



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:41 AM UTC

PDB ID : 2XDO / pdb_00002xdo
Title : Structure of the Tetracycline degrading Monooxygenase TetX2 from *Bacteroides thetaiotaomicron*
Authors : Volkers, G.; Palm, G.J.; Wright, G.D.; Hinrichs, W.
Deposited on : 2010-05-05
Resolution : 2.09 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

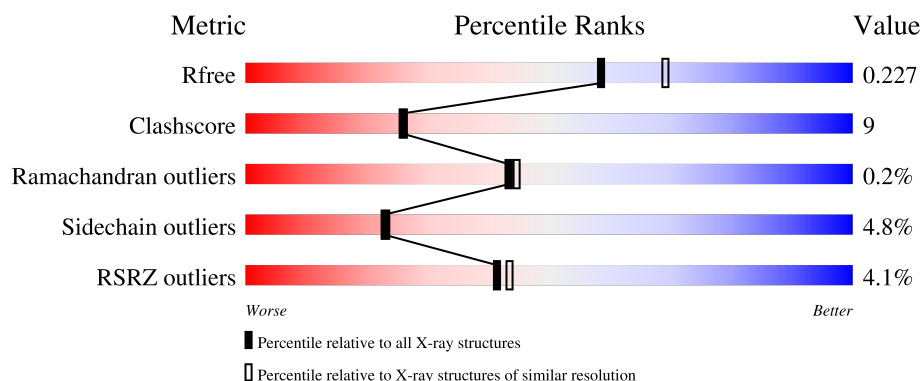
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	398	 5% 75% 12% • • 8%
1	B	398	 3% 77% 11% • • 8%
1	C	398	 4% 75% 14% • 8%
1	D	398	 4% 75% 13% • 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12183 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	367	Total	C	N	O	S	0	0	0
			2857	1812	486	547	12			
1	B	366	Total	C	N	O	S	0	0	0
			2841	1801	480	548	12			
1	C	365	Total	C	N	O	S	0	0	0
			2826	1791	478	545	12			
1	D	364	Total	C	N	O	S	0	0	0
			2811	1781	477	541	12			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	expression tag	UNP Q93L51
A	-8	GLY	-	expression tag	UNP Q93L51
A	-7	SER	-	expression tag	UNP Q93L51
A	-6	SER	-	expression tag	UNP Q93L51
A	-5	HIS	-	expression tag	UNP Q93L51
A	-4	HIS	-	expression tag	UNP Q93L51
A	-3	HIS	-	expression tag	UNP Q93L51
A	-2	HIS	-	expression tag	UNP Q93L51
A	-1	HIS	-	expression tag	UNP Q93L51
A	0	HIS	-	expression tag	UNP Q93L51
A	1	SER	-	expression tag	UNP Q93L51
A	2	SER	-	expression tag	UNP Q93L51
A	3	GLY	-	expression tag	UNP Q93L51
A	4	LEU	-	expression tag	UNP Q93L51
A	5	VAL	-	expression tag	UNP Q93L51
A	6	PRO	-	expression tag	UNP Q93L51
A	7	ARG	-	expression tag	UNP Q93L51
A	8	GLY	-	expression tag	UNP Q93L51
A	9	SER	-	expression tag	UNP Q93L51
A	10	HIS	-	expression tag	UNP Q93L51
B	-9	MET	-	expression tag	UNP Q93L51

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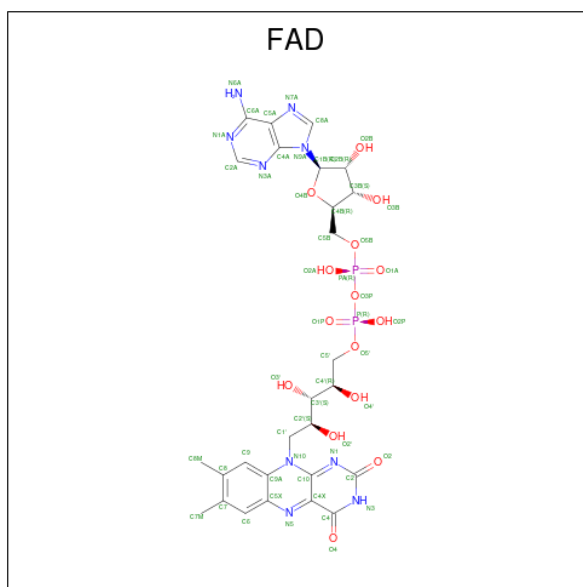
Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	GLY	-	expression tag	UNP Q93L51
B	-7	SER	-	expression tag	UNP Q93L51
B	-6	SER	-	expression tag	UNP Q93L51
B	-5	HIS	-	expression tag	UNP Q93L51
B	-4	HIS	-	expression tag	UNP Q93L51
B	-3	HIS	-	expression tag	UNP Q93L51
B	-2	HIS	-	expression tag	UNP Q93L51
B	-1	HIS	-	expression tag	UNP Q93L51
B	0	HIS	-	expression tag	UNP Q93L51
B	1	SER	-	expression tag	UNP Q93L51
B	2	SER	-	expression tag	UNP Q93L51
B	3	GLY	-	expression tag	UNP Q93L51
B	4	LEU	-	expression tag	UNP Q93L51
B	5	VAL	-	expression tag	UNP Q93L51
B	6	PRO	-	expression tag	UNP Q93L51
B	7	ARG	-	expression tag	UNP Q93L51
B	8	GLY	-	expression tag	UNP Q93L51
B	9	SER	-	expression tag	UNP Q93L51
B	10	HIS	-	expression tag	UNP Q93L51
C	-9	MET	-	expression tag	UNP Q93L51
C	-8	GLY	-	expression tag	UNP Q93L51
C	-7	SER	-	expression tag	UNP Q93L51
C	-6	SER	-	expression tag	UNP Q93L51
C	-5	HIS	-	expression tag	UNP Q93L51
C	-4	HIS	-	expression tag	UNP Q93L51
C	-3	HIS	-	expression tag	UNP Q93L51
C	-2	HIS	-	expression tag	UNP Q93L51
C	-1	HIS	-	expression tag	UNP Q93L51
C	0	HIS	-	expression tag	UNP Q93L51
C	1	SER	-	expression tag	UNP Q93L51
C	2	SER	-	expression tag	UNP Q93L51
C	3	GLY	-	expression tag	UNP Q93L51
C	4	LEU	-	expression tag	UNP Q93L51
C	5	VAL	-	expression tag	UNP Q93L51
C	6	PRO	-	expression tag	UNP Q93L51
C	7	ARG	-	expression tag	UNP Q93L51
C	8	GLY	-	expression tag	UNP Q93L51
C	9	SER	-	expression tag	UNP Q93L51
C	10	HIS	-	expression tag	UNP Q93L51
D	-9	MET	-	expression tag	UNP Q93L51
D	-8	GLY	-	expression tag	UNP Q93L51
D	-7	SER	-	expression tag	UNP Q93L51

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	SER	-	expression tag	UNP Q93L51
D	-5	HIS	-	expression tag	UNP Q93L51
D	-4	HIS	-	expression tag	UNP Q93L51
D	-3	HIS	-	expression tag	UNP Q93L51
D	-2	HIS	-	expression tag	UNP Q93L51
D	-1	HIS	-	expression tag	UNP Q93L51
D	0	HIS	-	expression tag	UNP Q93L51
D	1	SER	-	expression tag	UNP Q93L51
D	2	SER	-	expression tag	UNP Q93L51
D	3	GLY	-	expression tag	UNP Q93L51
D	4	LEU	-	expression tag	UNP Q93L51
D	5	VAL	-	expression tag	UNP Q93L51
D	6	PRO	-	expression tag	UNP Q93L51
D	7	ARG	-	expression tag	UNP Q93L51
D	8	GLY	-	expression tag	UNP Q93L51
D	9	SER	-	expression tag	UNP Q93L51
D	10	HIS	-	expression tag	UNP Q93L51

- 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		

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

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

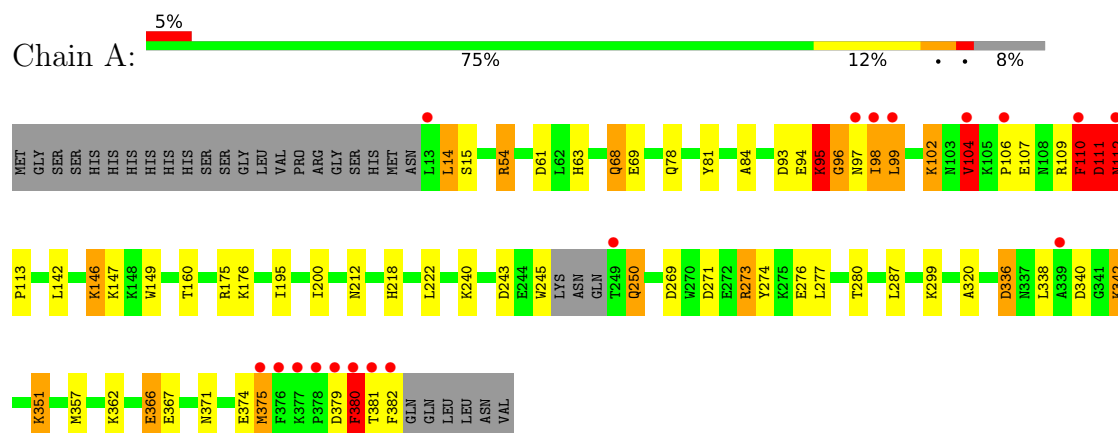
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	178	Total	O	0	0
			178	178		
4	B	174	Total	O	0	0
			174	174		
4	C	113	Total	O	0	0
			113	113		
4	D	106	Total	O	0	0
			106	106		

