



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:01 PM UTC

PDB ID : 3V3O / pdb_00003v3o
Title : Crystal structure of TetX2 T280A: an adaptive mutant in complex with tige-cycline
Authors : Walkiewicz, K.; Shamoo, Y.
Deposited on : 2011-12-13
Resolution : 2.90 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

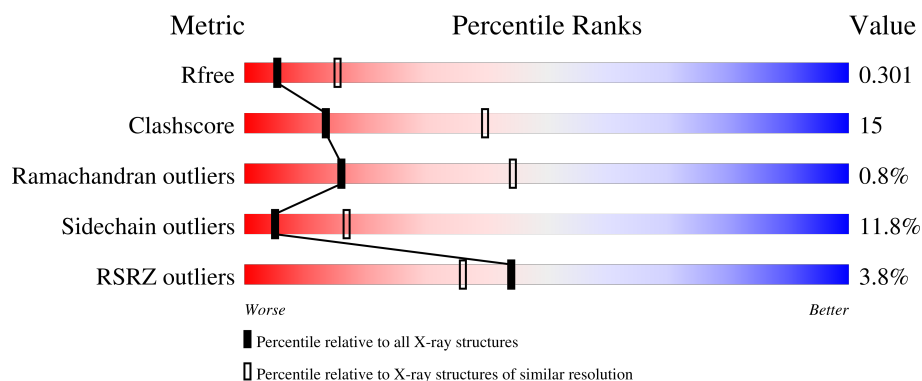
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

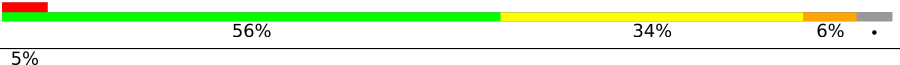
The reported resolution of this entry is 2.90 Å.

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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	378	
1	B	378	
1	C	378	
1	D	378	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11946 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 TetX2 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	S	0	0	0
			2895	1837	497	549	12			
1	B	365	Total	C	N	O	S	0	0	0
			2878	1826	492	548	12			
1	C	364	Total	C	N	O	S	0	0	0
			2866	1817	490	547	12			
1	D	364	Total	C	N	O	S	0	0	0
			2874	1823	492	547	12			

There are 12 discrepancies between the modelled and reference sequences:

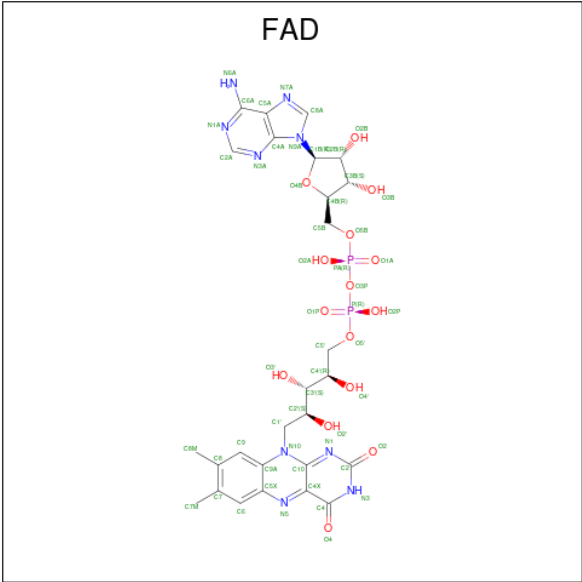
Chain	Residue	Modelled	Actual	Comment	Reference
A	94	LYS	GLU	engineered mutation	UNP Q93L51
A	266	LYS	GLU	engineered mutation	UNP Q93L51
A	280	ALA	THR	engineered mutation	UNP Q93L51
B	94	LYS	GLU	engineered mutation	UNP Q93L51
B	266	LYS	GLU	engineered mutation	UNP Q93L51
B	280	ALA	THR	engineered mutation	UNP Q93L51
C	94	LYS	GLU	engineered mutation	UNP Q93L51
C	266	LYS	GLU	engineered mutation	UNP Q93L51
C	280	ALA	THR	engineered mutation	UNP Q93L51
D	94	LYS	GLU	engineered mutation	UNP Q93L51
D	266	LYS	GLU	engineered mutation	UNP Q93L51
D	280	ALA	THR	engineered mutation	UNP Q93L51

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



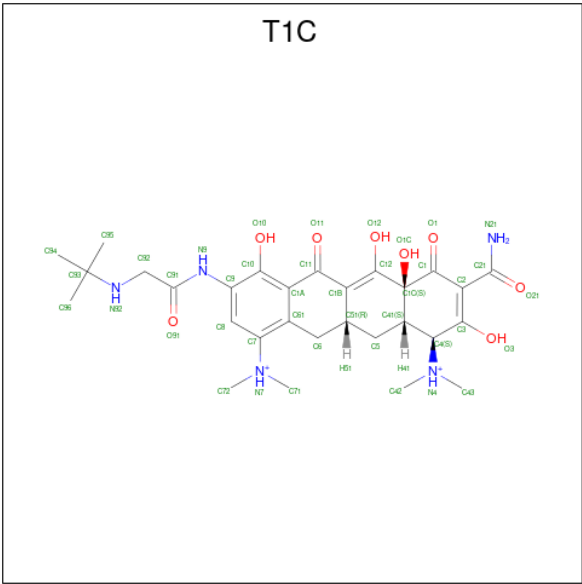
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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



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

- Molecule 4 is TIGECYCLINE (CCD ID: T1C) (formula: C₂₉H₄₁N₅O₈).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			42	29	5	8		
4	B	1	Total	C	N	O	0	0
			42	29	5	8		
4	C	1	Total	C	N	O	0	0
			42	29	5	8		
4	D	1	Total	C	N	O	0	0
			42	29	5	8		

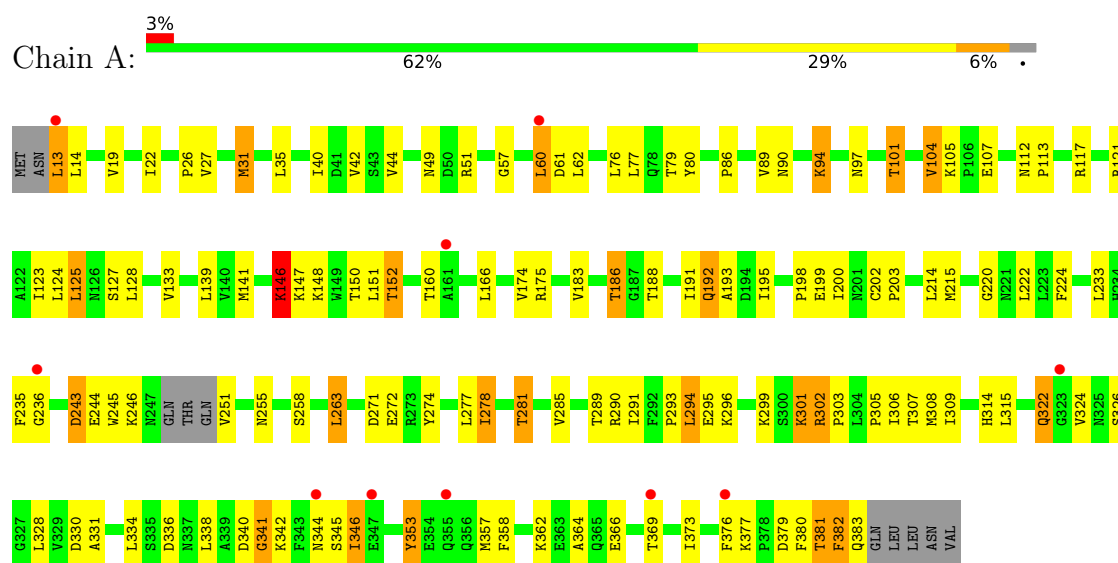
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	7	Total	O	0	0
			7	7		
5	B	9	Total	O	0	0
			9	9		
5	C	2	Total	O	0	0
			2	2		
5	D	5	Total	O	0	0
			5	5		

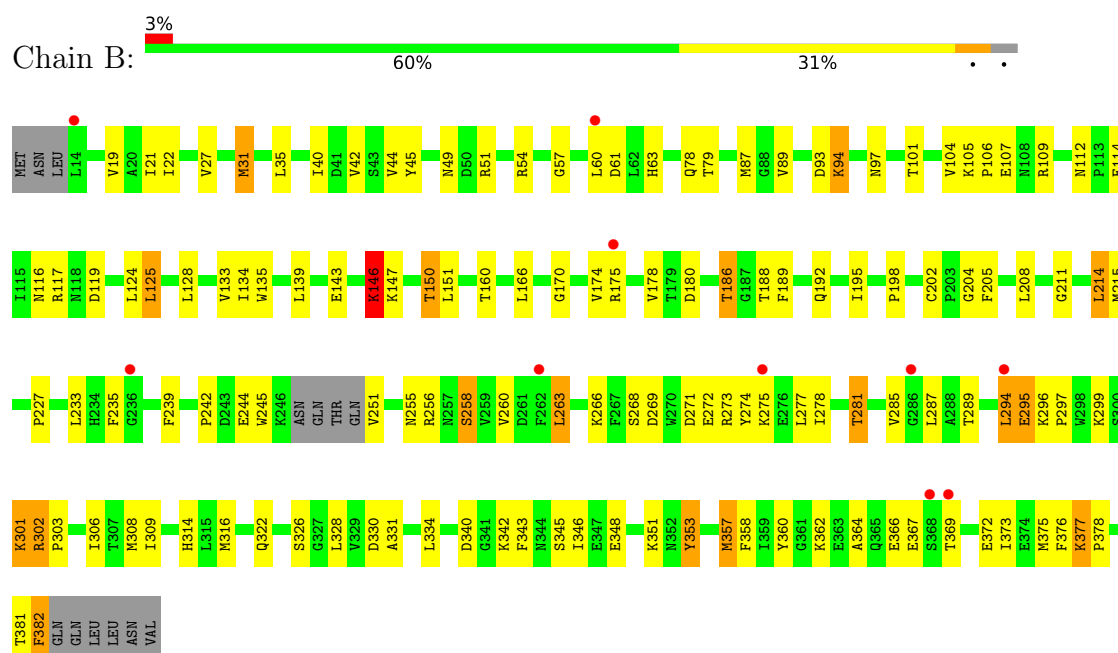
3 Residue-property plots [i](#)

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.

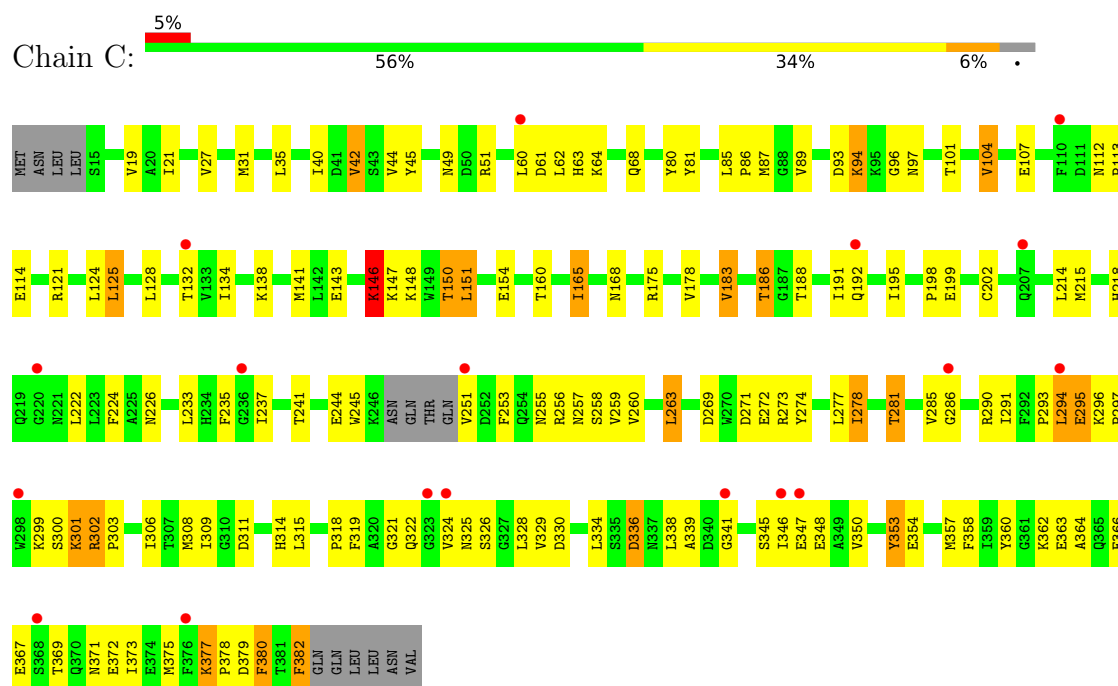
• Molecule 1: TetX2 protein



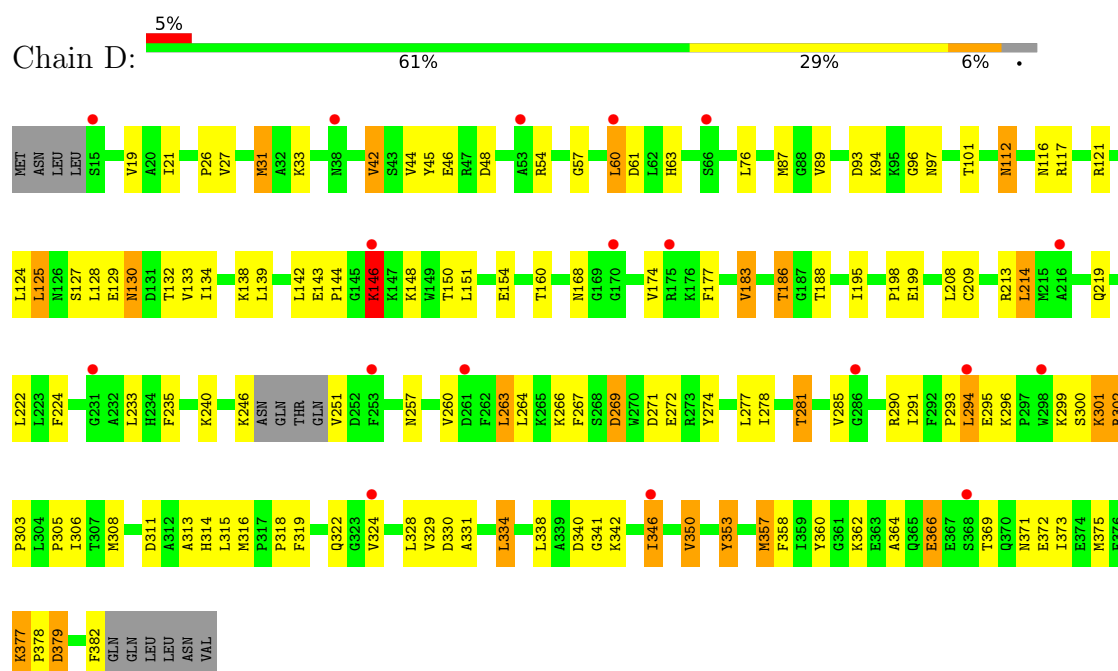
• Molecule 1: TetX2 protein



• Molecule 1: TetX2 protein



• Molecule 1: TetX2 protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	68.13Å 80.08Å 87.24Å 111.02° 89.97° 92.97°	Depositor
Resolution (Å)	48.95 – 2.90 48.95 – 2.90	Depositor EDS
% Data completeness (in resolution range)	93.4 (48.95-2.90) 93.5 (48.95-2.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.232 , 0.297 0.237 , 0.301	Depositor DCC
R_{free} test set	1824 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	58.8	Xtriage
Anisotropy	0.453	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 52.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11946	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.39% 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: T1C, FAD, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.69	0/2953	1.05	10/3991 (0.3%)
1	B	0.69	0/2936	1.04	9/3967 (0.2%)
1	C	0.59	0/2924	1.04	14/3952 (0.4%)
1	D	0.59	0/2932	0.99	9/3960 (0.2%)
All	All	0.64	0/11745	1.03	42/15870 (0.3%)

