



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 07:28 PM EDT

PDB ID : 3NS1 / pdb_00003ns1
Title : Crystal Structure of Bovine Xanthine Oxidase in Complex with 6-Mercaptopurine
Authors : Cao, H.; Pauff, J.M.; Hille, R.
Deposited on : 2010-07-01
Resolution : 2.60 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

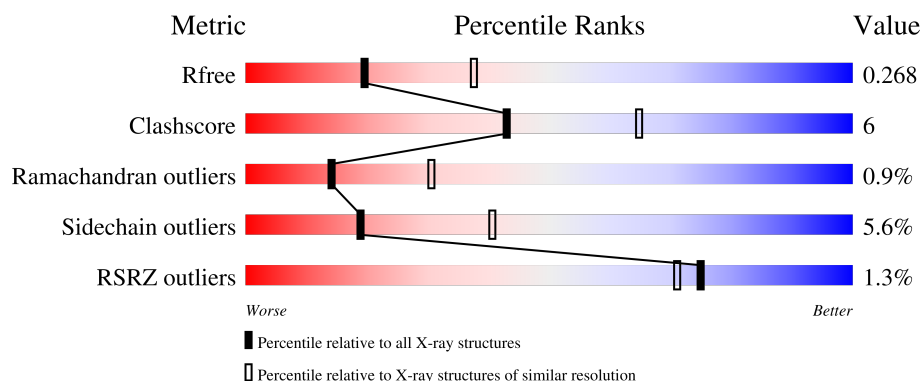
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	164	
1	J	164	
2	B	305	
2	K	305	
3	C	755	

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Mol	Chain	Length	Quality of chain
3	L	755	% 82% 15% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	PM6	C	1	-	X	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 19357 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 Xanthine dehydrogenase/oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	164	Total	C	N	O	S	0	0	0
			1255	788	225	230	12			
1	J	164	Total	C	N	O	S	0	0	0
			1255	788	225	230	12			

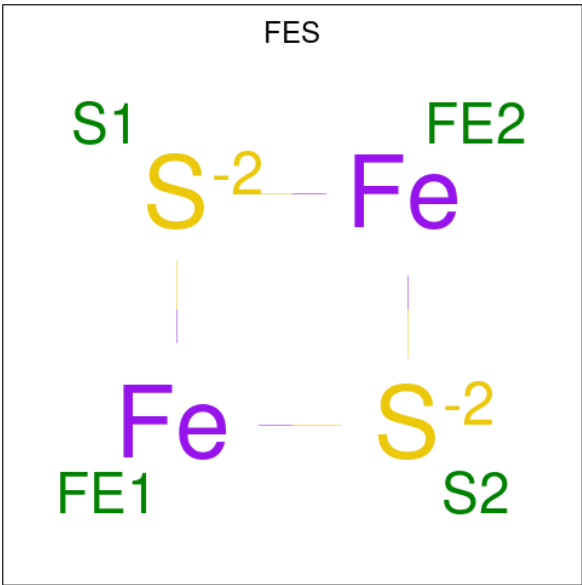
- Molecule 2 is a protein called Xanthine dehydrogenase/oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	305	Total	C	N	O	S	0	0	0
			2389	1539	402	435	13			
2	K	305	Total	C	N	O	S	0	0	0
			2389	1539	402	435	13			

- Molecule 3 is a protein called Xanthine dehydrogenase/oxidase.

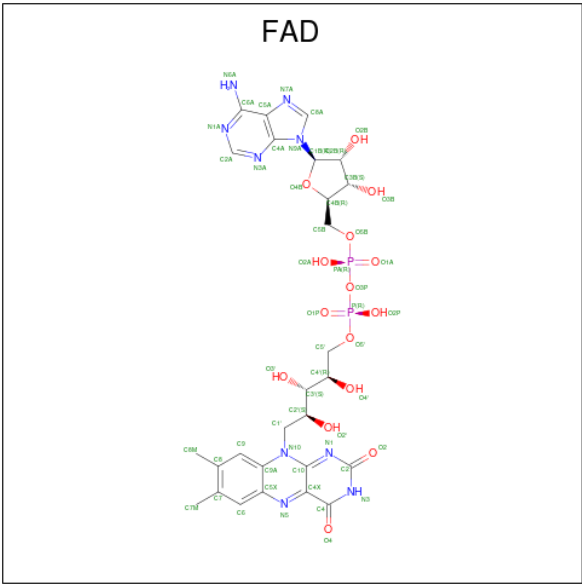
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	755	Total	C	N	O	S	0	0	0
			5823	3680	1003	1105	35			
3	L	745	Total	C	N	O	S	0	0	0
			5761	3643	992	1093	33			

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



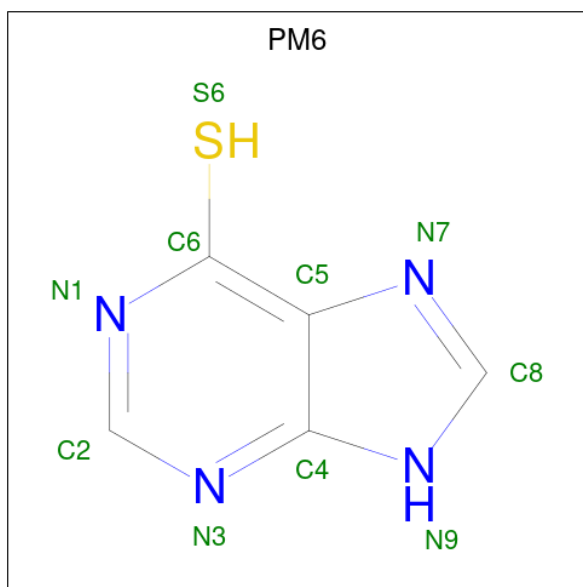
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			4	2	2		
4	A	1	Total	Fe	S	0	0
			4	2	2		
4	J	1	Total	Fe	S	0	0
			4	2	2		
4	J	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



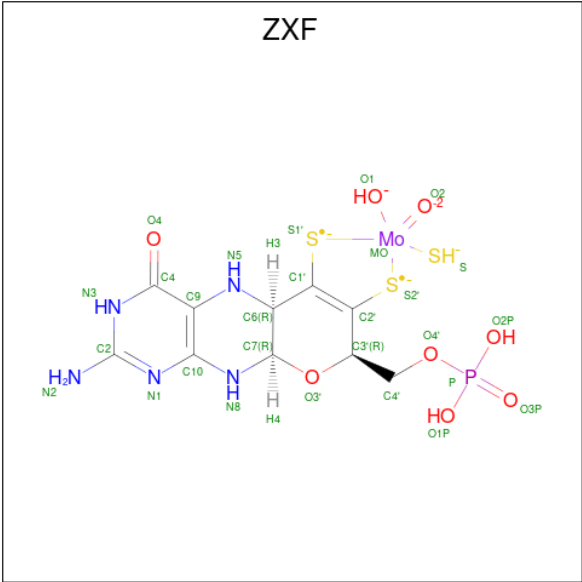
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	K	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 6 is 9H-purine-6-thiol (CCD ID: PM6) (formula: $C_5H_4N_4S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	S	0	0
			10	5	4	1		
6	L	1	Total	C	N	S	0	0
			10	5	4	1		

- Molecule 7 is Molybdopterin hydroxy-oxo-thiol-molybdenum (CCD ID: ZXF) (formula: $C_{10}H_{14}MoN_5O_8PS_3$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
7	C	1	Total	C	Mo	N	O	P	S	0	0
			28	10	1	5	8	1	3		
7	L	1	Total	C	Mo	N	O	P	S	0	0
			28	10	1	5	8	1	3		

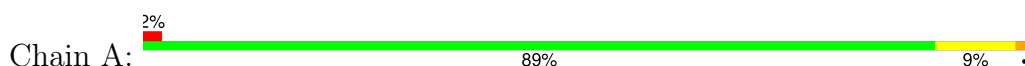
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	24	Total	O	0	0
			24	24		
8	B	15	Total	O	0	0
			15	15		
8	C	120	Total	O	0	0
			120	120		
8	J	14	Total	O	0	0
			14	14		
8	K	21	Total	O	0	0
			21	21		
8	L	93	Total	O	0	0
			93	93		

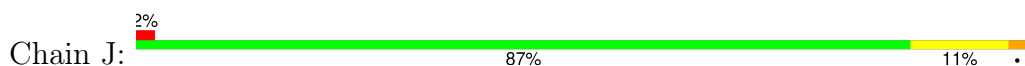
3 Residue-property plots

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.

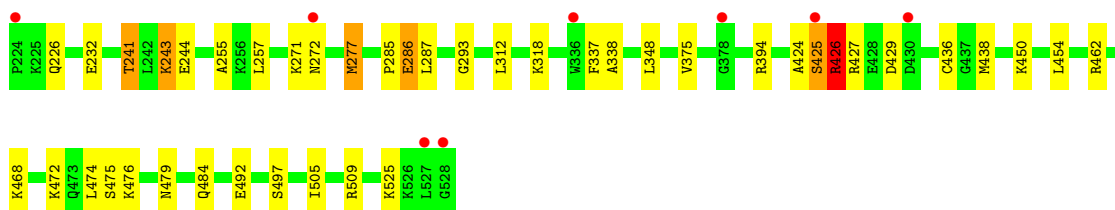
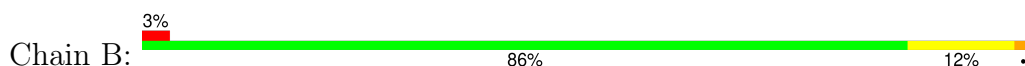
- Molecule 1: Xanthine dehydrogenase/oxidase



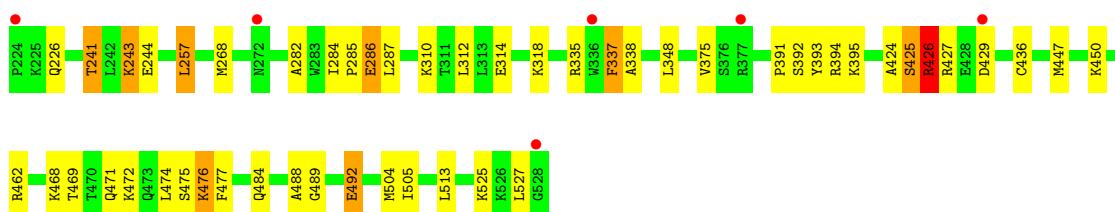
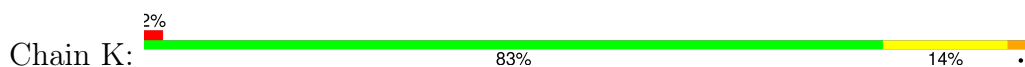
- Molecule 1: Xanthine dehydrogenase/oxidase



