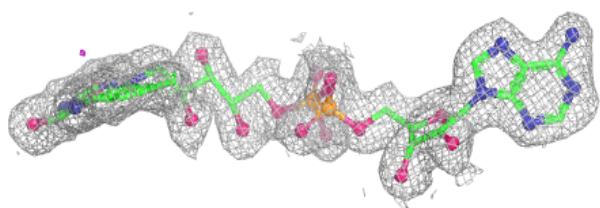
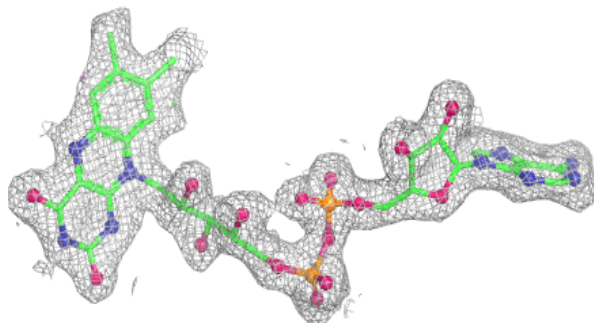
**Electron density around FAD D 801:**

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

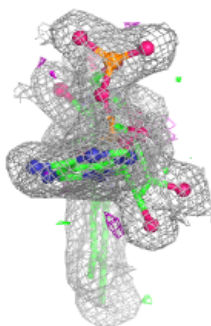
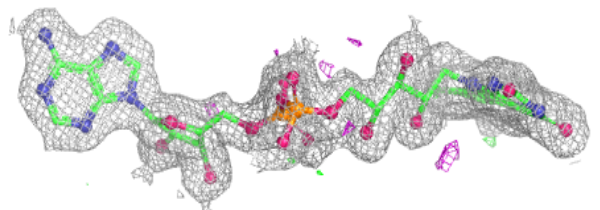
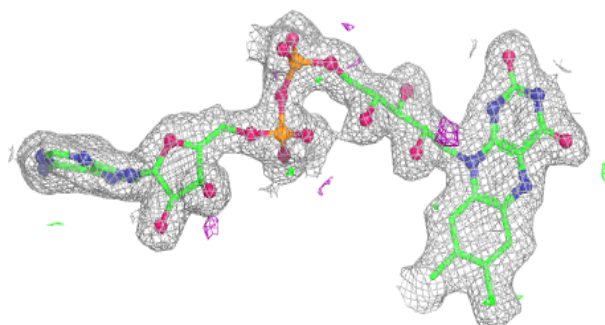


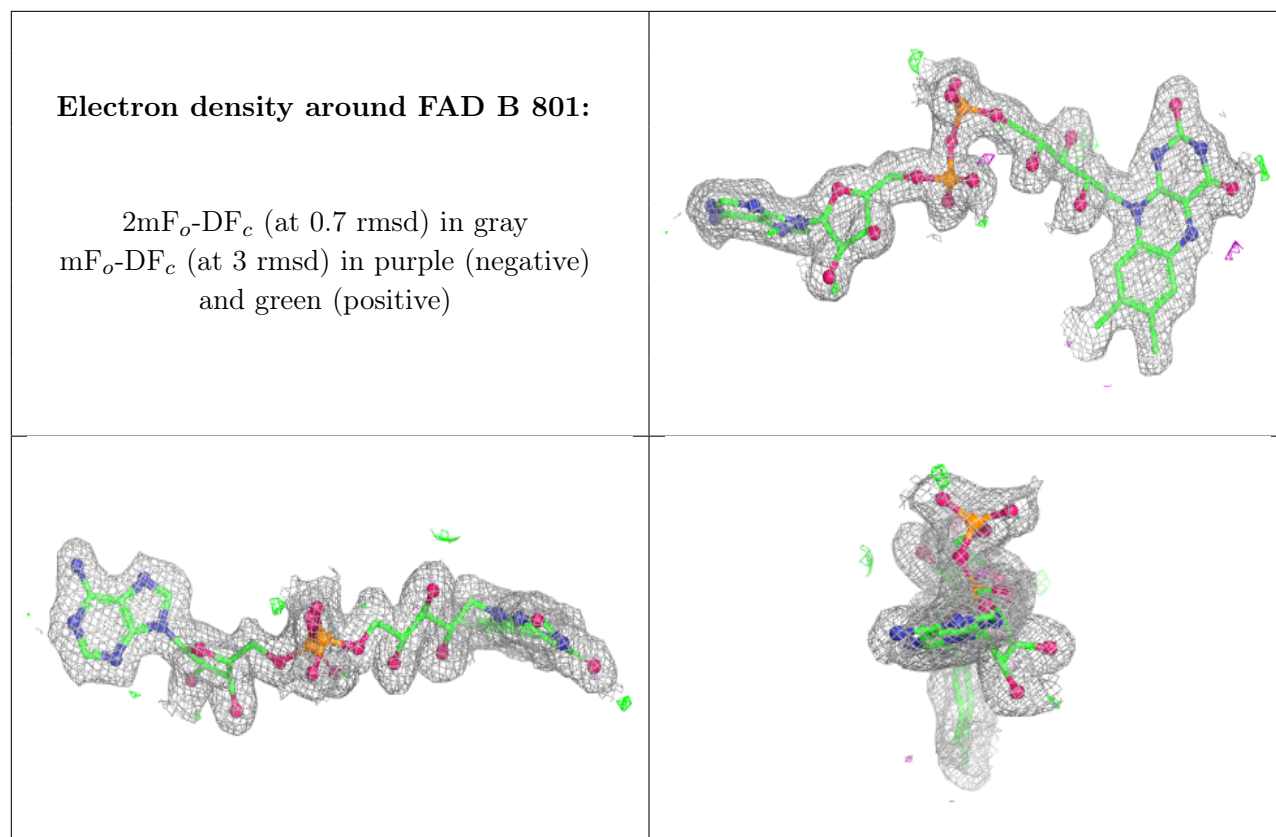
Electron density around FAD C 801:

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

**Electron density around FAD 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.