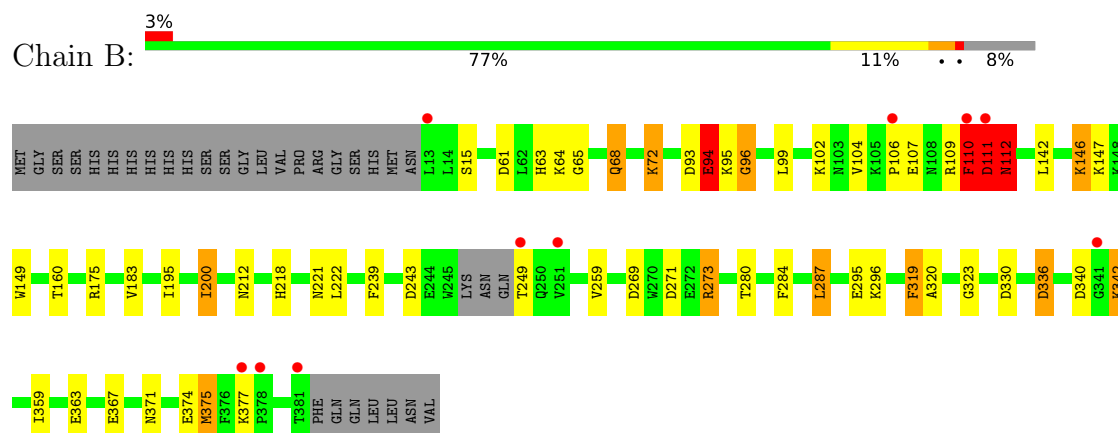
3 Residue-property plots

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

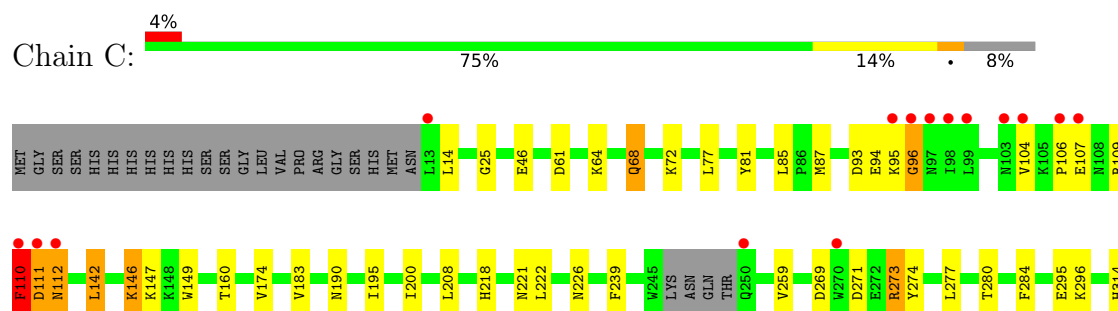
• Molecule 1: TETX2 PROTEIN



• Molecule 1: TETX2 PROTEIN

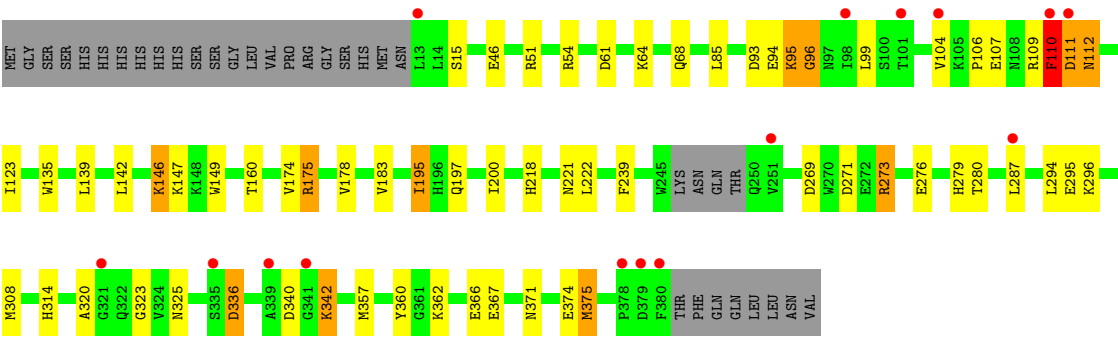


• Molecule 1: TETX2 PROTEIN





● 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	68.11Å 80.27Å 86.89Å 111.00° 90.23° 93.43°	Depositor
Resolution (Å)	40.54 – 2.09 40.54 – 2.09	Depositor EDS
% Data completeness (in resolution range)	90.5 (40.54-2.09) 63.1 (40.54-2.09)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.190 , 0.230 0.187 , 0.227	Depositor DCC
R_{free} test set	3252 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	33.2	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.4	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	0.95	EDS
Total number of atoms	12183	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.41% 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: SO4, 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	1.45	17/2915 (0.6%)	1.31	22/3949 (0.6%)
1	B	1.44	10/2898 (0.3%)	1.29	21/3929 (0.5%)
1	C	1.22	6/2883 (0.2%)	1.17	12/3912 (0.3%)
1	D	1.23	10/2868 (0.3%)	1.20	14/3892 (0.4%)
All	All	1.34	43/11564 (0.4%)	1.25	69/15682 (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	A	0	4
1	B	0	5
1	C	0	4
1	D	0	3
All	All	0	16

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	96	GLY	N-CA	13.41	1.56	1.44
1	D	96	GLY	N-CA	11.87	1.56	1.44
1	B	95	LYS	CA-C	11.57	1.63	1.52
1	A	95	LYS	N-CA	11.56	1.59	1.46
1	B	95	LYS	N-CA	10.25	1.58	1.46
1	B	96	GLY	N-CA	10.23	1.57	1.45
1	A	95	LYS	CA-C	10.18	1.62	1.52
1	D	95	LYS	CA-C	10.06	1.62	1.52
1	B	111	ASP	CA-CB	-8.34	1.40	1.53
1	C	110	PHE	N-CA	8.09	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	110	PHE	N-CA	7.96	1.56	1.46
1	A	110	PHE	N-CA	7.67	1.56	1.46
1	A	380	PHE	CE1-CZ	-7.54	1.16	1.38
1	A	104	VAL	CA-CB	7.53	1.65	1.54
1	C	183	VAL	CA-CB	7.53	1.61	1.54
1	D	95	LYS	N-CA	7.35	1.54	1.46
1	A	111	ASP	CA-C	-7.31	1.43	1.52
1	A	380	PHE	CG-CD2	-7.13	1.23	1.38
1	B	200	ILE	CA-CB	7.12	1.62	1.55
1	A	110	PHE	CA-C	-6.94	1.43	1.52
1	A	96	GLY	N-CA	6.83	1.53	1.45
1	B	110	PHE	N-CA	6.78	1.55	1.46
1	D	123	ILE	C-O	-6.73	1.16	1.24
1	A	112	ASN	CG-ND2	-6.46	1.19	1.33
1	A	250	GLN	N-CA	6.21	1.54	1.46
1	A	380	PHE	CE2-CZ	-6.11	1.20	1.38
1	B	111	ASP	CA-C	-6.02	1.45	1.52
1	C	95	LYS	CA-C	5.72	1.60	1.52
1	A	97	ASN	C-O	-5.69	1.17	1.24
1	B	183	VAL	CA-CB	5.66	1.60	1.54
1	C	95	LYS	N-CA	5.66	1.53	1.46
1	D	68	GLN	CD-OE1	-5.50	1.13	1.23
1	D	68	GLN	CD-NE2	-5.46	1.21	1.33
1	B	68	GLN	CD-OE1	-5.35	1.13	1.23
1	D	54	ARG	C-O	-5.29	1.17	1.23
1	D	183	VAL	CA-CB	5.19	1.59	1.54
1	A	68	GLN	CD-NE2	-5.17	1.22	1.33
1	B	363	GLU	N-CA	-5.17	1.40	1.46
1	C	68	GLN	CD-NE2	-5.13	1.22	1.33
1	A	54	ARG	C-O	-5.10	1.17	1.24
1	D	197	GLN	N-CA	5.07	1.50	1.46
1	A	98	ILE	N-CA	-5.07	1.40	1.46
1	A	61	ASP	N-CA	-5.06	1.39	1.46

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	LYS	N-CA-C	14.23	131.19	112.12
1	B	111	ASP	N-CA-C	-12.22	90.65	107.88
1	D	111	ASP	N-CA-C	-11.79	90.27	108.42
1	C	111	ASP	N-CA-C	-10.68	93.97	108.38
1	A	111	ASP	N-CA-C	-10.47	93.12	107.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	95	LYS	N-CA-C	10.40	126.06	112.12
1	B	96	GLY	N-CA-C	10.23	129.06	112.89
1	D	95	LYS	N-CA-C	10.07	125.61	112.12
1	A	96	GLY	N-CA-C	9.48	127.86	112.89
1	A	110	PHE	N-CA-C	-9.46	101.15	112.89
1	B	110	PHE	N-CA-C	-8.32	102.57	112.89
1	D	96	GLY	N-CA-C	8.03	125.27	112.58
1	B	175	ARG	NE-CZ-NH1	7.17	128.67	121.50
1	B	175	ARG	NE-CZ-NH2	-7.03	112.88	119.20
1	A	175	ARG	NE-CZ-NH2	-6.89	113.00	119.20
1	C	96	GLY	N-CA-C	6.81	124.50	112.64
1	A	175	ARG	NE-CZ-NH1	6.79	128.29	121.50
1	A	15	SER	N-CA-C	6.68	119.13	111.11
1	D	110	PHE	N-CA-C	-6.54	104.56	112.54
1	A	110	PHE	N-CA-CB	6.52	121.03	110.40
1	C	110	PHE	N-CA-C	-6.43	104.92	112.89
1	A	95	LYS	CA-C-N	6.31	130.39	121.30
1	A	95	LYS	C-N-CA	6.31	130.39	121.30
1	C	95	LYS	N-CA-C	6.22	124.05	110.80
1	D	15	SER	N-CA-C	6.09	118.42	111.11
1	B	95	LYS	CA-C-N	6.05	130.01	121.30
1	B	95	LYS	C-N-CA	6.05	130.01	121.30
1	A	380	PHE	CA-C-N	5.97	128.59	120.54
1	A	380	PHE	C-N-CA	5.97	128.59	120.54
1	B	110	PHE	N-CA-CB	5.86	119.96	110.40
1	B	112	ASN	CB-CA-C	5.81	121.62	110.17
1	B	200	ILE	N-CA-C	-5.79	106.17	111.67
1	A	104	VAL	CB-CA-C	5.77	120.02	111.31
1	D	95	LYS	CA-C-N	5.65	128.12	122.30
1	D	95	LYS	C-N-CA	5.65	128.12	122.30
1	B	175	ARG	CD-NE-CZ	5.63	132.28	124.40
1	B	64	LYS	CA-C-N	-5.61	108.32	121.34
1	B	64	LYS	C-N-CA	-5.61	108.32	121.34
1	A	112	ASN	CB-CA-C	5.56	121.13	110.17
1	C	377	LYS	CA-C-N	5.55	125.22	119.56
1	C	377	LYS	C-N-CA	5.55	125.22	119.56
1	A	366	GLU	CB-CA-C	-5.37	102.45	110.88
1	A	102	LYS	CA-C-N	-5.36	113.76	121.42
1	A	102	LYS	C-N-CA	-5.36	113.76	121.42
1	C	85	LEU	CA-C-N	-5.35	114.41	119.76
1	C	85	LEU	C-N-CA	-5.35	114.41	119.76
1	A	98	ILE	N-CA-C	-5.32	107.19	113.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	377	LYS	CA-C-N	5.31	126.48	119.84
1	B	377	LYS	C-N-CA	5.31	126.48	119.84
1	D	175	ARG	NE-CZ-NH2	-5.30	114.43	119.20
1	D	178	VAL	N-CA-C	-5.26	106.01	111.58
1	C	377	LYS	N-CA-C	-5.24	101.93	109.48
1	D	46	GLU	CA-C-N	5.19	127.24	120.28
1	D	46	GLU	C-N-CA	5.19	127.24	120.28
1	B	319	PHE	N-CA-C	5.16	117.65	111.71
1	A	380	PHE	CD1-CG-CD2	-5.15	110.87	118.60
1	C	46	GLU	CA-C-N	5.12	127.10	120.44
1	C	46	GLU	C-N-CA	5.12	127.10	120.44
1	A	240	LYS	N-CA-C	-5.12	102.70	110.28
1	A	104	VAL	CA-CB-CG2	5.06	119.00	110.40
1	D	85	LEU	CA-C-N	-5.05	114.71	119.76
1	D	85	LEU	C-N-CA	-5.05	114.71	119.76
1	B	330	ASP	N-CA-C	-5.05	105.78	111.28
1	B	15	SER	CA-C-N	-5.04	115.15	122.86
1	B	15	SER	C-N-CA	-5.04	115.15	122.86
1	D	112	ASN	N-CA-C	5.02	120.91	109.81
1	A	175	ARG	CD-NE-CZ	5.02	131.43	124.40
1	C	25	GLY	N-CA-C	-5.02	106.16	112.23
1	B	287	LEU	CA-CB-CG	5.02	133.87	116.30

