Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2023 – 05:25 PM EDT

PDB ID	:	3B9J
Title	:	Structure of Xanthine Oxidase with 2-hydroxy-6-methylpurine
Authors	:	Pauff, J.M.; Zhang, J.; Bell, C.E.; Hille, R.
Deposited on	:	2007-11-05
Resolution	:	2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

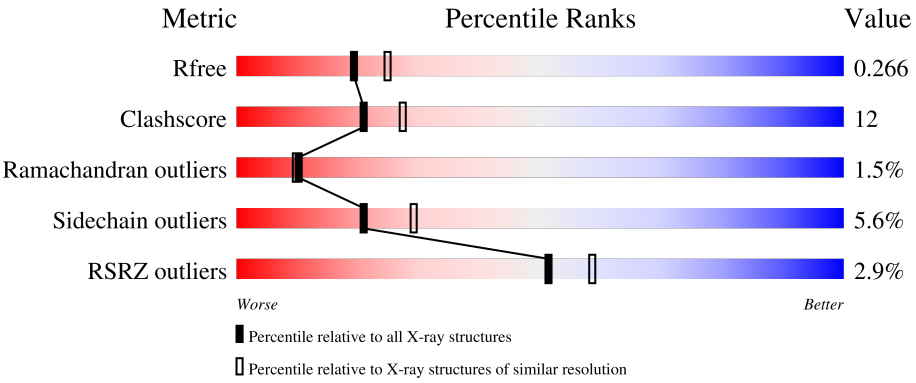
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	219	60% 12% 26%
1	I	219	4% 61% 10% 26%
2	B	350	2% 70% 15% 13%
2	J	350	3% 72% 13% 13%
3	C	763	3% 76% 19%

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Mol	Chain	Length	Quality of chain
3	K	763	

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	MOS	C	1334	-	-	X	-
8	MOS	K	1334	-	-	X	-
9	290	C	1335	-	-	X	-
9	290	K	1335	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 19847 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 oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	0	0	0
			1239	778	222	227	12			
1	I	162	Total	C	N	O	S	0	0	0
			1215	764	214	225	12			

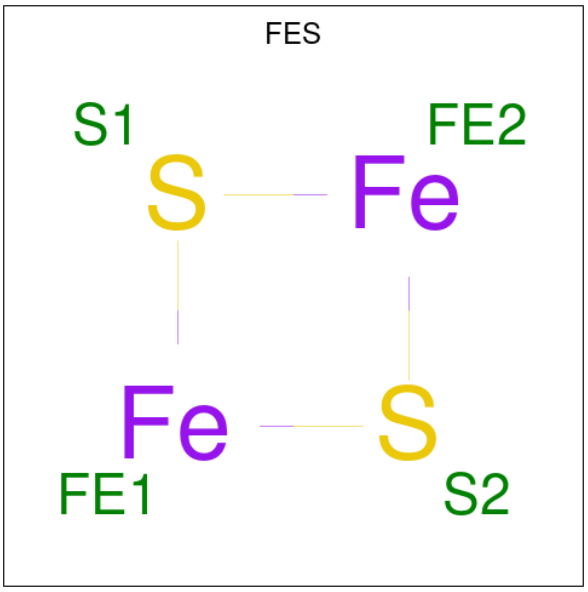
- Molecule 2 is a protein called xanthine oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	305	Total	C	N	O	S	0	0	0
			2381	1533	400	435	13			
2	J	305	Total	C	N	O	S	0	0	0
			2356	1516	393	434	13			

- Molecule 3 is a protein called xanthine oxidase.

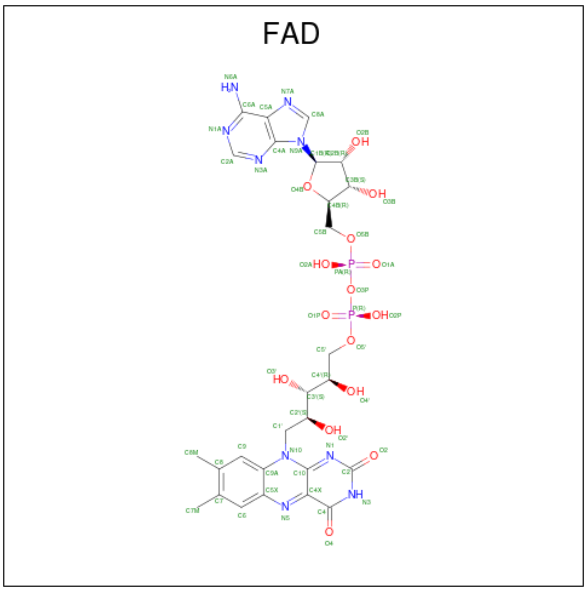
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	758	Total	C	N	O	S	0	0	0
			5835	3688	1005	1107	35			
3	K	747	Total	C	N	O	S	0	0	0
			5759	3645	987	1093	34			

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

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

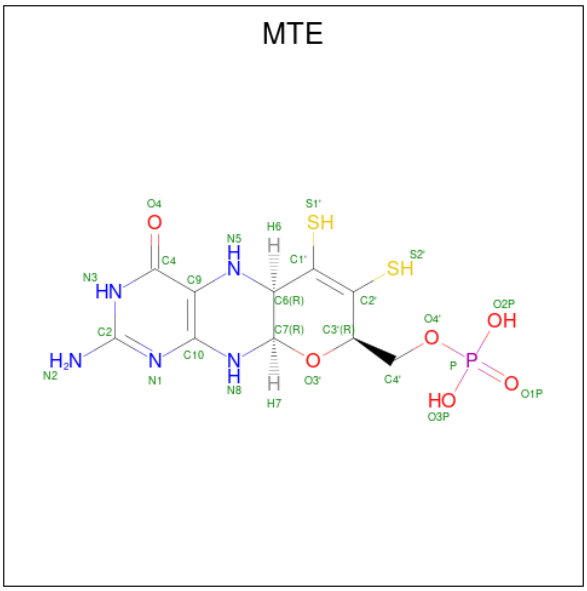


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	J	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

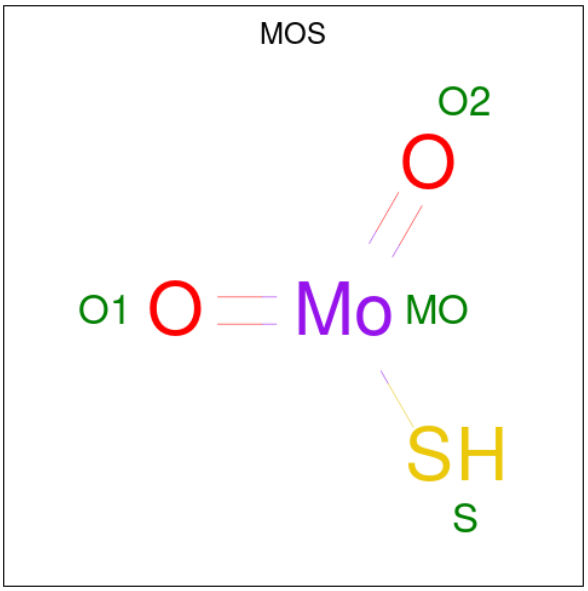
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	Ca	0	0
			1	1		

- Molecule 7 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: $C_{10}H_{14}N_5O_6PS_2$).



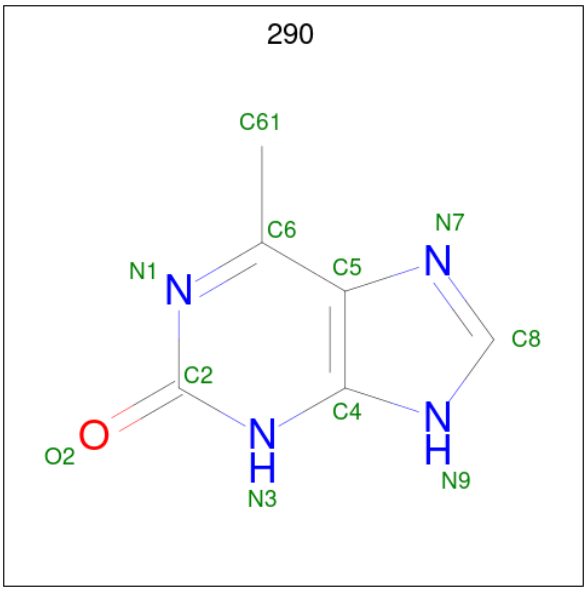
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	C	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
7	K	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		

- Molecule 8 is DIOXOTHIOMOLYBDENUM(VI) ION (three-letter code: MOS) (formula: $HMoO_2S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	1	Total	Mo	O	S	0	0
			4	1	2	1		
8	K	1	Total	Mo	O	S	0	0
			4	1	2	1		

- Molecule 9 is 6-methyl-3,9-dihydro-2H-purin-2-one (three-letter code: 290) (formula: $C_6H_6N_4O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	C	1	Total	C	N	O	0	0
			11	6	4	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	K	1	Total	C	N	O	0	0
			11	6	4	1		

- Molecule 10 is water.

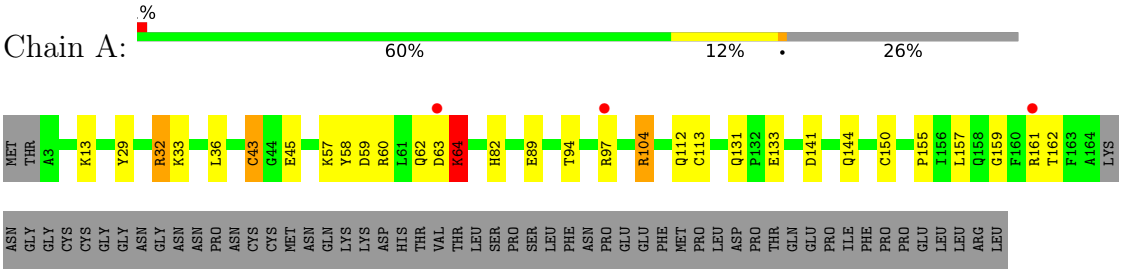
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	68	Total	O	0	0
			68	68		
10	B	87	Total	O	0	0
			87	87		
10	C	247	Total	O	0	0
			247	247		
10	I	73	Total	O	0	0
			73	73		
10	J	90	Total	O	0	0
			90	90		
10	K	296	Total	O	0	0
			296	296		

3 Residue-property plots (i)

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

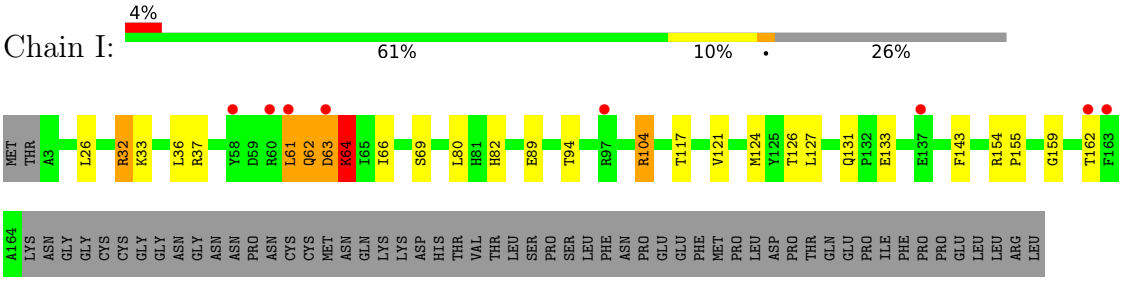
• Molecule 1: xanthine oxidase

Chain A:



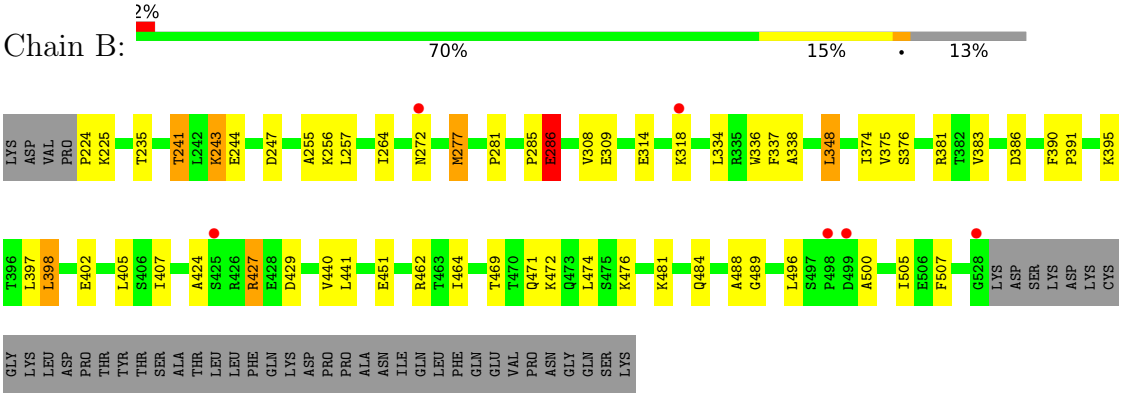
• Molecule 1: xanthine oxidase

Chain I:



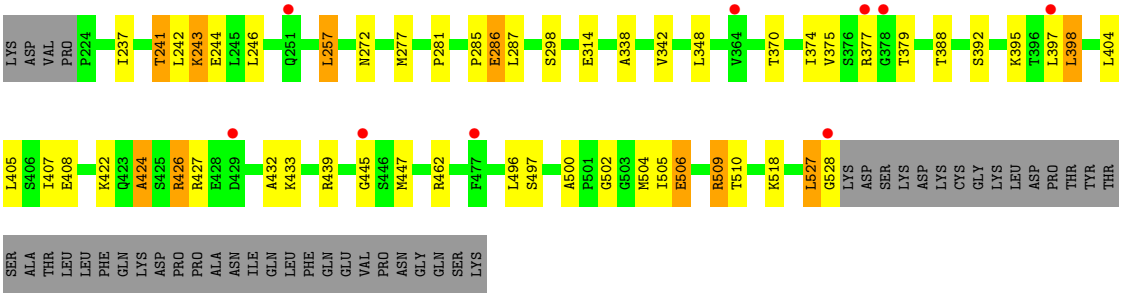
• Molecule 2: xanthine oxidase

Chain B:



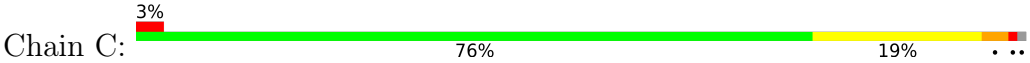
• Molecule 2: xanthine oxidase

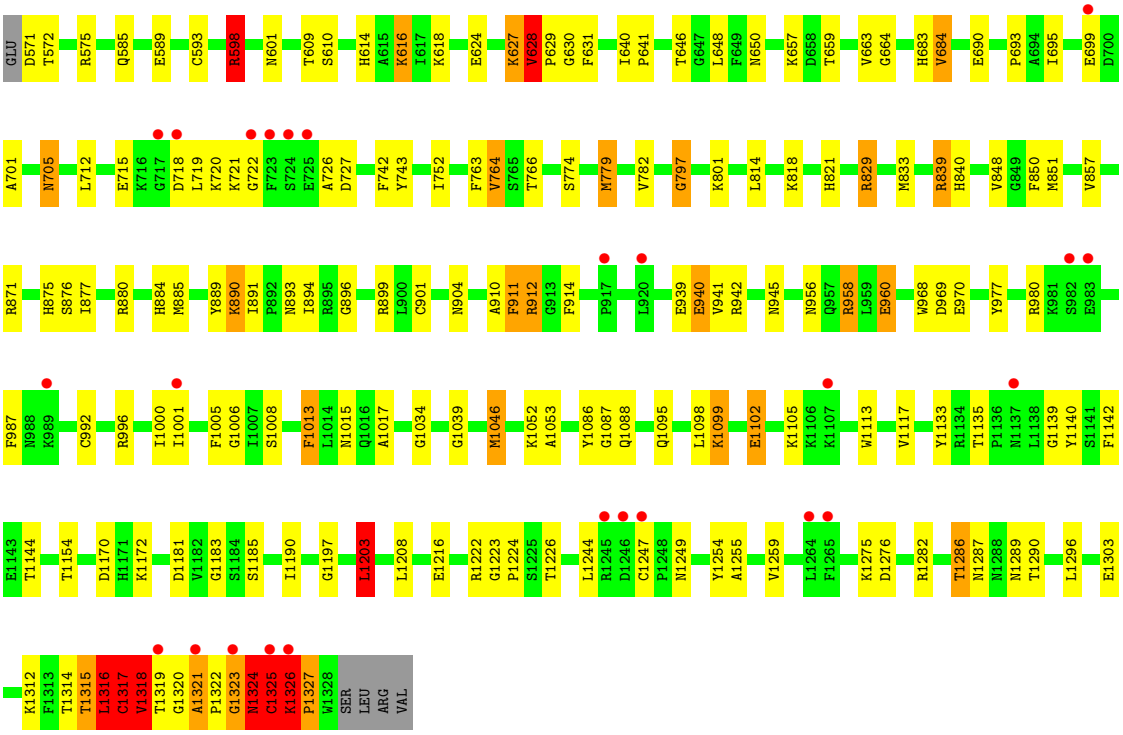
Chain J:



• Molecule 3: xanthine oxidase

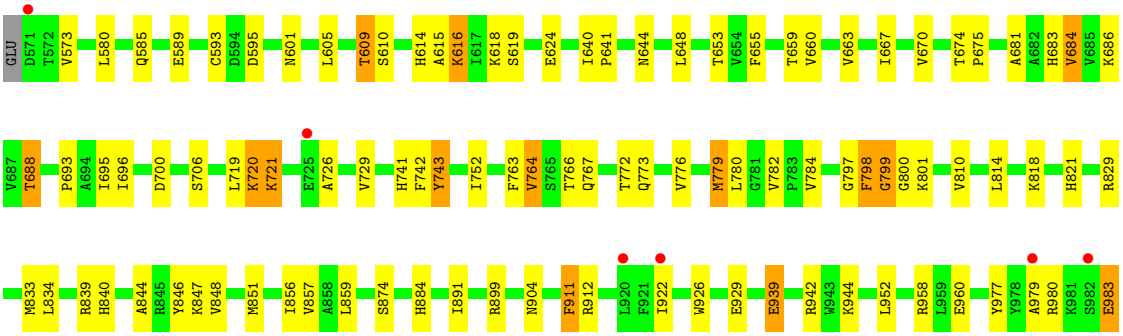
Chain C:

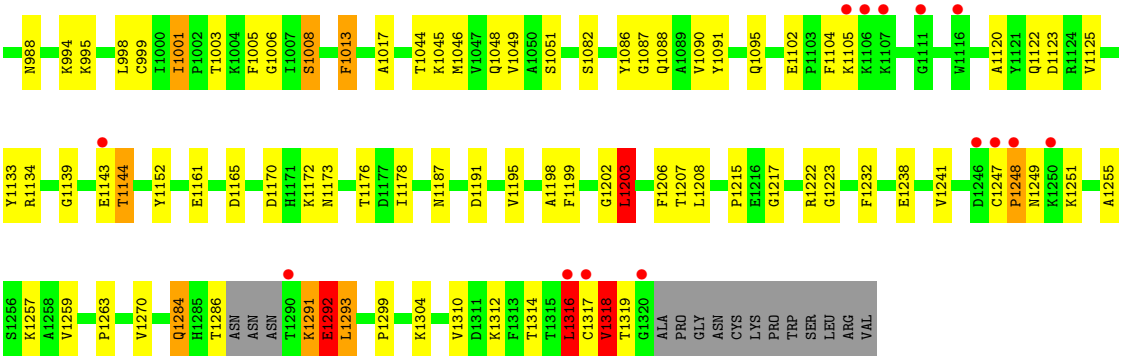




• Molecule 3: xanthine oxidase

Chain K:




N988 K994 K995 L998 C999 I1000 I1001 P1002 T1003 K1004 F1005 G1006 I1007 S1008 F1013 A1017 T1044 K1045 M1046 V1047 Q1048 V1049 A1050 S1051 S1082 Y1086 G1087 Q1088 A1089 V1090 Y1091 Q1095 E1102 P1103 F1104 K1105 K1106 K1107 G1111 W1116 A1120 Y1121 Q1122 D1123 R1124 V1125
Y1133 R1134 G1139 E1143 T1144 Y1152 E1161 D1165 D1170 H1171 K1172 N1173 T1176 D1177 I1178 N1187 D1191 V1195 A1198 F1199 G1202 L1203 F1206 T1207 L1208 P1215 E1216 G1217 R1222 G1223 F1232 E1238 V1241 D1246 C1247 P1248 N1249 K1250 K1251 A1255
S1256 K1257 A1258 V1259 P1263 V1270 Q1284 H1285 T1286 ASN ASN ASN T1290 K1291 E1292 L1293 P1299 K1304 V1310 D1311 K1312 F1313 T1314 T1315 L1316 C1317 V1318 T1319 G1320 ALA PRO GLY ASN CYS LYS PRO TRP SER LEU ARG VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	133.19Å 73.79Å 146.50Å 90.00° 98.87° 90.00°	Depositor
Resolution (Å)	144.34 – 2.30 33.59 – 2.23	Depositor EDS
% Data completeness (in resolution range)	96.2 (144.34-2.30) 94.6 (33.59-2.23)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.17 (at 2.22Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.194 , 0.263 0.197 , 0.266	Depositor DCC
R_{free} test set	6568 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	26.1	Xtriage
Anisotropy	0.786	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 47.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	19847	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MTE, FES, 290, MOS, CA, FAD

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	0.84	0/1261	0.90	4/1702 (0.2%)
1	I	0.78	0/1237	0.85	2/1672 (0.1%)
2	B	0.77	0/2430	0.80	2/3282 (0.1%)
2	J	0.72	1/2403 (0.0%)	0.78	2/3248 (0.1%)
3	C	0.83	4/5963 (0.1%)	0.93	16/8078 (0.2%)
3	K	0.78	1/5885 (0.0%)	0.85	8/7971 (0.1%)
All	All	0.79	6/19179 (0.0%)	0.86	34/25953 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	I	0	1
3	C	3	10
3	K	0	5
All	All	3	17

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	593	CYS	CB-SG	-6.74	1.70	1.82
3	K	593	CYS	CB-SG	-6.64	1.71	1.82
3	C	992	CYS	CB-SG	-6.30	1.71	1.82
2	J	314	GLU	CG-CD	5.70	1.60	1.51
3	C	699	GLU	CG-CD	5.22	1.59	1.51
3	C	1102	GLU	CG-CD	5.10	1.59	1.51

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	K	839	ARG	NE-CZ-NH2	-10.28	115.16	120.30
1	I	32	ARG	NE-CZ-NH2	-10.17	115.21	120.30
1	A	32	ARG	NE-CZ-NH2	-10.06	115.27	120.30
3	C	1326	LYS	N-CA-C	9.29	136.07	111.00
1	I	32	ARG	NE-CZ-NH1	9.20	124.90	120.30
3	C	628	VAL	N-CA-C	8.60	134.23	111.00
3	K	839	ARG	NE-CZ-NH1	8.44	124.52	120.30
3	C	829	ARG	NE-CZ-NH2	-8.17	116.22	120.30
1	A	32	ARG	NE-CZ-NH1	7.37	123.98	120.30
3	C	1318	VAL	N-CA-C	7.30	130.71	111.00
3	C	1316	LEU	N-CA-CB	-7.03	96.34	110.40
3	K	1203	LEU	CA-CB-CG	6.82	130.99	115.30
3	C	839	ARG	NE-CZ-NH1	6.77	123.69	120.30
3	C	1316	LEU	CA-CB-CG	6.46	130.15	115.30
3	C	1318	VAL	CB-CA-C	-6.44	99.16	111.40
3	C	1203	LEU	CA-CB-CG	6.43	130.08	115.30
3	C	1327	PRO	N-CA-CB	6.41	110.99	103.30
3	C	839	ARG	NE-CZ-NH2	-6.30	117.15	120.30
2	J	439	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	A	32	ARG	CG-CD-NE	-5.97	99.26	111.80
2	B	398	LEU	CA-CB-CG	5.86	128.77	115.30
3	K	595	ASP	CB-CG-OD1	5.59	123.33	118.30
2	B	386	ASP	CB-CG-OD1	5.54	123.28	118.30
3	C	1325	CYS	N-CA-C	-5.50	96.16	111.00
1	A	97	ARG	NE-CZ-NH1	5.39	123.00	120.30
3	C	1316	LEU	CB-CA-C	-5.39	99.95	110.20
2	J	398	LEU	CA-CB-CG	5.39	127.70	115.30
3	K	980	ARG	NE-CZ-NH2	-5.31	117.64	120.30
3	K	942	ARG	NE-CZ-NH1	5.27	122.94	120.30
3	K	980	ARG	NE-CZ-NH1	5.25	122.92	120.30
3	C	942	ARG	NE-CZ-NH1	5.15	122.88	120.30
3	K	798	PHE	CA-C-N	5.09	126.38	116.20
3	C	598	ARG	CG-CD-NE	-5.08	101.13	111.80
3	C	1316	LEU	CA-C-N	5.03	128.26	117.20

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	1315	THR	CA
3	C	1319	THR	CA
3	C	1326	LYS	CA

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	64	LYS	Peptide
3	C	1314	THR	Peptide
3	C	1315	THR	Peptide
3	C	1316	LEU	Peptide
3	C	1317	CYS	Peptide,Mainchain
3	C	1318	VAL	Peptide
3	C	1324	ASN	Peptide
3	C	627	LYS	Peptide
3	C	628	VAL	Peptide
3	C	630	GLY	Peptide
1	I	62	GLN	Peptide
3	K	1291	LYS	Peptide
3	K	1292	GLU	Peptide
3	K	1318	VAL	Peptide
3	K	798	PHE	Peptide
3	K	799	GLY	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1239	0	1245	26	0
1	I	1215	0	1201	19	0
2	B	2381	0	2437	58	0
2	J	2356	0	2394	48	0
3	C	5835	0	5747	162	0
3	K	5759	0	5679	156	0
4	A	8	0	0	0	0
4	I	8	0	0	0	0
5	B	53	0	31	2	0
5	J	53	0	31	3	0
6	C	1	0	0	0	0
7	C	24	0	10	0	0
7	K	24	0	10	2	0
8	C	4	0	0	7	0
8	K	4	0	0	8	0
9	C	11	0	6	4	0
9	K	11	0	6	5	0
10	A	68	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	B	87	0	0	6	0
10	C	247	0	0	22	0
10	I	73	0	0	2	0
10	J	90	0	0	5	0
10	K	296	0	0	15	0
All	All	19847	0	18797	461	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 12.

