



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:06 PM GMT

PDB ID : 3SR6  
Title : Crystal Structure of Reduced Bovine Xanthine Oxidase in Complex with Arsenite  
Authors : Cao, H.; Hille, R.  
Deposited on : 2011-07-07  
Resolution : 2.10 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

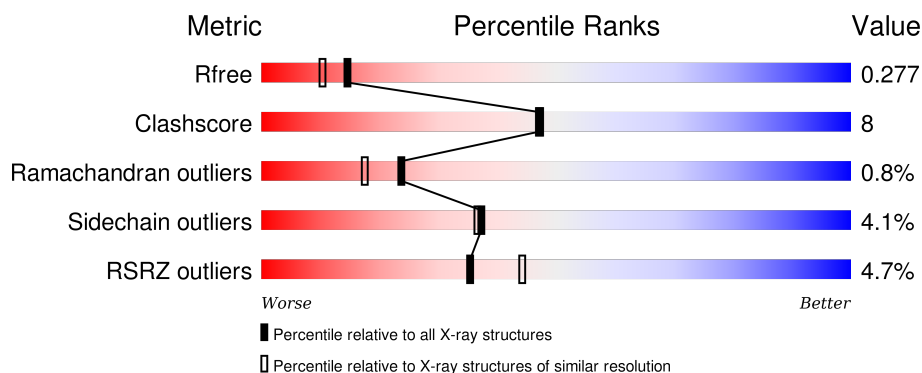
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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>5%</div> <div>82%</div> <div>18%</div> </div>
1	J	164	<div> <div>7%</div> <div>83%</div> <div>16%</div> </div>
2	B	305	<div> <div>8%</div> <div>86%</div> <div>11%</div> </div>
2	K	305	<div> <div>7%</div> <div>86%</div> <div>12%</div> </div>
3	C	745	<div> <div>3%</div> <div>82%</div> <div>16%</div> </div>

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Mol	Chain	Length	Quality of chain
3	L	745	

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	RMO	C	1317	-	-	X	-
7	RMO	L	1317	-	-	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 19834 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			

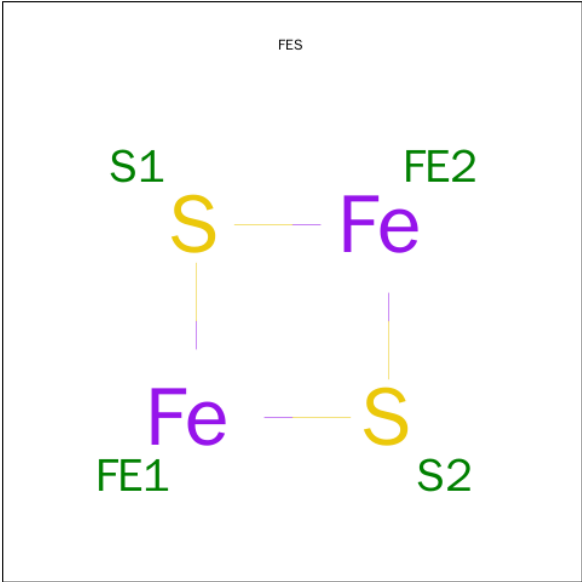
- Molecule 2 is a protein called Xanthine dehydrogenase/oxidase.

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.

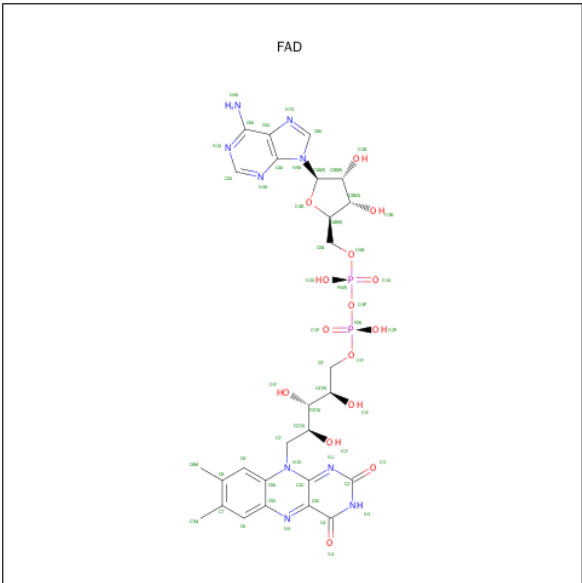
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	745	Total	C	N	O	S	0	0	0
			5761	3643	992	1093	33			
3	L	745	Total	C	N	O	S	0	0	0
			5761	3643	992	1093	33			

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



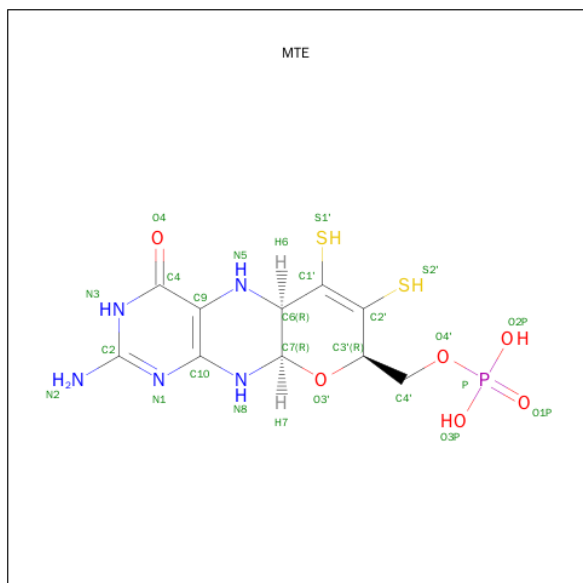
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			4	2	2		
4	A	1	Total	Fe	S	0	0
			4	2	2		
4	J	1	Total	Fe	S	0	0
			4	2	2		
4	J	1	Total	Fe	S	0	0
			4	2	2		

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



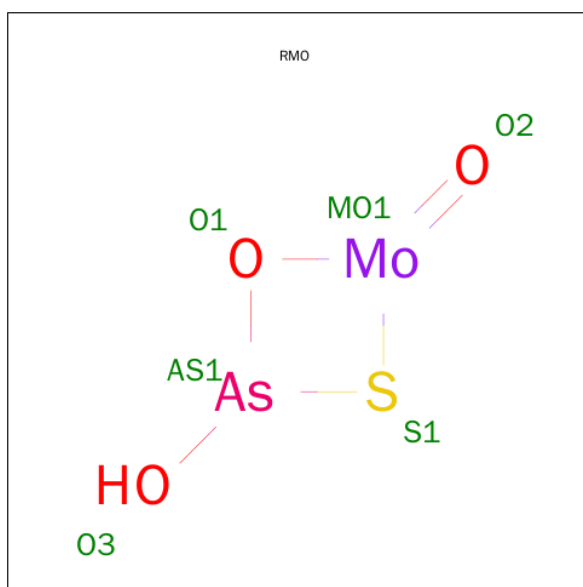
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	K	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- 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<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>6</sub>P S<sub>2</sub>).



