



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:03 AM GMT

PDB ID : 3NVZ  
Title : Crystal Structure of Bovine Xanthine Oxidase in Complex with Indole-3-Aldehyde  
Authors : Cao, H.; Hille, R.  
Deposited on : 2010-07-08  
Resolution : 1.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

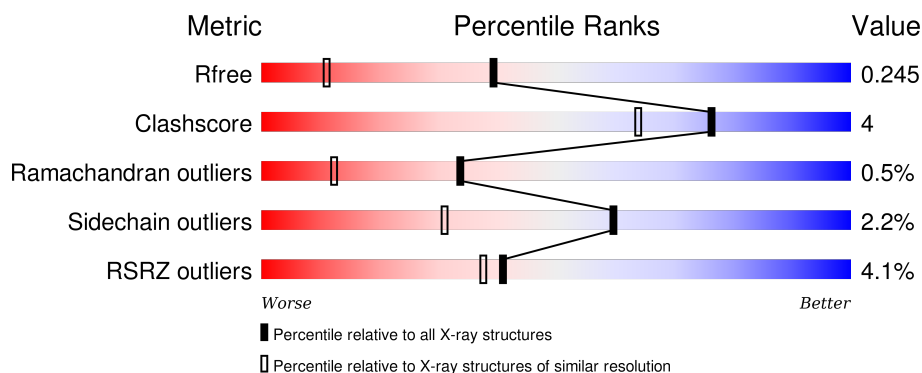
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



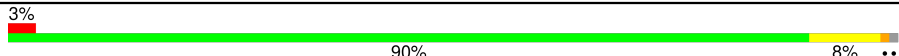
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2475 (1.60-1.60)
Clashscore	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)
RSRZ outliers	91569	2479 (1.60-1.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>4%</div> <div>94%</div> <div>5%</div> </div>
1	J	164	<div> <div>9%</div> <div>90%</div> <div>10%</div> </div>
2	B	305	<div> <div>5%</div> <div>89%</div> <div>9%</div> </div>
2	K	305	<div> <div>10%</div> <div>94%</div> <div>6%</div> </div>
3	C	755	<div> <div>%</div> <div>90%</div> <div>9%</div> </div>

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Mol	Chain	Length	Quality of chain
3	L	755	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	I3A	C	1	-	-	-	X
8	I3A	L	1	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 20672 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Xanthine dehydrogenase/oxidase.

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

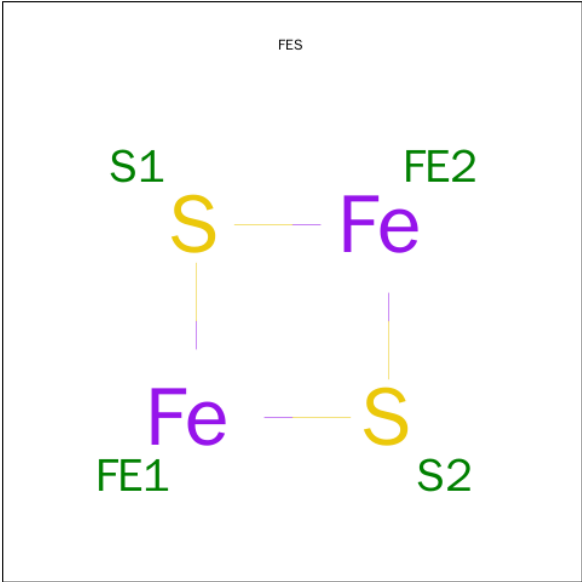
- Molecule 2 is a protein called Xanthine dehydrogenase/oxidase.

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

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

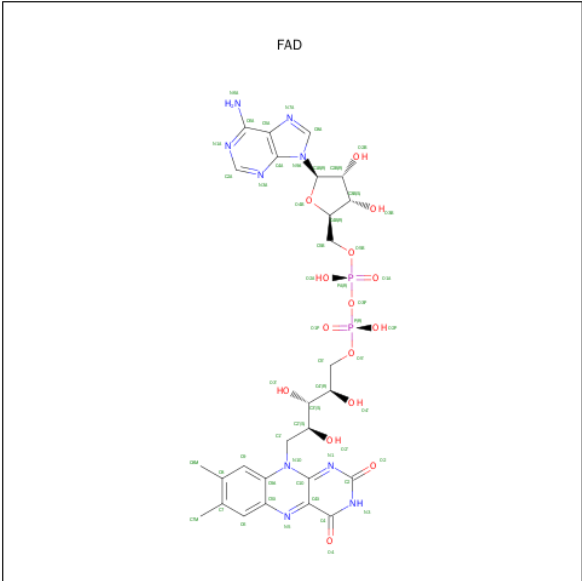
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	755	Total	C	N	O	S	0	0	0
			5823	3680	1003	1105	35			
3	L	745	Total	C	N	O	S	0	0	0
			5761	3643	992	1093	33			

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



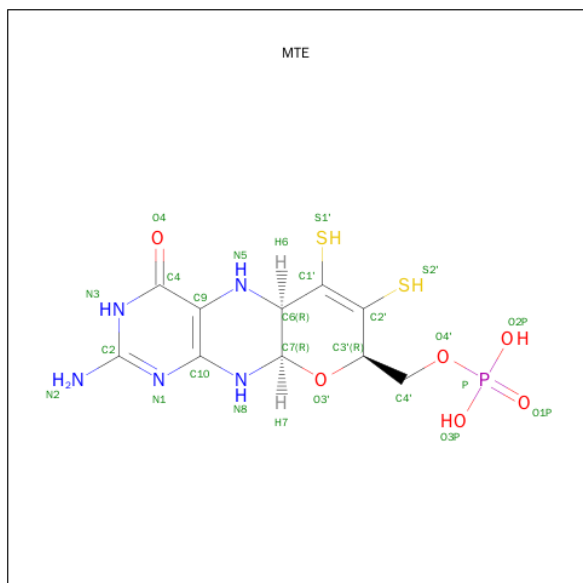
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			4	2	2		
4	A	1	Total	Fe	S	0	0
			4	2	2		
4	J	1	Total	Fe	S	0	0
			4	2	2		
4	J	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



