



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 03:35 PM EDT

PDB ID : 3NRZ / pdb_00003nrz
Title : Crystal Structure of Bovine Xanthine Oxidase in Complex with Hypoxanthine
Authors : Cao, H.; Pauff, J.M.; Hille, R.
Deposited on : 2010-07-01
Resolution : 1.80 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

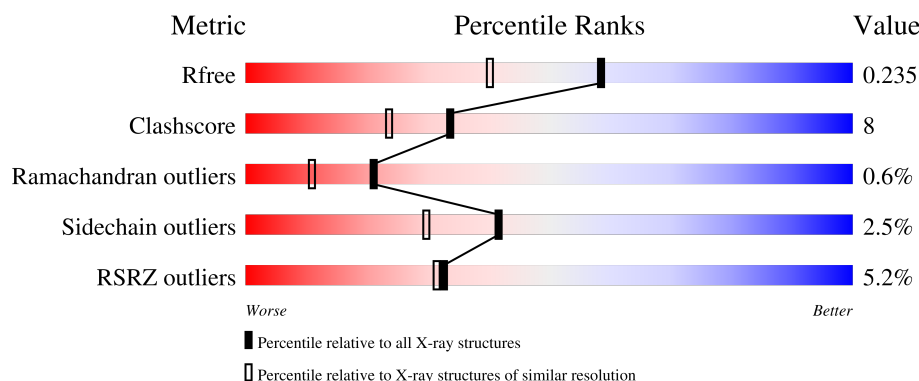
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	9% 93% 5%
1	J	164	7% 91% 9%
2	B	305	9% 84% 14%
2	K	305	9% 87% 11%
3	C	756	3% 82% 16%

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Mol	Chain	Length	Quality of chain
3	L	756	3% 86% 11% ..

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 20353 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			

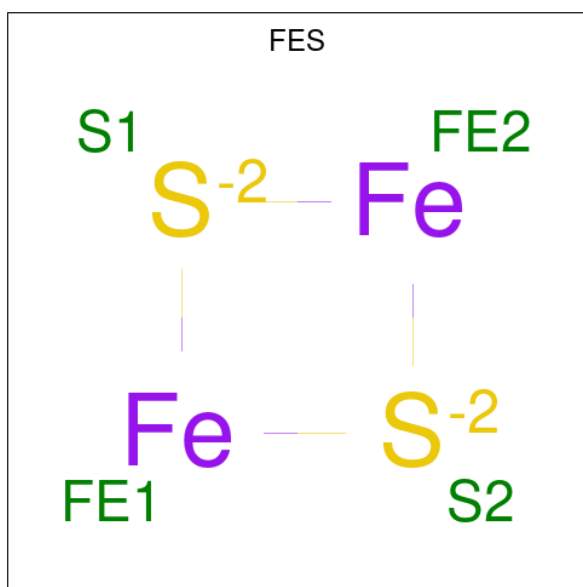
- Molecule 2 is a protein called Xanthine dehydrogenase/oxidase.

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.

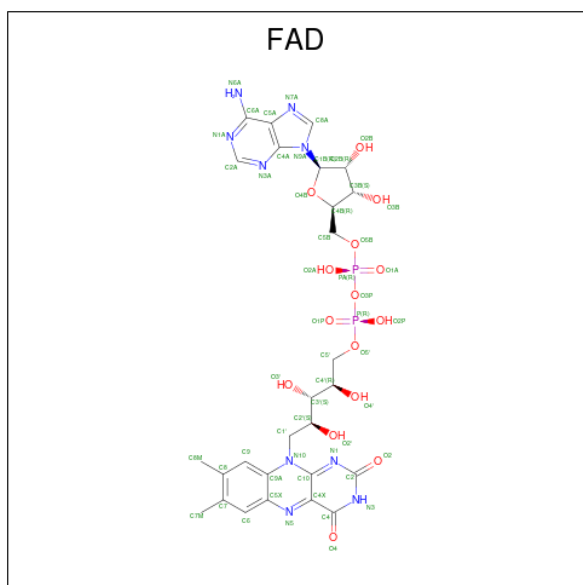
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	756	Total	C	N	O	S	0	0	0
			5832	3686	1005	1106	35			
3	L	745	Total	C	N	O	S	0	0	0
			5761	3643	992	1093	33			

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



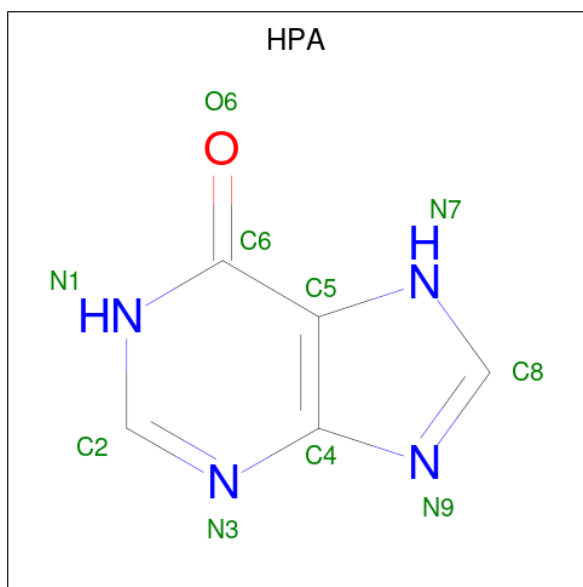
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 4	Fe 2	S 2	0	0
4	A	1	Total 4	Fe 2	S 2	0	0
4	J	1	Total 4	Fe 2	S 2	0	0
4	J	1	Total 4	Fe 2	S 2	0	0

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$).



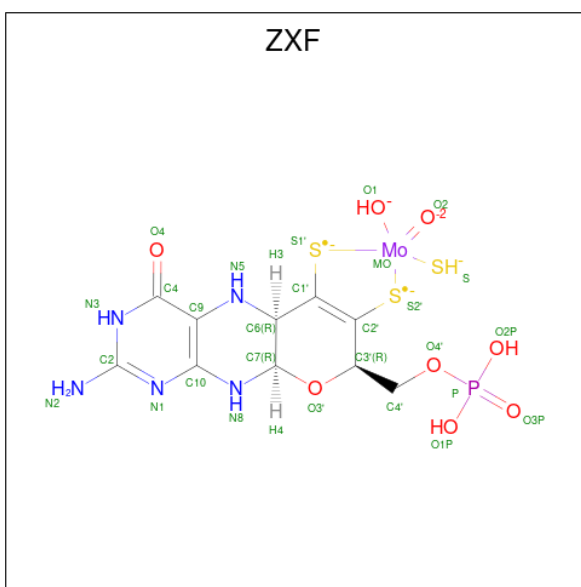
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	K	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 6 is HYPOXANTHINE (CCD ID: HPA) (formula: $C_5H_4N_4O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			10	5	4	1		
6	L	1	Total	C	N	O	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 28	C 10	Mo 1	N 5	O 8	P 1	S 3	0	0
7	L	1	Total 28	C 10	Mo 1	N 5	O 8	P 1	S 3	0	0

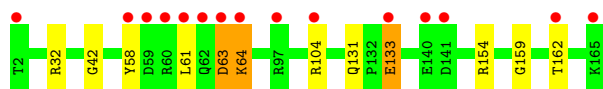
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	114	Total O 114 114	0	0
8	B	114	Total O 114 114	0	0
8	C	436	Total O 436 436	0	0
8	J	98	Total O 98 98	0	0
8	K	75	Total O 75 75	0	0
8	L	437	Total O 437 437	0	0

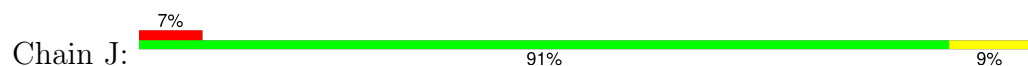
3 Residue-property plots [i](#)

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

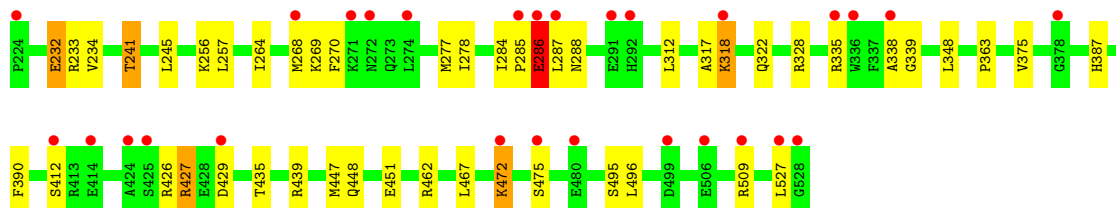
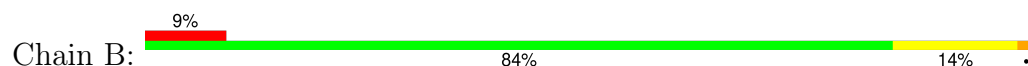
- Molecule 1: Xanthine dehydrogenase/oxidase



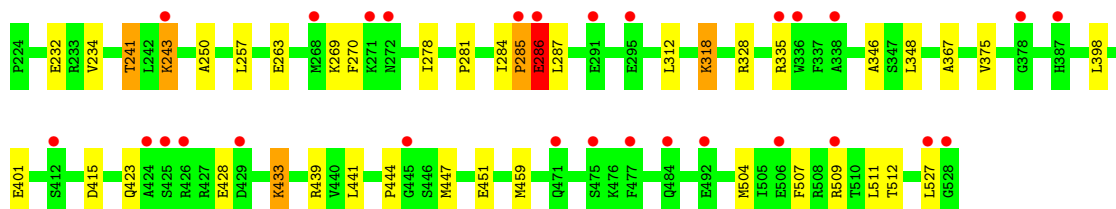
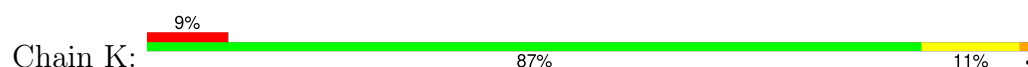
- Molecule 1: Xanthine dehydrogenase/oxidase