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

- Molecule 7 is [ARSENOTHIONITO(2-)-KAPPA 2 O,S](OXO)MOLYBDENUM (three-letter code: RMO) (formula: AsHMoO<sub>3</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total	As	Mo	O	S	0	0
			6	1	1	3	1		
7	L	1	Total	As	Mo	O	S	0	0
			6	1	1	3	1		

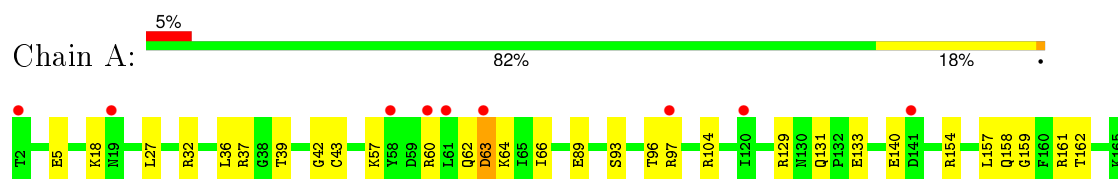
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	63	Total	O	0	0
			63	63		
8	B	88	Total	O	0	0
			88	88		
8	C	299	Total	O	0	0
			299	299		
8	J	51	Total	O	0	0
			51	51		
8	K	82	Total	O	0	0
			82	82		
8	L	259	Total	O	0	0
			259	259		

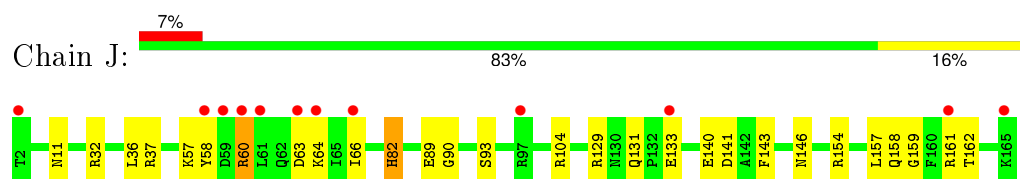
### 3 Residue-property plots [i](#)

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.

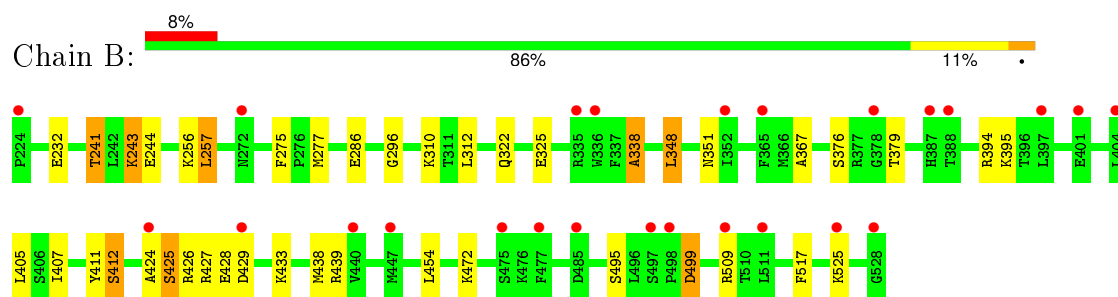
- Molecule 1: Xanthine dehydrogenase/oxidase



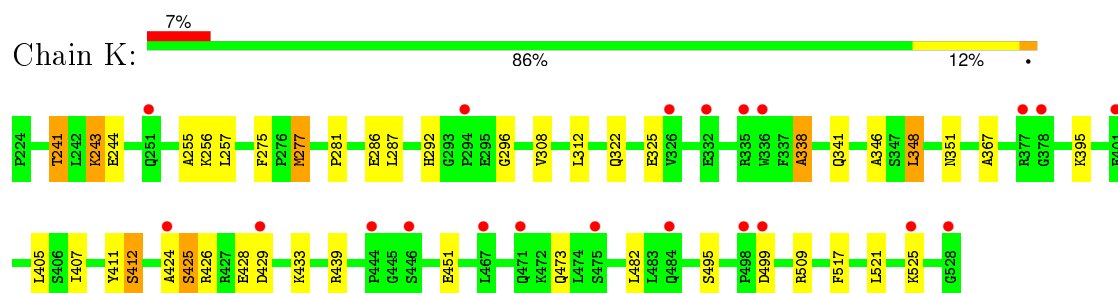
- Molecule 1: Xanthine dehydrogenase/oxidase



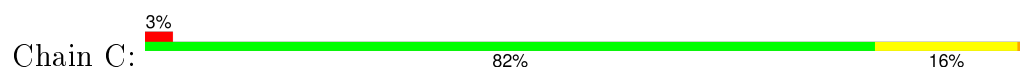
- Molecule 2: Xanthine dehydrogenase/oxidase



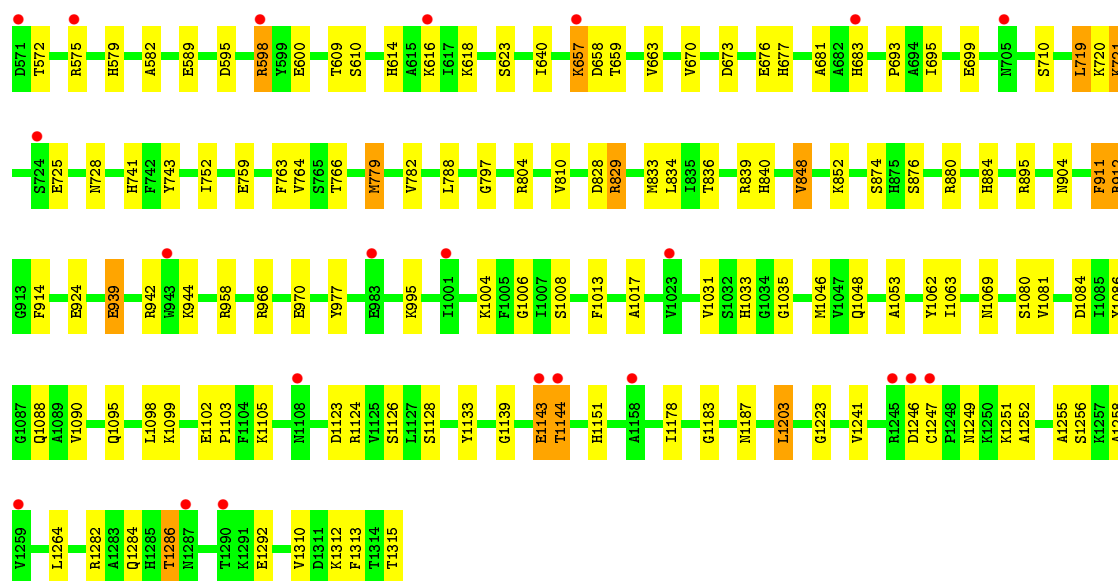
- Molecule 2: Xanthine dehydrogenase/oxidase



