



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 03:14 PM EDT

PDB ID : 3NVV / pdb_00003nvv
Title : Crystal Structure of Bovine Xanthine Oxidase in Complex with Arsenite
Authors : Cao, H.; Hille, R.
Deposited on : 2010-07-08
Resolution : 1.82 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

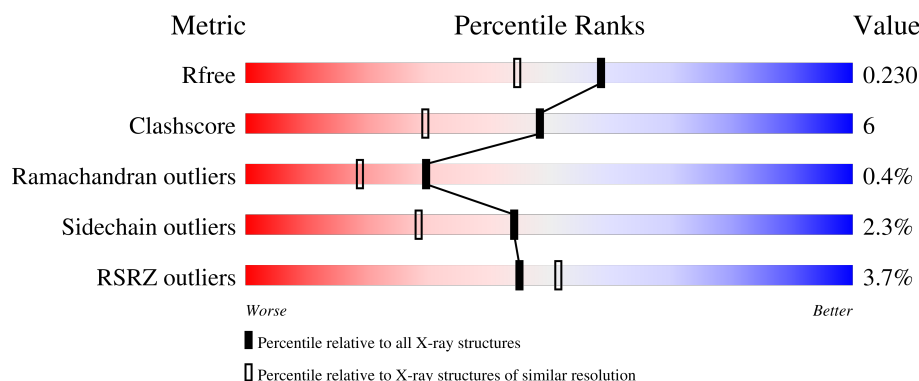
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.82 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	1112 (1.82-1.82)
Clashscore	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)

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	3% 88% 11% .
1	J	164	7% 85% 13% .
2	B	334	8% 90% 9% .
2	K	334	8% 81% 10% 9% .
3	C	755	% 88% 11% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	L	755	2% 86% 11% ..

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 20671 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			

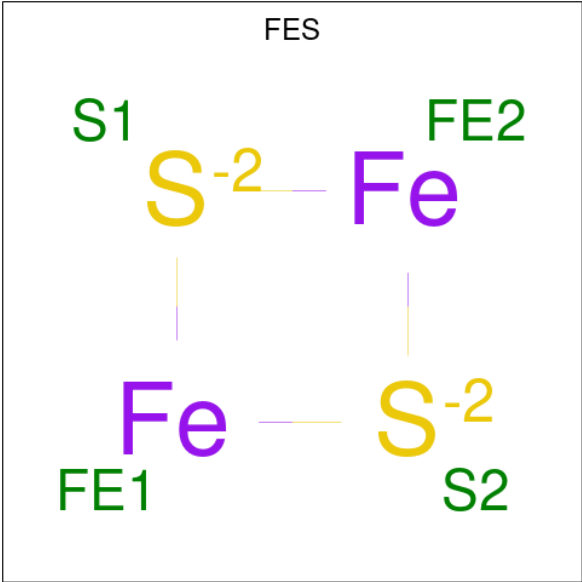
- Molecule 2 is a protein called Xanthine dehydrogenase/oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	334	Total	C	N	O	S	0	0	0
			2630	1700	437	479	14			
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.

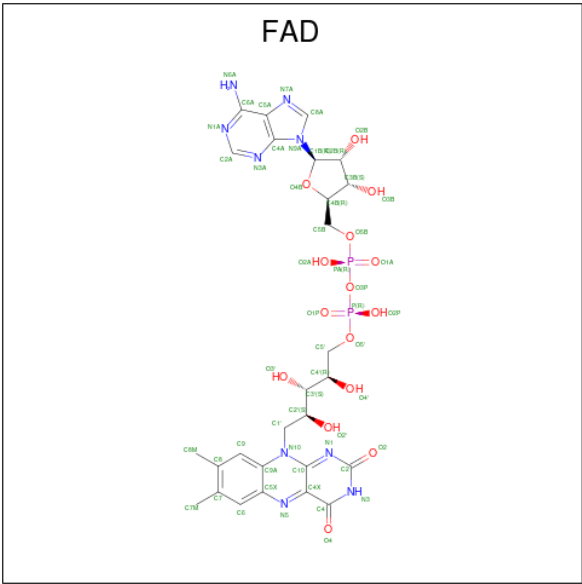
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	755	Total	C	N	O	S	0	0	0
			5823	3680	1003	1105	35			
3	L	745	Total	C	N	O	S	0	0	0
			5761	3643	992	1093	33			

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



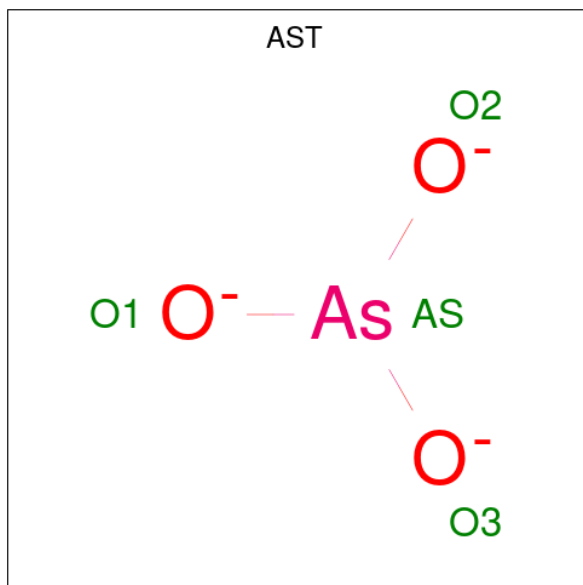
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			4	2	2		
4	A	1	Total	Fe	S	0	0
			4	2	2		
4	J	1	Total	Fe	S	0	0
			4	2	2		
4	J	1	Total	Fe	S	0	0
			4	2	2		

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



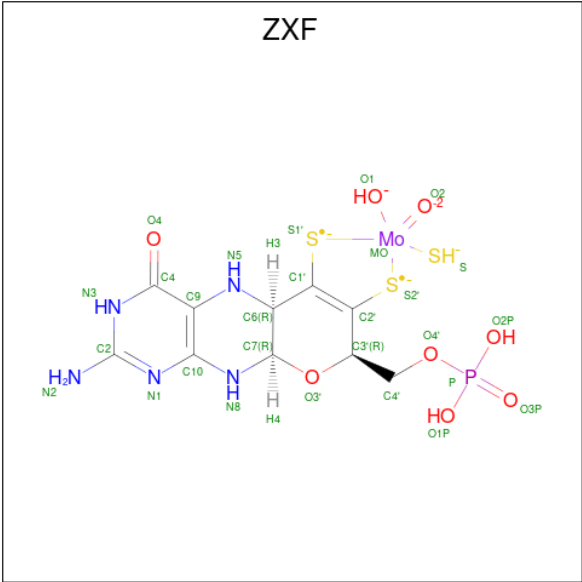
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	K	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 6 is ARSENITE (CCD ID: AST) (formula: AsO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	As	O	0	0
			3	1	2		
6	L	1	Total	As	O	0	0
			3	1	2		

- Molecule 7 is Molybdopterin hydroxy-oxo-thiol-molybdenum (CCD ID: ZXF) (formula: $\text{C}_{10}\text{H}_{14}\text{MoN}_5\text{O}_8\text{PS}_3$).



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		

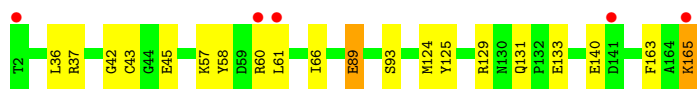
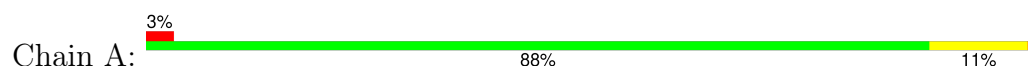
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	94	Total	O	0	0
			94	94		
8	B	137	Total	O	0	0
			137	137		
8	C	465	Total	O	0	0
			465	465		
8	J	99	Total	O	0	0
			99	99		
8	K	105	Total	O	0	0
			105	105		
8	L	474	Total	O	0	0
			474	474		

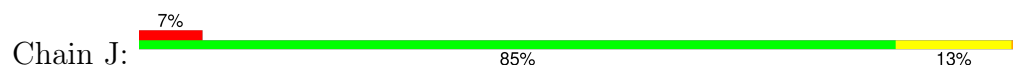
3 Residue-property plots [i](#)

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

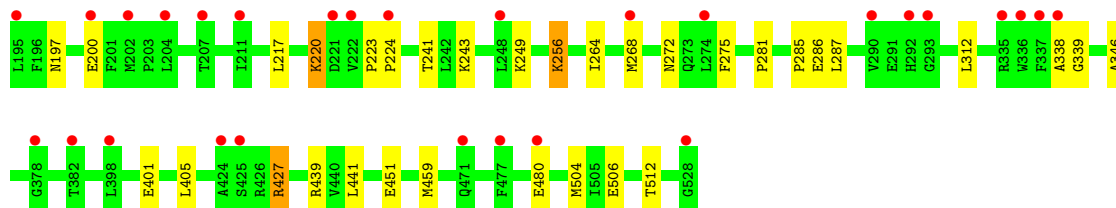
- Molecule 1: Xanthine dehydrogenase/oxidase