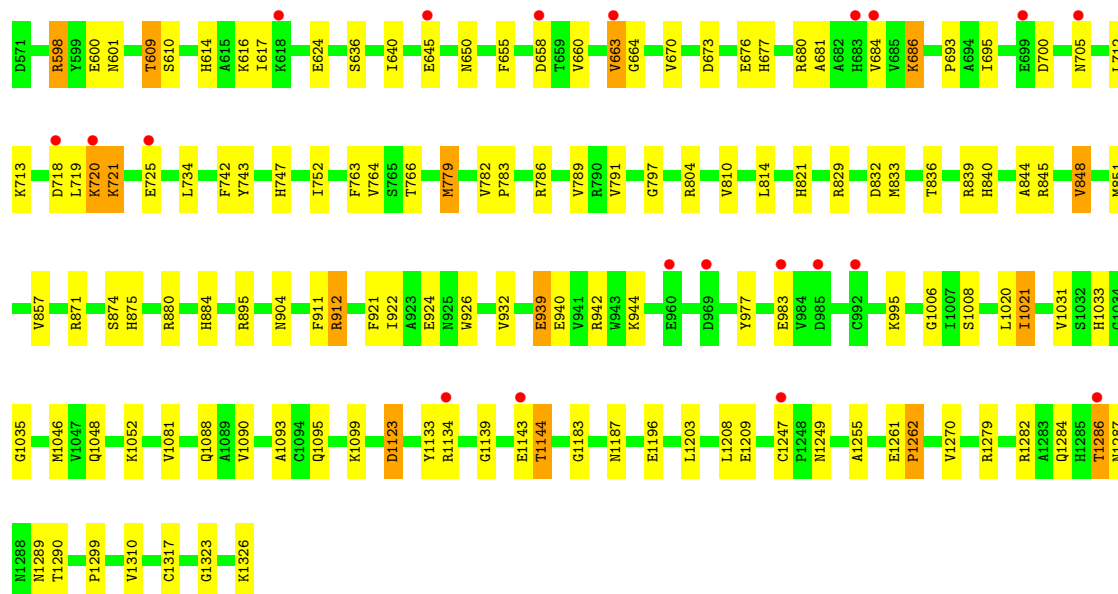
- Molecule 2: Xanthine dehydrogenase/oxidase



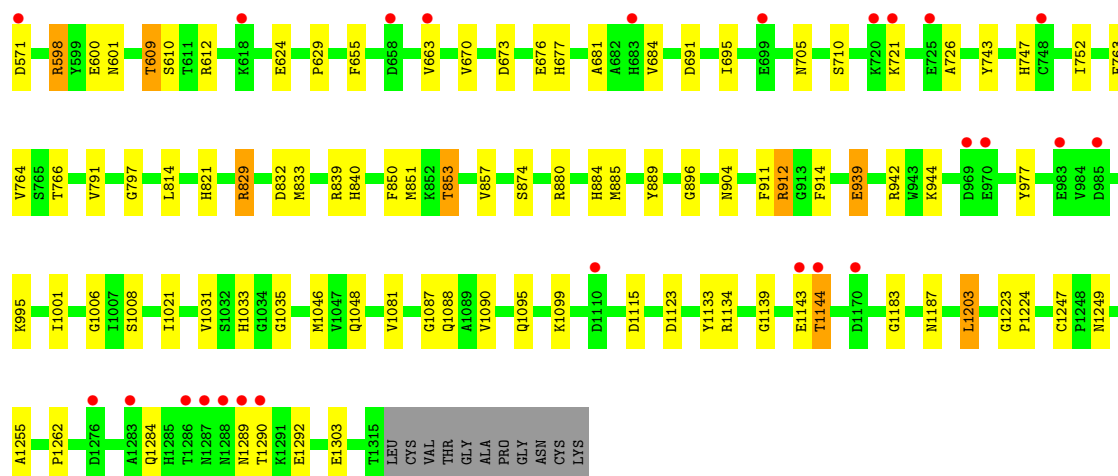
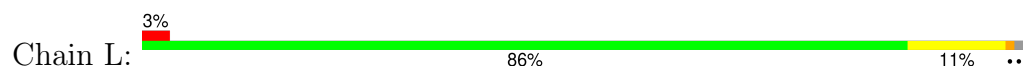
- Molecule 2: Xanthine dehydrogenase/oxidase



- 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	133.02Å 73.64Å 138.70Å 90.00° 97.05° 90.00°	Depositor
Resolution (Å)	23.50 – 1.80 23.50 – 1.80	Depositor EDS
% Data completeness (in resolution range)	95.1 (23.50-1.80) 95.1 (23.50-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.197 , 0.234 0.196 , 0.235	Depositor DCC
R_{free} test set	11843 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	20.4	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.010 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20353	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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, FAD, ZXF, HPA

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	0.76	0/1277	0.90	0/1723
1	J	0.71	0/1277	0.86	0/1723
2	B	0.61	0/2438	0.87	2/3290 (0.1%)
2	K	0.58	0/2438	0.85	1/3290 (0.0%)
3	C	0.73	0/5960	0.89	5/8072 (0.1%)
3	L	0.71	0/5888	0.88	3/7974 (0.0%)
All	All	0.69	0/19278	0.88	11/26072 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	1262	PRO	N-CA-C	7.16	119.43	110.70
3	C	839	ARG	NE-CZ-NH2	-6.96	112.94	119.20
3	L	839	ARG	NE-CZ-NH2	-6.71	113.17	119.20
3	C	663	VAL	N-CA-C	6.38	119.98	111.17
2	K	285	PRO	N-CA-C	-6.12	102.24	111.41
3	C	1262	PRO	N-CA-C	6.07	118.10	110.70
3	C	720	LYS	N-CA-C	-5.87	101.15	109.96
3	L	829	ARG	NE-CZ-NH2	-5.83	113.96	119.20
2	B	335	ARG	N-CA-C	5.56	117.03	110.97
3	C	839	ARG	CG-CD-NE	-5.44	100.04	112.00
2	B	286	GLU	N-CA-C	-5.33	99.45	110.80

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	11	0
1	J	1255	0	1265	10	0
2	B	2389	0	2459	38	0
2	K	2389	0	2459	39	0
3	C	5832	0	5759	119	1
3	L	5761	0	5685	86	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	3	0
6	C	10	0	4	1	0
6	L	10	0	4	0	0
7	C	28	0	0	2	0
7	L	28	0	0	1	0
8	A	114	0	0	3	1
8	B	114	0	0	12	0
8	C	436	0	0	13	0
8	J	98	0	0	1	0
8	K	75	0	0	5	0
8	L	437	0	0	9	0
All	All	20353	0	18962	291	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 8.