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	109	ARG	Peptide
1	A	110	PHE	Peptide
1	A	111	ASP	Peptide
1	A	94	GLU	Peptide
1	B	109	ARG	Peptide
1	B	110	PHE	Peptide
1	B	111	ASP	Peptide
1	B	249	THR	Peptide
1	B	94	GLU	Peptide
1	C	109	ARG	Peptide
1	C	110	PHE	Peptide
1	C	111	ASP	Peptide
1	C	94	GLU	Peptide
1	D	109	ARG	Peptide
1	D	111	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	D	94	GLU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2857	0	2760	79	0
1	B	2841	0	2735	54	0
1	C	2826	0	2710	47	0
1	D	2811	0	2688	44	0
2	A	53	0	31	1	0
2	B	53	0	31	0	0
2	C	53	0	31	0	0
2	D	53	0	31	1	0
3	A	15	0	0	1	0
3	B	20	0	0	0	0
3	C	15	0	0	0	0
3	D	15	0	0	0	0
4	A	178	0	0	12	0
4	B	174	0	0	13	0
4	C	113	0	0	5	0
4	D	106	0	0	5	0
All	All	12183	0	11017	214	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 (214) 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:A:96:GLY:HA2	4:A:2045:HOH:O	1.28	1.26
1:B:96:GLY:HA2	4:B:2042:HOH:O	1.24	1.25
1:C:96:GLY:HA2	4:C:2030:HOH:O	1.37	1.22
1:D:96:GLY:HA2	4:D:2031:HOH:O	1.35	1.22
1:A:99:LEU:HD23	4:A:2040:HOH:O	1.39	1.16
1:A:104:VAL:HG23	1:A:106:PRO:HD2	1.33	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:104:VAL:HG12	1:D:106:PRO:HD2	1.17	1.11
1:B:104:VAL:HG12	1:B:106:PRO:HD2	1.26	1.10
1:C:104:VAL:HG12	1:C:106:PRO:HD2	1.11	1.08
1:A:380:PHE:CD1	1:A:382:PHE:HB3	1.94	1.03
1:A:146:LYS:HD2	1:A:147:LYS:H	1.24	0.99
1:B:146:LYS:HD2	1:B:147:LYS:H	1.26	0.97
1:A:98:ILE:HG21	1:B:359:ILE:HG23	1.49	0.95
1:D:146:LYS:HD2	1:D:147:LYS:H	1.31	0.91
1:A:104:VAL:CG2	1:A:106:PRO:HD2	2.01	0.91
1:A:98:ILE:CG2	1:B:359:ILE:HG23	2.00	0.90
1:A:99:LEU:CD2	4:A:2040:HOH:O	2.04	0.90
1:C:146:LYS:HD2	1:C:147:LYS:H	1.36	0.89
1:A:375:MET:HA	1:A:380:PHE:CD2	2.08	0.89
1:A:99:LEU:HD12	4:B:2162:HOH:O	1.74	0.86
1:A:379:ASP:O	1:A:381:THR:N	2.10	0.84
1:C:104:VAL:CG1	1:C:106:PRO:HD2	2.03	0.82
1:C:104:VAL:HG12	1:C:106:PRO:CD	2.04	0.82
1:A:379:ASP:CB	1:B:65:GLY:HA3	2.12	0.79
1:D:271:ASP:OD1	1:D:273:ARG:HD3	1.84	0.77
1:A:218:HIS:HD2	4:B:2165:HOH:O	1.70	0.75
1:D:61:ASP:HB2	1:D:112:ASN:HB2	1.71	0.73
1:A:271:ASP:OD1	1:A:273:ARG:HD3	1.88	0.72
1:D:362:LYS:O	1:D:366:GLU:HG2	1.89	0.72
1:A:381:THR:N	1:A:382:PHE:HA	2.04	0.72
1:D:104:VAL:HG12	1:D:106:PRO:CD	2.10	0.71
1:B:271:ASP:OD1	1:B:273:ARG:HD3	1.89	0.71
1:C:61:ASP:HB2	1:C:112:ASN:HB2	1.73	0.71
1:B:110:PHE:HA	4:B:2048:HOH:O	1.91	0.70
1:D:104:VAL:CG1	1:D:106:PRO:HD2	2.10	0.70
1:D:107:GLU:HA	1:D:110:PHE:HB3	1.72	0.70
1:A:107:GLU:CA	4:A:2051:HOH:O	2.38	0.70
1:A:99:LEU:CD1	4:B:2162:HOH:O	2.34	0.70
1:C:341:GLY:HA3	4:C:2105:HOH:O	1.92	0.70
1:A:195:ILE:HD12	1:A:280:THR:HG23	1.72	0.70
1:D:195:ILE:HD12	1:D:280:THR:HG23	1.73	0.70
1:A:95:LYS:O	4:A:2045:HOH:O	2.08	0.69
1:C:107:GLU:HA	1:C:110:PHE:HB3	1.73	0.69
1:A:380:PHE:CE1	1:A:382:PHE:HB3	2.27	0.69
1:A:107:GLU:CB	4:A:2051:HOH:O	2.41	0.68
1:B:104:VAL:HG12	1:B:106:PRO:CD	2.16	0.68
1:A:362:LYS:O	1:A:366:GLU:HG2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:LYS:HD2	1:A:95:LYS:H	1.59	0.68
1:C:222:LEU:HD23	1:C:375:MET:HE2	1.74	0.68
1:A:222:LEU:HD23	1:A:375:MET:HE2	1.76	0.67
1:C:195:ILE:HD12	1:C:280:THR:HG23	1.74	0.67
1:C:96:GLY:HA3	4:C:2031:HOH:O	1.93	0.67
1:C:271:ASP:OD1	1:C:273:ARG:HD3	1.94	0.67
1:B:104:VAL:CG1	1:B:106:PRO:HD2	2.15	0.67
1:A:107:GLU:HA	1:A:110:PHE:HB3	1.75	0.67
1:B:222:LEU:HD23	1:B:375:MET:HE2	1.76	0.66
1:A:222:LEU:CD2	1:A:375:MET:HE2	2.26	0.66
1:B:195:ILE:HD12	1:B:280:THR:HG23	1.77	0.66
1:C:107:GLU:CA	1:C:110:PHE:HB3	2.26	0.66
1:A:95:LYS:HB3	1:A:271:ASP:HB2	1.77	0.65
1:D:107:GLU:CA	1:D:110:PHE:HB3	2.27	0.65
1:D:222:LEU:HD23	1:D:375:MET:HE2	1.78	0.65
1:D:146:LYS:HD2	1:D:147:LYS:N	2.10	0.65
1:C:342:LYS:HB2	1:C:342:LYS:NZ	2.12	0.65
1:B:218:HIS:HD2	4:B:2121:HOH:O	1.79	0.64
1:A:218:HIS:HE1	1:A:269:ASP:OD2	1.80	0.64
1:A:342:LYS:HB2	1:A:342:LYS:NZ	2.12	0.64
1:B:319:PHE:HB2	4:B:2167:HOH:O	1.98	0.64
1:B:102:LYS:HD3	1:B:212:ASN:HD21	1.62	0.63
1:D:96:GLY:HA3	4:D:2032:HOH:O	1.96	0.63
1:A:107:GLU:CA	1:A:110:PHE:HB3	2.29	0.63
1:A:375:MET:HA	1:A:380:PHE:CE2	2.33	0.63
1:B:342:LYS:HB2	1:B:342:LYS:NZ	2.13	0.63
1:D:342:LYS:NZ	1:D:342:LYS:HB2	2.13	0.63
1:A:54:ARG:HB2	3:A:391:SO4:O4	1.99	0.62
1:A:98:ILE:HG21	1:B:359:ILE:CG2	2.24	0.62
1:C:93:ASP:OD1	1:C:96:GLY:N	2.31	0.62
1:A:93:ASP:OD1	1:A:96:GLY:N	2.32	0.62
1:D:93:ASP:OD1	1:D:96:GLY:N	2.33	0.62
1:A:98:ILE:HG22	1:B:359:ILE:HG23	1.80	0.62
1:B:96:GLY:CA	4:B:2042:HOH:O	2.06	0.61
1:C:269:ASP:HB2	4:C:2081:HOH:O	2.01	0.60
1:B:146:LYS:HD2	1:B:147:LYS:N	2.07	0.60
1:A:146:LYS:HD2	1:A:147:LYS:N	2.06	0.59
1:B:93:ASP:OD1	1:B:96:GLY:N	2.35	0.59
1:B:107:GLU:HA	1:B:110:PHE:HB3	1.83	0.59
1:A:107:GLU:HB3	4:A:2051:HOH:O	2.01	0.59
1:B:342:LYS:HB2	1:B:342:LYS:HZ2	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:GLU:CA	1:B:110:PHE:HB3	2.33	0.58
1:D:221:ASN:HD22	1:D:239:PHE:HB3	1.69	0.58
1:D:95:LYS:O	4:D:2031:HOH:O	2.17	0.57
1:C:295:GLU:HG3	1:C:296:LYS:H	1.69	0.57
1:A:69:GLU:OE2	4:A:2029:HOH:O	2.17	0.57
1:A:95:LYS:HD2	1:A:95:LYS:N	2.19	0.57
1:A:380:PHE:CE1	1:A:382:PHE:CB	2.87	0.57
1:C:362:LYS:O	1:C:366:GLU:HG2	2.04	0.57
1:A:99:LEU:HB2	1:B:359:ILE:HG12	1.86	0.57
1:C:380:PHE:O	1:C:381:THR:HG23	2.04	0.57
1:A:342:LYS:HB2	1:A:342:LYS:HZ2	1.69	0.56
1:B:94:GLU:OE2	1:B:218:HIS:CD2	2.58	0.56