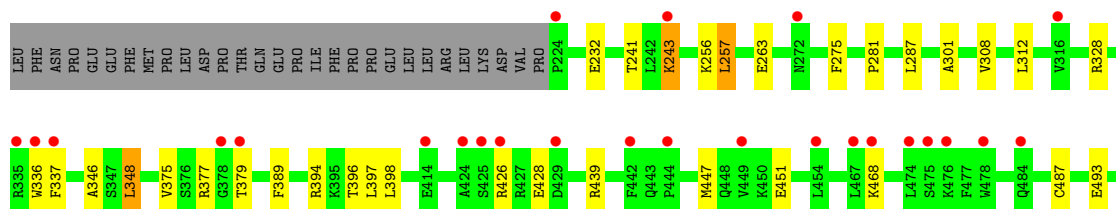
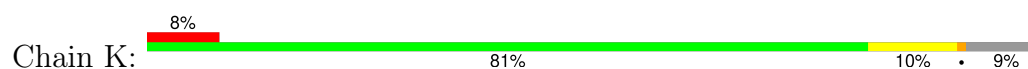
- Molecule 1: Xanthine dehydrogenase/oxidase

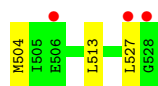


- Molecule 2: Xanthine dehydrogenase/oxidase

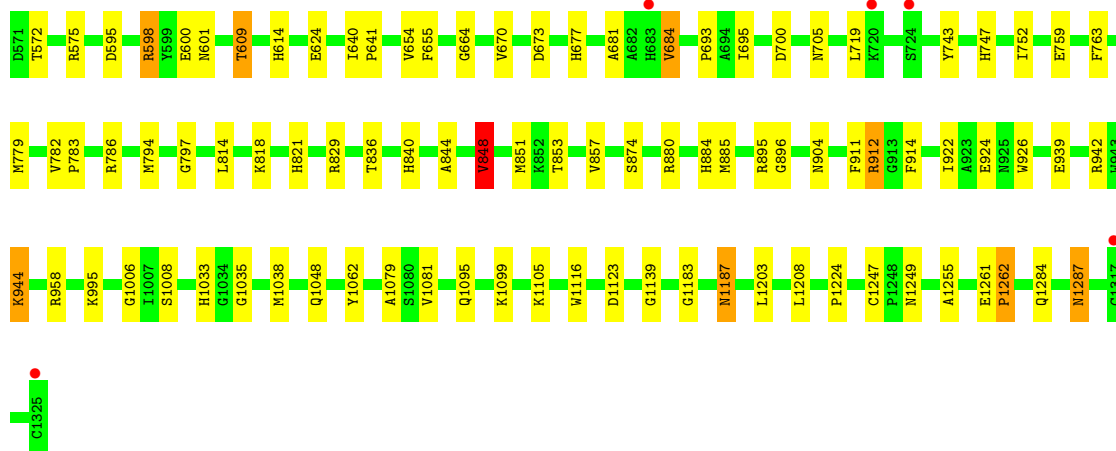
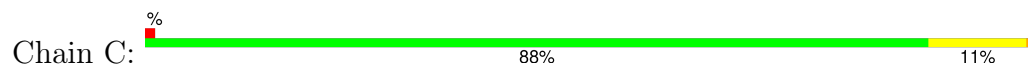


- Molecule 2: Xanthine dehydrogenase/oxidase

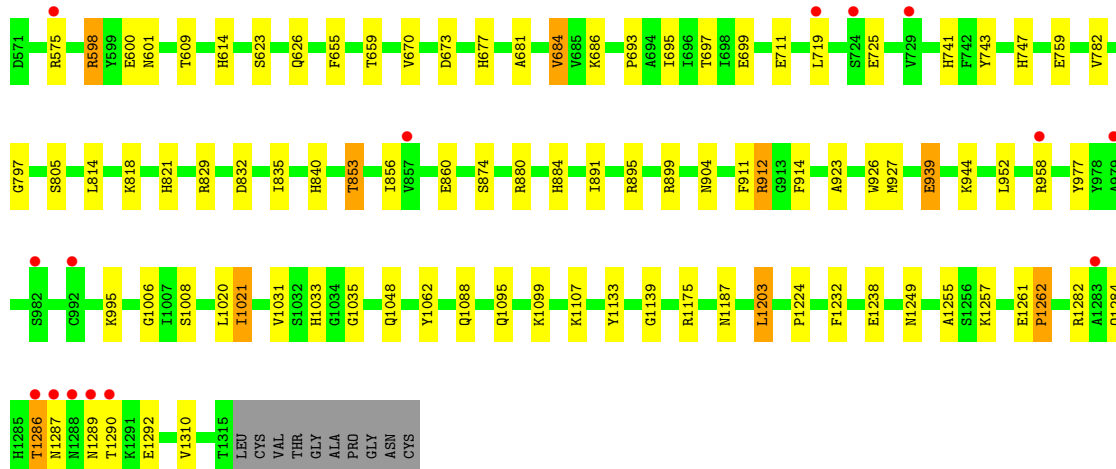
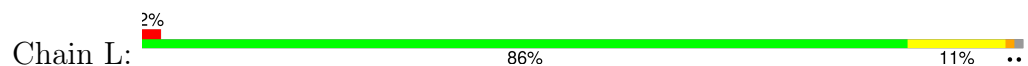




• Molecule 3: Xanthine dehydrogenase/oxidase



• Molecule 3: Xanthine dehydrogenase/oxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	132.77Å 73.42Å 138.16Å 90.00° 96.93° 90.00°	Depositor
Resolution (Å)	131.80 – 1.82 131.80 – 1.82	Depositor EDS
% Data completeness (in resolution range)	97.2 (131.80-1.82) 97.2 (131.80-1.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 1.82Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.193 , 0.229 0.193 , 0.230	Depositor DCC
R_{free} test set	11464 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	20.2	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.016 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20671	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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: FES, ZXF, AST, 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	0.73	0/1277	0.85	0/1723
1	J	0.72	0/1277	0.84	0/1723
2	B	0.59	0/2689	0.83	0/3637
2	K	0.56	0/2438	0.83	0/3290
3	C	0.75	0/5951	0.88	5/8061 (0.1%)
3	L	0.69	0/5888	0.86	3/7974 (0.0%)
All	All	0.69	0/19520	0.86	8/26408 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	1262	PRO	N-CA-C	7.84	120.27	110.70
3	C	848	VAL	CB-CA-C	-6.75	100.56	110.62
3	C	1262	PRO	N-CA-C	6.07	118.10	110.70
3	L	891	ILE	CA-C-N	5.72	125.40	119.05
3	L	891	ILE	C-N-CA	5.72	125.40	119.05
3	C	654	VAL	N-CA-C	-5.64	105.22	110.53
3	C	1187	ASN	CA-C-N	5.01	124.79	119.28
3	C	1187	ASN	C-N-CA	5.01	124.79	119.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1255	0	1265	13	0
1	J	1255	0	1265	20	0
2	B	2630	0	2697	20	0
2	K	2389	0	2459	25	0
3	C	5823	0	5744	78	1
3	L	5761	0	5685	71	0
4	A	8	0	0	0	0
4	J	8	0	0	0	0
5	B	53	0	31	1	0
5	K	53	0	31	3	0
6	C	3	0	0	1	0
6	L	3	0	0	1	0
7	C	28	0	0	1	0
7	L	28	0	0	1	0
8	A	94	0	0	0	0
8	B	137	0	0	3	0
8	C	465	0	0	4	0
8	J	99	0	0	1	0
8	K	105	0	0	1	0
8	L	474	0	0	3	1
All	All	20671	0	19177	213	1