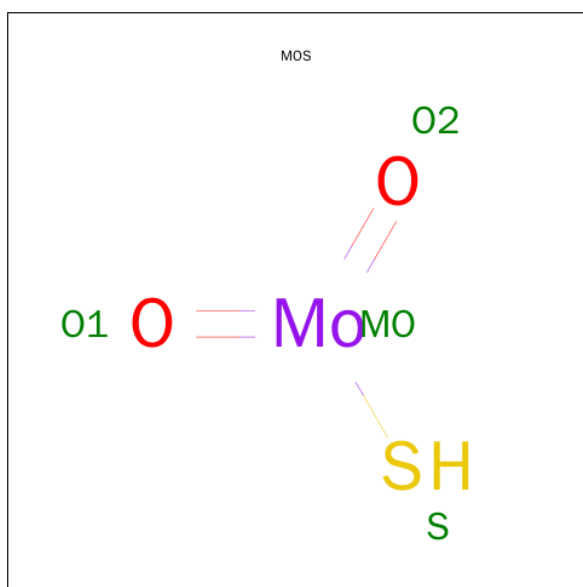
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	K	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 6 is PHOSPHONIC ACIDMONO-(2-AMINO-5,6-DIMERCAPTO-4-OXO-3,7,8A, 9,10,10A-HEXAHYDRO-4H-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-7-YLMETHYL) ESTER (three-letter code: MTE) (formula:  $C_{10}H_{14}N_5O_6P S_2$ ).



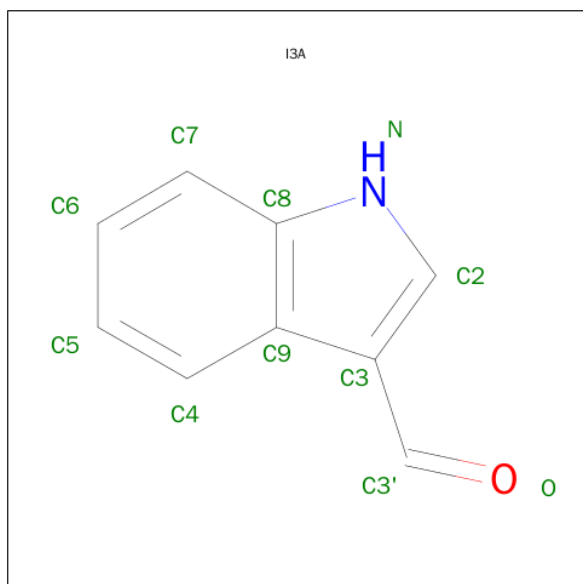
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	C	1	Total 24	C 10	N 5	O 6	P 1	S 2	0	0
6	L	1	Total 24	C 10	N 5	O 6	P 1	S 2	0	0

- Molecule 7 is DIOXOTHIOMOLYBDENUM(VI) ION (three-letter code: MOS) (formula:  $HMoO_2S$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	Mo	O	S	0	0
			4	1	2	1		
7	L	1	Total	Mo	O	S	0	0
			4	1	2	1		

- Molecule 8 is 1H-INDOLE-3-CARBALDEHYDE (three-letter code: I3A) (formula: C<sub>9</sub>H<sub>7</sub>NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	1	Total	C	N	O	0	0
			11	9	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	L	1	Total	C	N	O	0	0
			11	9	1	1		

- Molecule 9 is water.

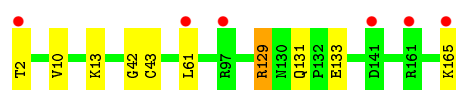
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	114	Total	O	0	0
			114	114		
9	B	192	Total	O	0	0
			192	192		
9	C	538	Total	O	0	0
			538	538		
9	J	111	Total	O	0	0
			111	111		
9	K	151	Total	O	0	0
			151	151		
9	L	494	Total	O	0	0
			494	494		



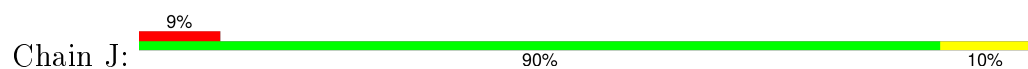
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

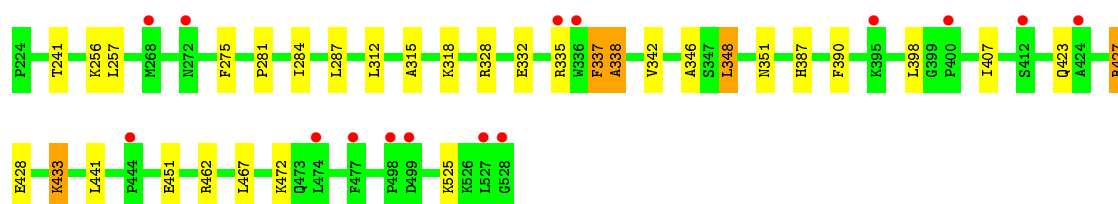
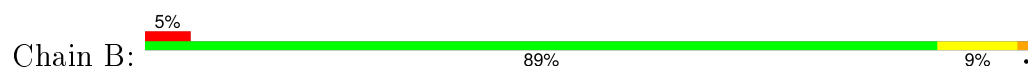
- Molecule 1: Xanthine dehydrogenase/oxidase



