



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:56 am GMT

PDB ID : 3NVW
Title : Crystal Structure of Bovine Xanthine Oxidase in Complex with Guanine
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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

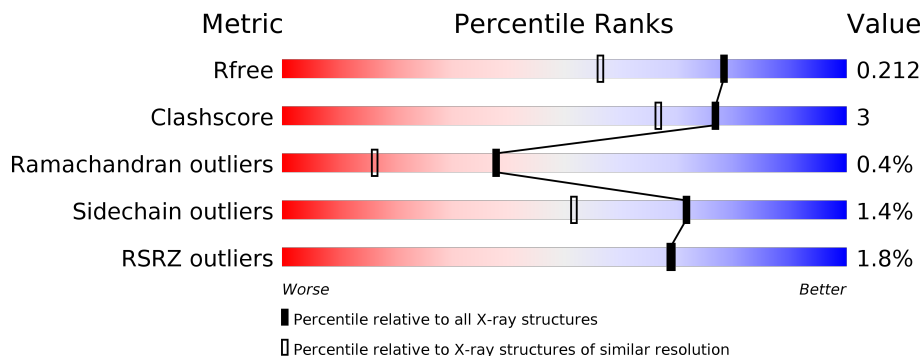
1 Overall quality at a glance

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}	100719	2696 (1.60-1.60)
Clashscore	112137	2967 (1.60-1.60)
Ramachandran outliers	110173	2887 (1.60-1.60)
Sidechain outliers	110143	2886 (1.60-1.60)
RSRZ outliers	101464	2714 (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 ≥ 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>2%</div> <div> <div></div> <div>95%</div> <div>5%</div> </div> </div>
1	J	164	<div> <div>6%</div> <div> <div></div> <div>94%</div> <div>6%</div> </div> </div>
2	B	334	<div> <div>3%</div> <div> <div></div> <div>93%</div> <div>7%</div> </div> </div>
2	K	334	<div> <div>4%</div> <div> <div></div> <div>84%</div> <div>7%</div> <div>9%</div> </div> </div>
3	C	756	<div> <div></div> <div> <div></div> <div>90%</div> <div>9%</div> </div> </div>
3	L	756	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>7%</div> </div> </div>

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
7	MOS	C	1328	-	-	-	X
7	MOS	L	1328	-	-	-	X
8	GUN	C	503	-	-	-	X
8	GUN	L	503	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 21495 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			

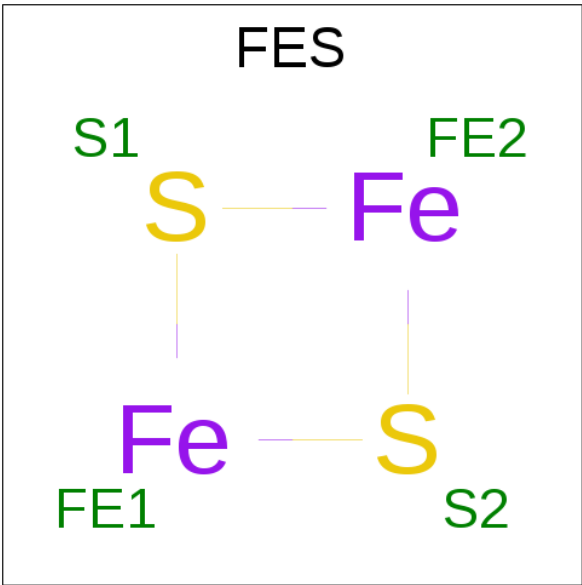
- Molecule 2 is a protein called Xanthine dehydrogenase/oxidase.

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.

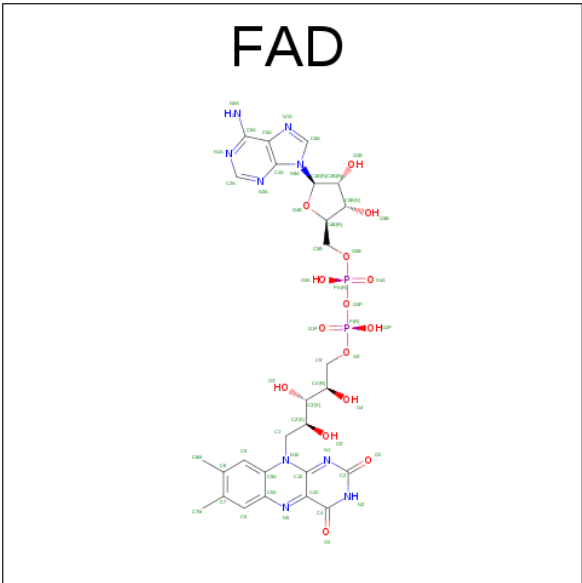
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	756	Total	C	N	O	S	0	0	0
			5832	3686	1005	1106	35			
3	L	745	Total	C	N	O	S	0	0	0
			5761	3643	992	1093	33			