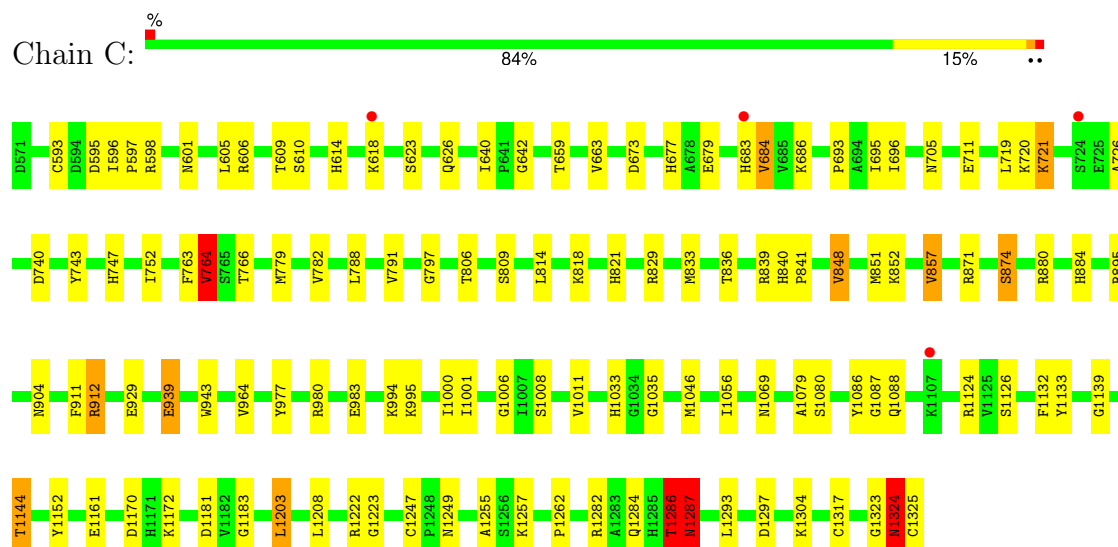
- Molecule 2: Xanthine dehydrogenase/oxidase



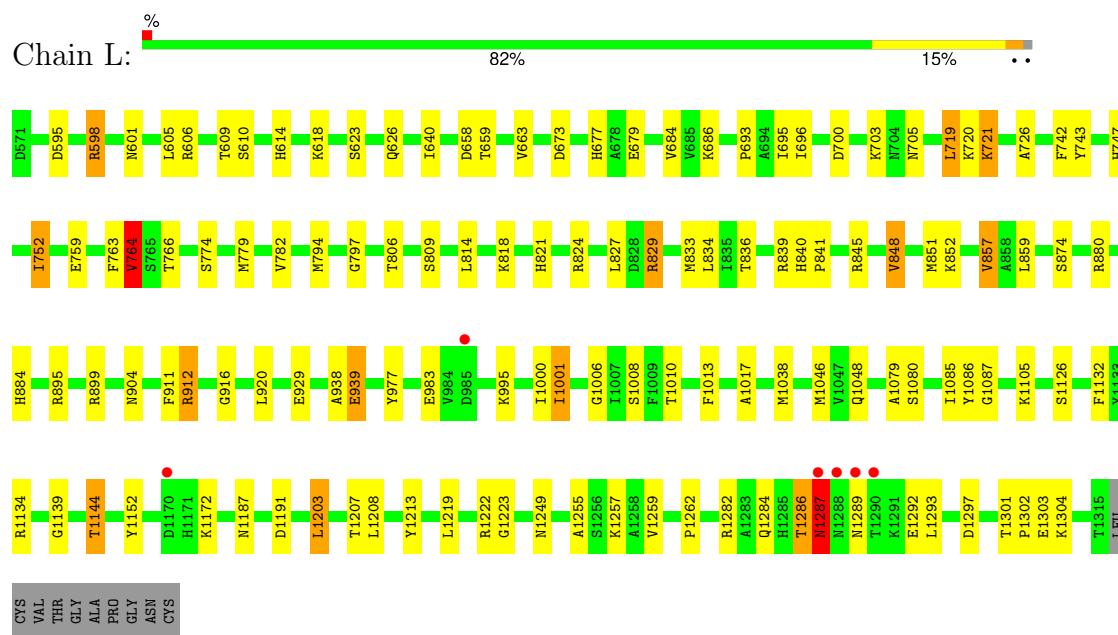
- Molecule 2: Xanthine dehydrogenase/oxidase



- Molecule 3: Xanthine dehydrogenase/oxidase



• Molecule 3: Xanthine dehydrogenase/oxidase



CYS
VAL
THR
GLY
ALA
PRO
GLY
ASN
CYS

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	134.64Å 73.93Å 140.35Å 90.00° 97.01° 90.00°	Depositor
Resolution (Å)	45.50 – 2.60 45.50 – 2.60	Depositor EDS
% Data completeness (in resolution range)	92.4 (45.50-2.60) 92.2 (45.50-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.72 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.217 , 0.269 0.217 , 0.268	Depositor DCC
R_{free} test set	3922 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	34.7	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	19357	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PM6, FAD, FES, ZXF

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	1.01	0/1277	1.07	3/1723 (0.2%)
1	J	1.01	0/1277	1.05	6/1723 (0.3%)
2	B	0.86	1/2438 (0.0%)	1.09	9/3290 (0.3%)
2	K	0.91	0/2438	1.05	6/3290 (0.2%)
3	C	0.99	3/5951 (0.1%)	1.12	17/8061 (0.2%)
3	L	1.00	1/5888 (0.0%)	1.09	10/7974 (0.1%)
All	All	0.97	5/19269 (0.0%)	1.09	51/26061 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1144	THR	CA-CB	6.12	1.63	1.53
3	L	1144	THR	CA-CB	6.04	1.63	1.53
3	C	1011	VAL	CA-C	5.84	1.57	1.53
3	C	964	VAL	CA-CB	5.12	1.57	1.53
2	B	293	GLY	N-CA	5.04	1.50	1.43

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	848	VAL	CB-CA-C	-8.38	98.13	110.62
2	B	286	GLU	N-CA-C	-7.92	93.94	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	484	GLN	N-CA-C	7.42	120.43	111.82
2	K	436	CYS	N-CA-C	7.26	120.10	109.07
2	B	436	CYS	N-CA-C	7.25	120.21	108.76
3	L	1262	PRO	N-CA-C	7.18	119.46	110.70
3	C	642	GLY	N-CA-C	7.04	116.61	110.21
2	K	286	GLU	N-CA-C	-6.96	95.98	110.80
3	C	1262	PRO	N-CA-C	6.82	119.03	110.70
2	B	505	ILE	N-CA-C	6.75	116.90	110.42
3	C	1324	ASN	CA-C-N	6.53	133.45	121.70
3	C	1324	ASN	C-N-CA	6.53	133.45	121.70
3	C	943	TRP	N-CA-C	6.51	118.04	111.07
1	A	141	ASP	N-CA-C	6.42	120.38	112.54
3	C	764	VAL	N-CA-C	6.38	117.90	108.45
1	J	131	GLN	CA-C-N	6.30	126.21	119.28
1	J	131	GLN	C-N-CA	6.30	126.21	119.28
3	C	1286	THR	N-CA-C	6.10	120.56	111.96
2	B	394	ARG	N-CA-C	6.07	119.91	111.90
2	K	505	ILE	N-CA-C	5.79	117.22	110.62
2	B	497	SER	CA-C-N	5.76	125.44	119.56
2	B	497	SER	C-N-CA	5.76	125.44	119.56
3	C	1170	ASP	N-CA-C	5.75	118.17	110.35
3	L	752	ILE	N-CA-C	5.73	113.73	107.60
3	L	1001	ILE	CA-C-N	5.68	126.86	120.66
3	L	1001	ILE	C-N-CA	5.68	126.86	120.66
1	A	164	ALA	CA-C-N	5.64	131.86	121.70
1	A	164	ALA	C-N-CA	5.64	131.86	121.70
3	L	764	VAL	N-CA-C	5.56	116.68	108.45
3	C	1325	CYS	N-CA-C	5.51	126.43	111.00
3	C	964	VAL	N-CA-CB	5.43	113.92	110.50
2	B	293	GLY	N-CA-C	5.42	118.50	112.00
3	C	1056	ILE	CB-CA-C	5.38	114.60	109.33
3	C	874	SER	N-CA-C	5.36	117.81	111.33
1	J	153	TYR	N-CA-C	5.24	121.96	110.80
2	B	479	ASN	N-CA-C	5.24	115.97	108.74
3	C	791	VAL	CB-CA-C	-5.21	104.47	110.41
3	C	1287	ASN	N-CA-C	5.21	115.01	108.45
2	K	484	GLN	CB-CA-C	-5.20	102.72	110.88
3	L	938	ALA	N-CA-C	5.16	116.59	111.07
2	K	394	ARG	N-CA-C	5.15	118.83	112.24
3	C	711	GLU	N-CA-C	5.14	117.93	110.42
3	L	759	GLU	N-CA-C	5.13	117.48	110.24
3	C	593	CYS	N-CA-C	5.12	117.25	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	1287	ASN	N-CA-C	5.11	115.03	108.34
1	J	164	ALA	CA-C-N	5.09	130.87	121.70
1	J	164	ALA	C-N-CA	5.09	130.87	121.70
3	L	824	ARG	N-CA-C	5.06	116.68	109.14
1	J	130	ASN	N-CA-C	-5.02	107.28	113.41
3	L	1013	PHE	N-CA-C	5.01	118.88	112.87
2	K	282	ALA	N-CA-C	5.01	117.39	111.33

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	1324	ASN	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	1255	0	1265	6	0
1	J	1255	0	1265	9	0
2	B	2389	0	2459	20	0
2	K	2389	0	2459	32	0
3	C	5823	0	5746	79	0
3	L	5761	0	5685	95	0
4	A	8	0	0	0	0
4	J	8	0	0	0	0
5	B	53	0	31	0	0
5	K	53	0	31	1	0
6	C	10	0	4	1	0
6	L	10	0	4	1	0
7	C	28	0	0	3	0
7	L	28	0	0	2	0
8	A	24	0	0	1	0
8	B	15	0	0	0	0
8	C	120	0	0	0	0
8	J	14	0	0	0	0
8	K	21	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	L	93	0	0	4	0
All	All	19357	0	18949	236	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 6.

