



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:50 PM UTC

PDB ID : 3B9J / pdb_00003b9j
Title : Structure of Xanthine Oxidase with 2-hydroxy-6-methylpurine
Authors : Paufl, 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

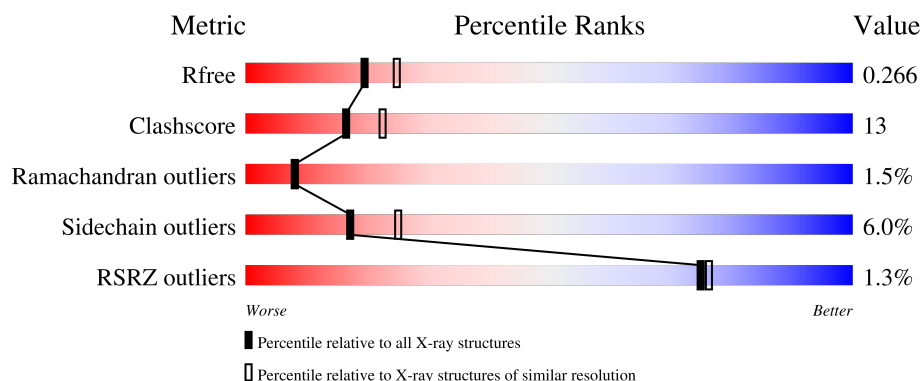
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 $\leq 5\%$. 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	219	2% 60% 12% 26%
1	I	219	2% 60% 11% 26%
2	B	350	2% 70% 15% 13%
2	J	350	2% 71% 14% 13%
3	C	763	2% 75% 19% ..

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Mol	Chain	Length	Quality of chain
3	K	763	% 73% 21% • •

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			

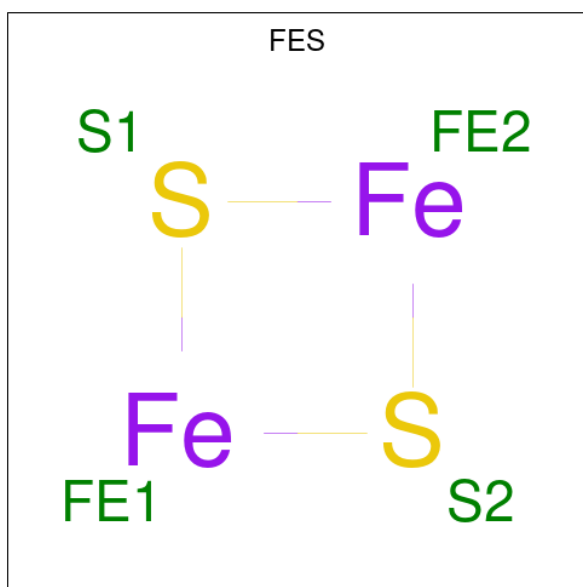
- Molecule 2 is a protein called xanthine oxidase.

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.

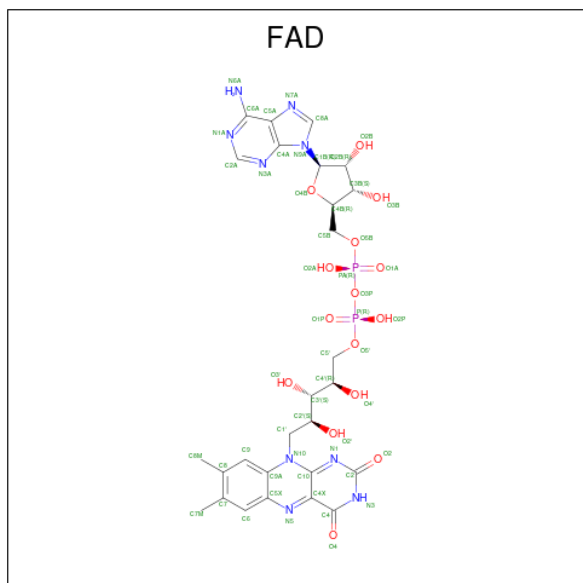
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	758	Total	C	N	O	S	0	0	0
			5835	3688	1005	1107	35			
3	K	747	Total	C	N	O	S	0	0	0
			5759	3645	987	1093	34			

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



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

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$).