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



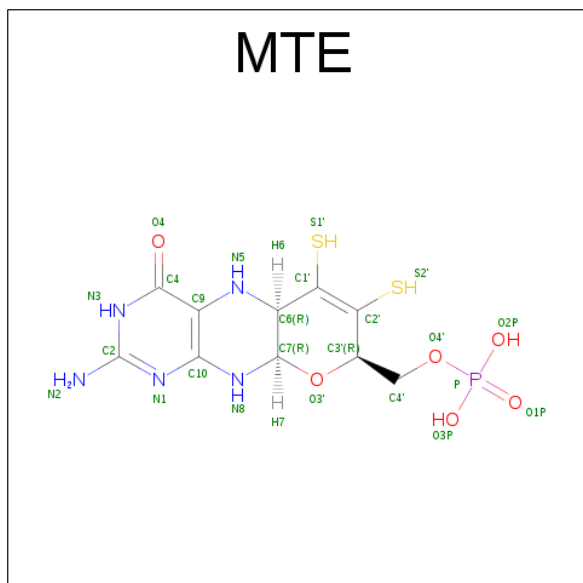
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			4	2	2		
4	A	1	Total	Fe	S	0	0
			4	2	2		
4	J	1	Total	Fe	S	0	0
			4	2	2		
4	J	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



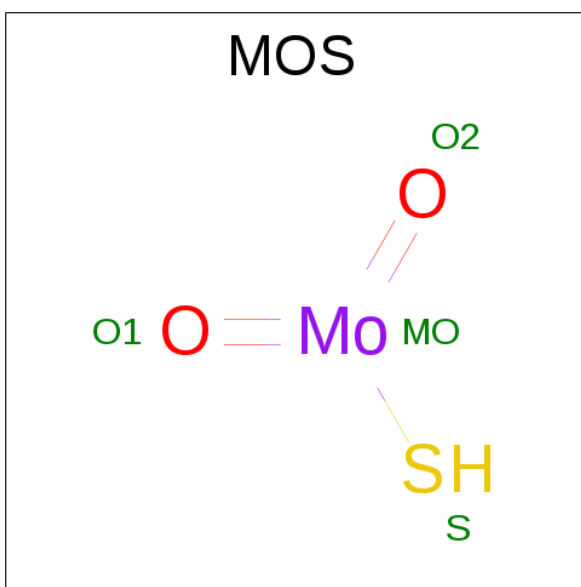
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	K	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 6 is 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: $C_{10}H_{14}N_5O_6PS_2$).



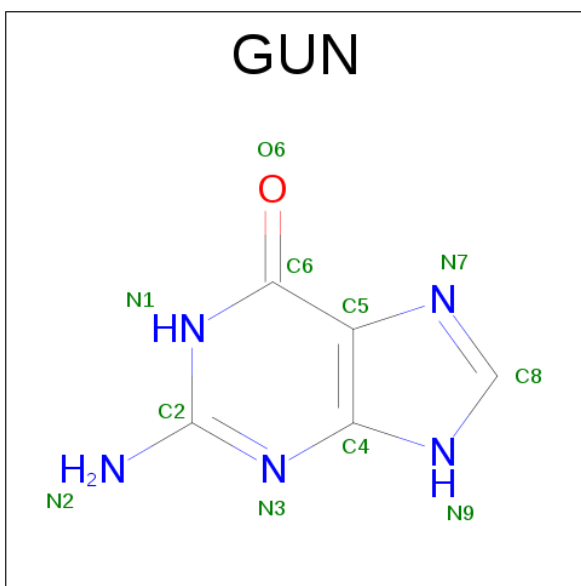
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	C	1	Total 24	C 10	N 5	O 6	P 1	S 2	0	0
6	L	1	Total 24	C 10	N 5	O 6	P 1	S 2	0	0

- 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 GUANINE (three-letter code: GUN) (formula: $C_5H_5N_5O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	1	Total	C	N	O	0	0
			11	5	5	1		
8	L	1	Total	C	N	O	0	0
			11	5	5	1		

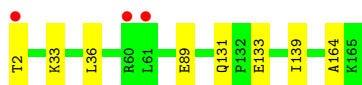
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	149	Total 149	O 149	0	0
9	B	273	Total 273	O 273	0	0
9	C	724	Total 724	O 724	0	0
9	J	134	Total 134	O 134	0	0
9	K	219	Total 219	O 219	0	0
9	L	674	Total 674	O 674	0	0

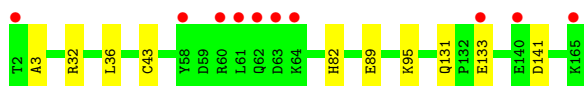
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

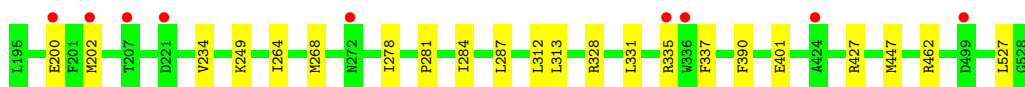
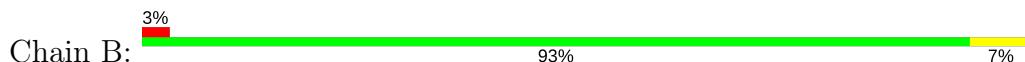
- Molecule 1: Xanthine dehydrogenase/oxidase