All (236) 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)
2:K:241:THR:HG23	2:K:243:LYS:HD3	1.20	1.15
3:C:995:LYS:HZ1	3:C:1284:GLN:NE2	1.52	1.08
3:L:779:MET:HE1	3:L:814:LEU:HD13	1.32	1.07
2:B:426:ARG:HG3	2:B:426:ARG:HH11	1.01	1.05
2:K:426:ARG:HH11	2:K:426:ARG:HG2	0.98	1.05
2:K:426:ARG:HG2	2:K:426:ARG:NH1	1.66	1.01
3:C:995:LYS:NZ	3:C:1284:GLN:HE21	1.62	0.98
3:C:779:MET:HE1	3:C:814:LEU:HD13	1.48	0.93
2:B:426:ARG:HG3	2:B:426:ARG:NH1	1.71	0.93
2:B:241:THR:HG22	2:B:244:GLU:H	1.34	0.92
3:L:995:LYS:HZ3	3:L:1284:GLN:NE2	1.69	0.91
2:K:241:THR:HG22	2:K:244:GLU:H	1.37	0.90
3:L:995:LYS:HZ3	3:L:1284:GLN:HE21	1.17	0.89
2:B:243:LYS:H	2:B:243:LYS:HD3	1.37	0.88
3:C:851:MET:HE3	3:C:857:VAL:HG21	1.55	0.88
2:B:241:THR:HG23	2:B:243:LYS:HD3	1.56	0.88
3:L:995:LYS:NZ	3:L:1284:GLN:NE2	2.25	0.85
3:L:851:MET:HE3	3:L:857:VAL:HG21	1.57	0.85
3:L:995:LYS:NZ	3:L:1284:GLN:HE21	1.74	0.84
3:L:779:MET:CE	3:L:814:LEU:HD13	2.08	0.84
3:C:1046:MET:HE1	3:C:1087:GLY:HA2	1.61	0.83
3:L:720:LYS:O	3:L:721:LYS:CB	2.25	0.82
3:L:1046:MET:HE1	3:L:1087:GLY:HA2	1.62	0.80
1:A:131:GLN:HE21	1:A:133:GLU:H	1.27	0.79
3:L:610:SER:O	3:L:663:VAL:O	2.02	0.78
3:L:829:ARG:CG	3:L:833:MET:HE2	2.14	0.78
2:K:426:ARG:HH11	2:K:426:ARG:CG	1.90	0.77
2:K:241:THR:CG2	2:K:243:LYS:HD3	2.09	0.77
3:C:695:ILE:H	3:C:904:ASN:HD22	1.32	0.76
3:L:623:SER:HA	3:L:626:GLN:HE21	1.50	0.76
2:K:286:GLU:O	2:K:287:LEU:HB2	1.86	0.75
3:C:995:LYS:NZ	3:C:1284:GLN:NE2	2.26	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:884:HIS:HE1	3:C:1006:GLY:H	1.36	0.73
3:C:720:LYS:O	3:C:721:LYS:CB	2.36	0.72
3:L:695:ILE:H	3:L:904:ASN:HD22	1.38	0.71
3:C:610:SER:O	3:C:663:VAL:O	2.08	0.71
2:K:243:LYS:HD3	2:K:243:LYS:H	1.56	0.70
3:C:623:SER:HA	3:C:626:GLN:HE21	1.56	0.70
3:C:829:ARG:CG	3:C:833:MET:HE2	2.22	0.70
2:B:426:ARG:HH11	2:B:426:ARG:CG	1.91	0.69
3:C:640:ILE:HG12	3:C:779:MET:HE3	1.73	0.69
2:K:243:LYS:H	2:K:243:LYS:CD	2.06	0.69
3:L:829:ARG:HG3	3:L:833:MET:HE2	1.75	0.68
3:C:726:ALA:HA	3:C:851:MET:HE1	1.74	0.68
3:C:779:MET:CE	3:C:814:LEU:HD13	2.22	0.68
3:C:829:ARG:HG3	3:C:833:MET:HE2	1.76	0.68
3:C:1046:MET:HE1	3:C:1087:GLY:CA	2.24	0.68
2:B:285:PRO:O	2:B:286:GLU:HB2	1.94	0.67
3:L:829:ARG:HG2	3:L:833:MET:HE2	1.75	0.67
2:B:243:LYS:H	2:B:243:LYS:CD	2.08	0.66
3:L:1287:ASN:C	3:L:1287:ASN:HD22	2.05	0.65
3:C:995:LYS:HZ1	3:C:1284:GLN:HE21	0.77	0.65
3:L:640:ILE:HG23	3:L:779:MET:HE2	1.77	0.65
1:J:131:GLN:HE21	1:J:133:GLU:H	1.43	0.65
3:L:720:LYS:O	3:L:721:LYS:HB2	1.98	0.64
2:B:286:GLU:O	2:B:287:LEU:HB2	1.98	0.64
3:L:1046:MET:HE1	3:L:1087:GLY:CA	2.28	0.63
3:L:884:HIS:HE1	3:L:1006:GLY:H	1.48	0.62
3:C:884:HIS:CE1	3:C:1006:GLY:H	2.17	0.62
3:C:880:ARG:O	3:C:884:HIS:HD2	1.81	0.62
3:L:720:LYS:O	3:L:721:LYS:HB3	1.98	0.62
3:L:1152:TYR:CE1	3:L:1257:LYS:HG2	2.34	0.62
7:C:1326:ZXF:O2	7:C:1326:ZXF:MO	1.72	0.61
2:B:285:PRO:O	2:B:286:GLU:CB	2.48	0.61
7:L:1326:ZXF:O2	7:L:1326:ZXF:MO	1.72	0.60
2:B:272:ASN:ND2	3:C:683:HIS:CE1	2.69	0.60
3:L:764:VAL:HG22	3:L:766:THR:HG22	1.82	0.60
3:L:726:ALA:HA	3:L:851:MET:HE1	1.83	0.60
3:L:880:ARG:O	3:L:884:HIS:HD2	1.84	0.60
3:L:623:SER:HA	3:L:626:GLN:NE2	2.16	0.60
2:B:474:LEU:O	2:B:475:SER:HB2	2.01	0.59
3:C:833:MET:HE1	3:C:1223:GLY:HA2	1.83	0.59
3:C:1282:ARG:HA	3:C:1286:THR:HG23	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:673:ASP:OD2	3:L:677:HIS:HD2	1.85	0.59
3:L:1079:ALA:O	3:L:1080:SER:HB2	2.03	0.58
3:C:764:VAL:HG22	3:C:766:THR:HG22	1.85	0.58
3:C:939:GLU:HG2	3:C:977:TYR:CE2	2.38	0.58
3:L:840:HIS:HE1	3:L:874:SER:OG	1.86	0.57
3:L:1191:ASP:OD2	8:L:168:HOH:O	2.17	0.57
2:B:285:PRO:C	2:B:286:GLU:O	2.43	0.57
3:L:1282:ARG:O	3:L:1286:THR:HG23	2.03	0.57
3:L:747:HIS:CD2	3:L:836:THR:HG21	2.39	0.56
3:L:939:GLU:HG2	3:L:977:TYR:CE2	2.41	0.56
1:A:37:ARG:HD3	3:C:595:ASP:O	2.06	0.56
3:C:752:ILE:CD1	3:C:763:PHE:HE1	2.19	0.56
3:L:833:MET:HE1	3:L:1222:ARG:C	2.30	0.56
3:C:829:ARG:HG2	3:C:833:MET:HE2	1.87	0.55
3:L:833:MET:CE	3:L:1222:ARG:C	2.80	0.55
1:A:36:LEU:HD22	1:A:89:GLU:HG3	1.88	0.55
2:K:285:PRO:O	2:K:286:GLU:CB	2.54	0.55
3:L:598:ARG:NH2	8:L:509:HOH:O	2.41	0.54
3:L:752:ILE:CD1	3:L:763:PHE:HE1	2.21	0.54
3:L:848:VAL:HG13	3:L:859:LEU:HD13	1.90	0.54
3:C:1126:SER:HB2	3:L:1132:PHE:CD1	2.42	0.54
3:C:1046:MET:HE1	3:C:1086:TYR:C	2.33	0.54
3:L:601:ASN:HB2	3:L:821:HIS:CD2	2.44	0.53
3:L:833:MET:HE1	3:L:1223:GLY:HA2	1.90	0.52
3:C:840:HIS:HE1	3:C:874:SER:OG	1.92	0.52
3:C:726:ALA:HA	3:C:851:MET:CE	2.37	0.52
6:C:1:PM6:H8	7:C:1326:ZXF:O1	2.08	0.52
3:C:720:LYS:O	3:C:721:LYS:HB2	2.08	0.52
2:K:476:LYS:HG2	2:K:477:PHE:H	1.75	0.52
2:B:272:ASN:CG	3:C:683:HIS:NE2	2.68	0.52
3:C:614:HIS:HD2	3:C:693:PRO:O	1.93	0.51
3:C:1033:HIS:HD2	3:C:1035:GLY:H	1.58	0.51
2:K:450:LYS:O	2:K:474:LEU:HD22	2.11	0.51
3:C:1297:ASP:HB2	3:C:1304:LYS:HE2	1.93	0.51
2:K:474:LEU:O	2:K:475:SER:HB2	2.10	0.51
3:L:806:THR:HA	3:L:809:SER:HB2	1.92	0.51
2:K:426:ARG:NH1	2:K:426:ARG:CG	2.52	0.51
3:L:1282:ARG:NH2	3:L:1292:GLU:OE2	2.36	0.51
3:C:720:LYS:O	3:C:721:LYS:HB3	2.09	0.51
3:L:614:HIS:HD2	3:L:693:PRO:O	1.93	0.50
3:L:884:HIS:CE1	3:L:1006:GLY:H	2.28	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:1046:MET:HE1	3:L:1086:TYR:C	2.35	0.50
3:L:752:ILE:HD12	3:L:763:PHE:HE1	1.77	0.50
3:L:1297:ASP:HB2	3:L:1304:LYS:HE2	1.94	0.50
2:B:438:MET:HG2	2:B:454:LEU:HD22	1.94	0.49
1:J:99:HIS:CG	1:J:100:PRO:HD2	2.47	0.49
3:L:1203:LEU:HD12	3:L:1203:LEU:C	2.38	0.49
2:K:285:PRO:O	2:K:286:GLU:HB2	2.11	0.49