All (291) 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)
3:C:1081:VAL:HG21	8:C:1338:HOH:O	1.25	1.29
3:C:1052:LYS:HE3	8:C:1342:HOH:O	1.23	1.27
3:L:1081:VAL:HG21	8:L:1366:HOH:O	1.11	1.26
3:C:764:VAL:HB	8:C:1472:HOH:O	1.09	1.23
3:L:726:ALA:HA	3:L:851:MET:HE1	1.22	1.19
2:B:241:THR:HB	8:B:558:HOH:O	1.44	1.18
3:C:610:SER:O	3:C:663:VAL:O	1.63	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:779:MET:SD	8:C:445:HOH:O	2.07	1.10
3:L:764:VAL:HB	8:L:1469:HOH:O	0.93	1.09
3:L:598:ARG:NH2	8:L:1437:HOH:O	1.85	1.07
3:C:1046:MET:SD	8:C:1498:HOH:O	2.11	1.06
2:K:243:LYS:H	2:K:243:LYS:HD3	0.95	1.06
3:L:833:MET:SD	8:L:1426:HOH:O	2.11	1.06
1:A:162:THR:HB	8:A:630:HOH:O	1.51	1.05
2:K:243:LYS:HD3	2:K:243:LYS:N	1.70	1.05
3:C:598:ARG:NH2	8:C:1350:HOH:O	1.91	1.04
2:K:243:LYS:H	2:K:243:LYS:CD	1.71	0.99
2:B:286:GLU:N	8:B:641:HOH:O	1.96	0.98
3:C:924:GLU:OE1	3:C:942:ARG:NH1	1.96	0.98
3:L:610:SER:O	3:L:663:VAL:O	1.86	0.93
3:C:725:GLU:HG3	3:C:851:MET:HE1	1.49	0.93
3:L:1046:MET:HE2	3:L:1090:VAL:HG21	1.50	0.93
3:C:1286:THR:HG22	3:C:1310:VAL:O	1.70	0.92
3:L:624:GLU:HB2	3:L:684:VAL:CG1	2.00	0.90
3:C:1046:MET:CE	3:C:1090:VAL:HG21	2.00	0.90
2:K:241:THR:HB	8:K:88:HOH:O	1.69	0.90
3:C:884:HIS:HE1	3:C:1006:GLY:H	1.19	0.90
3:C:1143:GLU:O	3:C:1144:THR:HG23	1.73	0.89
3:C:779:MET:CG	8:C:445:HOH:O	2.20	0.88
3:C:1046:MET:HE2	3:C:1090:VAL:HG21	1.55	0.87
2:K:286:GLU:O	2:K:287:LEU:HB2	1.74	0.87
2:K:241:THR:CG2	2:K:243:LYS:HE2	2.04	0.87
3:L:726:ALA:HA	3:L:851:MET:CE	2.03	0.87
3:C:829:ARG:HG3	3:C:833:MET:HE3	1.57	0.85
3:L:851:MET:HE3	3:L:857:VAL:HG21	1.57	0.84
3:L:1046:MET:HE1	3:L:1087:GLY:HA2	1.59	0.84
3:C:1282:ARG:HA	3:C:1286:THR:HG23	1.57	0.84
3:L:1021:ILE:HD12	3:L:1031:VAL:HG22	1.58	0.83
3:L:1143:GLU:O	3:L:1144:THR:HG23	1.79	0.82
3:C:705:ASN:HB2	8:C:108:HOH:O	1.78	0.82
3:C:851:MET:HE2	3:C:857:VAL:HG21	1.64	0.80
1:A:159:GLY:O	1:A:162:THR:HG22	1.81	0.80
3:L:884:HIS:HE1	3:L:1006:GLY:H	1.29	0.79
3:L:1289:ASN:HB2	3:L:1292:GLU:HB2	1.65	0.79
2:B:338:ALA:C	8:B:1966:HOH:O	2.26	0.79
1:A:131:GLN:HE21	1:A:133:GLU:H	1.29	0.78
3:L:695:ILE:H	3:L:904:ASN:HD22	1.32	0.77
3:C:695:ILE:H	3:C:904:ASN:HD22	1.33	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:1115:ASP:OD1	8:L:1717:HOH:O	2.04	0.76
3:C:995:LYS:NZ	3:C:1284:GLN:HE21	1.85	0.75
3:C:1046:MET:CE	3:C:1090:VAL:CG2	2.63	0.75
2:B:285:PRO:HA	8:B:641:HOH:O	1.86	0.75
3:C:1033:HIS:HD2	3:C:1035:GLY:H	1.35	0.74
2:K:243:LYS:N	2:K:243:LYS:CD	2.41	0.74
3:L:1046:MET:HE2	3:L:1090:VAL:CG2	2.16	0.74
3:C:624:GLU:HB2	3:C:684:VAL:HG12	1.70	0.73
2:K:439:ARG:NH2	2:K:451:GLU:OE1	2.21	0.73
3:L:764:VAL:HG23	3:L:766:THR:HG22	1.69	0.73
3:L:1088:GLN:HG2	3:L:1133:TYR:CD1	2.24	0.72
2:K:241:THR:HG22	8:K:169:HOH:O	1.89	0.72
3:L:829:ARG:HG3	3:L:833:MET:HE3	1.72	0.71
1:A:32:ARG:NE	8:A:1088:HOH:O	2.05	0.71
3:C:1046:MET:HE2	3:C:1090:VAL:CG2	2.19	0.71
2:K:241:THR:HG21	2:K:243:LYS:HE2	1.72	0.70
3:C:884:HIS:CE1	3:C:1006:GLY:H	2.06	0.70
2:K:509:ARG:HG2	8:K:1267:HOH:O	1.93	0.69
3:L:851:MET:HE3	3:L:857:VAL:CG2	2.22	0.68
3:L:752:ILE:CD1	3:L:763:PHE:HE1	2.07	0.68
3:L:884:HIS:CE1	3:L:1006:GLY:H	2.09	0.67
3:C:764:VAL:HG23	3:C:766:THR:HG22	1.77	0.67
2:B:509:ARG:HG2	8:B:35:HOH:O	1.94	0.67
2:B:241:THR:CB	8:B:558:HOH:O	2.17	0.67
3:L:726:ALA:CA	3:L:851:MET:HE1	2.15	0.66
2:K:504:MET:HE2	3:L:1303:GLU:HB2	1.77	0.66
2:K:241:THR:HG22	2:K:243:LYS:HE2	1.78	0.66
3:C:829:ARG:CG	3:C:833:MET:HE3	2.26	0.66
3:C:845:ARG:NH1	8:C:1508:HOH:O	2.26	0.66
3:L:571:ASP:N	8:L:434:HOH:O	2.28	0.65
2:B:284:ILE:HG22	2:B:285:PRO:O	1.97	0.65
3:C:1287:ASN:HD22	3:C:1289:ASN:H	1.44	0.64
3:L:840:HIS:HE1	3:L:874:SER:OG	1.80	0.63
3:C:779:MET:HG2	8:C:445:HOH:O	1.89	0.63
3:C:840:HIS:HE1	3:C:874:SER:OG	1.81	0.63
3:L:939:GLU:HG2	3:L:977:TYR:CE2	2.34	0.63
2:B:339:GLY:N	8:B:1966:HOH:O	2.32	0.62
3:C:720:LYS:O	3:C:721:LYS:CB	2.47	0.62
3:C:640:ILE:HG12	3:C:779:MET:HE1	1.82	0.61
2:B:318:LYS:HD3	2:B:318:LYS:N	2.15	0.61
3:C:1048:GLN:HE22	3:C:1187:ASN:HD22	1.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:1046:MET:HE3	3:L:1046:MET:HA	1.81	0.61
2:B:286:GLU:O	2:B:287:LEU:HB2	1.99	0.61
7:C:1327:ZXF:O2	7:C:1327:ZXF:MO	1.72	0.60
7:L:1327:ZXF:O2	7:L:1327:ZXF:MO	1.72	0.60
1:A:32:ARG:NH1	3:C:676:GLU:OE2	2.33	0.60
3:C:1033:HIS:CD2	3:C:1035:GLY:H	2.19	0.60
3:C:782:VAL:CG1	3:C:786:ARG:HG3	2.32	0.60
1:J:32:ARG:NH1	3:L:676:GLU:OE2	2.33	0.60
2:B:285:PRO:C	2:B:286:GLU:O	2.42	0.60
3:L:995:LYS:NZ	3:L:1284:GLN:HE21	2.00	0.60
1:J:42:GLY:O	3:L:829:ARG:HD2	2.02	0.59
3:C:880:ARG:O	3:C:884:HIS:HD2	1.86	0.59
2:B:339:GLY:CA	8:B:1966:HOH:O	2.50	0.59
3:C:1249:ASN:O	3:C:1255:ALA:HA	2.03	0.58
6:C:1:HPA:H8	7:C:1327:ZXF:O1	2.02	0.58
3:L:1095:GLN:O	3:L:1099:LYS:HG2	2.03	0.58
3:C:1088:GLN:HG2	3:C:1133:TYR:CD1	2.38	0.58
3:C:1286:THR:O	3:C:1326:LYS:HD3	2.04	0.58
2:K:232:GLU:OE2	3:L:629:PRO:HG2	2.04	0.58
3:C:995:LYS:HZ1	3:C:1284:GLN:HE21	1.52	0.57
3:C:939:GLU:HG2	3:C:977:TYR:CE2	2.39	0.57
3:C:932:VAL:HG13	3:C:1279:ARG:HH21	1.68	0.57
3:L:1033:HIS:HD2	3:L:1035:GLY:H	1.52	0.57
2:K:285:PRO:O	2:K:286:GLU:HB2	2.04	0.56
1:A:42:GLY:O	3:C:829:ARG:HD2	2.06	0.55
2:K:285:PRO:O	2:K:286:GLU:CB	2.54	0.55
3:C:742:PHE:CE1	3:C:833:MET:CE	2.89	0.55
3:C:609:THR:HG23	3:C:664:GLY:HA2	1.87	0.55
3:C:713:LYS:HD2	3:C:895:ARG:NH1	2.22	0.55
3:L:764:VAL:CG2	3:L:766:THR:HG22	2.36	0.55
3:C:673:ASP:OD2	3:C:677:HIS:HD2	1.90	0.55
2:B:285:PRO:CA	8:B:641:HOH:O	2.50	0.55
2:K:509:ARG:HD2	8:K:1767:HOH:O	2.06	0.55
2:K:286:GLU:O	2:K:287:LEU:CB	2.47	0.55
3:C:782:VAL:HG12	3:C:783:PRO:HD2	1.87	0.54
3:C:695:ILE:HG23	3:C:700:ASP:HB3	1.88	0.54
3:L:624:GLU:HB2	3:L:684:VAL:HG12	1.88	0.54
3:C:624:GLU:HG3	3:C:686:LYS:NZ	2.23	0.54
3:L:1203:LEU:HD12	3:L:1203:LEU:C	2.33	0.54
3:C:782:VAL:HG12	3:C:786:ARG:HG3	1.89	0.53
1:J:36:LEU:HD22	1:J:89:GLU:HG3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:285:PRO:O	2:K:286:GLU:OE1	2.26	0.53
3:L:1134:ARG:NE	8:L:1420:HOH:O	2.41	0.53
2:B:495:SER:HB2	2:B:509:ARG:HH22	1.72	0.53
2:B:234:VAL:HG11	2:B:278:ILE:HD12	1.89	0.53
2:K:250:ALA:HA	2:K:401:GLU:HG2	1.90	0.53
3:L:670:VAL:HG11	3:L:681:ALA:HB3	1.90	0.53
3:C:1317:CYS:SG	3:C:1323:GLY:HA3	2.50	0.52
3:L:624:GLU:CB	3:L:684:VAL:CG1	2.84	0.52
3:C:764:VAL:CG2	3:C:766:THR:HG22	2.37	0.52
3:C:624:GLU:HB2	3:C:684:VAL:CG1	2.38	0.52
3:C:779:MET:HG2	3:C:810:VAL:HG13	1.92	0.52
3:C:1095:GLN:O	3:C:1099:LYS:HG2	2.08	0.52
3:L:829:ARG:CG	3:L:833:MET:HE3	2.38	0.52
3:C:1048:GLN:NE2	3:C:1187:ASN:HD22	2.08	0.52
3:C:712:LEU:HD21	3:C:875:HIS:CE1	2.45	0.52