All (461) 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)
8:K:1334:MOS:O1	9:K:1335:290:C8	1.75	1.32
3:K:833:MET:HE3	3:K:1222:ARG:C	1.51	1.31
3:K:1046:MET:HE1	3:K:1086:TYR:C	1.65	1.16
8:K:1334:MOS:O1	9:K:1335:290:H8	1.30	1.15
3:C:683:HIS:HB2	10:C:1420:HOH:O	1.46	1.12
3:C:571:ASP:N	10:C:1384:HOH:O	1.83	1.09
3:C:1321:ALA:HB3	3:C:1322:PRO:HA	1.33	1.09
3:C:1323:GLY:CA	3:C:1324:ASN:CB	2.30	1.08
3:K:1143:GLU:O	3:K:1144:THR:HG23	1.52	1.08
3:C:705:ASN:HB2	10:C:1457:HOH:O	1.52	1.08
3:C:1321:ALA:HB3	3:C:1322:PRO:CA	1.84	1.07
3:K:640:ILE:HG23	3:K:779:MET:CE	1.86	1.05
3:K:726:ALA:HA	3:K:851:MET:HE1	1.04	1.04
2:B:424:ALA:O	10:B:677:HOH:O	1.78	0.98
8:C:1334:MOS:S	9:C:1335:290:H8	2.04	0.98
3:C:641:PRO:HD2	3:C:779:MET:HE3	1.46	0.97
3:C:779:MET:HE2	3:C:779:MET:O	1.63	0.97
3:C:726:ALA:HA	3:C:851:MET:HE1	1.47	0.96
2:B:481:LYS:CB	10:B:648:HOH:O	2.13	0.95
3:C:610:SER:O	3:C:663:VAL:O	1.85	0.94
3:K:726:ALA:HA	3:K:851:MET:CE	1.97	0.92
3:C:641:PRO:HD2	3:C:779:MET:CE	2.00	0.92
3:C:833:MET:HE3	3:C:1222:ARG:C	1.90	0.91
2:J:375:VAL:HG21	2:J:405:LEU:HD22	1.49	0.91
3:K:1046:MET:CE	3:K:1086:TYR:C	2.39	0.90
3:K:767:GLN:HE22	3:K:799:GLY:CA	1.84	0.90
3:C:1323:GLY:HA3	3:C:1324:ASN:CB	1.98	0.90
3:K:720:LYS:O	3:K:721:LYS:HB2	1.71	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ASP:OD1	10:A:639:HOH:O	1.91	0.87
3:K:851:MET:CE	3:K:857:VAL:HG21	2.04	0.87
3:C:616:LYS:HD2	3:C:659:THR:HG22	1.53	0.87
3:C:1323:GLY:HA2	3:C:1324:ASN:CB	2.04	0.87
3:K:726:ALA:CA	3:K:851:MET:HE1	1.99	0.86
3:C:640:ILE:HG23	3:C:779:MET:CE	2.06	0.86
3:C:1322:PRO:O	3:C:1323:GLY:O	1.93	0.85
8:C:1334:MOS:O1	9:C:1335:290:C8	2.23	0.85
3:K:616:LYS:HD2	3:K:659:THR:HG22	1.59	0.84
3:K:833:MET:HE3	3:K:1222:ARG:O	1.77	0.84
3:K:640:ILE:HG23	3:K:779:MET:HE2	1.60	0.83
9:K:1335:290:H61	10:K:1624:HOH:O	1.77	0.83
3:K:767:GLN:HE22	3:K:799:GLY:HA3	1.41	0.83
2:B:441:LEU:CD2	2:B:451:GLU:OE1	2.27	0.82
2:J:404:LEU:HD21	2:J:407:ILE:HD11	1.61	0.82
3:C:833:MET:HE3	3:C:1222:ARG:O	1.79	0.82
2:B:441:LEU:HD22	2:B:451:GLU:OE1	1.80	0.82
3:C:705:ASN:CB	10:C:1457:HOH:O	2.13	0.82
3:K:851:MET:HE3	3:K:857:VAL:HG21	1.59	0.82
3:C:1316:LEU:O	3:C:1319:THR:OG1	1.98	0.81
3:K:779:MET:HE2	3:K:779:MET:O	1.79	0.81
3:K:618:LYS:HG2	3:K:688:THR:HG22	1.60	0.81
3:K:833:MET:HE3	3:K:1223:GLY:N	1.95	0.81
3:C:1046:MET:CE	3:C:1086:TYR:HB2	2.11	0.80
2:B:241:THR:HG22	2:B:244:GLU:H	1.45	0.80
3:C:705:ASN:OD1	10:C:1457:HOH:O	2.00	0.79
2:B:314:GLU:O	2:B:318:LYS:HD2	1.83	0.79
3:C:889:TYR:O	3:C:891:ILE:HD12	1.82	0.78
8:C:1334:MOS:O1	9:C:1335:290:H8	1.84	0.78
3:C:1046:MET:CE	3:C:1086:TYR:CB	2.61	0.78
3:K:610:SER:O	3:K:663:VAL:O	2.02	0.78
3:C:1046:MET:HE3	3:C:1086:TYR:C	2.05	0.77
2:B:241:THR:CG2	2:B:244:GLU:H	1.98	0.77
3:C:705:ASN:CG	10:C:1457:HOH:O	2.22	0.77
2:B:241:THR:HG23	2:B:243:LYS:HG2	1.67	0.77
3:C:1034:GLY:O	10:C:1545:HOH:O	2.02	0.77
3:K:1046:MET:HE1	3:K:1087:GLY:N	2.01	0.75
3:C:829:ARG:HG3	3:C:833:MET:HE2	1.66	0.75
8:K:1334:MOS:S	8:K:1334:MOS:O2	2.44	0.75
3:C:640:ILE:HG23	3:C:779:MET:HE2	1.67	0.75
3:C:726:ALA:HA	3:C:851:MET:CE	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1321:ALA:CB	3:C:1322:PRO:CA	2.60	0.75
2:J:257:LEU:O	5:J:606:FAD:H2B	1.87	0.75
2:B:241:THR:HG21	10:B:662:HOH:O	1.86	0.75
3:C:1282:ARG:HA	3:C:1286:THR:CG2	2.17	0.75
3:C:833:MET:HE1	3:C:1223:GLY:HA2	1.67	0.74
3:K:1292:GLU:HG3	3:K:1293:LEU:N	2.03	0.74
3:K:779:MET:HG2	3:K:810:VAL:HG13	1.67	0.74
3:K:618:LYS:CG	3:K:688:THR:HG22	2.17	0.74
1:A:161:ARG:HG2	10:A:657:HOH:O	1.88	0.73
2:J:241:THR:HG23	2:J:243:LYS:HE2	1.70	0.73
3:C:752:ILE:HD11	3:C:763:PHE:HE1	1.54	0.73
3:C:1095:GLN:O	3:C:1099:LYS:HG2	1.87	0.73
2:J:500:ALA:HB3	2:J:505:ILE:HD11	1.71	0.72
3:K:833:MET:CE	3:K:1222:ARG:C	2.46	0.72
2:B:429:ASP:OD2	3:C:1226:THR:HG21	1.90	0.72
2:B:285:PRO:O	2:B:286:GLU:HB2	1.89	0.72
3:C:1321:ALA:HB3	3:C:1322:PRO:C	2.10	0.71
3:C:940:GLU:OE2	10:C:1399:HOH:O	2.07	0.71
3:C:876:SER:HB2	10:C:1404:HOH:O	1.91	0.71
1:A:104:ARG:HD2	10:A:644:HOH:O	1.91	0.70
2:J:237:ILE:HD12	2:J:277:MET:CE	2.22	0.70
3:K:767:GLN:HE22	3:K:799:GLY:HA2	1.56	0.70
1:I:159:GLY:O	1:I:162:THR:HG22	1.91	0.70
3:C:1316:LEU:HD13	3:C:1316:LEU:H	1.56	0.70
3:K:764:VAL:HG22	3:K:766:THR:HG22	1.73	0.69
3:K:1143:GLU:O	3:K:1144:THR:CG2	2.35	0.69
2:B:285:PRO:O	2:B:286:GLU:CB	2.40	0.69
2:J:506:GLU:OE1	10:J:639:HOH:O	2.11	0.69
3:C:764:VAL:HG22	3:C:766:THR:HG22	1.74	0.68
2:J:241:THR:CG2	2:J:243:LYS:HG2	2.23	0.68
1:A:104:ARG:HD3	1:A:162:THR:HG21	1.74	0.68
3:K:779:MET:HG2	3:K:810:VAL:CG1	2.23	0.68
3:C:640:ILE:HG23	3:C:779:MET:HE3	1.76	0.68
3:C:829:ARG:CG	3:C:833:MET:HE2	2.24	0.67
1:A:104:ARG:CD	1:A:162:THR:HG21	2.23	0.67
2:B:314:GLU:O	2:B:318:LYS:CD	2.42	0.67
3:K:1249:ASN:O	3:K:1255:ALA:HA	1.95	0.66
3:C:833:MET:CE	3:C:1222:ARG:C	2.63	0.66
3:C:1046:MET:CE	3:C:1086:TYR:C	2.64	0.66
3:C:695:ILE:H	3:C:904:ASN:HD22	1.44	0.66
3:C:764:VAL:HG22	3:C:766:THR:CG2	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:683:HIS:CB	10:C:1420:HOH:O	2.20	0.65
2:B:424:ALA:HB2	3:C:1170:ASP:OD2	1.96	0.65
3:K:1102:GLU:OE1	3:K:1105:LYS:HD3	1.95	0.64
3:C:1046:MET:HE1	3:C:1087:GLY:N	2.12	0.64
3:C:1321:ALA:CB	3:C:1322:PRO:C	2.66	0.64
2:B:500:ALA:HB3	2:B:505:ILE:HD11	1.80	0.64
3:K:999:CYS:SG	3:K:1001:ILE:CD1	2.85	0.64
2:B:441:LEU:HD23	2:B:451:GLU:OE1	1.98	0.63
3:C:880:ARG:O	3:C:884:HIS:HD2	1.81	0.63
3:K:772:THR:O	3:K:776:VAL:HG23	1.98	0.63
3:K:851:MET:HE2	3:K:857:VAL:HG21	1.80	0.63
3:K:601:ASN:HD22	3:K:821:HIS:HD2	1.46	0.63
3:K:1292:GLU:HG3	3:K:1293:LEU:CA	2.28	0.63
3:C:970:GLU:OE1	10:C:1461:HOH:O	2.15	0.62
3:K:767:GLN:NE2	3:K:799:GLY:HA3	2.11	0.62
3:C:1140:TYR:OH	10:C:1496:HOH:O	2.14	0.62
2:J:281:PRO:HB2	2:J:287:LEU:CD1	2.28	0.62
2:J:447:MET:HG2	2:J:527:LEU:HD13	1.81	0.62
8:K:1334:MOS:S	8:K:1334:MOS:MO	2.11	0.62
2:B:374:ILE:HD13	2:B:398:LEU:HD23	1.81	0.62
3:K:1312:LYS:O	3:K:1318:VAL:HG22	2.00	0.62
3:K:720:LYS:O	3:K:721:LYS:CB	2.47	0.62
8:K:1334:MOS:O1	9:K:1335:290:N9	2.30	0.62
3:C:1088:GLN:HG2	3:C:1133:TYR:CE1	2.35	0.62
3:K:1046:MET:CE	3:K:1086:TYR:O	2.47	0.62
8:C:1334:MOS:S	8:C:1334:MOS:O2	2.58	0.61
3:K:1165:ASP:CB	10:K:1571:HOH:O	2.48	0.61
3:K:1165:ASP:HB2	10:K:1571:HOH:O	2.00	0.61
3:C:1282:ARG:HA	3:C:1286:THR:HG22	1.82	0.61
3:K:695:ILE:H	3:K:904:ASN:HD22	1.49	0.60
3:C:779:MET:HE2	3:C:779:MET:C	2.21	0.60
3:C:833:MET:HE1	3:C:1223:GLY:CA	2.30	0.60
8:C:1334:MOS:O2	8:C:1334:MOS:MO	1.73	0.60
2:J:272:ASN:ND2	3:K:683:HIS:CE1	2.68	0.60
3:K:1046:MET:HE1	3:K:1086:TYR:CA	2.31	0.60
3:K:1046:MET:HE1	3:K:1086:TYR:CB	2.31	0.60
3:K:573:VAL:HG23	10:K:1394:HOH:O	2.00	0.60
3:C:1185:SER:HA	10:C:1403:HOH:O	2.02	0.60
3:K:833:MET:CE	3:K:1223:GLY:N	2.64	0.60
1:I:36:LEU:HD22	1:I:89:GLU:HG3	1.83	0.60
2:J:285:PRO:O	2:J:286:GLU:CD	2.39	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:388:THR:O	2:J:397:LEU:HD22	2.02	0.60
1:I:26:LEU:HD22	1:I:80:LEU:HD11	1.83	0.59
3:C:752:ILE:CD1	3:C:763:PHE:HE1	2.16	0.59
3:C:1046:MET:HE3	3:C:1086:TYR:CB	2.32	0.59
3:C:1046:MET:CE	3:C:1087:GLY:N	2.66	0.59