1:A:98:ILE:CG2	1:B:359:ILE:HA	2.36	0.55
1:C:72:LYS:HG3	1:C:77:LEU:HD22	1.88	0.55
1:B:68:GLN:NE2	1:B:111:ASP:HA	2.22	0.55
1:A:95:LYS:N	1:A:95:LYS:CD	2.68	0.55
1:B:221:ASN:HD22	1:B:239:PHE:HB3	1.72	0.55
1:C:64:LYS:HD2	1:C:110:PHE:O	2.06	0.55
1:B:222:LEU:CD2	1:B:375:MET:HE2	2.36	0.55
1:C:68:GLN:NE2	1:C:81:TYR:OH	2.40	0.55
1:C:221:ASN:HD22	1:C:239:PHE:HB3	1.71	0.55
1:A:102:LYS:CD	1:A:212:ASN:HD21	2.20	0.55
1:C:222:LEU:CD2	1:C:375:MET:HE2	2.36	0.54
1:A:99:LEU:HD13	1:B:359:ILE:HD11	1.90	0.53
1:B:336:ASP:OD1	1:B:340:ASP:OD2	2.27	0.53
1:A:195:ILE:HD12	1:A:280:THR:CG2	2.38	0.53
1:C:146:LYS:HD2	1:C:147:LYS:N	2.15	0.53
1:C:314:HIS:NE2	1:C:330:ASP:OD2	2.33	0.53
1:D:271:ASP:OD1	1:D:273:ARG:CD	2.56	0.53
1:A:274:TYR:O	1:A:277:LEU:HB3	2.10	0.52
1:A:78:GLN:HG2	1:C:64:LYS:HB3	1.92	0.52
1:C:61:ASP:OD2	1:C:112:ASN:HB2	2.09	0.52
1:D:222:LEU:CD2	1:D:375:MET:HE2	2.40	0.51
1:D:61:ASP:OD2	1:D:112:ASN:HB2	2.12	0.50
1:A:107:GLU:HA	4:A:2051:HOH:O	2.08	0.50
1:C:195:ILE:HD12	1:C:280:THR:CG2	2.41	0.50
1:A:380:PHE:CE1	1:A:382:PHE:CG	3.00	0.49
1:A:149:TRP:O	1:A:160:THR:HA	2.12	0.49
1:C:221:ASN:ND2	1:C:239:PHE:HB3	2.27	0.49
1:A:98:ILE:HG23	1:B:359:ILE:HA	1.94	0.48
1:A:380:PHE:CD1	1:A:382:PHE:CB	2.84	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:TRP:O	1:C:160:THR:HA	2.13	0.48
1:C:271:ASP:OD1	1:C:273:ARG:CD	2.61	0.48
1:A:336:ASP:OD1	1:A:340:ASP:OD2	2.32	0.48
1:B:218:HIS:CD2	4:B:2121:HOH:O	2.62	0.48
1:B:259:VAL:HG11	1:B:284:PHE:CG	2.49	0.48
1:D:139:LEU:HD21	1:D:142:LEU:HD13	1.95	0.48
1:A:271:ASP:OD1	1:A:273:ARG:CD	2.59	0.47
1:A:380:PHE:CE1	1:A:382:PHE:CD2	3.02	0.47
1:C:320:ALA:HB2	1:C:371:ASN:CG	2.39	0.47
1:D:195:ILE:CD1	1:D:280:THR:HG23	2.43	0.47
1:D:107:GLU:HA	1:D:110:PHE:CB	2.44	0.47
1:D:195:ILE:HD12	1:D:280:THR:CG2	2.43	0.47
1:D:218:HIS:HE1	1:D:269:ASP:OD2	1.98	0.47
1:A:110:PHE:O	1:A:110:PHE:CD1	2.67	0.47
1:B:243:ASP:CB	4:B:2133:HOH:O	2.62	0.47
1:D:279:HIS:CE1	4:D:2083:HOH:O	2.68	0.47
1:D:294:LEU:HD11	1:D:314:HIS:HB3	1.96	0.47
1:C:342:LYS:HB2	1:C:342:LYS:HZ3	1.79	0.46
1:C:142:LEU:HD22	1:C:174:VAL:HG22	1.96	0.46
1:D:295:GLU:HG3	1:D:296:LYS:H	1.80	0.46
1:A:95:LYS:H	1:A:95:LYS:CD	2.27	0.46
1:B:107:GLU:HB2	1:B:110:PHE:CD2	2.51	0.46
1:C:107:GLU:HA	1:C:110:PHE:CB	2.45	0.46
1:D:149:TRP:O	1:D:160:THR:HA	2.16	0.46
1:B:107:GLU:O	1:B:110:PHE:HB3	2.17	0.45
1:B:243:ASP:HA	4:B:2133:HOH:O	2.16	0.45
1:B:218:HIS:HE1	1:B:269:ASP:OD2	2.00	0.45
1:B:221:ASN:ND2	1:B:239:PHE:HB3	2.32	0.45
1:C:274:TYR:O	1:C:277:LEU:HB3	2.16	0.45
1:D:221:ASN:ND2	1:D:239:PHE:HB3	2.30	0.45
1:B:149:TRP:O	1:B:160:THR:HA	2.17	0.45
1:C:87:MET:HE1	1:C:226:ASN:OD1	2.16	0.45
1:B:295:GLU:HG3	1:B:296:LYS:H	1.82	0.45
1:C:61:ASP:HB2	1:C:112:ASN:CB	2.46	0.45
1:A:351:LYS:HA	1:A:351:LYS:HD3	1.31	0.44
1:A:176:LYS:O	1:A:299:LYS:NZ	2.47	0.44
1:B:320:ALA:HB2	1:B:371:ASN:CG	2.43	0.44
1:A:63:HIS:HA	1:A:111:ASP:CB	2.48	0.44
1:A:243:ASP:OD1	1:A:243:ASP:N	2.51	0.44
1:A:68:GLN:NE2	1:A:81:TYR:OH	2.51	0.43
2:A:389:FAD:H1'1	2:A:389:FAD:H9	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:LYS:HZ3	1:D:146:LYS:HG3	1.71	0.43
1:A:84:ALA:HB1	1:A:113:PRO:HB2	2.00	0.43
1:A:371:ASN:OD1	1:A:375:MET:SD	2.77	0.43
1:B:342:LYS:NZ	1:B:342:LYS:CB	2.81	0.43
1:C:371:ASN:OD1	1:C:375:MET:SD	2.77	0.43
1:D:336:ASP:OD1	1:D:340:ASP:OD2	2.36	0.43
1:A:106:PRO:C	4:A:2051:HOH:O	2.61	0.42
1:B:63:HIS:HA	1:B:111:ASP:CB	2.49	0.42
1:B:110:PHE:CA	4:B:2048:HOH:O	2.58	0.42
1:D:342:LYS:HB2	1:D:342:LYS:HZ3	1.81	0.42
1:C:259:VAL:HG11	1:C:284:PHE:CG	2.55	0.42
1:D:64:LYS:HD2	1:D:110:PHE:O	2.20	0.42
1:D:175:ARG:HG2	1:D:308:MET:SD	2.60	0.42
1:B:72:LYS:HE2	1:B:72:LYS:HB2	1.81	0.42
1:B:110:PHE:CD1	1:B:110:PHE:O	2.72	0.42
1:C:218:HIS:HE1	1:C:269:ASP:OD2	2.02	0.42
1:A:107:GLU:N	4:A:2051:HOH:O	2.52	0.42
1:D:325:ASN:HB2	4:D:2099:HOH:O	2.20	0.42
1:B:61:ASP:OD2	1:B:112:ASN:HB2	2.19	0.41
1:C:208:LEU:HD21	4:C:2030:HOH:O	2.20	0.41
1:A:320:ALA:HB2	1:A:371:ASN:CG	2.45	0.41
1:B:271:ASP:OD1	1:B:273:ARG:CD	2.64	0.41
1:C:107:GLU:HB2	1:C:110:PHE:CD2	2.56	0.41
1:A:357:MET:C	1:A:357:MET:SD	3.03	0.41
1:D:320:ALA:HB2	1:D:371:ASN:CG	2.45	0.41
1:C:190:ASN:HD21	1:C:319:PHE:HZ	1.67	0.41
1:A:112:ASN:N	1:A:113:PRO:HD2	2.36	0.41
1:C:357:MET:HE3	1:C:357:MET:HB3	1.98	0.41
1:D:61:ASP:CB	1:D:112:ASN:HB2	2.47	0.41
1:A:98:ILE:CG2	1:B:359:ILE:CG2	2.86	0.41
1:A:104:VAL:H	1:A:107:GLU:HG2	1.85	0.41
1:A:146:LYS:HZ3	1:A:146:LYS:HG3	1.65	0.41
1:A:245:TRP:HA	1:A:250:GLN:HE21	1.86	0.41
1:C:336:ASP:OD1	1:C:340:ASP:OD2	2.38	0.41
1:D:357:MET:HA	1:D:360:TYR:CZ	2.56	0.41
1:A:14:LEU:HD11	1:A:338:LEU:HD22	2.03	0.41
1:B:243:ASP:CA	4:B:2133:HOH:O	2.69	0.41
1:D:104:VAL:H	1:D:107:GLU:HG2	1.86	0.40
1:D:142:LEU:HD22	1:D:174:VAL:HG22	2.03	0.40
1:D:323:GLY:HA3	2:D:389:FAD:H1'2	2.03	0.40
1:A:95:LYS:C	4:A:2045:HOH:O	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:MET:HE3	1:A:357:MET:HB3	1.98	0.40
1:B:68:GLN:HE22	1:B:111:ASP:HA	1.85	0.40
1:D:51:ARG:HB3	1:D:135:TRP:CZ2	2.56	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	363/398 (91%)	350 (96%)	12 (3%)	1 (0%)	36	36
1	B	362/398 (91%)	348 (96%)	12 (3%)	2 (1%)	21	18
1	C	361/398 (91%)	347 (96%)	14 (4%)	0	100	100
1	D	360/398 (90%)	346 (96%)	14 (4%)	0	100	100
All	All	1446/1592 (91%)	1391 (96%)	52 (4%)	3 (0%)	43	44