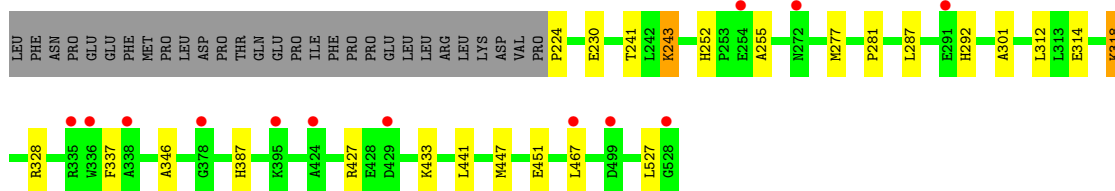
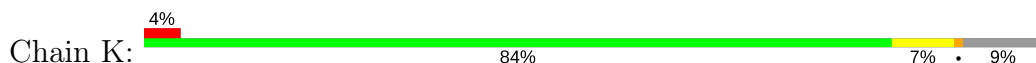
- Molecule 1: Xanthine dehydrogenase/oxidase



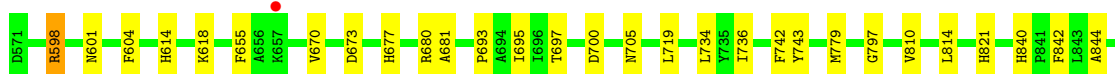
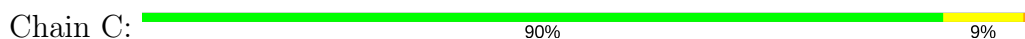
- Molecule 2: Xanthine dehydrogenase/oxidase

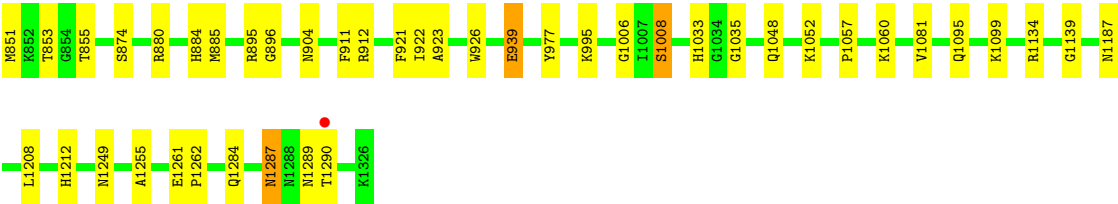


- Molecule 2: Xanthine dehydrogenase/oxidase

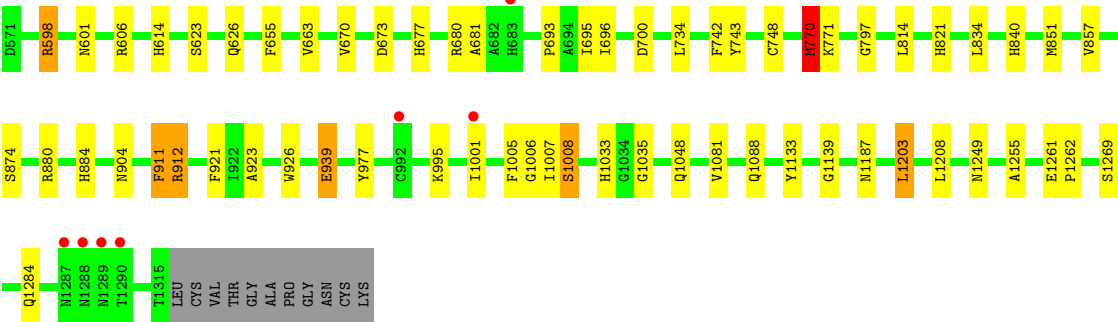
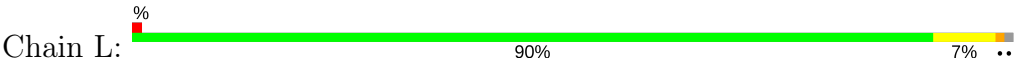


- Molecule 3: Xanthine dehydrogenase/oxidase





● 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	132.68Å 73.40Å 138.11Å 90.00° 96.97° 90.00°	Depositor
Resolution (Å)	131.70 – 1.60 131.70 – 1.60	Depositor EDS
% Data completeness (in resolution range)	96.5 (131.70-1.60) 96.5 (131.70-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.184 , 0.212 0.184 , 0.212	Depositor DCC
R_{free} test set	16908 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	13.8	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 56.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.017 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	21495	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.45	0/1277	0.61	0/1723
1	J	0.42	0/1277	0.56	0/1723
2	B	0.41	0/2689	0.55	0/3637
2	K	0.38	0/2438	0.54	0/3290
3	C	0.45	0/5960	0.59	0/8072
3	L	0.43	1/5888 (0.0%)	0.58	3/7974 (0.0%)
All	All	0.43	1/19529 (0.0%)	0.58	3/26419 (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	-5.93	1.72	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	1203	LEU	CA-CB-CG	7.00	131.39	115.30
3	L	770	MET	CG-SD-CE	-5.32	91.69	100.20
3	L	606	ARG	NE-CZ-NH2	-5.20	117.70	120.30

There are no chirality outliers.

