



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 05:29 PM EDT

PDB ID : 3NVY / pdb_00003nvY
Title : Crystal Structure of Bovine Xanthine Oxidase in Complex with Quercetin
Authors : Cao, H.; Hille, R.
Deposited on : 2010-07-08
Resolution : 2.00 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

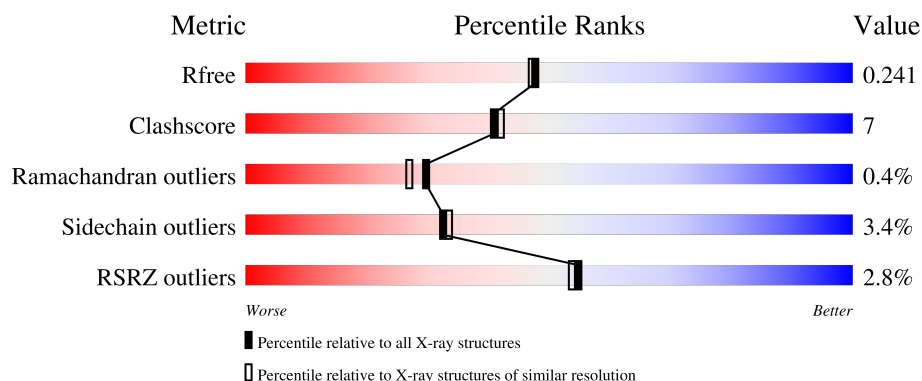
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	87% 10%
1	J	164	88% 12%
2	B	334	85% 13%
2	K	334	75% 14% 9%
3	C	756	86% 12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	L	756	2% 84% 13% ..

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 20401 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			

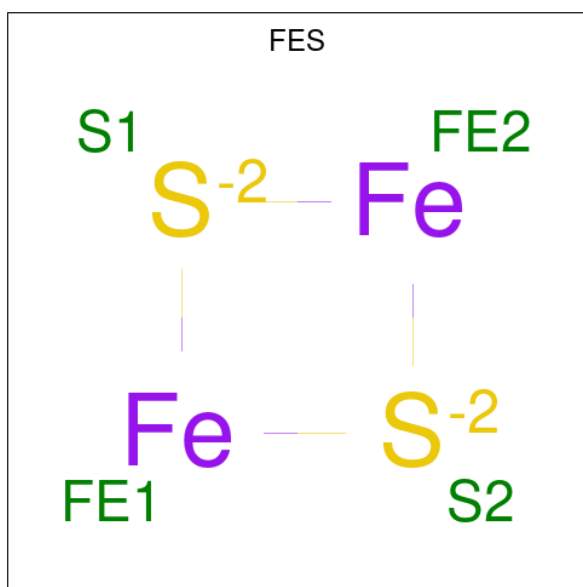
- Molecule 2 is a protein called Xanthine dehydrogenase/oxidase.

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.

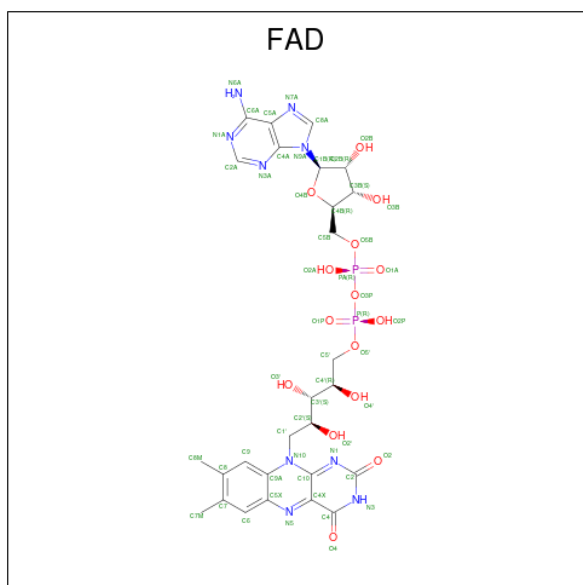
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	756	Total	C	N	O	S	0	0	0
			5832	3686	1005	1106	35			
3	L	745	Total	C	N	O	S	0	0	0
			5761	3643	992	1093	33			

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



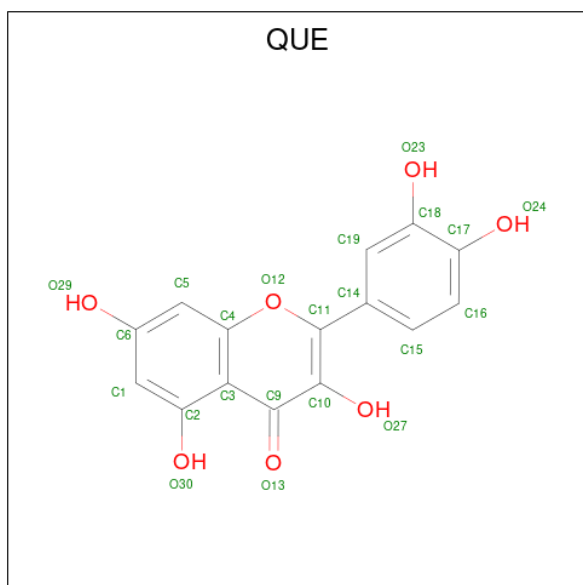
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 4	Fe 2	S 2	0	0
4	A	1	Total 4	Fe 2	S 2	0	0
4	J	1	Total 4	Fe 2	S 2	0	0
4	J	1	Total 4	Fe 2	S 2	0	0

- 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 3,5,7,3',4'-PENTAHYDROXYFLAVONE (CCD ID: QUE) (formula: $C_{15}H_{10}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			22	15	7		
6	L	1	Total	C	O	0	0
			22	15	7		

- Molecule 7 is Molybdopterin hydroxy-oxo-thiol-molybdenum (CCD ID: HOH) (formula: H_2O).

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		

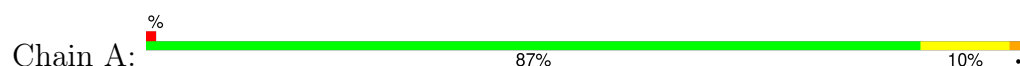
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	79	Total 79	O 79	0	0
8	B	114	Total 114	O 114	0	0
8	C	369	Total 369	O 369	0	0
8	J	84	Total 84	O 84	0	0
8	K	66	Total 66	O 66	0	0
8	L	345	Total 345	O 345	0	0

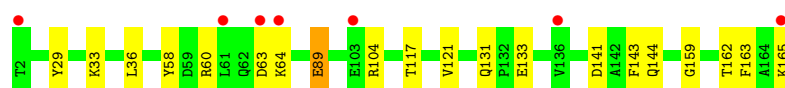
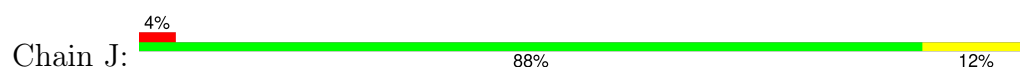
3 Residue-property plots [i](#)

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.

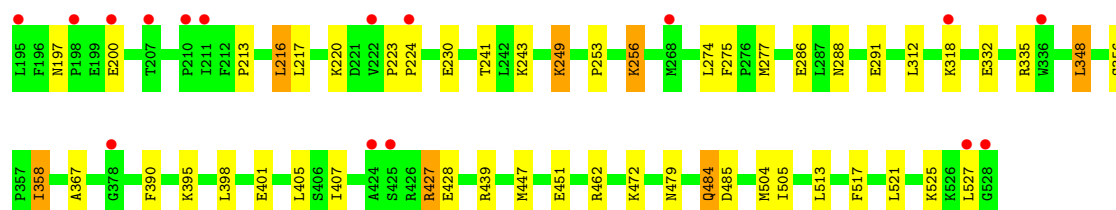
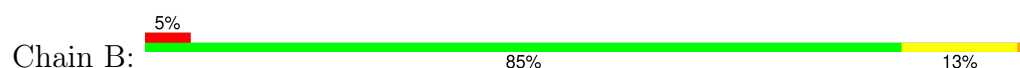
- Molecule 1: Xanthine dehydrogenase/oxidase



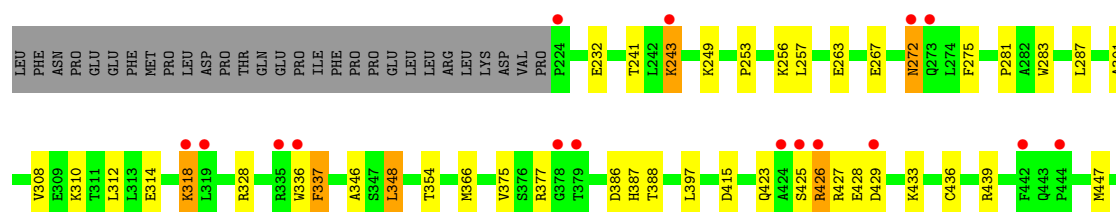
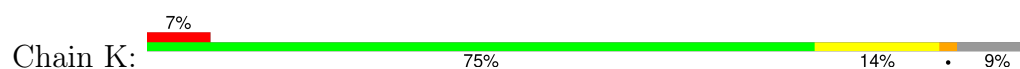
- Molecule 1: Xanthine dehydrogenase/oxidase



- Molecule 2: Xanthine dehydrogenase/oxidase

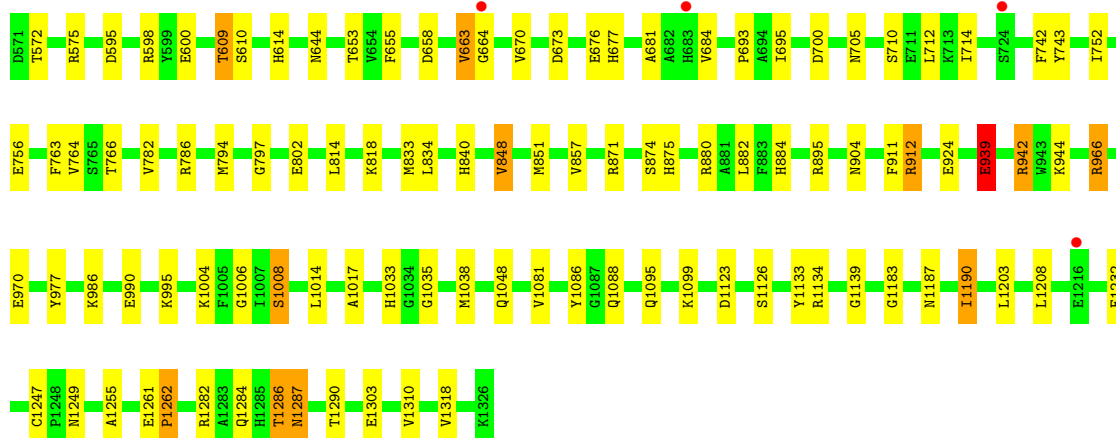
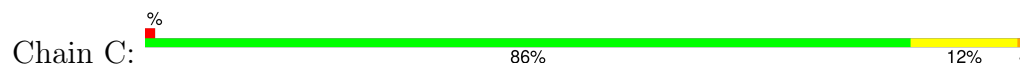