2:K:425:SER:O	2:K:426:ARG:CB	2.60	0.49
3:L:1048:GLN:HE22	3:L:1187:ASN:HD22	1.60	0.49
3:L:726:ALA:HA	3:L:851:MET:CE	2.43	0.49
2:B:232:GLU:OE2	3:C:677:HIS:HE1	1.96	0.49
3:C:673:ASP:OD2	3:C:677:HIS:HD2	1.96	0.49
3:L:1282:ARG:HA	3:L:1286:THR:HG23	1.94	0.49
3:C:684:VAL:O	3:C:684:VAL:HG13	2.13	0.48
3:C:1287:ASN:C	3:C:1287:ASN:HD22	2.21	0.48
3:C:1203:LEU:C	3:C:1203:LEU:HD12	2.38	0.48
3:L:911:PHE:HD2	3:L:912:ARG:N	2.11	0.48
1:J:63:ASP:C	1:J:63:ASP:OD1	2.57	0.48
3:L:1249:ASN:O	3:L:1255:ALA:HA	2.14	0.48
3:C:1124:ARG:HB3	3:L:1134:ARG:HG3	1.96	0.48
3:C:601:ASN:HB2	3:C:821:HIS:CD2	2.48	0.48
3:C:747:HIS:CD2	3:C:836:THR:HG21	2.49	0.48
3:C:1249:ASN:O	3:C:1255:ALA:HA	2.14	0.48
3:C:839:ARG:O	3:C:841:PRO:HD3	2.14	0.47
1:J:74:LEU:O	1:J:76:PRO:HD3	2.15	0.47
3:C:1183:GLY:HA2	3:C:1247:CYS:O	2.14	0.47
1:J:62:GLN:O	1:J:63:ASP:HB3	2.13	0.47
3:L:640:ILE:HG12	3:L:779:MET:HE3	1.96	0.47
3:C:1046:MET:HE1	3:C:1087:GLY:N	2.30	0.47
2:K:469:THR:HG23	2:K:489:GLY:HA3	1.97	0.47
3:L:839:ARG:O	3:L:841:PRO:HD3	2.15	0.47
2:B:425:SER:O	2:B:426:ARG:HB2	2.13	0.47
3:C:605:LEU:C	3:C:605:LEU:HD23	2.39	0.47
3:C:806:THR:HA	3:C:809:SER:HB2	1.96	0.47
3:C:1079:ALA:O	3:C:1080:SER:HB2	2.14	0.47
3:C:833:MET:HE1	3:C:1223:GLY:CA	2.44	0.47
3:C:623:SER:HA	3:C:626:GLN:NE2	2.28	0.47
3:L:833:MET:HE1	3:L:1223:GLY:CA	2.45	0.47
3:C:719:LEU:CD1	3:C:895:ARG:HB2	2.45	0.46
1:J:49:GLY:C	1:J:51:CYS:H	2.22	0.46
3:L:1213:TYR:CE2	3:L:1219:LEU:HD13	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1152:TYR:CE1	3:C:1257:LYS:HG2	2.50	0.46
3:L:995:LYS:HZ1	3:L:1284:GLN:NE2	2.09	0.46
2:K:257:LEU:O	5:K:606:FAD:H2B	2.16	0.46
3:L:695:ILE:H	3:L:904:ASN:ND2	2.10	0.46
3:L:833:MET:CE	3:L:1222:ARG:O	2.63	0.46
3:C:1317:CYS:SG	3:C:1323:GLY:HA3	2.56	0.46
3:C:719:LEU:HD11	3:C:895:ARG:HB2	1.97	0.46
1:J:49:GLY:C	1:J:51:CYS:N	2.74	0.46
3:C:1126:SER:HB2	3:L:1132:PHE:CE1	2.51	0.45
3:C:1046:MET:HE1	3:C:1086:TYR:O	2.16	0.45
3:L:606:ARG:HD3	3:L:679:GLU:HA	1.98	0.45
3:L:1203:LEU:O	3:L:1207:THR:OG1	2.32	0.45
2:B:474:LEU:O	2:B:475:SER:CB	2.65	0.45
1:A:142:ALA:HB1	8:A:174:HOH:O	2.15	0.45
3:L:601:ASN:HB2	3:L:821:HIS:HD2	1.80	0.45
3:C:740:ASP:OD2	3:C:833:MET:HG2	2.17	0.45
2:K:471:GLN:NE2	2:K:474:LEU:HD12	2.31	0.45
3:L:1046:MET:HE1	3:L:1086:TYR:O	2.16	0.45
3:C:911:PHE:HD2	3:C:912:ARG:N	2.15	0.45
3:C:1282:ARG:O	3:C:1286:THR:HG23	2.17	0.45
2:K:310:LYS:HE3	2:K:314:GLU:OE2	2.17	0.45
3:L:833:MET:HE3	3:L:1222:ARG:O	2.17	0.45
3:C:788:LEU:HD13	3:C:1069:ASN:HB3	1.99	0.45
2:K:391:PRO:HD2	2:K:395:LYS:O	2.17	0.44
3:L:1301:THR:HB	3:L:1302:PRO:HD2	1.98	0.44
3:C:1132:PHE:CD1	3:L:1126:SER:HB2	2.53	0.44
2:K:392:SER:O	2:K:393:TYR:C	2.59	0.44
3:L:845:ARG:HD2	8:L:1347:HOH:O	2.17	0.44
3:C:1282:ARG:HA	3:C:1286:THR:CG2	2.47	0.44
3:L:840:HIS:CE1	3:L:874:SER:OG	2.70	0.44
3:L:605:LEU:C	3:L:605:LEU:HD23	2.42	0.44
3:C:833:MET:CE	3:C:1222:ARG:C	2.91	0.44
2:K:447:MET:HG2	2:K:527:LEU:HD13	2.00	0.43
3:C:880:ARG:O	3:C:884:HIS:CD2	2.68	0.43
3:C:1088:GLN:HG2	3:C:1133:TYR:CD1	2.53	0.43
2:K:268:MET:CE	8:K:536:HOH:O	2.67	0.43
3:L:719:LEU:CD1	3:L:895:ARG:HB2	2.48	0.43
3:L:1287:ASN:ND2	3:L:1289:ASN:H	2.17	0.43
3:C:980:ARG:NH1	3:C:1161:GLU:OE1	2.52	0.43
1:J:36:LEU:HD22	1:J:89:GLU:HG3	1.99	0.43
1:A:62:GLN:O	1:A:63:ASP:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:880:ARG:O	3:L:884:HIS:CD2	2.69	0.43
3:L:794:MET:HE3	3:L:1038:MET:HB3	2.01	0.43
3:L:601:ASN:O	3:L:821:HIS:HD2	2.02	0.43
2:K:268:MET:HE1	8:K:536:HOH:O	2.18	0.42
7:L:1326:ZXF:O2	7:L:1326:ZXF:S	2.77	0.42
2:K:504:MET:HG2	3:L:1303:GLU:CD	2.45	0.42
3:L:827:LEU:HA	8:L:1338:HOH:O	2.19	0.42
3:C:833:MET:HE1	3:C:1222:ARG:C	2.44	0.42
3:L:833:MET:HE1	3:L:1223:GLY:N	2.35	0.42
3:L:929:GLU:HG2	3:L:1293:LEU:HD22	2.01	0.42
3:C:752:ILE:HD12	3:C:763:PHE:HE1	1.85	0.42
3:L:700:ASP:HA	3:L:703:LYS:HE3	2.01	0.42
3:L:1010:THR:HG23	6:L:1:PM6:S6	2.59	0.42
1:A:96:THR:OG1	1:A:97:ARG:N	2.52	0.42
3:L:1191:ASP:OD1	3:L:1259:VAL:HG11	2.20	0.42
2:B:255:ALA:HB2	2:B:277:MET:HG2	2.02	0.41
3:C:596:ILE:HA	3:C:597:PRO:HD3	1.95	0.41
1:J:37:ARG:HD3	3:L:595:ASP:O	2.20	0.41
2:K:243:LYS:CD	2:K:243:LYS:N	2.80	0.41
2:K:284:ILE:HB	2:K:287:LEU:HD12	2.02	0.41
3:C:994:LYS:O	3:C:995:LYS:HD3	2.20	0.41
3:L:779:MET:SD	3:L:779:MET:C	3.03	0.41
2:B:450:LYS:O	2:B:474:LEU:HD22	2.20	0.41
2:K:285:PRO:C	2:K:286:GLU:O	2.61	0.41
3:L:719:LEU:HD11	3:L:895:ARG:HB2	2.03	0.41
3:L:752:ILE:HD12	3:L:763:PHE:CE1	2.56	0.41
3:L:851:MET:HE3	3:L:857:VAL:CG2	2.41	0.41
3:L:663:VAL:HG12	3:L:834:LEU:HD11	2.03	0.41
3:L:764:VAL:HG22	3:L:766:THR:CG2	2.50	0.41
3:L:916:GLY:O	3:L:920:LEU:HG	2.19	0.41
3:L:1017:ALA:HB2	3:L:1085:ILE:HD12	2.03	0.41
2:K:337:PHE:CD2	2:K:337:PHE:C	2.99	0.41
3:C:1181:ASP:OD1	3:C:1181:ASP:C	2.63	0.40
3:C:929:GLU:HG2	3:C:1293:LEU:HD22	2.03	0.40
7:C:1326:ZXF:O2	7:C:1326:ZXF:S	2.79	0.40
3:C:684:VAL:O	3:C:684:VAL:CG1	2.69	0.40
3:L:1287:ASN:C	3:L:1287:ASN:ND2	2.74	0.40
3:C:606:ARG:HD3	3:C:679:GLU:HA	2.03	0.40
2:K:476:LYS:HG2	2:K:477:PHE:N	2.36	0.40
2:K:488:ALA:O	2:K:492:GLU:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	162/164 (99%)	152 (94%)	9 (6%)	1 (1%)	21	42
1	J	162/164 (99%)	152 (94%)	9 (6%)	1 (1%)	21	42
2	B	303/305 (99%)	280 (92%)	19 (6%)	4 (1%)	9	21
2	K	303/305 (99%)	279 (92%)	19 (6%)	5 (2%)	7	15
3	C	753/755 (100%)	723 (96%)	25 (3%)	5 (1%)	18	38
3	L	743/755 (98%)	705 (95%)	33 (4%)	5 (1%)	18	38
All	All	2426/2448 (99%)	2291 (94%)	114 (5%)	21 (1%)	14	30