1:J:159:GLY:O	1:J:162:THR:HG22	2.10	0.52
1:J:131:GLN:HE21	1:J:133:GLU:H	1.56	0.52
3:C:983:GLU:HG2	8:C:1917:HOH:O	2.09	0.52
3:C:742:PHE:CE1	3:C:833:MET:HE1	2.46	0.51
3:C:609:THR:HG22	8:C:1982:HOH:O	2.10	0.51
3:C:848:VAL:HG21	3:C:926:TRP:HB2	1.91	0.51
2:B:363:PRO:HG2	2:B:435:THR:HG23	1.93	0.51
3:C:995:LYS:HZ3	3:C:1284:GLN:HE21	1.57	0.51
3:L:752:ILE:HD12	3:L:763:PHE:HE1	1.75	0.51
2:B:447:MET:HG2	2:B:527:LEU:HD13	1.92	0.51
3:C:752:ILE:CD1	3:C:763:PHE:HE1	2.24	0.51
3:L:612:ARG:NH1	3:L:691:ASP:OD1	2.40	0.51
3:C:851:MET:CE	3:C:857:VAL:HG21	2.38	0.51
3:L:601:ASN:O	3:L:821:HIS:HD2	1.93	0.50
3:C:617:ILE:HD11	3:C:660:VAL:HG13	1.92	0.50
3:L:829:ARG:HG3	3:L:833:MET:CE	2.40	0.50
2:B:285:PRO:C	8:B:641:HOH:O	2.46	0.50
3:C:601:ASN:O	3:C:821:HIS:HD2	1.95	0.50
3:C:719:LEU:HD11	3:C:895:ARG:HB3	1.94	0.50
3:C:742:PHE:HE1	3:C:833:MET:HE1	1.76	0.49
3:L:853:THR:HG22	3:L:944:LYS:NZ	2.27	0.49
3:L:880:ARG:O	3:L:884:HIS:HD2	1.94	0.49
1:A:131:GLN:NE2	1:A:133:GLU:H	2.06	0.49
3:C:616:LYS:HD2	3:C:658:ASP:O	2.13	0.49
3:C:924:GLU:OE1	3:C:942:ARG:CZ	2.57	0.49
3:C:614:HIS:HD2	3:C:693:PRO:O	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:718:ASP:OD1	3:C:720:LYS:O	2.31	0.49
2:K:504:MET:CE	3:L:1303:GLU:HB2	2.41	0.49
3:C:645:GLU:OE2	3:C:650:ASN:HB3	2.13	0.49
3:L:655:PHE:HE1	3:L:814:LEU:HD23	1.78	0.49
3:L:1249:ASN:O	3:L:1255:ALA:HA	2.13	0.49
2:B:245:LEU:HD11	2:B:257:LEU:HD21	1.94	0.49
2:B:439:ARG:NH2	2:B:451:GLU:OE1	2.46	0.48
2:K:284:ILE:HG22	2:K:285:PRO:O	2.13	0.48
3:L:1048:GLN:HE22	3:L:1187:ASN:HD22	1.58	0.48
3:C:742:PHE:CE1	3:C:833:MET:HE2	2.48	0.48
3:C:1020:LEU:C	3:C:1021:ILE:HD13	2.38	0.48
3:C:1088:GLN:HG2	3:C:1133:TYR:CE1	2.49	0.48
3:L:995:LYS:HZ1	3:L:1284:GLN:HE21	1.60	0.48
2:B:232:GLU:OE2	3:C:680:ARG:NH1	2.47	0.48
1:J:97:ARG:HG2	1:J:97:ARG:HH11	1.78	0.48
3:L:764:VAL:HG23	3:L:791:VAL:HG22	1.96	0.48
3:L:609:THR:HG22	8:L:60:HOH:O	2.13	0.47
3:L:684:VAL:CG1	3:L:684:VAL:O	2.62	0.47
3:L:833:MET:HE1	3:L:1223:GLY:HA2	1.95	0.47
3:C:734:LEU:HD21	3:C:921:PHE:CE2	2.48	0.47
3:L:1183:GLY:HA2	3:L:1247:CYS:O	2.15	0.47
2:B:427:ARG:HD2	8:B:531:HOH:O	2.13	0.47
3:C:764:VAL:HG23	3:C:791:VAL:HG22	1.95	0.47
2:K:447:MET:HG2	2:K:527:LEU:HD13	1.97	0.47
3:C:747:HIS:HD2	3:C:832:ASP:OD1	1.98	0.47
3:C:1209:GLU:O	3:C:1299:PRO:HG3	2.15	0.47
2:K:423:GLN:HB3	2:K:433:LYS:HG2	1.97	0.47
2:K:459:MET:HE2	2:K:512:THR:HG21	1.97	0.47
3:C:670:VAL:HG11	3:C:681:ALA:HB3	1.97	0.46
2:K:241:THR:CB	8:K:88:HOH:O	2.42	0.46
3:C:598:ARG:HD3	3:L:600:GLU:OE2	2.16	0.46
1:A:154:ARG:NE	3:C:1196:GLU:OE2	2.46	0.46
3:C:1134:ARG:NH1	3:L:1123:ASP:O	2.48	0.46
1:J:45:GLU:CD	3:L:1224:PRO:HD2	2.40	0.46
3:L:624:GLU:HB2	3:L:684:VAL:HG11	1.94	0.46
1:A:104:ARG:HE	1:A:162:THR:HG21	1.81	0.46
3:C:995:LYS:NZ	3:C:1284:GLN:NE2	2.59	0.46
3:C:939:GLU:H	3:C:939:GLU:CD	2.23	0.45
3:C:1183:GLY:HA2	3:C:1247:CYS:O	2.17	0.45
3:C:1021:ILE:HG12	3:C:1093:ALA:CB	2.47	0.45
3:L:752:ILE:CD1	3:L:763:PHE:CE1	2.95	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:32:ARG:NH1	8:J:315:HOH:O	2.39	0.45
3:L:624:GLU:HB2	3:L:684:VAL:HG13	1.92	0.45
3:L:1088:GLN:HG2	3:L:1133:TYR:CE1	2.52	0.45
3:C:844:ALA:HB2	3:C:922:ILE:HD13	1.98	0.45
3:L:889:TYR:OH	3:L:942:ARG:HD3	2.17	0.45
2:B:285:PRO:O	2:B:286:GLU:HB2	2.17	0.44
2:K:415:ASP:OD2	2:K:444:PRO:HA	2.18	0.44
2:B:264:ILE:O	2:B:268:MET:HG3	2.17	0.44
3:C:1048:GLN:HE22	3:C:1187:ASN:HB2	1.82	0.44
3:L:609:THR:CG2	8:L:60:HOH:O	2.64	0.44
3:L:673:ASP:OD2	3:L:677:HIS:HD2	2.00	0.44
3:L:911:PHE:O	3:L:912:ARG:C	2.59	0.44
3:L:684:VAL:HG12	3:L:684:VAL:O	2.16	0.44
3:L:747:HIS:HD2	3:L:832:ASP:OD1	2.01	0.44
2:K:269:LYS:HG2	2:K:270:PHE:CE1	2.52	0.44
3:C:695:ILE:H	3:C:904:ASN:ND2	2.10	0.44
3:C:624:GLU:HB3	3:C:684:VAL:HG11	2.00	0.44
2:B:285:PRO:O	2:B:286:GLU:CB	2.65	0.43
3:C:680:ARG:O	3:C:684:VAL:HG23	2.18	0.43
3:C:1261:GLU:N	3:C:1262:PRO:CD	2.81	0.43
2:K:346:ALA:HB1	5:K:606:FAD:H4'	2.00	0.43
2:B:390:PHE:O	2:B:462:ARG:HD2	2.17	0.43
2:K:257:LEU:O	5:K:606:FAD:H2B	2.19	0.43
3:L:752:ILE:HD12	3:L:763:PHE:CE1	2.53	0.43
2:B:232:GLU:HG2	2:B:233:ARG:HG3	2.00	0.43
3:L:850:PHE:C	3:L:851:MET:HE2	2.44	0.43
2:B:286:GLU:C	2:B:288:ASN:H	2.27	0.43
2:B:448:GLN:HE21	2:B:475:SER:HB2	1.84	0.43
3:C:764:VAL:HG21	3:C:789:VAL:CG1	2.49	0.43
3:C:782:VAL:CG1	3:C:783:PRO:HD2	2.48	0.43
3:C:1033:HIS:HD2	3:C:1035:GLY:N	2.10	0.43
2:K:263:GLU:HB3	5:K:606:FAD:H52A	2.01	0.43
3:L:1033:HIS:CD2	3:L:1035:GLY:H	2.34	0.43
2:B:269:LYS:HG2	2:B:270:PHE:CE1	2.54	0.43
2:B:472:LYS:O	2:B:472:LYS:HG3	2.12	0.43
2:K:367:ALA:O	2:K:439:ARG:HD3	2.19	0.43
3:L:880:ARG:HD2	3:L:914:PHE:HB3	2.01	0.43
2:B:322:GLN:O	2:B:412:SER:HB3	2.19	0.42
3:C:655:PHE:HE1	3:C:814:LEU:CD2	2.32	0.42
2:K:318:LYS:HD3	2:K:318:LYS:N	2.34	0.42
2:K:441:LEU:HB3	2:K:451:GLU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:624:GLU:HG3	3:C:686:LYS:HZ1	1.83	0.42
3:C:1021:ILE:HG12	3:C:1093:ALA:HB1	2.01	0.42
2:B:317:ALA:C	2:B:318:LYS:HD3	2.44	0.42
3:C:1021:ILE:HD12	3:C:1031:VAL:HG13	2.01	0.42
3:C:624:GLU:CB	3:C:684:VAL:CG1	2.96	0.42
2:B:496:LEU:H	2:B:509:ARG:NH2	2.17	0.42
3:C:1203:LEU:HD13	3:C:1270:VAL:HG21	2.01	0.42
3:L:670:VAL:HG11	3:L:681:ALA:CB	2.50	0.42
3:L:655:PHE:CE1	3:L:814:LEU:HD23	2.54	0.42
1:A:58:TYR:CE1	1:A:63:ASP:O	2.73	0.42
3:C:1123:ASP:O	3:L:1134:ARG:CZ	2.68	0.42
2:K:507:PHE:CZ	2:K:511:LEU:HD11	2.55	0.42
3:L:840:HIS:CE1	3:L:874:SER:OG	2.67	0.42
3:C:720:LYS:O	3:C:721:LYS:HB3	2.19	0.41
3:C:940:GLU:O	3:C:944:LYS:HG3	2.20	0.41
1:J:124:MET:HE2	1:J:163:PHE:CD1	2.54	0.41
3:L:1048:GLN:HE22	3:L:1187:ASN:HB2	1.85	0.41
2:K:241:THR:HG22	2:K:243:LYS:CE	2.49	0.41
2:K:281:PRO:HB2	2:K:287:LEU:CD1	2.50	0.41
2:B:387:HIS:CE1	2:B:467:LEU:HD11	2.56	0.41
2:B:426:ARG:NH2	2:B:429:ASP:O	2.53	0.41
3:C:911:PHE:O	3:C:912:ARG:C	2.64	0.41
2:K:232:GLU:OE1	3:L:677:HIS:HE1	2.02	0.41
3:C:752:ILE:HD11	3:C:763:PHE:HE1	1.85	0.41
3:L:885:MET:SD	3:L:896:GLY:HA3	2.60	0.41
2:B:284:ILE:O	2:B:286:GLU:O	2.37	0.41
3:C:601:ASN:HB2	3:C:821:HIS:CD2	2.56	0.41
3:C:995:LYS:HZ1	3:C:1284:GLN:NE2	2.16	0.41
1:J:74:LEU:O	1:J:76:PRO:HD3	2.21	0.41
3:L:995:LYS:NZ	3:L:1284:GLN:NE2	2.67	0.41
1:A:32:ARG:NH2	8:A:1088:HOH:O	2.54	0.40
2:B:375:VAL:HG13	8:B:560:HOH:O	2.21	0.40
2:K:234:VAL:HG11	2:K:278:ILE:HD12	2.03	0.40
3:C:600:GLU:HG2	3:L:598:ARG:O	2.22	0.40
3:C:720:LYS:O	3:C:721:LYS:HB2	2.20	0.40
3:L:1048:GLN:NE2	3:L:1187:ASN:HD22	2.18	0.40
3:C:804:ARG:HG3	3:C:836:THR:O	2.21	0.40
3:C:1134:ARG:NH1	8:C:1926:HOH:O	2.53	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:871:ARG:NH1	8:A:173:HOH:O[1_565]	2.17	0.03