- Molecule 2: Xanthine dehydrogenase/oxidase

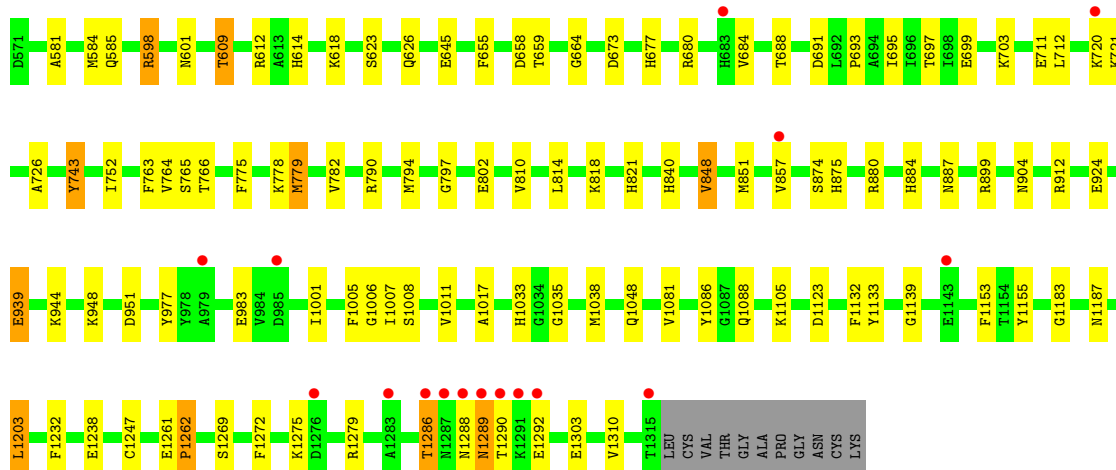
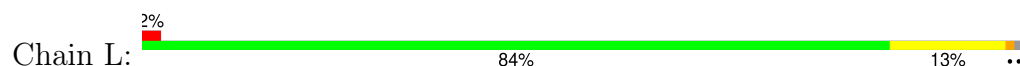




• Molecule 3: Xanthine dehydrogenase/oxidase



• 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	132.69Å 73.40Å 138.21Å 90.00° 97.13° 90.00°	Depositor
Resolution (Å)	101.50 – 2.00 101.50 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.2 (101.50-2.00) 98.2 (101.50-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.34 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.192 , 0.237 0.195 , 0.241	Depositor DCC
R_{free} test set	8835 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.013 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20401	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% 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, QUE, 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	0.89	0/1277	0.96	2/1723 (0.1%)
1	J	0.84	0/1277	0.92	1/1723 (0.1%)
2	B	0.72	0/2689	0.91	1/3637 (0.0%)
2	K	0.70	0/2438	0.91	3/3290 (0.1%)
3	C	0.91	2/5960 (0.0%)	1.01	10/8072 (0.1%)
3	L	0.87	1/5888 (0.0%)	0.96	7/7974 (0.1%)
All	All	0.84	3/19529 (0.0%)	0.96	24/26419 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1190	ILE	CA-CB	6.10	1.61	1.54
3	C	664	GLY	N-CA	5.63	1.53	1.45
3	L	779	MET	SD-CE	-5.06	1.67	1.79

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	848	VAL	CB-CA-C	-8.68	97.69	110.62
3	C	663	VAL	CA-C-N	-8.24	105.27	121.41
3	C	663	VAL	C-N-CA	-8.24	105.27	121.41
3	L	848	VAL	CB-CA-C	-7.76	99.15	110.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	663	VAL	O-C-N	-7.62	114.32	121.94
1	J	64	LYS	N-CA-C	6.56	118.33	110.19
3	C	1262	PRO	N-CA-C	6.22	118.29	110.70
3	C	942	ARG	NE-CZ-NH1	-6.13	115.37	121.50
1	A	131	GLN	CA-C-N	5.97	125.65	119.56
1	A	131	GLN	C-N-CA	5.97	125.65	119.56
2	K	505	ILE	N-CA-C	5.61	115.81	110.42
2	B	479	ASN	N-CA-C	5.58	115.48	108.45
3	L	1262	PRO	CA-C-N	-5.37	114.14	119.56
3	L	1262	PRO	C-N-CA	-5.37	114.14	119.56
3	C	939	GLU	CB-CA-C	-5.28	102.03	110.79
2	K	436	CYS	N-CA-C	5.28	117.28	108.99
3	C	944	LYS	CB-CA-C	-5.22	101.80	110.68
3	L	1288	ASN	N-CA-C	5.19	119.60	113.16
3	L	1275	LYS	CA-C-N	5.17	127.47	120.38
3	L	1275	LYS	C-N-CA	5.17	127.47	120.38
3	C	942	ARG	NE-CZ-NH2	5.17	123.85	119.20
2	K	429	ASP	N-CA-C	5.12	116.55	111.07
3	C	966	ARG	N-CA-C	5.10	116.53	111.07
3	L	743	TYR	N-CA-C	-5.04	103.13	110.24

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	164	ALA	Peptide

5.2 Too-close contacts [i](#)

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	17	1
1	J	1255	0	1265	16	0
2	B	2630	0	2697	28	0
2	K	2389	0	2459	37	0
3	C	5832	0	5759	78	1
3	L	5761	0	5685	81	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	22	0	7	4	0
6	L	22	0	7	3	0
7	C	28	0	0	0	0
7	L	28	0	0	0	0
8	A	79	0	0	2	0
8	B	114	0	0	4	0
8	C	369	0	0	10	0
8	J	84	0	0	2	0
8	K	66	0	0	1	0
8	L	345	0	0	7	0
All	All	20401	0	19206	251	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 7.