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 (213) 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:243:LYS:HD3	2:K:243:LYS:H	1.05	1.12
3:C:641:PRO:HD2	3:C:779:MET:CE	1.84	1.06
2:K:243:LYS:HD3	2:K:243:LYS:N	1.75	0.99
3:C:641:PRO:HD2	3:C:779:MET:HE1	1.43	0.99
3:C:924:GLU:OE1	3:C:942:ARG:NH1	1.97	0.96
3:L:952:LEU:CD2	3:L:958:ARG:HG2	1.97	0.95
2:K:241:THR:HB	2:K:243:LYS:HE2	1.49	0.94
3:L:1088:GLN:HG2	3:L:1133:TYR:CD1	2.04	0.91
3:L:697:THR:HB	3:L:699:GLU:OE1	1.72	0.88
2:K:243:LYS:H	2:K:243:LYS:CD	1.81	0.83
1:J:57:LYS:HE2	1:J:66:ILE:HD11	1.59	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:884:HIS:HE1	3:C:1006:GLY:H	1.23	0.81
3:L:695:ILE:H	3:L:904:ASN:HD22	1.27	0.80
1:A:131:GLN:HE21	1:A:133:GLU:H	1.28	0.80
1:J:104:ARG:HH11	1:J:162:THR:HG23	1.45	0.80
3:C:641:PRO:HD2	3:C:779:MET:HE2	1.64	0.79
3:L:856:ILE:HD11	3:L:927:MET:HE1	1.66	0.77
3:L:884:HIS:HE1	3:L:1006:GLY:H	1.31	0.76
3:C:695:ILE:H	3:C:904:ASN:HD22	1.33	0.75
1:A:57:LYS:HE2	1:A:66:ILE:HD11	1.66	0.75
1:J:159:GLY:O	1:J:162:THR:HG22	1.86	0.75
3:C:884:HIS:CE1	3:C:1006:GLY:H	2.05	0.75
3:L:1289:ASN:HB2	3:L:1292:GLU:HB2	1.70	0.74
1:J:131:GLN:HE21	1:J:133:GLU:H	1.36	0.74
3:L:952:LEU:HD23	3:L:958:ARG:HG2	1.69	0.74
3:C:640:ILE:HG23	3:C:779:MET:HE2	1.68	0.74
2:K:439:ARG:NH2	2:K:451:GLU:OE1	2.19	0.73
3:C:575:ARG:HD2	8:C:365:HOH:O	1.93	0.69
3:C:851:MET:HE2	3:C:857:VAL:HG11	1.74	0.69
1:J:134:PRO:O	1:J:165:LYS:HA	1.93	0.69
3:C:995:LYS:NZ	3:C:1284:GLN:HE21	1.91	0.68
2:B:439:ARG:NH2	2:B:451:GLU:OE1	2.24	0.68
3:C:1287:ASN:C	3:C:1287:ASN:HD22	2.01	0.67
3:L:1020:LEU:C	3:L:1021:ILE:HD13	2.20	0.67
3:C:673:ASP:OD2	3:C:677:HIS:HD2	1.76	0.67
3:L:995:LYS:NZ	3:L:1284:GLN:HE21	1.92	0.67
3:L:623:SER:HA	3:L:626:GLN:HE21	1.60	0.67
3:L:699:GLU:H	3:L:699:GLU:CD	2.03	0.66
3:C:640:ILE:HG23	3:C:779:MET:CE	2.25	0.65
3:C:572:THR:HA	3:C:575:ARG:HD3	1.77	0.65
3:L:952:LEU:HD21	3:L:958:ARG:HG2	1.75	0.65
3:C:840:HIS:HE1	3:C:874:SER:OG	1.79	0.65
3:L:856:ILE:CD1	3:L:927:MET:HE1	2.27	0.64
3:C:779:MET:CE	3:C:814:LEU:HD13	2.27	0.64
3:L:853:THR:HG22	3:L:944:LYS:HZ3	1.62	0.64
3:L:884:HIS:CE1	3:L:1006:GLY:H	2.13	0.63
3:L:673:ASP:OD2	3:L:677:HIS:HD2	1.82	0.61
2:K:243:LYS:N	2:K:243:LYS:CD	2.54	0.61
7:C:1326:ZXF:MO	7:C:1326:ZXF:O2	1.72	0.61
3:L:995:LYS:HZ1	3:L:1284:GLN:HE21	1.49	0.61
1:J:104:ARG:HD3	1:J:162:THR:HG21	1.82	0.61
3:C:601:ASN:O	3:C:821:HIS:HD2	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:705:ASN:HB2	8:C:114:HOH:O	2.01	0.60
7:L:1326:ZXF:O2	7:L:1326:ZXF:MO	1.73	0.58
2:B:217:LEU:O	2:B:220:LYS:HD2	2.04	0.58
3:L:914:PHE:CD1	6:L:1:AST:AS	3.17	0.58
3:L:1021:ILE:HD12	3:L:1031:VAL:HA	1.86	0.58
2:K:281:PRO:HB2	2:K:287:LEU:HD12	1.85	0.57
3:L:853:THR:HG22	3:L:944:LYS:NZ	2.19	0.57
3:L:840:HIS:HE1	3:L:874:SER:OG	1.87	0.57
3:C:752:ILE:CD1	3:C:763:PHE:HE1	2.18	0.57
2:B:241:THR:HG22	2:B:243:LYS:H	1.70	0.56
3:L:1033:HIS:HD2	3:L:1035:GLY:H	1.52	0.56
3:L:601:ASN:O	3:L:821:HIS:HD2	1.87	0.56
3:L:614:HIS:HD2	3:L:693:PRO:O	1.88	0.56
3:C:995:LYS:HZ3	3:C:1284:GLN:HE21	1.54	0.55
1:J:164:ALA:HB1	1:J:165:LYS:HG3	1.89	0.55
3:L:880:ARG:O	3:L:884:HIS:HD2	1.88	0.55
3:C:609:THR:HG22	8:C:338:HOH:O	2.07	0.55
3:C:609:THR:HG23	3:C:664:GLY:HA2	1.89	0.55
3:C:880:ARG:O	3:C:884:HIS:HD2	1.89	0.55
3:L:939:GLU:HG2	3:L:977:TYR:CE2	2.42	0.54
3:C:942:ARG:HH11	3:C:942:ARG:HG2	1.73	0.54
3:C:1048:GLN:HE22	3:C:1187:ASN:HD22	1.56	0.54
2:K:232:GLU:OE1	3:L:677:HIS:HE1	1.91	0.53
3:C:655:PHE:HE1	3:C:814:LEU:HD23	1.73	0.53
2:K:394:ARG:NH2	8:K:1351:HOH:O	2.41	0.53
2:B:264:ILE:O	2:B:268:MET:HG3	2.08	0.53
3:C:1033:HIS:HD2	3:C:1035:GLY:H	1.56	0.53
3:C:670:VAL:HG11	3:C:681:ALA:HB3	1.90	0.52
2:K:287:LEU:HD22	2:K:301:ALA:HB3	1.91	0.52
3:C:614:HIS:HD2	3:C:693:PRO:O	1.92	0.52
3:C:782:VAL:CG1	3:C:786:ARG:HG3	2.40	0.52
3:L:1088:GLN:HG2	3:L:1133:TYR:CE1	2.43	0.52
1:A:42:GLY:O	3:C:829:ARG:HD2	2.11	0.51
3:C:624:GLU:CB	3:C:684:VAL:CG1	2.87	0.51
3:C:914:PHE:CD1	6:C:1:AST:AS	3.24	0.51
3:L:670:VAL:HG11	3:L:681:ALA:HB3	1.92	0.51
1:A:125:TYR:CZ	1:A:129:ARG:HD2	2.46	0.51
3:C:779:MET:HE3	3:C:814:LEU:HD13	1.91	0.51
2:K:447:MET:HG2	2:K:527:LEU:HD13	1.93	0.51
3:C:655:PHE:HE1	3:C:814:LEU:CD2	2.24	0.51
3:C:779:MET:HE1	3:C:814:LEU:HD13	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:43:CYS:HA	3:L:829:ARG:HB2	1.92	0.50
1:J:104:ARG:HH11	1:J:162:THR:CG2	2.20	0.50
1:A:36:LEU:HD22	1:A:89:GLU:HG3	1.92	0.50
2:B:338:ALA:C	8:B:2064:HOH:O	2.55	0.50
3:C:624:GLU:HB2	3:C:684:VAL:CG1	2.42	0.50
3:L:1286:THR:OG1	3:L:1287:ASN:N	2.44	0.50
2:B:480:GLU:HG2	8:B:602:HOH:O	2.13	0.49
3:C:782:VAL:CG1	3:C:783:PRO:HD2	2.42	0.49
1:A:43:CYS:HA	3:C:829:ARG:HB2	1.95	0.49
3:L:719:LEU:HD11	3:L:895:ARG:CB	2.43	0.49
3:C:600:GLU:HG2	3:L:598:ARG:O	2.13	0.48
3:C:719:LEU:HD11	3:C:895:ARG:CB	2.42	0.48
1:J:42:GLY:O	3:L:829:ARG:HD2	2.13	0.48
3:L:1020:LEU:O	3:L:1021:ILE:HD13	2.13	0.48
3:L:1048:GLN:HE22	3:L:1187:ASN:HD22	1.61	0.48
3:C:705:ASN:O	3:C:705:ASN:CG	2.56	0.48
3:L:623:SER:HA	3:L:626:GLN:NE2	2.28	0.48
3:C:1062:TYR:OH	3:L:759:GLU:OE2	2.30	0.48
3:L:719:LEU:HD13	3:L:860:GLU:OE2	2.14	0.48
3:C:885:MET:SD	3:C:896:GLY:HA3	2.54	0.48
1:J:29:TYR:CD1	1:J:33:LYS:HD3	2.49	0.48
2:K:257:LEU:O	5:K:606:FAD:H2B	2.14	0.47
2:B:249:LYS:HG2	2:B:401:GLU:O	2.14	0.47
3:C:640:ILE:HG12	3:C:779:MET:HE3	1.96	0.47
3:C:695:ILE:HG23	3:C:700:ASP:HB3	1.97	0.47
1:A:61:LEU:HD21	2:B:285:PRO:HA	1.95	0.47
2:K:308:VAL:HG21	2:K:348:LEU:HG	1.96	0.47
3:C:911:PHE:O	3:C:912:ARG:C	2.57	0.47
3:C:884:HIS:HE1	3:C:1006:GLY:N	2.02	0.47
2:B:427:ARG:NE	2:B:504:MET:HE3	2.29	0.47
2:B:441:LEU:HB3	2:B:451:GLU:HB2	1.95	0.47
3:C:794:MET:HE3	3:C:1038:MET:HB3	1.96	0.47
3:C:641:PRO:CD	3:C:779:MET:HE1	2.29	0.47
1:J:45:GLU:CD	3:L:1224:PRO:HD2	2.40	0.46
1:J:104:ARG:NH1	1:J:162:THR:HG23	2.23	0.46
3:C:1095:GLN:O	3:C:1099:LYS:HG2	2.16	0.46
2:B:506:GLU:HG2	8:C:493:HOH:O	2.15	0.46
3:L:1282:ARG:NH2	3:L:1292:GLU:OE2	2.34	0.46
2:B:339:GLY:CA	8:B:2064:HOH:O	2.63	0.46
3:C:609:THR:CG2	3:C:664:GLY:HA2	2.45	0.46
3:L:1107:LYS:NZ	8:L:1489:HOH:O	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:624:GLU:HB3	3:C:684:VAL:CG1	2.46	0.46
3:L:1033:HIS:CD2	3:L:1035:GLY:H	2.31	0.45
2:K:337:PHE:O	2:K:337:PHE:HD2	2.00	0.45
2:K:256:LYS:HE3	2:K:275:PHE:CE2	2.52	0.45
1:A:165:LYS:HD3	1:A:165:LYS:HA	1.67	0.45
1:J:36:LEU:HD22	1:J:89:GLU:HG3	1.99	0.45
3:C:624:GLU:HB3	3:C:684:VAL:HG11	1.98	0.45
3:C:1261:GLU:N	3:C:1262:PRO:CD	2.80	0.45
3:L:655:PHE:HE1	3:L:814:LEU:HD23	1.82	0.45
3:L:880:ARG:HD2	3:L:914:PHE:HB3	1.99	0.45
3:L:1257:LYS:HE3	8:L:2028:HOH:O	2.17	0.45
3:C:1033:HIS:CD2	3:C:1035:GLY:H	2.34	0.45
1:J:29:TYR:HA	1:J:33:LYS:HD2	2.00	0.44
3:L:1095:GLN:O	3:L:1099:LYS:HG2	2.17	0.44
3:L:1249:ASN:O	3:L:1255:ALA:HA	2.17	0.44
2:K:346:ALA:HB1	5:K:606:FAD:H4'	1.99	0.44
2:B:459:MET:HE2	2:B:512:THR:HG21	1.99	0.44
2:K:377:ARG:HE	2:K:377:ARG:HB3	1.56	0.44
3:L:609:THR:HG21	3:L:835:ILE:HD11	1.99	0.44
3:L:1203:LEU:C	3:L:1203:LEU:HD12	2.42	0.44
1:A:37:ARG:HD3	3:C:595:ASP:O	2.17	0.44
3:C:1048:GLN:NE2	3:C:1187:ASN:HD22	2.15	0.44
3:C:1079:ALA:O	3:C:1081:VAL:HG13	2.17	0.44
3:C:1105:LYS:HG2	3:C:1116:TRP:CD2	2.52	0.44
3:C:853:THR:HG22	3:C:944:LYS:HD3	2.00	0.44
1:J:144:GLN:HE22	2:K:336:TRP:HA	1.84	0.43
3:C:624:GLU:HB2	3:C:684:VAL:HG13	2.01	0.43
3:C:1249:ASN:O	3:C:1255:ALA:HA	2.18	0.43
2:K:257:LEU:HD13	2:K:281:PRO:HG3	2.00	0.43
3:L:711:GLU:HA	3:L:899:ARG:HD2	2.00	0.43
1:A:45:GLU:CD	3:C:1224:PRO:HD2	2.43	0.43
3:C:782:VAL:HG12	3:C:786:ARG:HG3	2.01	0.43
2:K:389:PHE:O	2:K:396:THR:HA	2.18	0.43
3:C:782:VAL:HG12	3:C:783:PRO:HD2	2.01	0.43
3:C:995:LYS:HZ1	3:C:1284:GLN:HE21	1.66	0.43
3:C:1183:GLY:HA2	3:C:1247:CYS:O	2.19	0.43
3:L:1175:ARG:HA	3:L:1238:GLU:O	2.19	0.43
3:L:1261:GLU:N	3:L:1262:PRO:CD	2.82	0.43
1:A:58:TYR:CD2	2:B:220:LYS:HG3	2.54	0.42
3:C:1287:ASN:C	3:C:1287:ASN:ND2	2.72	0.42
2:K:468:LYS:HG2	2:K:493:GLU:CD	2.44	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:1282:ARG:HA	3:L:1286:THR:HG23	2.01	0.42
3:L:747:HIS:HD1	3:L:805:SER:HA	1.84	0.42
2:B:223:PRO:HA	2:B:224:PRO:HD3	1.97	0.42
1:J:37:ARG:NH1	8:J:2129:HOH:O	2.26	0.42
1:J:74:LEU:O	1:J:76:PRO:HD3	2.19	0.42
3:C:844:ALA:HB2	3:C:922:ILE:HD13	2.02	0.42
3:C:747:HIS:CD2	3:C:836:THR:HG21	2.55	0.42
3:L:719:LEU:HD11	3:L:895:ARG:HB2	2.00	0.42
3:L:747:HIS:HD2	3:L:832:ASP:OD1	2.03	0.42
3:C:601:ASN:O	3:C:821:HIS:CD2	2.70	0.42
1:A:36:LEU:HD22	1:A:89:GLU:CG	2.50	0.42
2:K:487:CYS:HA	2:K:513:LEU:HD22	2.01	0.42
3:L:741:HIS:HA	3:L:911:PHE:CE1	2.55	0.42
3:L:923:ALA:HA	3:L:926:TRP:NE1	2.35	0.42
1:J:59:ASP:HB3	1:J:62:GLN:HB2	2.02	0.41
3:L:856:ILE:HD11	3:L:927:MET:CE	2.41	0.41
3:L:911:PHE:O	3:L:912:ARG:C	2.63	0.41
2:K:337:PHE:CD2	2:K:337:PHE:C	2.98	0.41
2:B:197:ASN:O	2:B:200:GLU:HG2	2.21	0.41
3:L:719:LEU:HD11	3:L:895:ARG:HB3	2.02	0.41
2:B:281:PRO:HB2	2:B:287:LEU:HD13	2.03	0.41
2:B:286:GLU:HB3	2:B:405:LEU:HD11	2.03	0.41
2:B:346:ALA:HB1	5:B:606:FAD:H4'	2.03	0.41
3:C:719:LEU:HD11	3:C:895:ARG:HB3	2.03	0.41
3:C:759:GLU:OE2	3:L:1062:TYR:OH	2.32	0.41
3:L:684:VAL:O	3:L:686:LYS:HD2	2.21	0.41
1:J:143:PHE:HB3	3:L:1232:PHE:CE1	2.56	0.41
1:A:124:MET:HE2	1:A:163:PHE:CD1	2.57	0.40
2:K:504:MET:HE2	8:L:524:HOH:O	2.20	0.40
3:C:598:ARG:HD3	3:L:600:GLU:OE2	2.21	0.40
3:L:601:ASN:HB2	3:L:821:HIS:CD2	2.56	0.40
2:B:256:LYS:HG3	2:B:275:PHE:CG	2.56	0.40
3:C:848:VAL:HG21	3:C:926:TRP:HB2	2.04	0.40
2:K:263:GLU:HB3	5:K:606:FAD:H52A	2.03	0.40
3:L:695:ILE:H	3:L:904:ASN:ND2	2.07	0.40
3:L:1048:GLN:HE22	3:L:1187:ASN:HB2	1.87	0.40
3:L:1286:THR:HG22	3:L:1310:VAL:O	2.20	0.40
3:C:1048:GLN:HE22	3:C:1187:ASN:HB2	1.87	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:958:ARG:NH2	8:L:1506:HOH:O[2_655]	1.88	0.32