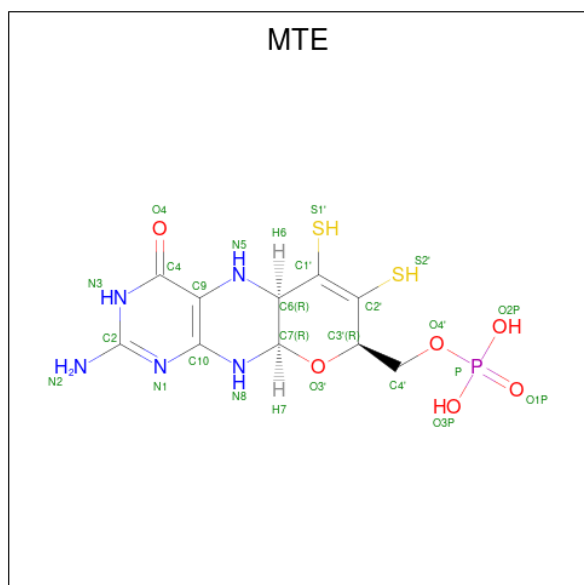


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	J	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

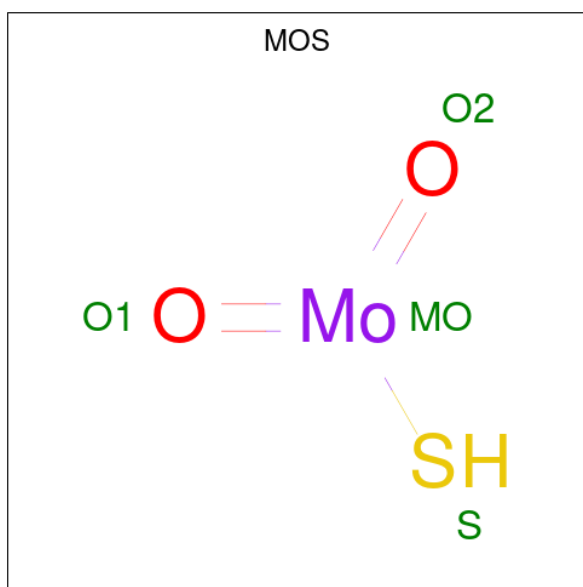
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	Ca	0	0
			1	1		

- 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 (CCD ID: MTE) (formula: C₁₀H₁₄N₅O₆PS₂).



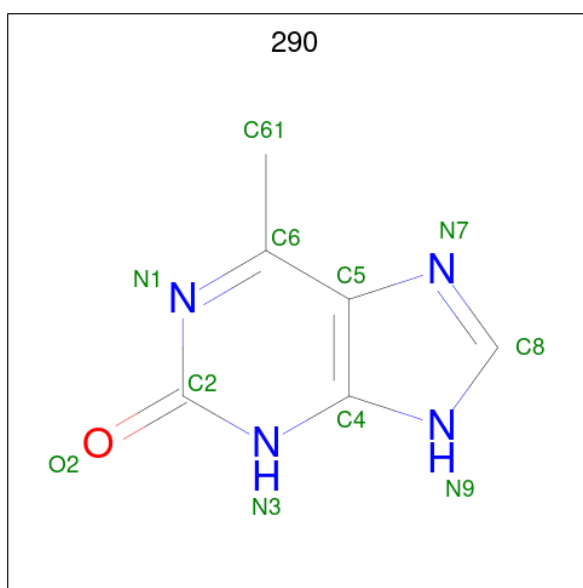
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	C	1	Total 24	C 10	N 5	O 6	P 1	S 2	0	0
7	K	1	Total 24	C 10	N 5	O 6	P 1	S 2	0	0

- Molecule 8 is DIOXOTHIOMOLYBDENUM(VI) ION (CCD ID: MOS) (formula: HMoO₂S).



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 (CCD ID: 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		
9	K	1	Total	C	N	O	0	0
			11	6	4	1		

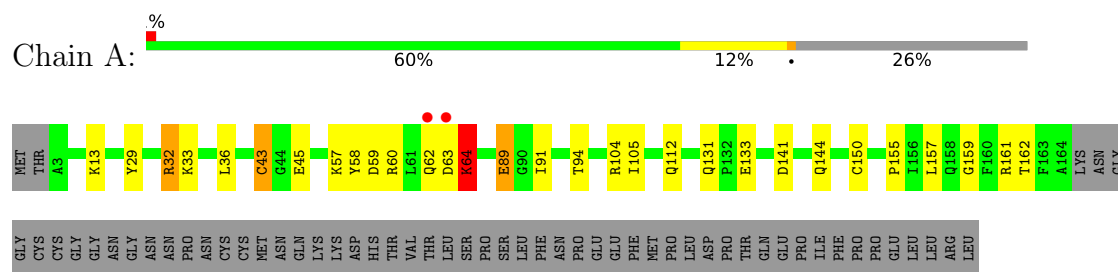
- Molecule 10 is water.