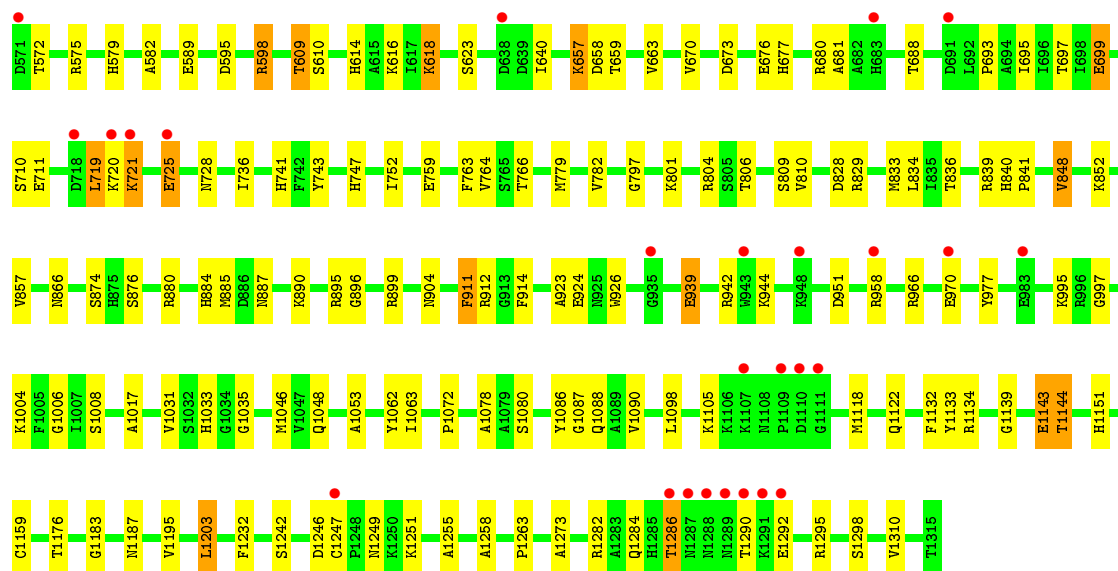
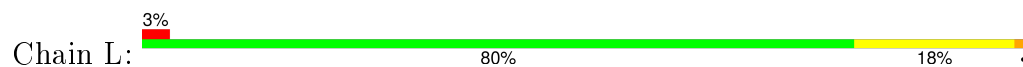
- Molecule 3: Xanthine dehydrogenase/oxidase







• 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, $\alpha$ , $\beta$ , $\gamma$	133.05Å 73.24Å 138.02Å 90.00° 96.80° 90.00°	Depositor
Resolution (Å)	22.10 – 2.10 22.07 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.8 (22.10-2.10) 95.9 (22.07-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.12 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.225 , 0.272 0.229 , 0.277	Depositor DCC
$R_{free}$ test set	7451 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.7	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 49.9	EDS
Estimated twinning fraction	0.033 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	1 of 147820 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	19834	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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: MTE, RMO, 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	0.68	0/1277	0.68	0/1723
1	J	0.64	0/1277	0.70	0/1723
2	B	0.57	0/2438	0.65	0/3290
2	K	0.59	0/2438	0.64	0/3290
3	C	0.66	1/5888 (0.0%)	0.74	5/7974 (0.1%)
3	L	0.68	1/5888 (0.0%)	0.75	4/7974 (0.1%)
All	All	0.65	2/19206 (0.0%)	0.72	9/25974 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	699	GLU	CG-CD	5.21	1.59	1.51
3	C	699	GLU	CG-CD	5.07	1.59	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	839	ARG	NE-CZ-NH2	-11.94	114.33	120.30
3	L	839	ARG	NE-CZ-NH1	8.98	124.79	120.30
3	C	839	ARG	NE-CZ-NH2	-7.54	116.53	120.30
3	C	829	ARG	NE-CZ-NH2	-6.18	117.21	120.30
3	L	1203	LEU	CA-CB-CG	6.15	129.45	115.30
3	C	1203	LEU	CA-CB-CG	5.74	128.50	115.30
3	C	848	VAL	CB-CA-C	-5.69	100.59	111.40
3	C	839	ARG	NE-CZ-NH1	5.52	123.06	120.30
3	L	848	VAL	CB-CA-C	-5.18	101.56	111.40

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	21	0
1	J	1255	0	1265	19	0
2	B	2389	0	2459	34	0
2	K	2389	0	2459	33	0
3	C	5761	0	5685	97	0
3	L	5761	0	5685	97	0
4	A	8	0	0	0	0
4	J	8	0	0	0	0
5	B	53	0	31	2	0
5	K	53	0	31	2	0
6	C	24	0	10	0	0
6	L	24	0	10	0	0
7	C	6	0	0	2	0
7	L	6	0	0	3	0
8	A	63	0	0	1	0
8	B	88	0	0	6	0
8	C	299	0	0	9	0
8	J	51	0	0	3	0
8	K	82	0	0	3	0
8	L	259	0	0	6	0
All	All	19834	0	18900	285	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 8.