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	57	GLY	N-CA-C	-7.99	103.90	112.04
1	C	341	GLY	N-CA-C	-7.70	102.46	115.62
1	C	278	ILE	N-CA-C	7.56	118.30	110.36
1	C	302	ARG	CA-C-N	7.50	127.87	119.32
1	C	302	ARG	C-N-CA	7.50	127.87	119.32
1	C	27	VAL	N-CA-C	7.49	117.61	110.42
1	B	27	VAL	N-CA-C	7.19	117.32	110.42
1	B	302	ARG	CA-C-N	7.17	127.50	119.32
1	B	302	ARG	C-N-CA	7.17	127.50	119.32
1	A	57	GLY	N-CA-C	-7.09	104.81	112.04
1	A	341	GLY	N-CA-C	-7.05	104.52	115.73
1	A	27	VAL	N-CA-C	7.03	117.17	110.42
1	D	302	ARG	CA-C-N	6.79	127.06	119.32
1	D	302	ARG	C-N-CA	6.79	127.06	119.32
1	D	27	VAL	N-CA-C	6.62	116.77	110.42
1	D	377	LYS	CA-C-N	6.61	128.10	119.84
1	D	377	LYS	C-N-CA	6.61	128.10	119.84
1	B	57	GLY	CA-C-O	-6.54	117.74	122.45
1	D	341	GLY	N-CA-C	-6.53	105.36	115.73
1	A	302	ARG	CA-C-N	6.51	126.74	119.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	302	ARG	C-N-CA	6.51	126.74	119.32
1	B	377	LYS	CA-C-N	6.46	127.92	119.84
1	B	377	LYS	C-N-CA	6.46	127.92	119.84
1	C	377	LYS	CA-C-N	6.16	127.53	119.84
1	C	377	LYS	C-N-CA	6.16	127.53	119.84
1	A	377	LYS	CA-C-N	6.01	127.35	119.84
1	A	377	LYS	C-N-CA	6.01	127.35	119.84
1	C	168	ASN	N-CA-C	5.86	120.69	112.72
1	A	105	LYS	CA-C-N	5.84	126.25	119.47
1	A	105	LYS	C-N-CA	5.84	126.25	119.47
1	D	168	ASN	N-CA-C	5.76	119.07	112.97
1	D	57	GLY	N-CA-C	-5.54	106.39	112.04
1	C	132	THR	N-CA-C	-5.47	105.48	111.82
1	C	241	THR	CA-C-N	5.35	125.36	119.90
1	C	241	THR	C-N-CA	5.35	125.36	119.90
1	C	226	ASN	CA-C-N	5.29	124.98	119.64
1	C	226	ASN	C-N-CA	5.29	124.98	119.64
1	D	112	ASN	N-CA-C	5.11	116.12	108.76
1	C	273	ARG	N-CA-C	5.08	116.90	111.36
1	B	105	LYS	CA-C-N	5.03	126.13	119.84
1	B	105	LYS	C-N-CA	5.03	126.13	119.84
1	A	278	ILE	N-CA-C	5.02	115.63	110.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2895	0	2859	83	0
1	B	2878	0	2842	82	0
1	C	2866	0	2820	91	0
1	D	2874	0	2842	86	0
2	A	10	0	0	0	0
2	B	20	0	0	0	0
3	A	53	0	31	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	53	0	31	2	0
3	C	53	0	31	2	0
3	D	53	0	31	2	0
4	A	42	0	41	7	0
4	B	42	0	40	2	0
4	C	42	0	41	1	0
4	D	42	0	41	4	0
5	A	7	0	0	0	0
5	B	9	0	0	2	0
5	C	2	0	0	0	0
5	D	5	0	0	1	0
All	All	11946	0	11650	346	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 15.