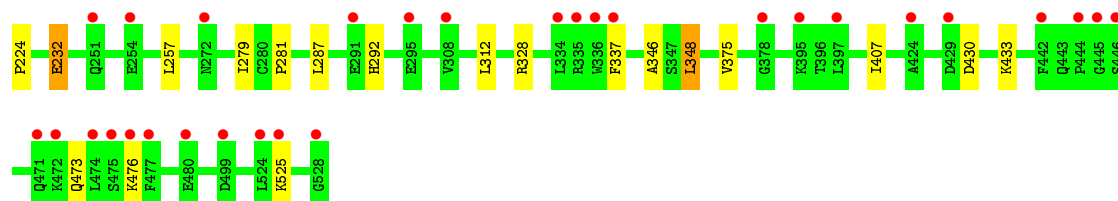
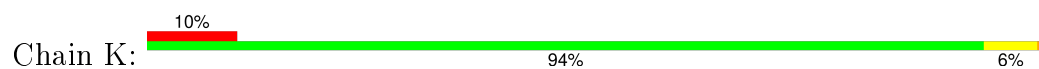
- Molecule 1: Xanthine dehydrogenase/oxidase



- Molecule 2: Xanthine dehydrogenase/oxidase

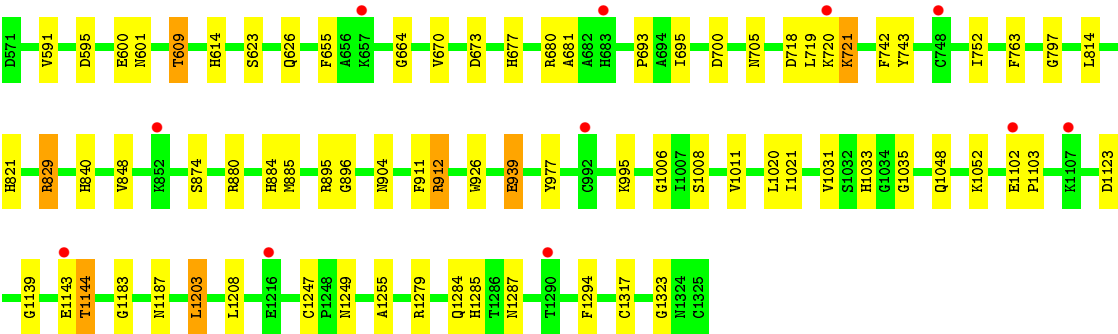


- Molecule 2: Xanthine dehydrogenase/oxidase

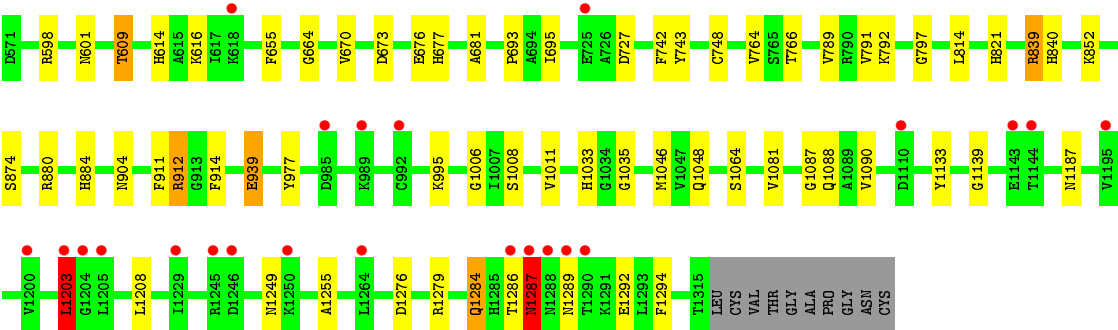
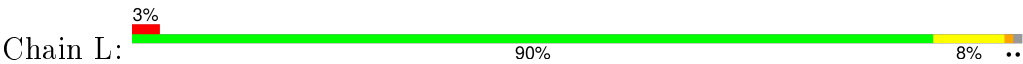


- Molecule 3: Xanthine dehydrogenase/oxidase





● 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, $\alpha$ , $\beta$ , $\gamma$	133.41Å 73.70Å 138.92Å 90.00° 97.12° 90.00°	Depositor
Resolution (Å)	45.20 – 1.60 45.18 – 1.60	Depositor EDS
% Data completeness (in resolution range)	96.5 (45.20-1.60) 96.2 (45.18-1.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.09 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.215 , 0.246 0.213 , 0.245	Depositor DCC
$R_{free}$ test set	17094 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.1	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 54.7	EDS
Estimated twinning fraction	0.008 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 339739 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	20672	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MOS, I3A, FES, FAD, MTE

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	0.59	0/1277	0.66	0/1723
1	J	0.56	0/1277	0.61	0/1723
2	B	0.51	0/2438	0.59	0/3290
2	K	0.47	0/2438	0.57	0/3290
3	C	0.59	0/5951	0.68	4/8061 (0.0%)
3	L	0.57	1/5888 (0.0%)	0.65	3/7974 (0.0%)
All	All	0.56	1/19269 (0.0%)	0.64	7/26061 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	748	CYS	CB-SG	-6.14	1.71	1.82