All (285) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:243:LYS:HD3	2:K:243:LYS:H	1.20	1.04
3:C:1315:THR:CA	8:C:1464:HOH:O	2.06	1.00
3:L:924:GLU:OE1	3:L:942:ARG:NH1	1.95	0.99
3:C:924:GLU:OE1	3:C:942:ARG:NH1	1.96	0.98
2:B:243:LYS:H	2:B:243:LYS:HD3	1.26	0.97
2:K:241:THR:HG23	2:K:243:LYS:HG2	1.46	0.95
3:C:1315:THR:C	8:C:1464:HOH:O	2.06	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:241:THR:HG22	2:B:244:GLU:HG3	1.48	0.92
2:K:241:THR:CG2	2:K:243:LYS:HG2	2.00	0.90
2:B:241:THR:HG23	2:B:243:LYS:HG2	1.54	0.89
1:J:60:ARG:HA	8:J:293:HOH:O	1.71	0.88
3:L:890:LYS:HD3	8:L:116:HOH:O	1.74	0.88
2:B:241:THR:CG2	2:B:243:LYS:HG2	2.05	0.86
2:K:495:SER:HB2	2:K:509:ARG:HH22	1.40	0.86
2:B:495:SER:HB2	2:B:509:ARG:HH22	1.41	0.86
1:J:104:ARG:HH11	1:J:162:THR:HG23	1.39	0.85
2:B:427:ARG:HD2	8:B:529:HOH:O	1.76	0.83
2:K:241:THR:HG22	2:K:244:GLU:HG3	1.60	0.83
3:C:1286:THR:HG22	3:C:1310:VAL:O	1.78	0.83
1:A:104:ARG:HH11	1:A:162:THR:HG23	1.44	0.82
3:C:695:ILE:H	3:C:904:ASN:HD22	1.26	0.82
3:C:1282:ARG:HA	3:C:1286:THR:HG23	1.63	0.81
3:L:572:THR:HA	3:L:575:ARG:HD3	1.63	0.80
3:C:884:HIS:HE1	3:C:1006:GLY:H	1.29	0.80
1:A:131:GLN:HE21	1:A:133:GLU:H	1.29	0.80
2:K:243:LYS:HD3	2:K:243:LYS:N	1.98	0.79
3:L:695:ILE:H	3:L:904:ASN:HD22	1.29	0.79
3:L:764:VAL:HG23	3:L:766:THR:HG22	1.65	0.79
2:K:243:LYS:CD	2:K:243:LYS:H	1.91	0.77
2:B:243:LYS:N	2:B:243:LYS:HD3	1.99	0.77
3:L:720:LYS:O	3:L:721:LYS:CB	2.33	0.76
1:A:93:SER:HB2	3:C:589:GLU:OE1	1.86	0.76
3:L:884:HIS:HE1	3:L:1006:GLY:H	1.35	0.75
3:C:1315:THR:O	8:C:1464:HOH:O	2.04	0.75
1:J:93:SER:HB2	3:L:589:GLU:OE1	1.86	0.74
3:C:572:THR:HA	3:C:575:ARG:HD3	1.69	0.74
3:C:1315:THR:HA	8:C:1464:HOH:O	1.76	0.74
3:L:880:ARG:O	3:L:884:HIS:HD2	1.68	0.74
3:L:779:MET:HG2	3:L:810:VAL:HG13	1.70	0.74
2:B:241:THR:CG2	2:B:244:GLU:HG3	2.18	0.74
2:B:310:LYS:HE3	8:B:97:HOH:O	1.88	0.73
2:K:495:SER:HB2	2:K:509:ARG:NH2	2.04	0.72
1:J:131:GLN:HE21	1:J:133:GLU:H	1.36	0.72
3:C:764:VAL:HG23	3:C:766:THR:HG22	1.73	0.71
3:L:1282:ARG:HA	3:L:1286:THR:HG23	1.71	0.70
3:C:720:LYS:O	3:C:721:LYS:CB	2.38	0.69
2:B:499:ASP:OD1	8:B:550:HOH:O	2.11	0.69
3:L:663:VAL:HG12	3:L:834:LEU:HD11	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:752:ILE:CD1	3:C:763:PHE:HE1	2.06	0.68
3:L:680:ARG:NH2	8:L:1323:HOH:O	2.27	0.67
2:B:322:GLN:O	2:B:412:SER:HB3	1.94	0.67
2:K:241:THR:HG22	2:K:244:GLU:H	1.60	0.67
1:A:32:ARG:NH1	3:C:676:GLU:OE2	2.21	0.67
2:B:495:SER:HB2	2:B:509:ARG:NH2	2.09	0.67
3:C:939:GLU:HG2	3:C:977:TYR:CE2	2.29	0.66
3:C:880:ARG:O	3:C:884:HIS:HD2	1.78	0.66
7:L:1317:RMO:MO1	7:L:1317:RMO:O2	1.66	0.66
2:B:243:LYS:H	2:B:243:LYS:CD	1.96	0.66
3:L:764:VAL:CG2	3:L:766:THR:HG22	2.25	0.65
1:A:36:LEU:HD22	1:A:89:GLU:HG3	1.77	0.65
1:J:104:ARG:NH1	1:J:162:THR:HG23	2.12	0.65
2:B:241:THR:HG22	2:B:244:GLU:H	1.62	0.64
3:L:1088:GLN:HG2	3:L:1133:TYR:CD1	2.32	0.64
3:L:939:GLU:HG2	3:L:977:TYR:CE2	2.33	0.64
3:C:779:MET:HG2	3:C:810:VAL:HG13	1.79	0.64
7:C:1317:RMO:MO1	7:C:1317:RMO:O2	1.66	0.64
3:L:1286:THR:HG22	3:L:1310:VAL:O	1.98	0.64
3:L:958:ARG:NH1	8:L:1334:HOH:O	2.19	0.64
2:K:241:THR:CG2	2:K:244:GLU:HG3	2.27	0.64
1:J:159:GLY:O	1:J:162:THR:HG22	1.98	0.63
3:C:673:ASP:OD2	3:C:677:HIS:HD2	1.81	0.63
3:L:880:ARG:O	3:L:884:HIS:CD2	2.52	0.63
3:C:663:VAL:HG12	3:C:834:LEU:HD11	1.80	0.62
3:L:840:HIS:HE1	3:L:874:SER:OG	1.81	0.62
1:A:159:GLY:O	1:A:162:THR:HG22	1.99	0.62
1:J:57:LYS:HE2	1:J:66:ILE:HD11	1.82	0.62
3:C:1249:ASN:O	3:C:1255:ALA:HA	1.99	0.62
2:K:322:GLN:O	2:K:412:SER:HB3	2.00	0.61
3:C:884:HIS:CE1	3:C:1006:GLY:H	2.15	0.61
3:L:1088:GLN:HG2	3:L:1133:TYR:CE1	2.36	0.61
1:A:104:ARG:NH1	1:A:162:THR:HG23	2.14	0.60
2:B:424:ALA:O	2:B:425:SER:HB3	2.02	0.60
3:C:640:ILE:HG12	3:C:779:MET:HE1	1.84	0.59
3:L:610:SER:O	3:L:663:VAL:O	2.20	0.59
3:L:1249:ASN:O	3:L:1255:ALA:HA	2.03	0.59
3:L:951:ASP:HB3	8:L:116:HOH:O	2.03	0.59
3:L:609:THR:HG22	8:L:59:HOH:O	2.01	0.58
3:L:720:LYS:O	3:L:721:LYS:HB3	2.04	0.58
3:C:720:LYS:O	3:C:721:LYS:HB3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:424:ALA:O	2:K:425:SER:HB3	2.04	0.58
2:B:325:GLU:HB2	2:B:412:SER:OG	2.03	0.58
2:K:325:GLU:HB2	2:K:412:SER:OG	2.03	0.58
3:L:752:ILE:CD1	3:L:763:PHE:HE1	2.16	0.58
1:J:82:HIS:HE1	8:J:172:HOH:O	1.87	0.58
3:L:880:ARG:HD2	3:L:914:PHE:HB3	1.86	0.57
3:C:995:LYS:NZ	3:C:1284:GLN:HE21	2.02	0.57
2:K:241:THR:HG23	2:K:243:LYS:CG	2.27	0.57
3:L:1046:MET:HE1	3:L:1090:VAL:HB	1.86	0.57
1:J:104:ARG:HD3	1:J:162:THR:HG21	1.87	0.57
1:A:104:ARG:HD3	1:A:162:THR:HG21	1.86	0.57
3:C:640:ILE:HG12	3:C:779:MET:CE	2.34	0.57
3:C:600:GLU:HG2	3:L:598:ARG:O	2.05	0.56
3:C:840:HIS:HE1	3:C:874:SER:OG	1.87	0.56
3:C:752:ILE:HD11	3:C:763:PHE:HE1	1.71	0.55
3:C:1088:GLN:HG2	3:C:1133:TYR:CD1	2.42	0.55
3:C:1033:HIS:HD2	3:C:1035:GLY:H	1.53	0.55
3:L:806:THR:HA	3:L:809:SER:HB2	1.88	0.54
3:C:1123:ASP:O	3:L:1134:ARG:NH1	2.40	0.54
1:A:157:LEU:O	1:A:161:ARG:HB2	2.07	0.54
3:C:610:SER:O	3:C:663:VAL:O	2.26	0.54
3:C:598:ARG:CD	8:C:1422:HOH:O	2.55	0.54
3:C:1282:ARG:NH2	3:C:1292:GLU:OE2	2.30	0.54
3:L:720:LYS:O	3:L:721:LYS:HB2	2.08	0.54
1:J:36:LEU:HD22	1:J:89:GLU:HG3	1.90	0.54
3:L:1046:MET:CE	3:L:1087:GLY:HA2	2.38	0.53
1:A:57:LYS:HE2	1:A:66:ILE:HD11	1.91	0.53
2:K:424:ALA:O	2:K:425:SER:CB	2.56	0.53
3:L:995:LYS:NZ	3:L:1284:GLN:HE21	2.07	0.53
2:K:338:ALA:N	8:K:214:HOH:O	2.43	0.52
3:C:670:VAL:HG11	3:C:681:ALA:HB3	1.91	0.52
2:B:394:ARG:HD2	8:B:530:HOH:O	2.09	0.52
1:A:154:ARG:NH1	1:A:158:GLN:OE1	2.43	0.52
3:L:887:ASN:ND2	3:L:924:GLU:OE2	2.43	0.51
1:J:37:ARG:HD3	3:L:595:ASP:O	2.10	0.51
3:C:759:GLU:OE2	3:L:1062:TYR:OH	2.25	0.51
3:L:711:GLU:HA	3:L:899:ARG:HD2	1.93	0.51
2:K:257:LEU:O	5:K:606:FAD:H2B	2.10	0.51
3:C:598:ARG:HD2	8:C:1422:HOH:O	2.09	0.51
2:B:257:LEU:O	5:B:606:FAD:H2B	2.11	0.51
8:B:544:HOH:O	3:C:683:HIS:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:241:THR:HG23	2:B:243:LYS:CG	2.34	0.50
3:C:1062:TYR:OH	3:L:759:GLU:OE2	2.25	0.50
3:C:1046:MET:HE1	3:C:1090:VAL:HB	1.94	0.50
3:L:673:ASP:OD2	3:L:677:HIS:HD2	1.94	0.50
3:C:1128:SER:HB2	3:L:1072:PRO:HG3	1.93	0.50
3:C:764:VAL:CG2	3:C:766:THR:HG22	2.41	0.49
2:B:424:ALA:O	2:B:425:SER:CB	2.60	0.49
2:K:241:THR:HG21	2:K:243:LYS:HG2	1.90	0.49
3:C:695:ILE:H	3:C:904:ASN:ND2	2.04	0.49
3:L:840:HIS:CE1	3:L:874:SER:OG	2.64	0.49
3:L:579:HIS:HB3	3:L:582:ALA:HB2	1.94	0.49
3:C:741:HIS:HA	3:C:911:PHE:CE1	2.46	0.49
3:C:876:SER:HB3	3:C:914:PHE:HE2	1.77	0.49
3:C:598:ARG:NE	8:C:1422:HOH:O	2.45	0.49
1:A:43:CYS:HA	3:C:829:ARG:HB2	1.94	0.48
2:B:296:GLY:HA2	2:B:411:TYR:CD1	2.47	0.48
3:C:728:ASN:HD21	3:C:852:LYS:HD3	1.77	0.48