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	721	LYS
3	C	1008	SER
2	K	426	ARG
3	L	721	LYS
3	L	1008	SER
2	B	338	ALA
2	B	426	ARG
3	L	1139	GLY
3	C	912	ARG
2	K	424	ALA
2	K	425	SER
2	B	424	ALA
2	B	425	SER
2	K	338	ALA
3	L	797	GLY
3	L	912	ARG
1	A	61	LEU
3	C	797	GLY
1	J	61	LEU
2	K	335	ARG

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Mol	Chain	Res	Type
3	C	1139	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	137/137 (100%)	129 (94%)	8 (6%)	18	39
1	J	137/137 (100%)	129 (94%)	8 (6%)	18	39
2	B	261/261 (100%)	240 (92%)	21 (8%)	11	25
2	K	261/261 (100%)	242 (93%)	19 (7%)	13	29
3	C	631/631 (100%)	604 (96%)	27 (4%)	26	51
3	L	624/631 (99%)	592 (95%)	32 (5%)	21	45
All	All	2051/2058 (100%)	1936 (94%)	115 (6%)	19	40

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	33	LYS
1	A	63	ASP
1	A	64	LYS
1	A	89	GLU
1	A	97	ARG
1	A	140	GLU
1	A	162	THR
2	B	226	GLN
2	B	241	THR
2	B	243	LYS
2	B	257	LEU
2	B	271	LYS
2	B	277	MET
2	B	312	LEU
2	B	318	LYS
2	B	337	PHE

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Mol	Chain	Res	Type
2	B	348	LEU
2	B	375	VAL
2	B	426	ARG
2	B	427	ARG
2	B	429	ASP
2	B	462	ARG
2	B	468	LYS
2	B	472	LYS
2	B	476	LYS
2	B	492	GLU
2	B	509	ARG
2	B	525	LYS
3	C	598	ARG
3	C	609	THR
3	C	618	LYS
3	C	659	THR
3	C	684	VAL
3	C	686	LYS
3	C	696	ILE
3	C	705	ASN
3	C	743	TYR
3	C	764	VAL
3	C	782	VAL
3	C	818	LYS
3	C	848	VAL
3	C	852	LYS
3	C	857	VAL
3	C	871	ARG
3	C	939	GLU
3	C	983	GLU
3	C	1000	ILE
3	C	1001	ILE
3	C	1144	THR
3	C	1172	LYS
3	C	1203	LEU
3	C	1208	LEU
3	C	1286	THR
3	C	1287	ASN
3	C	1324	ASN
1	J	33	LYS
1	J	63	ASP
1	J	64	LYS

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Mol	Chain	Res	Type
1	J	89	GLU
1	J	97	ARG
1	J	133	GLU
1	J	140	GLU
1	J	162	THR
2	K	226	GLN
2	K	241	THR
2	K	243	LYS
2	K	257	LEU
2	K	312	LEU
2	K	318	LYS
2	K	337	PHE
2	K	348	LEU
2	K	375	VAL
2	K	426	ARG
2	K	427	ARG
2	K	429	ASP
2	K	462	ARG
2	K	468	LYS
2	K	472	LYS
2	K	476	LYS
2	K	492	GLU
2	K	513	LEU
2	K	525	LYS
3	L	598	ARG
3	L	609	THR
3	L	618	LYS
3	L	658	ASP
3	L	659	THR
3	L	684	VAL
3	L	686	LYS
3	L	696	ILE
3	L	705	ASN
3	L	719	LEU
3	L	742	PHE
3	L	743	TYR
3	L	764	VAL
3	L	774	SER
3	L	782	VAL
3	L	818	LYS
3	L	829	ARG
3	L	848	VAL

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Mol	Chain	Res	Type
3	L	852	LYS
3	L	857	VAL
3	L	899	ARG
3	L	939	GLU
3	L	983	GLU
3	L	1000	ILE
3	L	1001	ILE
3	L	1105	LYS
3	L	1144	THR
3	L	1172	LYS
3	L	1203	LEU
3	L	1208	LEU
3	L	1286	THR
3	L	1287	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	146	ASN
2	B	226	GLN
2	B	261	ASN
2	B	272	ASN
2	B	351	ASN
2	B	471	GLN
3	C	585	GLN
3	C	614	HIS
3	C	626	GLN
3	C	677	HIS
3	C	728	ASN
3	C	821	HIS
3	C	830	ASN
3	C	840	HIS
3	C	884	HIS
3	C	904	ASN
3	C	956	ASN
3	C	1016	GLN
3	C	1033	HIS
3	C	1048	GLN
3	C	1069	ASN
3	C	1284	GLN
3	C	1287	ASN

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Mol	Chain	Res	Type
1	J	109	HIS
1	J	131	GLN
2	K	261	ASN
2	K	351	ASN
2	K	471	GLN
3	L	614	HIS
3	L	626	GLN
3	L	677	HIS
3	L	728	ASN
3	L	821	HIS
3	L	840	HIS
3	L	884	HIS
3	L	904	ASN
3	L	1016	GLN
3	L	1033	HIS
3	L	1048	GLN
3	L	1220	HIS
3	L	1284	GLN
3	L	1285	HIS
3	L	1287	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FES	J	602	1	0,4,4	-	-	-		
6	PM6	L	1	-	10,11,11	3.23	4 (40%)	13,15,15	2.50	5 (38%)
4	FES	J	601	1	0,4,4	-	-	-		
7	ZXF	C	1326	-	24,31,31	3.65	5 (20%)	22,52,52	2.98	8 (36%)
7	ZXF	L	1326	-	24,31,31	3.80	4 (16%)	22,52,52	2.50	10 (45%)
6	PM6	C	1	-	10,11,11	3.37	5 (50%)	13,15,15	2.49	7 (53%)
5	FAD	K	606	-	58,58,58	1.14	5 (8%)	85,89,89	1.81	21 (24%)
4	FES	A	601	1	0,4,4	-	-	-		
4	FES	A	602	1	0,4,4	-	-	-		
5	FAD	B	606	-	58,58,58	1.50	7 (12%)	85,89,89	1.79	19 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FES	J	602	1	-	-	0/1/1/1
6	PM6	L	1	-	-	-	0/2/2/2
4	FES	J	601	1	-	-	0/1/1/1
7	ZXF	C	1326	-	-	1/6/46/46	0/4/4/4
7	ZXF	L	1326	-	-	1/6/46/46	0/4/4/4
6	PM6	C	1	-	-	-	0/2/2/2
5	FAD	K	606	-	-	7/34/50/50	0/6/6/6
4	FES	A	601	1	-	-	0/1/1/1
4	FES	A	602	1	-	-	0/1/1/1
5	FAD	B	606	-	-	3/34/50/50	0/6/6/6

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	1326	ZXF	MO-S2'	14.59	2.60	2.39
7	L	1326	ZXF	MO-S2'	13.35	2.58	2.39
7	L	1326	ZXF	MO-S1'	9.83	2.53	2.39
7	C	1326	ZXF	C9-C10	7.82	1.52	1.38
6	C	1	PM6	C5-C6	7.32	1.49	1.39
6	L	1	PM6	C5-C6	6.70	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	1326	ZXF	C9-C10	6.40	1.49	1.38
6	L	1	PM6	C5-C4	5.62	1.48	1.39
5	B	606	FAD	P-O3P	5.34	1.65	1.59
6	C	1	PM6	C5-C4	5.31	1.47	1.39
7	C	1326	ZXF	MO-S1'	4.82	2.46	2.39
5	B	606	FAD	C4X-N5	4.15	1.39	1.30
5	B	606	FAD	PA-O3P	4.00	1.63	1.59
5	K	606	FAD	C4X-N5	3.59	1.38	1.30
7	L	1326	ZXF	C9-C4	3.41	1.52	1.41
5	K	606	FAD	C2A-N1A	3.12	1.39	1.33
5	B	606	FAD	C2A-N1A	3.11	1.39	1.33
7	C	1326	ZXF	C9-C4	3.01	1.50	1.41
6	C	1	PM6	C8-N7	2.98	1.38	1.32
6	C	1	PM6	C6-N1	2.94	1.37	1.33
6	L	1	PM6	C8-N7	2.79	1.37	1.32
6	L	1	PM6	C6-N1	2.67	1.37	1.33
5	K	606	FAD	C10-N1	2.62	1.38	1.33
5	B	606	FAD	C10-N1	2.62	1.38	1.33
5	K	606	FAD	C2A-N3A	2.56	1.38	1.33
5	K	606	FAD	C8A-N7A	2.28	1.36	1.31
5	B	606	FAD	C2A-N3A	2.23	1.37	1.33
5	B	606	FAD	C8A-N7A	2.07	1.35	1.31
6	C	1	PM6	C2-N3	2.04	1.37	1.33
7	C	1326	ZXF	C4-N3	-2.04	1.35	1.38