2:J:504:MET:HE1	10:K:1613:HOH:O	2.03	0.59
2:J:241:THR:HG22	2:J:244:GLU:H	1.68	0.59
3:K:1120:ALA:HB1	3:K:1125:VAL:HB	1.84	0.59
3:C:839:ARG:NH2	3:C:912:ARG:O	2.35	0.58
2:J:342:VAL:HG21	5:J:606:FAD:HM73	1.85	0.58
3:C:571:ASP:OD1	3:C:1052:LYS:HD2	2.03	0.58
3:C:598:ARG:NH2	10:C:1413:HOH:O	2.31	0.58
3:C:958:ARG:HE	3:C:960:GLU:HG2	1.67	0.58
3:K:1292:GLU:HG3	3:K:1293:LEU:HA	1.85	0.58
2:B:488:ALA:HA	3:C:1319:THR:HG22	1.86	0.58
3:K:1017:ALA:HB1	3:K:1086:TYR:CD2	2.39	0.58
2:B:375:VAL:HG21	2:B:405:LEU:HD22	1.86	0.58
3:C:1088:GLN:HG2	3:C:1133:TYR:CD1	2.38	0.58
2:J:338:ALA:HB1	2:J:342:VAL:HB	1.85	0.58
2:B:391:PRO:HG3	2:B:397:LEU:CD1	2.34	0.57
2:B:241:THR:CG2	2:B:243:LYS:HG2	2.34	0.57
2:J:237:ILE:HD12	2:J:277:MET:HE2	1.86	0.57
3:K:640:ILE:HG12	3:K:779:MET:HE1	1.87	0.57
3:C:624:GLU:HB2	3:C:684:VAL:HG13	1.87	0.57
3:K:833:MET:HE1	3:K:1223:GLY:HA2	1.85	0.57
3:C:840:HIS:CD2	3:C:877:ILE:HD13	2.40	0.56
2:J:374:ILE:HD13	2:J:398:LEU:CD2	2.35	0.56
3:K:884:HIS:CE1	3:K:1006:GLY:H	2.24	0.56
3:C:601:ASN:HD22	3:C:821:HIS:HD2	1.52	0.56
2:B:241:THR:HG22	2:B:244:GLU:HB2	1.88	0.56
3:K:1046:MET:HE3	3:K:1086:TYR:O	2.06	0.56
3:K:640:ILE:HG23	3:K:779:MET:HE3	1.85	0.56
3:K:695:ILE:HG23	3:K:700:ASP:HB3	1.86	0.56
2:B:255:ALA:HB2	2:B:277:MET:HG2	1.88	0.55
1:A:131:GLN:HE21	1:A:133:GLU:H	1.53	0.55
3:C:885:MET:SD	3:C:896:GLY:HA3	2.46	0.55
1:A:94:THR:OG1	3:C:589:GLU:OE2	2.22	0.55
3:C:1046:MET:HE1	3:C:1086:TYR:HB2	1.89	0.55
2:J:404:LEU:CD2	2:J:407:ILE:HD11	2.34	0.55
8:K:1334:MOS:S	9:K:1335:290:H8	2.47	0.55
2:B:471:GLN:NE2	2:B:474:LEU:HD12	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:764:VAL:HG22	3:K:766:THR:CG2	2.36	0.55
2:B:348:LEU:HD13	2:B:407:ILE:HD13	1.89	0.55
3:C:1322:PRO:C	3:C:1323:GLY:O	2.46	0.55
2:J:528:GLY:HA3	10:J:617:HOH:O	2.07	0.55
3:K:696:ILE:HD12	3:K:1217:GLY:HA3	1.89	0.54
3:K:884:HIS:HE1	3:K:1005:PHE:HA	1.73	0.54
2:J:496:LEU:HB3	2:J:505:ILE:HD12	1.88	0.54
3:K:856:ILE:HG22	3:K:891:ILE:HG23	1.90	0.54
3:C:1282:ARG:CA	3:C:1286:THR:CG2	2.85	0.54
3:C:1322:PRO:O	3:C:1323:GLY:C	2.45	0.54
3:K:773:GLN:HG2	3:K:784:VAL:HG13	1.89	0.53
2:B:264:ILE:HD11	5:B:606:FAD:H3B	1.91	0.53
3:C:720:LYS:HD2	10:C:1532:HOH:O	2.09	0.53
2:J:285:PRO:O	2:J:286:GLU:OE1	2.25	0.53
2:J:375:VAL:CG2	2:J:405:LEU:HD22	2.30	0.53
3:K:833:MET:CE	3:K:1222:ARG:O	2.51	0.53
3:C:1317:CYS:SG	3:C:1323:GLY:HA2	2.48	0.53
1:I:131:GLN:HE21	1:I:133:GLU:H	1.57	0.53
2:J:281:PRO:HB2	2:J:287:LEU:HD12	1.90	0.53
1:A:144:GLN:HE22	2:B:336:TRP:HA	1.74	0.53
3:C:1282:ARG:HG2	3:C:1286:THR:HG21	1.91	0.53
3:C:1259:VAL:O	3:C:1259:VAL:HG22	2.07	0.53
3:C:884:HIS:HE1	3:C:1006:GLY:H	1.55	0.53
3:K:884:HIS:HE1	3:K:1006:GLY:H	1.56	0.53
3:C:585:GLN:NE2	10:C:1576:HOH:O	2.41	0.52
2:J:241:THR:HG21	2:J:243:LYS:HG2	1.90	0.52
2:J:432:ALA:HB2	2:J:502:GLY:HA3	1.91	0.52
3:K:1165:ASP:CA	10:K:1571:HOH:O	2.56	0.52
2:B:224:PRO:N	10:B:642:HOH:O	2.42	0.52
2:J:241:THR:CG2	2:J:243:LYS:HE2	2.37	0.52
2:B:257:LEU:O	5:B:606:FAD:H2B	2.09	0.52
1:I:143:PHE:HB3	3:K:1232:PHE:CE1	2.45	0.52
3:K:779:MET:CG	3:K:810:VAL:HG13	2.37	0.52
1:A:63:ASP:O	1:A:64:LYS:O	2.28	0.52
1:A:161:ARG:CG	10:A:657:HOH:O	2.55	0.52
2:B:500:ALA:HB3	2:B:505:ILE:CD1	2.40	0.52
3:C:609:THR:HG22	10:C:1359:HOH:O	2.10	0.52
3:C:1113:TRP:O	3:C:1117:VAL:HG23	2.08	0.52
3:C:1316:LEU:H	3:C:1316:LEU:CD1	2.23	0.52
1:A:104:ARG:NE	1:A:162:THR:HG21	2.25	0.51
3:K:585:GLN:NE2	10:K:1596:HOH:O	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:285:PRO:O	2:B:286:GLU:OE1	2.27	0.51
3:C:1249:ASN:O	3:C:1255:ALA:HA	2.09	0.51
1:I:32:ARG:NH2	10:I:619:HOH:O	2.42	0.51
3:K:833:MET:HE3	3:K:1222:ARG:CA	2.37	0.51
3:K:851:MET:HE2	3:K:857:VAL:CG2	2.40	0.51
2:B:374:ILE:HG23	2:B:398:LEU:HD22	1.93	0.51
3:C:987:PHE:CD2	3:C:996:ARG:HG3	2.46	0.51
8:C:1334:MOS:S	9:C:1335:290:C8	2.88	0.51
3:K:1198:ALA:HB3	3:K:1263:PRO:HB2	1.93	0.51
3:C:572:THR:HA	3:C:575:ARG:HD3	1.92	0.51
3:C:1203:LEU:HD13	10:C:1454:HOH:O	2.10	0.51
3:C:1282:ARG:CA	3:C:1286:THR:HG23	2.40	0.51
3:C:797:GLY:HA2	3:C:801:LYS:HD2	1.92	0.50
3:C:779:MET:HE3	3:C:814:LEU:HD13	1.93	0.50
2:B:241:THR:HG23	2:B:243:LYS:H	1.76	0.50
2:J:392:SER:OG	2:J:395:LYS:HD3	2.12	0.50
3:K:609:THR:CG2	10:K:1499:HOH:O	2.60	0.50
3:K:610:SER:OG	3:K:660:VAL:HG21	2.11	0.50
3:K:1316:LEU:HD12	3:K:1316:LEU:O	2.12	0.50
2:J:237:ILE:HD12	2:J:277:MET:HE1	1.93	0.50
3:K:1046:MET:CE	3:K:1087:GLY:N	2.68	0.50
3:K:994:LYS:HE3	10:K:1571:HOH:O	2.11	0.50
1:A:112:GLN:HB3	3:C:1039:GLY:O	2.11	0.50
3:K:1259:VAL:HG22	3:K:1259:VAL:O	2.11	0.50
3:K:999:CYS:SG	3:K:1001:ILE:HD12	2.51	0.50
3:C:712:LEU:HD21	3:C:875:HIS:CE1	2.47	0.50
3:C:1046:MET:HE3	3:C:1086:TYR:HB3	1.94	0.50
2:B:390:PHE:O	2:B:462:ARG:HD2	2.12	0.49
3:C:683:HIS:CG	3:C:683:HIS:O	2.65	0.49
3:C:1282:ARG:O	3:C:1286:THR:HG23	2.12	0.49
2:J:422:LYS:CB	10:J:618:HOH:O	2.59	0.49
3:C:833:MET:CE	3:C:1223:GLY:N	2.76	0.49
3:K:766:THR:HA	3:K:801:LYS:HB3	1.94	0.49
1:I:37:ARG:NH1	10:I:608:HOH:O	2.44	0.49
8:K:1334:MOS:O1	8:K:1334:MOS:S	2.71	0.49
3:C:1312:LYS:HB2	3:C:1318:VAL:HG13	1.94	0.49
3:C:1327:PRO:CB	10:C:1489:HOH:O	2.60	0.49
3:K:1152:TYR:CE1	3:K:1257:LYS:HG2	2.47	0.49
2:B:484:GLN:HG3	3:C:1319:THR:O	2.13	0.49
2:J:504:MET:CE	10:K:1613:HOH:O	2.60	0.49
3:K:640:ILE:HG12	3:K:779:MET:CE	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:952:LEU:HD23	3:K:952:LEU:N	2.28	0.49
1:I:63:ASP:O	1:I:64:LYS:O	2.31	0.48
3:K:614:HIS:HD2	3:K:693:PRO:O	1.96	0.48
3:C:1013:PHE:CD1	3:C:1013:PHE:C	2.86	0.48
3:C:1088:GLN:CG	3:C:1133:TYR:CD1	2.96	0.48
3:C:970:GLU:OE1	3:C:1244:LEU:HD12	2.13	0.48
3:K:1045:LYS:O	3:K:1049:VAL:HG23	2.13	0.48
3:K:605:LEU:HD23	3:K:605:LEU:C	2.34	0.48
2:J:392:SER:OG	2:J:395:LYS:CE	2.61	0.48
3:C:779:MET:O	3:C:779:MET:CE	2.50	0.48
3:C:941:VAL:O	3:C:945:ASN:ND2	2.38	0.48
1:I:62:GLN:O	1:I:64:LYS:HD2	2.14	0.48
2:B:391:PRO:HG3	2:B:397:LEU:HD12	1.94	0.47
3:C:624:GLU:CB	3:C:684:VAL:HG13	2.44	0.47
3:C:1312:LYS:HD2	3:C:1318:VAL:CG1	2.44	0.47
3:K:624:GLU:HB2	3:K:684:VAL:HG13	1.96	0.47
3:K:1207:THR:HG21	3:K:1270:VAL:HG12	1.96	0.47
1:A:62:GLN:HG3	10:A:620:HOH:O	2.14	0.47
2:B:507:PHE:HB2	3:C:1303:GLU:HG3	1.97	0.47
3:K:743:TYR:O	3:K:829:ARG:NH2	2.34	0.47
1:A:43:CYS:HA	3:C:829:ARG:HB2	1.96	0.47
2:B:272:ASN:ND2	3:C:683:HIS:CE1	2.82	0.47
3:K:580:LEU:HG	3:K:1044:THR:HG23	1.96	0.47
3:K:939:GLU:HG2	3:K:977:TYR:CE2	2.49	0.47
2:J:342:VAL:HG21	5:J:606:FAD:C7M	2.44	0.47
3:C:1275:LYS:HG3	3:C:1296:LEU:HD23	1.97	0.47
3:C:752:ILE:HD11	3:C:763:PHE:CE1	2.43	0.47
3:C:1312:LYS:HB3	3:C:1326:LYS:HD3	1.95	0.47
3:C:884:HIS:CE1	3:C:1006:GLY:H	2.32	0.47
3:K:1143:GLU:C	3:K:1144:THR:HG23	2.30	0.47
3:K:1173:ASN:HB3	10:K:1543:HOH:O	2.15	0.47
3:K:995:LYS:NZ	3:K:1284:GLN:HE21	2.13	0.47
1:A:157:LEU:O	1:A:161:ARG:HG3	2.14	0.46
2:B:376:SER:HB3	2:B:402:GLU:HG2	1.96	0.46
3:C:1140:TYR:HE2	3:C:1142:PHE:CD1	2.34	0.46
2:J:374:ILE:HD13	2:J:398:LEU:HD23	1.97	0.46
2:B:309:GLU:HB2	2:B:334:LEU:HD13	1.97	0.46
2:B:272:ASN:ND2	3:C:683:HIS:NE2	2.63	0.46
2:J:241:THR:HG23	2:J:243:LYS:HG2	1.96	0.46
3:K:660:VAL:HG11	3:K:667:ILE:HD11	1.97	0.46