All (251) 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:L:726:ALA:HA	3:L:851:MET:HE1	1.22	1.12
2:K:243:LYS:H	2:K:243:LYS:HD3	0.97	1.11
3:L:779:MET:HG3	3:L:810:VAL:CG1	1.84	1.08
3:L:851:MET:HE3	3:L:857:VAL:HG21	1.25	1.07
1:J:165:LYS:HD3	8:J:167:HOH:O	1.58	1.04
3:C:851:MET:HE2	3:C:857:VAL:HG11	1.37	1.02
3:C:742:PHE:CE1	3:C:833:MET:CE	2.44	1.00
2:K:243:LYS:HD3	2:K:243:LYS:N	1.75	1.00
3:L:779:MET:HG3	3:L:810:VAL:HG13	1.43	1.00
2:K:243:LYS:H	2:K:243:LYS:CD	1.73	0.99
3:C:924:GLU:OE1	3:C:942:ARG:NH1	1.96	0.99
3:L:726:ALA:HA	3:L:851:MET:CE	1.93	0.98
3:C:742:PHE:HE1	3:C:833:MET:HE1	1.26	0.98
3:C:742:PHE:CE1	3:C:833:MET:HE1	2.02	0.93
3:C:1282:ARG:HA	3:C:1286:THR:HG23	1.54	0.90
1:J:165:LYS:HA	8:J:167:HOH:O	1.73	0.89
3:C:884:HIS:HE1	3:C:1006:GLY:H	1.23	0.85
3:L:851:MET:HE3	3:L:857:VAL:CG2	2.05	0.84
3:L:695:ILE:H	3:L:904:ASN:HD22	1.27	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ARG:HH11	1:A:162:THR:HG23	1.47	0.79
1:A:131:GLN:HE21	1:A:133:GLU:H	1.29	0.78
3:C:705:ASN:HB2	8:C:119:HOH:O	1.84	0.78
3:C:695:ILE:H	3:C:904:ASN:HD22	1.32	0.76
3:L:1289:ASN:HB2	3:L:1292:GLU:HB2	1.67	0.76
2:K:241:THR:HB	2:K:243:LYS:HE2	1.67	0.76
3:C:764:VAL:HG23	3:C:766:THR:HG22	1.66	0.76
3:C:802:GLU:OE1	6:C:1356:QUE:O27	2.05	0.75
3:C:742:PHE:CD1	3:C:833:MET:CE	2.70	0.75
3:C:1286:THR:HG22	3:C:1310:VAL:O	1.86	0.74
3:C:1088:GLN:HG2	3:C:1133:TYR:CD1	2.22	0.73
3:C:600:GLU:HG2	3:L:598:ARG:O	1.87	0.73
3:C:742:PHE:CD1	3:C:833:MET:HE2	2.24	0.73
1:J:104:ARG:HD3	1:J:162:THR:HG21	1.70	0.73
3:L:802:GLU:OE1	6:L:1356:QUE:O27	2.07	0.72
1:A:159:GLY:O	1:A:162:THR:HG22	1.88	0.71
3:L:884:HIS:HE1	3:L:1006:GLY:H	1.36	0.71
3:L:1088:GLN:HG2	3:L:1133:TYR:CD1	2.25	0.71
3:C:752:ILE:CD1	3:C:763:PHE:HE1	2.05	0.70
1:J:104:ARG:HH11	1:J:162:THR:HG23	1.56	0.70
2:B:472:LYS:HZ1	2:B:485:ASP:HB3	1.58	0.69
3:C:712:LEU:HD21	3:C:875:HIS:CE1	2.27	0.69
2:K:480:GLU:CD	2:K:480:GLU:H	2.01	0.69
1:J:131:GLN:HE21	1:J:133:GLU:H	1.42	0.68
1:A:32:ARG:NH1	3:C:676:GLU:OE2	2.27	0.68
3:C:884:HIS:CE1	3:C:1006:GLY:H	2.09	0.68
3:L:752:ILE:CD1	3:L:763:PHE:HE1	2.07	0.68
2:B:447:MET:HG2	2:B:527:LEU:HD13	1.77	0.67
2:B:197:ASN:O	2:B:200:GLU:HG2	1.95	0.67
1:J:159:GLY:O	1:J:162:THR:HG22	1.96	0.66
2:K:425:SER:O	2:K:426:ARG:HB3	1.95	0.66
3:C:752:ILE:HD12	3:C:763:PHE:HE1	1.62	0.65
3:L:884:HIS:CE1	3:L:1006:GLY:H	2.15	0.65
2:B:288:ASN:OD1	8:B:903:HOH:O	2.15	0.65
3:L:645:GLU:HG3	3:L:778:LYS:NZ	2.11	0.64
3:C:764:VAL:CG2	3:C:766:THR:HG22	2.27	0.64
2:K:257:LEU:O	5:K:606:FAD:H2B	1.97	0.64
2:B:472:LYS:NZ	2:B:485:ASP:HB3	2.13	0.64
3:L:840:HIS:HE1	3:L:874:SER:OG	1.81	0.64
3:L:764:VAL:HG23	3:L:766:THR:HG22	1.80	0.63
3:C:794:MET:HE3	3:C:1038:MET:HB3	1.79	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:287:LEU:HD22	2:K:301:ALA:HB3	1.79	0.63
8:C:1357:ZXF:S	8:C:1357:ZXF:MO	2.09	0.63
2:B:504:MET:HE2	3:C:1303:GLU:HB2	1.81	0.62
3:L:726:ALA:CA	3:L:851:MET:HE1	2.13	0.62
3:L:1289:ASN:ND2	3:L:1289:ASN:H	1.96	0.62
8:C:1357:ZXF:MO	8:C:1357:ZXF:O2	1.71	0.61
3:C:840:HIS:HE1	3:C:874:SER:OG	1.82	0.61
3:C:1033:HIS:HD2	3:C:1035:GLY:H	1.47	0.61
8:L:1357:ZXF:MO	8:L:1357:ZXF:S	2.10	0.61
2:B:217:LEU:O	2:B:220:LYS:HG2	2.00	0.61
3:C:610:SER:O	3:C:663:VAL:O	2.19	0.61
3:L:614:HIS:HD2	3:L:693:PRO:O	1.84	0.61
3:C:1134:ARG:NE	8:C:1383:HOH:O	2.33	0.61
3:L:711:GLU:HA	3:L:899:ARG:HD2	1.82	0.60
3:C:712:LEU:HD21	3:C:875:HIS:HE1	1.66	0.60
8:L:1357:ZXF:MO	8:L:1357:ZXF:O2	1.72	0.60
3:L:645:GLU:HG3	3:L:778:LYS:HZ1	1.66	0.60
3:L:673:ASP:OD2	3:L:677:HIS:HD2	1.84	0.60
3:C:1282:ARG:CA	3:C:1286:THR:HG23	2.31	0.59
3:C:673:ASP:OD2	3:C:677:HIS:HD2	1.85	0.59
3:L:655:PHE:HE1	3:L:814:LEU:HD23	1.67	0.59
3:C:609:THR:HG22	8:C:16:HOH:O	2.02	0.59
2:K:310:LYS:O	2:K:314:GLU:HG2	2.02	0.59
3:L:939:GLU:HG2	3:L:977:TYR:CE2	2.37	0.59
2:K:232:GLU:OE2	3:L:677:HIS:HE1	1.86	0.58
3:C:1282:ARG:HA	3:C:1286:THR:CG2	2.32	0.58
3:C:670:VAL:HG11	3:C:681:ALA:HB3	1.86	0.57
3:C:995:LYS:NZ	3:C:1284:GLN:HE21	2.03	0.57
3:L:697:THR:HB	3:L:699:GLU:OE1	2.05	0.56
2:K:281:PRO:HB2	2:K:287:LEU:HD12	1.86	0.56
6:C:1356:QUE:O27	6:C:1356:QUE:H19	2.05	0.56
3:L:752:ILE:HD12	3:L:763:PHE:HE1	1.69	0.56
2:B:428:GLU:HG3	8:B:146:HOH:O	2.05	0.56
3:C:1095:GLN:O	3:C:1099:LYS:HG2	2.06	0.56
3:C:1088:GLN:HG2	3:C:1133:TYR:CE1	2.40	0.55
1:J:144:GLN:HE22	2:K:336:TRP:HA	1.71	0.55
3:C:1033:HIS:CD2	3:C:1035:GLY:H	2.24	0.55
1:A:37:ARG:HD3	3:C:595:ASP:O	2.07	0.55
3:C:705:ASN:OD1	8:C:395:HOH:O	2.18	0.55
1:A:139:ILE:HD12	1:A:164:ALA:HB2	1.89	0.55
3:L:1048:GLN:HE22	3:L:1187:ASN:HD22	1.54	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:614:HIS:HD2	3:C:693:PRO:O	1.90	0.54
3:C:695:ILE:HG23	3:C:700:ASP:HB3	1.89	0.54
3:L:609:THR:HG22	8:L:357:HOH:O	2.07	0.54
3:L:1286:THR:HG21	3:L:1310:VAL:HB	1.90	0.54
2:B:253:PRO:HB3	2:B:401:GLU:HG2	1.90	0.54
2:B:439:ARG:NH2	2:B:451:GLU:OE1	2.41	0.54
3:L:699:GLU:H	3:L:699:GLU:CD	2.16	0.54
3:L:712:LEU:HD21	3:L:875:HIS:CE1	2.43	0.53
2:B:348:LEU:HD13	2:B:407:ILE:HD13	1.89	0.53
2:K:281:PRO:HB2	2:K:287:LEU:CD1	2.38	0.53
3:L:1001:ILE:HD12	3:L:1269:SER:HA	1.88	0.53
3:C:742:PHE:HD1	3:C:833:MET:HE2	1.73	0.53
2:K:439:ARG:NH2	2:K:451:GLU:OE1	2.35	0.53
1:J:58:TYR:CE1	1:J:63:ASP:O	2.62	0.53
6:L:1356:QUE:O27	6:L:1356:QUE:H19	2.08	0.53
3:L:1088:GLN:HG2	3:L:1133:TYR:CE1	2.43	0.53
1:A:32:ARG:NH2	8:A:700:HOH:O	2.35	0.52
2:K:263:GLU:HB3	5:K:606:FAD:H52A	1.91	0.52
1:A:164:ALA:O	1:A:165:LYS:HB2	2.09	0.52
3:L:779:MET:CG	3:L:810:VAL:CG1	2.74	0.52
1:A:104:ARG:NH1	1:A:162:THR:HG23	2.21	0.51
3:C:880:ARG:O	3:C:884:HIS:HD2	1.93	0.51
3:L:1286:THR:HG22	3:L:1310:VAL:O	2.10	0.51
3:C:1287:ASN:C	3:C:1287:ASN:HD22	2.18	0.51
2:K:447:MET:HG2	2:K:527:LEU:HD13	1.93	0.51