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

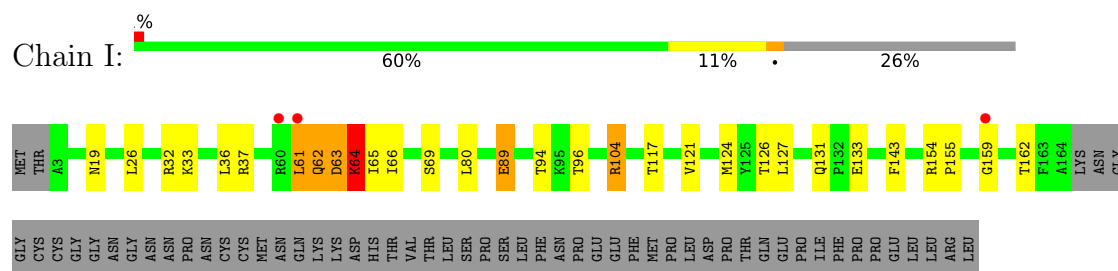
3 Residue-property plots [i](#)

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

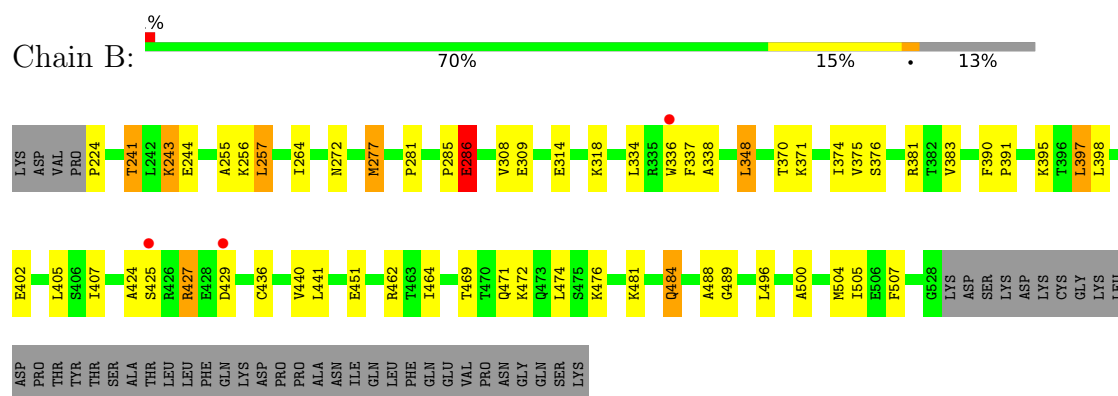
- Molecule 1: xanthine oxidase



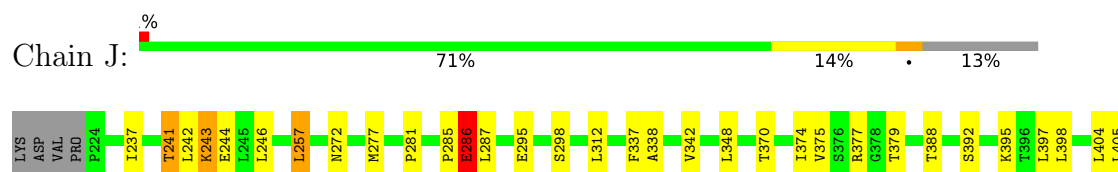