1:I:104:ARG:HD3	1:I:162:THR:CG2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:911:PHE:O	3:C:912:ARG:C	2.54	0.46
3:C:890:LYS:NZ	10:C:1453:HOH:O	2.30	0.46
1:I:104:ARG:HD3	1:I:162:THR:HG21	1.97	0.46
1:A:36:LEU:HD22	1:A:89:GLU:HG3	1.97	0.46
3:C:1324:ASN:O	3:C:1325:CYS:O	2.34	0.46
10:J:668:HOH:O	3:K:683:HIS:HB2	2.16	0.46
3:K:1291:LYS:O	3:K:1292:GLU:O	2.33	0.46
3:K:859:LEU:HD22	3:K:926:TRP:CZ2	2.51	0.46
3:K:1102:GLU:OE1	3:K:1102:GLU:HA	2.16	0.46
3:K:1247:CYS:N	3:K:1248:PRO:CD	2.79	0.46
1:A:159:GLY:O	1:A:162:THR:HG22	2.15	0.46
3:C:1216:GLU:H	3:C:1216:GLU:CD	2.19	0.46
1:I:61:LEU:C	1:I:63:ASP:H	2.20	0.46
3:K:614:HIS:O	3:K:615:ALA:HB2	2.15	0.45
3:K:696:ILE:HD12	3:K:1217:GLY:CA	2.45	0.45
2:J:370:THR:HG23	2:J:408:GLU:O	2.16	0.45
2:B:395:LYS:HD2	10:B:663:HOH:O	2.15	0.45
2:B:308:VAL:HG21	2:B:348:LEU:HG	1.98	0.45
3:C:1053:ALA:O	3:C:1098:LEU:HD11	2.16	0.45
3:K:1316:LEU:HA	10:K:1552:HOH:O	2.16	0.45
3:C:601:ASN:HB2	3:C:821:HIS:CD2	2.51	0.45
2:B:257:LEU:HD13	2:B:281:PRO:HG3	1.99	0.45
2:J:242:LEU:O	2:J:246:LEU:HG	2.16	0.45
3:C:939:GLU:HG2	3:C:977:TYR:CE2	2.51	0.45
3:C:1102:GLU:OE1	3:C:1105:LYS:NZ	2.51	0.44
3:C:718:ASP:O	3:C:893:ASN:HB3	2.17	0.44
3:C:1320:GLY:HA2	3:C:1321:ALA:HA	1.82	0.44
2:B:395:LYS:CD	10:B:663:HOH:O	2.65	0.44
3:K:655:PHE:HE1	3:K:814:LEU:HD23	1.82	0.44
2:B:374:ILE:CG2	2:B:398:LEU:HD22	2.47	0.44
3:K:767:GLN:NE2	3:K:799:GLY:CA	2.67	0.44
3:K:848:VAL:HG21	3:K:926:TRP:HB2	1.99	0.44
3:K:1299:PRO:O	3:K:1304:LYS:HD2	2.18	0.44
3:C:722:GLY:CA	3:C:857:VAL:HG12	2.48	0.44
3:C:880:ARG:O	3:C:884:HIS:CD2	2.65	0.44
3:K:648:LEU:HD12	3:K:648:LEU:HA	1.90	0.44
3:K:958:ARG:HE	3:K:960:GLU:HG2	1.82	0.44
3:K:1104:PHE:CE1	3:K:1125:VAL:HG21	2.52	0.44
3:K:1176:THR:HG21	3:K:1199:PHE:CZ	2.53	0.44
2:B:427:ARG:O	2:B:427:ARG:HG2	2.18	0.44
2:J:518:LYS:NZ	3:K:1165:ASP:OD2	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:663:VAL:HG12	3:K:834:LEU:HD11	1.99	0.44
3:K:1143:GLU:O	3:K:1143:GLU:HG3	2.17	0.44
2:J:424:ALA:CB	3:K:1170:ASP:OD1	2.66	0.44
3:K:1088:GLN:HG2	3:K:1133:TYR:CD1	2.53	0.44
3:C:1015:ASN:HB3	3:C:1135:THR:HB	1.99	0.43
3:C:1154:THR:HG23	3:C:1181:ASP:O	2.18	0.43
3:K:641:PRO:HG2	3:K:780:LEU:HA	1.99	0.43
2:B:488:ALA:HA	3:C:1319:THR:CG2	2.47	0.43
3:C:628:VAL:HA	3:C:629:PRO:HD3	1.91	0.43
3:K:846:TYR:OH	3:K:929:GLU:OE1	2.30	0.43
3:K:979:ALA:O	3:K:983:GLU:OE2	2.36	0.43
3:K:1082:SER:HB2	7:K:1333:MTE:O3P	2.18	0.43
3:C:968:TRP:CH2	3:C:1000:ILE:HG23	2.54	0.43
2:B:381:ARG:NH1	2:B:383:VAL:HG11	2.33	0.43
2:B:496:LEU:HB3	2:B:505:ILE:HD12	1.99	0.43
3:C:1046:MET:CE	3:C:1086:TYR:HB3	2.44	0.43
1:A:58:TYR:OH	1:A:63:ASP:HA	2.19	0.43
1:A:104:ARG:HD3	1:A:162:THR:CG2	2.43	0.43
1:A:59:ASP:O	1:A:63:ASP:O	2.36	0.43
2:B:241:THR:HG22	2:B:244:GLU:CB	2.47	0.43
3:C:720:LYS:HG3	3:C:720:LYS:O	2.18	0.43
3:K:644:ASN:O	3:K:653:THR:HA	2.19	0.43
7:K:1333:MTE:S1'	8:K:1334:MOS:S	3.17	0.43
3:C:980:ARG:NH2	10:C:1503:HOH:O	2.46	0.43
1:I:94:THR:OG1	3:K:589:GLU:OE2	2.27	0.43
2:B:337:PHE:O	2:B:338:ALA:C	2.55	0.43
2:J:338:ALA:CB	2:J:342:VAL:HB	2.49	0.43
3:K:797:GLY:O	3:K:800:GLY:HA3	2.19	0.43
3:K:844:ALA:HB2	3:K:922:ILE:HD13	2.01	0.43
3:K:1191:ASP:O	3:K:1195:VAL:HG23	2.18	0.43
3:K:1091:TYR:O	3:K:1095:GLN:HG2	2.19	0.43
3:K:1317:CYS:C	3:K:1319:THR:HA	2.39	0.43
3:C:618:LYS:HE3	3:C:690:GLU:OE1	2.19	0.42
3:C:609:THR:CG2	3:C:664:GLY:HA2	2.49	0.42
2:J:374:ILE:CG2	2:J:398:LEU:HD22	2.49	0.42
3:K:856:ILE:CG2	3:K:891:ILE:HG23	2.48	0.42
3:K:1178:ILE:HD12	3:K:1241:VAL:HG22	2.01	0.42
2:B:235:THR:HB	2:B:277:MET:HE3	2.02	0.42
1:I:143:PHE:HB3	3:K:1232:PHE:CD1	2.55	0.42
3:K:640:ILE:HG23	3:K:779:MET:HE1	1.91	0.42
3:K:1284:GLN:O	3:K:1284:GLN:HG3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:641:PRO:CD	3:C:779:MET:CE	2.87	0.42
3:C:727:ASP:H	3:C:851:MET:HE2	1.84	0.42
1:I:124:MET:CE	1:I:127:LEU:HD23	2.50	0.42
2:J:424:ALA:HB2	3:K:1170:ASP:OD1	2.19	0.42
3:K:1044:THR:O	3:K:1048:GLN:HG3	2.19	0.42
3:K:1318:VAL:N	3:K:1319:THR:HA	2.34	0.42
3:K:1088:GLN:HG2	3:K:1133:TYR:CE1	2.55	0.42
1:A:45:GLU:CD	3:C:1224:PRO:HD2	2.40	0.42
3:K:1292:GLU:O	3:K:1293:LEU:HG	2.20	0.42
1:A:150:CYS:O	3:C:1197:GLY:HA3	2.20	0.42
1:I:69:SER:N	1:I:126:THR:HG21	2.35	0.42
3:K:1203:LEU:HD13	10:K:1481:HOH:O	2.18	0.42
2:B:285:PRO:O	2:B:286:GLU:CD	2.58	0.42
2:B:464:ILE:HD13	2:B:464:ILE:HG21	1.82	0.42
3:C:1046:MET:HE2	3:C:1086:TYR:HB2	1.94	0.42
1:I:117:THR:O	1:I:121:VAL:HG23	2.20	0.42
3:K:840:HIS:HE1	3:K:874:SER:OG	2.02	0.42
3:K:1165:ASP:HA	10:K:1571:HOH:O	2.18	0.42
3:C:646:THR:O	3:C:650:ASN:HA	2.19	0.42
3:C:1319:THR:HA	3:C:1320:GLY:HA2	1.84	0.42
1:I:124:MET:HE1	1:I:127:LEU:HD23	2.01	0.42
3:K:752:ILE:HD12	3:K:763:PHE:HE1	1.84	0.42
3:K:999:CYS:SG	3:K:1001:ILE:HD11	2.58	0.42
1:A:29:TYR:CZ	1:A:33:LYS:HD2	2.55	0.41
2:B:314:GLU:O	2:B:318:LYS:HD3	2.20	0.41
3:C:614:HIS:HD2	3:C:693:PRO:O	2.03	0.41
3:C:833:MET:HE1	3:C:1223:GLY:N	2.35	0.41
3:K:719:LEU:HD23	3:K:719:LEU:HA	1.96	0.41
3:C:648:LEU:HB2	10:C:1490:HOH:O	2.20	0.41
2:J:370:THR:CG2	2:J:407:ILE:HG23	2.50	0.41
3:K:609:THR:HG23	10:K:1499:HOH:O	2.19	0.41
3:K:741:HIS:HA	3:K:911:PHE:CE1	2.56	0.41
3:C:1183:GLY:HA2	3:C:1247:CYS:O	2.21	0.41
3:K:1013:PHE:CD1	3:K:1013:PHE:C	2.94	0.41
3:K:998:LEU:CD1	3:K:1161:GLU:HB2	2.51	0.41
1:A:155:PRO:HG3	10:A:634:HOH:O	2.20	0.41
3:C:701:ALA:CB	3:C:901:CYS:HB3	2.51	0.41
3:C:884:HIS:HE1	3:C:1005:PHE:HA	1.86	0.41
1:A:32:ARG:HG2	3:C:598:ARG:NH2	2.35	0.41
2:B:469:THR:HG23	2:B:489:GLY:HA3	2.03	0.41
3:K:1202:GLY:O	3:K:1206:PHE:CD1	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:722:GLY:HA2	3:C:857:VAL:HG12	2.03	0.41
2:J:285:PRO:O	2:J:286:GLU:CB	2.69	0.41
2:J:374:ILE:HG23	2:J:398:LEU:HD22	2.02	0.41
2:J:510:THR:HG21	3:K:1314:THR:HG22	2.03	0.41
3:K:729:VAL:HG11	3:K:847:LYS:HE2	2.03	0.41
3:C:641:PRO:HD2	3:C:779:MET:HE1	1.91	0.41
3:C:779:MET:CE	3:C:779:MET:C	2.88	0.41
3:C:1017:ALA:HB1	3:C:1086:TYR:CD2	2.56	0.41
3:C:850:PHE:CD2	3:C:850:PHE:N	2.89	0.40
3:C:1254:TYR:O	3:C:1255:ALA:HB3	2.22	0.40
3:K:670:VAL:HG11	3:K:681:ALA:HB3	2.02	0.40
3:K:674:THR:HB	3:K:675:PRO:HD2	2.01	0.40
2:J:509:ARG:HG2	10:J:640:HOH:O	2.21	0.40
2:B:440:VAL:O	2:B:440:VAL:HG13	2.21	0.40
3:C:880:ARG:HD2	3:C:914:PHE:HB3	2.03	0.40
3:C:910:ALA:HB1	8:C:1334:MOS:S	2.61	0.40
1:I:154:ARG:N	1:I:155:PRO:HD2	2.36	0.40
3:K:833:MET:HE1	3:K:1223:GLY:CA	2.50	0.40
3:K:1048:GLN:HE22	3:K:1187:ASN:HD22	1.68	0.40
3:K:988:ASN:O	3:K:995:LYS:NZ	2.55	0.40
3:K:1046:MET:HE3	3:K:1090:VAL:CG2	2.52	0.40
1:A:104:ARG:NH1	10:A:646:HOH:O	2.54	0.40
3:K:1286:THR:HG22	3:K:1310:VAL:O	2.21	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	160/219 (73%)	151 (94%)	7 (4%)	2 (1%)	12 12
1	I	160/219 (73%)	150 (94%)	7 (4%)	3 (2%)	8 7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	303/350 (87%)	286 (94%)	16 (5%)	1 (0%)	41 50
2	J	303/350 (87%)	286 (94%)	12 (4%)	5 (2%)	9 8
3	C	756/763 (99%)	710 (94%)	30 (4%)	16 (2%)	7 5
3	K	743/763 (97%)	704 (95%)	29 (4%)	10 (1%)	12 12
All	All	2425/2664 (91%)	2287 (94%)	101 (4%)	37 (2%)	10 10