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	380	PHE
1	B	112	ASN
1	B	323	GLY

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	303/345 (88%)	285 (94%)	18 (6%)	18	16
1	B	301/345 (87%)	286 (95%)	15 (5%)	22	22
1	C	298/345 (86%)	286 (96%)	12 (4%)	28	29
1	D	295/345 (86%)	282 (96%)	13 (4%)	25	26
All	All	1197/1380 (87%)	1139 (95%)	58 (5%)	23	23

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	95	LYS
1	A	99	LEU
1	A	104	VAL
1	A	110	PHE
1	A	112	ASN
1	A	142	LEU
1	A	146	LYS
1	A	200	ILE
1	A	273	ARG
1	A	276	GLU
1	A	287	LEU
1	A	336	ASP
1	A	342	LYS
1	A	351	LYS
1	A	367	GLU
1	A	374	GLU
1	A	375	MET
1	B	72	LYS
1	B	94	GLU
1	B	99	LEU
1	B	110	PHE
1	B	112	ASN
1	B	142	LEU
1	B	146	LYS
1	B	200	ILE
1	B	273	ARG
1	B	287	LEU
1	B	336	ASP
1	B	342	LYS
1	B	367	GLU
1	B	374	GLU
1	B	375	MET

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Mol	Chain	Res	Type
1	C	14	LEU
1	C	110	PHE
1	C	112	ASN
1	C	142	LEU
1	C	146	LYS
1	C	200	ILE
1	C	273	ARG
1	C	336	ASP
1	C	342	LYS
1	C	367	GLU
1	C	374	GLU
1	C	375	MET
1	D	99	LEU
1	D	110	PHE
1	D	146	LYS
1	D	195	ILE
1	D	200	ILE
1	D	273	ARG
1	D	276	GLU
1	D	287	LEU
1	D	336	ASP
1	D	342	LYS
1	D	367	GLU
1	D	374	GLU
1	D	375	MET

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	38	ASN
1	A	49	ASN
1	A	68	GLN
1	A	130	ASN
1	A	190	ASN
1	A	212	ASN
1	A	218	HIS
1	A	221	ASN
1	A	250	GLN
1	A	356	GLN
1	A	370	GLN
1	B	38	ASN
1	B	49	ASN

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Mol	Chain	Res	Type
1	B	130	ASN
1	B	190	ASN
1	B	201	ASN
1	B	212	ASN
1	B	218	HIS
1	B	219	GLN
1	B	221	ASN
1	B	356	GLN
1	C	38	ASN
1	C	49	ASN
1	C	68	GLN
1	C	130	ASN
1	C	190	ASN
1	C	218	HIS
1	C	221	ASN
1	C	279	HIS
1	C	356	GLN
1	D	38	ASN
1	D	49	ASN
1	D	78	GLN
1	D	130	ASN
1	D	190	ASN
1	D	201	ASN
1	D	207	GLN
1	D	212	ASN
1	D	218	HIS
1	D	221	ASN
1	D	279	HIS
1	D	356	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

17 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	B	392	-	4,4,4	0.34	0	6,6,6	0.36	0
3	SO4	A	392	-	4,4,4	0.35	0	6,6,6	0.38	0
3	SO4	B	391	-	4,4,4	0.22	0	6,6,6	0.38	0
2	FAD	A	389	-	58,58,58	1.42	10 (17%)	85,89,89	2.17	25 (29%)
3	SO4	C	392	-	4,4,4	0.20	0	6,6,6	0.65	0
3	SO4	D	393	-	4,4,4	0.29	0	6,6,6	0.41	0
3	SO4	A	393	-	4,4,4	0.39	0	6,6,6	0.33	0
3	SO4	C	391	-	4,4,4	0.29	0	6,6,6	0.58	0
3	SO4	D	391	-	4,4,4	0.39	0	6,6,6	0.47	0
3	SO4	D	392	-	4,4,4	0.32	0	6,6,6	0.27	0
3	SO4	A	391	-	4,4,4	0.43	0	6,6,6	0.67	0
2	FAD	B	389	-	58,58,58	1.70	8 (13%)	85,89,89	2.09	24 (28%)
3	SO4	B	394	-	4,4,4	0.48	0	6,6,6	0.16	0
3	SO4	C	393	-	4,4,4	0.15	0	6,6,6	0.31	0
3	SO4	B	393	-	4,4,4	0.58	0	6,6,6	0.47	0
2	FAD	D	389	-	58,58,58	1.55	7 (12%)	85,89,89	1.90	22 (25%)
2	FAD	C	389	-	58,58,58	1.51	9 (15%)	85,89,89	2.19	26 (30%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	B	389	-	-	1/34/50/50	0/6/6/6
2	FAD	D	389	-	-	2/34/50/50	0/6/6/6
2	FAD	A	389	-	-	2/34/50/50	0/6/6/6
2	FAD	C	389	-	-	0/34/50/50	0/6/6/6

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	389	FAD	PA-O3P	6.57	1.66	1.59
2	B	389	FAD	P-O3P	5.87	1.65	1.59
2	D	389	FAD	C8A-N7A	4.74	1.40	1.31
2	D	389	FAD	C2A-N3A	4.05	1.41	1.33
2	C	389	FAD	C2A-N3A	4.04	1.41	1.33
2	D	389	FAD	C2A-N1A	3.86	1.40	1.33
2	C	389	FAD	C4X-N5	3.67	1.38	1.30
2	B	389	FAD	C4X-N5	3.64	1.38	1.30
2	C	389	FAD	PA-O3P	3.60	1.63	1.59
2	A	389	FAD	P-O3P	3.58	1.63	1.59
2	A	389	FAD	C1'-C2'	3.58	1.57	1.52
2	C	389	FAD	C8A-N7A	3.57	1.38	1.31
2	D	389	FAD	C1'-C2'	3.57	1.57	1.52
2	D	389	FAD	C4X-N5	3.55	1.38	1.30
2	A	389	FAD	C4X-N5	3.36	1.38	1.30
2	A	389	FAD	C2A-N1A	3.21	1.39	1.33
2	B	389	FAD	C1'-C2'	3.14	1.57	1.52
2	C	389	FAD	C2A-N1A	3.13	1.39	1.33
2	A	389	FAD	C2A-N3A	3.09	1.39	1.33
2	C	389	FAD	C1'-C2'	2.92	1.56	1.52
2	B	389	FAD	C5'-C4'	2.86	1.55	1.51
2	C	389	FAD	C10-N1	2.85	1.39	1.33
2	B	389	FAD	C2A-N1A	2.80	1.38	1.33
2	B	389	FAD	C8A-N7A	2.71	1.36	1.31
2	D	389	FAD	C8A-N9A	2.44	1.41	1.37
2	C	389	FAD	C8A-N9A	2.38	1.41	1.37
2	A	389	FAD	C6-C5X	2.34	1.43	1.40
2	A	389	FAD	P-O2P	-2.34	1.44	1.55
2	A	389	FAD	C4-N3	-2.24	1.34	1.38
2	A	389	FAD	C4A-N3A	2.17	1.38	1.34
2	C	389	FAD	C9A-N10	-2.13	1.37	1.41
2	D	389	FAD	C5A-C4A	2.11	1.42	1.39
2	B	389	FAD	C9A-N10	-2.03	1.37	1.41
2	A	389	FAD	C8A-N9A	2.02	1.41	1.37