There are no planarity outliers.

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	3	0
1	J	1255	0	1265	9	0
2	B	2630	0	2697	13	0
2	K	2389	0	2459	22	0
3	C	5832	0	5759	51	0
3	L	5761	0	5685	38	0
4	A	8	0	0	0	0
4	J	8	0	0	0	0
5	B	53	0	31	0	0
5	K	53	0	31	1	0
6	C	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	5	0	0
8	L	11	0	5	0	0
9	A	149	0	0	0	0
9	B	273	0	0	2	0
9	C	724	0	0	7	0
9	J	134	0	0	2	0
9	K	219	0	0	4	0
9	L	674	0	0	4	0
All	All	21495	0	19222	134	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 3.

All (134) 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:475:HOH:O	1.20	1.27
2:K:255:ALA:HB2	2:K:277:MET:CE	1.94	0.95
3:L:770:MET:HG3	3:L:771:LYS:N	1.84	0.93
3:L:1001:ILE:HD12	3:L:1269:SER:HA	1.63	0.81
3:L:695:ILE:H	3:L:904:ASN:HD22	1.32	0.77
1:A:131:GLN:HE21	1:A:133:GLU:H	1.30	0.76
3:C:695:ILE:H	3:C:904:ASN:HD22	1.32	0.76
2:K:255:ALA:HB2	2:K:277:MET:HE3	1.69	0.75
3:C:884:HIS:HE1	3:C:1006:GLY:H	1.32	0.75
3:L:1088:GLN:HG2	3:L:1133:TYR:CD1	2.22	0.73
3:L:884:HIS:HE1	3:L:1006:GLY:H	1.35	0.73
1:J:3:ALA:HB2	2:K:230:GLU:HG2	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:314:GLU:O	2:K:318:LYS:HD2	1.88	0.72
2:K:427:ARG:HD2	9:K:537:HOH:O	1.92	0.70
1:J:141:ASP:O	9:J:956:HOH:O	2.08	0.70
3:C:680:ARG:NH2	9:C:1817:HOH:O	2.20	0.70
1:J:95:LYS:HE3	9:L:1408:HOH:O	1.92	0.69
3:C:695:ILE:HG23	3:C:700:ASP:HB3	1.75	0.68
3:C:884:HIS:CE1	3:C:1006:GLY:H	2.13	0.67
3:C:673:ASP:OD2	3:C:677:HIS:HD2	1.79	0.65
3:C:1033:HIS:HD2	3:C:1035:GLY:H	1.43	0.65
3:L:884:HIS:CE1	3:L:1006:GLY:H	2.15	0.65
3:C:614:HIS:HD2	3:C:693:PRO:O	1.80	0.64
3:L:770:MET:HG3	3:L:771:LYS:H	1.62	0.64
1:J:95:LYS:NZ	9:J:850:HOH:O	2.24	0.63
3:C:705:ASN:HB2	9:C:44:HOH:O	1.99	0.62
7:C:1328:MOS:MO	7:C:1328:MOS:O2	1.71	0.62
3:C:840:HIS:HE1	3:C:874:SER:OG	1.82	0.61
7:L:1328:MOS:MO	7:L:1328:MOS:O2	1.72	0.61
3:L:939:GLU:HG2	3:L:977:TYR:CE2	2.36	0.61
3:L:840:HIS:HE1	3:L:874:SER:OG	1.83	0.60
3:C:851:MET:HB2	3:C:853:THR:HG22	1.83	0.60
1:J:131:GLN:HE21	1:J:133:GLU:H	1.50	0.60
3:C:719:LEU:HD11	3:C:895:ARG:CB	2.32	0.59
3:C:719:LEU:HD11	3:C:895:ARG:HB3	1.84	0.59
3:L:1033:HIS:HD2	3:L:1035:GLY:H	1.51	0.59
3:C:1033:HIS:CD2	3:C:1035:GLY:H	2.21	0.58
2:K:255:ALA:CB	2:K:277:MET:HE3	2.32	0.58
2:B:331:LEU:O	2:B:335:ARG:HG2	2.03	0.58