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	LYS
2	B	286	GLU
3	C	1316	LEU
3	C	1317	CYS
3	C	1323	GLY
3	C	1324	ASN
1	I	61	LEU
1	I	64	LYS
2	J	286	GLU
2	J	426	ARG
3	K	1292	GLU
3	K	1293	LEU
3	C	631	PHE
3	C	721	LYS
3	C	1008	SER
3	C	1139	GLY
3	C	1321	ALA
3	C	1326	LYS
3	K	721	LYS
3	K	912	ARG
3	K	1008	SER
3	K	1139	GLY
3	K	1144	THR
1	A	43	CYS
3	C	912	ARG
3	C	956	ASN
1	I	63	ASP
2	J	445	GLY
3	C	1325	CYS
2	J	527	LEU
3	C	628	VAL
3	K	1251	LYS

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Mol	Chain	Res	Type
3	K	1316	LEU
3	C	894	ILE
2	J	424	ALA
3	K	1248	PRO
3	C	797	GLY

5.3.2 Protein sidechains (i)

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	135/187 (72%)	128 (95%)	7 (5%)	23	32
1	I	130/187 (70%)	125 (96%)	5 (4%)	33	47
2	B	259/302 (86%)	248 (96%)	11 (4%)	30	42
2	J	254/302 (84%)	240 (94%)	14 (6%)	21	30
3	C	630/639 (99%)	589 (94%)	41 (6%)	17	23
3	K	623/639 (98%)	588 (94%)	35 (6%)	21	29
All	All	2031/2256 (90%)	1918 (94%)	113 (6%)	21	29

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LYS
1	A	57	LYS
1	A	60	ARG
1	A	64	LYS
1	A	82	HIS
1	A	104	ARG
1	A	113	CYS
2	B	225	LYS
2	B	241	THR
2	B	243	LYS
2	B	247	ASP
2	B	256	LYS
2	B	277	MET

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Mol	Chain	Res	Type
2	B	286	GLU
2	B	348	LEU
2	B	427	ARG
2	B	472	LYS
2	B	476	LYS
3	C	598	ARG
3	C	616	LYS
3	C	627	LYS
3	C	657	LYS
3	C	684	VAL
3	C	705	ASN
3	C	715	GLU
3	C	719	LEU
3	C	742	PHE
3	C	743	TYR
3	C	764	VAL
3	C	774	SER
3	C	779	MET
3	C	782	VAL
3	C	818	LYS
3	C	848	VAL
3	C	871	ARG
3	C	890	LYS
3	C	899	ARG
3	C	911	PHE
3	C	940	GLU
3	C	958	ARG
3	C	960	GLU
3	C	969	ASP
3	C	1001	ILE
3	C	1013	PHE
3	C	1046	MET
3	C	1099	LYS
3	C	1144	THR
3	C	1172	LYS
3	C	1190	ILE
3	C	1203	LEU
3	C	1208	LEU
3	C	1276	ASP
3	C	1286	THR
3	C	1287	ASN
3	C	1289	ASN

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Mol	Chain	Res	Type
3	C	1290	THR
3	C	1315	THR
3	C	1316	LEU
3	C	1326	LYS
1	I	33	LYS
1	I	64	LYS
1	I	66	ILE
1	I	82	HIS
1	I	104	ARG
2	J	241	THR
2	J	243	LYS
2	J	257	LEU
2	J	298	SER
2	J	348	LEU
2	J	377	ARG
2	J	379	THR
2	J	426	ARG
2	J	427	ARG
2	J	433	LYS
2	J	462	ARG
2	J	497	SER
2	J	506	GLU
2	J	509	ARG
3	K	609	THR
3	K	616	LYS
3	K	619	SER
3	K	684	VAL
3	K	686	LYS
3	K	688	THR
3	K	706	SER
3	K	720	LYS
3	K	742	PHE
3	K	743	TYR
3	K	764	VAL
3	K	779	MET
3	K	782	VAL
3	K	818	LYS
3	K	899	ARG
3	K	911	PHE
3	K	939	GLU
3	K	944	LYS
3	K	983	GLU

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Mol	Chain	Res	Type
3	K	1001	ILE
3	K	1003	THR
3	K	1008	SER
3	K	1013	PHE
3	K	1051	SER
3	K	1122	GLN
3	K	1123	ASP
3	K	1134	ARG
3	K	1172	LYS
3	K	1203	LEU
3	K	1208	LEU
3	K	1215	PRO
3	K	1238	GLU
3	K	1284	GLN
3	K	1316	LEU
3	K	1318	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	144	GLN
2	B	272	ASN
2	B	273	GLN
2	B	471	GLN
2	B	473	GLN
3	C	585	GLN
3	C	614	HIS
3	C	626	GLN
3	C	677	HIS
3	C	821	HIS
3	C	840	HIS
3	C	875	HIS
3	C	884	HIS
3	C	904	ASN
3	C	1016	GLN
3	C	1033	HIS
3	C	1048	GLN
3	C	1212	HIS
3	C	1284	GLN
3	C	1287	ASN
3	C	1289	ASN

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Mol	Chain	Res	Type
1	I	82	HIS
1	I	131	GLN
1	I	146	ASN
2	J	272	ASN
2	J	351	ASN
2	J	473	GLN
3	K	614	HIS
3	K	626	GLN
3	K	677	HIS
3	K	683	HIS
3	K	767	GLN
3	K	821	HIS
3	K	840	HIS
3	K	884	HIS
3	K	904	ASN
3	K	1033	HIS
3	K	1048	GLN
3	K	1122	GLN
3	K	1284	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 for Mogul analysis.

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	-	-	-		
5	FAD	B	606	-	53,58,58	1.13	3 (5%)	68,89,89	1.71	15 (22%)
8	MOS	K	1334	7	0,3,3	-	-	-		
9	290	C	1335	-	7,12,12	1.29	1 (14%)	8,17,17	2.68	4 (50%)
4	FES	A	602	1	0,4,4	-	-	-		
9	290	K	1335	-	7,12,12	1.09	0	8,17,17	2.91	3 (37%)
4	FES	I	602	1	0,4,4	-	-	-		
8	MOS	C	1334	7	0,3,3	-	-	-		
5	FAD	J	606	-	53,58,58	1.22	4 (7%)	68,89,89	1.60	12 (17%)
7	MTE	K	1333	8	21,26,26	1.39	2 (9%)	21,40,40	2.54	9 (42%)
7	MTE	C	1333	8	21,26,26	1.84	3 (14%)	21,40,40	2.57	9 (42%)
4	FES	I	601	1	0,4,4	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FES	A	601	1	-	-	0/1/1/1
5	FAD	B	606	-	-	0/30/50/50	0/6/6/6
9	290	C	1335	-	-	-	0/2/2/2
4	FES	A	602	1	-	-	0/1/1/1
9	290	K	1335	-	-	-	0/2/2/2
4	FES	I	602	1	-	-	0/1/1/1
5	FAD	J	606	-	-	4/30/50/50	0/6/6/6
7	MTE	K	1333	8	-	3/6/34/34	0/3/3/3
7	MTE	C	1333	8	-	1/6/34/34	0/3/3/3
4	FES	I	601	1	-	-	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	1333	MTE	C9-C4	5.99	1.49	1.41
7	K	1333	MTE	C9-C4	4.55	1.47	1.41
5	J	606	FAD	C4X-N5	4.30	1.39	1.30
7	C	1333	MTE	C7-C6	-3.90	1.50	1.53
5	B	606	FAD	C4X-N5	3.71	1.38	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	606	FAD	C2A-N1A	3.44	1.40	1.33
5	J	606	FAD	C2A-N3A	3.34	1.37	1.32
5	J	606	FAD	C10-N1	3.25	1.39	1.33
7	C	1333	MTE	C9-C10	3.23	1.47	1.41
7	K	1333	MTE	C9-C10	3.00	1.47	1.41
5	B	606	FAD	C2A-N1A	2.55	1.38	1.33
5	B	606	FAD	C2A-N3A	2.26	1.35	1.32
9	C	1335	290	C6-N1	2.19	1.35	1.32

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	1333	MTE	C4-C9-N5	7.90	125.75	119.12
5	B	606	FAD	N3A-C2A-N1A	-7.41	117.10	128.68
7	K	1333	MTE	C4-C9-N5	7.37	125.31	119.12
5	J	606	FAD	N3A-C2A-N1A	-6.63	118.32	128.68
9	K	1335	290	C61-C6-N1	5.16	122.83	116.71
9	C	1335	290	C61-C6-N1	4.69	122.27	116.71
9	K	1335	290	N3-C4-N9	4.21	128.04	123.18
7	K	1333	MTE	C2-N3-C4	4.00	122.28	115.93
9	C	1335	290	C2-N1-C6	3.98	122.62	118.82
7	C	1333	MTE	C2-N3-C4	3.81	121.98	115.93
5	B	606	FAD	C4X-C10-N10	3.63	121.79	116.48
9	K	1335	290	C2-N1-C6	3.55	122.21	118.82
5	B	606	FAD	C1B-N9A-C4A	-3.53	120.44	126.64
7	C	1333	MTE	O3'-C7-N8	3.39	112.05	108.57
7	K	1333	MTE	C2-N1-C10	3.37	122.10	114.54
7	K	1333	MTE	N2-C2-N3	3.24	122.29	117.25
5	J	606	FAD	C5A-C6A-N6A	-3.18	115.52	120.35
5	B	606	FAD	O5'-C5'-C4'	-3.17	100.89	109.36
5	B	606	FAD	C2A-N1A-C6A	3.06	123.99	118.75
7	C	1333	MTE	O4'-P-O1P	-3.06	97.89	106.47
5	J	606	FAD	O3'-C3'-C2'	-2.81	102.01	108.81
7	K	1333	MTE	N1-C2-N3	-2.67	121.23	125.42
5	B	606	FAD	C10-C4X-N5	-2.66	119.21	124.86
5	J	606	FAD	O4'-C4'-C3'	2.58	115.37	109.10
5	J	606	FAD	C9A-C5X-N5	-2.56	119.65	122.43
5	B	606	FAD	C4-C4X-N5	2.51	121.80	118.23
5	B	606	FAD	C10-N1-C2	2.41	121.73	116.90
7	K	1333	MTE	O2P-P-O4'	-2.40	100.34	106.73
5	J	606	FAD	C4X-C4-N3	2.40	119.29	113.19
7	C	1333	MTE	C2-N1-C10	2.38	119.88	114.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	606	FAD	O4'-C4'-C3'	2.36	114.85	109.10
7	C	1333	MTE	O2P-P-O1P	2.34	119.85	110.68
7	K	1333	MTE	C10-N8-C7	-2.31	119.14	123.67
7	K	1333	MTE	O2P-P-O1P	2.29	119.64	110.68
7	C	1333	MTE	C10-C9-C4	2.28	116.60	114.57
5	J	606	FAD	C4'-C3'-C2'	-2.28	108.62	113.36
5	B	606	FAD	C4X-C4-N3	2.25	118.91	113.19
5	J	606	FAD	O4-C4-C4X	-2.25	120.64	126.60
7	K	1333	MTE	O3P-P-O4'	-2.24	100.77	106.73
9	C	1335	290	C61-C6-C5	2.22	121.77	117.53
9	C	1335	290	N3-C4-N9	2.19	125.72	123.18
5	B	606	FAD	O2'-C2'-C1'	2.14	114.97	109.80
5	B	606	FAD	C4X-C10-N1	-2.12	119.81	124.73
5	J	606	FAD	C10-C4X-N5	-2.11	120.37	124.86
5	J	606	FAD	C10-N1-C2	2.08	121.06	116.90
5	B	606	FAD	O4-C4-C4X	-2.06	121.13	126.60
7	C	1333	MTE	O2P-P-O4'	-2.06	101.26	106.73
5	B	606	FAD	N6A-C6A-N1A	2.05	122.82	118.57
5	B	606	FAD	O2-C2-N3	2.04	122.62	118.65
5	J	606	FAD	C4X-C10-N1	-2.03	120.02	124.73
7	C	1333	MTE	C9-C4-N3	-2.02	118.26	124.01
5	J	606	FAD	O2'-C2'-C1'	2.00	114.64	109.80

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	1333	MTE	C3'-C4'-O4'-P
7	K	1333	MTE	C4'-O4'-P-O2P
5	J	606	FAD	C2'-C3'-C4'-C5'
7	K	1333	MTE	C4'-O4'-P-O3P
5	J	606	FAD	C2'-C3'-C4'-O4'
7	K	1333	MTE	C3'-C4'-O4'-P
5	J	606	FAD	O3'-C3'-C4'-C5'
5	J	606	FAD	P-O3P-PA-O2A

There are no ring outliers.