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	389	FAD	N3A-C2A-N1A	-7.56	117.14	128.58
2	C	389	FAD	N3A-C2A-N1A	-7.11	117.82	128.58
2	A	389	FAD	N9A-C8A-N7A	-6.60	104.57	113.94
2	B	389	FAD	N9A-C8A-N7A	-6.35	104.92	113.94
2	A	389	FAD	N3A-C2A-N1A	-6.27	119.08	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	389	FAD	N9A-C8A-N7A	-6.21	105.13	113.94
2	C	389	FAD	C4-N3-C2	-5.55	115.79	125.64
2	D	389	FAD	N9A-C8A-N7A	-5.36	106.33	113.94
2	B	389	FAD	O3P-PA-O1A	-5.22	95.01	110.70
2	D	389	FAD	C5'-C4'-C3'	-5.01	102.77	112.22
2	A	389	FAD	C4A-N9A-C8A	4.96	110.95	105.74
2	A	389	FAD	C5X-C9A-N10	4.96	122.45	117.97
2	C	389	FAD	C4A-N9A-C8A	4.90	110.88	105.74
2	D	389	FAD	N3A-C2A-N1A	-4.60	121.62	128.58
2	A	389	FAD	C5A-N7A-C8A	4.54	110.59	103.45
2	A	389	FAD	C5'-C4'-C3'	-4.24	104.22	112.22
2	D	389	FAD	C5A-C4A-N3A	-4.11	121.06	126.72
2	D	389	FAD	C4X-C10-N10	4.02	122.24	116.48
2	B	389	FAD	C4A-N9A-C8A	3.96	109.90	105.74
2	A	389	FAD	O3P-PA-O1A	-3.94	98.85	110.70
2	B	389	FAD	C5A-N7A-C8A	3.90	109.58	103.45
2	A	389	FAD	C4X-C10-N10	3.87	122.02	116.48
2	D	389	FAD	C5A-N7A-C8A	3.84	109.49	103.45
2	C	389	FAD	C4X-C4-N3	3.76	122.82	113.25
2	B	389	FAD	C4-C4X-N5	3.76	123.40	118.21
2	C	389	FAD	O3P-PA-O1A	-3.72	99.51	110.70
2	B	389	FAD	C4X-C10-N10	3.70	121.78	116.48
2	A	389	FAD	O4B-C1B-N9A	-3.69	101.01	108.09
2	B	389	FAD	C1'-N10-C9A	3.68	127.79	120.63
2	C	389	FAD	C5A-C4A-N3A	-3.60	121.76	126.72
2	C	389	FAD	O2-C2-N1	-3.59	115.84	121.80
2	C	389	FAD	C2A-N3A-C4A	3.55	120.51	111.83
2	A	389	FAD	C9A-C5X-N5	-3.52	118.72	122.45
2	C	389	FAD	C4X-C10-N10	3.48	121.46	116.48
2	B	389	FAD	C10-C4X-N5	-3.36	117.95	124.81
2	C	389	FAD	C5A-N7A-C8A	3.36	108.72	103.45
2	D	389	FAD	O2-C2-N1	-3.35	116.24	121.80
2	A	389	FAD	O2A-PA-O3P	3.34	116.29	107.27
2	C	389	FAD	C5'-C4'-C3'	-3.32	105.95	112.22
2	B	389	FAD	C2A-N1A-C6A	3.28	124.12	118.73
2	C	389	FAD	C9A-C5X-N5	-3.26	118.99	122.45
2	C	389	FAD	C10-C4X-N5	-3.22	118.23	124.81
2	B	389	FAD	C2A-N3A-C4A	3.19	119.62	111.83
2	A	389	FAD	O3B-C3B-C4B	-3.18	101.95	111.08
2	B	389	FAD	C9A-C5X-N5	-3.16	119.10	122.45
2	A	389	FAD	C9-C9A-N10	-3.12	117.66	121.85
2	D	389	FAD	C4A-N9A-C8A	3.08	108.97	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	389	FAD	C1'-N10-C9A	3.05	126.56	120.63
2	B	389	FAD	C4-N3-C2	-3.04	120.24	125.64
2	C	389	FAD	C4-C4X-N5	3.03	122.40	118.21
2	B	389	FAD	O2-C2-N1	-2.91	116.97	121.80
2	A	389	FAD	N3A-C4A-N9A	2.89	132.09	127.17
2	A	389	FAD	C2A-N3A-C4A	2.88	118.86	111.83
2	C	389	FAD	N3A-C4A-N9A	2.87	132.05	127.17
2	A	389	FAD	C5A-C4A-N3A	-2.85	122.80	126.72
2	C	389	FAD	O4'-C4'-C3'	2.85	115.91	109.25
2	D	389	FAD	C2A-N3A-C4A	2.83	118.74	111.83
2	A	389	FAD	O2-C2-N1	-2.81	117.13	121.80
2	B	389	FAD	C5A-C4A-N3A	-2.79	122.87	126.72
2	B	389	FAD	O2P-P-O3P	-2.76	99.82	107.27
2	D	389	FAD	C4-N3-C2	-2.73	120.79	125.64
2	D	389	FAD	C5X-C9A-N10	2.72	120.42	117.97
2	A	389	FAD	C6-C5X-C9A	2.68	122.73	119.05
2	D	389	FAD	N3A-C4A-N9A	2.63	131.63	127.17
2	A	389	FAD	C5X-C6-C7	-2.61	115.98	120.83
2	D	389	FAD	C10-C4X-N5	-2.60	119.51	124.81
2	A	389	FAD	C9A-N10-C10	-2.59	116.80	120.75
2	D	389	FAD	O3P-PA-O1A	-2.58	102.95	110.70
2	A	389	FAD	C4-N3-C2	-2.54	121.12	125.64
2	A	389	FAD	C8M-C8-C9	-2.52	115.12	119.57
2	C	389	FAD	O3'-C3'-C2'	-2.52	103.20	108.93
2	B	389	FAD	C5X-C9A-N10	2.51	120.24	117.97
2	B	389	FAD	C4X-C4-N3	2.49	119.60	113.25
2	A	389	FAD	O2'-C2'-C3'	-2.45	103.52	109.25
2	B	389	FAD	O5B-PA-O1A	2.39	118.39	108.94
2	C	389	FAD	O5B-PA-O1A	2.37	118.35	108.94
2	D	389	FAD	C4A-C5A-N7A	-2.36	107.88	110.58
2	C	389	FAD	C4A-N9A-C1B	-2.36	121.12	126.63
2	D	389	FAD	O4-C4-C4X	-2.34	120.35	126.53
2	C	389	FAD	O4-C4-C4X	-2.31	120.45	126.53
2	C	389	FAD	C4'-C3'-C2'	2.30	117.40	113.57
2	C	389	FAD	O3B-C3B-C4B	-2.27	104.56	111.08
2	B	389	FAD	O4B-C1B-N9A	-2.26	103.75	108.09
2	D	389	FAD	C6-C5X-C9A	2.25	122.14	119.05
2	C	389	FAD	C1'-N10-C9A	2.25	125.01	120.63
2	B	389	FAD	C5X-N5-C4X	2.21	121.67	118.09
2	D	389	FAD	C4A-N9A-C1B	-2.19	121.52	126.63
2	A	389	FAD	C10-C4X-N5	-2.18	120.35	124.81
2	B	389	FAD	C6-C5X-C9A	2.16	122.01	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	389	FAD	O5B-PA-O1A	2.14	117.43	108.94
2	B	389	FAD	C9-C8-C7	2.14	122.82	119.69
2	B	389	FAD	O3P-P-O1P	2.13	117.11	110.70
2	C	389	FAD	C4X-C10-N1	-2.11	119.41	124.59
2	A	389	FAD	C2A-N1A-C6A	2.08	122.14	118.73
2	C	389	FAD	O2P-P-O1P	-2.05	102.92	112.44
2	D	389	FAD	C4-C4X-N5	2.03	121.01	118.21
2	D	389	FAD	C9-C8-C7	2.01	122.64	119.69

There are no chirality outliers.

All (5) torsion outliers are listed below:

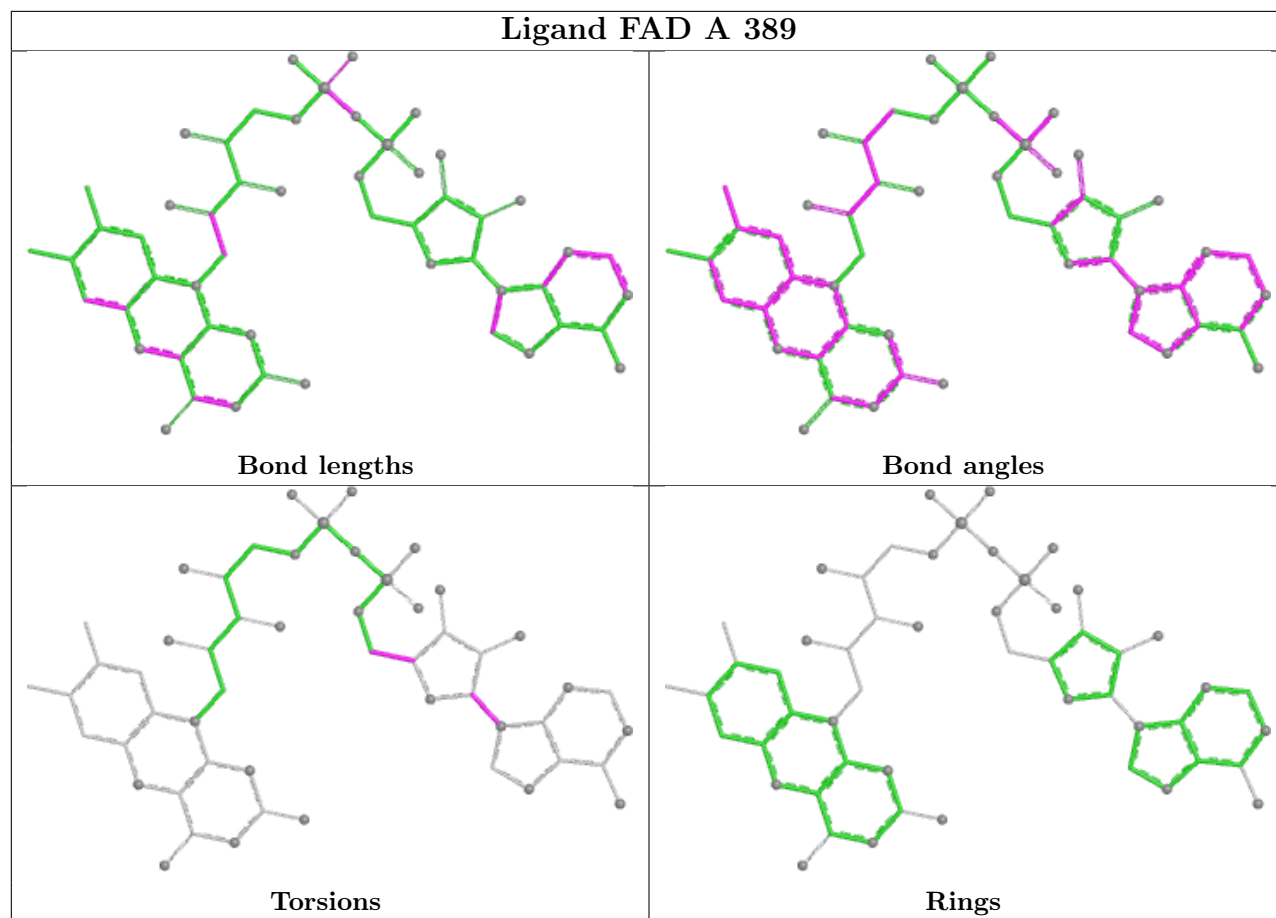
Mol	Chain	Res	Type	Atoms
2	A	389	FAD	C2B-C1B-N9A-C8A
2	B	389	FAD	C2B-C1B-N9A-C8A
2	D	389	FAD	C2B-C1B-N9A-C8A
2	A	389	FAD	O4B-C4B-C5B-O5B
2	D	389	FAD	O4B-C4B-C5B-O5B