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%)	155 (96%)	6 (4%)	1 (1%)	21	11
1	J	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
2	B	303/305 (99%)	291 (96%)	12 (4%)	0	100	100
2	K	303/305 (99%)	292 (96%)	10 (3%)	1 (0%)	36	25
3	C	754/756 (100%)	733 (97%)	15 (2%)	6 (1%)	16	6
3	L	743/756 (98%)	724 (97%)	13 (2%)	6 (1%)	16	6
All	All	2427/2450 (99%)	2349 (97%)	64 (3%)	14 (1%)	21	11

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	721	LYS
3	C	1008	SER
3	C	1144	THR
3	L	721	LYS
3	L	1008	SER
3	L	1144	THR
3	L	912	ARG
1	A	64	LYS
3	C	912	ARG
2	K	286	GLU
3	L	1139	GLY
3	L	797	GLY
3	C	797	GLY
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%)	133 (97%)	4 (3%)	37	25
1	J	137/137 (100%)	135 (98%)	2 (2%)	57	49
2	B	261/261 (100%)	250 (96%)	11 (4%)	26	14
2	K	261/261 (100%)	249 (95%)	12 (5%)	24	12
3	C	632/632 (100%)	619 (98%)	13 (2%)	47	36
3	L	624/632 (99%)	614 (98%)	10 (2%)	55	47
All	All	2052/2060 (100%)	2000 (98%)	52 (2%)	42	30

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	LEU
1	A	63	ASP
1	A	64	LYS
1	A	133	GLU
2	B	232	GLU
2	B	241	THR
2	B	256	LYS
2	B	277	MET
2	B	286	GLU
2	B	312	LEU
2	B	318	LYS
2	B	328	ARG
2	B	348	LEU
2	B	427	ARG
2	B	472	LYS
3	C	598	ARG
3	C	609	THR
3	C	636	SER
3	C	686	LYS
3	C	743	TYR
3	C	779	MET
3	C	848	VAL

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Mol	Chain	Res	Type
3	C	939	GLU
3	C	1021	ILE
3	C	1123	ASP
3	C	1208	LEU
3	C	1286	THR
3	C	1290	THR
1	J	89	GLU
1	J	93	SER
2	K	241	THR
2	K	243	LYS
2	K	286	GLU
2	K	312	LEU
2	K	318	LYS
2	K	328	ARG
2	K	335	ARG
2	K	348	LEU
2	K	375	VAL
2	K	398	LEU
2	K	428	GLU
2	K	433	LYS
3	L	598	ARG
3	L	609	THR
3	L	705	ASN
3	L	710	SER
3	L	743	TYR
3	L	853	THR
3	L	939	GLU
3	L	1001	ILE
3	L	1203	LEU
3	L	1290	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	144	GLN
1	A	146	ASN
2	B	226	GLN
2	B	261	ASN
2	B	351	ASN
2	B	448	GLN
2	B	471	GLN

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Mol	Chain	Res	Type
2	B	473	GLN
3	C	585	GLN
3	C	614	HIS
3	C	626	GLN
3	C	677	HIS
3	C	705	ASN
3	C	821	HIS
3	C	840	HIS
3	C	884	HIS
3	C	904	ASN
3	C	1033	HIS
3	C	1048	GLN
3	C	1212	HIS
3	C	1220	HIS
3	C	1284	GLN
3	C	1287	ASN
3	C	1307	ASN
1	J	71	ASN
1	J	131	GLN
1	J	144	GLN
1	J	146	ASN
2	K	226	GLN
2	K	261	ASN
2	K	333	GLN
2	K	351	ASN
2	K	473	GLN
3	L	585	GLN
3	L	614	HIS
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	1033	HIS
3	L	1048	GLN
3	L	1088	GLN
3	L	1173	ASN
3	L	1212	HIS
3	L	1220	HIS
3	L	1284	GLN
3	L	1288	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
5	FAD	B	606	-	58,58,58	1.10	5 (8%)	85,89,89	1.62	14 (16%)
6	HPA	L	1	-	10,11,11	1.79	2 (20%)	11,15,15	2.10	5 (45%)
4	FES	A	602	1	0,4,4	-	-	-	-	-
4	FES	J	601	1	0,4,4	-	-	-	-	-
7	ZXF	C	1327	-	24,31,31	1.49	3 (12%)	22,52,52	2.00	10 (45%)
7	ZXF	L	1327	-	24,31,31	1.92	3 (12%)	22,52,52	2.51	9 (40%)
4	FES	A	601	1	0,4,4	-	-	-	-	-
6	HPA	C	1	-	10,11,11	2.21	3 (30%)	11,15,15	2.64	6 (54%)
4	FES	J	602	1	0,4,4	-	-	-	-	-
5	FAD	K	606	-	58,58,58	1.14	5 (8%)	85,89,89	1.62	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
5	FAD	B	606	-	-	1/34/50/50	0/6/6/6
6	HPA	L	1	-	-	-	0/2/2/2
4	FES	A	602	1	-	-	0/1/1/1
7	ZXF	C	1327	-	-	2/6/46/46	0/4/4/4
4	FES	J	601	1	-	-	0/1/1/1
7	ZXF	L	1327	-	-	3/6/46/46	0/4/4/4
4	FES	A	601	1	-	-	0/1/1/1
6	HPA	C	1	-	-	-	0/2/2/2
4	FES	J	602	1	-	-	0/1/1/1
5	FAD	K	606	-	-	0/34/50/50	0/6/6/6

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	1327	ZXF	C9-C10	5.79	1.48	1.38
7	L	1327	ZXF	MO-S2'	5.60	2.47	2.39
7	C	1327	ZXF	C9-C10	5.41	1.47	1.38
6	C	1	HPA	C2-N3	4.22	1.37	1.30
6	C	1	HPA	C8-N7	-4.08	1.28	1.35
5	K	606	FAD	C4X-N5	3.95	1.39	1.30
5	B	606	FAD	C4X-N5	3.77	1.38	1.30
6	L	1	HPA	C8-N7	-3.23	1.29	1.35
6	L	1	HPA	C2-N3	3.19	1.36	1.30
5	B	606	FAD	C10-N1	3.11	1.39	1.33
5	K	606	FAD	C2A-N3A	3.02	1.39	1.33
5	B	606	FAD	C2A-N3A	2.94	1.39	1.33
5	K	606	FAD	C2A-N1A	2.93	1.39	1.33
5	K	606	FAD	C10-N1	2.84	1.39	1.33
5	B	606	FAD	C2A-N1A	2.73	1.38	1.33
5	K	606	FAD	C8A-N7A	2.58	1.36	1.31
7	C	1327	ZXF	C9-C4	2.51	1.49	1.41
5	B	606	FAD	P-O3P	2.31	1.62	1.59
7	C	1327	ZXF	C4-N3	-2.30	1.34	1.38
7	L	1327	ZXF	C9-C4	2.28	1.48	1.41
6	C	1	HPA	C5-C6	-2.04	1.35	1.41

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	606	FAD	N3A-C2A-N1A	-6.09	119.36	128.58
5	K	606	FAD	N3A-C2A-N1A	-6.09	119.37	128.58
7	L	1327	ZXF	C1'-C2'-S2'	5.76	123.42	120.15
6	C	1	HPA	O6-C6-C5	-4.90	115.44	127.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	1327	ZXF	C2-N1-C10	4.49	121.28	113.36
5	K	606	FAD	C5A-C4A-N3A	-4.22	120.90	126.72
7	L	1327	ZXF	C2'-C1'-S1'	4.20	122.53	120.15
7	C	1327	ZXF	C2-N1-C10	4.11	120.61	113.36
5	B	606	FAD	C5A-C4A-N3A	-4.09	121.09	126.72
5	K	606	FAD	N9A-C8A-N7A	-4.06	108.18	113.94
5	B	606	FAD	N9A-C8A-N7A	-3.81	108.53	113.94
6	C	1	HPA	C2-N1-C6	-3.55	120.23	125.09
5	B	606	FAD	C5A-N7A-C8A	3.52	108.99	103.45
5	K	606	FAD	C2A-N3A-C4A	3.48	120.33	111.83
6	C	1	HPA	O6-C6-N1	3.46	127.38	120.75
7	C	1327	ZXF	O2P-P-O4'	-3.37	97.88	106.67
5	B	606	FAD	C2A-N3A-C4A	3.32	119.94	111.83
5	K	606	FAD	C5A-N7A-C8A	3.30	108.64	103.45
7	L	1327	ZXF	O2P-P-O4'	-3.30	98.07	106.67
7	L	1327	ZXF	C4-C9-N5	3.16	124.89	116.27
6	C	1	HPA	C5-C6-N1	3.16	117.18	110.26
6	L	1	HPA	O6-C6-C5	-3.15	119.65	127.26
5	B	606	FAD	C4-N3-C2	-3.12	120.10	125.64
6	L	1	HPA	N1-C2-N3	-3.09	121.94	125.50
7	C	1327	ZXF	O4-C4-C9	-3.07	119.86	127.26
6	L	1	HPA	C5-C6-N1	3.04	116.92	110.26
6	L	1	HPA	C2-N1-C6	-3.02	120.95	125.09
7	L	1327	ZXF	O4-C4-C9	-2.98	120.08	127.26
6	C	1	HPA	C8-N9-C4	2.93	107.94	102.89
7	L	1327	ZXF	O3'-C3'-C2'	2.92	113.21	109.09
5	K	606	FAD	N3A-C4A-N9A	2.87	132.06	127.17
7	C	1327	ZXF	O1P-P-O2P	2.85	118.50	107.80
5	B	606	FAD	N3A-C4A-N9A	2.80	131.92	127.17
5	K	606	FAD	C4-N3-C2	-2.78	120.71	125.64
5	K	606	FAD	C4X-C4-N3	2.74	120.22	113.25
7	L	1327	ZXF	C9-C4-N3	2.69	119.51	112.13
7	C	1327	ZXF	C7-C6-N5	2.69	110.50	107.87
5	B	606	FAD	C4X-C4-N3	2.65	120.01	113.25
5	K	606	FAD	C4-C4X-N5	2.54	121.72	118.21
5	B	606	FAD	C4A-C5A-N7A	-2.53	107.69	110.58
5	K	606	FAD	C4X-C10-N10	2.52	120.09	116.48
5	K	606	FAD	C5'-C4'-C3'	-2.51	107.49	112.22
5	K	606	FAD	C10-C4X-N5	-2.50	119.70	124.81
5	B	606	FAD	C9A-C5X-N5	-2.48	119.83	122.45
5	B	606	FAD	C10-C4X-N5	-2.47	119.76	124.81
7	C	1327	ZXF	O1P-P-O4'	-2.45	100.27	106.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	1327	ZXF	O3'-C3'-C2'	2.41	112.49	109.09
5	B	606	FAD	C4X-C10-N10	2.40	119.91	116.48
5	B	606	FAD	O2A-PA-O3P	2.35	113.63	107.27
5	K	606	FAD	C9A-C5X-N5	-2.35	119.96	122.45
5	B	606	FAD	C4X-C10-N1	-2.26	119.04	124.59
5	K	606	FAD	C4A-N9A-C8A	2.25	108.10	105.74
7	C	1327	ZXF	C9-C4-N3	2.24	118.27	112.13
5	K	606	FAD	C4A-C5A-N7A	-2.23	108.03	110.58
5	K	606	FAD	O3'-C3'-C2'	-2.22	103.88	108.93
7	C	1327	ZXF	C4-C9-N5	2.22	122.32	116.27
6	L	1	HPA	C8-N9-C4	2.21	106.70	102.89
6	C	1	HPA	N1-C2-N3	-2.21	122.96	125.50
5	K	606	FAD	O2A-PA-O3P	2.20	113.21	107.27
7	L	1327	ZXF	O1P-P-O2P	2.19	116.01	107.80
5	K	606	FAD	C1'-C2'-C3'	-2.14	103.86	109.66
5	K	606	FAD	O4-C4-C4X	-2.05	121.12	126.53
7	C	1327	ZXF	C2'-C1'-S1'	2.01	121.29	120.15