- Molecule 1: xanthine oxidase

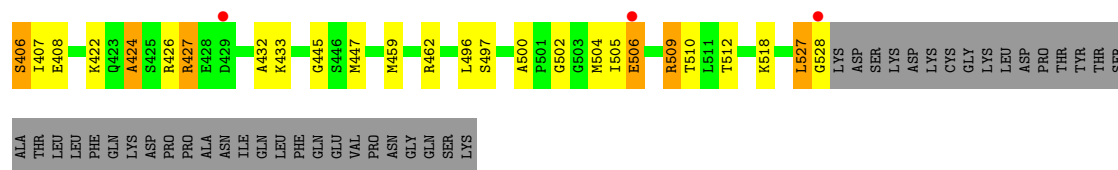


- Molecule 2: xanthine oxidase

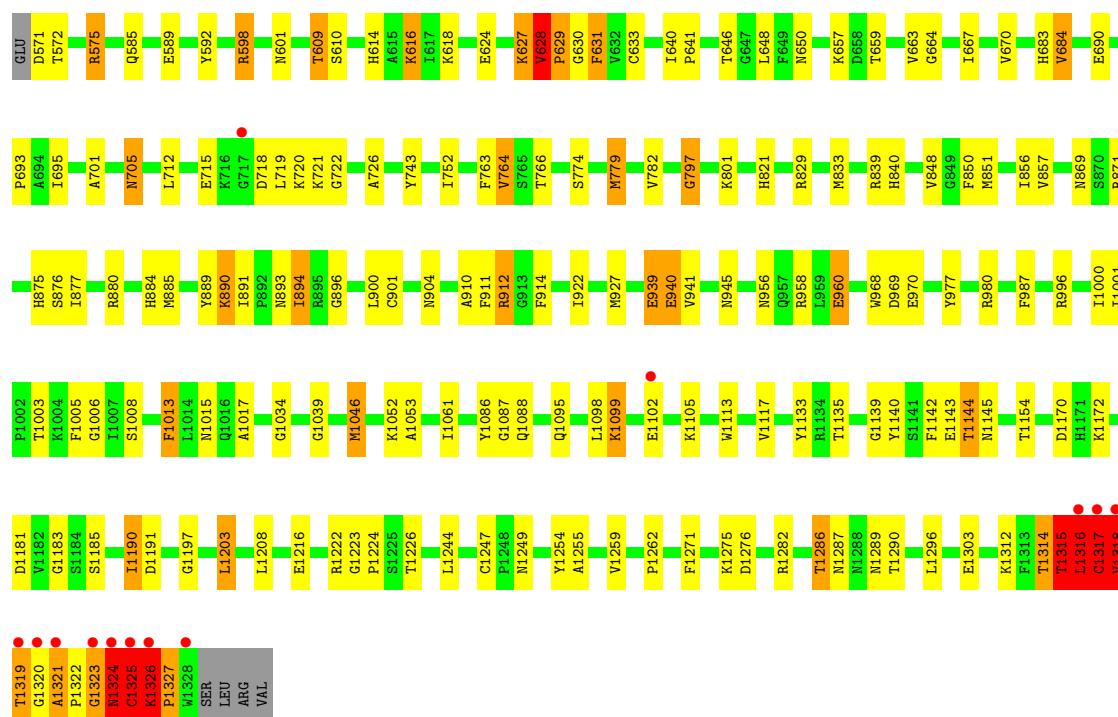
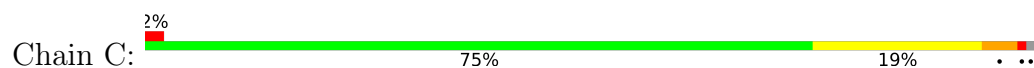


- Molecule 2: xanthine oxidase

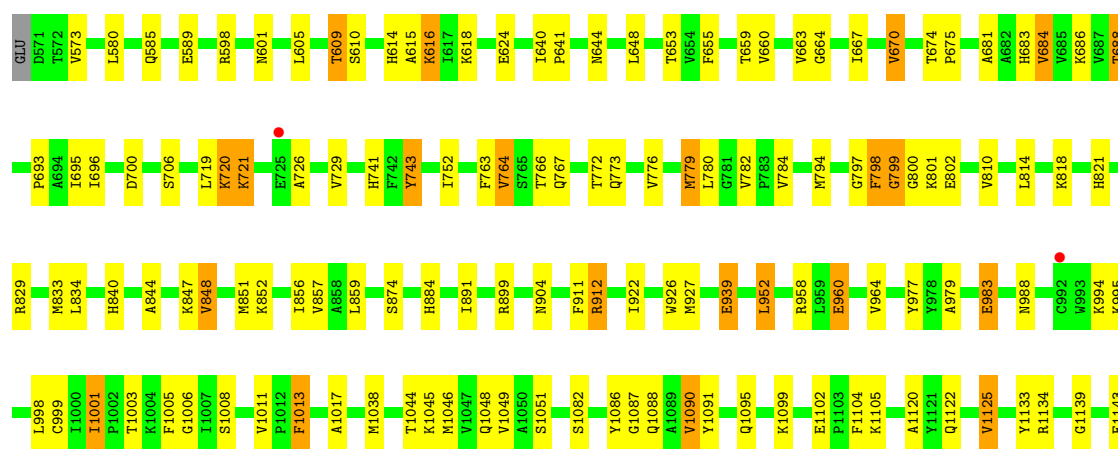
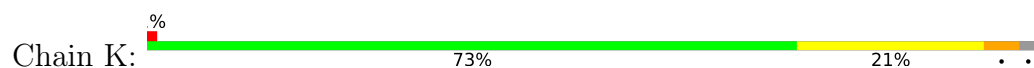