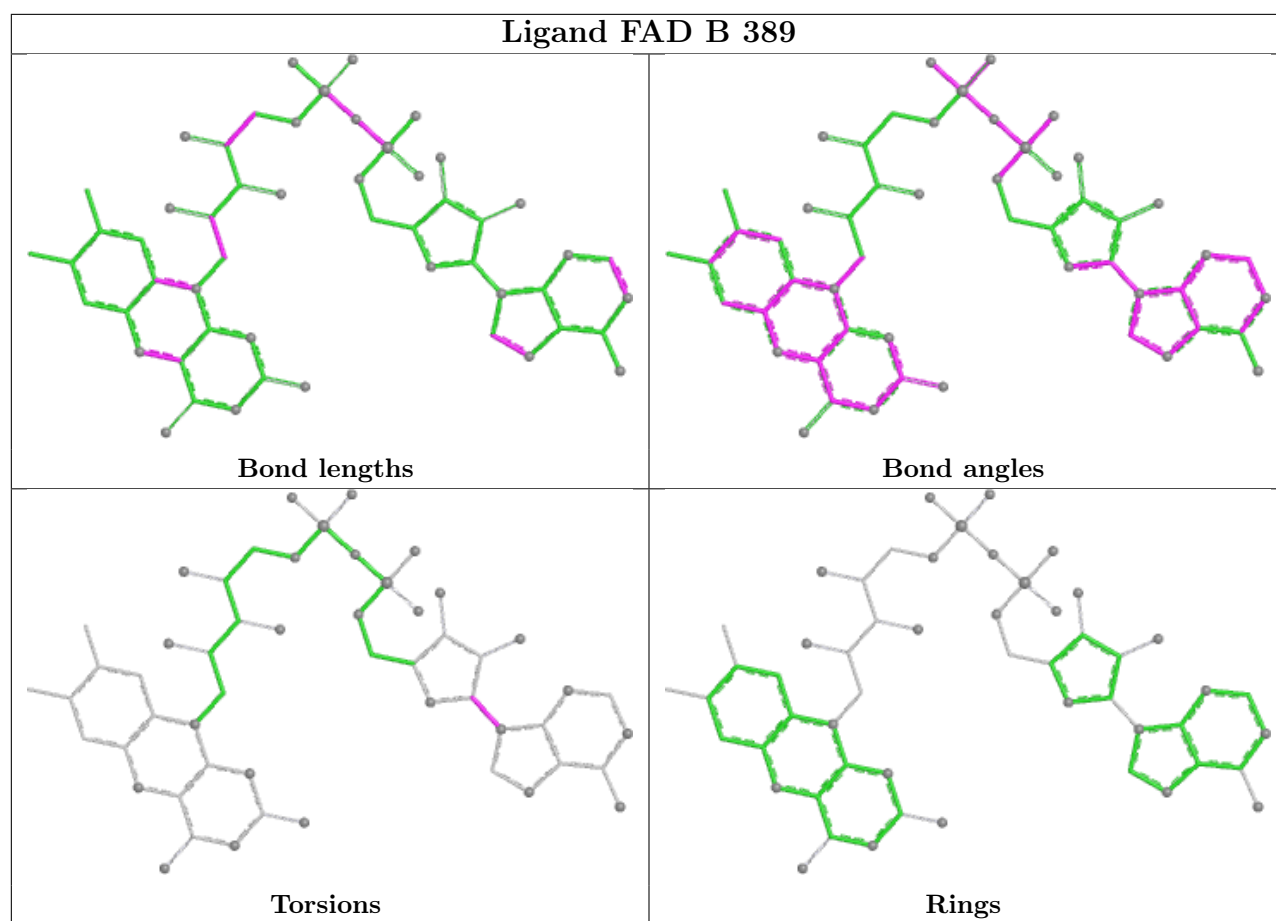
There are no ring outliers.

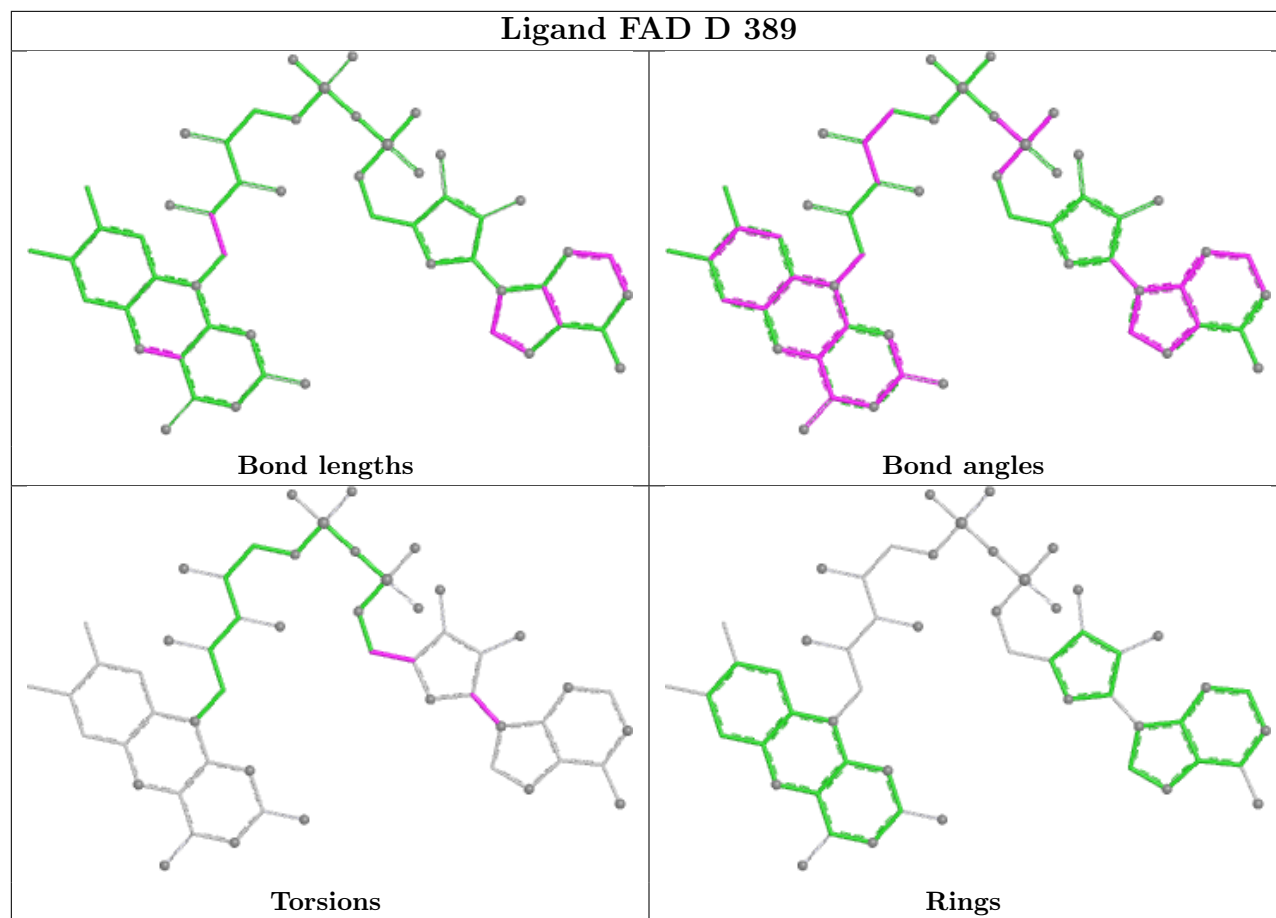
3 monomers are involved in 3 short contacts:

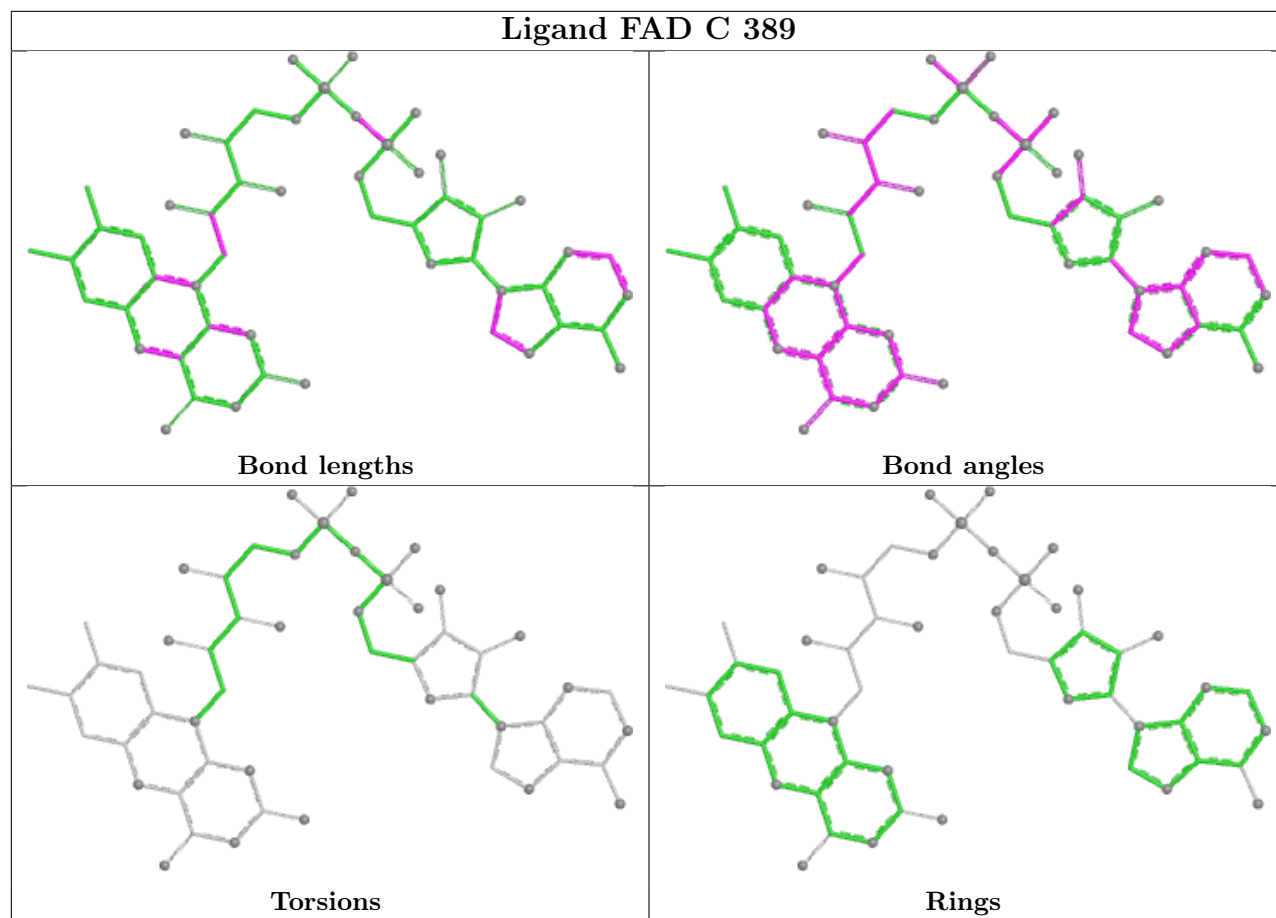
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	389	FAD	1	0
3	A	391	SO4	1	0
2	D	389	FAD	1	0