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	829	ARG	NE-CZ-NH2	-13.21	113.69	120.30
3	C	829	ARG	NE-CZ-NH1	11.19	125.90	120.30
3	L	839	ARG	NE-CZ-NH2	-10.14	115.23	120.30
3	L	839	ARG	NE-CZ-NH1	7.92	124.26	120.30
3	C	1203	LEU	CA-CB-CG	7.54	132.63	115.30
3	L	1203	LEU	CA-CB-CG	6.79	130.91	115.30
3	C	829	ARG	CD-NE-CZ	5.44	131.22	123.60

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	5	0
1	J	1255	0	1265	16	0
2	B	2389	0	2459	21	0
2	K	2389	0	2459	8	0
3	C	5823	0	5746	55	0
3	L	5761	0	5685	45	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	1	0
6	C	24	0	10	0	0
6	L	24	0	10	0	0
7	C	4	0	0	1	0
7	L	4	0	0	1	0
8	C	11	0	7	2	0
8	L	11	0	7	1	0
9	A	114	0	0	0	0
9	B	192	0	0	4	0
9	C	538	0	0	4	0
9	J	111	0	0	6	0
9	K	151	0	0	2	0
9	L	494	0	0	3	0
All	All	20672	0	18975	146	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (146) 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:1052:LYS:HE3	9:C:1502:HOH:O	1.11	1.22
3:L:1081:VAL:HG21	9:L:1363:HOH:O	1.03	1.19
2:B:241:THR:HB	9:B:752:HOH:O	1.03	1.18
3:L:764:VAL:HB	9:L:1454:HOH:O	0.94	1.11
3:C:1143:GLU:O	3:C:1144:THR:HG23	1.62	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1102:GLU:HG2	3:C:1103:PRO:HD3	1.54	0.87
1:J:32:ARG:NE	9:J:1229:HOH:O	1.92	0.86
3:C:884:HIS:HE1	3:C:1006:GLY:H	1.22	0.85
1:J:104:ARG:HH11	1:J:162:THR:HG23	1.42	0.84
1:A:131:GLN:HE21	1:A:133:GLU:H	1.27	0.82
3:L:695:ILE:H	3:L:904:ASN:HD22	1.29	0.80
3:L:1088:GLN:HG2	3:L:1133:TYR:CD1	2.17	0.79
3:C:680:ARG:NH2	9:C:2132:HOH:O	2.13	0.79
3:C:695:ILE:H	3:C:904:ASN:HD22	1.33	0.77
3:C:1033:HIS:HD2	3:C:1035:GLY:H	1.33	0.75
3:L:884:HIS:HE1	3:L:1006:GLY:H	1.35	0.73
3:C:1317:CYS:SG	3:C:1323:GLY:HA3	2.32	0.70
1:A:42:GLY:O	3:C:829:ARG:HD2	1.90	0.70
3:C:884:HIS:CE1	3:C:1006:GLY:H	2.08	0.69
3:C:705:ASN:OD1	9:C:1525:HOH:O	2.10	0.69
1:J:131:GLN:HE21	1:J:133:GLU:H	1.41	0.68
1:J:159:GLY:O	1:J:162:THR:HG22	1.93	0.68
3:C:1033:HIS:CD2	3:C:1035:GLY:H	2.13	0.67
3:L:840:HIS:HE1	3:L:874:SER:OG	1.77	0.67
3:L:1046:MET:HE2	3:L:1090:VAL:HG21	1.76	0.66
3:L:884:HIS:CE1	3:L:1006:GLY:H	2.15	0.65
3:C:601:ASN:O	3:C:821:HIS:HD2	1.80	0.64
3:L:1011:VAL:HG23	8:L:1:I3A:H5	1.80	0.64
3:C:695:ILE:HG23	3:C:700:ASP:HB3	1.80	0.63
3:C:720:LYS:O	3:C:721:LYS:CB	2.47	0.63
3:C:1011:VAL:HG23	8:C:1:I3A:H5	1.81	0.62
3:C:939:GLU:HG2	3:C:977:TYR:CE2	2.35	0.62
1:J:57:LYS:HE2	1:J:66:ILE:HD11	1.81	0.61
1:J:104:ARG:HD3	1:J:162:THR:HG21	1.82	0.61
3:C:995:LYS:NZ	3:C:1284:GLN:HE21	1.98	0.61
3:C:623:SER:HA	3:C:626:GLN:HE21	1.66	0.61
3:C:752:ILE:CD1	3:C:763:PHE:HE1	2.12	0.61
7:L:1327:MOS:MO	7:L:1327:MOS:O2	1.72	0.60
3:L:1046:MET:HE1	3:L:1090:VAL:HB	1.82	0.60
3:C:609:THR:HG23	3:C:664:GLY:HA2	1.84	0.60
3:C:840:HIS:HE1	3:C:874:SER:OG	1.85	0.60
3:L:609:THR:HG22	9:L:500:HOH:O	2.01	0.60
3:L:995:LYS:NZ	3:L:1284:GLN:HE21	2.00	0.59
3:C:752:ILE:HD11	3:C:763:PHE:HE1	1.67	0.59
1:J:104:ARG:NH1	1:J:162:THR:HG23	2.14	0.59
3:L:609:THR:HG23	3:L:664:GLY:HA2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:1033:HIS:HD2	3:L:1035:GLY:H	1.51	0.58
9:B:1039:HOH:O	3:C:680:ARG:HG2	2.04	0.57
2:K:281:PRO:HB2	2:K:287:LEU:CD1	2.35	0.57
3:C:673:ASP:OD2	3:C:677:HIS:HD2	1.88	0.56
3:C:1048:GLN:HE22	3:C:1187:ASN:HD22	1.53	0.56
1:J:32:ARG:CZ	9:J:1229:HOH:O	2.44	0.56
3:C:718:ASP:OD2	3:C:720:LYS:O	2.24	0.56
3:L:673:ASP:OD2	3:L:677:HIS:HD2	1.89	0.55
3:C:719:LEU:HD12	3:C:895:ARG:NH1	2.21	0.55
3:L:764:VAL:HG23	3:L:791:VAL:HG22	1.87	0.55
2:B:315:ALA:HA	2:B:318:LYS:HE2	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	0.55
3:C:848:VAL:HG21	3:C:926:TRP:HB2	1.88	0.55
3:L:764:VAL:HG23	3:L:766:THR:HG22	1.88	0.55
3:C:720:LYS:O	3:C:721:LYS:HB2	2.07	0.54
3:L:727:ASP:HB3	3:L:852:LYS:HE2	1.90	0.54
2:B:241:THR:HG23	9:B:138:HOH:O	2.08	0.54
1:J:32:ARG:NH2	9:J:1229:HOH:O	2.42	0.53
3:L:764:VAL:HG21	3:L:789:VAL:CG1	2.39	0.53
3:C:670:VAL:HG11	3:C:681:ALA:HB3	1.90	0.52