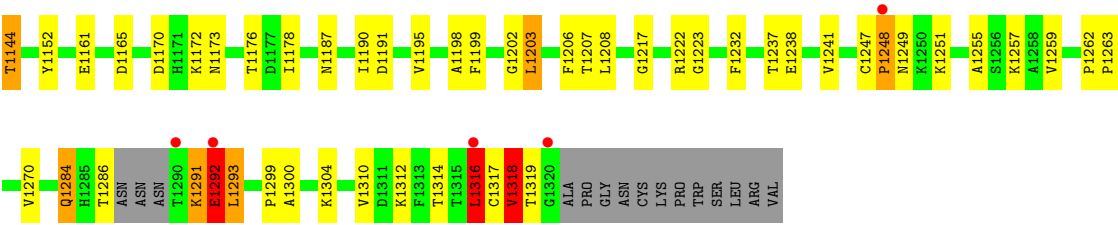


• Molecule 3: xanthine oxidase



• Molecule 3: xanthine oxidase





4 Data and refinement statistics

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 – 2.30 144.34 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.2 (144.34-2.30) 96.2 (144.34-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (4.77%)	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 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 290, CA, MOS, FES, MTE, 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	1.10	2/1261 (0.2%)	1.07	1/1702 (0.1%)
1	I	1.00	1/1237 (0.1%)	1.01	1/1672 (0.1%)
2	B	0.96	0/2430	1.04	2/3282 (0.1%)
2	J	0.91	0/2403	1.01	1/3248 (0.0%)
3	C	1.08	7/5963 (0.1%)	1.19	23/8078 (0.3%)
3	K	1.00	4/5885 (0.1%)	1.09	6/7971 (0.1%)
All	All	1.02	14/19179 (0.1%)	1.10	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 (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1315	THR	CA-C	-6.54	1.44	1.52
1	I	96	THR	CA-C	6.15	1.55	1.52
1	A	91	ILE	CA-CB	5.67	1.61	1.54
1	A	105	ILE	CA-CB	5.63	1.62	1.54
3	C	1315	THR	CA-CB	-5.61	1.44	1.53
3	K	964	VAL	CA-C	5.55	1.57	1.52
3	C	894	ILE	CA-CB	5.39	1.61	1.54
3	C	1190	ILE	CA-CB	5.39	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	1300	ALA	CA-CB	5.33	1.60	1.52
3	C	1318	VAL	CA-CB	5.24	1.61	1.54
3	C	1319	THR	N-CA	-5.23	1.39	1.46
3	K	1125	VAL	CA-CB	5.09	1.60	1.54
3	K	664	GLY	N-CA	5.03	1.52	1.45
3	C	922	ILE	CA-C	5.00	1.58	1.52

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1318	VAL	N-CA-C	18.24	130.71	113.20
3	C	628	VAL	N-CA-C	11.74	134.23	108.88
3	C	1318	VAL	CB-CA-C	-11.66	99.16	110.70
3	C	1314	THR	N-CA-C	9.25	121.13	111.14
3	C	1326	LYS	N-CA-C	8.96	136.07	111.00
3	C	1316	LEU	N-CA-CB	-8.38	96.34	110.49
3	K	1262	PRO	N-CA-C	8.10	120.58	110.70
3	C	1262	PRO	N-CA-C	7.38	119.70	110.70
3	K	1318	VAL	N-CA-C	7.31	120.23	111.09
3	C	667	ILE	CB-CA-C	-7.30	104.50	111.44
3	C	1325	CYS	N-CA-C	-6.87	96.16	110.80
3	C	1318	VAL	N-CA-CB	-6.78	102.29	112.67
3	C	629	PRO	N-CA-C	-6.64	99.73	110.55
3	K	798	PHE	N-CA-C	6.36	122.75	113.40
3	C	631	PHE	N-CA-C	6.26	124.14	110.80
3	C	1317	CYS	N-CA-C	6.25	124.12	110.80
2	B	425	SER	N-CA-C	6.09	119.04	109.96
3	C	592	TYR	N-CA-C	-5.93	101.42	110.14
2	B	436	CYS	N-CA-C	5.82	117.91	109.07
1	A	32	ARG	CG-CD-NE	-5.79	99.26	112.00
3	C	1316	LEU	N-CA-C	5.74	123.02	110.80
3	C	1327	PRO	N-CA-CB	5.74	110.99	103.42
3	C	869	ASN	N-CA-C	5.63	119.24	112.93
3	C	1325	CYS	CA-C-N	5.51	131.63	121.70
3	C	1325	CYS	C-N-CA	5.51	131.63	121.70
3	K	1011	VAL	CA-C-N	5.31	124.76	119.24
3	K	1011	VAL	C-N-CA	5.31	124.76	119.24
2	J	406	SER	N-CA-C	5.31	117.13	109.07
3	C	1316	LEU	CB-CA-C	-5.26	99.95	110.42
3	C	633	CYS	N-CA-C	5.17	115.99	108.14
3	C	1316	LEU	O-C-N	-5.13	115.76	122.59
3	K	1090	VAL	CB-CA-C	-5.10	105.18	112.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	19	ASN	N-CA-C	5.08	116.53	110.44
3	C	575	ARG	CB-CA-C	5.04	115.66	108.76