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	1326	ZXF	C2'-C1'-S1'	8.15	124.78	120.15
5	B	606	FAD	N3A-C2A-N1A	-7.31	117.52	128.58
7	C	1326	ZXF	C1'-C2'-S2'	6.39	123.78	120.15
5	K	606	FAD	N3A-C2A-N1A	-6.06	119.41	128.58
6	C	1	PM6	C6-C5-N7	5.88	137.35	132.88
6	L	1	PM6	C6-C5-N7	5.59	137.13	132.88
7	L	1326	ZXF	C2-N1-C10	5.40	122.89	113.36
7	L	1326	ZXF	C1'-C2'-S2'	4.63	122.78	120.15
5	K	606	FAD	C4-N3-C2	-4.39	117.85	125.64
7	C	1326	ZXF	O3'-C7-N8	4.23	112.44	108.61
5	K	606	FAD	N9A-C8A-N7A	-4.15	108.05	113.94
5	B	606	FAD	C5X-C9A-N10	4.14	121.71	117.97
6	L	1	PM6	N1-C2-N3	-4.01	122.50	128.58
7	L	1326	ZXF	O3'-C7-N8	3.81	112.06	108.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	606	FAD	N9A-C8A-N7A	-3.73	108.64	113.94
5	B	606	FAD	C4-N3-C2	-3.67	119.12	125.64
7	C	1326	ZXF	O3'-C3'-C2'	3.59	114.16	109.09
5	B	606	FAD	C2A-N3A-C4A	3.42	120.19	111.83
5	K	606	FAD	C4X-C4-N3	3.37	121.83	113.25
7	C	1326	ZXF	C2-N1-C10	3.37	119.30	113.36
7	L	1326	ZXF	C4-C9-N5	3.28	125.22	116.27
5	K	606	FAD	O4-C4-C4X	-3.27	117.90	126.53
5	K	606	FAD	O4'-C4'-C3'	3.27	116.89	109.25
5	K	606	FAD	C5A-C4A-N3A	-3.26	122.22	126.72
5	K	606	FAD	C5A-N7A-C8A	3.24	108.54	103.45
5	K	606	FAD	O3'-C3'-C2'	-3.21	101.64	108.93
5	B	606	FAD	C9A-C5X-N5	-3.16	119.10	122.45
5	K	606	FAD	O2A-PA-O3P	3.15	115.79	107.27
5	B	606	FAD	C5A-C4A-N3A	-3.07	122.49	126.72
5	B	606	FAD	C8M-C8-C9	-2.96	114.35	119.57
6	C	1	PM6	C5-C4-N3	-2.93	121.41	126.75
6	C	1	PM6	N1-C2-N3	-2.92	124.17	128.58
5	B	606	FAD	C6-C5X-C9A	2.91	123.05	119.05
5	K	606	FAD	C2A-N3A-C4A	2.89	118.90	111.83
5	B	606	FAD	C4X-C4-N3	2.84	120.47	113.25
7	C	1326	ZXF	O2P-P-O4'	-2.81	99.35	106.67
7	L	1326	ZXF	O4-C4-C9	-2.80	120.50	127.26
5	K	606	FAD	C4X-C10-N10	2.79	120.48	116.48
5	K	606	FAD	C9A-C5X-N5	-2.77	119.52	122.45
5	B	606	FAD	C4A-N9A-C8A	2.73	108.61	105.74
5	B	606	FAD	O4-C4-C4X	-2.71	119.38	126.53
6	L	1	PM6	C5-C4-N3	-2.69	121.85	126.75
6	C	1	PM6	C5-N7-C8	2.67	106.50	103.48
5	B	606	FAD	N3A-C4A-N9A	2.67	131.71	127.17
6	L	1	PM6	N9-C4-N3	2.66	131.00	126.69
5	B	606	FAD	O2A-PA-O3P	2.65	114.45	107.27
6	L	1	PM6	C2-N1-C6	2.63	122.14	116.23
7	C	1326	ZXF	C4-C9-N5	2.61	123.39	116.27
5	B	606	FAD	C4X-C10-N1	-2.61	118.20	124.59
6	C	1	PM6	C4-C5-N7	-2.60	107.06	110.67
7	L	1326	ZXF	O2P-P-O4'	-2.58	99.95	106.67
5	K	606	FAD	C4A-N9A-C8A	2.53	108.40	105.74
5	B	606	FAD	C5A-N7A-C8A	2.50	107.38	103.45
5	B	606	FAD	C4-C4X-C10	2.49	121.21	116.93
5	K	606	FAD	N3A-C4A-N9A	2.47	131.36	127.17
7	C	1326	ZXF	O3'-C7-C6	-2.43	107.34	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	1326	ZXF	N2-C2-N3	2.43	121.88	116.76
5	K	606	FAD	O5'-C5'-C4'	-2.39	102.98	109.36
5	B	606	FAD	C2A-N1A-C6A	2.38	122.64	118.73
7	L	1326	ZXF	O3'-C7-C6	-2.34	107.40	108.96
5	K	606	FAD	O2P-P-O3P	2.33	113.57	107.27
5	K	606	FAD	C10-C4X-N5	-2.32	120.08	124.81
5	B	606	FAD	O3P-P-O1P	2.30	117.62	110.70
5	K	606	FAD	C5A-C6A-N6A	-2.25	117.73	123.29
7	L	1326	ZXF	O4'-C4'-C3'	2.24	114.10	108.58
6	C	1	PM6	N9-C4-N3	2.11	130.10	126.69
6	C	1	PM6	C5-C4-N9	2.10	108.48	105.67
5	K	606	FAD	C4'-C3'-C2'	2.06	117.00	113.57
7	L	1326	ZXF	C9-C4-N3	2.05	117.75	112.13
5	K	606	FAD	C4X-C10-N1	-2.03	119.61	124.59

There are no chirality outliers.

All (12) torsion outliers are listed below:

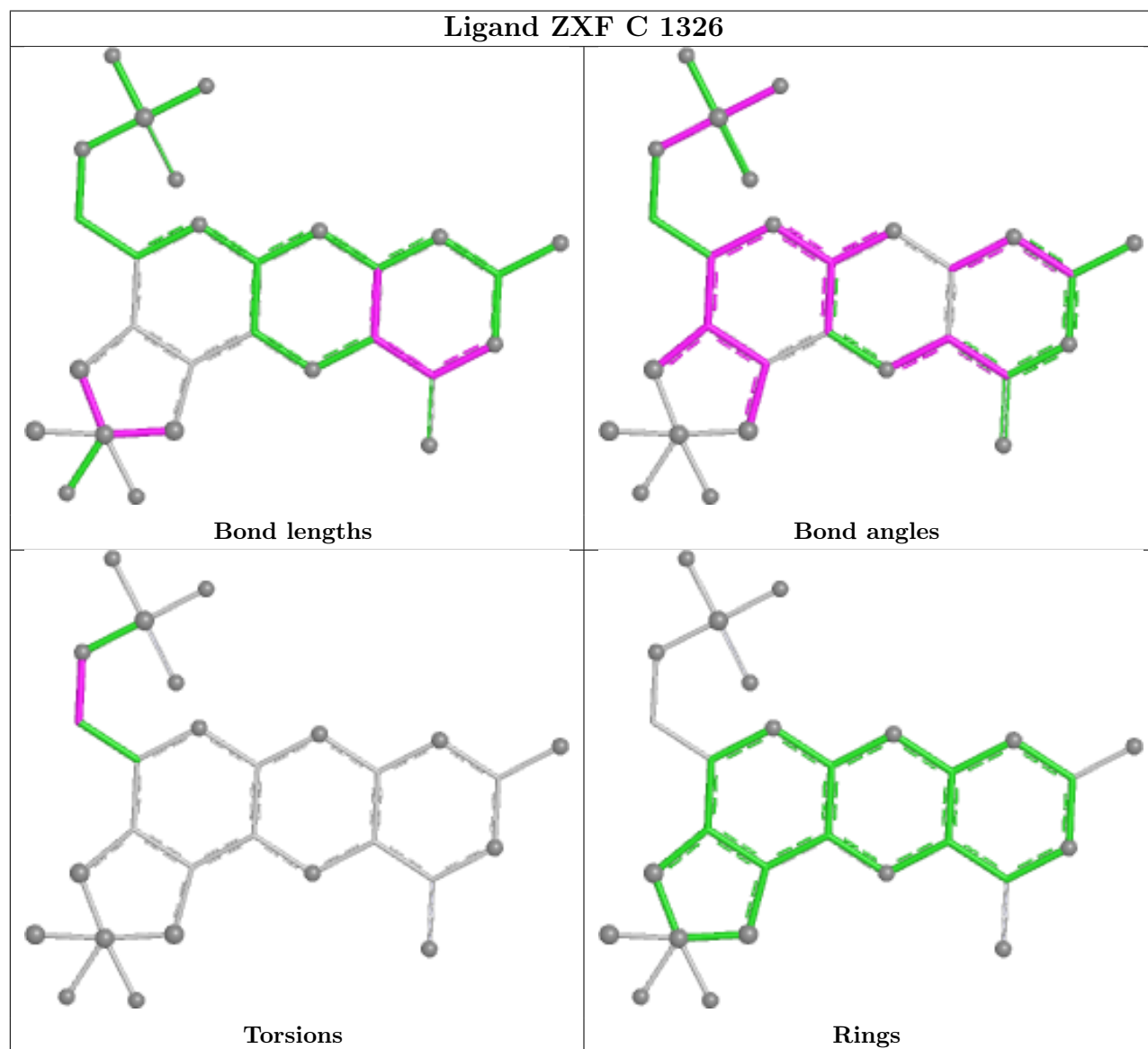
Mol	Chain	Res	Type	Atoms
5	B	606	FAD	C5B-O5B-PA-O1A
5	K	606	FAD	C5B-O5B-PA-O1A
5	K	606	FAD	C5B-O5B-PA-O3P
5	K	606	FAD	C1'-C2'-C3'-O3'
7	L	1326	ZXF	C3'-C4'-O4'-P
5	K	606	FAD	O2'-C2'-C3'-O3'
5	B	606	FAD	O4B-C4B-C5B-O5B
5	K	606	FAD	O4B-C4B-C5B-O5B
5	B	606	FAD	C3B-C4B-C5B-O5B
5	K	606	FAD	O2'-C2'-C3'-C4'
5	K	606	FAD	C3B-C4B-C5B-O5B
7	C	1326	ZXF	C3'-C4'-O4'-P

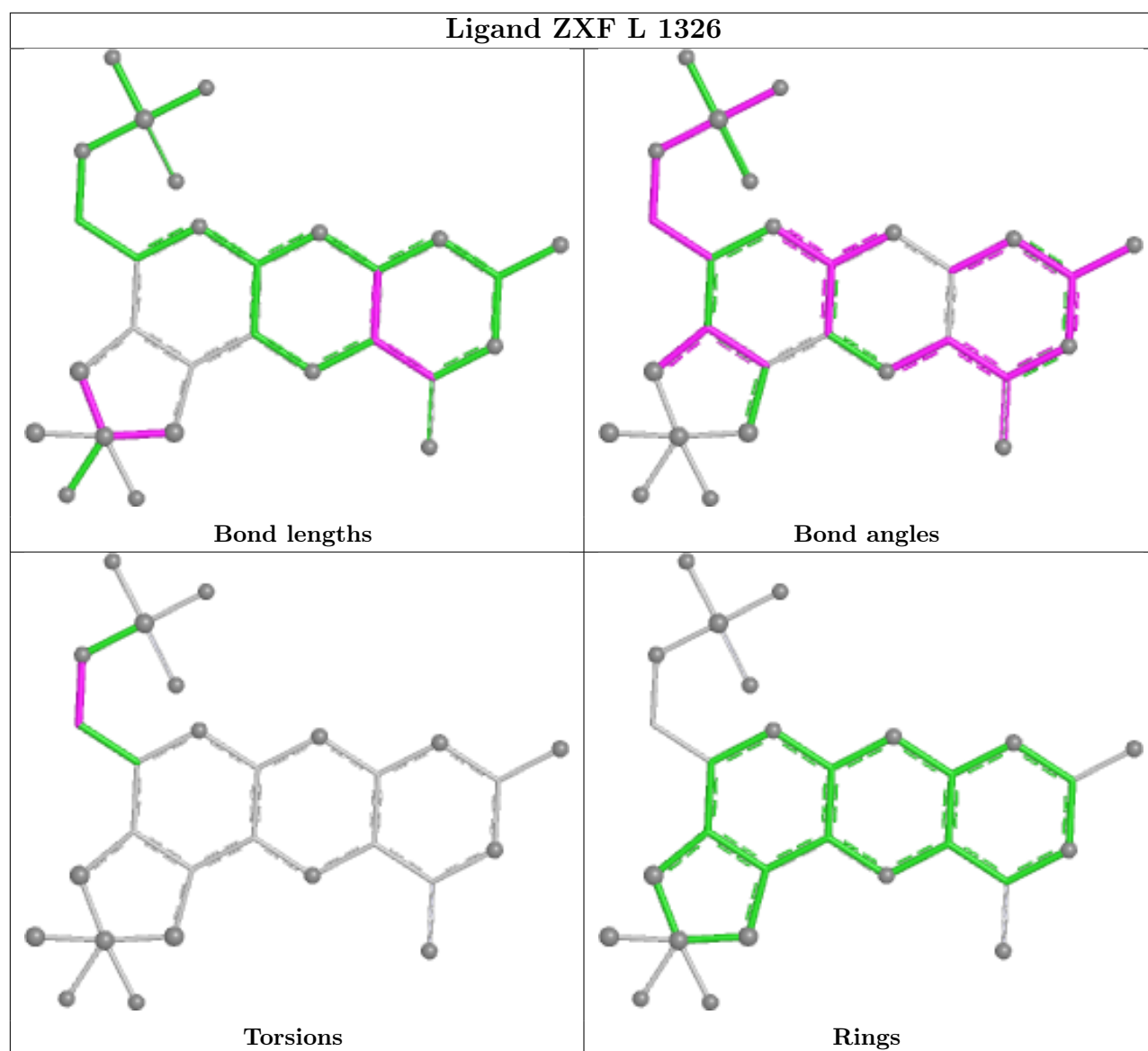
There are no ring outliers.