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	1327	ZXF	C4'-O4'-P-O1P
7	L	1327	ZXF	C4'-O4'-P-O1P
7	L	1327	ZXF	C4'-O4'-P-O2P
7	C	1327	ZXF	C3'-C4'-O4'-P
5	B	606	FAD	C5B-O5B-PA-O1A
7	L	1327	ZXF	C3'-C4'-O4'-P

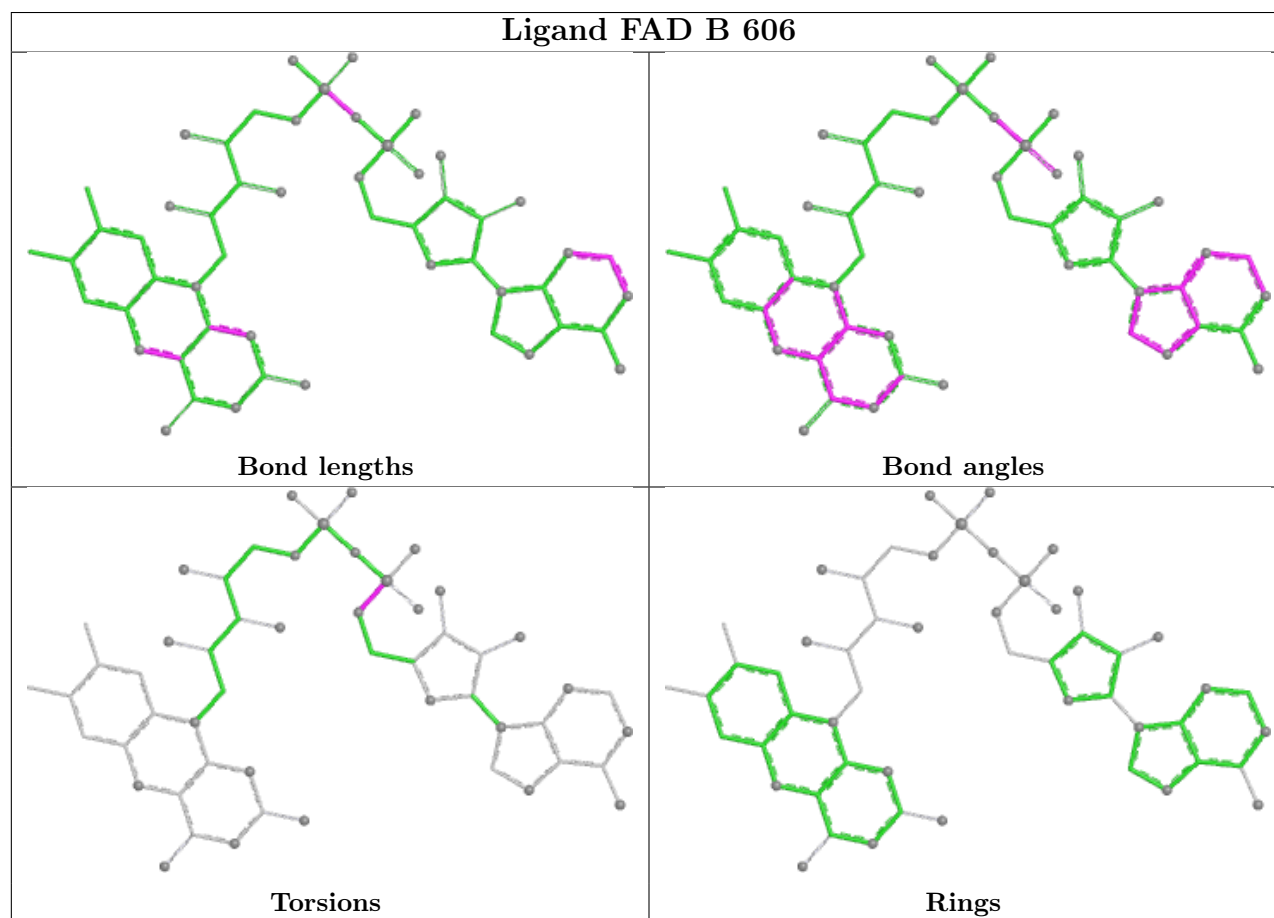
There are no ring outliers.

4 monomers are involved in 6 short contacts:

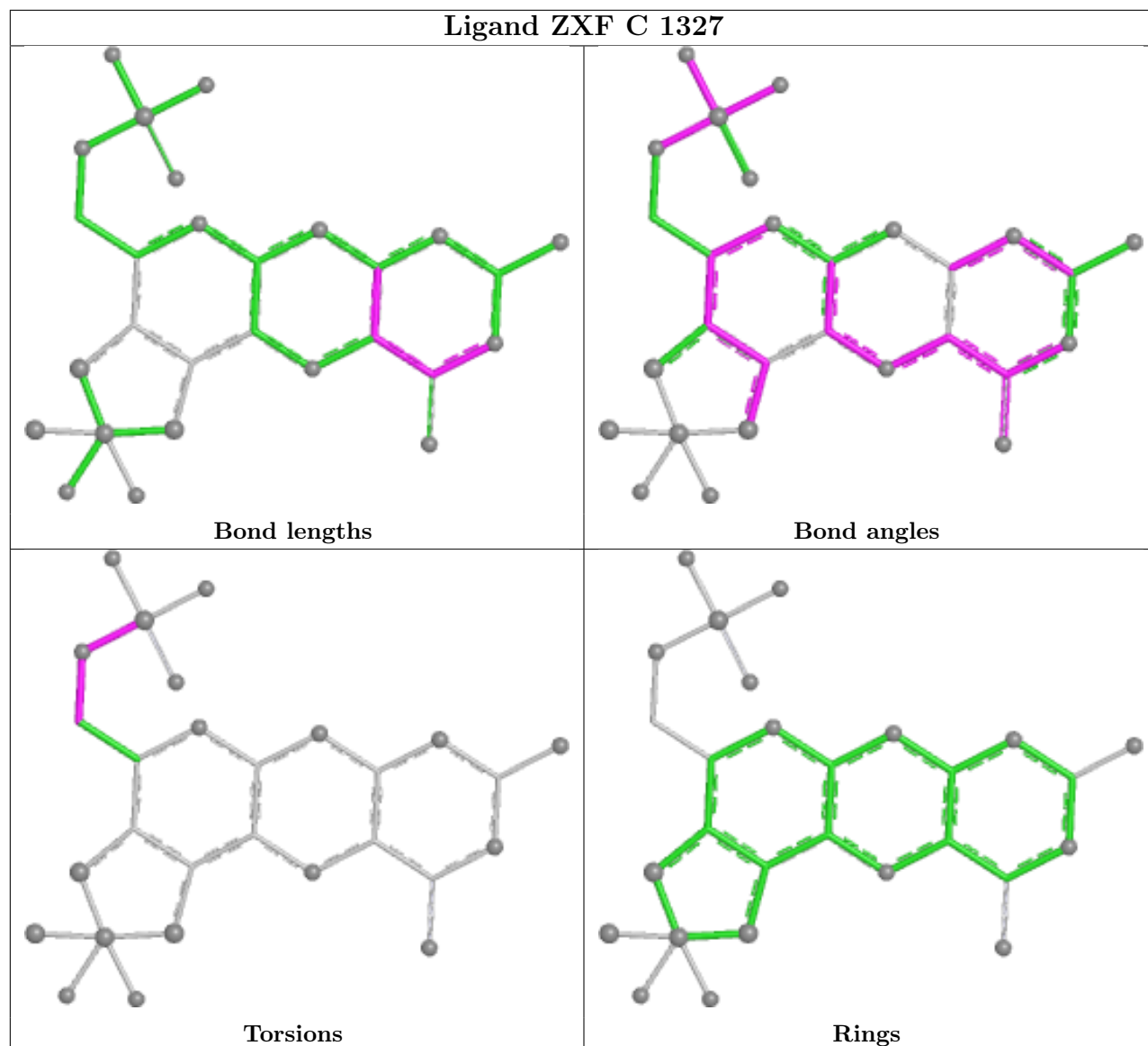
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	1327	ZXF	2	0
7	L	1327	ZXF	1	0
6	C	1	HPA	1	0
5	K	606	FAD	3	0

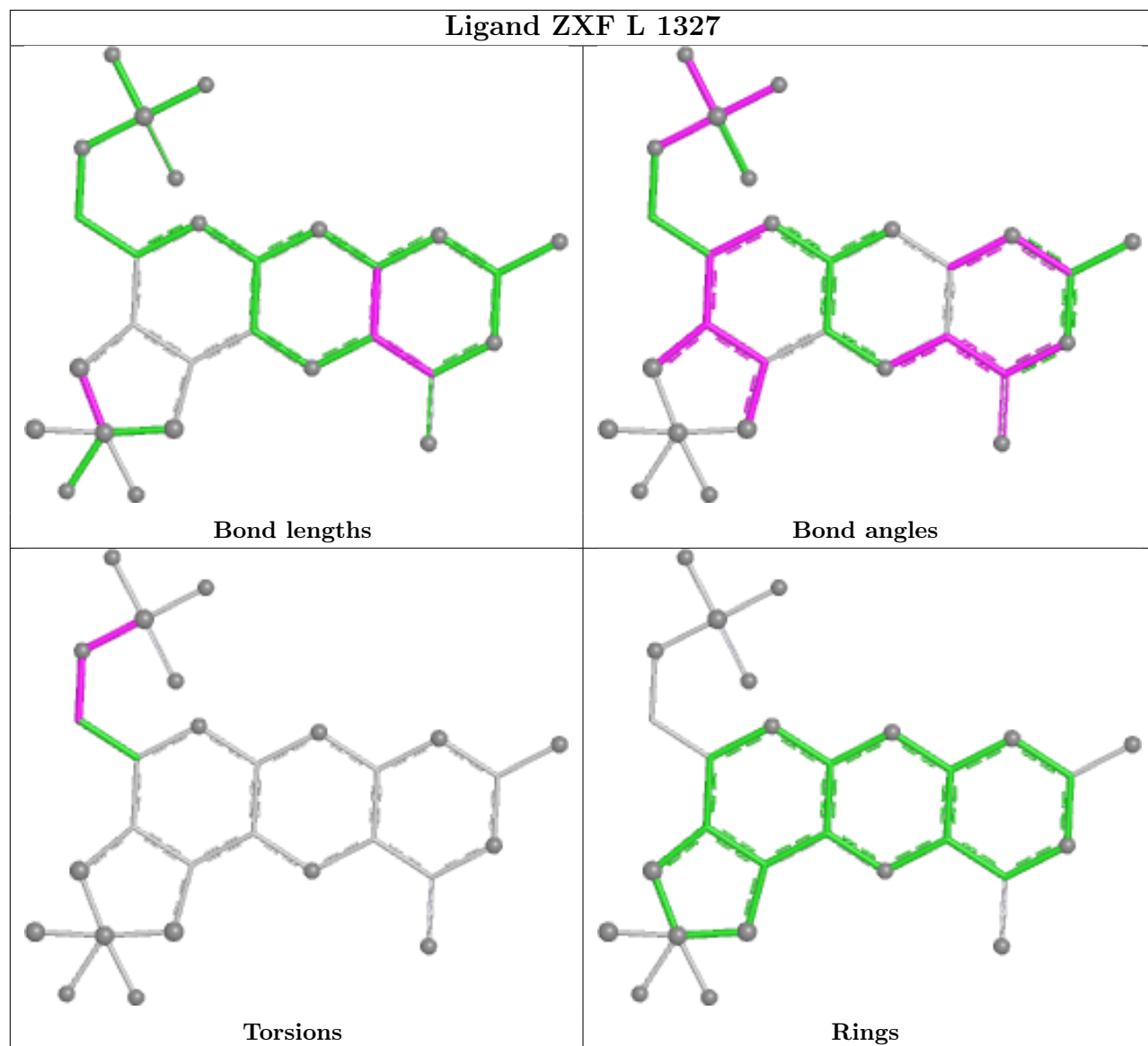
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