2:K:256:LYS:HE3	2:K:275:PHE:CE2	2.45	0.51
3:L:880:ARG:O	3:L:884:HIS:HD2	1.93	0.50
3:L:1203:LEU:HD12	3:L:1203:LEU:C	2.37	0.50
3:L:1289:ASN:H	3:L:1289:ASN:HD22	1.58	0.50
2:K:314:GLU:O	2:K:318:LYS:HD3	2.11	0.50
3:C:742:PHE:HE1	3:C:833:MET:CE	1.95	0.49
3:C:752:ILE:HD12	3:C:763:PHE:CE1	2.43	0.49
3:C:986:LYS:NZ	3:C:990:GLU:OE2	2.42	0.49
2:B:213:PRO:HB2	2:B:216:LEU:HB2	1.94	0.49
3:L:840:HIS:CE1	3:L:874:SER:OG	2.64	0.49
2:B:484:GLN:HG2	3:C:1318:VAL:O	2.11	0.49
1:J:104:ARG:HH11	1:J:162:THR:CG2	2.22	0.49
3:C:1014:LEU:HD11	6:C:1356:QUE:C19	2.43	0.49
8:L:1357:ZXF:S	8:L:1357:ZXF:O1	2.71	0.49
3:C:1261:GLU:N	3:C:1262:PRO:CD	2.75	0.48
3:C:1126:SER:HB2	3:L:1132:PHE:CD1	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:752:ILE:HD11	3:L:763:PHE:HE1	1.79	0.48
3:L:612:ARG:NH1	3:L:691:ASP:OD1	2.43	0.48
3:L:1038:MET:HG3	8:L:1357:ZXF:C4	2.42	0.48
3:C:572:THR:HA	3:C:575:ARG:HD3	1.95	0.48
2:K:308:VAL:HG21	2:K:348:LEU:HG	1.96	0.48
3:L:752:ILE:HD12	3:L:763:PHE:CE1	2.48	0.48
1:A:33:LYS:NZ	8:A:298:HOH:O	2.47	0.47
3:C:1282:ARG:HG2	3:C:1286:THR:HG21	1.96	0.47
1:J:36:LEU:HD22	1:J:89:GLU:HG3	1.97	0.47
3:L:765:SER:OG	3:L:794:MET:HG2	2.14	0.47
3:C:1048:GLN:HE22	3:C:1187:ASN:HD22	1.61	0.47
2:K:243:LYS:N	2:K:243:LYS:CD	2.47	0.47
3:L:1033:HIS:HD2	3:L:1035:GLY:H	1.62	0.47
2:K:283:TRP:HB2	8:K:114:HOH:O	2.14	0.47
1:A:104:ARG:HD3	1:A:162:THR:HG21	1.97	0.47
3:C:1249:ASN:O	3:C:1255:ALA:HA	2.15	0.46
2:K:504:MET:HG2	3:L:1303:GLU:CD	2.40	0.46
3:L:775:PHE:O	3:L:779:MET:HB2	2.14	0.46
3:C:1017:ALA:HB1	3:C:1086:TYR:CD2	2.51	0.46
1:A:9:PHE:CD1	2:B:216:LEU:HG	2.50	0.46
3:L:720:LYS:HD3	8:L:1730:HOH:O	2.16	0.46
1:J:159:GLY:O	1:J:162:THR:CG2	2.63	0.46
3:L:779:MET:HG3	3:L:810:VAL:HG11	1.89	0.46
3:C:1286:THR:CG2	3:C:1310:VAL:O	2.61	0.46
3:L:623:SER:HA	3:L:626:GLN:HE21	1.81	0.46
3:L:601:ASN:O	3:L:821:HIS:HD2	1.99	0.45
3:C:742:PHE:CE1	3:C:833:MET:HE3	2.41	0.45
3:C:782:VAL:CG1	3:C:786:ARG:HG3	2.46	0.45
3:C:752:ILE:CD1	3:C:763:PHE:CE1	2.92	0.45
1:J:29:TYR:CZ	1:J:33:LYS:HD2	2.52	0.45
3:L:680:ARG:HG2	8:L:1468:HOH:O	2.15	0.45
3:C:1134:ARG:CZ	8:C:1383:HOH:O	2.65	0.45
3:L:618:LYS:HD3	3:L:688:THR:HG21	1.98	0.45
3:L:695:ILE:H	3:L:904:ASN:ND2	2.04	0.45
3:C:966:ARG:O	3:C:970:GLU:HG3	2.16	0.45
3:L:1279:ARG:NH2	3:L:1290:THR:O	2.49	0.45
8:C:1357:ZXF:S	8:C:1357:ZXF:O2	2.75	0.45
1:J:104:ARG:HD2	1:J:163:PHE:CE1	2.51	0.45
2:B:256:LYS:HG3	2:B:275:PHE:CG	2.53	0.44
2:B:517:PHE:CZ	2:B:521:LEU:HD11	2.52	0.44
1:J:165:LYS:HD3	1:J:165:LYS:HA	1.86	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:505:ILE:HG12	8:B:155:HOH:O	2.17	0.44
3:L:1033:HIS:CD2	3:L:1035:GLY:H	2.36	0.44
3:L:948:LYS:O	3:L:951:ASP:HB2	2.18	0.44
2:K:346:ALA:HB1	5:K:606:FAD:H4'	2.00	0.43
3:L:1007:ILE:HG22	3:L:1081:VAL:HG12	2.00	0.43
2:K:423:GLN:HB3	2:K:433:LYS:HG2	2.00	0.43
2:B:241:THR:HG22	2:B:243:LYS:H	1.83	0.43
3:C:644:ASN:O	3:C:653:THR:HA	2.19	0.43
8:C:1357:ZXF:S	8:C:1357:ZXF:S1'	3.17	0.43
3:C:802:GLU:OE1	6:C:1356:QUE:O13	2.36	0.43
2:K:479:ASN:OD1	2:K:481:LYS:HB3	2.19	0.43
2:K:480:GLU:CD	2:K:480:GLU:N	2.74	0.43
3:L:1001:ILE:HD11	3:L:1272:PHE:CD1	2.54	0.43
3:C:663:VAL:HG12	3:C:834:LEU:HD11	2.00	0.42
3:C:1008:SER:HA	3:C:1081:VAL:HG11	2.01	0.42
3:C:851:MET:HE2	3:C:857:VAL:CG1	2.27	0.42
1:A:36:LEU:HD22	1:A:89:GLU:HG3	2.01	0.42
3:C:714:ILE:HD12	3:C:882:LEU:HB3	2.02	0.42
3:C:911:PHE:O	3:C:912:ARG:C	2.62	0.42
2:K:249:LYS:NZ	2:K:253:PRO:O	2.51	0.42
2:K:287:LEU:CD2	2:K:301:ALA:HB3	2.48	0.42
3:L:1007:ILE:CG2	3:L:1081:VAL:HG12	2.50	0.42
2:B:427:ARG:HD3	8:B:146:HOH:O	2.20	0.42
3:C:1134:ARG:NH1	3:L:1123:ASP:O	2.51	0.42
3:L:1048:GLN:NE2	3:L:1187:ASN:HD22	2.17	0.42
1:A:143:PHE:HB3	3:C:1232:PHE:CE1	2.55	0.42
3:C:655:PHE:HE1	3:C:814:LEU:HD23	1.85	0.42
2:K:426:ARG:HB2	2:K:433:LYS:HG3	2.00	0.42
2:K:337:PHE:C	2:K:337:PHE:CD2	2.98	0.42
3:C:655:PHE:HE1	3:C:814:LEU:CD2	2.32	0.42
2:K:386:ASP:OD2	2:K:388:THR:HG23	2.20	0.42
3:L:884:HIS:HE1	3:L:1005:PHE:HA	1.84	0.42
3:L:1017:ALA:HB1	3:L:1086:TYR:CD2	2.54	0.42
2:K:263:GLU:HG3	2:K:267:GLU:OE2	2.20	0.42
2:K:366:MET:HE2	2:K:387:HIS:HA	2.01	0.42
1:J:117:THR:O	1:J:121:VAL:HG23	2.19	0.41
3:L:887:ASN:ND2	3:L:924:GLU:OE2	2.53	0.41
3:L:581:ALA:O	3:L:585:GLN:HG3	2.20	0.41
3:L:609:THR:HG23	3:L:664:GLY:HA2	2.02	0.41
1:A:165:LYS:HD3	1:A:165:LYS:HA	1.89	0.41
3:L:1261:GLU:N	3:L:1262:PRO:CD	2.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:THR:HG23	2:B:230:GLU:OE1	2.19	0.41
2:B:223:PRO:HA	2:B:224:PRO:HD3	1.97	0.41
2:B:390:PHE:O	2:B:462:ARG:HD2	2.20	0.41
3:L:1183:GLY:HA2	3:L:1247:CYS:O	2.21	0.41
2:K:500:ALA:HA	2:K:501:PRO:HD2	1.82	0.41
2:B:367:ALA:O	2:B:439:ARG:HD3	2.20	0.41
3:C:756:GLU:HB3	3:L:584:MET:SD	2.61	0.41
2:K:263:GLU:HG2	2:K:354:THR:OG1	2.21	0.41
3:L:711:GLU:HA	3:L:899:ARG:CD	2.48	0.41
2:K:377:ARG:HE	2:K:377:ARG:HB3	1.35	0.41
2:B:356:SER:OG	2:B:358:ILE:HD12	2.20	0.41
3:C:1183:GLY:HA2	3:C:1247:CYS:O	2.20	0.41
1:J:143:PHE:HB3	3:L:1232:PHE:CE1	2.56	0.41
3:L:763:PHE:CE2	3:L:790:ARG:HD3	2.56	0.41
1:A:108:SER:O	1:A:109:HIS:HB2	2.20	0.41
2:B:318:LYS:HD3	2:B:318:LYS:N	2.36	0.41
3:L:703:LYS:O	3:L:703:LYS:HG2	2.21	0.41
2:B:249:LYS:HD2	2:B:249:LYS:HA	1.76	0.40
3:C:1287:ASN:HB2	8:C:123:HOH:O	2.20	0.40
3:L:884:HIS:CE1	3:L:1005:PHE:HA	2.56	0.40
2:B:332:GLU:HA	2:B:335:ARG:HG3	2.03	0.40
2:B:286:GLU:HB3	2:B:405:LEU:HD11	2.03	0.40
3:L:1153:PHE:HB2	3:L:1155:TYR:CZ	2.56	0.40
3:C:939:GLU:HG2	3:C:977:TYR:CE2	2.57	0.40
2:K:272:ASN:HD22	2:K:272:ASN:HA	1.76	0.40
3:L:1011:VAL:HG21	6:L:1356:QUE:C15	2.51	0.40
3:L:601:ASN:HB2	3:L:821:HIS:CD2	2.56	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)
1:A:63:ASP:OD2	3:C:871:ARG:NH1[1_545]	2.06	0.14