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

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	20	0
2	B	2381	0	2437	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	2356	0	2394	50	0
3	C	5835	0	5747	173	0
3	K	5759	0	5679	167	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	7	0
10	A	68	0	0	7	0
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	17	0
All	All	19847	0	18797	487	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 13.

All (487) 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:1046:MET:HE1	3:K:1086:TYR:C	1.55	1.30
3:C:640:ILE:HG23	3:C:779:MET:HE3	1.21	1.20
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:K:851:MET:HE3	3:K:857:VAL:HG21	1.10	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
2:J:237:ILE:HD12	2:J:277:MET:HE1	1.37	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:640:ILE:HG23	3:K:779:MET:CE	1.86	1.05
3:K:1046:MET:HE1	3:K:1087:GLY:N	1.75	1.00
3:C:779:MET:HE2	3:C:779:MET:O	1.60	0.99
3:K:726:ALA:HA	3:K:851:MET:HE1	1.41	0.99
2:B:424:ALA:O	10:B:677:HOH:O	1.78	0.98
3:C:726:ALA:HA	3:C:851:MET:HE1	1.40	0.98
8:C:1334:MOS:S	9:C:1335:290:H8	2.04	0.98
3:C:1046:MET:HE1	3:C:1087:GLY:N	1.79	0.97
3:K:1046:MET:CE	3:K:1086:TYR:C	2.39	0.95
2:B:481:LYS:CB	10:B:648:HOH:O	2.13	0.95
3:K:726:ALA:HA	3:K:851:MET:CE	1.97	0.94
3:C:610:SER:O	3:C:663:VAL:O	1.85	0.94
3:C:641:PRO:HD2	3:C:779:MET:CE	2.00	0.92
2:J:375:VAL:HG21	2:J:405:LEU:HD22	1.49	0.91
3:K:833:MET:HE3	3:K:1222:ARG:C	1.96	0.91
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:C:641:PRO:HD2	3:C:779:MET:HE1	1.51	0.88
3:K:720:LYS:O	3:K:721:LYS:HB2	1.71	0.88
3:K:833:MET:CE	3:K:1222:ARG:C	2.46	0.88
1:A:141:ASP:OD1	10:A:639:HOH:O	1.91	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:C:829:ARG:CG	3:C:833:MET:HE2	2.05	0.87
3:K:851:MET:HE3	3:K:857:VAL:CG2	2.02	0.86
3:C:640:ILE:HG23	3:C:779:MET:CE	2.06	0.85
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:C:1046:MET:HE1	3:C:1086:TYR:C	2.02	0.85
3:C:779:MET:HE2	3:C:779:MET:C	2.01	0.85
3:K:616:LYS:HD2	3:K:659:THR:HG22	1.59	0.84
3:C:829:ARG:HG3	3:C:833:MET:HE2	1.57	0.84
3:K:833:MET:HE1	3:K:1223:GLY:N	1.91	0.84
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:K:779:MET:HE2	3:K:779:MET:O	1.78	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:C:705:ASN:CG	10:C:1457:HOH:O	2.22	0.82
3:C:1316:LEU:O	3:C:1319:THR:OG1	1.98	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:618:LYS:HG2	3:K:688:THR:HG22	1.60	0.81
3:C:833:MET:HE1	3:C:1223:GLY:HA2	1.63	0.80
3:K:833:MET:HE1	3:K:1223:GLY:CA	2.10	0.80
3:C:1046:MET:CE	3:C:1086:TYR:HB2	2.11	0.80
3:K:1046:MET:HE1	3:K:1086:TYR:O	1.82	0.80
2:B:241:THR:HG22	2:B:244:GLU:H	1.45	0.80
3:K:640:ILE:HG23	3:K:779:MET:HE2	1.62	0.79
3:K:851:MET:CE	3:K:857:VAL:HG21	2.04	0.79
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:833:MET:HE1	3:C:1223:GLY:CA	2.13	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
2:B:241:THR:CG2	2:B:244:GLU:H	1.98	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:C:1321:ALA:HB3	3:C:1322:PRO:C	2.10	0.76
3:C:833:MET:HE1	3:C:1223:GLY:N	2.01	0.75
3:K:833:MET:HE3	3:K:1222:ARG:O	1.86	0.75
3:K:829:ARG:CG	3:K:833:MET:HE2	2.17	0.75
8:K:1334:MOS:S	8:K:1334:MOS:O2	2.44	0.75
3:C:726:ALA:HA	3:C:851:MET:CE	2.16	0.75