3:C:670:VAL:HG11	3:C:681:ALA:HB3	1.85	0.57
3:C:601:ASN:O	3:C:821:HIS:HD2	1.86	0.57
3:L:673:ASP:OD2	3:L:677:HIS:HD2	1.87	0.57
3:L:1033:HIS:CD2	3:L:1035:GLY:H	2.23	0.57
1:J:95:LYS:CE	9:L:1408:HOH:O	2.52	0.57
1:A:139:ILE:HD12	1:A:164:ALA:HB2	1.86	0.56
3:L:601:ASN:O	3:L:821:HIS:HD2	1.89	0.55
2:B:427:ARG:HD2	9:B:568:HOH:O	2.07	0.55
2:K:241:THR:HB	2:K:243:LYS:HE2	1.89	0.55
3:L:770:MET:CG	3:L:771:LYS:N	2.66	0.54
3:L:851:MET:CE	3:L:857:VAL:HG11	2.37	0.54
2:K:252:HIS:HB2	2:K:277:MET:HE1	1.90	0.54
3:L:995:LYS:NZ	3:L:1284:GLN:HE21	2.06	0.53
3:C:1048:GLN:HE22	3:C:1187:ASN:HD22	1.55	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:939:GLU:HG2	3:C:977:TYR:CE2	2.44	0.52
2:K:287:LEU:HD22	2:K:301:ALA:HB3	1.90	0.52
2:K:281:PRO:HB2	2:K:287:LEU:HD12	1.91	0.52
3:L:623:SER:HA	3:L:626:GLN:HE21	1.74	0.52
2:B:390:PHE:O	2:B:462:ARG:HD2	2.10	0.51
3:C:995:LYS:NZ	3:C:1284:GLN:HE21	2.08	0.51
3:L:880:ARG:O	3:L:884:HIS:HD2	1.94	0.50
2:B:447:MET:HG2	2:B:527:LEU:HD13	1.94	0.49
3:C:880:ARG:O	3:C:884:HIS:HD2	1.95	0.49
3:C:655:PHE:HE1	3:C:814:LEU:HD23	1.78	0.49
2:B:249:LYS:HG2	2:B:401:GLU:O	2.13	0.49
3:C:853:THR:HG23	3:C:855:THR:H	1.76	0.49
3:C:598:ARG:HD2	3:C:604:PHE:CZ	2.48	0.49
2:B:281:PRO:HB2	2:B:287:LEU:CD1	2.43	0.49
3:C:680:ARG:HG2	9:C:1532:HOH:O	2.14	0.48
2:K:252:HIS:HB3	2:K:277:MET:HE2	1.94	0.48
3:C:1095:GLN:O	3:C:1099:LYS:HG2	2.13	0.48
2:K:292:HIS:HE1	9:K:564:HOH:O	1.95	0.48
3:C:821:HIS:HE1	9:C:2949:HOH:O	1.96	0.48
3:L:655:PHE:HE1	3:L:814:LEU:HD23	1.79	0.48
3:L:670:VAL:HG11	3:L:681:ALA:HB3	1.95	0.48
2:B:337:PHE:O	9:B:2882:HOH:O	2.20	0.47
2:B:281:PRO:HB2	2:B:287:LEU:HD13	1.96	0.47
2:K:441:LEU:HB3	2:K:451:GLU:HB2	1.95	0.47
3:C:1287:ASN:HD22	3:C:1289:ASN:H	1.61	0.47
2:B:427:ARG:HD3	3:C:1212:HIS:CD2	2.50	0.47
3:C:779:MET:SD	3:C:810:VAL:CG1	3.02	0.47
1:J:36:LEU:HD22	1:J:89:GLU:HG3	1.96	0.47
3:L:1001:ILE:CD1	3:L:1269:SER:HA	2.38	0.47
3:L:695:ILE:HG23	3:L:700:ASP:HB3	1.97	0.46
3:C:697:THR:O	3:C:700:ASP:HB2	2.15	0.46
2:K:447:MET:HG2	2:K:527:LEU:HD13	1.96	0.46
3:C:1134:ARG:NE	9:C:546:HOH:O	2.48	0.46
2:K:252:HIS:CB	2:K:277:MET:CE	2.94	0.46
3:L:1048:GLN:HE22	3:L:1187:ASN:HD22	1.61	0.46
3:C:885:MET:SD	3:C:896:GLY:HA3	2.56	0.45
3:L:1007:ILE:O	3:L:1008:SER:HB3	2.17	0.45
2:K:346:ALA:HB1	5:K:606:FAD:H4'	1.99	0.45