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%)	157 (97%)	5 (3%)	0	100	100
1	J	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
2	B	332/334 (99%)	315 (95%)	17 (5%)	0	100	100
2	K	303/334 (91%)	289 (95%)	13 (4%)	1 (0%)	36	35
3	C	754/756 (100%)	727 (96%)	23 (3%)	4 (0%)	24	21
3	L	743/756 (98%)	722 (97%)	16 (2%)	5 (1%)	18	14
All	All	2456/2508 (98%)	2365 (96%)	81 (3%)	10 (0%)	30	27

All (10) 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
2	K	426	ARG
3	L	721	LYS
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	40
1	J	137/137 (100%)	134 (98%)	3 (2%)	45	50
2	B	290/290 (100%)	275 (95%)	15 (5%)	21	18

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	K	261/290 (90%)	248 (95%)	13 (5%)	22	20
3	C	632/632 (100%)	614 (97%)	18 (3%)	38	41
3	L	624/632 (99%)	607 (97%)	17 (3%)	39	42
All	All	2081/2118 (98%)	2011 (97%)	70 (3%)	32	33

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LYS
1	A	89	GLU
1	A	97	ARG
1	A	140	GLU
2	B	216	LEU
2	B	249	LYS
2	B	256	LYS
2	B	274	LEU
2	B	277	MET
2	B	291	GLU
2	B	312	LEU
2	B	348	LEU
2	B	358	ILE
2	B	395	LYS
2	B	398	LEU
2	B	427	ARG
2	B	484	GLN
2	B	513	LEU
2	B	525	LYS
3	C	598	ARG
3	C	609	THR
3	C	658	ASP
3	C	684	VAL
3	C	710	SER
3	C	743	TYR
3	C	818	LYS
3	C	848	VAL
3	C	895	ARG
3	C	939	GLU
3	C	1004	LYS
3	C	1123	ASP
3	C	1190	ILE
3	C	1203	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	1208	LEU
3	C	1286	THR
3	C	1287	ASN
3	C	1290	THR
1	J	60	ARG
1	J	89	GLU
1	J	141	ASP
2	K	243	LYS
2	K	272	ASN
2	K	312	LEU
2	K	318	LYS
2	K	328	ARG
2	K	337	PHE
2	K	348	LEU
2	K	375	VAL
2	K	397	LEU
2	K	415	ASP
2	K	427	ARG
2	K	428	GLU
2	K	499	ASP
3	L	598	ARG
3	L	609	THR
3	L	658	ASP
3	L	659	THR
3	L	684	VAL
3	L	743	TYR
3	L	782	VAL
3	L	818	LYS
3	L	848	VAL
3	L	939	GLU
3	L	944	LYS
3	L	983	GLU
3	L	1105	LYS
3	L	1203	LEU
3	L	1238	GLU
3	L	1286	THR
3	L	1289	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	71	ASN
1	A	82	HIS
1	A	131	GLN
1	A	144	GLN
1	A	146	ASN
2	B	252	HIS
2	B	261	ASN
2	B	288	ASN
2	B	322	GLN
2	B	351	ASN
3	C	614	HIS
3	C	626	GLN
3	C	650	ASN
3	C	677	HIS
3	C	821	HIS
3	C	840	HIS
3	C	875	HIS
3	C	884	HIS
3	C	904	ASN
3	C	1033	HIS
3	C	1048	GLN
3	C	1173	ASN
3	C	1212	HIS
3	C	1220	HIS
3	C	1284	GLN
3	C	1285	HIS
3	C	1287	ASN
1	J	82	HIS
1	J	131	GLN
1	J	144	GLN
1	J	146	ASN
2	K	226	GLN
2	K	261	ASN
2	K	272	ASN
2	K	273	GLN
2	K	292	HIS
2	K	322	GLN
2	K	351	ASN
3	L	585	GLN
3	L	614	HIS
3	L	626	GLN
3	L	677	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	1151	HIS
3	L	1220	HIS
3	L	1288	ASN
3	L	1289	ASN
3	L	1307	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
8	ZXF	L	1357	-	24,31,31	1.98	4 (16%)	22,52,52	2.07	9 (40%)
4	FES	J	601	1	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FAD	K	606	-	58,58,58	1.22	7 (12%)	85,89,89	1.73	21 (24%)
5	FAD	B	606	-	58,58,58	0.96	3 (5%)	85,89,89	1.62	11 (12%)
6	QUE	C	1356	-	24,24,24	3.34	5 (20%)	36,36,36	2.09	11 (30%)
6	QUE	L	1356	-	24,24,24	3.44	4 (16%)	36,36,36	1.81	10 (27%)
8	ZXF	C	1357	-	24,31,31	1.86	4 (16%)	22,52,52	2.10	9 (40%)
4	FES	A	602	1	0,4,4	-	-	-	-	-
4	FES	J	602	1	0,4,4	-	-	-	-	-
4	FES	A	601	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
8	ZXF	L	1357	-	-	2/6/46/46	0/4/4/4
4	FES	J	601	1	-	-	0/1/1/1
5	FAD	K	606	-	-	0/34/50/50	0/6/6/6
5	FAD	B	606	-	-	1/34/50/50	0/6/6/6
6	QUE	C	1356	-	-	0/4/4/4	0/3/3/3
6	QUE	L	1356	-	-	0/4/4/4	0/3/3/3
8	ZXF	C	1357	-	-	1/6/46/46	0/4/4/4
4	FES	A	602	1	-	-	0/1/1/1
4	FES	J	602	1	-	-	0/1/1/1
4	FES	A	601	1	-	-	0/1/1/1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	1356	QUE	C10-C11	13.82	1.49	1.36
6	C	1356	QUE	C10-C11	13.20	1.49	1.36
8	L	1357	ZXF	C9-C10	6.58	1.49	1.38
6	L	1356	QUE	C18-C17	5.87	1.50	1.40
8	C	1357	ZXF	C9-C10	5.78	1.48	1.38
6	C	1356	QUE	C3-C2	5.34	1.49	1.41
6	L	1356	QUE	C3-C2	5.21	1.49	1.41
6	C	1356	QUE	C18-C17	4.97	1.48	1.40
6	L	1356	QUE	C3-C4	4.77	1.49	1.40
6	C	1356	QUE	C3-C4	4.68	1.48	1.40
8	L	1357	ZXF	MO-S1'	-4.63	2.32	2.39
8	C	1357	ZXF	MO-S2'	-4.06	2.33	2.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	606	FAD	C4X-N5	3.86	1.39	1.30
5	K	606	FAD	C2A-N1A	3.62	1.40	1.33
5	B	606	FAD	C4X-N5	3.59	1.38	1.30
5	K	606	FAD	C2A-N3A	3.22	1.39	1.33
6	C	1356	QUE	C14-C11	2.85	1.51	1.47
5	K	606	FAD	C10-N1	2.81	1.38	1.33
8	C	1357	ZXF	O4-C4	2.78	1.28	1.23
5	K	606	FAD	C2'-C3'	-2.70	1.48	1.53
5	B	606	FAD	C2A-N3A	2.52	1.38	1.33
5	K	606	FAD	C8A-N7A	2.41	1.36	1.31
8	L	1357	ZXF	C10-N8	-2.19	1.33	1.35
5	K	606	FAD	C5A-N7A	-2.06	1.35	1.39
5	B	606	FAD	C2A-N1A	2.05	1.37	1.33
8	L	1357	ZXF	MO-S2'	-2.04	2.36	2.39
8	C	1357	ZXF	MO-S1'	-2.02	2.36	2.39

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	606	FAD	N3A-C2A-N1A	-6.65	118.51	128.58
6	C	1356	QUE	O12-C11-C14	6.43	119.89	110.87
6	L	1356	QUE	O12-C11-C14	5.17	118.12	110.87
5	K	606	FAD	N3A-C2A-N1A	-4.75	121.39	128.58
6	C	1356	QUE	O12-C4-C5	4.69	122.47	115.83
5	K	606	FAD	C5A-C4A-N3A	-4.44	120.60	126.72
5	K	606	FAD	O3'-C3'-C2'	-4.33	99.09	108.93
6	C	1356	QUE	C14-C11-C10	-4.09	122.01	128.44
5	K	606	FAD	N9A-C8A-N7A	-4.00	108.26	113.94
6	L	1356	QUE	C14-C11-C10	-3.92	122.27	128.44
5	B	606	FAD	C5A-C4A-N3A	-3.83	121.44	126.72
5	K	606	FAD	C5'-C4'-C3'	-3.79	105.08	112.22
8	C	1357	ZXF	O3'-C7-C6	-3.75	106.46	108.96
8	C	1357	ZXF	C2-N1-C10	3.73	119.93	113.36
8	L	1357	ZXF	C2-N1-C10	3.68	119.85	113.36
8	C	1357	ZXF	C7-C6-N5	3.65	111.45	107.87
5	B	606	FAD	O2P-P-O3P	3.61	117.03	107.27
5	B	606	FAD	C2A-N3A-C4A	3.55	120.51	111.83
8	L	1357	ZXF	O3'-C3'-C2'	3.55	114.10	109.09
6	L	1356	QUE	C11-C10-C9	-3.53	119.00	121.52
5	K	606	FAD	C5A-N7A-C8A	3.52	108.99	103.45
5	K	606	FAD	C1'-C2'-C3'	-3.37	100.52	109.66
5	B	606	FAD	N9A-C8A-N7A	-3.34	109.20	113.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	1356	QUE	O12-C4-C5	3.32	120.54	115.83
8	L	1357	ZXF	O4-C4-C9	-3.26	119.41	127.26
6	C	1356	QUE	C5-C6-C1	3.22	124.89	120.47
5	K	606	FAD	C4-N3-C2	-3.20	119.95	125.64
8	C	1357	ZXF	O3'-C7-N8	3.20	111.51	108.61
5	K	606	FAD	N3A-C4A-N9A	3.09	132.41	127.17
8	L	1357	ZXF	C2'-C1'-S1'	3.01	121.86	120.15
8	L	1357	ZXF	O1P-P-O4'	-2.93	99.03	106.67
8	L	1357	ZXF	C7-C6-N5	2.92	110.73	107.87
8	C	1357	ZXF	O2P-P-O4'	-2.92	99.06	106.67
5	B	606	FAD	C4X-C10-N10	2.90	120.64	116.48
5	K	606	FAD	C4X-C4-N3	2.90	120.64	113.25
6	C	1356	QUE	C4-O12-C11	2.89	125.11	120.67
5	K	606	FAD	C2A-N3A-C4A	2.89	118.89	111.83
5	K	606	FAD	O2A-PA-O3P	2.84	114.94	107.27
6	C	1356	QUE	C2-C3-C4	2.82	120.10	117.41
8	L	1357	ZXF	C1'-C2'-S2'	2.77	121.72	120.15
5	B	606	FAD	C5A-N7A-C8A	2.73	107.73	103.45
6	L	1356	QUE	C1-C2-C3	-2.68	117.92	120.92
5	K	606	FAD	C4X-C10-N10	2.68	120.32	116.48
5	B	606	FAD	N3A-C4A-N9A	2.67	131.71	127.17
6	C	1356	QUE	C5-C4-C3	-2.66	117.16	121.79
5	K	606	FAD	O2P-P-O3P	2.63	114.38	107.27
5	K	606	FAD	C6A-C5A-C4A	2.58	120.71	117.18
5	K	606	FAD	C10-C4X-N5	-2.57	119.55	124.81
5	B	606	FAD	C10-C4X-N5	-2.57	119.57	124.81
5	K	606	FAD	C4-C4X-N5	2.56	121.75	118.21
8	C	1357	ZXF	O4-C4-C9	-2.50	121.22	127.26
8	C	1357	ZXF	O1P-P-O2P	2.48	117.11	107.80
5	B	606	FAD	O2A-PA-O3P	2.43	113.85	107.27
6	C	1356	QUE	O12-C11-C10	-2.42	117.90	120.19
6	C	1356	QUE	C11-C10-C9	-2.34	119.85	121.52
8	L	1357	ZXF	C4-C9-N5	2.33	122.62	116.27
5	K	606	FAD	O5'-C5'-C4'	-2.32	103.16	109.36
6	L	1356	QUE	C5-C6-C1	2.30	123.63	120.47
5	B	606	FAD	C2A-N1A-C6A	2.29	122.50	118.73
6	C	1356	QUE	C14-C19-C18	2.23	122.04	120.09
8	L	1357	ZXF	C9-C4-N3	2.23	118.24	112.13
8	C	1357	ZXF	C4-C9-N5	2.21	122.28	116.27
6	C	1356	QUE	C1-C2-C3	-2.20	118.46	120.92
5	K	606	FAD	C4A-C5A-N7A	-2.17	108.10	110.58
6	L	1356	QUE	C4-O12-C11	2.16	123.98	120.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	1356	QUE	C2-C3-C4	2.16	119.47	117.41
5	K	606	FAD	C5A-C6A-N6A	-2.09	118.11	123.29
6	L	1356	QUE	C4-C3-C9	-2.08	117.52	120.03
8	C	1357	ZXF	C9-C4-N3	2.07	117.82	112.13
5	K	606	FAD	O4'-C4'-C3'	2.07	114.09	109.25
6	L	1356	QUE	C5-C4-C3	-2.05	118.21	121.79

There are no chirality outliers.