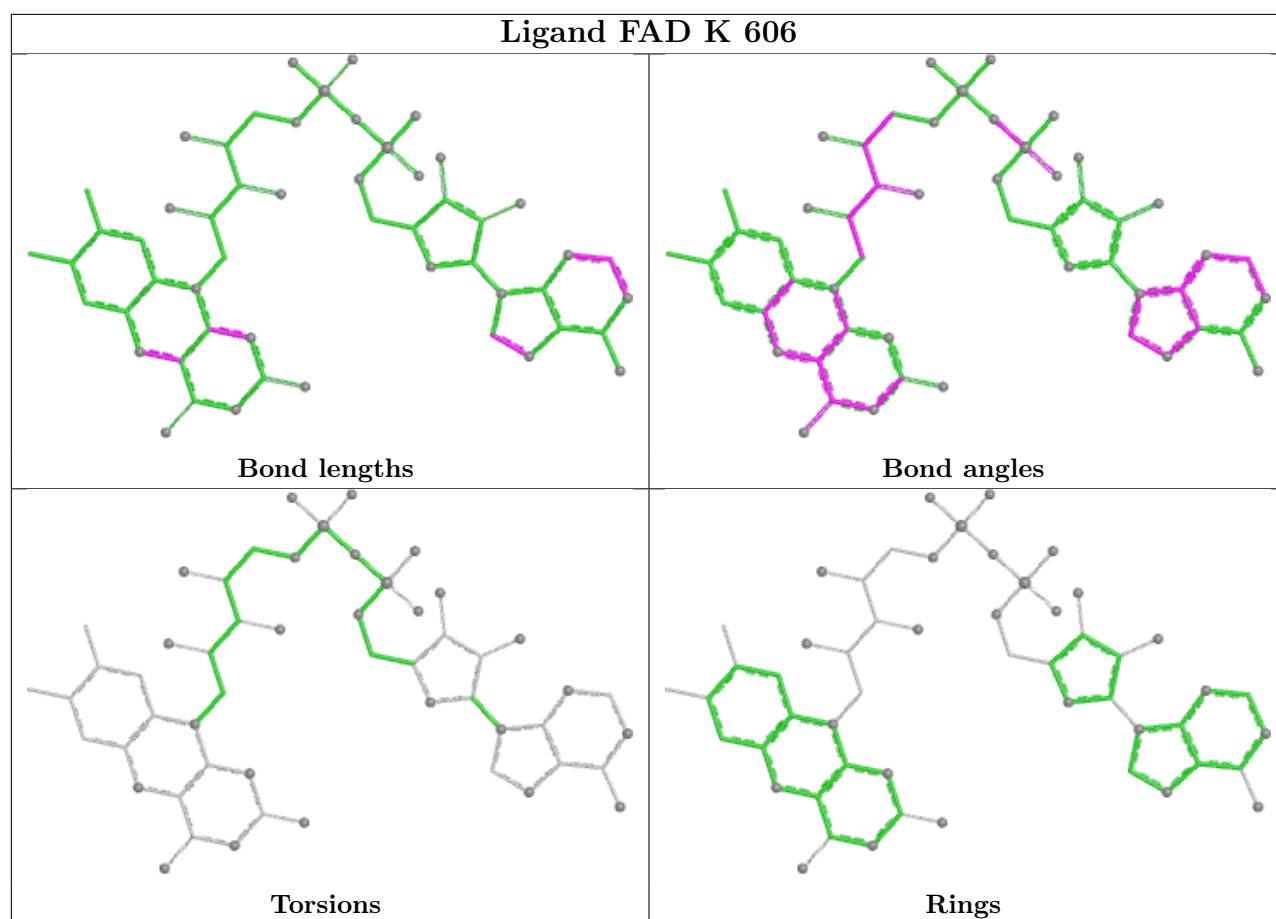
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



Ligand ZXF C 1327







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%)	0.15	15 (9%)	15 13	8, 19, 36, 45	0
1	J	164/164 (100%)	0.16	12 (7%)	21 19	11, 21, 41, 52	0
2	B	305/305 (100%)	0.66	28 (9%)	14 12	16, 27, 41, 45	0
2	K	305/305 (100%)	0.79	28 (9%)	14 12	19, 32, 44, 50	0
3	C	756/756 (100%)	-0.08	20 (2%)	57 57	10, 18, 30, 38	0
3	L	745/756 (98%)	0.02	25 (3%)	48 48	10, 20, 33, 56	0
All	All	2439/2450 (99%)	0.18	128 (5%)	33 31	8, 21, 39, 56	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	63	ASP	7.2
2	K	528	GLY	6.7
1	A	61	LEU	6.4
2	B	424	ALA	5.5
2	B	336	TRP	5.0
2	K	336	TRP	4.9
1	J	2	THR	4.9
1	J	63	ASP	4.7
3	C	1286	THR	4.6
2	B	338	ALA	4.4
2	K	425	SER	4.3
2	B	528	GLY	4.3
3	L	1290	THR	4.2
2	K	429	ASP	4.1
1	A	2	THR	4.1
1	A	141	ASP	4.0
1	J	61	LEU	4.0
3	L	985	ASP	3.9
2	K	424	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
3	C	1143	GLU	3.8
2	B	412	SER	3.8
2	K	506	GLU	3.6
2	K	378	GLY	3.6
3	L	969	ASP	3.6
2	B	272	ASN	3.5
3	L	1288	ASN	3.5
2	B	285	PRO	3.5
1	A	97	ARG	3.5
3	C	618	LYS	3.5
1	J	62	GLN	3.4
1	J	58	TYR	3.4
3	C	683	HIS	3.4
2	B	506	GLU	3.3
3	C	725	GLU	3.3
2	K	412	SER	3.2
3	C	1247	CYS	3.2
2	B	425	SER	3.2
2	B	509	ARG	3.1
2	B	378	GLY	3.1
3	C	720	LYS	3.0
3	C	969	ASP	3.0
3	L	1287	ASN	3.0
2	B	292	HIS	2.9
3	L	683	HIS	2.9
3	L	721	LYS	2.9
2	B	499	ASP	2.9
1	A	140	GLU	2.9
2	K	272	ASN	2.8
1	A	60	ARG	2.8
1	A	133	GLU	2.8
2	K	477	PHE	2.8
2	B	287	LEU	2.8
1	J	141	ASP	2.8
3	L	1144	THR	2.8
3	L	1143	GLU	2.7
2	B	224	PRO	2.7
3	C	663	VAL	2.7
2	K	338	ALA	2.6
2	K	291	GLU	2.6
3	L	725	GLU	2.6
2	B	318	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
2	K	285	PRO	2.6
1	A	64	LYS	2.6
2	B	271	LYS	2.6
1	A	58	TYR	2.6
2	B	286	GLU	2.6
2	B	472	LYS	2.6
3	C	699	GLU	2.5
2	K	484	GLN	2.5
3	L	983	GLU	2.5
3	C	684	VAL	2.5
3	L	1289	ASN	2.4
3	L	748	CYS	2.4
2	K	527	LEU	2.4
3	L	720	LYS	2.4
2	K	475	SER	2.4
1	J	64	LYS	2.4
2	K	335	ARG	2.4
1	J	165	LYS	2.4
2	B	335	ARG	2.3
3	C	645	GLU	2.3
3	C	983	GLU	2.3
2	K	471	GLN	2.3
2	K	268	MET	2.3
2	K	445	GLY	2.3
1	A	165	LYS	2.3
3	C	658	ASP	2.3
3	C	960	GLU	2.3
2	B	475	SER	2.3
2	K	492	GLU	2.3
3	L	970	GLU	2.2
1	A	59	ASP	2.2
3	C	985	ASP	2.2
1	A	162	THR	2.2
1	J	60	ARG	2.2
3	L	1283	ALA	2.2
2	B	268	MET	2.2
2	B	527	LEU	2.2
2	K	286	GLU	2.2
3	L	1276	ASP	2.2
2	K	387	HIS	2.1
2	B	291	GLU	2.1
2	K	295	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
3	L	658	ASP	2.1
3	C	992	CYS	2.1
3	C	1134	ARG	2.1
3	C	705	ASN	2.1
3	C	718	ASP	2.1
3	L	1170	ASP	2.1
2	K	271	LYS	2.1
2	B	414	GLU	2.1
2	B	429	ASP	2.1
3	L	1110	ASP	2.1
1	A	104	ARG	2.1
3	L	1286	THR	2.1
3	L	663	VAL	2.1
2	K	509	ARG	2.1
3	L	618	LYS	2.0
1	J	162	THR	2.0
1	A	62	GLN	2.0
1	J	136	VAL	2.0
2	B	274	LEU	2.0
2	K	426	ARG	2.0
3	L	571	ASP	2.0
2	B	480	GLU	2.0
3	L	699	GLU	2.0
2	K	243	LYS	2.0
1	J	104	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