All (346) 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:B:61:ASP:HB2	1:B:112:ASN:HB2	1.52	0.92
1:B:330:ASP:HB2	1:B:353:TYR:HE1	1.41	0.85
1:B:78:GLN:HG2	1:C:64:LYS:HB3	1.61	0.83
1:B:186:THR:HG22	1:B:188:THR:H	1.45	0.80
1:D:293:PRO:HB2	1:D:295:GLU:HG2	1.62	0.80
1:C:263:LEU:HB3	1:C:278:ILE:HD13	1.64	0.79
1:A:294:LEU:HD21	1:A:314:HIS:HB3	1.65	0.77
1:C:322:GLN:HG2	1:C:364:ALA:HB1	1.65	0.77
1:A:35:LEU:HD22	1:A:40:ILE:HD12	1.65	0.76
1:A:146:LYS:HE3	1:A:147:LYS:H	1.51	0.75
1:D:330:ASP:HB2	1:D:353:TYR:HE1	1.53	0.72
1:D:322:GLN:HG2	1:D:364:ALA:HB1	1.72	0.72
1:C:293:PRO:HB2	1:C:295:GLU:HG2	1.71	0.72
1:C:330:ASP:HB2	1:C:353:TYR:HE1	1.54	0.71
1:C:186:THR:HG22	1:C:188:THR:H	1.56	0.71
1:A:307:THR:HG21	1:A:334:LEU:HD11	1.73	0.70
1:A:166:LEU:HD21	1:A:174:VAL:HG23	1.74	0.70
1:D:186:THR:HG22	1:D:188:THR:H	1.55	0.70
1:C:148:LYS:HD3	1:C:160:THR:HB	1.74	0.70
1:B:93:ASP:OD1	1:B:97:ASN:N	2.22	0.69
1:A:235:PHE:HZ	1:A:281:THR:HG21	1.57	0.69
1:B:117:ARG:NH2	3:B:403:FAD:O2'	2.20	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:VAL:HB	1:A:133:VAL:HG22	1.73	0.69
1:C:61:ASP:HB2	1:C:112:ASN:HB2	1.75	0.69
1:A:61:ASP:HB2	1:A:112:ASN:HB2	1.74	0.68
1:D:330:ASP:HB2	1:D:353:TYR:CE1	2.29	0.67
1:B:146:LYS:HE3	1:B:147:LYS:H	1.58	0.67
1:C:21:ILE:HB	1:C:44:VAL:HG22	1.78	0.66
1:D:235:PHE:HZ	1:D:281:THR:HG21	1.60	0.66
1:A:330:ASP:HB2	1:A:353:TYR:HE1	1.61	0.66
1:B:295:GLU:HG3	1:B:296:LYS:H	1.60	0.65
1:B:21:ILE:HB	1:B:44:VAL:HG22	1.77	0.65
1:B:35:LEU:HD22	1:B:40:ILE:HD12	1.78	0.65
1:A:305:PRO:HB3	1:A:346:ILE:HD12	1.78	0.64
1:D:263:LEU:HB3	1:D:278:ILE:HD13	1.78	0.64
1:A:222:LEU:HD23	1:A:224:PHE:CZ	2.33	0.63
1:A:186:THR:HG22	1:A:188:THR:H	1.62	0.63
1:D:44:VAL:HB	1:D:133:VAL:HG22	1.80	0.63
1:A:293:PRO:HB2	1:A:295:GLU:HG2	1.81	0.62
1:D:290:ARG:HB2	1:D:315:LEU:HD21	1.81	0.62
1:D:302:ARG:NH2	1:D:306:ILE:O	2.25	0.62
1:B:94:LYS:O	1:B:271:ASP:N	2.32	0.61
1:D:121:ARG:HG2	1:D:125:LEU:HD22	1.81	0.61
1:A:299:LYS:O	1:A:302:ARG:HD2	2.00	0.61
1:A:31:MET:HG3	1:A:309:ILE:CD1	2.30	0.61
1:C:373:ILE:HG22	1:C:377:LYS:HE2	1.81	0.61
1:A:148:LYS:HD3	1:A:160:THR:HB	1.82	0.60
1:B:208:LEU:HD23	1:B:214:LEU:HD21	1.82	0.60
1:C:31:MET:HG3	1:C:309:ILE:HD13	1.83	0.60
1:B:348:GLU:HA	1:B:351:LYS:HE3	1.83	0.60
1:B:330:ASP:HB2	1:B:353:TYR:CE1	2.31	0.60
1:A:31:MET:HE1	1:A:334:LEU:HD22	1.82	0.59
1:B:211:GLY:O	5:B:505:HOH:O	2.17	0.59
1:D:21:ILE:HB	1:D:44:VAL:HG22	1.84	0.59
1:C:345:SER:O	1:C:348:GLU:HG2	2.02	0.59
1:D:369:THR:O	1:D:373:ILE:HG12	2.03	0.59
1:D:19:VAL:HB	1:D:42:VAL:HG13	1.85	0.58
1:D:33:LYS:HE2	1:D:127:SER:HB2	1.86	0.58
1:D:219:GLN:NE2	1:D:269:ASP:OD2	2.36	0.58
1:D:271:ASP:OD1	1:D:272:GLU:N	2.36	0.58
1:B:175:ARG:HG2	1:B:308:MET:SD	2.43	0.58
1:A:107:GLU:OE1	1:A:107:GLU:N	2.35	0.57
1:B:180:ASP:OD1	1:B:296:LYS:NZ	2.24	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:GLN:OE1	1:C:81:TYR:OH	2.18	0.57
1:D:314:HIS:NE2	1:D:330:ASP:OD2	2.32	0.57
1:C:244:GLU:HG3	1:C:245:TRP:CD1	2.40	0.56
1:D:294:LEU:HD21	1:D:314:HIS:HB3	1.87	0.56
1:D:295:GLU:HG3	1:D:296:LYS:H	1.70	0.56
1:A:330:ASP:HB2	1:A:353:TYR:CE1	2.40	0.56
1:C:334:LEU:O	1:C:338:LEU:HG	2.05	0.56
1:C:377:LYS:O	1:C:379:ASP:N	2.38	0.56
1:D:130:ASN:OD1	1:D:130:ASN:N	2.37	0.56
3:B:403:FAD:H2'	3:B:403:FAD:N1	2.21	0.56
1:A:271:ASP:OD1	1:A:272:GLU:N	2.38	0.56
1:D:334:LEU:O	1:D:338:LEU:HG	2.05	0.55
1:D:377:LYS:O	1:D:379:ASP:N	2.39	0.55
1:A:290:ARG:HB2	1:A:315:LEU:HD21	1.89	0.55
1:C:271:ASP:OD1	1:C:272:GLU:N	2.38	0.55
1:D:117:ARG:NH2	3:D:402:FAD:O2'	2.26	0.55
1:A:97:ASN:ND2	1:B:366:GLU:HG2	2.21	0.55
1:D:366:GLU:HA	1:D:369:THR:HG22	1.88	0.55
1:C:31:MET:HG3	1:C:309:ILE:CD1	2.37	0.55
1:D:357:MET:HA	1:D:360:TYR:CZ	2.42	0.54
1:C:198:PRO:HB3	1:C:233:LEU:HB2	1.89	0.54
1:C:45:TYR:HE1	1:C:134:ILE:HD12	1.72	0.54
1:B:235:PHE:HZ	1:B:281:THR:HG21	1.73	0.54
1:D:300:SER:H	1:D:301:LYS:HE3	1.72	0.54
1:B:44:VAL:HB	1:B:133:VAL:HG22	1.89	0.54
1:D:209:CYS:HA	1:D:214:LEU:HD23	1.90	0.54
1:D:93:ASP:OD1	1:D:97:ASN:N	2.40	0.53
1:D:277:LEU:O	1:D:281:THR:HG22	2.08	0.53
1:A:60:LEU:HD22	1:A:117:ARG:HG2	1.91	0.53
1:A:222:LEU:HD23	1:A:224:PHE:HZ	1.71	0.53
1:A:86:PRO:HB2	1:A:104:VAL:HG11	1.90	0.53
1:A:94:LYS:O	1:A:271:ASP:N	2.40	0.53
1:D:60:LEU:HG	1:D:324:VAL:HG11	1.89	0.53
1:A:381:THR:O	1:A:382:PHE:HB2	2.08	0.53
1:C:358:PHE:O	1:C:362:LYS:HB2	2.08	0.53
1:D:129:GLU:O	1:D:132:THR:OG1	2.16	0.52
1:B:271:ASP:OD1	1:B:272:GLU:N	2.42	0.52
1:D:324:VAL:HG12	3:D:402:FAD:O2	2.09	0.52
4:A:404:T1C:O11	4:A:404:T1C:O12	2.15	0.52
1:B:244:GLU:HG3	1:B:245:TRP:CD1	2.45	0.52
1:C:375:MET:HG2	1:C:380:PHE:CZ	2.45	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:LEU:HB3	1:A:278:ILE:HD13	1.91	0.52
1:C:369:THR:HA	1:C:372:GLU:HG2	1.91	0.52
1:B:348:GLU:HA	1:B:351:LYS:HB3	1.92	0.51
1:C:357:MET:HA	1:C:360:TYR:CZ	2.46	0.51
1:B:294:LEU:HD21	1:B:314:HIS:HB3	1.92	0.51
1:D:142:LEU:HD12	1:D:174:VAL:HB	1.93	0.51
1:D:358:PHE:O	1:D:362:LYS:HB2	2.11	0.51
1:A:26:PRO:HD2	3:A:403:FAD:O1P	2.11	0.51
1:C:124:LEU:O	1:C:128:LEU:HG	2.11	0.51
1:D:199:GLU:H	1:D:199:GLU:CD	2.18	0.51
1:A:383:GLN:HB3	4:A:404:T1C:H963	1.93	0.51
1:C:321:GLY:O	1:C:325:ASN:ND2	2.44	0.51
1:A:324:VAL:O	1:A:328:LEU:N	2.37	0.51
1:C:324:VAL:HG12	3:C:402:FAD:O2	2.11	0.50
1:D:61:ASP:HB2	1:D:112:ASN:HB2	1.93	0.50
1:B:314:HIS:NE2	1:B:330:ASP:OD2	2.37	0.50
1:C:255:ASN:O	1:C:258:SER:HB3	2.12	0.50
1:A:31:MET:HG3	1:A:309:ILE:HD13	1.92	0.50
1:D:318:PRO:HD2	1:D:319:PHE:CE2	2.45	0.50
1:A:198:PRO:HB3	1:A:233:LEU:HB2	1.93	0.50
1:A:175:ARG:HG2	1:A:308:MET:CE	2.42	0.50
1:A:202:CYS:SG	1:A:233:LEU:HD13	2.52	0.50
1:B:263:LEU:HD23	1:B:278:ILE:HG23	1.94	0.50
1:A:324:VAL:HG12	3:A:403:FAD:O2	2.12	0.50
1:B:268:SER:O	1:B:275:LYS:NZ	2.41	0.50
1:B:357:MET:HE3	1:B:358:PHE:CD1	2.47	0.50
1:B:358:PHE:O	1:B:362:LYS:HB2	2.12	0.50
1:A:77:LEU:HD12	1:A:80:TYR:HD2	1.77	0.49
1:B:31:MET:HG3	1:B:309:ILE:HD12	1.93	0.49
1:D:124:LEU:O	1:D:128:LEU:HG	2.12	0.49
1:C:143:GLU:O	1:C:150:THR:N	2.35	0.49
1:C:314:HIS:NE2	1:C:330:ASP:OD2	2.43	0.49
1:B:214:LEU:HD12	1:B:215:MET:N	2.27	0.49
1:A:328:LEU:O	1:A:331:ALA:HB3	2.13	0.49
1:C:253:PHE:CE2	1:C:286:GLY:HA3	2.48	0.49
1:C:302:ARG:NH2	1:C:306:ILE:O	2.37	0.49
1:A:62:LEU:HB2	1:A:80:TYR:CZ	2.48	0.49
1:A:255:ASN:O	1:A:258:SER:HB3	2.11	0.49
1:C:87:MET:HB3	1:C:87:MET:HE3	1.75	0.48
1:C:222:LEU:O	1:C:237:ILE:HA	2.13	0.48
4:D:401:T1C:O11	4:D:401:T1C:O12	2.27	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:PHE:O	1:A:362:LYS:HB2	2.12	0.48
1:A:86:PRO:HA	1:A:113:PRO:HA	1.95	0.48
1:A:236:GLY:HA3	4:A:404:T1C:H421	1.96	0.48
1:A:243:ASP:OD1	1:A:243:ASP:N	2.47	0.48
1:A:308:MET:O	1:A:353:TYR:OH	2.20	0.48
1:B:166:LEU:HD21	1:B:174:VAL:HG23	1.96	0.48
1:C:371:ASN:O	1:C:375:MET:HG3	2.13	0.48
1:D:146:LYS:HB2	1:D:146:LYS:NZ	2.28	0.48
1:D:302:ARG:HA	1:D:303:PRO:HD3	1.71	0.48
1:D:316:MET:HE1	1:D:364:ALA:HB1	1.96	0.48
1:D:324:VAL:O	1:D:328:LEU:N	2.35	0.48
1:B:375:MET:C	1:B:377:LYS:H	2.22	0.48
1:C:45:TYR:CE1	1:C:134:ILE:HD12	2.49	0.48
1:D:371:ASN:O	1:D:375:MET:HG3	2.13	0.48
1:C:86:PRO:HA	1:C:113:PRO:HA	1.95	0.48
1:C:277:LEU:O	1:C:281:THR:HG22	2.14	0.48
1:D:146:LYS:H	1:D:146:LYS:HG3	1.44	0.48
4:B:405:T1C:O11	4:B:405:T1C:O12	2.21	0.47
1:A:166:LEU:HD13	1:A:306:ILE:HD11	1.96	0.47
1:C:324:VAL:O	1:C:328:LEU:N	2.36	0.47
1:C:330:ASP:HB2	1:C:353:TYR:CE1	2.44	0.47
1:C:363:GLU:O	1:C:367:GLU:HG3	2.14	0.47
1:A:302:ARG:NH2	1:A:306:ILE:O	2.34	0.47
1:A:244:GLU:HG3	1:A:245:TRP:CD1	2.49	0.47
1:B:45:TYR:CE1	1:B:134:ILE:HD12	2.50	0.47
1:B:107:GLU:OE1	1:B:107:GLU:N	2.41	0.47
1:B:116:ASN:HB3	1:B:119:ASP:OD2	2.14	0.47
1:B:215:MET:HB3	1:B:382:PHE:CZ	2.49	0.47
1:C:86:PRO:HB2	1:C:104:VAL:HG11	1.95	0.47
1:D:87:MET:HE2	1:D:213:ARG:HG2	1.96	0.47
1:A:76:LEU:HD13	1:A:123:ILE:HG22	1.97	0.47
1:B:345:SER:O	1:B:348:GLU:HG2	2.15	0.47
1:D:31:MET:HE3	1:D:31:MET:O	2.14	0.47
1:B:255:ASN:O	1:B:258:SER:HB3	2.15	0.47
1:B:296:LYS:HG2	1:B:297:PRO:O	2.15	0.47
1:B:322:GLN:HG2	1:B:364:ALA:HB1	1.97	0.47
1:C:87:MET:HG3	1:C:114:GLU:HG3	1.97	0.47
1:D:45:TYR:HE1	1:D:134:ILE:HD12	1.79	0.46
4:A:404:T1C:H433	4:A:404:T1C:H41	1.62	0.46
1:C:299:LYS:O	1:C:302:ARG:HD2	2.15	0.46
1:C:318:PRO:O	4:C:401:T1C:H433	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:PHE:CZ	1:A:281:THR:HG21	2.45	0.46
1:A:277:LEU:O	1:A:281:THR:HG22	2.16	0.46
1:A:340:ASP:HB3	1:A:342:LYS:HB2	1.96	0.46
1:B:87:MET:HE1	1:B:227:PRO:HD2	1.96	0.46
1:C:146:LYS:H	1:C:146:LYS:HG3	1.37	0.46
1:D:198:PRO:HB3	1:D:233:LEU:HB2	1.97	0.46
1:B:277:LEU:O	1:B:281:THR:HG22	2.15	0.46
1:A:191:ILE:C	1:A:192:GLN:HG2	2.41	0.46
1:B:328:LEU:O	1:B:331:ALA:HB3	2.16	0.46
1:A:90:ASN:OD1	1:A:101:THR:HB	2.16	0.46
1:C:257:ASN:HA	1:C:260:VAL:HB	1.97	0.46
1:D:308:MET:O	1:D:313:ALA:HB2	2.16	0.46
1:A:215:MET:HG2	1:A:224:PHE:HD2	1.80	0.46
1:D:46:GLU:HG3	1:D:48:ASP:H	1.81	0.46
1:D:144:PRO:HD3	1:D:177:PHE:CE2	2.51	0.46
1:D:148:LYS:HD3	1:D:160:THR:HB	1.98	0.46
1:D:198:PRO:HD2	1:D:199:GLU:OE1	2.16	0.46
1:B:189:PHE:HB3	1:B:239:PHE:CE1	2.51	0.46
1:C:138:LYS:HD3	1:C:154:GLU:OE1	2.15	0.46
1:D:144:PRO:HD3	1:D:177:PHE:HE2	1.81	0.46
1:A:295:GLU:HG3	1:A:296:LYS:H	1.81	0.46
1:B:198:PRO:HG3	1:B:233:LEU:H	1.80	0.46
1:C:296:LYS:HZ3	1:C:299:LYS:HG3	1.81	0.46
1:B:106:PRO:HA	1:B:109:ARG:HE	1.81	0.45
1:A:224:PHE:HB2	4:A:404:T1C:H423	1.98	0.45
1:B:316:MET:HE1	1:B:364:ALA:C	2.40	0.45
1:C:198:PRO:HD2	1:C:199:GLU:OE1	2.16	0.45
1:A:307:THR:OG1	1:A:308:MET:N	2.39	0.45
1:C:183:VAL:HG21	1:C:290:ARG:HD3	1.98	0.45
1:C:202:CYS:SG	1:C:233:LEU:HD13	2.57	0.45
1:C:357:MET:HA	1:C:360:TYR:CE2	2.52	0.45
1:D:63:HIS:CD2	4:D:401:T1C:H961	2.51	0.45
1:C:215:MET:HB3	1:C:382:PHE:CZ	2.52	0.45
1:D:299:LYS:O	1:D:302:ARG:HD2	2.17	0.45
1:D:369:THR:HA	1:D:372:GLU:HG2	1.99	0.45
1:B:124:LEU:O	1:B:128:LEU:HG	2.16	0.45
1:C:35:LEU:HD22	1:C:40:ILE:HD12	1.98	0.45
1:B:301:LYS:H	1:B:301:LYS:HD2	1.81	0.45
1:B:343:PHE:CE1	1:B:348:GLU:HG3	2.51	0.45
1:C:198:PRO:HG3	1:C:233:LEU:H	1.81	0.45
1:B:150:THR:HA	1:B:160:THR:HG22	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:ARG:O	1:B:260:VAL:HG23	2.16	0.45
1:A:328:LEU:HD23	1:A:328:LEU:HA	1.85	0.45
1:B:22:ILE:HG21	1:B:139:LEU:HD22	1.98	0.45
1:D:87:MET:HE3	1:D:87:MET:HB3	1.70	0.45
1:A:220:GLY:HA2	1:A:376:PHE:HA	1.99	0.44
1:C:222:LEU:HB3	1:C:224:PHE:HE1	1.82	0.44
1:D:96:GLY:O	1:D:208:LEU:HD11	2.17	0.44
1:D:138:LYS:HD3	1:D:154:GLU:OE1	2.17	0.44
1:B:186:THR:HB	1:B:289:THR:O	2.17	0.44
4:B:405:T1C:H423	4:B:405:T1C:H41	1.66	0.44
1:D:300:SER:N	1:D:301:LYS:HE3	2.32	0.44
1:C:222:LEU:HB3	1:C:224:PHE:CE1	2.52	0.44
1:C:369:THR:O	1:C:373:ILE:HG12	2.16	0.44
1:C:360:TYR:O	1:C:363:GLU:HB3	2.17	0.44
1:D:274:TYR:O	1:D:277:LEU:HB2	2.17	0.44
1:D:375:MET:HG3	1:D:375:MET:H	1.58	0.44
1:A:263:LEU:HD12	1:A:263:LEU:HA	1.80	0.44
1:C:178:VAL:HG22	1:C:306:ILE:HG23	2.00	0.44
1:B:263:LEU:HB3	1:B:278:ILE:HD13	1.98	0.44
1:C:274:TYR:O	1:C:277:LEU:HB2	2.17	0.44
1:D:340:ASP:HB3	1:D:342:LYS:H	1.81	0.44
1:A:199:GLU:H	1:A:199:GLU:CD	2.25	0.43
1:A:236:GLY:HA3	4:A:404:T1C:C42	2.48	0.43
1:C:21:ILE:HG12	1:C:165:ILE:HB	1.99	0.43
1:C:373:ILE:O	1:C:377:LYS:HG3	2.17	0.43
1:D:305:PRO:HB3	1:D:346:ILE:HD12	2.00	0.43
1:A:121:ARG:HG2	1:A:125:LEU:HD22	2.01	0.43
1:B:22:ILE:HD11	1:B:151:LEU:HD23	2.01	0.43
1:C:61:ASP:OD2	1:C:63:HIS:NE2	2.51	0.43
1:D:183:VAL:HG21	1:D:290:ARG:HD3	2.00	0.43
1:A:76:LEU:HD21	1:A:127:SER:HB3	1.99	0.43
1:A:186:THR:HB	1:A:289:THR:O	2.19	0.43
1:C:296:LYS:HG2	1:C:297:PRO:O	2.18	0.43
1:D:31:MET:HE2	1:D:31:MET:HB3	1.68	0.43
1:A:274:TYR:O	1:A:277:LEU:HB2	2.19	0.43
4:A:404:T1C:H951	4:A:404:T1C:H922	1.78	0.43
1:D:301:LYS:CD	1:D:301:LYS:H	2.32	0.43
1:B:170:GLY:O	1:B:175:ARG:NH2	2.42	0.43
1:C:93:ASP:OD1	1:C:96:GLY:N	2.52	0.43
1:D:257:ASN:HA	1:D:260:VAL:HB	2.01	0.43
1:D:26:PRO:HD3	5:D:503:HOH:O	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:328:LEU:O	1:D:331:ALA:HB3	2.18	0.43
1:A:141:MET:HB3	1:A:152:THR:HG23	2.01	0.42
1:B:87:MET:HG3	1:B:114:GLU:HG3	2.01	0.42
1:B:372:GLU:O	1:B:376:PHE:HD2	2.02	0.42
1:D:208:LEU:HD23	1:D:214:LEU:HD21	2.01	0.42
1:B:54:ARG:HH21	1:D:54:ARG:NE	2.17	0.42
1:B:362:LYS:O	1:B:366:GLU:HB2	2.19	0.42
1:D:264:LEU:HD23	1:D:264:LEU:HA	1.87	0.42
1:A:322:GLN:HG2	1:A:364:ALA:HB1	2.01	0.42
1:C:141:MET:HE2	1:C:141:MET:HB3	1.87	0.42
1:C:256:ARG:O	1:C:260:VAL:HG23	2.19	0.42
1:A:22:ILE:HG21	1:A:139:LEU:HD22	2.00	0.42
1:A:146:LYS:HE3	1:A:146:LYS:HB2	1.80	0.42
1:A:369:THR:O	1:A:373:ILE:HG12	2.19	0.42
1:B:299:LYS:O	1:B:302:ARG:HD2	2.19	0.42
1:A:299:LYS:HB3	1:A:301:LYS:HD2	2.01	0.42
1:D:222:LEU:HD21	1:D:375:MET:HE2	2.01	0.42
1:B:369:THR:O	1:B:373:ILE:HG12	2.20	0.42
1:C:235:PHE:HZ	1:C:281:THR:HG21	1.84	0.42
1:D:308:MET:O	1:D:353:TYR:OH	2.35	0.42
1:A:302:ARG:HA	1:A:303:PRO:HD3	1.73	0.42
1:B:204:GLY:HA3	1:B:273:ARG:HG2	2.02	0.42
1:B:343:PHE:CD1	1:B:348:GLU:HG3	2.53	0.42
1:C:302:ARG:HA	1:C:303:PRO:HD3	1.72	0.42
1:A:200:ILE:O	1:A:203:PRO:HD3	2.19	0.42
1:B:61:ASP:OD2	1:B:63:HIS:NE2	2.53	0.42
1:C:318:PRO:HD2	1:C:319:PHE:CE2	2.54	0.42
1:B:180:ASP:H	1:B:296:LYS:NZ	2.18	0.42
1:B:202:CYS:SG	1:B:233:LEU:HD13	2.60	0.42
1:C:146:LYS:HB2	1:C:147:LYS:H	1.72	0.42
1:C:296:LYS:NZ	1:C:299:LYS:HG3	2.34	0.42
1:A:198:PRO:HG3	1:A:233:LEU:H	1.84	0.42
1:B:205:PHE:HD2	1:B:233:LEU:HD11	1.85	0.42
1:B:274:TYR:O	1:B:277:LEU:HB2	2.20	0.42
1:C:151:LEU:HD23	1:C:151:LEU:N	2.35	0.42
1:D:224:PHE:HB2	4:D:401:T1C:O3	2.20	0.42
1:A:193:ALA:HB3	1:A:235:PHE:CE1	2.55	0.41
1:B:125:LEU:HD21	1:B:135:TRP:CZ2	2.55	0.41
1:B:125:LEU:HD21	1:B:135:TRP:HZ2	1.84	0.41
1:C:199:GLU:CD	1:C:199:GLU:H	2.28	0.41
1:A:124:LEU:O	1:A:128:LEU:HG	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:ARG:HG2	1:C:125:LEU:HD22	2.02	0.41
3:C:402:FAD:H2'	3:C:402:FAD:N1	2.35	0.41
1:D:45:TYR:CE1	1:D:134:ILE:HD12	2.55	0.41
1:D:188:THR:HA	1:D:240:LYS:HA	2.01	0.41
1:D:346:ILE:O	1:D:350:VAL:HG13	2.20	0.41
1:B:178:VAL:HG22	1:B:306:ILE:HG23	2.01	0.41
1:B:340:ASP:HB3	1:B:342:LYS:H	1.86	0.41
1:C:175:ARG:HG2	1:C:308:MET:CE	2.50	0.41
1:C:294:LEU:HD12	1:C:294:LEU:HA	1.92	0.41
1:C:354:GLU:HA	1:C:357:MET:HG2	2.02	0.41
1:C:107:GLU:OE1	1:C:107:GLU:N	2.48	0.41
1:C:259:VAL:O	1:C:263:LEU:HB2	2.20	0.41
4:D:401:T1C:H41	4:D:401:T1C:H433	1.72	0.41
1:A:121:ARG:O	1:A:125:LEU:HB2	2.20	0.41
1:B:302:ARG:HA	1:B:303:PRO:HD3	1.75	0.41
1:B:266:LYS:NZ	5:B:506:HOH:O	2.31	0.41
1:C:62:LEU:HB2	1:C:80:TYR:CZ	2.56	0.41
1:C:290:ARG:HB2	1:C:315:LEU:HD21	2.02	0.41
1:A:35:LEU:HD21	1:A:338:LEU:HD12	2.03	0.41
1:C:94:LYS:HD2	1:C:218:HIS:CE1	2.56	0.41
1:C:300:SER:H	1:C:301:LYS:NZ	2.19	0.41
1:C:336:ASP:O	1:C:339:ALA:N	2.54	0.41
1:A:13:LEU:HB2	1:A:341:GLY:HA2	2.03	0.41
1:C:85:LEU:O	1:C:87:MET:HG2	2.21	0.41
1:A:344:ASN:CG	1:A:345:SER:N	2.79	0.40
1:B:330:ASP:HB3	1:B:360:TYR:OH	2.21	0.40
1:C:93:ASP:OD1	1:C:97:ASN:N	2.46	0.40
1:D:266:LYS:HB3	1:D:267:PHE:HD1	1.86	0.40
1:D:269:ASP:OD1	1:D:269:ASP:N	2.48	0.40
1:B:54:ARG:HE	1:D:54:ARG:HE	1.69	0.40
1:A:94:LYS:NZ	1:B:367:GLU:OE2	2.55	0.40
1:B:143:GLU:O	1:B:150:THR:N	2.33	0.40
1:D:334:LEU:HD22	1:D:338:LEU:HD11	2.02	0.40
1:B:242:PRO:HG2	1:B:245:TRP:CZ2	2.56	0.40
1:C:19:VAL:HB	1:C:42:VAL:HG13	2.04	0.40
1:C:191:ILE:C	1:C:192:GLN:HG2	2.47	0.40
1:D:76:LEU:HD21	1:D:127:SER:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	364/378 (96%)	337 (93%)	24 (7%)	3 (1%)	16	44
1	B	361/378 (96%)	333 (92%)	24 (7%)	4 (1%)	11	36
1	C	360/378 (95%)	329 (91%)	28 (8%)	3 (1%)	16	44
1	D	360/378 (95%)	334 (93%)	24 (7%)	2 (1%)	21	51
All	All	1445/1512 (96%)	1333 (92%)	100 (7%)	12 (1%)	16	44