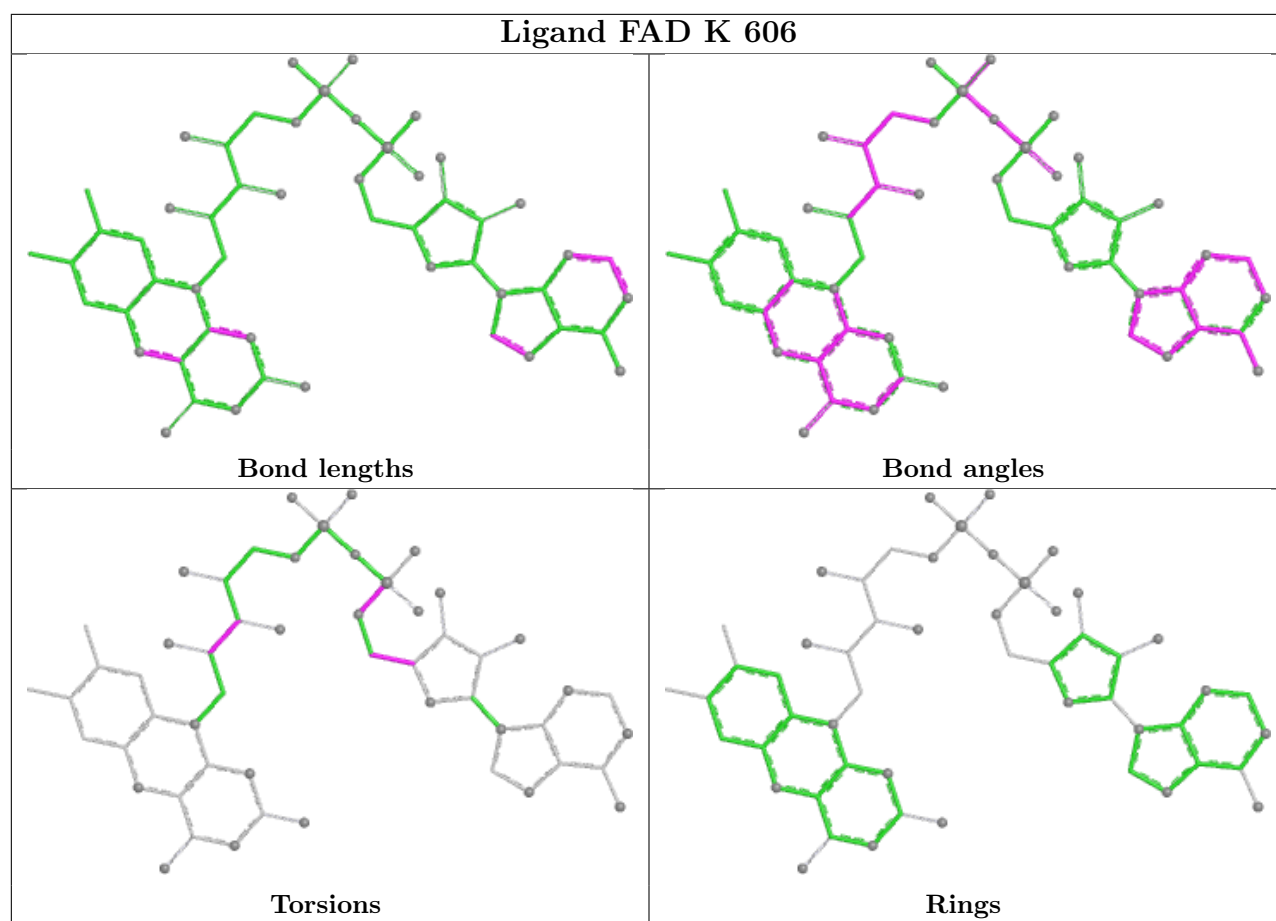
5 monomers are involved in 7 short contacts:

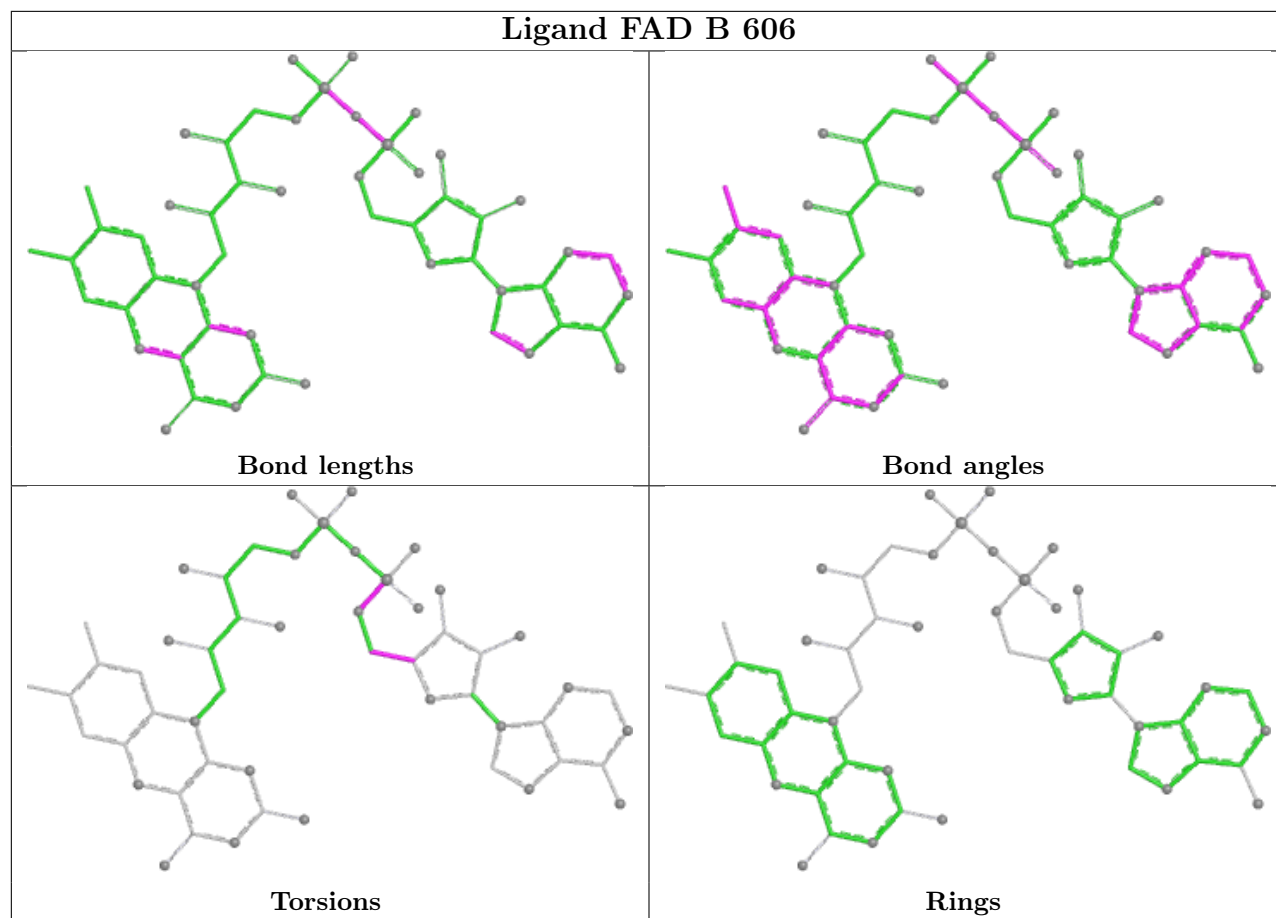
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	1	PM6	1	0
7	C	1326	ZXF	3	0
7	L	1326	ZXF	2	0
6	C	1	PM6	1	0
5	K	606	FAD	1	0

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	164/164 (100%)	-0.11	3 (1%) 67 63	14, 24, 42, 55	0
1	J	164/164 (100%)	-0.19	4 (2%) 59 54	14, 24, 42, 56	0
2	B	305/305 (100%)	0.21	8 (2%) 57 51	22, 34, 47, 50	0
2	K	305/305 (100%)	0.21	6 (1%) 65 60	22, 34, 47, 51	0
3	C	755/755 (100%)	-0.30	4 (0%) 87 85	13, 22, 36, 49	0
3	L	745/755 (98%)	-0.31	6 (0%) 82 80	13, 22, 36, 49	0
All	All	2438/2448 (99%)	-0.16	31 (1%) 75 71	13, 25, 43, 56	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	61	LEU	5.3
1	A	63	ASP	4.1
2	K	528	GLY	3.8
3	L	1288	ASN	3.8
2	K	336	TRP	3.8
2	B	528	GLY	3.7
1	J	60	ARG	3.5
2	B	527	LEU	3.5
2	B	336	TRP	3.5
2	K	224	PRO	3.3
3	L	985	ASP	3.3
3	L	1290	THR	3.2
3	C	724	SER	2.9
2	B	224	PRO	2.9
2	B	272	ASN	2.8
2	B	425	SER	2.5
1	J	2	THR	2.5
3	L	1287	ASN	2.5
1	A	60	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
2	K	272	ASN	2.3
1	J	63	ASP	2.3
2	K	377	ARG	2.2
3	L	1170	ASP	2.2
2	B	378	GLY	2.2
3	C	618	LYS	2.1
3	C	683	HIS	2.1
3	L	1289	ASN	2.1
1	J	165	LYS	2.1
2	K	429	ASP	2.1
2	B	430	ASP	2.0
3	C	1107	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