All (4) torsion outliers are listed below:

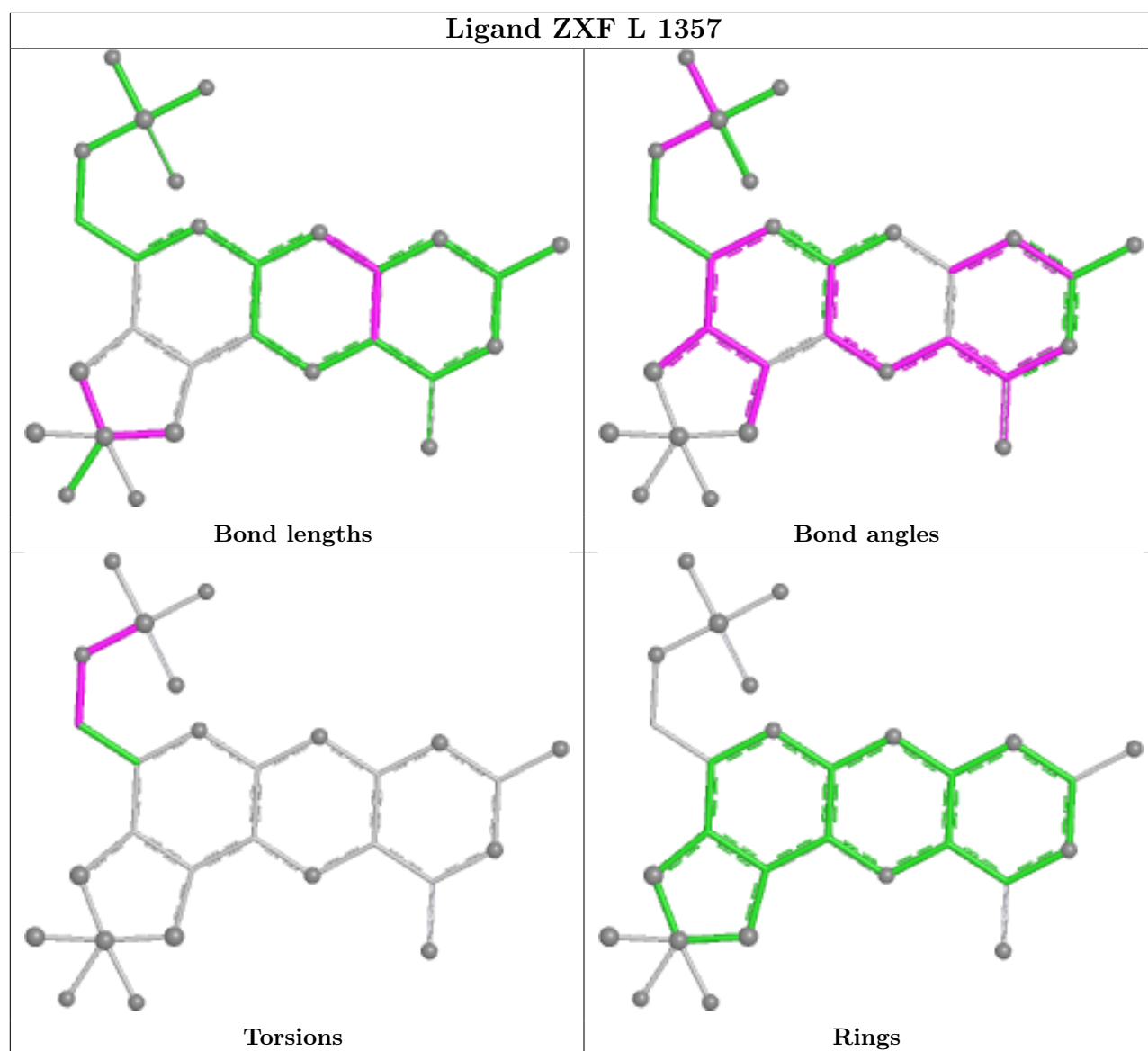
Mol	Chain	Res	Type	Atoms
8	L	1357	ZXF	C3'-C4'-O4'-P
5	B	606	FAD	C5B-O5B-PA-O1A
8	C	1357	ZXF	C3'-C4'-O4'-P
8	L	1357	ZXF	C4'-O4'-P-O1P

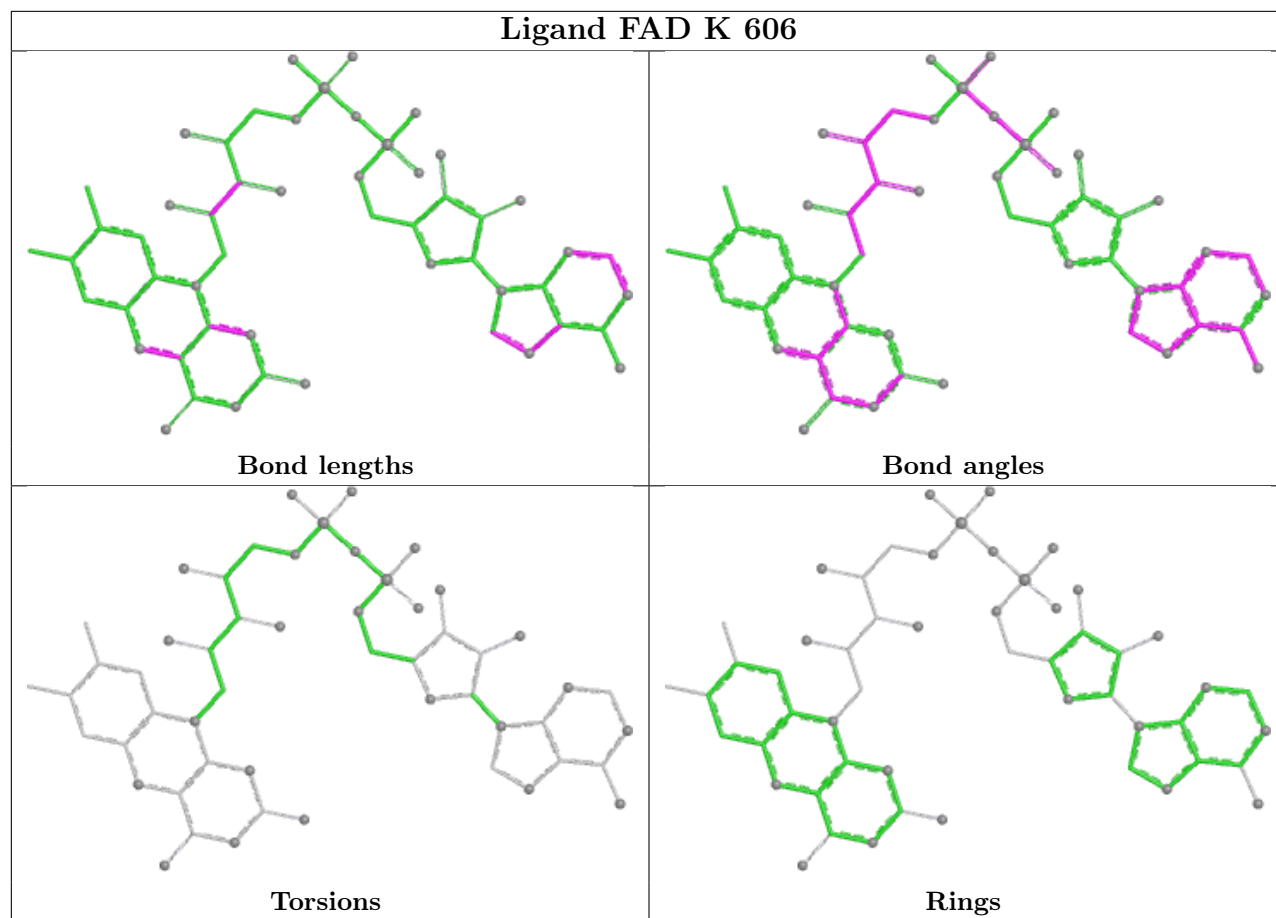
There are no ring outliers.

5 monomers are involved in 18 short contacts:

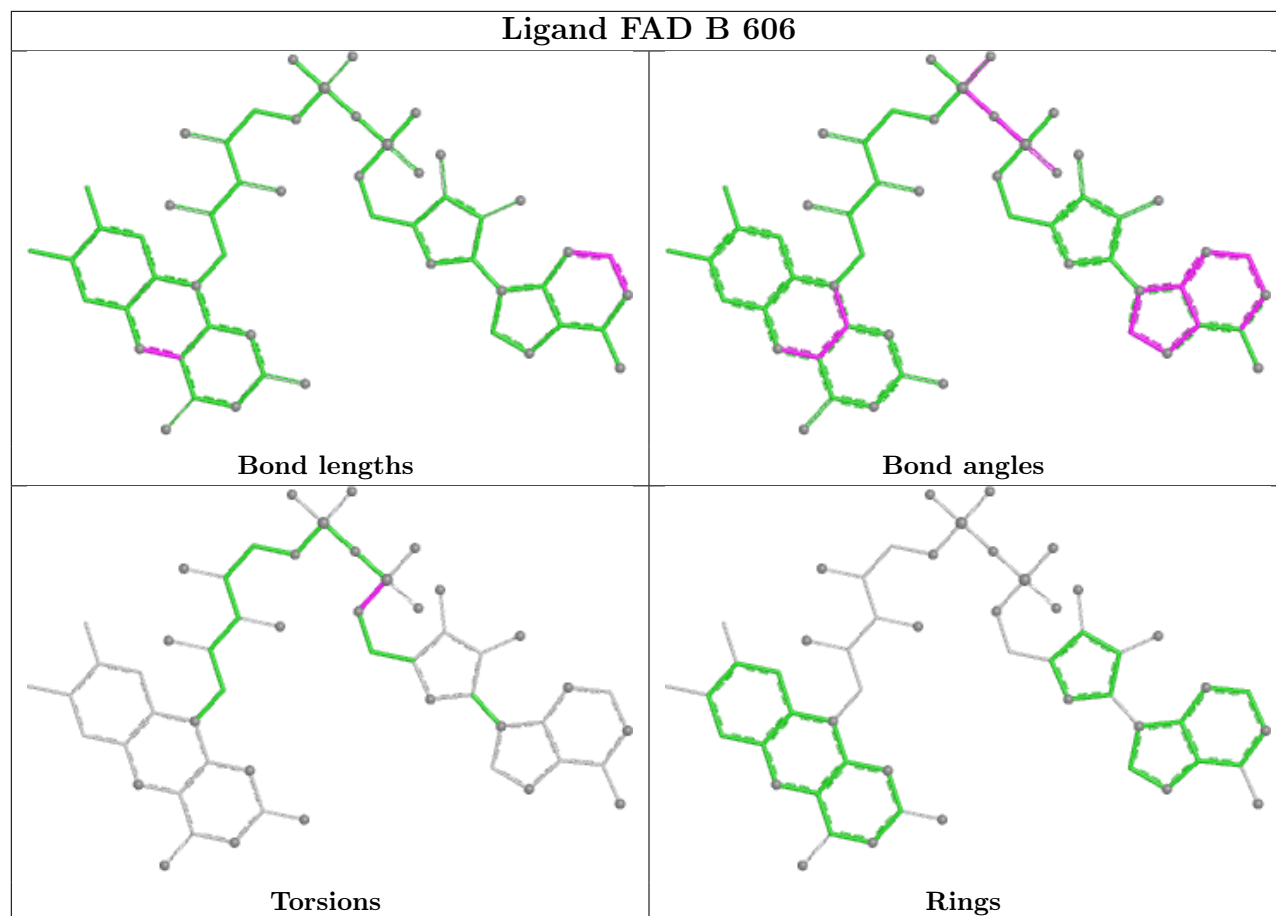
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	L	1357	ZXF	4	0
5	K	606	FAD	3	0
6	C	1356	QUE	4	0
6	L	1356	QUE	3	0
8	C	1357	ZXF	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