2:K:348:LEU:HD13	2:K:407:ILE:HD13	1.91	0.52
3:L:880:ARG:O	3:L:884:HIS:HD2	1.93	0.51
3:L:1249:ASN:O	3:L:1255:ALA:HA	2.11	0.51
3:L:655:PHE:HE1	3:L:814:LEU:HD23	1.75	0.51
3:C:614:HIS:HD2	3:C:693:PRO:O	1.93	0.51
3:L:609:THR:CG2	3:L:664:GLY:HA2	2.40	0.51
3:L:1046:MET:CE	3:L:1090:VAL:HG21	2.41	0.50
3:L:1048:GLN:HE22	3:L:1187:ASN:HD22	1.57	0.50
2:B:332:GLU:HA	2:B:335:ARG:HG3	1.93	0.50
3:C:600:GLU:HG2	3:L:598:ARG:O	2.12	0.50
2:B:256:LYS:HG3	2:B:275:PHE:CD2	2.47	0.50
3:C:1285:HIS:HD2	9:C:334:HOH:O	1.95	0.49
3:C:995:LYS:HZ3	3:C:1284:GLN:HE21	1.60	0.49
2:K:292:HIS:HE1	9:K:543:HOH:O	1.95	0.49
2:B:427:ARG:HG2	2:B:428:GLU:HG2	1.94	0.49
3:C:1021:ILE:HD12	3:C:1031:VAL:HG22	1.94	0.48
3:L:792:LYS:NZ	3:L:1064:SER:O	2.41	0.48
1:A:10:VAL:O	1:A:13:LYS:HG2	2.13	0.48
3:L:1286:THR:OG1	3:L:1287:ASN:N	2.47	0.48
3:L:1033:HIS:CD2	3:L:1035:GLY:H	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:63:ASP:O	1:J:64:LYS:HG3	2.14	0.47
3:L:614:HIS:HD2	3:L:693:PRO:O	1.97	0.47
3:L:601:ASN:O	3:L:821:HIS:HD2	1.98	0.47
2:K:224:PRO:N	9:K:812:HOH:O	2.47	0.47
3:L:839:ARG:NH2	3:L:912:ARG:O	2.39	0.46
3:C:1102:GLU:HG2	3:C:1103:PRO:CD	2.36	0.46
3:C:601:ASN:HB2	3:C:821:HIS:CD2	2.51	0.46
3:C:1011:VAL:CG2	8:C:1:I3A:H5	2.45	0.46
3:C:912:ARG:N	7:C:1327:MOS:S	2.89	0.46
2:B:256:LYS:HG3	2:B:275:PHE:CG	2.51	0.46
3:C:1048:GLN:NE2	3:C:1187:ASN:HD22	2.14	0.45
2:B:427:ARG:O	2:B:427:ARG:HG2	2.16	0.45
3:L:995:LYS:HZ1	3:L:1284:GLN:HE21	1.65	0.45
3:C:1249:ASN:O	3:C:1255:ALA:HA	2.17	0.45
3:C:1143:GLU:O	3:C:1144:THR:CG2	2.50	0.45
1:J:104:ARG:HD3	1:J:162:THR:CG2	2.47	0.45
3:L:1279:ARG:HG2	3:L:1294:PHE:HE2	1.82	0.44
1:J:32:ARG:NH1	3:L:676:GLU:OE2	2.50	0.44
2:B:281:PRO:HB2	2:B:287:LEU:CD1	2.48	0.44
2:B:284:ILE:HB	2:B:287:LEU:HD12	1.99	0.44
2:B:390:PHE:O	2:B:462:ARG:HD2	2.18	0.44
2:B:423:GLN:HB3	2:B:433:LYS:HG2	1.99	0.44
3:L:609:THR:HG23	3:L:664:GLY:CA	2.47	0.43
3:C:1020:LEU:C	3:C:1021:ILE:HD13	2.39	0.43
2:K:473:GLN:O	2:K:476:LYS:HB2	2.19	0.43
1:J:95:LYS:NZ	9:J:708:HOH:O	2.45	0.43
3:C:655:PHE:HE1	3:C:814:LEU:HD23	1.83	0.43
3:C:1183:GLY:HA2	3:C:1247:CYS:O	2.18	0.43
3:C:601:ASN:O	3:C:821:HIS:CD2	2.68	0.42
1:J:95:LYS:CE	9:J:708:HOH:O	2.66	0.42
3:C:752:ILE:HD11	3:C:763:PHE:CE1	2.51	0.42
2:B:441:LEU:HB3	2:B:451:GLU:HB2	2.01	0.42
1:J:32:ARG:NH1	9:J:684:HOH:O	2.47	0.42
2:B:342:VAL:HG23	9:B:942:HOH:O	2.20	0.42
3:C:609:THR:CG2	3:C:664:GLY:HA2	2.49	0.42
3:L:670:VAL:HG11	3:L:681:ALA:HB3	2.02	0.42
2:B:337:PHE:O	2:B:338:ALA:O	2.37	0.42
3:L:1203:LEU:C	3:L:1203:LEU:HD12	2.40	0.42
3:L:1046:MET:HA	3:L:1046:MET:CE	2.50	0.41
2:B:348:LEU:HD13	2:B:407:ILE:HD13	2.02	0.41
3:C:1021:ILE:CD1	3:C:1031:VAL:HG13	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:281:PRO:HB2	2:B:287:LEU:HD13	2.02	0.41
3:L:1289:ASN:HB3	3:L:1292:GLU:HB2	2.02	0.41
1:J:36:LEU:HD22	1:J:89:GLU:HG3	2.02	0.41
2:B:387:HIS:CE1	2:B:467:LEU:HD11	2.55	0.41
3:L:1046:MET:CE	3:L:1087:GLY:HA2	2.51	0.41
2:B:346:ALA:HB1	5:B:606:FAD:H4'	2.03	0.41
3:C:885:MET:SD	3:C:896:GLY:HA3	2.60	0.41
1:A:43:CYS:HA	3:C:829:ARG:HB2	2.02	0.41
3:L:840:HIS:CE1	3:L:874:SER:OG	2.67	0.41
2:K:257:LEU:HA	2:K:279:ILE:O	2.21	0.41
1:A:129:ARG:HA	1:A:129:ARG:HD3	1.78	0.41
2:B:257:LEU:HD13	2:B:281:PRO:HG3	2.01	0.41
3:L:880:ARG:HD2	3:L:914:PHE:HB3	2.03	0.40
2:K:346:ALA:HB1	5:K:606:FAD:H4'	2.03	0.40
3:C:1279:ARG:HG2	3:C:1294:PHE:HE2	1.85	0.40
2:K:232:GLU:OE1	3:L:677:HIS:HE1	2.03	0.40
2:B:338:ALA:HB1	2:B:342:VAL:HB	2.03	0.40
3:C:591:VAL:HG13	3:C:595:ASP:HB2	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
1	J	162/164 (99%)	157 (97%)	5 (3%)	0	100	100
2	B	303/305 (99%)	295 (97%)	7 (2%)	1 (0%)	46	23
2	K	303/305 (99%)	296 (98%)	7 (2%)	0	100	100
3	C	753/755 (100%)	733 (97%)	14 (2%)	6 (1%)	24	6
3	L	743/755 (98%)	728 (98%)	10 (1%)	5 (1%)	26	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2426/2448 (99%)	2365 (98%)	49 (2%)	12 (0%)	34 12