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	162/164 (99%)	158 (98%)	4 (2%)	0	100	100
1	J	162/164 (99%)	157 (97%)	4 (2%)	1 (1%)	21	11
2	B	332/334 (99%)	317 (96%)	15 (4%)	0	100	100
2	K	303/334 (91%)	290 (96%)	13 (4%)	0	100	100
3	C	753/755 (100%)	736 (98%)	13 (2%)	4 (0%)	24	14
3	L	743/755 (98%)	722 (97%)	17 (2%)	4 (0%)	24	14
All	All	2455/2506 (98%)	2380 (97%)	66 (3%)	9 (0%)	30	19

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	1008	SER
3	L	1008	SER
3	C	912	ARG
3	L	912	ARG
3	L	1139	GLY
3	C	1139	GLY
1	J	43	CYS
3	L	797	GLY
3	C	797	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	137/137 (100%)	132 (96%)	5 (4%)	31	13
1	J	137/137 (100%)	136 (99%)	1 (1%)	76	70
2	B	290/290 (100%)	285 (98%)	5 (2%)	53	41
2	K	261/290 (90%)	250 (96%)	11 (4%)	26	10
3	C	631/631 (100%)	619 (98%)	12 (2%)	50	37
3	L	624/631 (99%)	610 (98%)	14 (2%)	45	30
All	All	2080/2116 (98%)	2032 (98%)	48 (2%)	44	28

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	ARG
1	A	89	GLU
1	A	93	SER
1	A	140	GLU
1	A	165	LYS
2	B	220	LYS
2	B	256	LYS
2	B	272	ASN
2	B	312	LEU
2	B	427	ARG
3	C	598	ARG
3	C	609	THR
3	C	684	VAL
3	C	743	TYR
3	C	818	LYS
3	C	848	VAL
3	C	939	GLU
3	C	944	LYS
3	C	1123	ASP
3	C	1203	LEU
3	C	1208	LEU
3	C	1287	ASN
1	J	89	GLU
2	K	243	LYS
2	K	257	LEU
2	K	312	LEU
2	K	328	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	K	348	LEU
2	K	375	VAL
2	K	379	THR
2	K	397	LEU
2	K	398	LEU
2	K	426	ARG
2	K	428	GLU
3	L	575	ARG
3	L	598	ARG
3	L	659	THR
3	L	684	VAL
3	L	725	GLU
3	L	743	TYR
3	L	782	VAL
3	L	818	LYS
3	L	853	THR
3	L	939	GLU
3	L	1021	ILE
3	L	1203	LEU
3	L	1286	THR
3	L	1290	THR