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: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
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:K:833:MET:HE1	3:K:1223:GLY:HA2	1.70	0.71
3:C:833:MET:CE	3:C:1222:ARG:C	2.63	0.71
3:C:940:GLU:OE2	10:C:1399:HOH:O	2.07	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:1046:MET:CE	3:C:1086:TYR:C	2.64	0.70
3:K:640:ILE:HG12	3:K:779:MET:HE3	1.71	0.70
3:K:1046:MET:HE2	3:K:1086:TYR:HB3	1.73	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
3:C:1321:ALA:CB	3:C:1322:PRO:C	2.66	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:K:1046:MET:HE2	3:K:1086:TYR:CB	2.24	0.68
1:A:104:ARG:CD	1:A:162:THR:HG21	2.23	0.67
3:K:1046:MET:HE3	3:K:1090:VAL:CG2	2.25	0.67
3:K:833:MET:HE1	3:K:1222:ARG:C	2.18	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: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
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:726:ALA:CA	3:K:851:MET:HE1	2.24	0.65
3:K:829:ARG:HG3	3:K:833:MET:HE2	1.79	0.65
2:J:285:PRO:O	2:J:286:GLU:CD	2.39	0.64
3:K:1102:GLU:OE1	3:K:1105:LYS:HD3	1.95	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
3:C:850:PHE:C	3:C:851:MET:HE2	2.22	0.63
3:K:641:PRO:HD2	3:K:779:MET:HE1	1.79	0.63
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:829:ARG:HG2	3:K:833:MET:HE2	1.80	0.63
3:C:829:ARG:HG2	3:C:833:MET:HE2	1.81	0.63
3:K:601:ASN:HD22	3:K:821:HIS:HD2	1.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:J:237:ILE:HD12	2:J:277:MET:CE	2.22	0.62
3:K:640:ILE:HG23	3:K:779:MET:HE1	1.80	0.62
3:K:779:MET:HE2	3:K:779:MET:C	2.24	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:HE3	3:K:1090:VAL:HG21	1.82	0.61
3:C:833:MET:HE1	3:C:1222:ARG:C	2.25	0.61
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
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:1087:GLY:CA	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
1:I:36:LEU:HD22	1:I:89:GLU:HG3	1.83	0.60
3:C:833:MET:HE3	3:C:1222:ARG:O	2.02	0.60
2:J:388:THR:O	2:J:397:LEU:HD22	2.02	0.60
1:I:124:MET:HE1	1:I:127:LEU:HD23	1.83	0.59
3:C:833:MET:HE3	3:C:1222:ARG:C	2.26	0.59
3:C:1322:PRO:C	3:C:1323:GLY:O	2.46	0.59
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:HB3	1.84	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:641:PRO:CD	3:C:779:MET:HE1	2.29	0.58
3:C:958:ARG:HE	3:C:960:GLU:HG2	1.67	0.58
3:C:1322:PRO:O	3:C:1323:GLY:C	2.45	0.58
3:K:1292:GLU:HG3	3:K:1293:LEU:HA	1.85	0.58
3:K:726:ALA:HA	3:K:851:MET:HE2	1.82	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
3:K:1046:MET:CE	3:K:1086:TYR:O	2.47	0.57
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
3:C:890:LYS:NZ	10:C:1453:HOH:O	2.30	0.57
3:C:624:GLU:HB2	3:C:684:VAL:HG13	1.87	0.57
3:C:840:HIS:CD2	3:C:877:ILE:HD13	2.40	0.56
2:J:427:ARG:CZ	2:J:504:MET:HE3	2.34	0.56
2:J:374:ILE:HD13	2:J:398:LEU:CD2	2.35	0.56
2:J:459:MET:HE2	2:J:512:THR:HG21	1.88	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: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
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
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:1046:MET:HE3	3:C:1086:TYR:CB	2.33	0.55
3:K:833:MET:CE	3:K:1222:ARG:O	2.51	0.55
2:J:528:GLY:HA3	10:J:617:HOH:O	2.07	0.55
3:C:1046:MET:HE2	3:C:1086:TYR:HB2	1.86	0.54
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