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	338	ALA
3	C	721	LYS
3	C	1008	SER
3	C	1144	THR
3	L	1008	SER
3	L	912	ARG
3	C	912	ARG
3	L	1139	GLY
3	L	1287	ASN
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%)	50 21
1	J	137/137 (100%)	134 (98%)	3 (2%)	60 31
2	B	261/261 (100%)	251 (96%)	10 (4%)	40 13
2	K	261/261 (100%)	252 (97%)	9 (3%)	44 16
3	C	631/631 (100%)	622 (99%)	9 (1%)	74 53
3	L	624/631 (99%)	613 (98%)	11 (2%)	66 41
All	All	2051/2058 (100%)	2005 (98%)	46 (2%)	60 31

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	61	LEU
1	A	129	ARG
1	A	165	LYS
2	B	312	LEU
2	B	328	ARG
2	B	337	PHE
2	B	348	LEU
2	B	351	ASN
2	B	398	LEU
2	B	427	ARG
2	B	433	LYS
2	B	472	LYS
2	B	525	LYS
3	C	609	THR
3	C	742	PHE
3	C	743	TYR
3	C	911	PHE
3	C	939	GLU
3	C	1123	ASP
3	C	1203	LEU
3	C	1208	LEU
3	C	1287	ASN
1	J	2	THR
1	J	82	HIS
1	J	93	SER
2	K	232	GLU
2	K	312	LEU
2	K	328	ARG
2	K	337	PHE
2	K	348	LEU
2	K	375	VAL
2	K	430	ASP
2	K	433	LYS
2	K	525	LYS
3	L	609	THR
3	L	616	LYS
3	L	742	PHE
3	L	743	TYR
3	L	911	PHE
3	L	939	GLU
3	L	1203	LEU
3	L	1208	LEU

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Mol	Chain	Res	Type
3	L	1276	ASP
3	L	1284	GLN
3	L	1287	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	144	GLN
1	A	146	ASN
2	B	272	ASN
2	B	351	ASN
3	C	614	HIS
3	C	626	GLN
3	C	677	HIS
3	C	683	HIS
3	C	821	HIS
3	C	840	HIS
3	C	884	HIS
3	C	904	ASN
3	C	1016	GLN
3	C	1033	HIS
3	C	1048	GLN
3	C	1284	GLN
3	C	1285	HIS
3	C	1287	ASN
3	C	1324	ASN
1	J	131	GLN
1	J	144	GLN
1	J	146	ASN
2	K	292	HIS
2	K	351	ASN
3	L	585	GLN
3	L	614	HIS
3	L	626	GLN
3	L	677	HIS
3	L	705	ASN
3	L	821	HIS
3	L	840	HIS
3	L	884	HIS
3	L	904	ASN
3	L	1016	GLN