7 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	606	FAD	2	0

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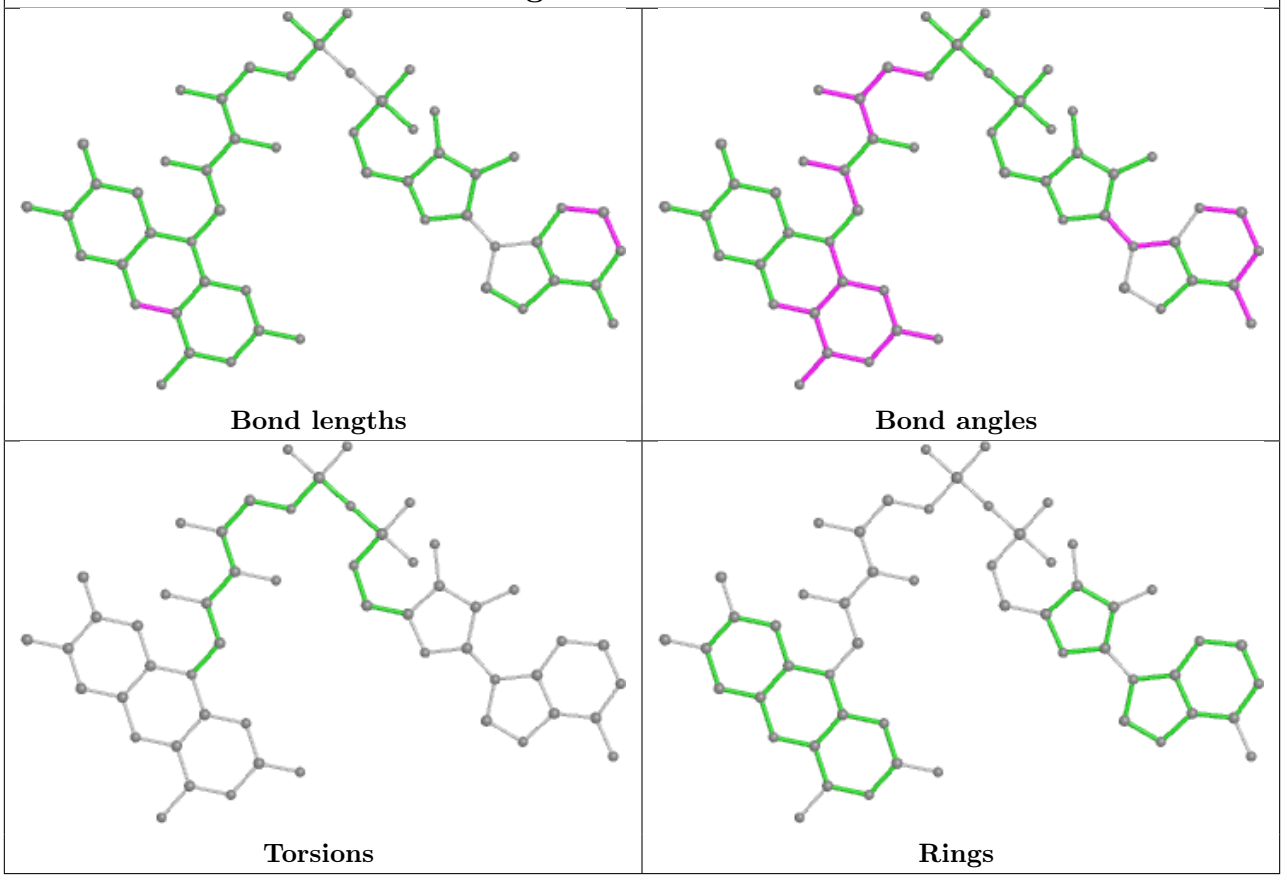
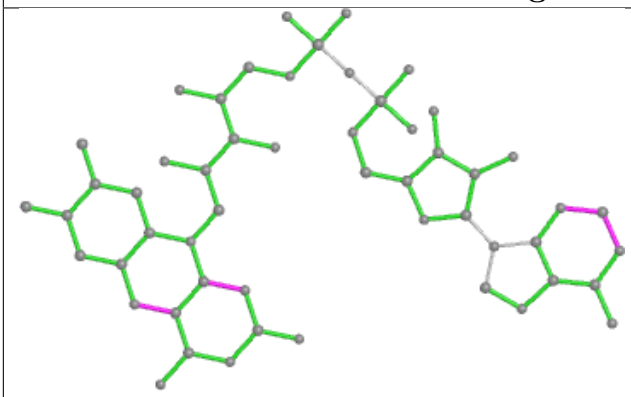
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	K	1334	MOS	8	0
9	C	1335	290	4	0
9	K	1335	290	5	0
8	C	1334	MOS	7	0
5	J	606	FAD	3	0
7	K	1333	MTE	2	0

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

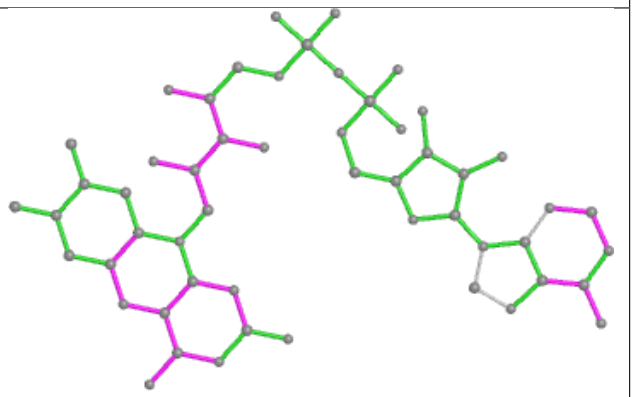
Ligand FAD B 606



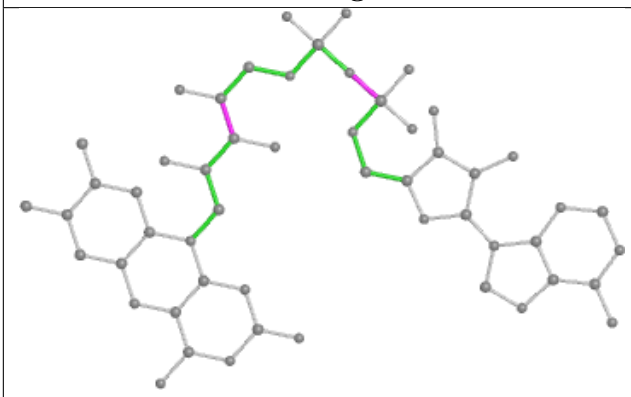
Ligand FAD J 606



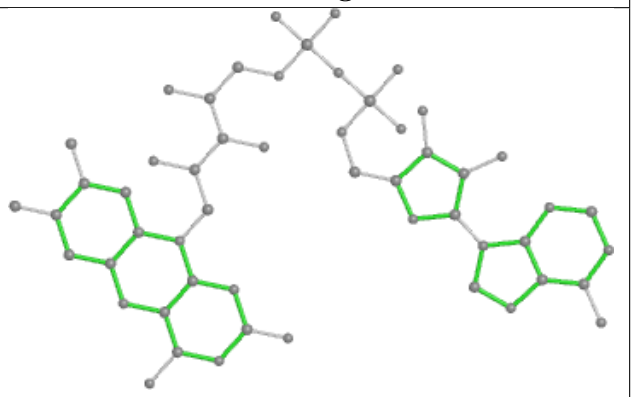
Bond lengths



Bond angles

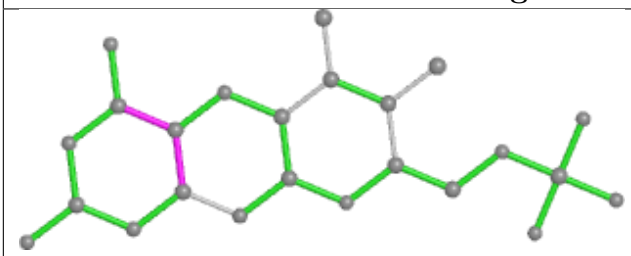


Torsions

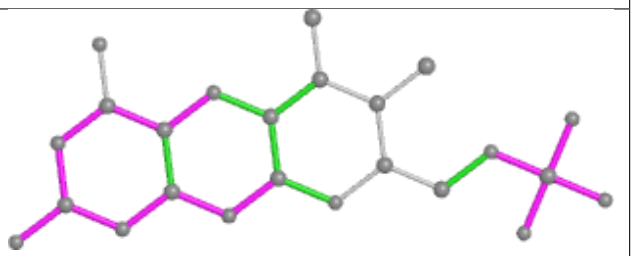


Rings

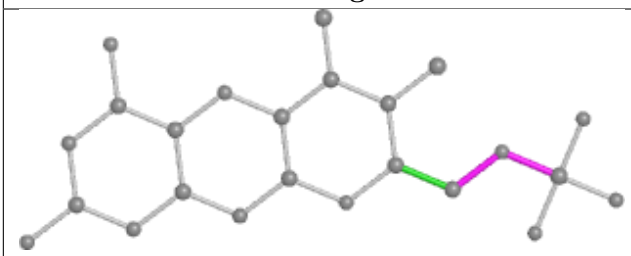
Ligand MTE K 1333



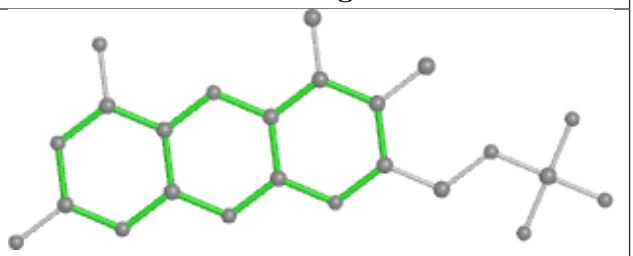
Bond lengths



Bond angles

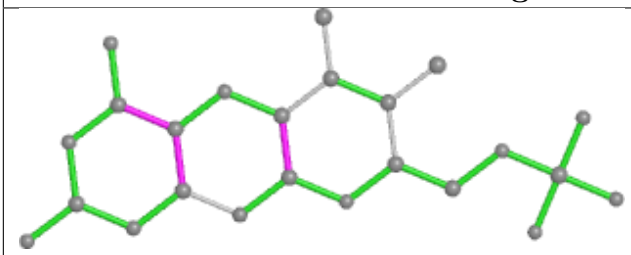


Torsions

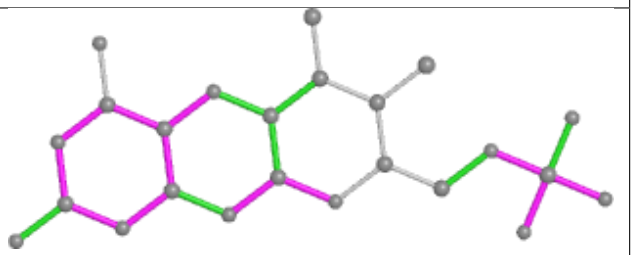


Rings

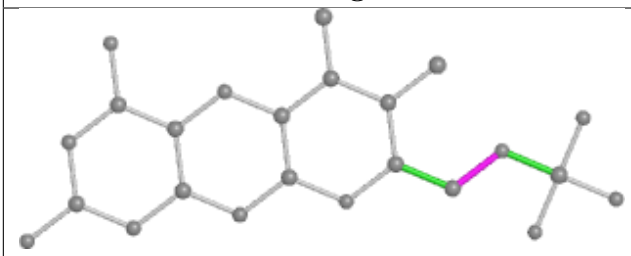
Ligand MTE C 1333



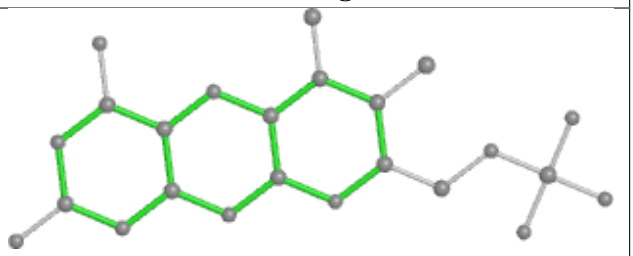
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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	162/219 (73%)	-0.15	3 (1%)	66	73	13, 21, 37, 50	0
1	I	162/219 (73%)	0.03	8 (4%)	29	36	17, 27, 44, 54	0
2	B	305/350 (87%)	0.00	6 (1%)	65	71	15, 28, 39, 43	0
2	J	305/350 (87%)	0.19	9 (2%)	50	57	22, 34, 44, 47	0
3	C	758/763 (99%)	0.11	25 (3%)	46	53	13, 25, 39, 51	0
3	K	747/763 (97%)	0.02	20 (2%)	54	62	12, 25, 40, 55	0
All	All	2439/2664 (91%)	0.06	71 (2%)	51	58	12, 26, 41, 55	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	1325	CYS	6.2
3	K	1248	PRO	5.3
2	J	429	ASP	4.0
3	K	1250	LYS	3.8
2	J	378	GLY	3.7
3	K	1316	LEU	3.7
2	J	528	GLY	3.6
2	B	425	SER	3.6
3	K	1290	THR	3.5
3	K	1111	GLY	3.5
3	K	1320	GLY	3.5
3	C	718	ASP	3.2
3	C	722	GLY	3.1
2	J	477	PHE	3.1
2	B	499	ASP	3.1
1	I	61	LEU	3.1
3	C	1323	GLY	3.1
3	C	724	SER	3.0
3	C	1264	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	I	162	THR	2.9
2	J	397	LEU	2.9
3	C	723	PHE	2.9
1	A	97	ARG	2.8
3	C	1246	ASP	2.8
3	C	1247	CYS	2.8
3	K	1143	GLU	2.8
3	K	1246	ASP	2.8
1	I	58	TYR	2.7
3	C	717	GLY	2.7
3	C	1245	ARG	2.7
3	C	920	LEU	2.7
3	C	725	GLU	2.6
3	C	1321	ALA	2.6
3	C	699	GLU	2.6
3	C	1319	THR	2.6
3	K	725	GLU	2.5
1	A	63	ASP	2.5
3	C	989	LYS	2.5
2	B	528	GLY	2.4
3	K	920	LEU	2.4
3	K	1106	LYS	2.4
2	J	377	ARG	2.3
3	K	1107	LYS	2.3
2	B	498	PRO	2.3
3	K	1116	TRP	2.3
3	C	982	SER	2.3
1	A	161	ARG	2.2
1	I	97	ARG	2.2
3	K	922	ILE	2.2
1	I	163	PHE	2.2
3	C	917	PRO	2.2
1	I	63	ASP	2.2
3	C	1326	LYS	2.2
3	C	1107	LYS	2.2
3	C	1001	ILE	2.2
2	J	251	GLN	2.2
1	I	60	ARG	2.1
3	K	982	SER	2.1
3	C	1137	ASN	2.1
2	J	364	VAL	2.1
3	K	979	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
2	J	445	GLY	2.1
3	K	1105	LYS	2.1
3	C	1265	PHE	2.1
3	K	571	ASP	2.1
3	K	1247	CYS	2.1
3	K	1317	CYS	2.1
2	B	272	ASN	2.0
1	I	137	GLU	2.0
3	C	983	GLU	2.0
2	B	318	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 monosaccharides in this entry.