3:C:1048:GLN:HE22	3:C:1187:ASN:HD22	1.62	0.48
3:C:880:ARG:HD2	3:C:914:PHE:HB3	1.95	0.48
3:L:1078:ALA:HB1	7:L:1317:RMO:O1	2.13	0.48
2:K:292:HIS:HE1	8:K:544:HOH:O	1.96	0.48
3:C:1178:ILE:HD12	3:C:1241:VAL:HG22	1.94	0.48
3:L:736:ILE:HG13	3:L:1298:SER:HB3	1.96	0.48
3:L:1017:ALA:HB1	3:L:1086:TYR:CD2	2.49	0.48
1:A:27:LEU:CD1	1:A:39:THR:HG22	2.43	0.48
3:L:1033:HIS:HD2	3:L:1035:GLY:H	1.60	0.48
3:L:1195:VAL:HA	3:L:1263:PRO:HG2	1.96	0.48
2:B:232:GLU:OE1	3:C:677:HIS:HE1	1.96	0.48
3:L:885:MET:SD	3:L:896:GLY:HA3	2.54	0.48
2:B:241:THR:HG21	2:B:243:LYS:HG2	1.91	0.47
3:L:1031:VAL:HB	3:L:1063:ILE:HG12	1.96	0.47
3:L:640:ILE:HG12	3:L:779:MET:HE1	1.96	0.47
3:L:728:ASN:HD21	3:L:852:LYS:HD3	1.79	0.47
3:L:1159:CYS:O	3:L:1176:THR:HA	2.15	0.47
3:C:958:ARG:HH11	3:C:958:ARG:HG2	1.80	0.47
2:B:256:LYS:HG3	2:B:275:PHE:CG	2.50	0.47
2:K:296:GLY:HA2	2:K:411:TYR:CD1	2.49	0.47
3:C:880:ARG:O	3:C:884:HIS:CD2	2.63	0.47
3:L:1282:ARG:NH2	3:L:1292:GLU:OE2	2.31	0.47
3:L:719:LEU:HD13	3:L:895:ARG:HB2	1.96	0.47
1:J:143:PHE:HB3	3:L:1232:PHE:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:1053:ALA:O	3:L:1098:LEU:HD11	2.15	0.47
2:K:346:ALA:HB1	5:K:606:FAD:H4'	1.95	0.47
3:C:1046:MET:HE2	3:C:1090:VAL:HG21	1.96	0.47
2:B:286:GLU:HB3	2:B:405:LEU:HD11	1.96	0.47
3:C:1264:LEU:HD23	3:C:1264:LEU:C	2.35	0.47
3:C:752:ILE:CD1	3:C:763:PHE:CE1	2.94	0.46
3:L:958:ARG:HH11	3:L:958:ARG:HG2	1.80	0.46
3:L:1143:GLU:O	3:L:1144:THR:HG23	2.15	0.46
3:L:876:SER:HB3	3:L:914:PHE:HE2	1.80	0.46
3:C:614:HIS:HD2	3:C:693:PRO:O	1.98	0.46
3:C:616:LYS:HD2	3:C:658:ASP:O	2.16	0.46
3:L:997:GLY:HA3	3:L:1273:ALA:O	2.16	0.46
3:C:1048:GLN:HE22	3:C:1187:ASN:HB2	1.80	0.46
3:C:1046:MET:CE	3:C:1090:VAL:HG21	2.46	0.46
2:B:509:ARG:HG2	8:B:108:HOH:O	2.16	0.46
3:L:1295:ARG:HA	8:L:264:HOH:O	2.14	0.46
3:L:884:HIS:CE1	3:L:1006:GLY:H	2.23	0.46
1:A:32:ARG:NH2	8:A:932:HOH:O	2.48	0.46
3:L:829:ARG:O	3:L:833:MET:HG3	2.16	0.46
3:L:1080:SER:HB3	3:L:1258:ALA:HB1	1.97	0.45
3:C:719:LEU:CD1	3:C:895:ARG:HB2	2.46	0.45
3:C:1126:SER:HB2	3:L:1132:PHE:CD1	2.51	0.45
3:L:923:ALA:HA	3:L:926:TRP:NE1	2.31	0.45
3:L:1048:GLN:HE22	3:L:1187:ASN:HB2	1.81	0.45
3:L:614:HIS:HD2	3:L:693:PRO:O	1.99	0.45
2:B:472:LYS:HE2	2:B:472:LYS:HB3	1.72	0.45
1:J:154:ARG:NH1	1:J:158:GLN:OE1	2.50	0.45
1:A:62:GLN:O	1:A:63:ASP:CB	2.64	0.45
3:C:1315:THR:HB	8:C:1464:HOH:O	2.16	0.45
1:A:62:GLN:O	1:A:63:ASP:HB3	2.17	0.45
3:L:1183:GLY:HA2	3:L:1247:CYS:O	2.17	0.45
3:L:1033:HIS:CD2	3:L:1035:GLY:H	2.35	0.45
2:K:348:LEU:HD13	2:K:407:ILE:HD13	1.98	0.45
3:C:833:MET:HE3	3:C:1223:GLY:HA2	1.98	0.45
1:A:42:GLY:O	3:C:829:ARG:HD2	2.17	0.44
1:J:157:LEU:O	1:J:161:ARG:HB2	2.16	0.44
3:C:1046:MET:HE1	3:C:1090:VAL:CG2	2.47	0.44
2:K:256:LYS:HG3	2:K:275:PHE:CG	2.51	0.44
2:K:255:ALA:HB2	2:K:277:MET:HG2	1.99	0.44
2:K:451:GLU:HG2	8:K:153:HOH:O	2.18	0.44
2:B:348:LEU:HD13	2:B:407:ILE:HD13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:32:ARG:NH1	3:L:676:GLU:OE2	2.42	0.44
1:J:104:ARG:HD3	1:J:162:THR:CG2	2.48	0.44
1:J:146:ASN:ND2	2:K:341:GLN:HE22	2.15	0.44
2:B:438:MET:HG2	2:B:454:LEU:HD22	2.00	0.44
3:C:1151:HIS:CD2	3:C:1251:LYS:HB3	2.53	0.44
3:C:995:LYS:HZ1	3:C:1284:GLN:HE21	1.66	0.44
3:C:1252:ALA:HB3	3:C:1256:SER:O	2.18	0.44
3:L:618:LYS:NZ	3:L:688:THR:HG21	2.33	0.44
3:C:720:LYS:O	3:C:721:LYS:HB2	2.16	0.43
3:L:1118:MET:O	3:L:1122:GLN:HG3	2.17	0.43
3:L:670:VAL:HG11	3:L:681:ALA:HB3	2.00	0.43
3:C:1017:ALA:HB1	3:C:1086:TYR:CD2	2.53	0.43
3:C:579:HIS:HB3	3:C:582:ALA:HB2	1.99	0.43
3:C:1282:ARG:HG2	3:C:1286:THR:HG21	2.01	0.43
3:C:840:HIS:CE1	3:C:874:SER:OG	2.70	0.43
3:C:719:LEU:HD13	3:C:895:ARG:HB2	1.99	0.43
2:K:308:VAL:HG21	2:K:348:LEU:HG	2.01	0.43
2:K:367:ALA:O	2:K:439:ARG:NH1	2.46	0.43
3:C:1031:VAL:HB	3:C:1063:ILE:HG12	2.00	0.43
3:C:1081:VAL:O	3:C:1084:ASP:HB2	2.19	0.43
3:L:697:THR:HB	3:L:699:GLU:OE1	2.19	0.42
3:L:640:ILE:HG12	3:L:779:MET:CE	2.48	0.42
3:L:1290:THR:C	3:L:1292:GLU:H	2.23	0.42
3:L:657:LYS:HB3	3:L:657:LYS:HE3	1.69	0.42
3:C:788:LEU:HD13	3:C:1069:ASN:HB3	2.01	0.42
3:C:1143:GLU:O	3:C:1144:THR:HG23	2.19	0.42
3:C:1095:GLN:O	3:C:1099:LYS:HG2	2.19	0.42
3:C:1312:LYS:HD3	8:C:415:HOH:O	2.18	0.42
1:J:58:TYR:HE2	8:J:293:HOH:O	2.02	0.42
7:L:1317:RMO:S1	7:L:1317:RMO:O2	2.78	0.42
3:C:1080:SER:HB3	3:C:1258:ALA:HB1	2.00	0.42
2:K:517:PHE:CZ	2:K:521:LEU:HD11	2.55	0.42
3:L:1046:MET:HE2	3:L:1090:VAL:HG21	2.02	0.42
3:L:1046:MET:HE1	3:L:1086:TYR:O	2.20	0.42
2:B:338:ALA:HB2	5:B:606:FAD:C6	2.50	0.42
2:B:517:PHE:CG	3:C:1313:PHE:CZ	3.08	0.42
3:L:804:ARG:HG3	3:L:836:THR:O	2.19	0.42
2:K:256:LYS:HG3	2:K:275:PHE:CD2	2.55	0.41
3:C:1053:ALA:O	3:C:1098:LEU:HD11	2.19	0.41
2:K:281:PRO:HB2	2:K:287:LEU:HD12	2.01	0.41
3:C:804:ARG:HG3	3:C:836:THR:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:THR:O	1:A:97:ARG:HG3	2.21	0.41
2:K:473:GLN:HE21	2:K:482:LEU:HD12	1.85	0.41
3:C:1183:GLY:HA2	3:C:1247:CYS:O	2.21	0.41
3:C:1102:GLU:N	3:C:1103:PRO:CD	2.84	0.41
1:A:5:GLU:HG2	1:A:18:LYS:HG2	2.02	0.41
3:L:958:ARG:CG	3:L:958:ARG:HH11	2.34	0.41
3:L:1143:GLU:O	3:L:1144:THR:CB	2.69	0.41
3:L:841:PRO:HD2	3:L:866:ASN:HB3	2.01	0.41
2:B:376:SER:OG	2:B:379:THR:OG1	2.30	0.41
2:K:286:GLU:HB3	2:K:405:LEU:HD11	2.03	0.41
3:C:914:PHE:CD1	7:C:1317:RMO:AS1	3.34	0.41
3:C:1124:ARG:HB3	3:L:1134:ARG:HG3	2.02	0.41
3:C:911:PHE:O	3:C:912:ARG:C	2.58	0.41
3:C:657:LYS:HB3	3:C:657:LYS:HE3	1.72	0.41
1:J:11:ASN:OD1	1:J:90:GLY:HA3	2.20	0.41
3:L:719:LEU:CD1	3:L:895:ARG:HB2	2.51	0.41
3:L:1048:GLN:HE22	3:L:1187:ASN:HD22	1.68	0.41
2:B:367:ALA:O	2:B:439:ARG:NH1	2.50	0.41
3:C:752:ILE:HD11	3:C:763:PHE:CE1	2.54	0.40
1:A:104:ARG:HD3	1:A:162:THR:CG2	2.51	0.40
3:L:1286:THR:CG2	3:L:1310:VAL:HB	2.51	0.40
3:L:1046:MET:CE	3:L:1090:VAL:HB	2.51	0.40
2:B:256:LYS:HG3	2:B:275:PHE:CD2	2.56	0.40
1:A:37:ARG:HD3	3:C:595:ASP:O	2.21	0.40
3:L:1151:HIS:CD2	3:L:1251:LYS:HB3	2.56	0.40
3:L:966:ARG:O	3:L:970:GLU:HB2	2.20	0.40
3:L:747:HIS:CE1	3:L:801:LYS:HG2	2.56	0.40
3:L:741:HIS:HA	3:L:911:PHE:CE1	2.57	0.40
3:C:876:SER:HB3	3:C:914:PHE:CE2	2.55	0.40
3:L:725:GLU:HG2	3:L:857:VAL:HG11	2.03	0.40
3:L:616:LYS:HD2	3:L:658:ASP:O	2.21	0.40
3:C:966:ARG:O	3:C:970:GLU:HB2	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%)	154 (95%)	6 (4%)	2 (1%)	16	10
1	J	162/164 (99%)	153 (94%)	7 (4%)	2 (1%)	16	10
2	B	303/305 (99%)	291 (96%)	10 (3%)	2 (1%)	26	21
2	K	303/305 (99%)	290 (96%)	11 (4%)	2 (1%)	26	21
3	C	743/745 (100%)	717 (96%)	20 (3%)	6 (1%)	24	17
3	L	743/745 (100%)	724 (97%)	13 (2%)	6 (1%)	24	17
All	All	2416/2428 (100%)	2329 (96%)	67 (3%)	20 (1%)	24	17