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Mol	Chain	Res	Type
3	L	1033	HIS
3	L	1048	GLN
3	L	1284	GLN
3	L	1287	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	FES	A	601	1	0,4,4	0.00	-	0,4,4	0.00	-
4	FES	A	602	1	0,4,4	0.00	-	0,4,4	0.00	-
5	FAD	B	606	-	48,58,58	1.23	5 (10%)	54,89,89	2.26	7 (12%)
8	I3A	C	1	-	11,12,12	1.50	3 (27%)	11,16,16	1.11	1 (9%)
6	MTE	C	1326	7	19,26,26	1.06	1 (5%)	19,40,40	2.16	7 (36%)
7	MOS	C	1327	6	0,3,3	0.00	-	0,3,3	0.00	-
4	FES	J	601	1	0,4,4	0.00	-	0,4,4	0.00	-
4	FES	J	602	1	0,4,4	0.00	-	0,4,4	0.00	-
5	FAD	K	606	-	48,58,58	1.29	5 (10%)	54,89,89	2.03	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	I3A	L	1	-	11,12,12	1.52	3 (27%)	11,16,16	0.74	0
6	MTE	L	1326	7	19,26,26	1.02	1 (5%)	19,40,40	1.87	4 (21%)
7	MOS	L	1327	6	0,3,3	0.00	-	0,3,3	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FES	A	601	1	-	0/0/4/4	0/1/1/1
4	FES	A	602	1	-	0/0/4/4	0/1/1/1
5	FAD	B	606	-	-	0/30/50/50	0/6/6/6
8	I3A	C	1	-	-	0/0/2/2	0/2/2/2
6	MTE	C	1326	7	-	0/6/34/34	0/3/3/3
7	MOS	C	1327	6	-	0/0/0/0	0/0/0/0
4	FES	J	601	1	-	0/0/4/4	0/1/1/1
4	FES	J	602	1	-	0/0/4/4	0/1/1/1
5	FAD	K	606	-	-	0/30/50/50	0/6/6/6
8	I3A	L	1	-	-	0/0/2/2	0/2/2/2
6	MTE	L	1326	7	-	0/6/34/34	0/3/3/3
7	MOS	L	1327	6	-	0/0/0/0	0/0/0/0

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	606	FAD	C2A-N1A	2.14	1.38	1.33
8	C	1	I3A	C6-C7	2.18	1.41	1.36
5	B	606	FAD	C1'-N10	2.30	1.50	1.48
8	C	1	I3A	C5-C4	2.32	1.42	1.36
8	L	1	I3A	C6-C7	2.34	1.42	1.36
8	L	1	I3A	C5-C4	2.42	1.42	1.36
5	K	606	FAD	C5X-N5	2.45	1.39	1.35
8	C	1	I3A	C3-C3'	2.46	1.54	1.46
8	L	1	I3A	C3-C3'	2.50	1.54	1.46
5	K	606	FAD	C2A-N1A	2.66	1.39	1.33
5	B	606	FAD	C4-N3	2.68	1.38	1.33
5	K	606	FAD	C4-N3	3.13	1.38	1.33
6	L	1326	MTE	C9-C10	3.24	1.48	1.41
6	C	1326	MTE	C9-C10	3.50	1.48	1.41
5	K	606	FAD	C2A-N3A	3.91	1.39	1.32
5	B	606	FAD	C2A-N3A	3.97	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	606	FAD	C4X-N5	4.13	1.39	1.33
5	K	606	FAD	C4X-N5	4.29	1.40	1.33