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	71	ASN
1	A	131	GLN
1	A	146	ASN
2	B	272	ASN
2	B	322	GLN
2	B	423	GLN
2	B	471	GLN
3	C	585	GLN
3	C	614	HIS
3	C	626	GLN
3	C	677	HIS
3	C	821	HIS
3	C	840	HIS
3	C	884	HIS
3	C	904	ASN
3	C	1033	HIS
3	C	1048	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	1088	GLN
3	C	1220	HIS
3	C	1284	GLN
3	C	1287	ASN
1	J	71	ASN
1	J	131	GLN
1	J	144	GLN
1	J	146	ASN
2	K	226	GLN
2	K	292	HIS
2	K	333	GLN
2	K	473	GLN
3	L	585	GLN
3	L	614	HIS
3	L	626	GLN
3	L	677	HIS
3	L	821	HIS
3	L	840	HIS
3	L	884	HIS
3	L	904	ASN
3	L	1033	HIS
3	L	1048	GLN
3	L	1212	HIS
3	L	1220	HIS
3	L	1284	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

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
7	ZXF	L	1326	6	24,31,31	1.68	3 (12%)	22,52,52	2.21	9 (40%)
6	AST	C	1	7	0,2,3	-	-	0,1,3	-	-
6	AST	L	1	7	0,2,3	-	-	0,1,3	-	-
4	FES	J	601	1	0,4,4	-	-	-	-	-
4	FES	A	601	1	0,4,4	-	-	-	-	-
5	FAD	K	606	-	58,58,58	1.13	6 (10%)	85,89,89	1.60	20 (23%)
7	ZXF	C	1326	6	24,31,31	1.82	4 (16%)	22,52,52	2.38	12 (54%)
5	FAD	B	606	-	58,58,58	1.10	6 (10%)	85,89,89	1.57	16 (18%)
4	FES	J	602	1	0,4,4	-	-	-	-	-
4	FES	A	602	1	0,4,4	-	-	-	-	-

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
7	ZXF	L	1326	6	-	1/6/46/46	0/4/4/4
4	FES	J	601	1	-	-	0/1/1/1
4	FES	A	601	1	-	-	0/1/1/1
5	FAD	K	606	-	-	2/34/50/50	0/6/6/6
7	ZXF	C	1326	6	-	1/6/46/46	0/4/4/4
5	FAD	B	606	-	-	0/34/50/50	0/6/6/6
4	FES	J	602	1	-	-	0/1/1/1
4	FES	A	602	1	-	-	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	1326	ZXF	C9-C10	6.14	1.49	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	1326	ZXF	C9-C10	5.27	1.47	1.38
7	C	1326	ZXF	MO-S2'	-4.88	2.32	2.39
5	B	606	FAD	C4X-N5	3.74	1.38	1.30
5	K	606	FAD	C4X-N5	3.58	1.38	1.30
5	B	606	FAD	C10-N1	3.28	1.39	1.33
5	K	606	FAD	C10-N1	2.96	1.39	1.33
5	K	606	FAD	C2A-N1A	2.82	1.38	1.33
5	K	606	FAD	C2A-N3A	2.64	1.38	1.33
5	K	606	FAD	C8A-N7A	2.63	1.36	1.31
5	B	606	FAD	C2A-N3A	2.48	1.38	1.33
7	C	1326	ZXF	MO-S1'	-2.43	2.35	2.39
5	B	606	FAD	C2A-N1A	2.38	1.38	1.33
5	B	606	FAD	P-O3P	2.32	1.62	1.59
7	L	1326	ZXF	C10-N8	-2.23	1.33	1.35
7	L	1326	ZXF	MO-S1'	-2.20	2.36	2.39
5	B	606	FAD	C8A-N7A	2.15	1.35	1.31
5	K	606	FAD	C5A-N7A	-2.10	1.35	1.39
7	C	1326	ZXF	O4-C4	2.02	1.27	1.23

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	606	FAD	N3A-C2A-N1A	-6.48	118.78	128.58
7	L	1326	ZXF	C2'-C1'-S1'	6.21	123.67	120.15
5	K	606	FAD	N3A-C2A-N1A	-5.39	120.42	128.58
7	C	1326	ZXF	C2-N1-C10	4.61	121.49	113.36
5	K	606	FAD	N9A-C8A-N7A	-4.28	107.86	113.94
5	B	606	FAD	C5A-C4A-N3A	-4.16	120.99	126.72
5	K	606	FAD	C5A-C4A-N3A	-4.04	121.16	126.72
7	C	1326	ZXF	O3'-C7-C6	-3.90	106.36	108.96
5	B	606	FAD	N9A-C8A-N7A	-3.65	108.76	113.94
7	L	1326	ZXF	C2-N1-C10	3.48	119.50	113.36
5	B	606	FAD	C2A-N3A-C4A	3.44	120.24	111.83
5	K	606	FAD	C5A-N7A-C8A	3.40	108.79	103.45
7	C	1326	ZXF	O4-C4-C9	-3.31	119.28	127.26
7	C	1326	ZXF	O2P-P-O4'	-3.07	98.67	106.67
7	L	1326	ZXF	C4-C9-N5	3.06	124.60	116.27
5	K	606	FAD	O3'-C3'-C2'	-3.05	102.00	108.93
5	K	606	FAD	C2A-N3A-C4A	3.00	119.15	111.83
5	B	606	FAD	N3A-C4A-N9A	2.97	132.21	127.17
7	C	1326	ZXF	O3'-C7-N8	2.83	111.18	108.61
5	K	606	FAD	C4-N3-C2	-2.81	120.66	125.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	606	FAD	N3A-C4A-N9A	2.78	131.90	127.17
7	L	1326	ZXF	C7-C6-N5	2.77	110.58	107.87
5	B	606	FAD	C5A-N7A-C8A	2.72	107.73	103.45
7	C	1326	ZXF	O1P-P-O2P	2.70	117.91	107.80
7	C	1326	ZXF	C1'-C2'-S2'	-2.69	118.62	120.15
7	L	1326	ZXF	O1P-P-O4'	-2.67	99.71	106.67
5	B	606	FAD	C4X-C4-N3	2.62	119.92	113.25
7	C	1326	ZXF	C9-C4-N3	2.60	119.26	112.13
5	K	606	FAD	C4X-C4-N3	2.58	119.82	113.25
7	C	1326	ZXF	C4-C9-N5	2.57	123.28	116.27
7	L	1326	ZXF	O4-C4-C9	-2.54	121.12	127.26
7	C	1326	ZXF	O1P-P-O4'	-2.52	100.11	106.67
5	B	606	FAD	C10-C4X-N5	-2.51	119.68	124.81
5	K	606	FAD	O2P-P-O3P	2.48	113.97	107.27
5	K	606	FAD	C10-C4X-N5	-2.45	119.81	124.81
5	K	606	FAD	C4X-C10-N10	2.45	119.98	116.48
7	C	1326	ZXF	O4'-C4'-C3'	2.42	114.54	108.58
5	B	606	FAD	C4-C4X-N5	2.39	121.50	118.21
5	B	606	FAD	O2A-PA-O3P	2.35	113.63	107.27
5	B	606	FAD	C4X-C10-N10	2.35	119.85	116.48
5	K	606	FAD	C4A-N9A-C8A	2.32	108.17	105.74
5	K	606	FAD	C5'-C4'-C3'	-2.31	107.87	112.22
7	L	1326	ZXF	C9-C4-N3	2.30	118.45	112.13
7	C	1326	ZXF	O3'-C3'-C2'	2.30	112.33	109.09
5	B	606	FAD	C1'-C2'-C3'	-2.28	103.48	109.66
5	B	606	FAD	C9A-C5X-N5	-2.26	120.06	122.45
7	L	1326	ZXF	O4'-C4'-C3'	2.24	114.10	108.58
5	K	606	FAD	C1'-C2'-C3'	-2.23	103.60	109.66
5	B	606	FAD	C4-N3-C2	-2.23	121.68	125.64
7	L	1326	ZXF	O3'-C3'-C2'	2.23	112.24	109.09
5	B	606	FAD	O2P-P-O3P	2.17	113.13	107.27
5	K	606	FAD	O2A-PA-O3P	2.09	112.91	107.27
5	K	606	FAD	C9A-C5X-N5	-2.08	120.25	122.45
5	K	606	FAD	C4A-C5A-N7A	-2.07	108.22	110.58
5	K	606	FAD	C4-C4X-N5	2.06	121.05	118.21
5	K	606	FAD	C6A-C5A-C4A	2.03	119.94	117.18
5	B	606	FAD	C5A-C6A-N6A	-2.00	118.32	123.29

There are no chirality outliers.