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	338	ALA
2	B	425	SER
3	C	721	LYS
2	K	338	ALA
2	K	425	SER
3	L	721	LYS
1	A	64	LYS
3	C	912	ARG
3	C	1008	SER
3	L	1008	SER
1	A	63	ASP
3	C	797	GLY
3	C	1144	THR
1	J	64	LYS
3	L	797	GLY
3	L	912	ARG
3	L	1144	THR
3	C	1139	GLY
1	J	63	ASP
3	L	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%)	134 (98%)	3 (2%)	60	64
1	J	137/137 (100%)	132 (96%)	5 (4%)	42	43
2	B	261/261 (100%)	246 (94%)	15 (6%)	25	22
2	K	261/261 (100%)	247 (95%)	14 (5%)	27	24
3	C	624/624 (100%)	600 (96%)	24 (4%)	40	40
3	L	624/624 (100%)	601 (96%)	23 (4%)	41	41
All	All	2044/2044 (100%)	1960 (96%)	84 (4%)	37	36

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	ARG
1	A	129	ARG
1	A	140	GLU
2	B	241	THR
2	B	243	LYS
2	B	257	LEU
2	B	277	MET
2	B	312	LEU
2	B	348	LEU
2	B	351	ASN
2	B	395	LYS
2	B	412	SER
2	B	426	ARG
2	B	428	GLU
2	B	429	ASP
2	B	433	LYS
2	B	499	ASP
2	B	525	LYS
3	C	598	ARG
3	C	609	THR
3	C	618	LYS
3	C	623	SER
3	C	657	LYS
3	C	659	THR
3	C	710	SER
3	C	719	LEU