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	606	FAD	N3A-C2A-N1A	-12.65	119.21	128.89
5	K	606	FAD	N3A-C2A-N1A	-11.56	120.04	128.89
5	B	606	FAD	C4X-C4-N3	-2.93	119.58	123.59
5	K	606	FAD	C4X-C4-N3	-2.78	119.78	123.59
6	C	1326	MTE	O3P-P-O4'	-2.73	98.71	106.56
8	C	1	I3A	C5-C4-C9	-2.58	117.23	120.88
6	C	1326	MTE	N3-C2-N1	-2.34	121.70	125.53
5	K	606	FAD	C4A-C5A-N7A	-2.13	107.52	109.48
6	L	1326	MTE	O2P-P-O4'	-2.09	100.55	106.56
5	K	606	FAD	C4-C4X-N5	2.02	121.17	118.72
6	C	1326	MTE	C10-C9-N5	2.05	121.44	118.85
5	B	606	FAD	C4-C4X-N5	2.10	121.27	118.72
6	C	1326	MTE	O3P-P-O2P	2.35	116.31	107.38
5	B	606	FAD	C2B-C1B-N9A	2.43	118.00	114.29
6	C	1326	MTE	C2-N1-C10	2.46	120.07	114.54
5	K	606	FAD	C4X-N5-C5X	2.55	119.70	116.76
6	L	1326	MTE	C2-N1-C10	2.79	120.80	114.54
6	C	1326	MTE	N8-C10-N1	3.14	121.61	116.62
5	B	606	FAD	C4X-N5-C5X	3.17	120.41	116.76
6	L	1326	MTE	N8-C10-N1	3.53	122.24	116.62
5	B	606	FAD	C1'-N10-C9A	3.61	122.91	118.86
6	L	1326	MTE	C4-N3-C2	4.51	122.19	115.94
5	K	606	FAD	C4-N3-C2	5.08	119.64	115.25
6	C	1326	MTE	C4-N3-C2	5.76	123.93	115.94
5	B	606	FAD	C4-N3-C2	5.99	120.43	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	606	FAD	1	0
8	C	1	I3A	2	0
7	C	1327	MOS	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	606	FAD	1	0
8	L	1	I3A	1	0
7	L	1327	MOS	1	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	164/164 (100%)	0.22	6 (3%) 45 43	10, 17, 32, 36	0
1	J	164/164 (100%)	0.49	14 (8%) 13 11	12, 19, 38, 49	0
2	B	305/305 (100%)	0.30	15 (4%) 33 30	14, 23, 34, 39	0
2	K	305/305 (100%)	0.49	30 (9%) 10 8	17, 27, 38, 42	0
3	C	755/755 (100%)	-0.00	11 (1%) 76 75	11, 16, 26, 34	0
3	L	745/755 (98%)	0.18	23 (3%) 52 50	11, 18, 30, 52	0
All	All	2438/2448 (99%)	0.20	99 (4%) 41 37	10, 19, 33, 52	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	58	TYR	13.5
3	L	1288	ASN	10.5
1	J	2	THR	7.2
1	J	61	LEU	6.8
3	L	1290	THR	6.7
1	J	165	LYS	6.3
3	L	1287	ASN	6.1
2	K	528	GLY	6.1
2	B	528	GLY	5.9
1	A	2	THR	5.2
2	K	477	PHE	4.9
3	L	985	ASP	4.9
2	K	272	ASN	4.3
1	J	97	ARG	4.1
1	A	61	LEU	4.1
2	K	499	ASP	4.0
3	L	1289	ASN	4.0
3	L	1110	ASP	4.0
3	L	1264	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
2	K	445	GLY	3.8
2	B	527	LEU	3.8
2	B	477	PHE	3.8
2	B	272	ASN	3.7
2	K	378	GLY	3.7
3	L	618	LYS	3.6
1	J	133	GLU	3.5
2	K	442	PHE	3.5
2	K	474	LEU	3.5
3	L	1143	GLU	3.4
2	K	335	ARG	3.4
2	K	395	LYS	3.3
2	K	475	SER	3.3
1	J	62	GLN	3.3
3	C	683	HIS	3.3
1	J	63	ASP	3.3
2	K	337	PHE	3.2
1	J	161	ARG	3.1
3	C	1143	GLU	3.1
2	B	498	PRO	3.0
2	K	429	ASP	3.0
3	C	720	LYS	3.0
2	B	335	ARG	3.0
2	K	471	GLN	2.9
3	L	1205	LEU	2.9
3	L	989	LYS	2.8
1	J	162	THR	2.8
3	C	1290	THR	2.8
2	B	424	ALA	2.7
2	B	474	LEU	2.7
2	B	499	ASP	2.7
3	L	1200	VAL	2.7
2	K	336	TRP	2.7
1	A	165	LYS	2.7
2	K	446	SER	2.7
1	J	132	PRO	2.6
1	A	97	ARG	2.6
1	J	60	ARG	2.5
2	K	397	LEU	2.5
3	L	1229	ILE	2.5
2	K	476	LYS	2.5
2	K	424	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
3	L	1144	THR	2.4
2	K	472	LYS	2.4
3	C	1107	LYS	2.4
3	C	1216	GLU	2.4
2	K	291	GLU	2.3
3	C	992	CYS	2.3
3	L	1204	GLY	2.3
3	L	1286	THR	2.3
1	A	161	ARG	2.3
2	K	251	GLN	2.3
2	B	395	LYS	2.3
1	J	64	LYS	2.3
1	J	163	PHE	2.3
3	L	725	GLU	2.2
2	B	268	MET	2.2
2	K	480	GLU	2.2
3	C	1102	GLU	2.2
2	B	444	PRO	2.2
2	K	525	LYS	2.2
3	L	1246	ASP	2.2
3	C	748	CYS	2.2
3	L	992	CYS	2.2
2	B	400	PRO	2.1
3	C	657	LYS	2.1
3	L	1250	LYS	2.1
2	K	295	GLU	2.1
3	C	852	LYS	2.1
2	K	308	VAL	2.1
2	K	444	PRO	2.1
2	K	334	LEU	2.1
2	K	524	LEU	2.1
2	B	412	SER	2.1
2	B	336	TRP	2.1
2	K	254	GLU	2.1
1	A	141	ASP	2.0
3	L	1195	VAL	2.0
3	L	1245	ARG	2.0
3	L	1203	LEU	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 [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
8	I3A	C	1	11/11	0.72	0.21	6.17	27,29,30,30	0
8	I3A	L	1	11/11	0.72	0.15	3.32	32,34,35,35	0
4	FES	J	601	4/4	0.99	0.10	-0.41	13,13,15,15	0
4	FES	A	601	4/4	1.00	0.10	-0.47	11,11,13,13	0
5	FAD	K	606	53/53	0.96	0.10	-0.49	16,21,23,25	0
5	FAD	B	606	53/53	0.97	0.09	-0.57	14,17,21,22	0
4	FES	A	602	4/4	0.99	0.10	-0.75	12,12,14,14	0
4	FES	J	602	4/4	0.99	0.09	-0.90	13,14,14,15	0
7	MOS	C	1327	4/4	0.98	0.10	-0.95	20,20,23,33	0
6	MTE	L	1326	24/24	0.98	0.09	-1.13	15,18,25,25	0
7	MOS	L	1327	4/4	0.98	0.10	-1.13	22,22,25,34	0
6	MTE	C	1326	24/24	0.97	0.08	-2.05	13,16,19,20	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.