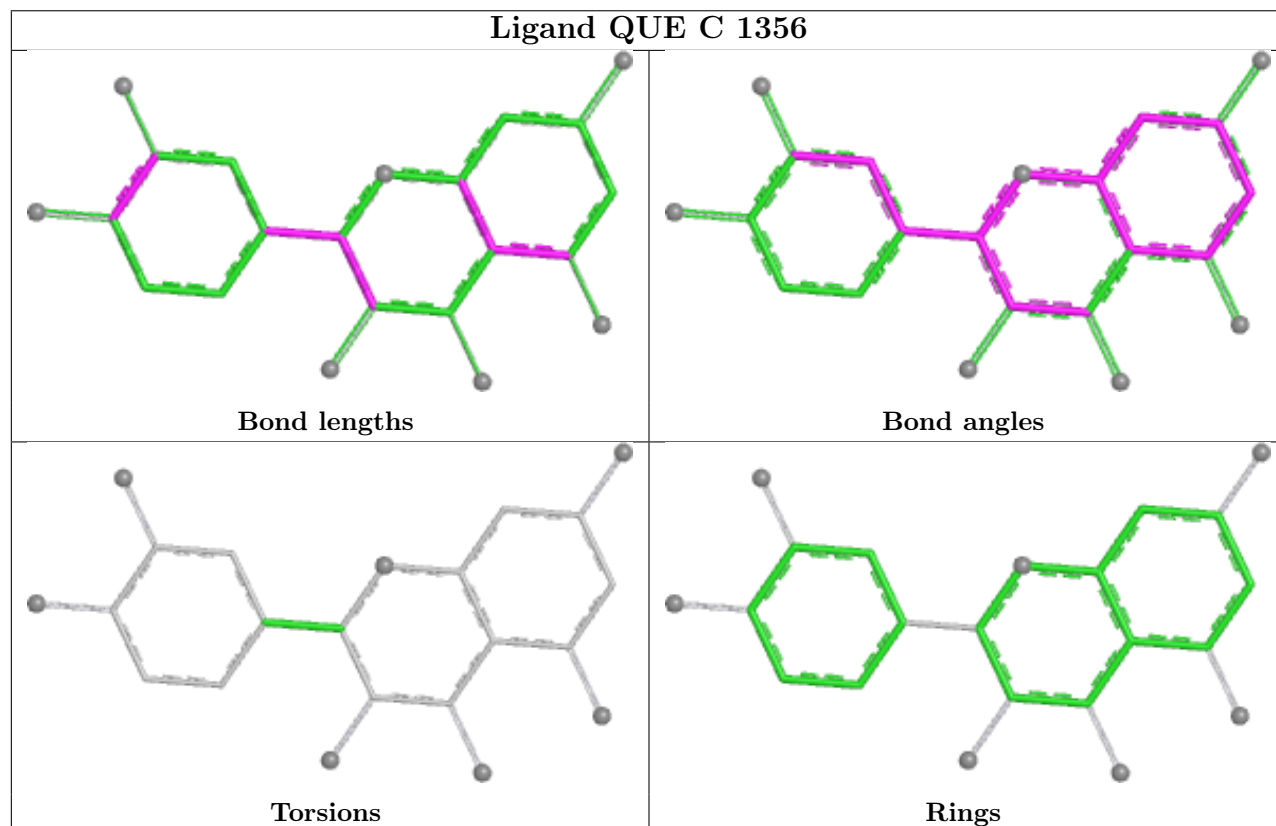


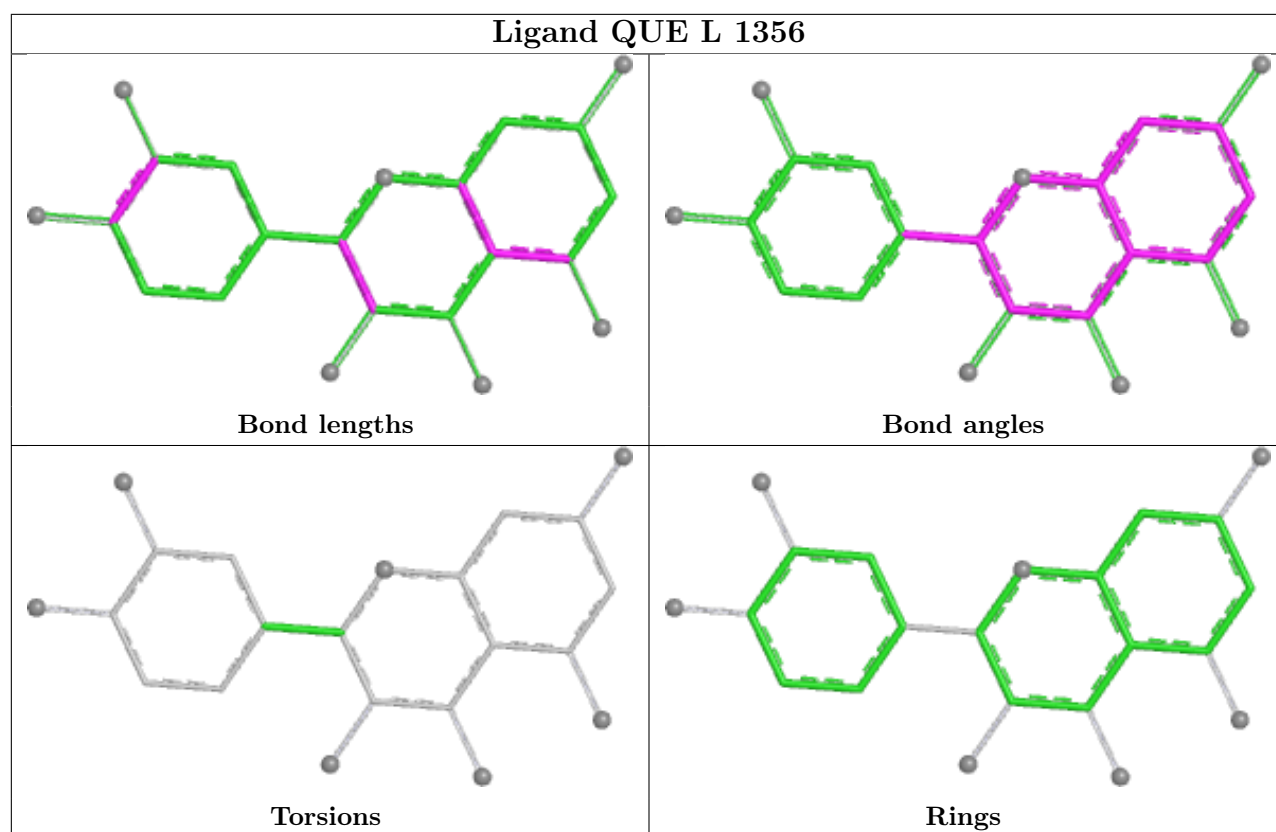


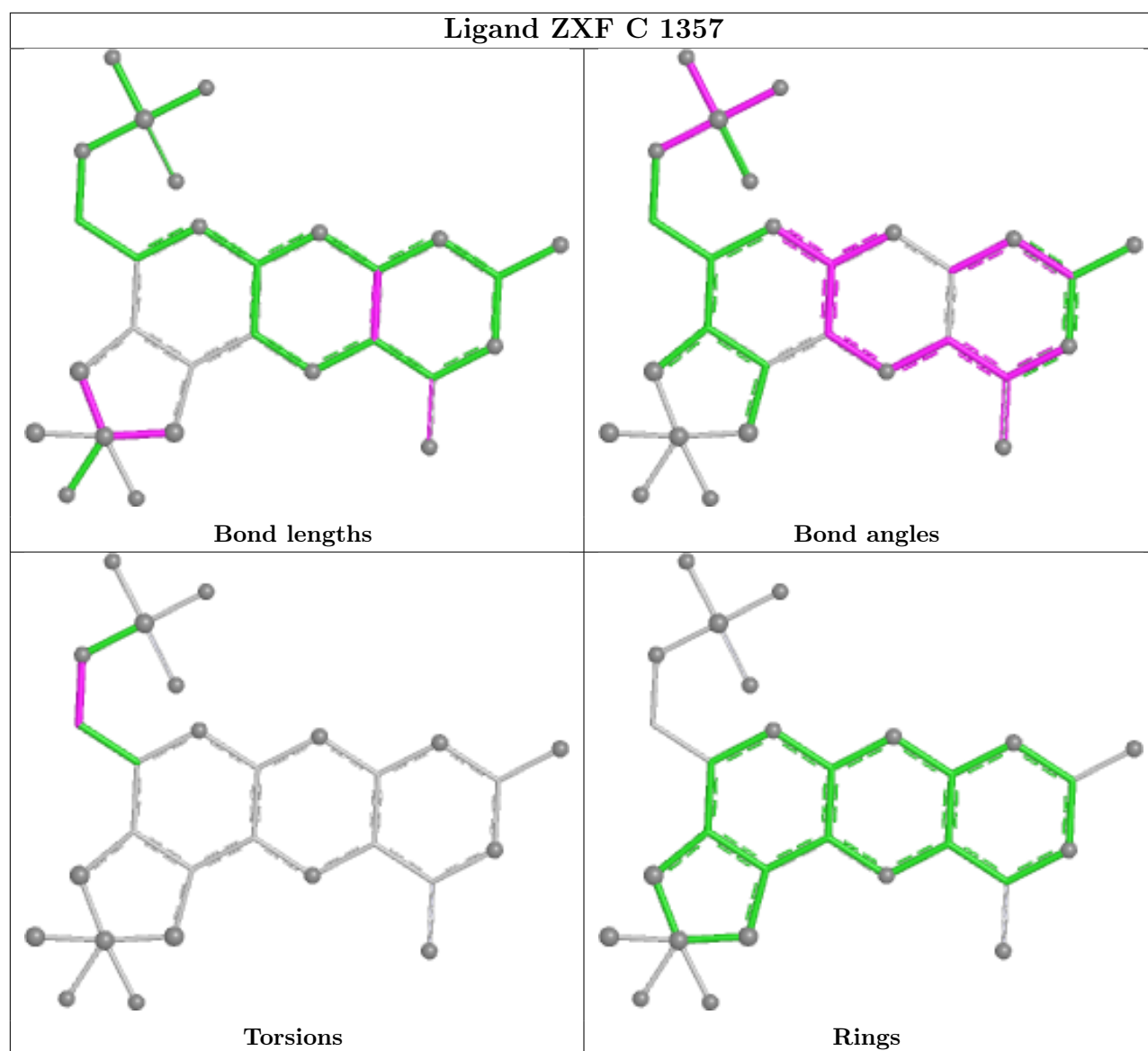
Ligand FAD B 606



Ligand QUE C 1356







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%)	-0.01	2 (1%) 76 76	11, 21, 38, 46	0
1	J	164/164 (100%)	0.13	7 (4%) 40 39	15, 25, 44, 59	0
2	B	334/334 (100%)	0.51	16 (4%) 35 34	18, 31, 46, 57	0
2	K	305/334 (91%)	0.79	23 (7%) 20 19	23, 37, 50, 58	0
3	C	756/756 (100%)	-0.26	4 (0%) 87 87	11, 20, 31, 37	0
3	L	745/756 (98%)	-0.05	16 (2%) 63 63	12, 22, 37, 68	0
All	All	2468/2508 (98%)	0.08	68 (2%) 55 54	11, 24, 43, 68	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	61	LEU	6.4
2	K	424	ALA	5.8
2	K	528	GLY	4.5
1	J	63	ASP	4.3
1	J	2	THR	3.9
3	L	1288	ASN	3.9
3	L	1287	ASN	3.7
2	K	425	SER	3.6
3	L	1289	ASN	3.6
2	K	484	GLN	3.6
1	A	141	ASP	3.5
3	L	1283	ALA	3.5
2	B	200	GLU	3.4
2	B	528	GLY	3.4
3	L	720	LYS	3.2
3	C	1216	GLU	3.2
3	L	1315	THR	3.1
2	K	336	TRP	3.1
2	K	272	ASN	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	L	1143	GLU	3.0
2	B	527	LEU	3.0
2	K	474	LEU	2.9
2	K	429	ASP	2.9
2	B	318	LYS	2.8
2	B	211	ILE	2.8
3	L	1290	THR	2.7
2	B	222	VAL	2.7
2	K	318	LYS	2.7
2	B	195	LEU	2.7
2	K	468	LYS	2.7
3	L	1286	THR	2.6
2	B	425	SER	2.6
1	J	64	LYS	2.6
1	J	165	LYS	2.5
2	K	335	ARG	2.4
2	K	442	PHE	2.4
2	K	224	PRO	2.4
2	B	378	GLY	2.3
1	J	103	GLU	2.3
2	B	424	ALA	2.3
1	J	61	LEU	2.3
3	L	1291	LYS	2.3
3	L	683	HIS	2.3
3	L	985	ASP	2.3
3	L	979	ALA	2.3
2	B	210	PRO	2.2
2	K	319	LEU	2.2
2	B	336	TRP	2.2
2	B	198	PRO	2.1
2	K	480	GLU	2.1
2	B	207	THR	2.1
2	K	444	PRO	2.1
3	L	857	VAL	2.1
3	C	724	SER	2.1
2	K	243	LYS	2.1
2	K	426	ARG	2.1
2	K	378	GLY	2.1
3	C	664	GLY	2.1
1	J	136	VAL	2.1
2	K	475	SER	2.1
3	L	1292	GLU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	L	1276	ASP	2.0
3	C	683	HIS	2.0