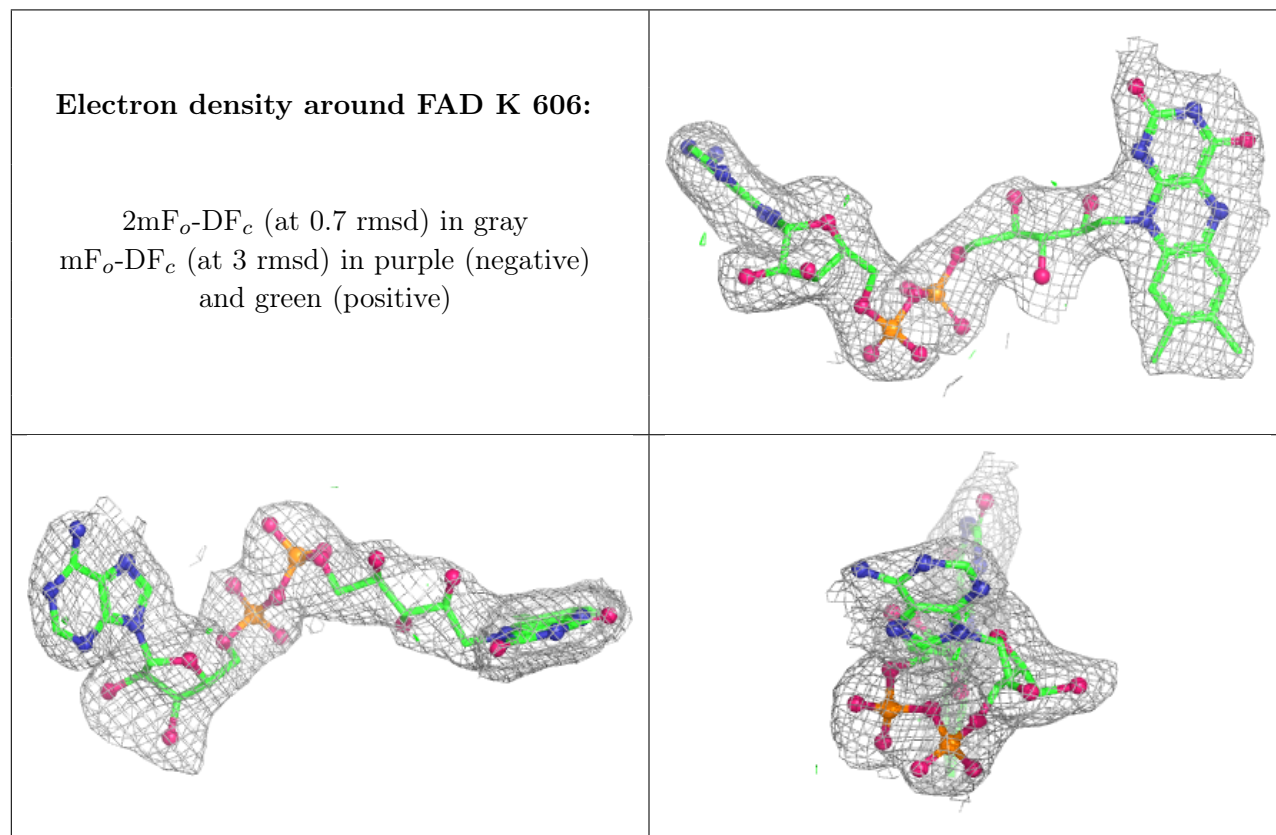
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

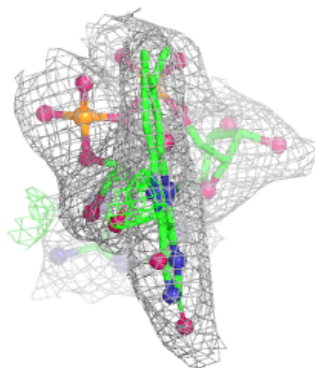
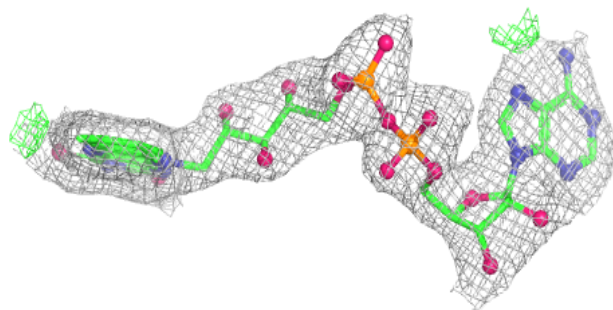
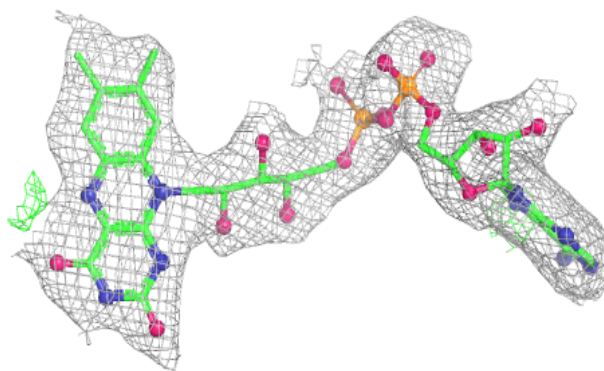
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	PM6	L	1	10/10	0.84	0.14	42,43,44,44	0
6	PM6	C	1	10/10	0.92	0.10	31,32,33,33	0
5	FAD	K	606	53/53	0.95	0.07	21,27,34,38	0
5	FAD	B	606	53/53	0.97	0.06	16,21,26,28	0
7	ZXF	C	1326	28/28	0.97	0.07	18,23,34,48	0
4	FES	J	601	4/4	0.98	0.03	14,14,15,19	0
7	ZXF	L	1326	28/28	0.98	0.08	24,29,39,45	0
4	FES	A	602	4/4	0.99	0.03	15,16,17,18	0
4	FES	A	601	4/4	0.99	0.02	12,12,14,17	0
4	FES	J	602	4/4	0.99	0.03	18,19,20,21	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.



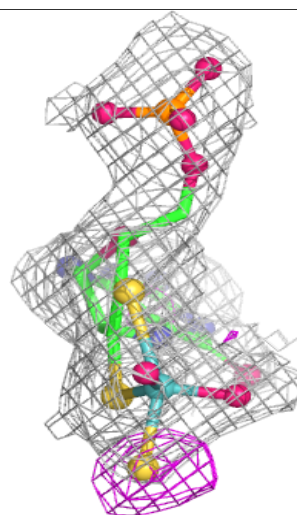
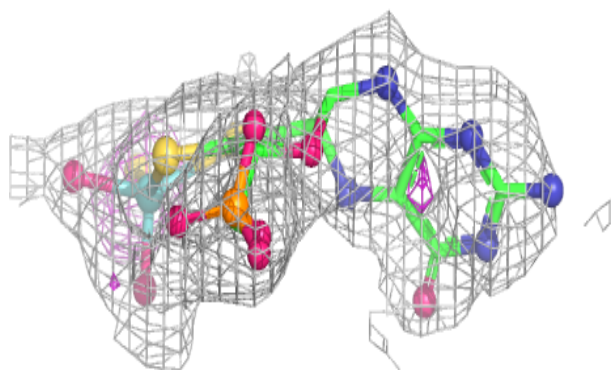
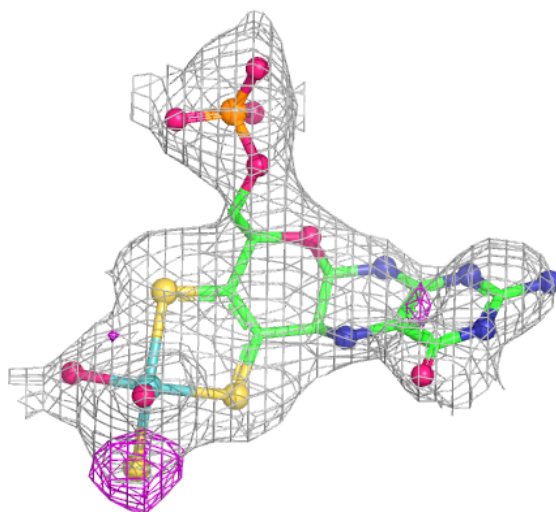
Electron density around FAD B 606:

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



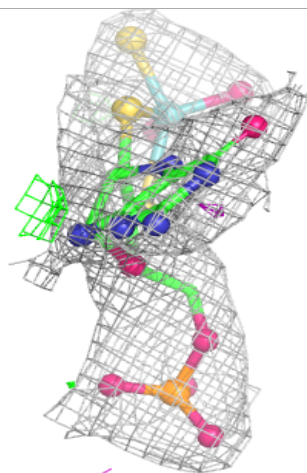
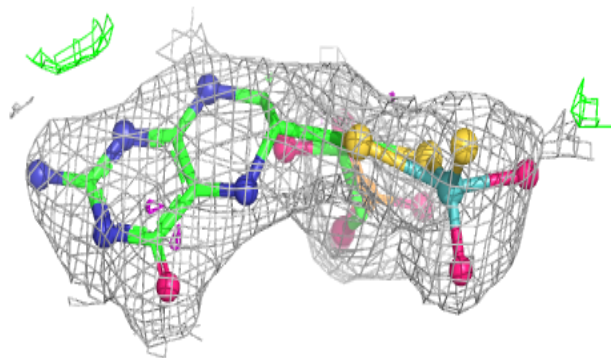
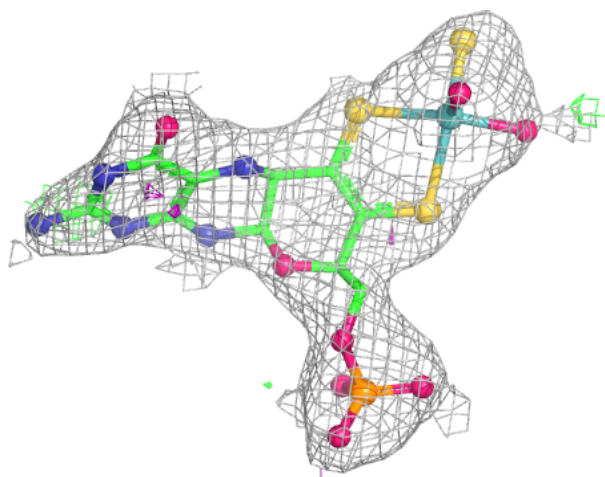
Electron density around ZXF C 1326:

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



Electron density around ZXF L 1326:

$2mF_o-DF_c$ (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.