All (4) torsion outliers are listed below:

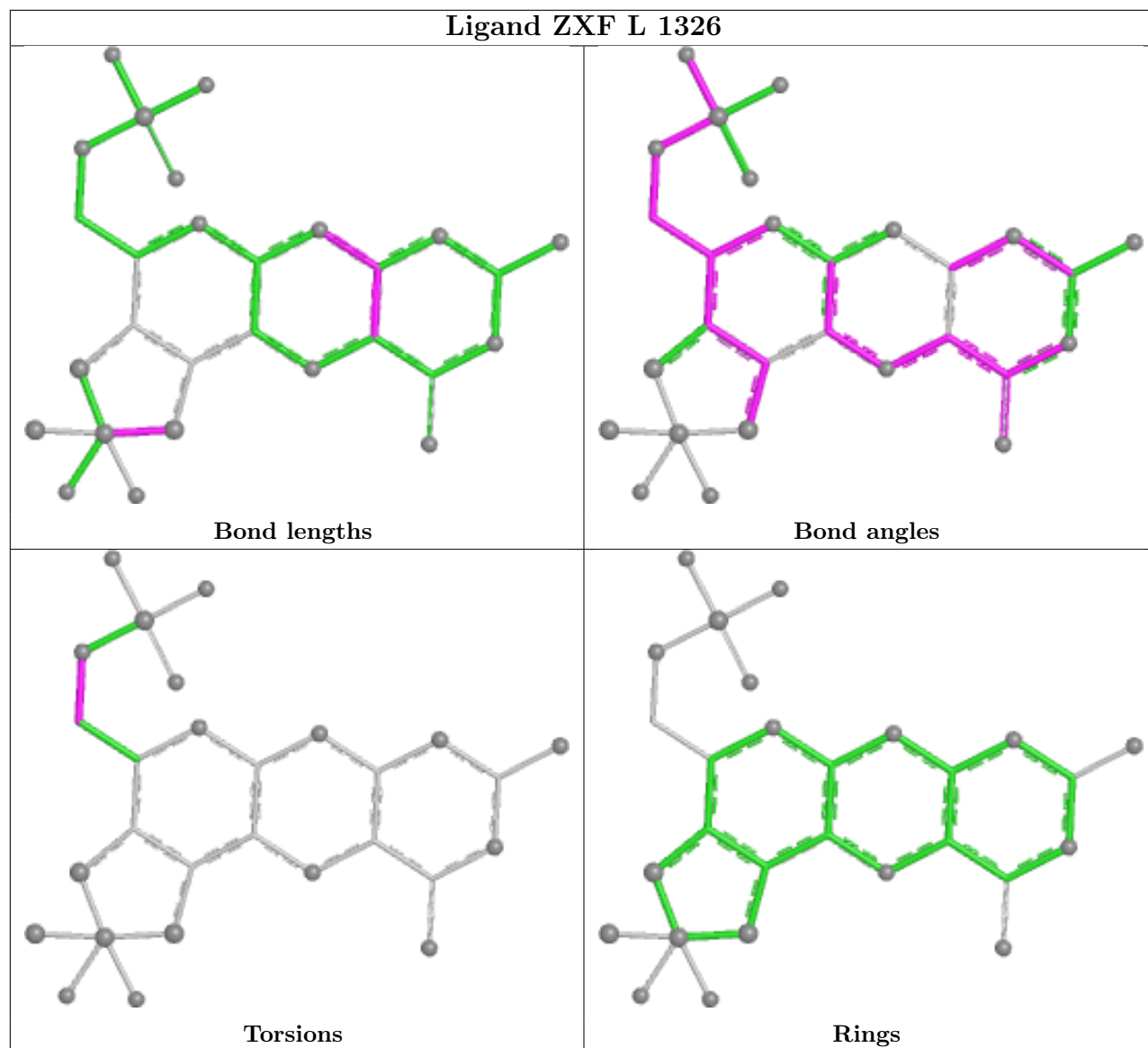
Mol	Chain	Res	Type	Atoms
7	L	1326	ZXF	C3'-C4'-O4'-P
7	C	1326	ZXF	C3'-C4'-O4'-P
5	K	606	FAD	C5B-O5B-PA-O1A
5	K	606	FAD	O4B-C4B-C5B-O5B

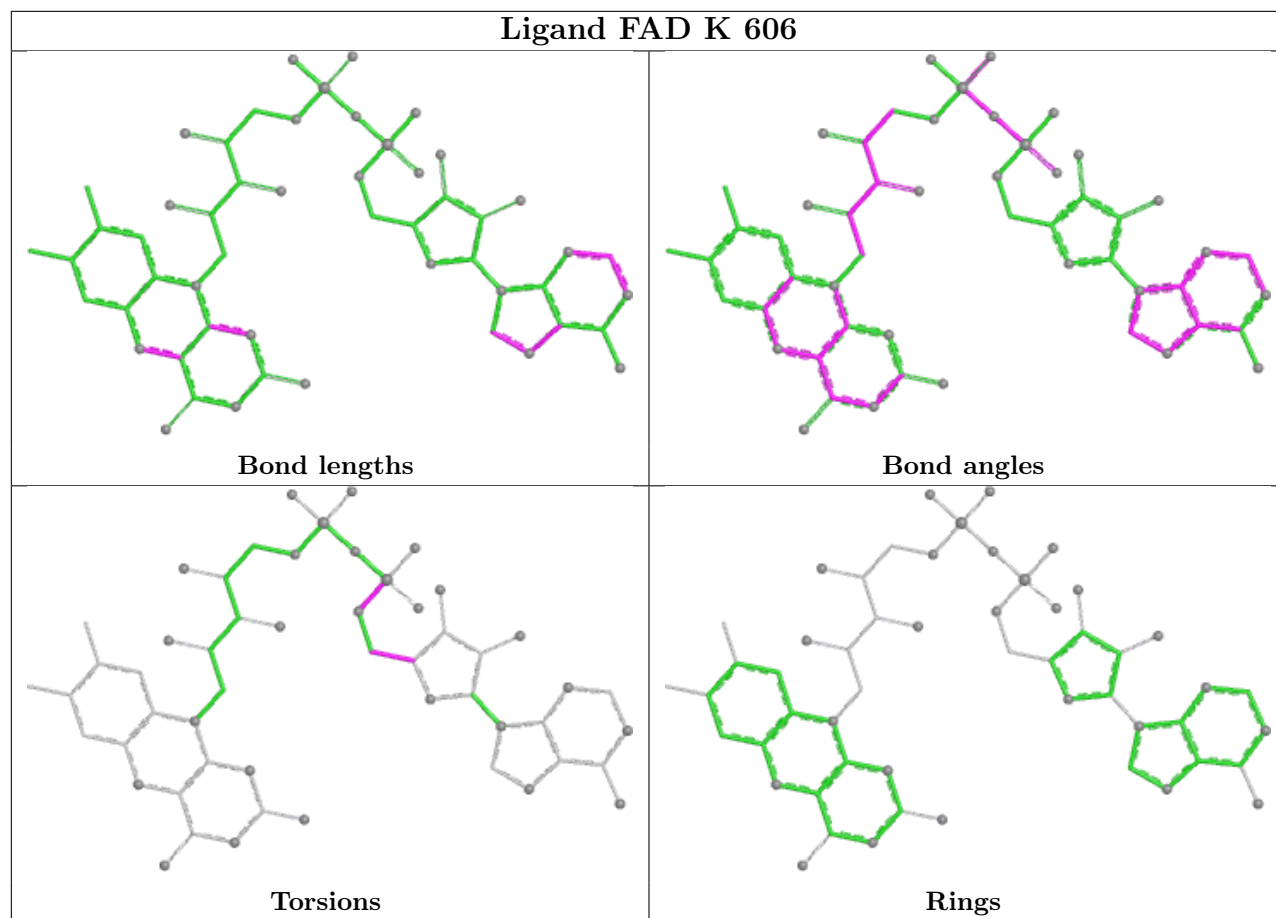
There are no ring outliers.

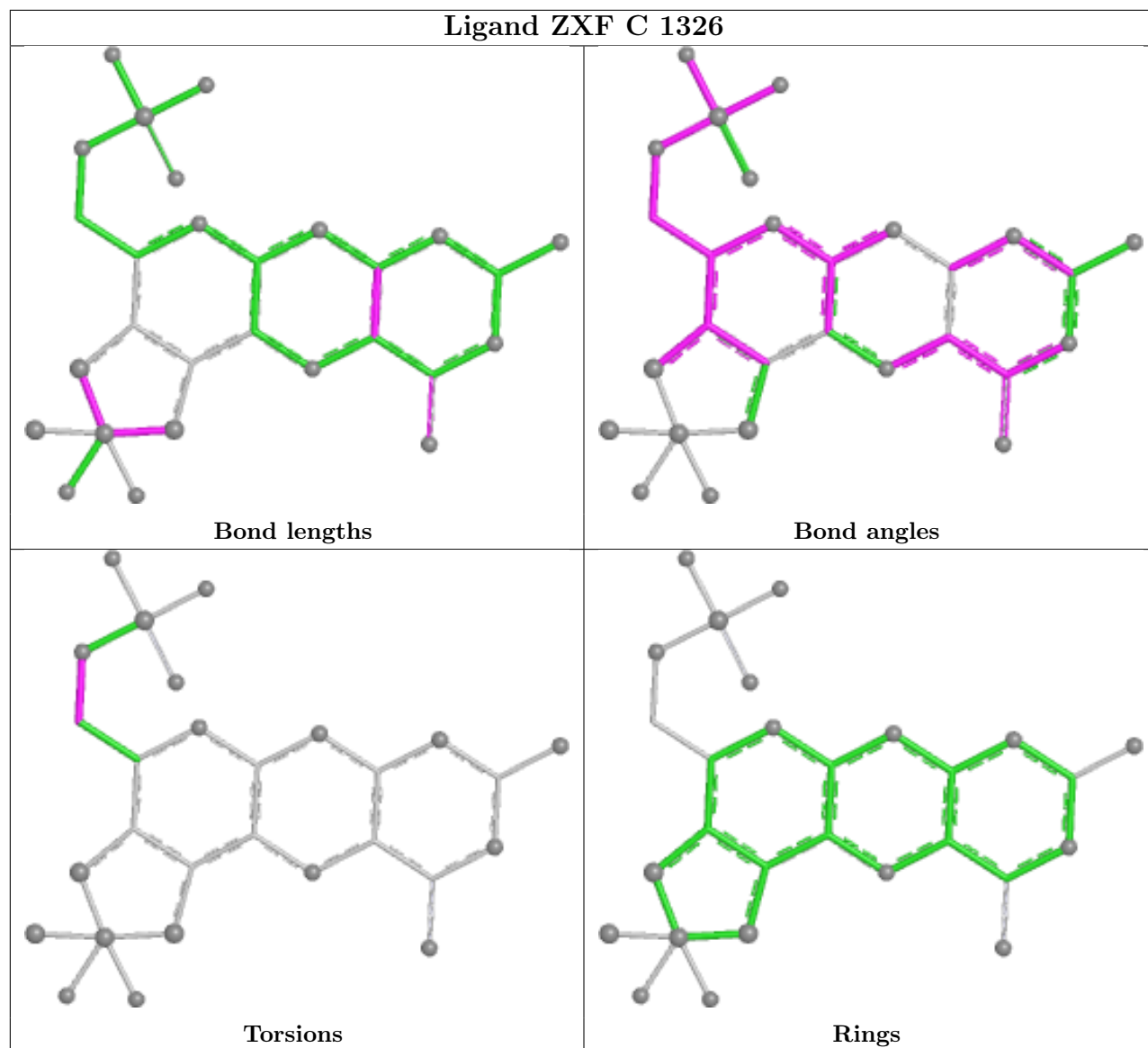
6 monomers are involved in 8 short contacts:

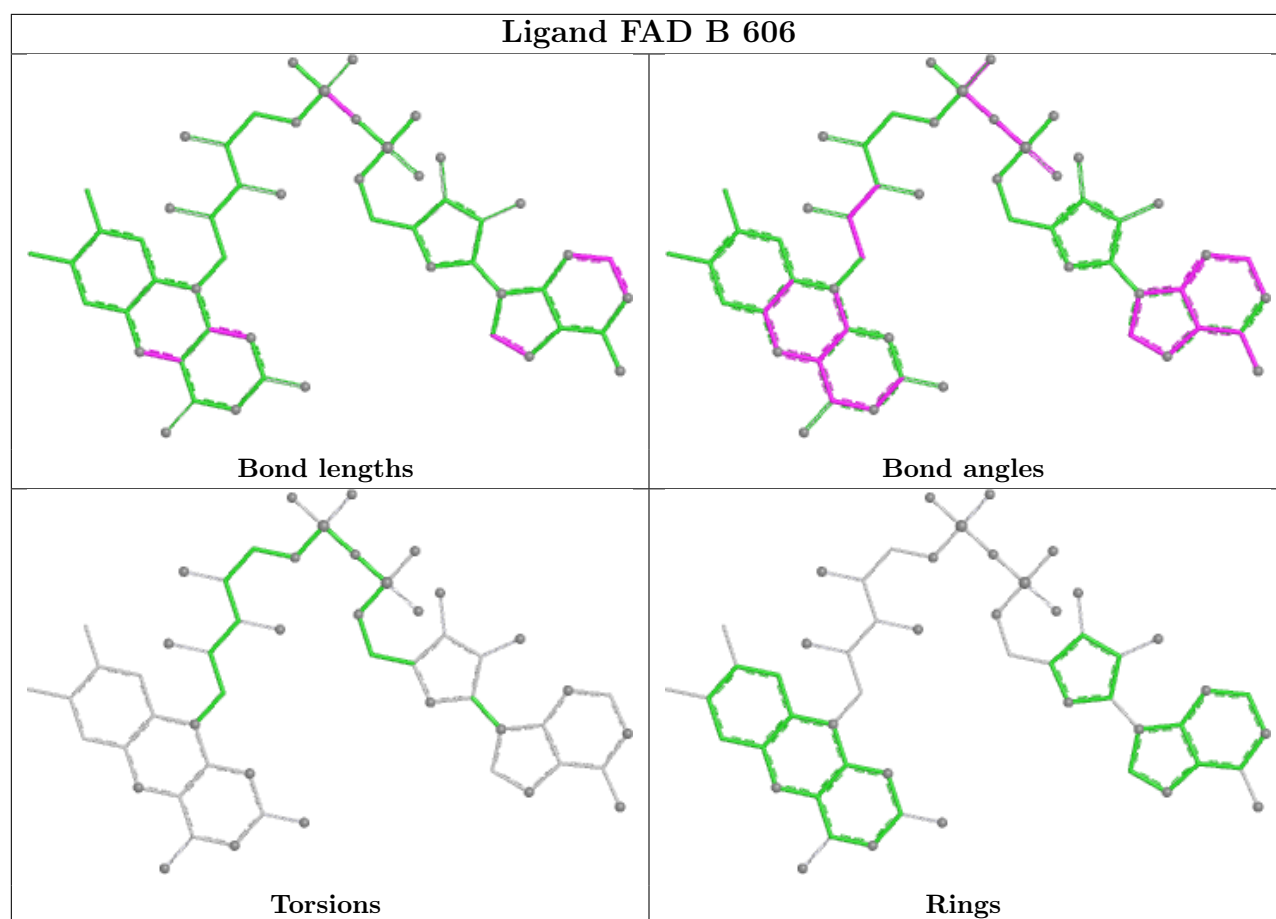
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	L	1326	ZXF	1	0
6	C	1	AST	1	0
6	L	1	AST	1	0
5	K	606	FAD	3	0
7	C	1326	ZXF	1	0
5	B	606	FAD	1	0

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%)	0.07	5 (3%)	52 59	10, 20, 34, 43	0
1	J	164/164 (100%)	0.22	11 (6%)	24 27	13, 22, 42, 52	0
2	B	334/334 (100%)	0.72	28 (8%)	17 19	17, 29, 42, 50	0
2	K	305/334 (91%)	0.83	28 (9%)	14 16	21, 33, 45, 49	0
3	C	755/755 (100%)	-0.20	5 (0%)	84 88	11, 18, 28, 35	0
3	L	745/755 (98%)	-0.02	15 (2%)	65 71	12, 20, 34, 60	0
All	All	2467/2506 (98%)	0.15	92 (3%)	45 51	10, 22, 40, 60	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	528	GLY	6.0
1	J	58	TYR	5.7
2	K	424	ALA	5.0
1	J	61	LEU	4.8
2	B	338	ALA	4.8
1	A	61	LEU	4.8
2	B	424	ALA	4.6
2	K	425	SER	4.3
3	L	1290	THR	4.0
2	B	425	SER	3.9
3	C	1325	CYS	3.8
2	K	224	PRO	3.8
3	L	1288	ASN	3.7
1	A	141	ASP	3.5
2	K	336	TRP	3.4
3	L	1287	ASN	3.4
2	K	429	ASP	3.3
2	K	414	GLU	3.2
1	A	2	THR	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	K	474	LEU	3.1
2	B	528	GLY	3.0
2	B	336	TRP	3.0
2	B	200	GLU	3.0
3	L	979	ALA	3.0
3	L	1289	ASN	3.0
2	B	207	THR	2.9
3	C	720	LYS	2.9
2	K	475	SER	2.9
2	B	292	HIS	2.8
3	C	1317	CYS	2.7
2	K	444	PRO	2.6
2	K	272	ASN	2.6
2	K	484	GLN	2.6
2	K	506	GLU	2.6
2	B	195	LEU	2.6
2	B	248	LEU	2.6
2	B	222	VAL	2.6
2	K	467	LEU	2.6
2	K	426	ARG	2.5
1	J	141	ASP	2.5
2	K	527	LEU	2.5
2	K	378	GLY	2.5
3	L	1286	THR	2.5
3	L	992	CYS	2.4
3	C	683	HIS	2.4
3	C	724	SER	2.4
2	B	268	MET	2.4
1	A	165	LYS	2.4
3	L	575	ARG	2.4
2	B	378	GLY	2.4
2	B	211	ILE	2.4
1	J	2	THR	2.4
2	K	379	THR	2.4
3	L	1283	ALA	2.4
2	K	335	ARG	2.4
1	J	136	VAL	2.4
2	K	243	LYS	2.4
2	B	221	ASP	2.3
1	J	164	ALA	2.3
2	K	449	VAL	2.3
2	B	398	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	L	982	SER	2.3
2	B	293	GLY	2.2
2	K	442	PHE	2.2
2	B	290	VAL	2.2
3	L	729	VAL	2.2
1	A	60	ARG	2.2
3	L	724	SER	2.2
2	K	478	TRP	2.2
3	L	958	ARG	2.2
1	J	162	THR	2.2
1	J	60	ARG	2.2
2	K	316	VAL	2.2
2	K	476	LYS	2.2
2	B	337	PHE	2.1
3	L	857	VAL	2.1
2	B	274	LEU	2.1
2	B	335	ARG	2.1
2	K	454	LEU	2.1
2	B	480	GLU	2.1
2	B	204	LEU	2.1
2	B	224	PRO	2.1
2	K	337	PHE	2.1
1	J	133	GLU	2.1
1	J	165	LYS	2.1
2	K	468	LYS	2.1
2	B	202	MET	2.1
1	J	33	LYS	2.0
2	B	471	GLN	2.0
3	L	719	LEU	2.0
2	B	477	PHE	2.0
2	B	382	THR	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](#)