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.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	367/398 (92%)	-0.03	18 (4%) 35 37	18, 32, 59, 84	0
1	B	366/398 (91%)	-0.17	10 (2%) 56 59	17, 33, 58, 80	0
1	C	365/398 (91%)	0.11	17 (4%) 36 38	22, 42, 73, 95	0
1	D	364/398 (91%)	0.26	15 (4%) 41 43	22, 44, 76, 101	0
All	All	1462/1592 (91%)	0.04	60 (4%) 41 43	17, 38, 68, 101	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	381	THR	6.9
1	A	379	ASP	5.8
1	A	110	PHE	5.6
1	B	110	PHE	5.5
1	C	110	PHE	5.2
1	A	382	PHE	5.1
1	A	378	PRO	4.7
1	A	377	LYS	4.7
1	A	376	PHE	4.5
1	A	380	PHE	4.3
1	D	110	PHE	4.2
1	C	103	ASN	4.0
1	D	339	ALA	3.9
1	D	380	PHE	3.9
1	C	95	LYS	3.8
1	B	106	PRO	3.8
1	B	341	GLY	3.7
1	C	98	ILE	3.4
1	A	375	MET	3.3
1	A	104	VAL	3.2
1	C	341	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	112	ASN	3.1
1	A	99	LEU	3.0
1	D	104	VAL	2.9
1	C	111	ASP	2.8
1	B	381	THR	2.8
1	C	378	PRO	2.8
1	D	379	ASP	2.8
1	A	106	PRO	2.7
1	D	321	GLY	2.7
1	D	111	ASP	2.6
1	A	249	THR	2.5
1	B	249	THR	2.5
1	A	13	LEU	2.5
1	C	96	GLY	2.5
1	D	335	SER	2.5
1	D	251	VAL	2.5
1	A	97	ASN	2.5
1	C	250	GLN	2.4
1	B	378	PRO	2.4
1	C	99	LEU	2.4
1	D	287	LEU	2.4
1	D	341	GLY	2.4
1	B	111	ASP	2.3
1	D	98	ILE	2.3
1	B	377	LYS	2.3
1	D	13	LEU	2.3
1	C	270	TRP	2.3
1	C	107	GLU	2.2
1	C	106	PRO	2.2
1	B	13	LEU	2.2
1	C	112	ASN	2.2
1	D	101	THR	2.2
1	D	378	PRO	2.1
1	B	251	VAL	2.1
1	A	339	ALA	2.1
1	C	13	LEU	2.1
1	A	98	ILE	2.1
1	C	104	VAL	2.1
1	C	97	ASN	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](#)

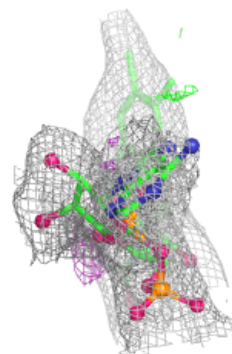
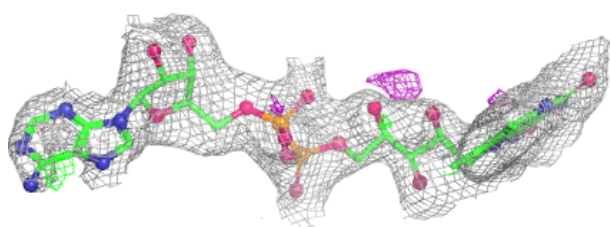
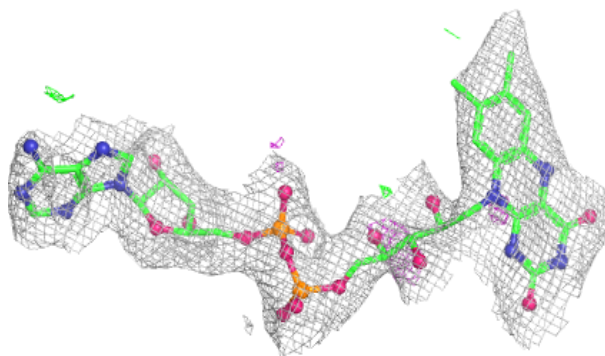
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	SO4	B	393	5/5	0.84	0.14	55,55,59,61	5
3	SO4	C	393	5/5	0.86	0.13	58,62,63,63	5
3	SO4	A	393	5/5	0.88	0.11	68,71,73,73	0
3	SO4	B	394	5/5	0.89	0.12	61,63,66,67	0
3	SO4	A	392	5/5	0.90	0.08	65,67,68,68	0
3	SO4	D	393	5/5	0.91	0.09	57,59,61,61	5
3	SO4	C	392	5/5	0.92	0.12	58,59,60,61	0
3	SO4	B	392	5/5	0.93	0.07	73,75,75,75	0
3	SO4	B	391	5/5	0.94	0.09	60,63,65,67	0
3	SO4	C	391	5/5	0.95	0.07	57,64,65,67	0
3	SO4	D	391	5/5	0.95	0.10	49,53,58,58	0
3	SO4	A	391	5/5	0.95	0.07	61,62,62,66	0
3	SO4	D	392	5/5	0.96	0.12	58,59,60,60	0
2	FAD	D	389	53/53	0.98	0.06	20,26,35,38	0
2	FAD	C	389	53/53	0.98	0.05	18,24,33,37	0
2	FAD	B	389	53/53	0.99	0.04	14,20,26,28	0
2	FAD	A	389	53/53	0.99	0.04	15,22,25,27	0

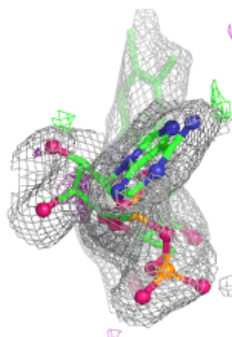
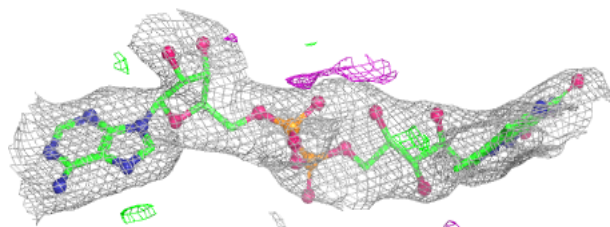
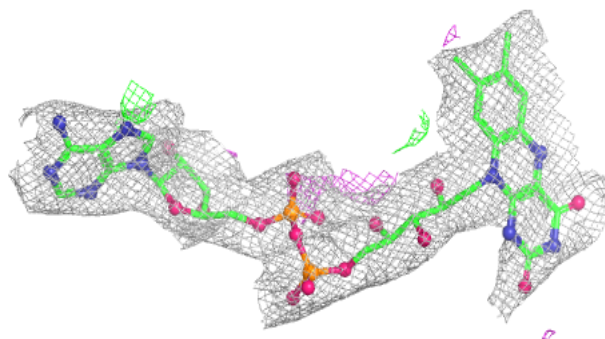
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD D 389:

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

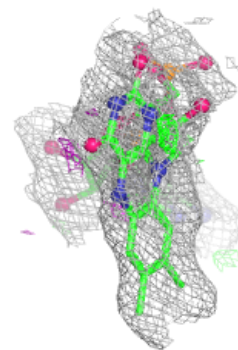
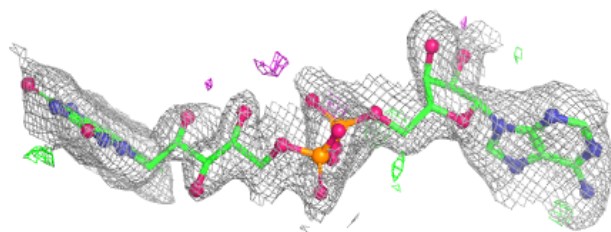
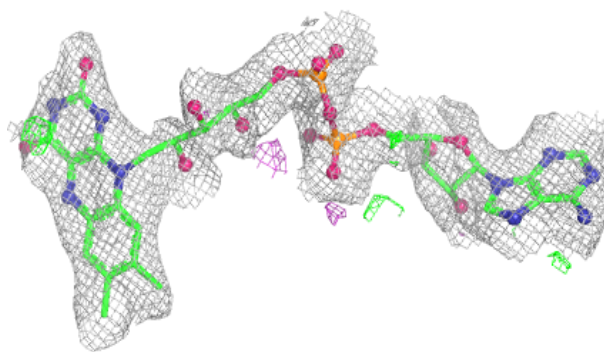
**Electron density around FAD C 389:**

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

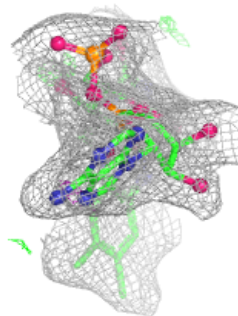
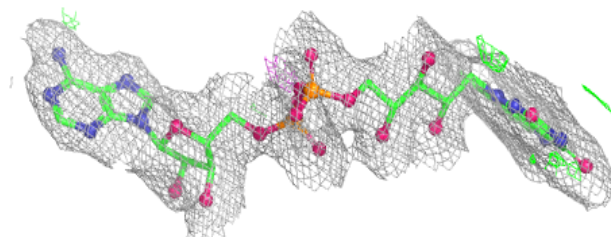
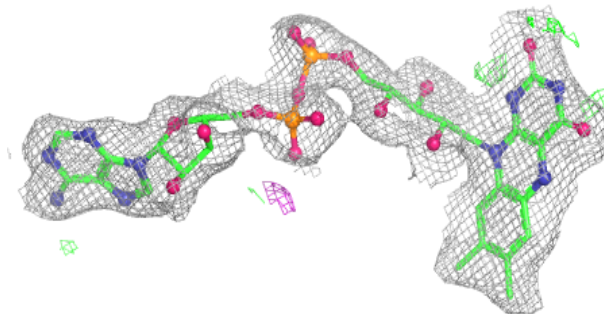


Electron density around FAD B 389:

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

**Electron density around FAD A 389:**

$2mF_o-DF_c$ (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.