2	B	268	MET	2.0
2	K	273	GLN	2.0
2	K	467	LEU	2.0
2	B	224	PRO	2.0
2	K	379	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](#)

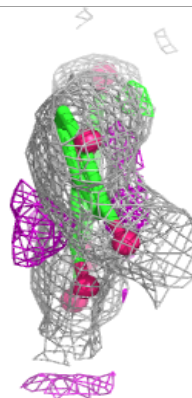
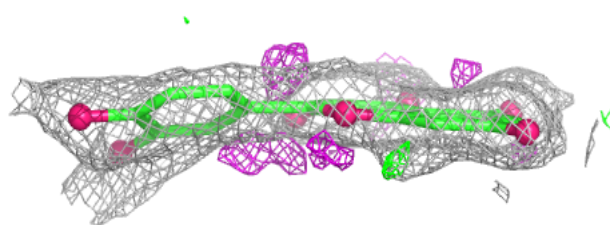
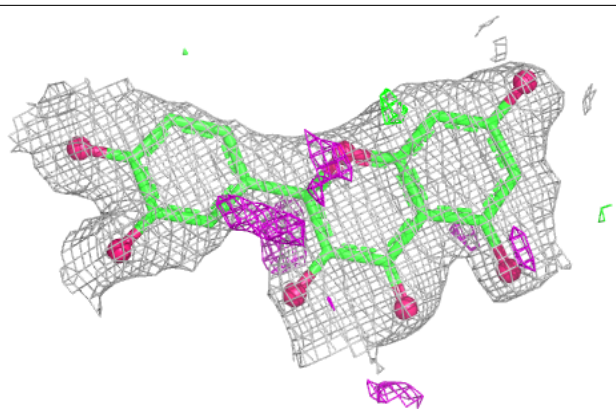
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	QUE	C	1356	22/22	0.84	0.12	35,37,38,40	0
6	QUE	L	1356	22/22	0.87	0.12	37,39,40,41	0
5	FAD	B	606	53/53	0.96	0.07	19,24,27,28	0
5	FAD	K	606	53/53	0.96	0.07	23,30,33,35	0
4	FES	J	602	4/4	0.98	0.04	17,17,18,18	0
4	FES	J	601	4/4	0.99	0.03	15,16,17,18	0
4	FES	A	602	4/4	0.99	0.03	15,15,17,18	0
8	ZXF	C	1357	28/28	0.99	0.05	12,14,21,34	0
8	ZXF	L	1357	28/28	0.99	0.05	13,17,28,35	0
4	FES	A	601	4/4	1.00	0.02	14,15,15,15	0

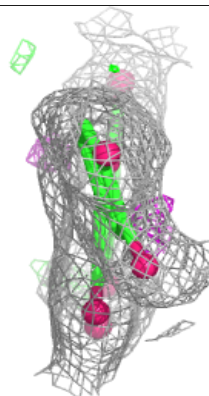
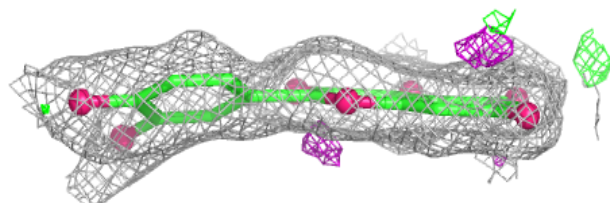
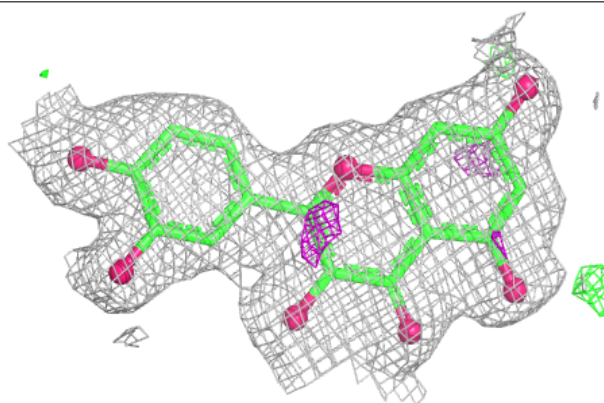
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around QUE C 1356:

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

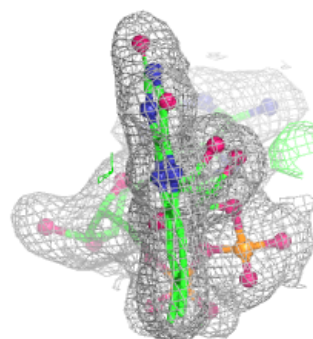
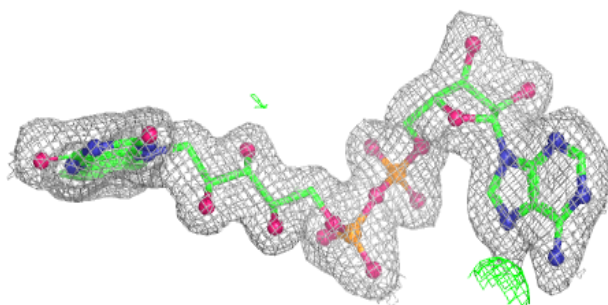
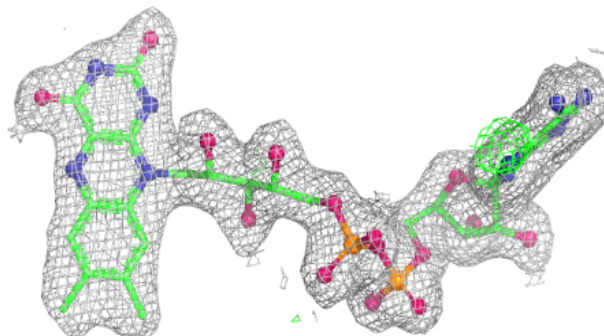
**Electron density around QUE L 1356:**

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

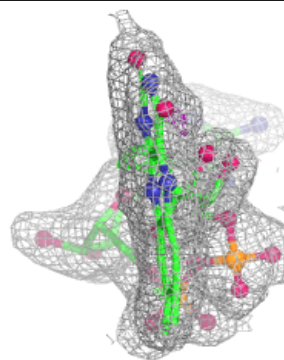
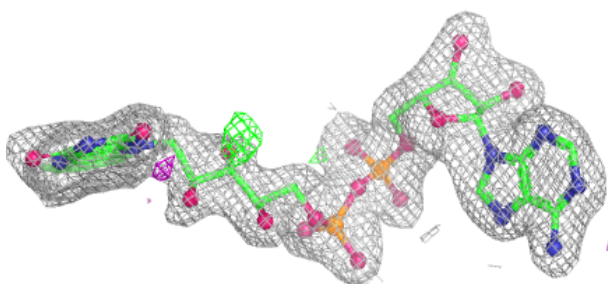
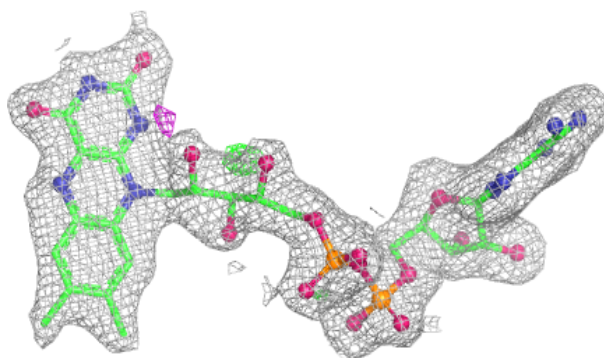


Electron density around FAD B 606:

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

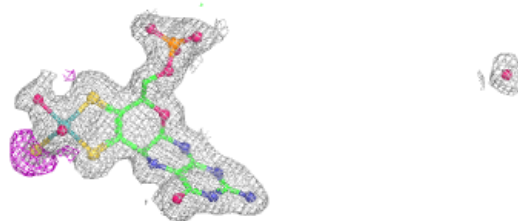
**Electron density around FAD K 606:**

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



Electron density around ZXF C 1357:

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

**Electron density around ZXF L 1357:**

$2mF_o-DF_c$ (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.