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	LYS
1	A	379	ASP
1	B	146	LYS
1	C	146	LYS
1	C	378	PRO
1	C	380	PHE
1	D	146	LYS
1	D	378	PRO
1	A	382	PHE
1	B	295	GLU
1	B	258	SER
1	B	378	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	314/327 (96%)	273 (87%)	41 (13%)	4	13
1	B	313/327 (96%)	280 (90%)	33 (10%)	6	22
1	C	311/327 (95%)	275 (88%)	36 (12%)	5	18
1	D	313/327 (96%)	276 (88%)	37 (12%)	5	17
All	All	1251/1308 (96%)	1104 (88%)	147 (12%)	5	17

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	14	LEU
1	A	19	VAL
1	A	31	MET
1	A	42	VAL
1	A	49	ASN
1	A	51	ARG
1	A	60	LEU
1	A	79	THR
1	A	89	VAL
1	A	94	LYS
1	A	101	THR
1	A	104	VAL
1	A	125	LEU
1	A	146	LYS
1	A	150	THR
1	A	151	LEU
1	A	152	THR
1	A	183	VAL
1	A	186	THR
1	A	192	GLN
1	A	195	ILE
1	A	214	LEU
1	A	243	ASP
1	A	246	LYS
1	A	251	VAL
1	A	263	LEU
1	A	281	THR
1	A	285	VAL
1	A	291	ILE
1	A	294	LEU
1	A	301	LYS
1	A	322	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	326	SER
1	A	336	ASP
1	A	346	ILE
1	A	353	TYR
1	A	357	MET
1	A	366	GLU
1	A	380	PHE
1	A	381	THR
1	B	19	VAL
1	B	31	MET
1	B	42	VAL
1	B	49	ASN
1	B	51	ARG
1	B	60	LEU
1	B	79	THR
1	B	89	VAL
1	B	94	LYS
1	B	101	THR
1	B	104	VAL
1	B	125	LEU
1	B	146	LYS
1	B	150	THR
1	B	186	THR
1	B	192	GLN
1	B	195	ILE
1	B	214	LEU
1	B	251	VAL
1	B	263	LEU
1	B	269	ASP
1	B	281	THR
1	B	285	VAL
1	B	287	LEU
1	B	294	LEU
1	B	301	LYS
1	B	326	SER
1	B	334	LEU
1	B	346	ILE
1	B	353	TYR
1	B	357	MET
1	B	381	THR
1	B	382	PHE
1	C	42	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	49	ASN
1	C	51	ARG
1	C	60	LEU
1	C	89	VAL
1	C	94	LYS
1	C	101	THR
1	C	104	VAL
1	C	125	LEU
1	C	146	LYS
1	C	150	THR
1	C	151	LEU
1	C	165	ILE
1	C	183	VAL
1	C	186	THR
1	C	195	ILE
1	C	214	LEU
1	C	251	VAL
1	C	263	LEU
1	C	269	ASP
1	C	281	THR
1	C	285	VAL
1	C	291	ILE
1	C	294	LEU
1	C	295	GLU
1	C	301	LYS
1	C	311	ASP
1	C	326	SER
1	C	329	VAL
1	C	336	ASP
1	C	346	ILE
1	C	347	GLU
1	C	350	VAL
1	C	353	TYR
1	C	366	GLU
1	C	382	PHE
1	D	31	MET
1	D	42	VAL
1	D	60	LEU
1	D	89	VAL
1	D	94	LYS
1	D	101	THR
1	D	116	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	125	LEU
1	D	130	ASN
1	D	139	LEU
1	D	143	GLU
1	D	146	LYS
1	D	150	THR
1	D	151	LEU
1	D	183	VAL
1	D	186	THR
1	D	195	ILE
1	D	214	LEU
1	D	246	LYS
1	D	251	VAL
1	D	263	LEU
1	D	269	ASP
1	D	281	THR
1	D	285	VAL
1	D	291	ILE
1	D	294	LEU
1	D	301	LYS
1	D	311	ASP
1	D	329	VAL
1	D	334	LEU
1	D	346	ILE
1	D	350	VAL
1	D	353	TYR
1	D	357	MET
1	D	366	GLU
1	D	379	ASP
1	D	382	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	HIS
1	A	97	ASN
1	B	103	ASN
1	B	196	HIS
1	B	201	ASN
1	C	38	ASN
1	C	108	ASN
1	C	201	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	218	HIS
1	C	325	ASN
1	D	37	GLN
1	D	63	HIS
1	D	201	ASN
1	D	325	ASN
1	D	355	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
2	SO4	A	402	-	4,4,4	0.29	0	6,6,6	0.13	0
2	SO4	B	402	-	4,4,4	0.35	0	6,6,6	0.39	0
3	FAD	A	403	-	58,58,58	1.86	12 (20%)	85,89,89	2.17	27 (31%)
2	SO4	B	404	-	4,4,4	0.26	0	6,6,6	0.12	0
4	T1C	A	404	-	45,45,45	3.74	22 (48%)	56,72,72	2.11	15 (26%)
4	T1C	B	405	-	45,45,45	3.69	23 (51%)	56,72,72	1.87	16 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	T1C	D	401	-	45,45,45	3.59	20 (44%)	56,72,72	1.64	14 (25%)
2	SO4	A	401	-	4,4,4	0.32	0	6,6,6	0.14	0
3	FAD	B	403	-	58,58,58	1.66	10 (17%)	85,89,89	1.77	23 (27%)
2	SO4	B	406	-	4,4,4	0.23	0	6,6,6	0.15	0
3	FAD	C	402	-	58,58,58	1.70	11 (18%)	85,89,89	1.98	23 (27%)
3	FAD	D	402	-	58,58,58	1.69	12 (20%)	85,89,89	2.06	23 (27%)
4	T1C	C	401	-	45,45,45	3.56	20 (44%)	56,72,72	1.65	15 (26%)
2	SO4	B	401	-	4,4,4	0.28	0	6,6,6	0.15	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FAD	A	403	-	-	2/34/50/50	0/6/6/6
4	T1C	A	404	-	-	10/22/80/80	0/4/4/4
4	T1C	B	405	-	-	4/22/80/80	0/4/4/4
4	T1C	D	401	-	-	5/22/80/80	0/4/4/4
3	FAD	B	403	-	-	10/34/50/50	0/6/6/6
3	FAD	C	402	-	-	7/34/50/50	0/6/6/6
3	FAD	D	402	-	-	9/34/50/50	0/6/6/6
4	T1C	C	401	-	-	7/22/80/80	0/4/4/4