2:B:284:ILE:HB	2:B:287:LEU:HD12	1.99	0.45
3:C:1008:SER:HA	3:C:1081:VAL:HG11	2.00	0.45
3:C:1048:GLN:NE2	3:C:1187:ASN:HD22	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:32:ARG:HD2	3:L:598:ARG:NH2	2.32	0.44
3:L:614:HIS:HD2	3:L:693:PRO:O	1.99	0.44
2:K:224:PRO:N	9:K:2913:HOH:O	2.50	0.44
2:B:313:LEU:HD21	2:B:335:ARG:HH12	1.83	0.44
3:L:923:ALA:HA	3:L:926:TRP:NE1	2.33	0.44
9:K:1960:HOH:O	3:L:680:ARG:HG2	2.18	0.44
2:B:264:ILE:HG22	2:B:268:MET:HE2	2.00	0.43
3:C:923:ALA:HA	3:C:926:TRP:NE1	2.33	0.43
2:K:252:HIS:HB2	2:K:277:MET:CE	2.48	0.43
3:C:1249:ASN:O	3:C:1255:ALA:HA	2.18	0.43
3:L:1249:ASN:O	3:L:1255:ALA:HA	2.18	0.43
3:L:939:GLU:H	3:L:939:GLU:CD	2.21	0.43
2:K:252:HIS:CB	2:K:277:MET:HE2	2.48	0.43
3:C:844:ALA:HB2	3:C:922:ILE:HD13	2.00	0.43
3:L:696:ILE:HG12	9:L:1602:HOH:O	2.19	0.42
2:K:255:ALA:HB2	2:K:277:MET:HE1	1.90	0.42
3:C:618:LYS:HA	3:C:618:LYS:HD3	1.88	0.42
3:L:1008:SER:HA	3:L:1081:VAL:HG11	2.02	0.42
3:C:939:GLU:HG2	3:C:977:TYR:CZ	2.55	0.42
2:K:387:HIS:CG	2:K:467:LEU:HD11	2.55	0.41
2:B:234:VAL:HG11	2:B:278:ILE:HD12	2.02	0.41
3:C:614:HIS:HE1	9:C:2711:HOH:O	2.02	0.41
3:C:1287:ASN:ND2	3:C:1289:ASN:H	2.17	0.41
3:L:734:LEU:HD21	3:L:921:PHE:CE2	2.56	0.41
3:C:655:PHE:HE1	3:C:814:LEU:CD2	2.34	0.41
1:J:3:ALA:HB2	2:K:230:GLU:CG	2.46	0.41
3:C:1261:GLU:N	3:C:1262:PRO:CD	2.84	0.41
3:C:995:LYS:HZ3	3:C:1284:GLN:HE21	1.68	0.41
3:L:884:HIS:HE1	3:L:1005:PHE:HA	1.86	0.41
3:L:911:PHE:O	3:L:912:ARG:C	2.59	0.41
3:C:779:MET:SD	3:C:810:VAL:HG12	2.60	0.40
3:C:939:GLU:H	3:C:939:GLU:CD	2.23	0.40
1:A:36:LEU:HD22	1:A:89:GLU:HG3	2.02	0.40
3:L:1261:GLU:N	3:L:1262:PRO:CD	2.85	0.40
3:L:663:VAL:HG12	3:L:834:LEU:HD11	2.04	0.40
3:C:736:ILE:CG2	3:C:842:PHE:HB2	2.52	0.40
3:C:1057:PRO:HD2	3:C:1060:LYS:HD2	2.02	0.40
3:C:1048:GLN:HE22	3:C:1187:ASN:HB2	1.86	0.40
3:C:734:LEU:HD21	3:C:921:PHE:CE2	2.56	0.40
3:L:770:MET:HG2	9:L:2880:HOH:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	162/164 (99%)	157 (97%)	5 (3%)	0	100	100
1	J	162/164 (99%)	157 (97%)	4 (2%)	1 (1%)	28	9
2	B	332/334 (99%)	326 (98%)	6 (2%)	0	100	100
2	K	303/334 (91%)	294 (97%)	9 (3%)	0	100	100
3	C	754/756 (100%)	734 (97%)	16 (2%)	4 (0%)	32	12
3	L	743/756 (98%)	726 (98%)	13 (2%)	4 (0%)	32	12
All	All	2456/2508 (98%)	2394 (98%)	53 (2%)	9 (0%)	38	16