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Mol	Chain	Res	Type
3	C	725	GLU
3	C	743	TYR
3	C	779	MET
3	C	782	VAL
3	C	828	ASP
3	C	848	VAL
3	C	911	PHE
3	C	939	GLU
3	C	944	LYS
3	C	1004	LYS
3	C	1013	PHE
3	C	1105	LYS
3	C	1143	GLU
3	C	1203	LEU
3	C	1246	ASP
3	C	1286	THR
1	J	60	ARG
1	J	82	HIS
1	J	129	ARG
1	J	140	GLU
1	J	141	ASP
2	K	241	THR
2	K	243	LYS
2	K	277	MET
2	K	312	LEU
2	K	348	LEU
2	K	351	ASN
2	K	395	LYS
2	K	412	SER
2	K	426	ARG
2	K	428	GLU
2	K	429	ASP
2	K	433	LYS
2	K	499	ASP
2	K	525	LYS
3	L	598	ARG
3	L	609	THR
3	L	618	LYS
3	L	623	SER
3	L	657	LYS
3	L	659	THR
3	L	710	SER

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Mol	Chain	Res	Type
3	L	719	LEU
3	L	725	GLU
3	L	743	TYR
3	L	782	VAL
3	L	828	ASP
3	L	848	VAL
3	L	911	PHE
3	L	939	GLU
3	L	944	LYS
3	L	1004	LYS
3	L	1105	LYS
3	L	1143	GLU
3	L	1203	LEU
3	L	1242	SER
3	L	1246	ASP
3	L	1286	THR

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	144	GLN
1	A	146	ASN
2	B	272	ASN
2	B	351	ASN
2	B	471	GLN
2	B	473	GLN
3	C	614	HIS
3	C	626	GLN
3	C	677	HIS
3	C	728	ASN
3	C	821	HIS
3	C	840	HIS
3	C	875	HIS
3	C	884	HIS
3	C	904	ASN
3	C	1016	GLN
3	C	1033	HIS
3	C	1048	GLN
3	C	1212	HIS
3	C	1284	GLN
1	J	82	HIS

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Mol	Chain	Res	Type
1	J	131	GLN
1	J	144	GLN
1	J	146	ASN
2	K	273	GLN
2	K	292	HIS
2	K	351	ASN
2	K	473	GLN
3	L	614	HIS
3	L	626	GLN
3	L	677	HIS
3	L	728	ASN
3	L	821	HIS
3	L	840	HIS
3	L	884	HIS
3	L	904	ASN
3	L	1033	HIS
3	L	1048	GLN
3	L	1284	GLN

### 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](#)

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	$\# Z  > 2$
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	1.21	5 (10%)	54,89,89	2.42	10 (18%)
6	MTE	C	1316	7	19,26,26	1.50	2 (10%)	19,40,40	2.30	7 (36%)
7	RMO	C	1317	6	0,6,6	0.00	-	0,8,8	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	1.24	6 (12%)	54,89,89	2.20	10 (18%)
6	MTE	L	1316	7	19,26,26	0.94	1 (5%)	19,40,40	2.14	6 (31%)
7	RMO	L	1317	6	0,6,6	0.00	-	0,8,8	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
6	MTE	C	1316	7	-	0/6/34/34	0/3/3/3
7	RMO	C	1317	6	-	0/0/8/8	0/0/1/1
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
6	MTE	L	1316	7	-	0/6/34/34	0/3/3/3
7	RMO	L	1317	6	-	0/0/8/8	0/0/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1316	MTE	C7-C6	-3.17	1.51	1.53
5	K	606	FAD	C5X-N5	2.09	1.38	1.35
5	B	606	FAD	C2A-N1A	2.28	1.38	1.33
5	K	606	FAD	C2A-N1A	2.32	1.38	1.33
5	B	606	FAD	C4X-N5	2.46	1.37	1.33
5	K	606	FAD	C1'-N10	2.61	1.51	1.48
5	K	606	FAD	C4-N3	2.70	1.38	1.33
6	L	1316	MTE	C9-C10	2.86	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	606	FAD	C1'-N10	2.87	1.51	1.48
5	B	606	FAD	C4-N3	3.28	1.39	1.33
5	K	606	FAD	C4X-N5	3.53	1.38	1.33
5	K	606	FAD	C2A-N3A	3.67	1.38	1.32
5	B	606	FAD	C2A-N3A	3.75	1.38	1.32
6	C	1316	MTE	C9-C10	4.12	1.50	1.41