All (130) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	404	T1C	C7-C61	12.72	1.55	1.40
4	B	405	T1C	C7-C61	12.34	1.55	1.40
4	C	401	T1C	C7-C61	11.39	1.54	1.40
4	D	401	T1C	C7-C61	11.28	1.54	1.40
4	C	401	T1C	O1-C1	10.63	1.40	1.22
4	A	404	T1C	O1-C1	10.57	1.40	1.22
4	D	401	T1C	O1-C1	10.43	1.40	1.22
4	B	405	T1C	O1-C1	10.38	1.40	1.22
4	A	404	T1C	O11-C11	8.03	1.40	1.23
4	B	405	T1C	O11-C11	7.92	1.39	1.23
4	C	401	T1C	O11-C11	7.79	1.39	1.23
4	D	401	T1C	O11-C11	7.77	1.39	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	401	T1C	C1A-C10	7.12	1.55	1.41
4	C	401	T1C	C1A-C10	6.93	1.54	1.41
4	B	405	T1C	C1A-C10	6.79	1.54	1.41
3	A	403	FAD	C10-N1	6.78	1.46	1.33
4	D	401	T1C	C91-N9	6.49	1.49	1.35
4	C	401	T1C	C91-N9	6.48	1.49	1.35
4	A	404	T1C	C1A-C10	6.43	1.53	1.41
4	B	405	T1C	C91-N9	6.39	1.49	1.35
3	D	402	FAD	C10-N1	6.32	1.46	1.33
3	B	403	FAD	C10-N1	6.29	1.46	1.33
4	A	404	T1C	C91-N9	6.21	1.48	1.35
3	C	402	FAD	C10-N1	6.17	1.45	1.33
4	A	404	T1C	C6-C61	4.94	1.58	1.51
4	B	405	T1C	C6-C61	4.91	1.58	1.51
4	C	401	T1C	C41-C4	4.61	1.59	1.54
4	B	405	T1C	C21-N21	4.57	1.46	1.33
4	D	401	T1C	C6-C61	4.52	1.58	1.51
4	A	404	T1C	C41-C4	4.46	1.58	1.54
4	D	401	T1C	C9-C10	4.28	1.46	1.40
4	C	401	T1C	C9-C10	4.23	1.46	1.40
4	D	401	T1C	C9-N9	4.23	1.50	1.41
4	B	405	T1C	C41-C4	4.17	1.58	1.54
4	C	401	T1C	C6-C61	4.15	1.57	1.51
4	D	401	T1C	C41-C4	4.12	1.58	1.54
4	D	401	T1C	C21-N21	4.07	1.45	1.33
4	A	404	T1C	C9-N9	4.06	1.49	1.41
4	A	404	T1C	C9-C10	3.99	1.46	1.40
4	C	401	T1C	C9-N9	3.97	1.49	1.41
3	B	403	FAD	C2B-C3B	-3.96	1.42	1.53
3	A	403	FAD	C2-N1	3.94	1.45	1.36
3	C	402	FAD	C2B-C3B	-3.94	1.42	1.53
4	B	405	T1C	C9-N9	3.85	1.49	1.41
4	C	401	T1C	C21-N21	3.83	1.44	1.33
4	A	404	T1C	C1C-C41	3.74	1.56	1.53
4	B	405	T1C	C9-C10	3.69	1.45	1.40
4	A	404	T1C	C21-N21	3.65	1.44	1.33
4	A	404	T1C	C51-C1B	-3.64	1.47	1.51
3	D	402	FAD	C2B-C3B	-3.61	1.43	1.53
4	B	405	T1C	O1C-C1C	-3.61	1.36	1.42
3	A	403	FAD	C2B-C3B	-3.49	1.43	1.53
3	A	403	FAD	PA-O3P	-3.47	1.55	1.59
4	B	405	T1C	C2-C21	3.43	1.54	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	404	T1C	O1C-C1C	-3.41	1.37	1.42
4	D	401	T1C	O1C-C1C	-3.39	1.37	1.42
4	C	401	T1C	O1C-C1C	-3.36	1.37	1.42
4	D	401	T1C	C51-C1B	-3.33	1.48	1.51
3	A	403	FAD	P-O3P	-3.27	1.56	1.59
3	D	402	FAD	C6A-N6A	3.26	1.42	1.34
4	B	405	T1C	C1C-C1	-3.18	1.50	1.55
3	A	403	FAD	C5X-N5	-3.17	1.33	1.39
3	A	403	FAD	C6A-N6A	3.15	1.42	1.34
3	C	402	FAD	C6A-N6A	3.10	1.42	1.34
3	B	403	FAD	C6A-N6A	3.09	1.42	1.34
3	B	403	FAD	C2-N1	3.05	1.43	1.36
4	A	404	T1C	C1C-C1	-3.01	1.51	1.55
4	B	405	T1C	C1C-C41	2.96	1.55	1.53
4	D	401	T1C	C8-C9	2.93	1.44	1.39
3	C	402	FAD	O4'-C4'	-2.91	1.37	1.43
3	B	403	FAD	C5X-N5	-2.89	1.34	1.39
4	D	401	T1C	C1C-C1	-2.88	1.51	1.55
4	A	404	T1C	C1B-C12	-2.88	1.32	1.36
4	A	404	T1C	C8-C7	2.84	1.44	1.39
4	C	401	T1C	C51-C1B	-2.82	1.48	1.51
3	D	402	FAD	C2-N1	2.82	1.43	1.36
3	D	402	FAD	C5X-N5	-2.79	1.34	1.39
3	D	402	FAD	C9A-N10	-2.79	1.36	1.41
4	B	405	T1C	C51-C1B	-2.75	1.48	1.51
4	B	405	T1C	C4-C3	2.73	1.57	1.51
4	A	404	T1C	C7-N7	2.72	1.49	1.42
3	C	402	FAD	C5X-N5	-2.69	1.34	1.39
3	C	402	FAD	C9A-N10	-2.65	1.36	1.41
3	D	402	FAD	C4X-N5	2.63	1.36	1.30
3	C	402	FAD	C2-N1	2.62	1.42	1.36
4	C	401	T1C	C8-C9	2.61	1.43	1.39
4	C	401	T1C	C1C-C41	2.60	1.55	1.53
4	A	404	T1C	C4-C3	2.56	1.56	1.51
4	A	404	T1C	C8-C9	2.54	1.43	1.39
4	D	401	T1C	C8-C7	2.51	1.43	1.39
3	B	403	FAD	C2'-C3'	2.51	1.57	1.53
3	A	403	FAD	C9-C9A	2.45	1.43	1.39
3	D	402	FAD	O4'-C4'	-2.44	1.38	1.43
3	C	402	FAD	C8A-N7A	2.43	1.36	1.31
3	C	402	FAD	C4X-N5	2.43	1.36	1.30
4	B	405	T1C	C8-C7	2.42	1.43	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	405	T1C	C7-N7	2.40	1.48	1.42
3	A	403	FAD	C2'-C3'	2.39	1.57	1.53
3	C	402	FAD	C2'-C3'	2.39	1.57	1.53
4	D	401	T1C	C1A-C61	-2.38	1.36	1.40
4	C	401	T1C	C1C-C1	-2.32	1.52	1.55
4	D	401	T1C	C2-C21	2.31	1.52	1.47
3	A	403	FAD	C5'-C4'	2.31	1.54	1.51
4	A	404	T1C	C1A-C61	-2.26	1.36	1.40
4	B	405	T1C	C6-C51	2.26	1.58	1.52
3	B	403	FAD	O4'-C4'	-2.25	1.38	1.43
4	A	404	T1C	O3-C3	2.25	1.40	1.32
4	C	401	T1C	C1A-C61	-2.24	1.36	1.40
4	B	405	T1C	C8-C9	2.22	1.43	1.39
3	A	403	FAD	O4'-C4'	-2.19	1.38	1.43
3	B	403	FAD	C4X-N5	2.18	1.35	1.30
4	D	401	T1C	C7-N7	2.18	1.48	1.42
3	A	403	FAD	C4X-N5	2.17	1.35	1.30
4	C	401	T1C	C4-C3	2.17	1.56	1.51
4	C	401	T1C	C7-N7	2.16	1.48	1.42
4	B	405	T1C	C1A-C61	-2.14	1.37	1.40
3	D	402	FAD	C8A-N9A	-2.11	1.34	1.37
4	D	401	T1C	C1C-C41	2.11	1.55	1.53
3	D	402	FAD	P-O1P	2.11	1.58	1.50
4	C	401	T1C	O3-C3	2.11	1.40	1.32
3	B	403	FAD	C5A-N7A	-2.11	1.35	1.39
3	C	402	FAD	P-O1P	2.11	1.58	1.50
3	D	402	FAD	C2'-C3'	2.10	1.57	1.53
4	C	401	T1C	C8-C7	2.08	1.43	1.39
3	B	403	FAD	C4A-N9A	-2.06	1.33	1.37
4	D	401	T1C	C4-C3	2.06	1.55	1.51
4	B	405	T1C	O3-C3	2.05	1.40	1.32
4	A	404	T1C	C2-C21	2.03	1.51	1.47
3	D	402	FAD	C2-N3	2.02	1.43	1.39
4	B	405	T1C	O12-C12	2.02	1.39	1.32

All (156) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	404	T1C	C41-C1C-C1	7.20	119.31	111.05
3	D	402	FAD	O2P-P-O5'	-6.32	78.92	107.57
3	A	403	FAD	O2P-P-O5'	-6.27	79.14	107.57
4	B	405	T1C	C41-C1C-C1	5.97	117.90	111.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	403	FAD	O2P-P-O3P	5.88	123.17	107.27
3	C	402	FAD	O2P-P-O5'	-5.68	81.84	107.57
3	D	402	FAD	N3A-C2A-N1A	-5.11	120.85	128.58
3	D	402	FAD	O4B-C1B-N9A	4.99	117.67	108.09
3	A	403	FAD	O5'-C5'-C4'	4.94	122.56	109.36
3	B	403	FAD	C5A-C4A-N3A	-4.94	119.92	126.72
3	C	402	FAD	C5A-C4A-N3A	-4.91	119.95	126.72
3	A	403	FAD	C5A-C4A-N3A	-4.72	120.22	126.72
4	A	404	T1C	C61-C7-N7	4.70	124.48	118.87
3	C	402	FAD	O2P-P-O3P	4.65	119.83	107.27
3	C	402	FAD	N3A-C2A-N1A	-4.47	121.82	128.58
4	A	404	T1C	C11-C1B-C12	-4.42	115.31	118.80
4	A	404	T1C	C1C-C1-C2	4.36	122.68	115.75
3	D	402	FAD	C5A-C4A-N3A	-4.32	120.76	126.72
3	C	402	FAD	O3P-P-O1P	4.28	123.58	110.70
3	D	402	FAD	N9A-C8A-N7A	-4.16	108.03	113.94
3	D	402	FAD	O5'-P-O1P	-4.14	92.54	108.94
3	D	402	FAD	O2P-P-O3P	4.11	118.38	107.27
3	A	403	FAD	N3A-C2A-N1A	-4.10	122.38	128.58
3	D	402	FAD	C4A-C5A-N7A	-4.10	105.90	110.58
3	C	402	FAD	O5'-P-O1P	-4.09	92.71	108.94
3	B	403	FAD	N3A-C2A-N1A	-4.01	122.51	128.58
3	A	403	FAD	N9A-C8A-N7A	-4.01	108.25	113.94
3	A	403	FAD	O2A-PA-O3P	3.98	118.03	107.27
4	B	405	T1C	C61-C7-N7	3.98	123.62	118.87
3	D	402	FAD	O3P-P-O1P	3.94	122.56	110.70
3	A	403	FAD	O5'-P-O1P	-3.87	93.61	108.94
4	B	405	T1C	C1C-C1-C2	3.86	121.88	115.75
3	A	403	FAD	O3P-PA-O1A	-3.85	99.12	110.70
3	B	403	FAD	N9A-C8A-N7A	-3.82	108.51	113.94
4	A	404	T1C	C21-C2-C1	-3.70	116.59	120.97
3	C	402	FAD	C4A-C5A-N7A	-3.60	106.47	110.58
3	C	402	FAD	O5'-C5'-C4'	3.57	118.88	109.36
4	A	404	T1C	O1C-C1C-C41	-3.56	101.42	109.30
4	D	401	T1C	C1C-C1-C2	3.56	121.41	115.75
3	D	402	FAD	C2A-N3A-C4A	3.52	120.42	111.83
3	B	403	FAD	C4A-C5A-N7A	-3.47	106.61	110.58
4	C	401	T1C	C1C-C41-C4	3.46	116.38	111.64
4	C	401	T1C	C51-C5-C41	-3.45	104.50	110.38
4	A	404	T1C	O12-C12-C1C	3.43	118.33	113.37
3	D	402	FAD	C5A-N7A-C8A	3.42	108.83	103.45
3	D	402	FAD	O5'-C5'-C4'	3.42	118.49	109.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	405	T1C	C21-C2-C1	-3.40	116.94	120.97
3	B	403	FAD	O2A-PA-O3P	3.40	116.46	107.27
4	B	405	T1C	C2-C21-N21	3.36	125.49	118.64
3	C	402	FAD	C2A-N3A-C4A	3.36	120.03	111.83
3	B	403	FAD	C2A-N3A-C4A	3.32	119.94	111.83
3	A	403	FAD	C4A-C5A-N7A	-3.29	106.81	110.58
3	C	402	FAD	N9A-C8A-N7A	-3.23	109.35	113.94
3	A	403	FAD	C5A-N7A-C8A	3.23	108.53	103.45
4	A	404	T1C	O3-C3-C2	-3.21	117.56	122.93
3	A	403	FAD	C4A-N9A-C8A	3.18	109.08	105.74
4	D	401	T1C	C41-C1C-C1	3.18	114.70	111.05
3	A	403	FAD	C1'-C2'-C3'	3.18	118.27	109.66
4	B	405	T1C	O21-C21-N21	-3.15	115.82	122.89
3	B	403	FAD	C5A-N7A-C8A	3.15	108.40	103.45
3	C	402	FAD	O4B-C1B-N9A	3.13	114.10	108.09
3	A	403	FAD	C2A-N3A-C4A	3.12	119.44	111.83
3	C	402	FAD	C10-C4X-N5	-3.11	118.46	124.81
3	A	403	FAD	N3A-C4A-N9A	3.11	132.46	127.17
3	A	403	FAD	C4X-C10-N1	-3.06	117.09	124.59
4	C	401	T1C	O3-C3-C2	-3.06	117.82	122.93
3	C	402	FAD	C5A-N7A-C8A	3.05	108.25	103.45
3	A	403	FAD	O4-C4-C4X	-3.05	118.48	126.53
3	C	402	FAD	C4X-C10-N10	3.02	120.80	116.48
3	A	403	FAD	C10-N1-C2	2.94	123.21	116.85
3	D	402	FAD	C10-C4X-N5	-2.92	118.85	124.81
3	B	403	FAD	N3A-C4A-N9A	2.91	132.11	127.17
3	A	403	FAD	C5'-C4'-C3'	2.90	117.69	112.22
4	D	401	T1C	O12-C12-C1B	-2.89	117.91	123.52
3	B	403	FAD	C1'-C2'-C3'	2.88	117.46	109.66
4	B	405	T1C	O12-C12-C1B	-2.85	117.99	123.52
4	D	401	T1C	O12-C12-C1C	2.84	117.48	113.37
3	D	402	FAD	C4A-N9A-C8A	2.83	108.71	105.74
4	D	401	T1C	C5-C41-C4	-2.80	109.69	113.73
3	A	403	FAD	C9-C9A-N10	2.79	125.60	121.85
4	B	405	T1C	O12-C12-C1C	2.77	117.38	113.37
3	B	403	FAD	C9-C9A-N10	2.77	125.58	121.85
3	B	403	FAD	C4X-C10-N1	-2.76	117.82	124.59
3	B	403	FAD	C10-N1-C2	2.73	122.77	116.85
4	C	401	T1C	C1C-C1-C2	2.73	120.09	115.75
4	D	401	T1C	O3-C3-C2	-2.71	118.39	122.93
4	A	404	T1C	C72-N7-C71	-2.71	107.49	116.18
3	B	403	FAD	C10-C4X-N5	-2.71	119.28	124.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	404	T1C	O1-C1-C2	-2.69	117.54	123.23
4	C	401	T1C	C5-C41-C4	-2.67	109.87	113.73
4	B	405	T1C	C11-C1B-C12	-2.67	116.69	118.80
4	A	404	T1C	O12-C12-C1B	-2.67	118.34	123.52
3	B	403	FAD	O5'-C5'-C4'	2.66	116.45	109.36
3	B	403	FAD	O4-C4-C4X	-2.65	119.54	126.53
4	C	401	T1C	C1-C1C-C12	2.64	112.97	109.88
3	B	403	FAD	C4A-N9A-C8A	2.63	108.50	105.74
3	B	403	FAD	O3P-P-O1P	2.63	118.62	110.70
4	D	401	T1C	O1-C1-C2	-2.62	117.69	123.23
3	A	403	FAD	C4-C4X-C10	2.61	121.41	116.93
3	C	402	FAD	N3A-C4A-N9A	2.59	131.57	127.17
3	C	402	FAD	C10-N1-C2	2.59	122.45	116.85
3	B	403	FAD	C4'-C3'-C2'	-2.57	109.30	113.57
3	C	402	FAD	C4X-C10-N1	-2.55	118.34	124.59
3	C	402	FAD	C1'-C2'-C3'	2.54	116.53	109.66
3	A	403	FAD	C4'-C3'-C2'	-2.53	109.36	113.57
3	A	403	FAD	C4X-C4-N3	2.51	119.65	113.25
3	B	403	FAD	O2P-P-O1P	-2.50	100.83	112.44
3	C	402	FAD	O2-C2-N3	2.50	123.37	118.58
3	D	402	FAD	C5A-C4A-N9A	2.48	108.52	105.81
4	C	401	T1C	C92-N92-C93	2.48	118.91	115.77
4	D	401	T1C	C6-C61-C1A	2.46	122.31	118.13
3	A	403	FAD	C10-C4X-N5	-2.45	119.80	124.81
3	C	402	FAD	C5A-C4A-N9A	2.45	108.48	105.81
4	C	401	T1C	C6-C61-C1A	2.44	122.28	118.13
3	D	402	FAD	O4-C4-C4X	-2.44	120.10	126.53
4	B	405	T1C	C72-N7-C71	-2.42	108.42	116.18
4	C	401	T1C	O12-C12-C1C	2.40	116.84	113.37
4	C	401	T1C	O12-C12-C1B	-2.37	118.92	123.52
4	B	405	T1C	C1A-C11-C1B	2.36	122.71	118.28
4	C	401	T1C	C92-C91-N9	2.35	120.72	114.84
3	A	403	FAD	O3'-C3'-C4'	2.34	114.25	108.93
4	D	401	T1C	O21-C21-N21	-2.33	117.66	122.89
4	B	405	T1C	C8-C7-N7	-2.33	117.27	120.89
4	B	405	T1C	O11-C11-C1B	-2.32	117.10	121.14
4	A	404	T1C	C8-C7-N7	-2.31	117.29	120.89
3	D	402	FAD	C6A-C5A-N7A	2.31	136.54	132.09
4	B	405	T1C	O1C-C1C-C41	-2.30	104.21	109.30
3	B	403	FAD	C4-C4X-C10	2.30	120.88	116.93
3	D	402	FAD	C10-N1-C2	2.30	121.83	116.85
3	D	402	FAD	O2-C2-N3	2.27	122.94	118.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	401	T1C	C21-C2-C1	-2.26	118.29	120.97
4	D	401	T1C	C1C-C41-C4	2.24	114.70	111.64
3	C	402	FAD	C4-C4X-C10	2.24	120.77	116.93
3	D	402	FAD	C4-C4X-N5	2.23	121.29	118.21
3	B	403	FAD	C4X-C10-N10	2.21	119.64	116.48
3	D	402	FAD	O4B-C4B-C5B	2.21	116.40	109.33
3	A	403	FAD	C9-C9A-C5X	-2.19	116.15	120.03
4	B	405	T1C	C5-C41-C4	-2.19	110.57	113.73
4	A	404	T1C	C5-C41-C4	-2.18	110.59	113.73
4	C	401	T1C	C2-C21-N21	2.17	123.07	118.64
3	A	403	FAD	C6-C5X-C9A	2.17	122.03	119.05
4	B	405	T1C	O1-C1-C2	-2.15	118.68	123.23
4	C	401	T1C	O21-C21-N21	-2.14	118.10	122.89
3	B	403	FAD	C4X-C4-N3	2.13	118.68	113.25
4	A	404	T1C	C61-C6-C51	2.12	115.93	113.12
3	C	402	FAD	O4B-C4B-C5B	2.11	116.09	109.33
4	C	401	T1C	C43-N4-C4	-2.11	109.30	114.10
4	D	401	T1C	O11-C11-C1B	-2.10	117.48	121.14
3	B	403	FAD	O2-C2-N3	2.10	122.62	118.58
4	A	404	T1C	C1C-C41-C4	2.10	114.50	111.64
4	D	401	T1C	C1A-C11-C1B	2.09	122.19	118.28
3	D	402	FAD	N3A-C4A-N9A	2.09	130.72	127.17
4	C	401	T1C	O1C-C1C-C12	-2.05	106.86	110.14
3	D	402	FAD	C4X-C10-N1	-2.04	119.58	124.59
3	C	402	FAD	O4-C4-C4X	-2.04	121.15	126.53
4	D	401	T1C	C11-C1B-C12	-2.01	117.21	118.80