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	912	ARG
3	C	1008	SER
3	L	1008	SER
3	L	912	ARG
3	L	1139	GLY
3	L	797	GLY
3	C	797	GLY
3	C	1139	GLY
1	J	43	CYS

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%)	135 (98%)	2 (2%)	70	48
1	J	137/137 (100%)	136 (99%)	1 (1%)	87	77
2	B	290/290 (100%)	286 (99%)	4 (1%)	71	52
2	K	261/290 (90%)	255 (98%)	6 (2%)	56	28
3	C	632/632 (100%)	624 (99%)	8 (1%)	73	55
3	L	624/632 (99%)	616 (99%)	8 (1%)	73	55
All	All	2081/2118 (98%)	2052 (99%)	29 (1%)	71	52

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	33	LYS
2	B	200	GLU
2	B	202	MET
2	B	312	LEU
2	B	328	ARG
3	C	598	ARG
3	C	742	PHE
3	C	743	TYR
3	C	911	PHE
3	C	939	GLU
3	C	1208	LEU
3	C	1287	ASN
3	C	1290	THR
1	J	82	HIS
2	K	243	LYS
2	K	312	LEU
2	K	318	LYS
2	K	328	ARG
2	K	337	PHE
2	K	433	LYS
3	L	598	ARG
3	L	742	PHE
3	L	743	TYR
3	L	770	MET
3	L	911	PHE
3	L	939	GLU
3	L	1203	LEU
3	L	1208	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	146	ASN
2	B	197	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	976	GLN
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
2	K	473	GLN
3	L	585	GLN
3	L	614	HIS
3	L	626	GLN
3	L	677	HIS
3	L	683	HIS
3	L	821	HIS
3	L	840	HIS
3	L	884	HIS
3	L	904	ASN
3	L	1016	GLN
3	L	1033	HIS
3	L	1048	GLN
3	L	1284	GLN
3	L	1287	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	-	51,58,58	1.31	7 (13%)	54,89,89	2.07	7 (12%)
6	MTE	C	1327	7	21,26,26	1.58	2 (9%)	19,40,40	1.98	6 (31%)
7	MOS	C	1328	6	0,3,3	0.00	-	0,3,3	0.00	-
8	GUN	C	503	-	9,12,12	1.72	2 (22%)	8,17,17	3.12	6 (75%)
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	-	51,58,58	1.35	6 (11%)	54,89,89	1.86	6 (11%)
6	MTE	L	1327	7	21,26,26	1.57	2 (9%)	19,40,40	1.92	5 (26%)
7	MOS	L	1328	6	0,3,3	0.00	-	0,3,3	0.00	-
8	GUN	L	503	-	9,12,12	1.73	2 (22%)	8,17,17	3.41	6 (75%)

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	-	-	0/28/50/50	0/6/6/6
6	MTE	C	1327	7	-	0/6/34/34	0/3/3/3
7	MOS	C	1328	6	-	0/0/0/0	0/0/0/0
8	GUN	C	503	-	-	0/0/0/0	0/2/2/2
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	-	-	0/28/50/50	0/6/6/6
6	MTE	L	1327	7	-	0/6/34/34	0/3/3/3
7	MOS	L	1328	6	-	0/0/0/0	0/0/0/0
8	GUN	L	503	-	-	0/0/0/0	0/2/2/2

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	606	FAD	C5X-N5	2.02	1.38	1.35
5	K	606	FAD	C5X-N5	2.20	1.38	1.35
5	B	606	FAD	C2A-N1A	2.41	1.38	1.33
5	B	606	FAD	C1'-N10	2.70	1.51	1.48
5	K	606	FAD	C2A-N1A	2.70	1.39	1.33
8	C	503	GUN	C5-C4	2.74	1.46	1.40
8	L	503	GUN	C5-C4	2.78	1.46	1.40
5	B	606	FAD	C4-N3	2.85	1.38	1.33
5	K	606	FAD	C4-N3	2.91	1.38	1.33
6	L	1327	MTE	C9-C10	3.54	1.48	1.41
5	B	606	FAD	C10-N1	3.70	1.38	1.33
5	B	606	FAD	C4X-N5	3.80	1.38	1.33
8	L	503	GUN	C6-C5	3.83	1.48	1.41
5	K	606	FAD	C2A-N3A	3.84	1.38	1.32
6	C	1327	MTE	C9-C10	3.90	1.48	1.41
5	B	606	FAD	C2A-N3A	3.91	1.38	1.32
8	C	503	GUN	C6-C5	3.95	1.48	1.41
5	K	606	FAD	C10-N1	4.30	1.39	1.33
5	K	606	FAD	C4X-N5	4.33	1.39	1.33
6	C	1327	MTE	C4-C9	5.29	1.47	1.41
6	L	1327	MTE	C4-C9	5.58	1.47	1.41