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	606	FAD	N3A-C2A-N1A	-12.38	119.42	128.89
5	K	606	FAD	N3A-C2A-N1A	-10.79	120.64	128.89
5	B	606	FAD	C4X-C4-N3	-3.61	118.65	123.59
5	K	606	FAD	C4X-C4-N3	-3.39	118.95	123.59
6	C	1316	MTE	O2P-P-O4'	-3.15	97.49	106.56
6	L	1316	MTE	O3'-C7-C6	-3.08	106.86	108.96
6	L	1316	MTE	O2P-P-O4'	-2.85	98.36	106.56
5	K	606	FAD	O3P-PA-O5B	-2.56	96.14	102.94
5	K	606	FAD	C4A-C5A-N7A	-2.21	107.45	109.48
5	K	606	FAD	C2B-C1B-N9A	2.11	117.51	114.29
6	C	1316	MTE	O2P-P-O1P	2.18	117.60	110.58
5	B	606	FAD	C4-C4X-C10	2.24	121.38	119.94
5	K	606	FAD	O2P-P-O3P	2.30	115.54	105.09
5	K	606	FAD	C5X-C9A-N10	2.35	119.40	117.62
5	B	606	FAD	C6-C5X-C9A	2.44	122.20	118.98
6	C	1316	MTE	C2-N1-C10	2.45	120.06	114.54
6	L	1316	MTE	O3P-P-O2P	2.58	117.20	107.38
5	K	606	FAD	C4X-N5-C5X	2.79	119.97	116.76
5	B	606	FAD	C4X-N5-C5X	2.81	120.00	116.76
6	C	1316	MTE	N2-C2-N1	2.83	121.88	117.20
6	C	1316	MTE	O3P-P-O2P	2.99	118.78	107.38
5	B	606	FAD	O4'-C4'-C3'	3.13	116.89	109.02
6	L	1316	MTE	C2-N1-C10	3.28	121.92	114.54
5	B	606	FAD	C2B-C1B-N9A	3.46	119.58	114.29
6	L	1316	MTE	N8-C10-N1	3.51	122.21	116.62
5	K	606	FAD	C1'-N10-C9A	3.52	122.81	118.86
6	C	1316	MTE	N8-C10-N1	4.01	123.01	116.62
6	L	1316	MTE	C4-N3-C2	4.04	121.54	115.94
5	B	606	FAD	C1'-N10-C9A	4.12	123.49	118.86
5	B	606	FAD	C5X-C9A-N10	4.34	120.92	117.62
5	B	606	FAD	C4-N3-C2	5.38	119.90	115.25
6	C	1316	MTE	C4-N3-C2	5.48	123.55	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	606	FAD	C4-N3-C2	6.67	121.01	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	606	FAD	2	0
7	C	1317	RMO	2	0
5	K	606	FAD	2	0
7	L	1317	RMO	3	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%)	0.41	9 (5%)	29 37	11, 22, 41, 56	0
1	J	164/164 (100%)	0.46	12 (7%)	18 24	11, 23, 41, 56	0
2	B	305/305 (100%)	0.63	25 (8%)	14 20	19, 30, 41, 46	0
2	K	305/305 (100%)	0.52	21 (6%)	20 27	19, 30, 41, 46	0
3	C	745/745 (100%)	0.23	22 (2%)	54 62	11, 22, 35, 48	0
3	L	745/745 (100%)	0.28	26 (3%)	48 57	11, 22, 35, 48	0
All	All	2428/2428 (100%)	0.36	115 (4%)	35 44	11, 24, 39, 56	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	1288	ASN	8.5
1	J	61	LEU	8.4
3	L	1290	THR	6.9
1	J	2	THR	6.6
1	J	60	ARG	6.1
1	J	58	TYR	5.4
2	B	528	GLY	4.8
3	L	1287	ASN	4.7
2	B	336	TRP	4.6
1	A	2	THR	4.5
1	A	58	TYR	4.4
1	J	59	ASP	4.3
2	K	335	ARG	4.1
2	K	528	GLY	4.1
1	J	63	ASP	4.0
1	A	61	LEU	3.9
1	J	97	ARG	3.8
3	C	943	TRP	3.7
3	L	935	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	335	ARG	3.7
3	L	1289	ASN	3.6
2	K	336	TRP	3.6
3	L	683	HIS	3.4
2	K	251	GLN	3.4
2	B	272	ASN	3.4
3	L	638	ASP	3.4
2	B	378	GLY	3.4
3	C	1158	ALA	3.3
2	B	365	PHE	3.3
3	L	1286	THR	3.3
1	A	97	ARG	3.2
3	L	718	ASP	3.2
1	J	133	GLU	3.2
3	L	1110	ASP	3.1
1	A	63	ASP	3.1
1	J	161	ARG	3.1
3	C	683	HIS	3.1
2	B	477	PHE	3.1
3	L	1291	LYS	3.0
1	J	165	LYS	3.0
2	B	497	SER	3.0
3	C	1144	THR	3.0
2	K	378	GLY	2.9
2	K	446	SER	2.9
3	C	1245	ARG	2.9
2	K	424	ALA	2.9
1	A	120	ILE	2.9
3	C	705	ASN	2.8
2	K	471	GLN	2.8
1	A	60	ARG	2.8
3	L	571	ASP	2.8
2	K	377	ARG	2.8
3	L	943	TRP	2.8
3	C	657	LYS	2.7
2	K	475	SER	2.7
3	C	1023	VAL	2.7
3	C	1108	ASN	2.7
2	K	429	ASP	2.6
2	B	224	PRO	2.6
3	L	1109	PRO	2.6
3	C	571	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
3	L	958	ARG	2.6
2	B	440	VAL	2.6
3	C	616	LYS	2.6
1	J	66	ILE	2.6
2	B	525	LYS	2.5
3	C	1247	CYS	2.5
3	L	691	ASP	2.5
2	B	509	ARG	2.5
2	K	332	GLU	2.5
3	C	1143	GLU	2.5
3	C	1246	ASP	2.5
3	L	1247	CYS	2.5
3	L	720	LYS	2.4
2	B	475	SER	2.4
2	B	424	ALA	2.4
1	J	64	LYS	2.4
3	C	1259	VAL	2.4
2	B	388	THR	2.4
2	B	401	GLU	2.3
3	C	983	GLU	2.3
3	L	725	GLU	2.3
3	L	1292	GLU	2.3
3	C	1290	THR	2.3
3	L	1111	GLY	2.2
2	K	294	PRO	2.2
2	B	429	ASP	2.2
3	C	1287	ASN	2.2
1	A	141	ASP	2.2
3	C	598	ARG	2.2
2	K	401	GLU	2.2
2	K	499	ASP	2.2
2	K	326	VAL	2.2
2	B	352	ILE	2.2
2	B	511	LEU	2.1
3	L	948	LYS	2.1
2	K	467	LEU	2.1
3	C	575	ARG	2.1
2	B	447	MET	2.1
2	B	404	LEU	2.1
3	C	1001	ILE	2.1
3	L	721	LYS	2.1
2	B	498	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
2	K	444	PRO	2.1
2	K	484	GLN	2.1
2	B	485	ASP	2.1
2	K	498	PRO	2.1
2	B	387	HIS	2.0
3	L	1107	LYS	2.0
1	A	19	ASN	2.0
2	B	397	LEU	2.0
3	L	970	GLU	2.0
3	L	983	GLU	2.0
3	C	724	SER	2.0
2	K	525	LYS	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, 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
6	MTE	L	1316	24/24	0.96	0.11	-0.25	13,17,29,30	0
4	FES	J	601	4/4	0.99	0.10	-0.42	14,14,14,17	0
4	FES	A	601	4/4	0.99	0.10	-0.69	10,12,14,15	0
5	FAD	K	606	53/53	0.97	0.09	-1.05	17,22,24,24	0
6	MTE	C	1316	24/24	0.97	0.09	-1.07	15,17,20,24	0
4	FES	A	602	4/4	0.98	0.08	-1.15	14,15,17,19	0
5	FAD	B	606	53/53	0.96	0.10	-1.18	14,20,24,28	0
7	RMO	L	1317	6/6	0.99	0.07	-1.61	22,24,39,40	0
4	FES	J	602	4/4	0.99	0.06	-1.66	12,13,14,15	0
7	RMO	C	1317	6/6	0.99	0.07	-2.38	25,29,37,40	0

## 6.5 Other polymers

There are no such residues in this entry.