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	403	FAD	C5'-O5'-P-O2P
3	A	403	FAD	C5'-O5'-P-O3P
3	B	403	FAD	C5'-O5'-P-O2P
3	B	403	FAD	C5'-O5'-P-O3P
3	B	403	FAD	PA-O3P-P-O5'
3	C	402	FAD	P-O3P-PA-O5B
3	D	402	FAD	C5B-O5B-PA-O1A
3	D	402	FAD	C5B-O5B-PA-O2A
3	D	402	FAD	C5B-O5B-PA-O3P
4	A	404	T1C	C41-C4-N4-C43
4	A	404	T1C	C3-C2-C21-O21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	404	T1C	C1-C2-C21-O21
4	B	405	T1C	C41-C4-N4-C42
4	C	401	T1C	C91-C92-N92-C93
4	D	401	T1C	C41-C4-N4-C43
4	B	405	T1C	C94-C93-N92-C92
3	D	402	FAD	O4B-C4B-C5B-O5B
4	B	405	T1C	C95-C93-N92-C92
4	A	404	T1C	N9-C91-C92-N92
4	A	404	T1C	O91-C91-C92-N92
3	D	402	FAD	C3B-C4B-C5B-O5B
4	C	401	T1C	O91-C91-C92-N92
4	C	401	T1C	N9-C91-C92-N92
3	D	402	FAD	P-O3P-PA-O5B
4	A	404	T1C	C3-C2-C21-N21
4	C	401	T1C	C3-C2-C21-N21
4	C	401	T1C	C3-C2-C21-O21
4	A	404	T1C	C91-C92-N92-C93
4	D	401	T1C	C10-C9-N9-C91
3	B	403	FAD	C5B-O5B-PA-O1A
3	B	403	FAD	C5'-O5'-P-O1P
3	C	402	FAD	C5B-O5B-PA-O2A
3	C	402	FAD	C5B-O5B-PA-O3P
4	A	404	T1C	C1-C2-C21-N21
4	C	401	T1C	C1-C2-C21-N21
3	B	403	FAD	P-O3P-PA-O2A
4	A	404	T1C	C61-C7-N7-C71
3	C	402	FAD	C2B-C1B-N9A-C8A
4	D	401	T1C	C8-C9-N9-C91
4	D	401	T1C	N9-C91-C92-N92
4	B	405	T1C	C96-C93-N92-C92
3	C	402	FAD	O4B-C1B-N9A-C8A
3	B	403	FAD	C2B-C1B-N9A-C8A
3	D	402	FAD	C2B-C1B-N9A-C8A
3	B	403	FAD	P-O3P-PA-O1A
3	C	402	FAD	P-O3P-PA-O1A
3	D	402	FAD	P-O3P-PA-O1A
3	C	402	FAD	O4B-C4B-C5B-O5B
4	D	401	T1C	O91-C91-C92-N92
4	C	401	T1C	C41-C4-N4-C42
4	A	404	T1C	C8-C7-N7-C71
3	B	403	FAD	O4B-C1B-N9A-C8A
3	D	402	FAD	O4B-C1B-N9A-C8A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	403	FAD	O4B-C4B-C5B-O5B

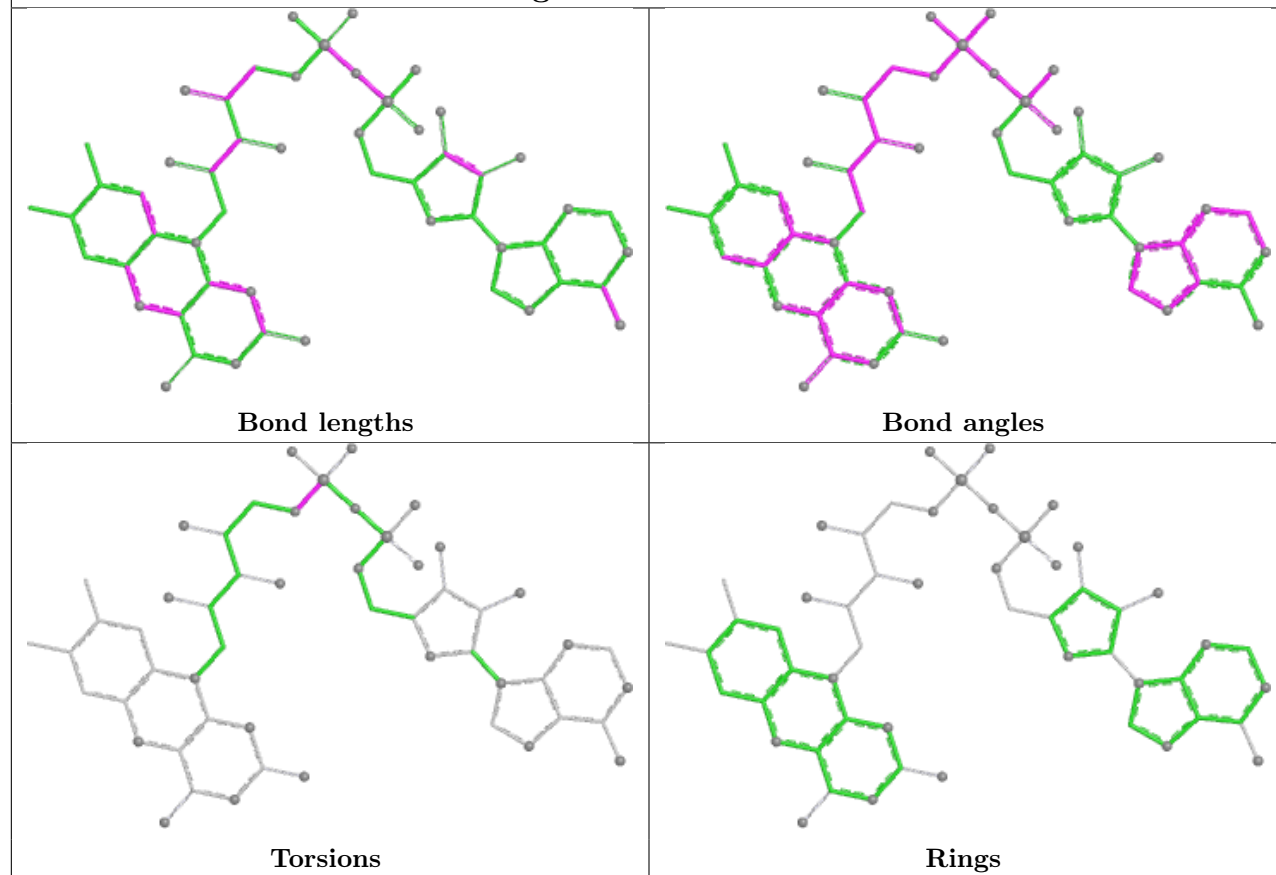
There are no ring outliers.

8 monomers are involved in 22 short contacts:

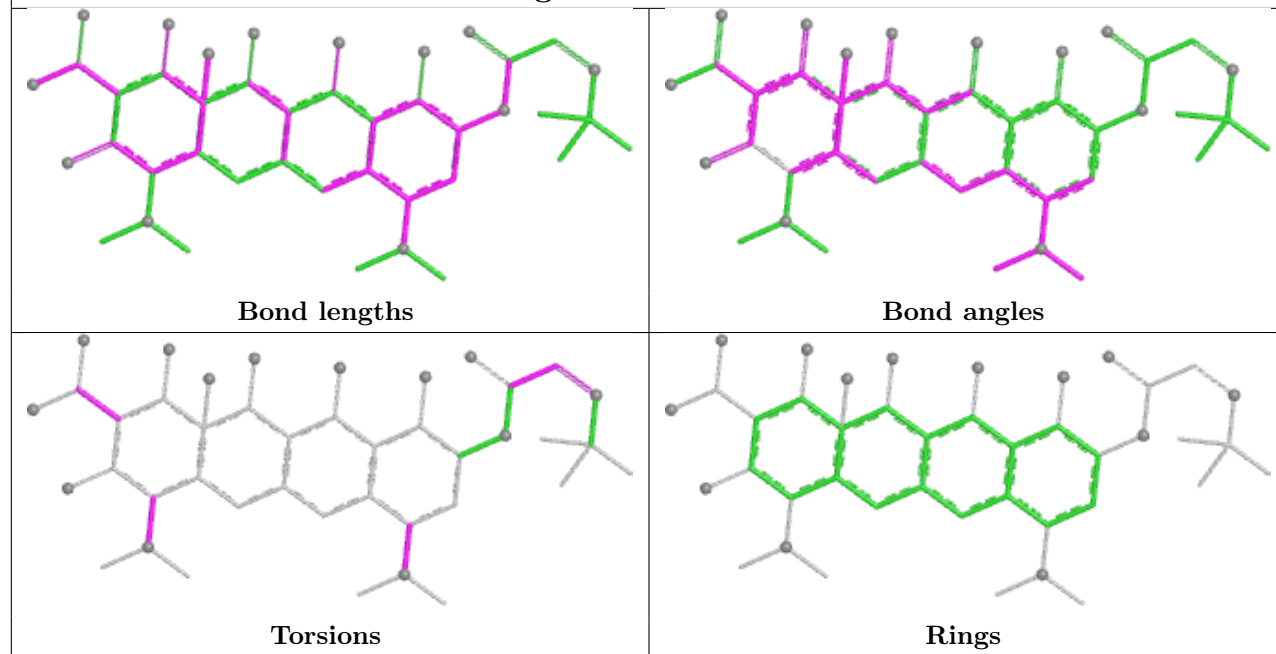
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	403	FAD	2	0
4	A	404	T1C	7	0
4	B	405	T1C	2	0
4	D	401	T1C	4	0
3	B	403	FAD	2	0
3	C	402	FAD	2	0
3	D	402	FAD	2	0
4	C	401	T1C	1	0

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.