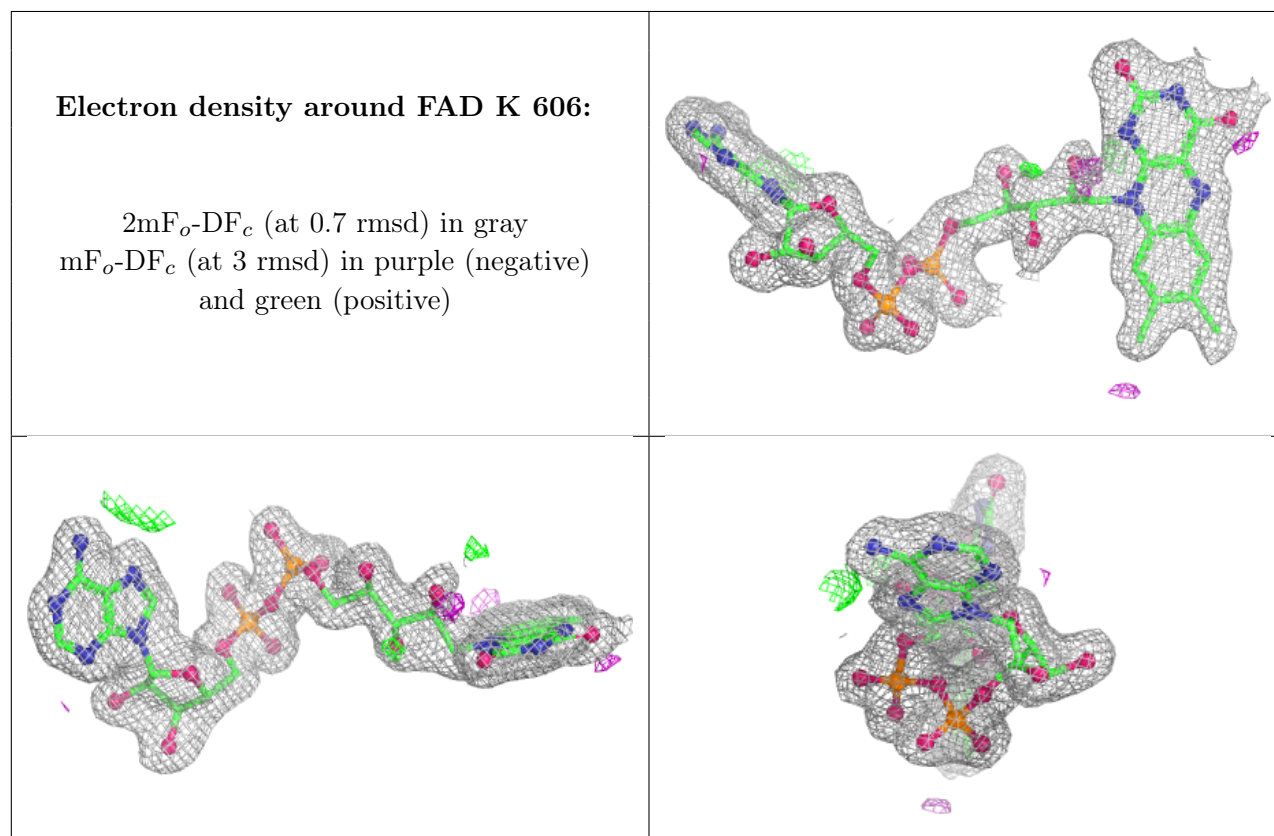
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

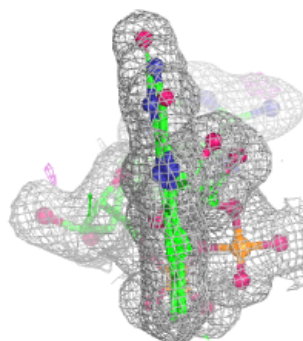
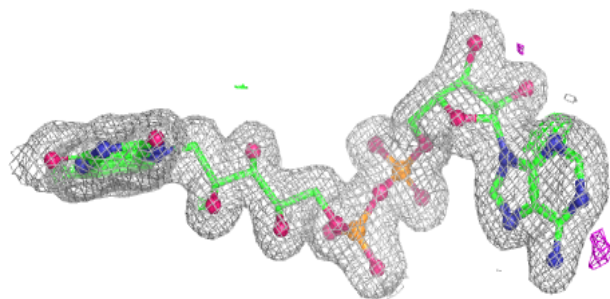
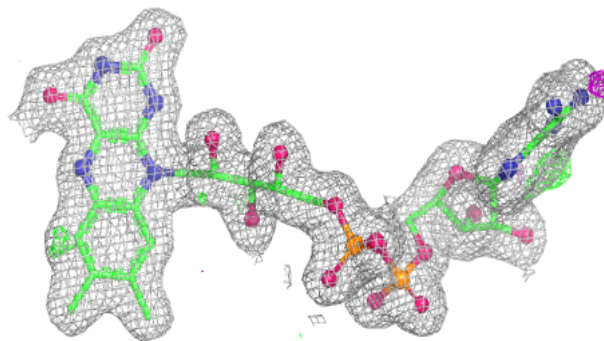
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	HPA	C	1	10/10	0.68	0.15	25,27,29,29	0
6	HPA	L	1	10/10	0.77	0.13	25,26,28,29	0
5	FAD	K	606	53/53	0.96	0.07	17,24,27,29	0
5	FAD	B	606	53/53	0.97	0.06	15,18,24,27	0
7	ZXF	C	1327	28/28	0.98	0.07	11,15,27,35	0
7	ZXF	L	1327	28/28	0.98	0.06	12,17,27,35	0
4	FES	J	602	4/4	0.99	0.03	13,13,14,14	0
4	FES	A	602	4/4	1.00	0.02	11,12,12,13	0
4	FES	J	601	4/4	1.00	0.02	11,11,12,13	0
4	FES	A	601	4/4	1.00	0.03	10,10,11,11	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.



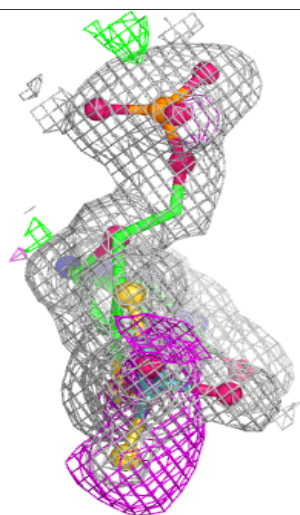
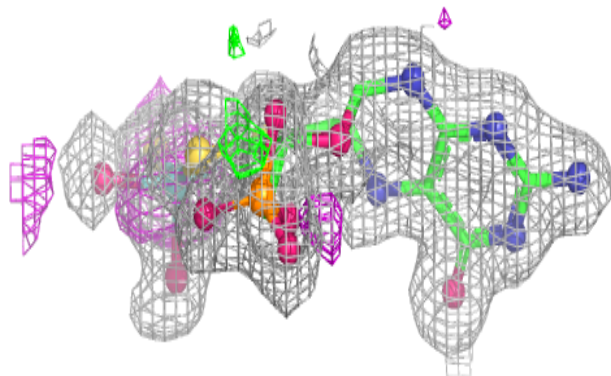
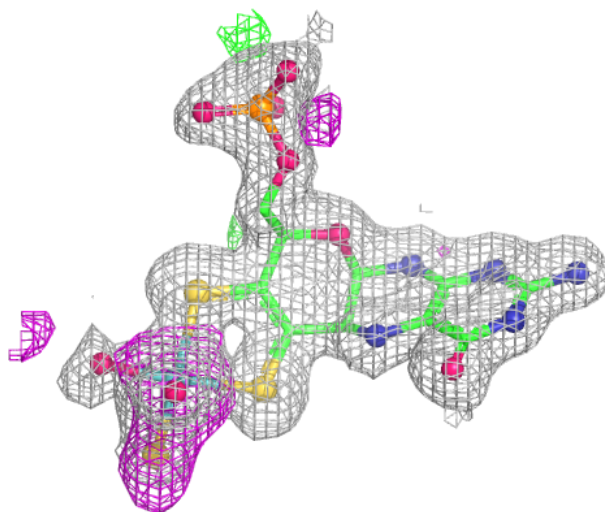
Electron density around FAD B 606:

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



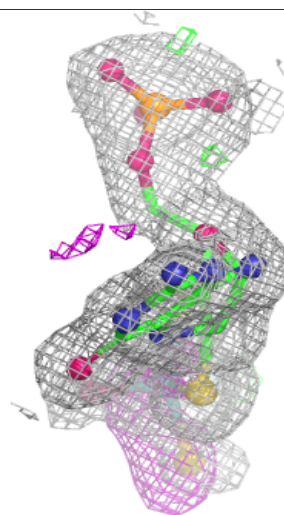
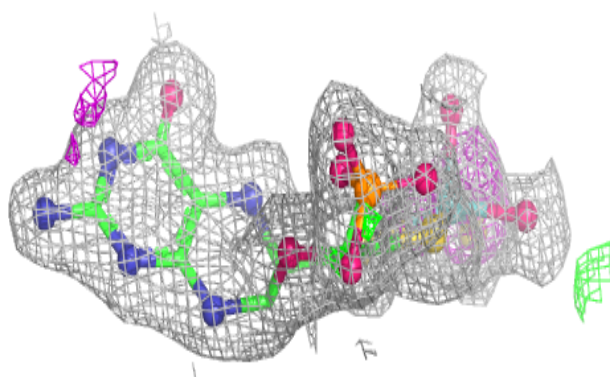
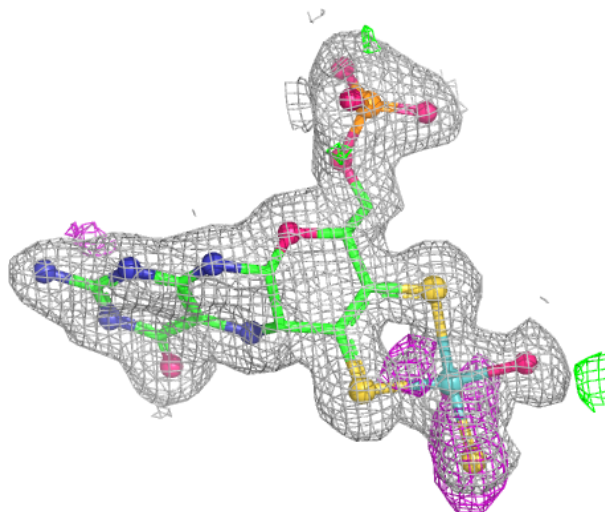
Electron density around ZXF C 1327:

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



Electron density around ZXF L 1327:

$2mF_o-DF_c$ (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.