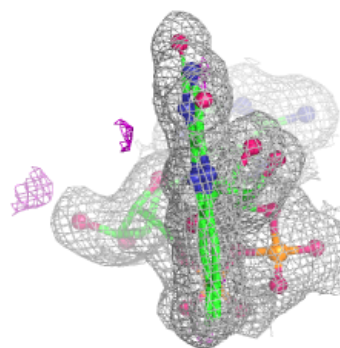
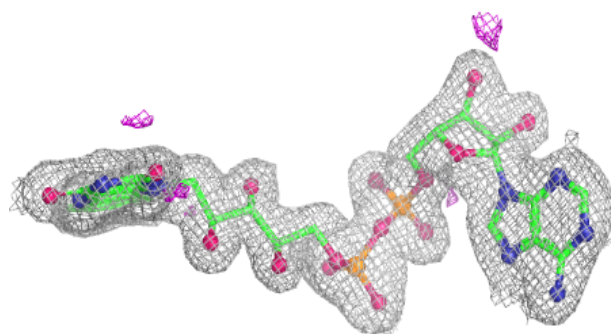
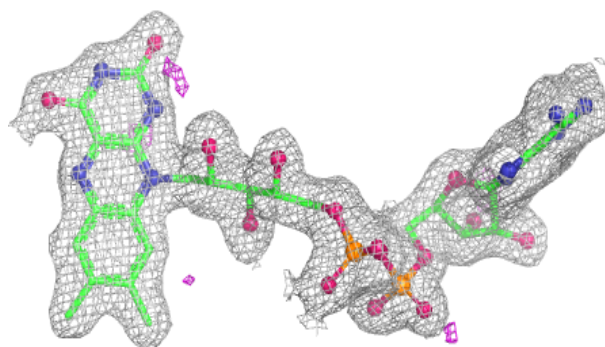
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
5	FAD	B	606	53/53	0.96	0.07	17,21,27,29	0
5	FAD	K	606	53/53	0.96	0.07	20,26,28,30	0
4	FES	J	602	4/4	0.99	0.03	15,15,16,16	0
4	FES	A	602	4/4	0.99	0.03	14,15,16,16	0
4	FES	J	601	4/4	0.99	0.03	14,14,16,16	0
6	AST	C	1	3/4	0.99	0.07	21,21,22,23	0
6	AST	L	1	3/4	0.99	0.07	26,26,26,31	0
7	ZXF	C	1326	28/28	0.99	0.05	9,13,20,32	0
7	ZXF	L	1326	28/28	0.99	0.04	12,15,20,29	0
4	FES	A	601	4/4	1.00	0.02	13,14,14,15	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.

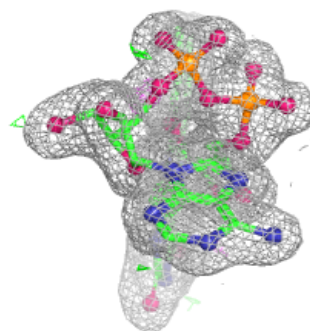
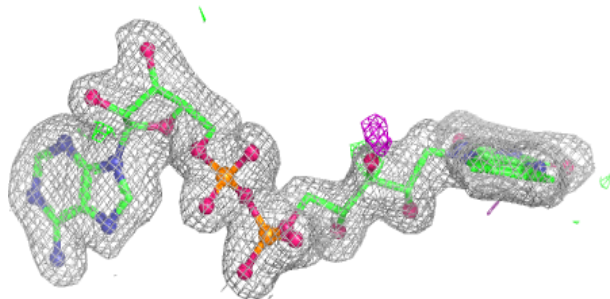
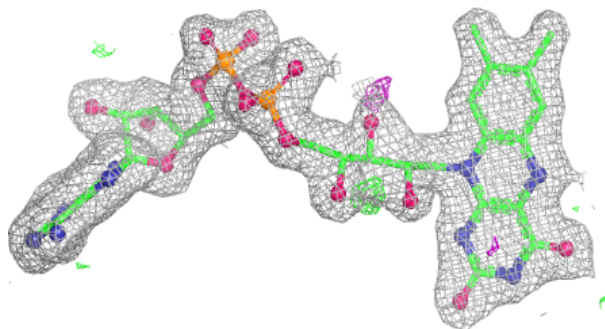
Electron density around FAD B 606:

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



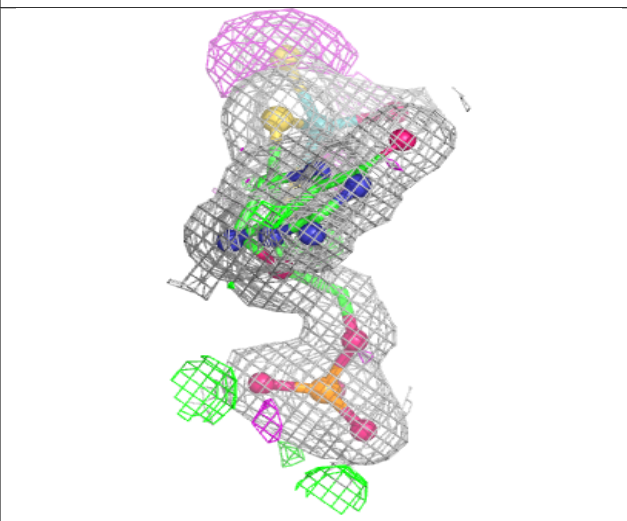
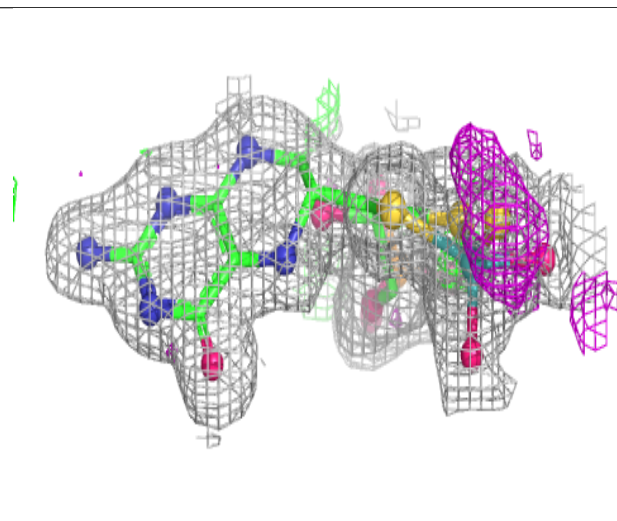
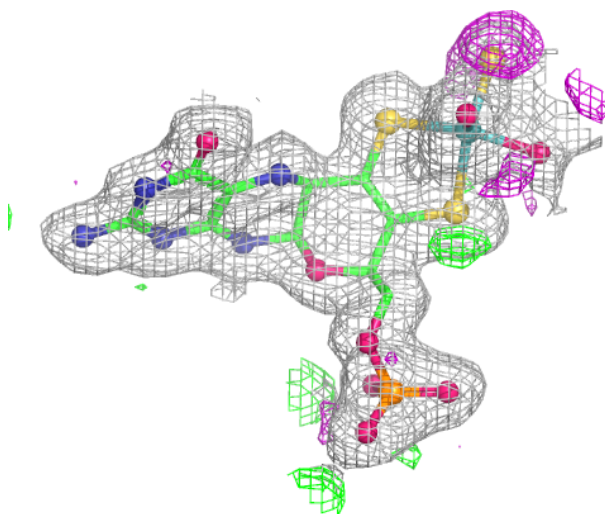
Electron density around FAD K 606:

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



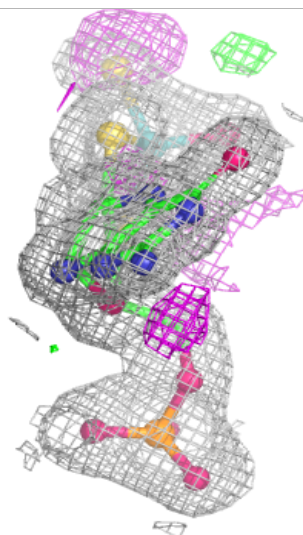
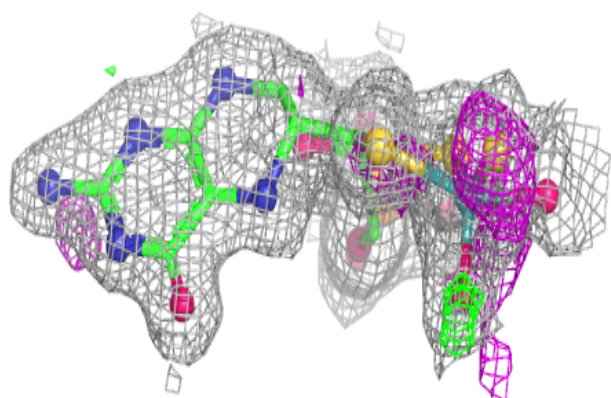
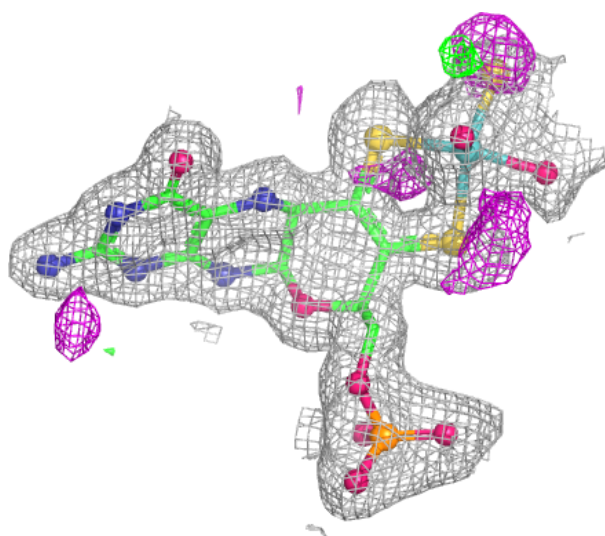
Electron density around ZXF C 1326:

$2mF_o-DF_c$ (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.