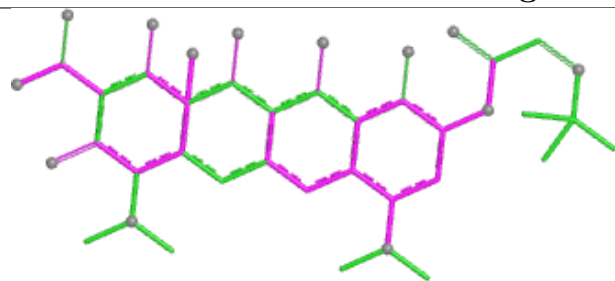
Ligand FAD A 403



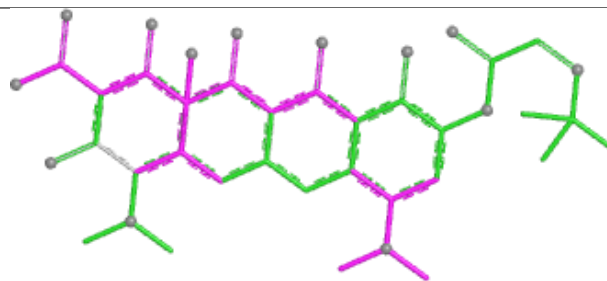
Ligand T1C A 404



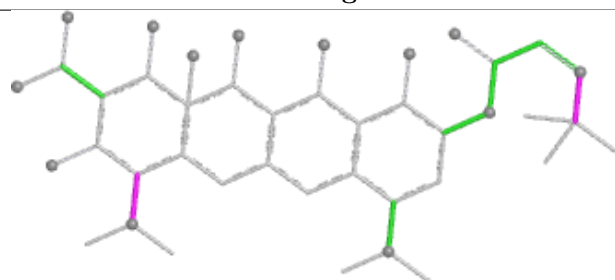
Ligand T1C B 405



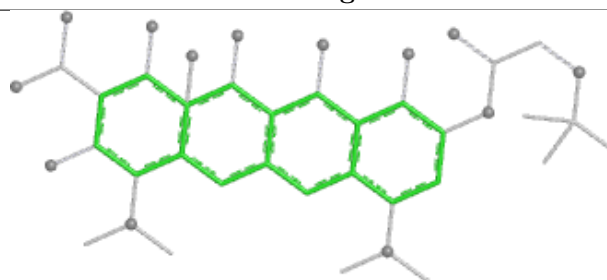
Bond lengths



Bond angles

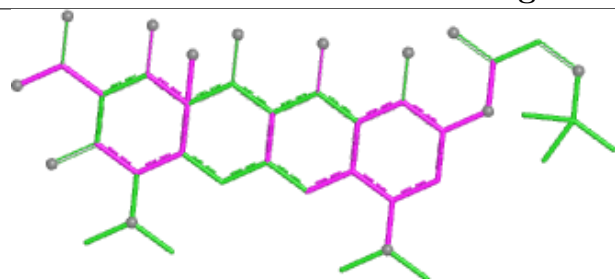


Torsions

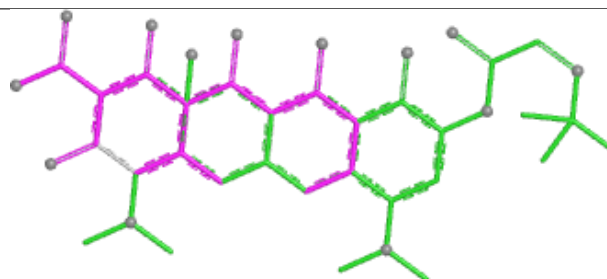


Rings

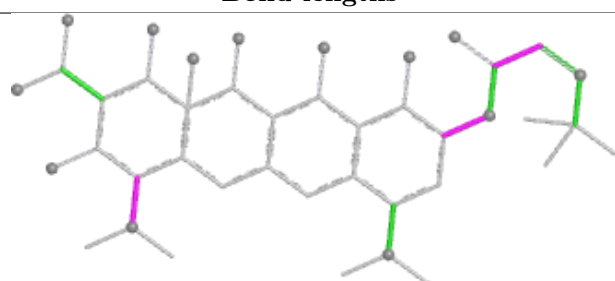
Ligand T1C D 401



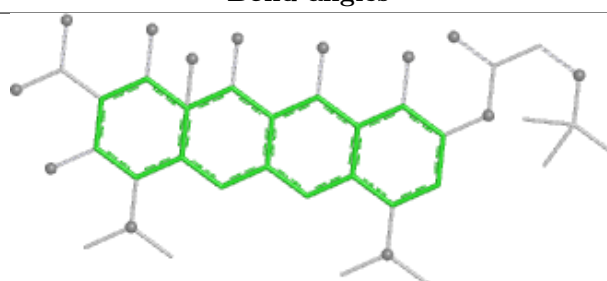
Bond lengths



Bond angles

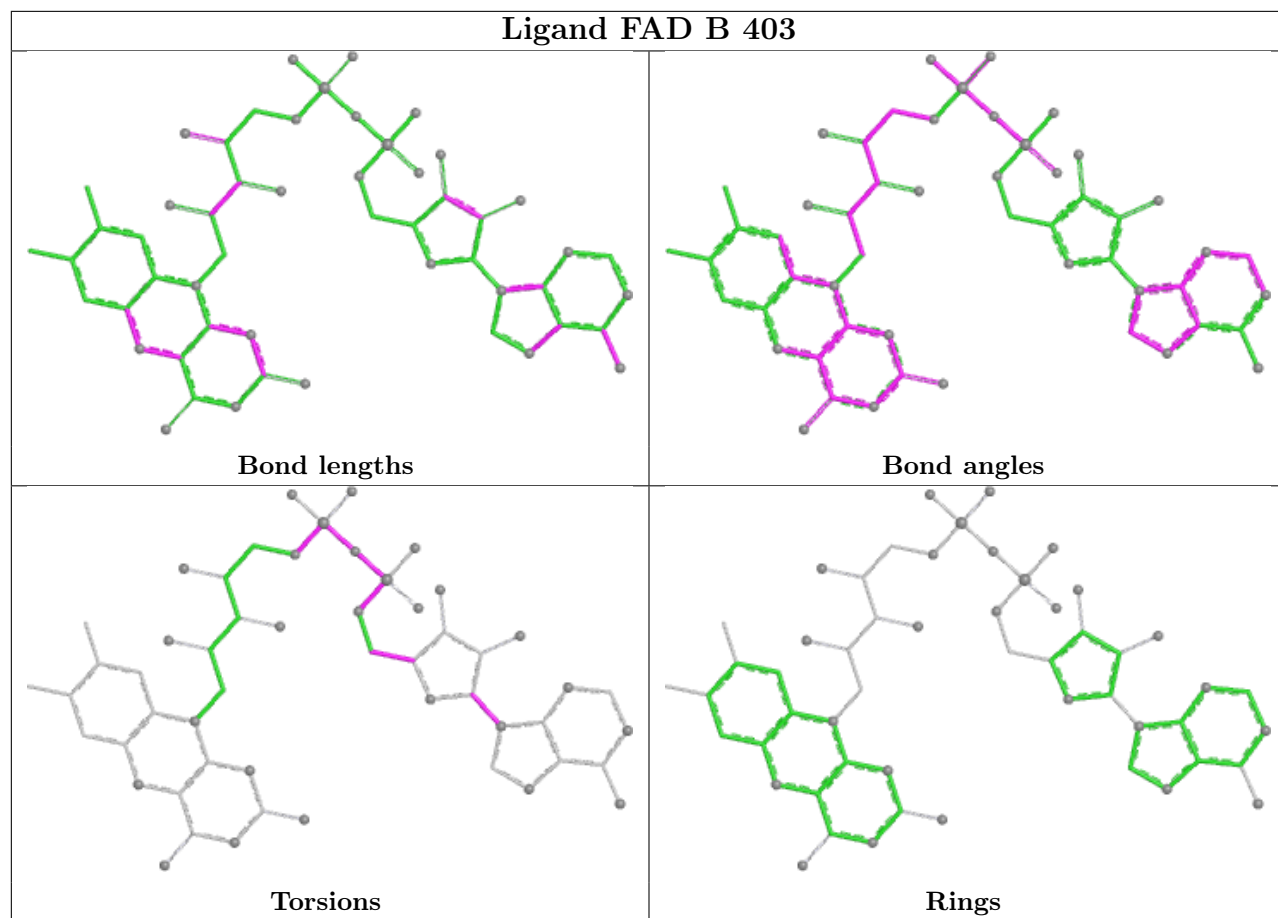


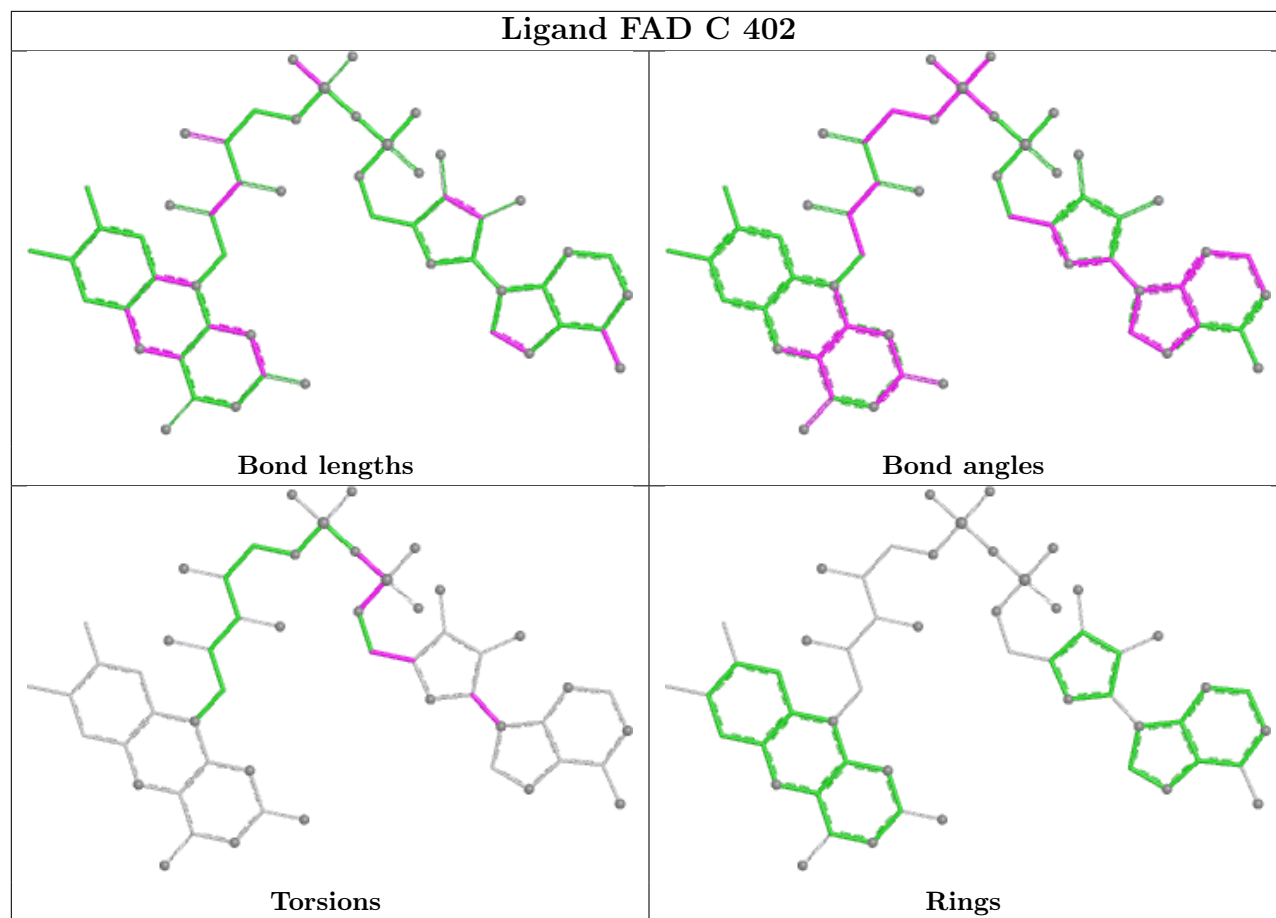
Torsions

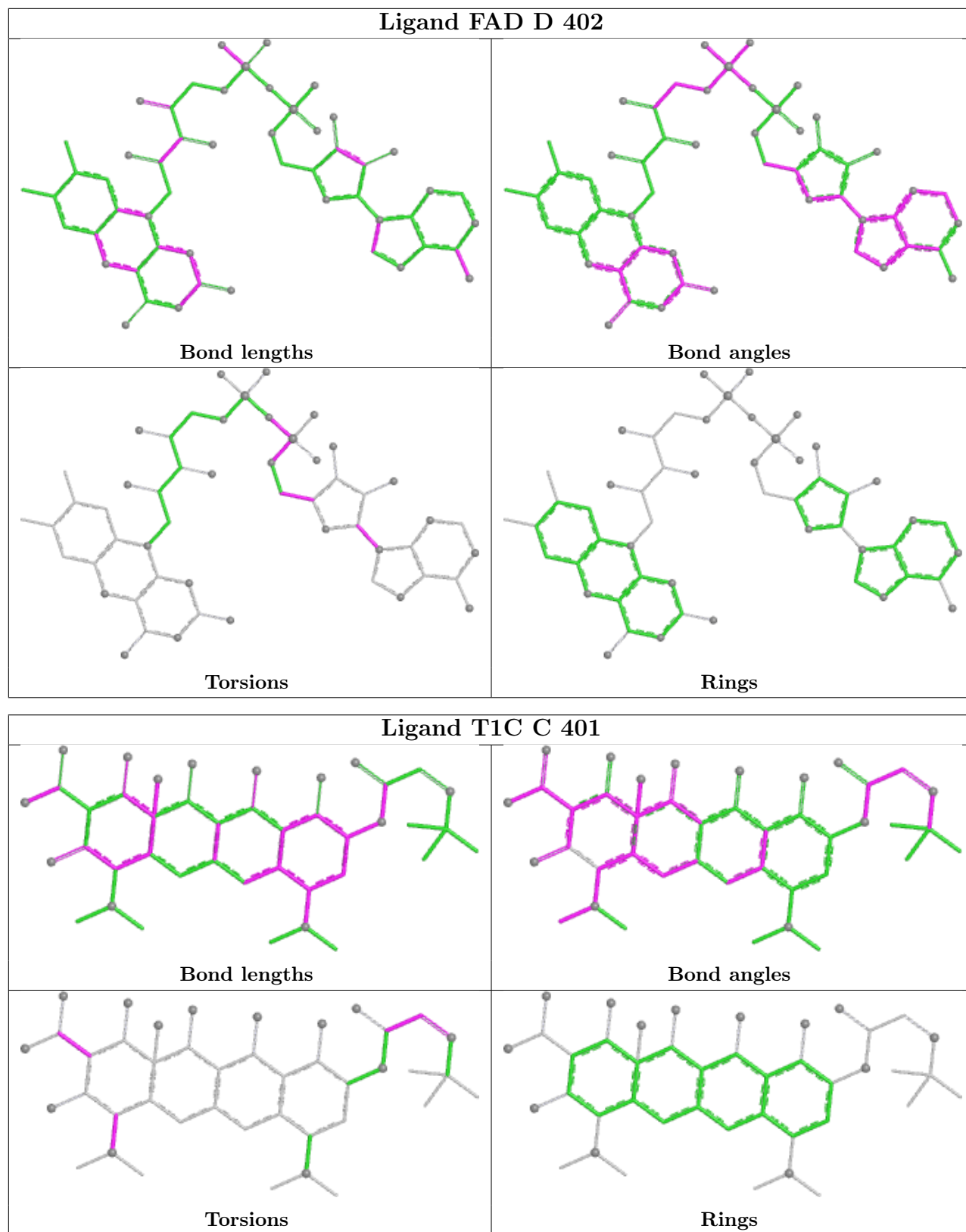


Rings

Ligand FAD B 403







5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	368/378 (97%)	0.48	10 (2%)	56 47	37, 58, 86, 113	0
1	B	365/378 (96%)	0.51	10 (2%)	56 47	37, 59, 88, 103	0
1	C	364/378 (96%)	0.72	18 (4%)	35 27	45, 73, 100, 112	0
1	D	364/378 (96%)	0.77	18 (4%)	35 27	46, 74, 101, 114	0
All	All	1461/1512 (96%)	0.62	56 (3%)	44 36	37, 66, 97, 114	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	60	LEU	4.5
1	C	286	GLY	3.7
1	B	286	GLY	3.6
1	D	60	LEU	3.6
1	A	13	LEU	3.3
1	C	368	SER	3.3
1	C	236	GLY	3.1
1	B	368	SER	3.1
1	C	294	LEU	3.0
1	C	341	GLY	2.9
1	D	294	LEU	2.8
1	D	286	GLY	2.8
1	B	14	LEU	2.6
1	C	346	ILE	2.6
1	D	231	GLY	2.5
1	C	110	PHE	2.5
1	C	324	VAL	2.4
1	D	253	PHE	2.4
1	C	60	LEU	2.4
1	C	323	GLY	2.4
1	D	146	LYS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	346	ILE	2.4
1	C	251	VAL	2.4
1	C	376	PHE	2.4
1	C	347	GLU	2.4
1	D	38	ASN	2.3
1	A	344	ASN	2.3
1	B	294	LEU	2.3
1	D	261	ASP	2.3
1	C	207	GLN	2.2
1	B	369	THR	2.2
1	A	376	PHE	2.2
1	B	262	PHE	2.2
1	A	60	LEU	2.2
1	C	192	GLN	2.2
1	A	347	GLU	2.2
1	D	216	ALA	2.2
1	B	275	LYS	2.1
1	A	323	GLY	2.1
1	C	220	GLY	2.1
1	D	170	GLY	2.1
1	D	368	SER	2.1
1	D	324	VAL	2.1
1	A	236	GLY	2.1
1	B	236	GLY	2.1
1	C	132	THR	2.1
1	C	298	TRP	2.1
1	D	175	ARG	2.1
1	A	355	GLN	2.1
1	A	369	THR	2.1
1	D	15	SER	2.0
1	D	66	SER	2.0
1	B	175	ARG	2.0
1	A	161	ALA	2.0
1	D	298	TRP	2.0
1	D	53	ALA	2.0

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

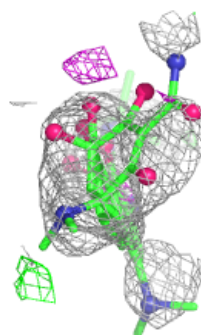
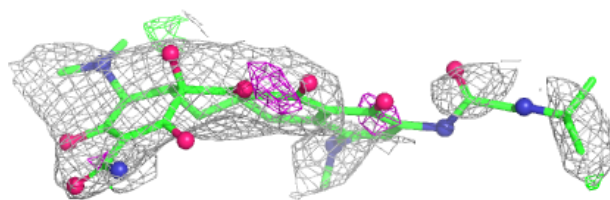
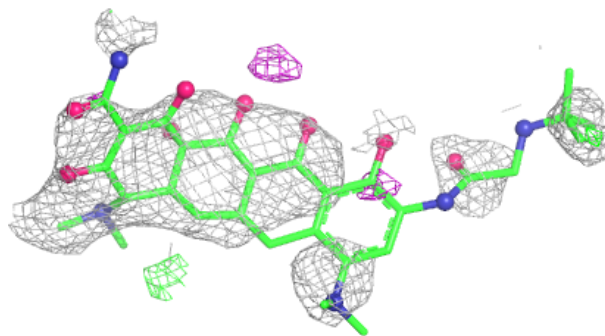
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	T1C	D	401	42/42	0.66	0.21	62,90,114,120	0