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	606	FAD	N3A-C2A-N1A	-10.64	119.59	128.86
5	K	606	FAD	N3A-C2A-N1A	-9.85	120.28	128.86
8	L	503	GUN	C6-C5-C4	-5.01	115.86	120.84
8	C	503	GUN	C6-C5-C4	-4.56	116.31	120.84
8	C	503	GUN	C5-C6-N1	-3.86	117.99	123.48
8	L	503	GUN	C5-C6-N1	-3.86	117.99	123.48
8	L	503	GUN	C4-C5-N7	-3.20	106.31	109.41
8	L	503	GUN	N3-C2-N1	-3.18	122.82	127.46
8	C	503	GUN	C4-C5-N7	-2.91	106.60	109.41
5	K	606	FAD	C4X-C4-N3	-2.70	119.63	123.48
8	C	503	GUN	N3-C2-N1	-2.68	123.54	127.46
6	L	1327	MTE	O3'-C7-C6	-2.60	107.23	108.96
6	C	1327	MTE	O3P-P-O4'	-2.53	100.01	106.73
5	B	606	FAD	C4X-C4-N3	-2.42	120.03	123.48
6	C	1327	MTE	N3-C2-N1	-2.32	121.68	125.45
6	L	1327	MTE	C10-N8-C7	-2.27	119.23	123.67
6	L	1327	MTE	C9-C4-N3	-2.00	118.02	123.91
6	C	1327	MTE	C9-C4-N3	-2.00	118.03	123.91
5	K	606	FAD	C5X-C9A-N10	2.16	119.26	117.66
5	B	606	FAD	C4-C4X-N5	2.28	121.18	118.68
6	C	1327	MTE	C2-N1-C10	2.33	119.77	114.51
6	C	1327	MTE	N8-C10-N1	2.40	121.53	116.90
6	L	1327	MTE	C2-N1-C10	2.45	120.03	114.51
5	K	606	FAD	C1'-N10-C9A	2.71	120.83	118.35
5	B	606	FAD	C5X-C9A-N10	2.75	119.70	117.66
8	C	503	GUN	C2-N3-C4	2.91	118.55	115.16
5	K	606	FAD	C4X-N5-C5X	3.10	120.03	116.76
5	B	606	FAD	C4X-N5-C5X	3.13	120.06	116.76
8	L	503	GUN	C2-N3-C4	3.33	119.05	115.16
8	C	503	GUN	C6-N1-C2	4.17	122.06	116.06
8	L	503	GUN	C6-N1-C2	4.48	122.51	116.06
6	L	1327	MTE	C4-N3-C2	4.84	123.02	116.06
5	B	606	FAD	C1'-N10-C9A	5.15	123.07	118.35
6	C	1327	MTE	C4-N3-C2	5.52	124.00	116.06
5	K	606	FAD	C4-N3-C2	6.08	120.48	115.16
5	B	606	FAD	C4-N3-C2	6.16	120.55	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	1328	MOS	1	0
5	K	606	FAD	1	0
7	L	1328	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, 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%)	-0.24	3 (1%) 69 69	7, 13, 25, 34	0
1	J	164/164 (100%)	-0.04	10 (6%) 22 21	9, 16, 33, 43	0
2	B	334/334 (100%)	-0.04	9 (2%) 55 54	11, 19, 29, 40	0
2	K	305/334 (91%)	0.18	13 (4%) 36 34	14, 23, 33, 37	0
3	C	756/756 (100%)	-0.39	2 (0%) 93 93	6, 12, 21, 25	0
3	L	745/756 (98%)	-0.32	7 (0%) 84 85	7, 14, 25, 45	0
All	All	2468/2508 (98%)	-0.22	44 (1%) 69 69	6, 15, 29, 45	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	58	TYR	9.1
1	J	61	LEU	9.0
3	L	1288	ASN	8.7
3	L	1290	THR	6.5
1	J	2	THR	6.3
2	K	336	TRP	5.9
2	K	528	GLY	5.5
1	A	2	THR	5.5
1	A	61	LEU	5.4
3	L	1289	ASN	5.1
3	L	1287	ASN	4.5
2	B	424	ALA	4.3
2	K	378	GLY	3.9
1	J	60	ARG	3.9
2	K	338	ALA	3.7
2	B	272	ASN	3.7
2	K	272	ASN	3.7
1	J	62	GLN	3.6
2	K	254	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
2	K	424	ALA	3.4
1	J	165	LYS	3.4
2	K	335	ARG	3.3
1	J	63	ASP	3.2
2	K	429	ASP	3.2
2	B	202	MET	3.1
1	J	64	LYS	3.1
2	K	499	ASP	3.1
3	C	657	LYS	2.9
1	A	60	ARG	2.7
2	B	499	ASP	2.5
3	C	1290	THR	2.5
2	K	395	LYS	2.4
3	L	683	HIS	2.4
1	J	140	GLU	2.4
2	B	207	THR	2.4
2	B	335	ARG	2.3
1	J	133	GLU	2.3
2	K	467	LEU	2.1
2	K	291	GLU	2.1
2	B	221	ASP	2.1
3	L	992	CYS	2.1
3	L	1001	ILE	2.1
2	B	200	GLU	2.0
2	B	336	TRP	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 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, 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	LLDF	B-factors(\AA^2)	Q<0.9
8	GUN	C	503	11/11	0.89	0.12	2.74	17,18,19,19	0
8	GUN	L	503	11/11	0.90	0.11	2.47	18,19,20,20	0
7	MOS	L	1328	4/4	0.99	0.08	2.30	12,12,12,22	0
7	MOS	C	1328	4/4	1.00	0.08	2.22	11,12,15,23	0
4	FES	A	602	4/4	1.00	0.07	1.05	9,9,10,10	0
4	FES	J	601	4/4	0.99	0.07	0.85	9,10,10,10	0
6	MTE	L	1327	24/24	0.99	0.07	0.78	8,10,12,13	0
4	FES	A	601	4/4	1.00	0.08	0.72	7,8,8,9	0
4	FES	J	602	4/4	0.99	0.06	-0.02	10,10,10,11	0
6	MTE	C	1327	24/24	0.99	0.07	-0.08	6,8,10,11	0
5	FAD	B	606	53/53	0.97	0.06	-0.57	10,12,15,16	0
5	FAD	K	606	53/53	0.97	0.07	-0.63	13,17,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.