6.4 Ligands (i)

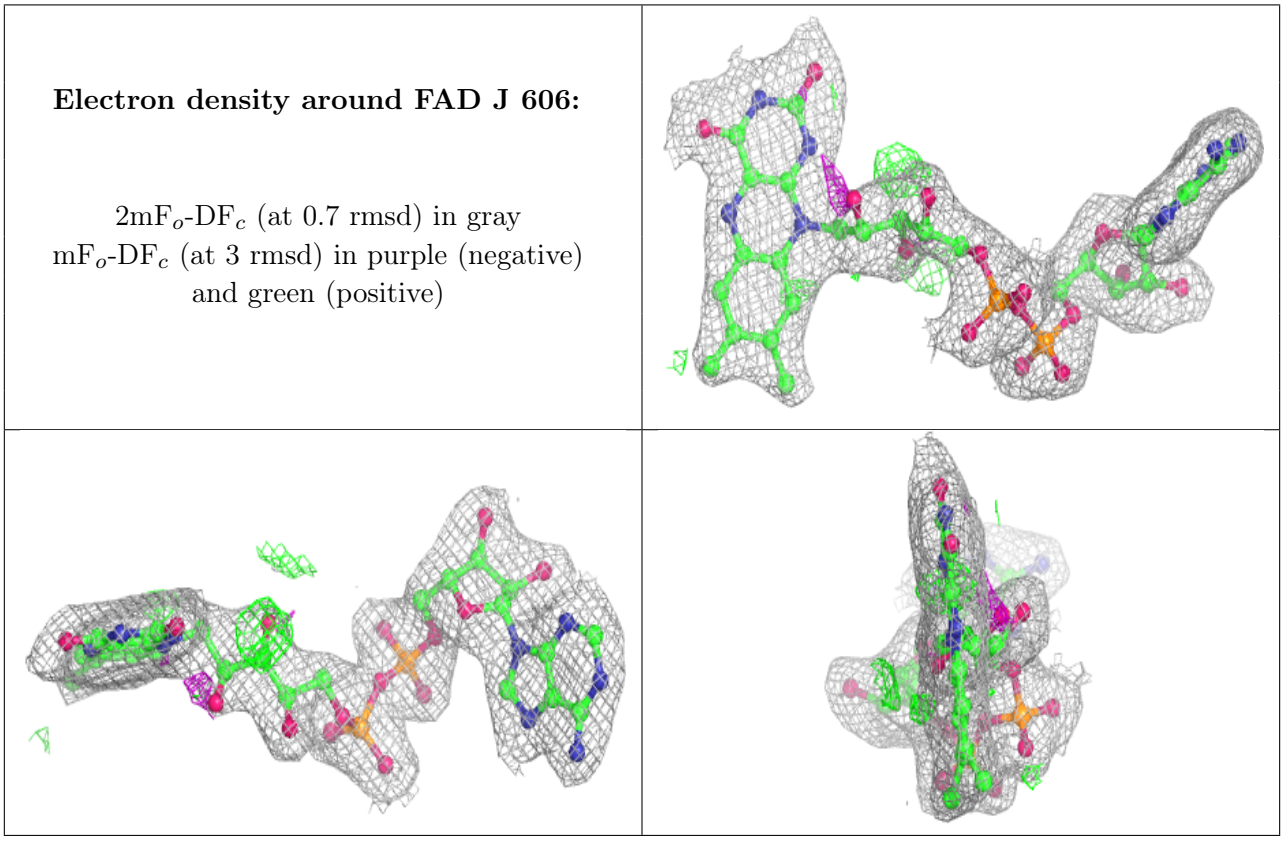
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	CA	C	1	1/1	0.86	0.27	49,49,49,49	0
9	290	C	1335	11/11	0.86	0.17	30,31,32,32	0
9	290	K	1335	11/11	0.94	0.13	19,21,22,23	0
5	FAD	J	606	53/53	0.96	0.12	19,25,30,37	0
7	MTE	K	1333	24/24	0.96	0.10	27,29,32,35	0
7	MTE	C	1333	24/24	0.97	0.10	20,24,29,32	0
5	FAD	B	606	53/53	0.97	0.12	13,22,25,27	0
8	MOS	K	1334	4/4	0.98	0.12	40,44,45,46	0
8	MOS	C	1334	4/4	0.99	0.11	42,45,48,49	0
4	FES	I	602	4/4	0.99	0.10	19,19,19,20	0
4	FES	A	602	4/4	0.99	0.10	13,14,16,18	0
4	FES	I	601	4/4	0.99	0.09	19,19,20,21	0
4	FES	A	601	4/4	1.00	0.09	13,16,18,18	0

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

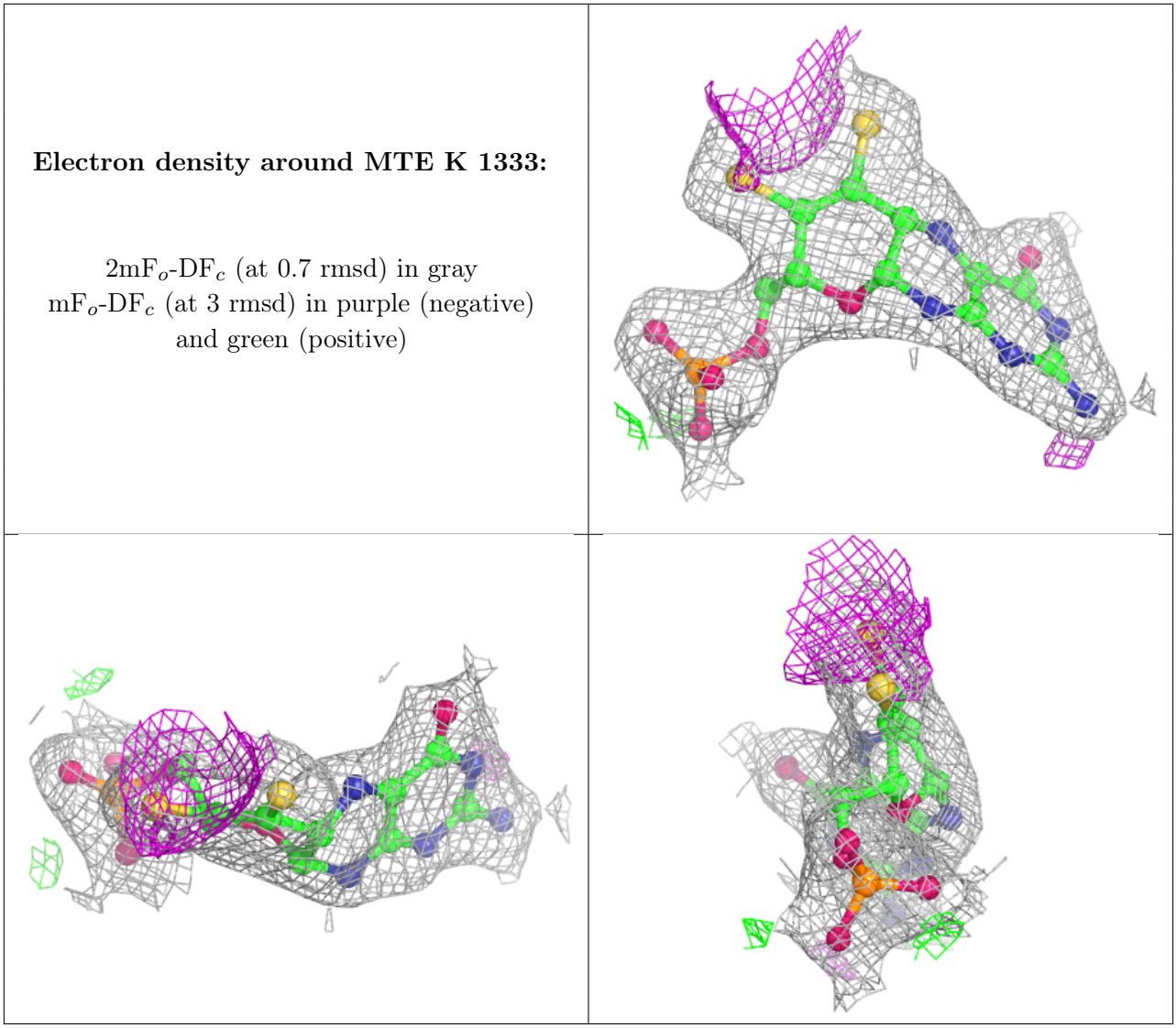
Electron density around FAD J 606:

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



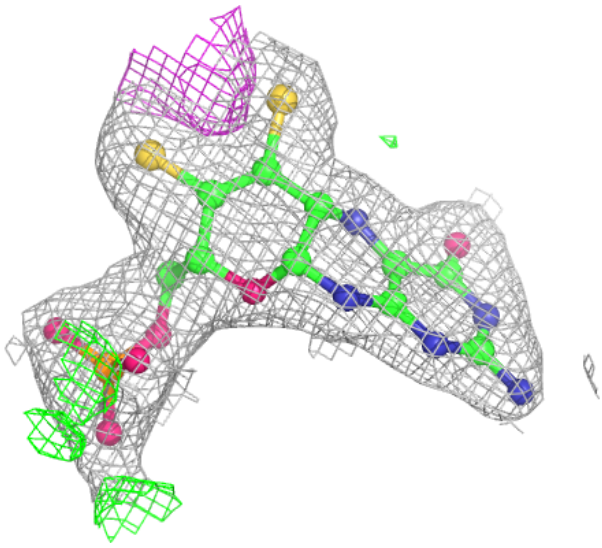
Electron density around MTE K 1333:

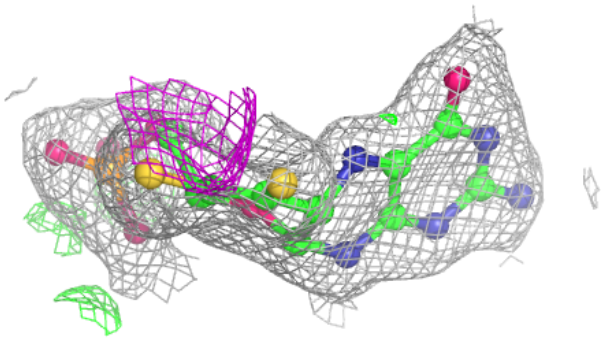
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around MTE C 1333:

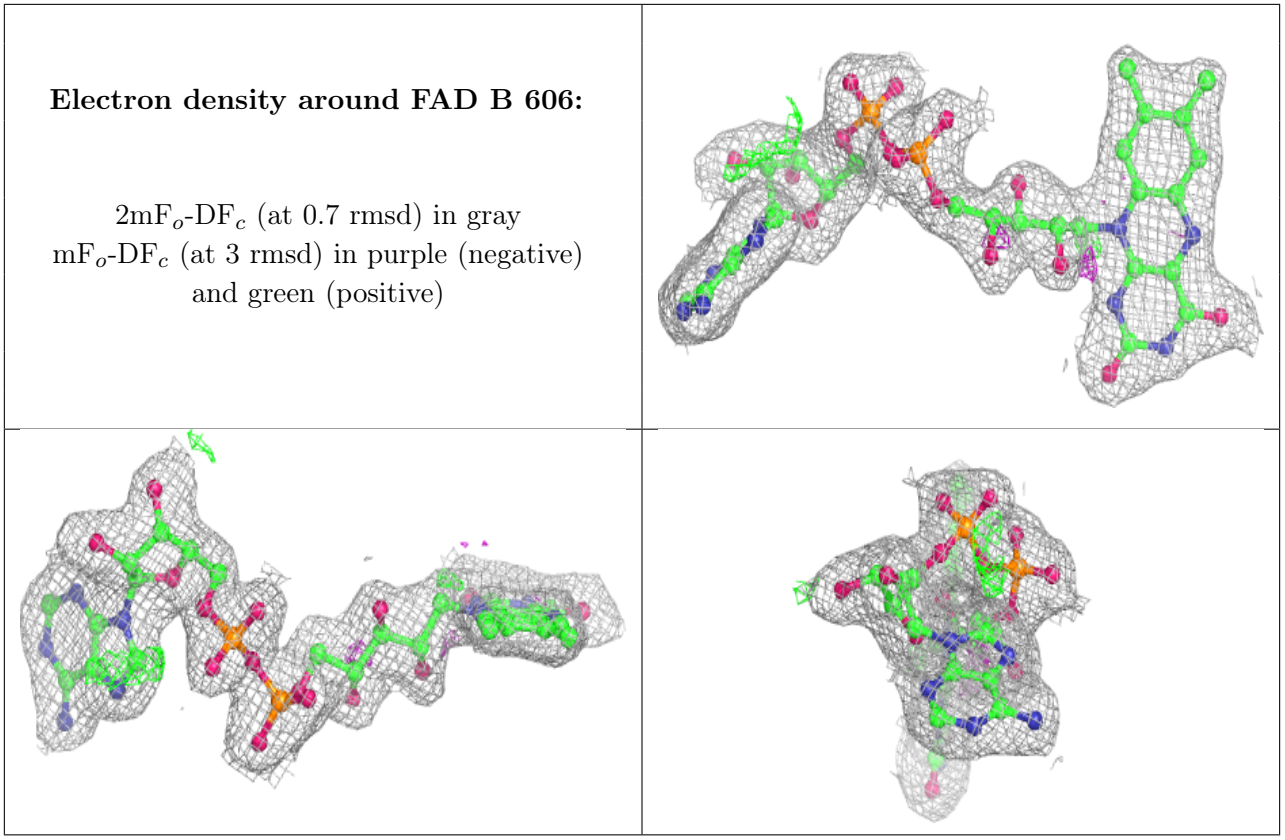
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around FAD B 606:

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



6.5 Other polymers (i)

There are no such residues in this entry.