4	T1C	B	405	42/42	0.73	0.19	41,77,98,109	0
4	T1C	C	401	42/42	0.73	0.18	62,86,114,117	0
4	T1C	A	404	42/42	0.73	0.18	44,65,81,87	0
2	SO4	A	402	5/5	0.81	0.11	68,70,85,88	0
2	SO4	B	401	5/5	0.86	0.13	74,85,87,93	0
2	SO4	B	404	5/5	0.87	0.14	79,79,87,95	0
2	SO4	B	406	5/5	0.89	0.13	58,64,81,86	0
3	FAD	C	402	53/53	0.90	0.11	41,58,72,77	0
3	FAD	D	402	53/53	0.90	0.12	42,56,77,83	0
2	SO4	A	401	5/5	0.92	0.13	61,71,78,93	0
3	FAD	A	403	53/53	0.93	0.09	32,47,62,68	0
3	FAD	B	403	53/53	0.93	0.10	30,46,61,75	0
2	SO4	B	402	5/5	0.94	0.12	63,66,72,85	0

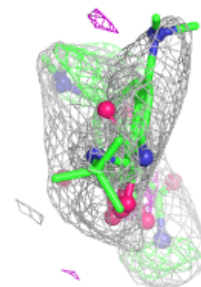
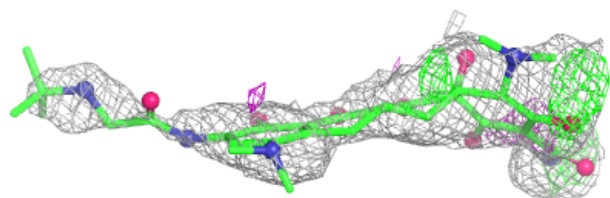
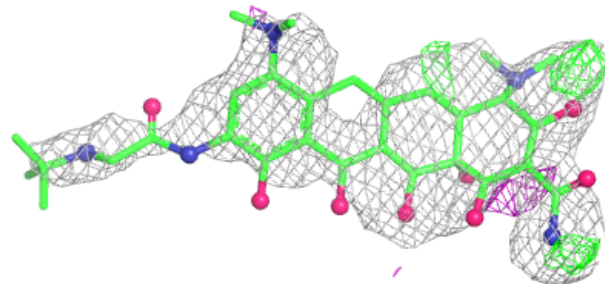
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around T1C D 401:

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

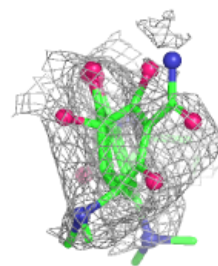
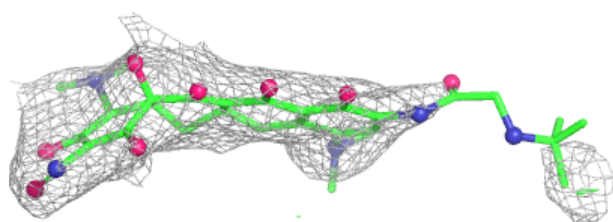
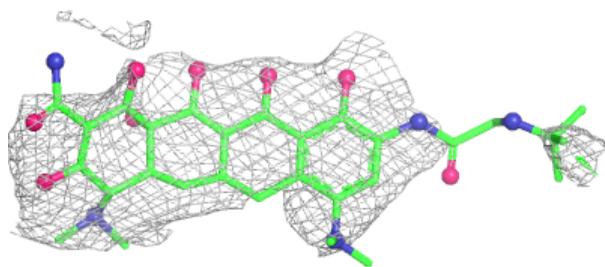
**Electron density around T1C B 405:**

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

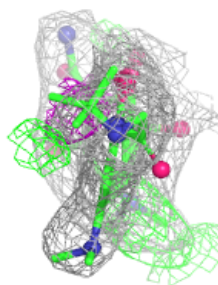
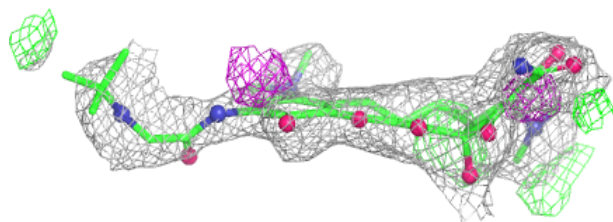
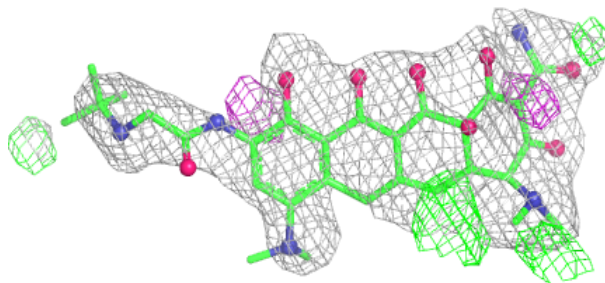


Electron density around T1C C 401:

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

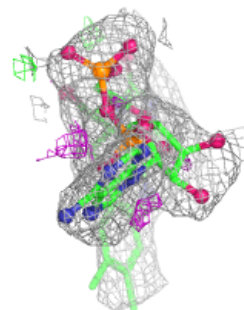
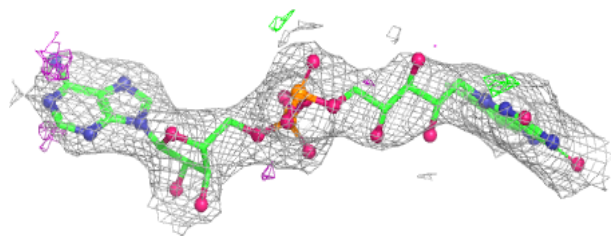
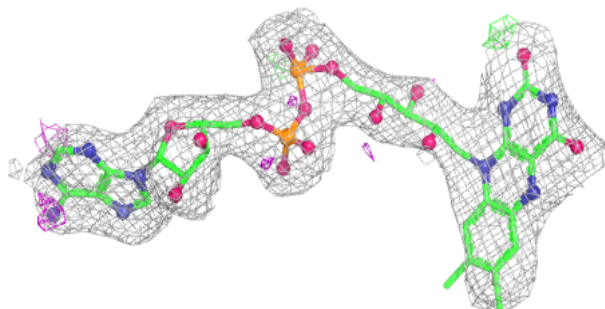
**Electron density around T1C A 404:**

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

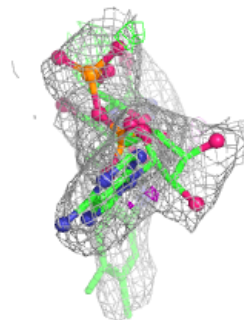
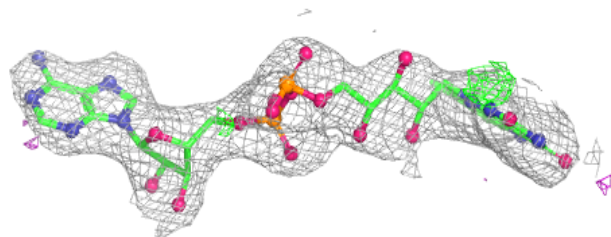
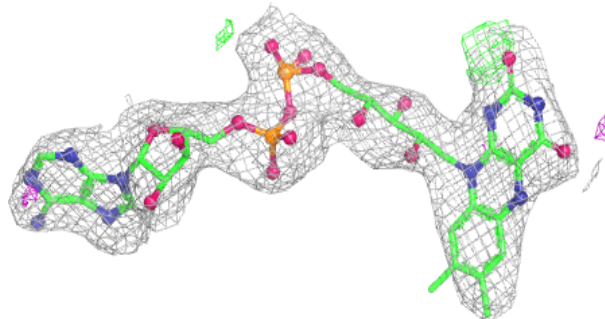


Electron density around FAD C 402:

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

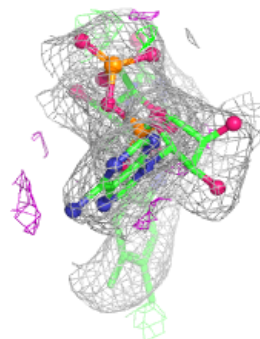
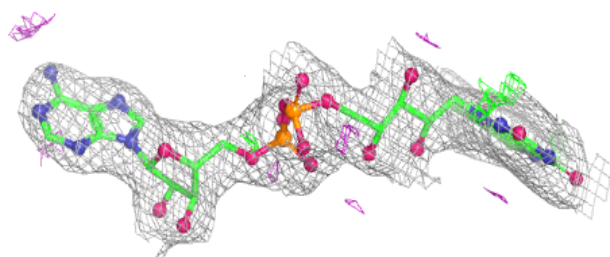
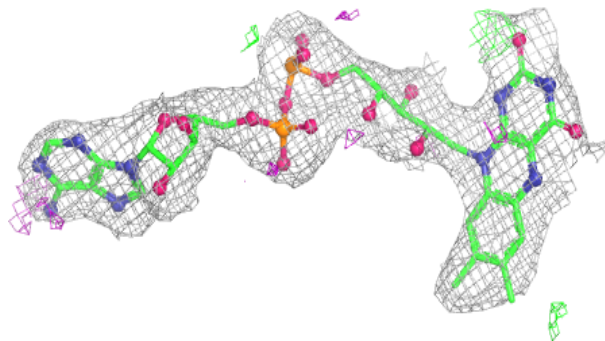
**Electron density around FAD D 402:**

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

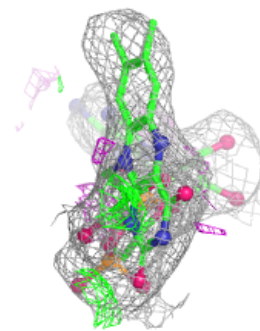
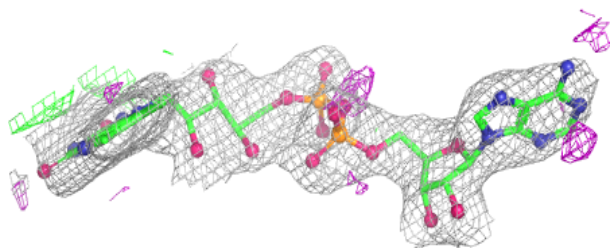
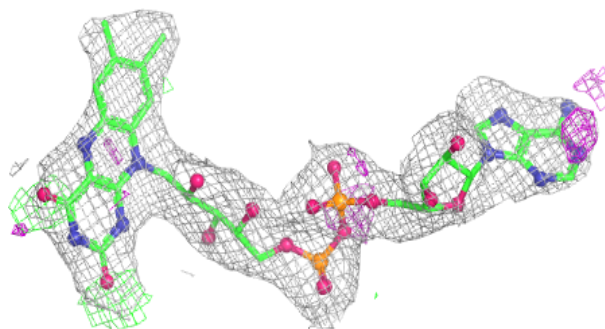


Electron density around FAD A 403:

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

**Electron density around FAD B 403:**

$2mF_o-DF_c$ (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.