3:K:605:LEU:HD23	3:K:605:LEU:C	2.34	0.53
1:A:144:GLN:HE22	2:B:336:TRP:HA	1.74	0.53
3:C:641:PRO:HD2	3:C:779:MET:HE3	1.85	0.53
3:C:1013:PHE:CD1	3:C:1013:PHE:C	2.86	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
3:K:794:MET:HE3	3:K:1038:MET:HB3	1.92	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
2:B:285:PRO:O	2:B:286:GLU:OE1	2.27	0.51
3:K:1143:GLU:C	3:K:1144:THR:HG23	2.30	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:1198:ALA:HB3	3:K:1263:PRO:HB2	1.93	0.51
2:B:427:ARG:CZ	2:B:504:MET:HE3	2.40	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:1216:GLU:H	3:C:1216:GLU:CD	2.19	0.50
2:B:241:THR:HG23	2:B:243:LYS:H	1.76	0.50
1:I:61:LEU:C	1:I:63:ASP:H	2.20	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:342:VAL:HG21	5:J:606:FAD:HM71	1.92	0.50
3:C:911:PHE:O	3:C:912:ARG:C	2.54	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
2:B:390:PHE:O	2:B:462:ARG:HD2	2.12	0.49
3:C:683:HIS:O	3:C:683:HIS:CG	2.65	0.49
3:C:851:MET:HE2	3:C:851:MET:N	2.27	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: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:C:833:MET:CE	3:C:1222:ARG:O	2.60	0.49
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: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:926:TRP:CZ3	3:K:927:MET:HE2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:392:SER:OG	2:J:395:LYS:CE	2.61	0.48
3:K:802:GLU:OE2	9:K:1335:290:H61	2.14	0.48
3:K:1317:CYS:C	3:K:1319:THR:HA	2.39	0.48
3:C:941:VAL:O	3:C:945:ASN:ND2	2.38	0.48
2:B:337:PHE:O	2:B:338:ALA:C	2.55	0.48
1:I:62:GLN:O	1:I:64:LYS:HD2	2.14	0.48
3:K:1299:PRO:O	3:K:1304:LYS:NZ	2.45	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
1:A:45:GLU:CD	3:C:1224:PRO:HD2	2.40	0.47
3:C:884:HIS:CE1	3:C:1006:GLY:H	2.32	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:285:PRO:O	2:B:286:GLU:CD	2.58	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
9:K:1335:290:C61	10:K:1624:HOH:O	2.62	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
1:I:104:ARG:HD3	1:I:162:THR:HG21	1.97	0.46
2:J:427:ARG:NE	2:J:504:MET:HE3	2.31	0.46
1:A:36:LEU:HD22	1:A:89:GLU:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1046:MET:CE	3:C:1087:GLY:N	2.66	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
3:K:1013:PHE:CD1	3:K:1013:PHE:C	2.94	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
9:K:1335:290:H61B	10:K:1624:HOH:O	2.15	0.45
2:B:257:LEU:HD13	2:B:281:PRO:HG3	1.99	0.45
3:K:1046:MET:HE3	3:K:1090:VAL:HG23	1.99	0.45
3:C:851:MET:HE2	3:C:851:MET:HA	1.98	0.45
3:C:856:ILE:HD13	3:C:927:MET:HE1	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
2:J:504:MET:HE2	10:K:1613:HOH:O	2.16	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
1:I:154:ARG:HD2	1:I:154:ARG:C	2.43	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:640:ILE:HG12	3:K:779:MET:CE	2.43	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
2:J:518:LYS:NZ	3:K:1165:ASP:OD2	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:851:MET:HE2	3:C:851:MET:CA	2.48	0.43
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:C:1185:SER:OG	3:C:1191:ASP:OD2	2.31	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
3:C:1143:GLU:C	3:C:1145:ASN:H	2.25	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:726:ALA:CA	3:C:851:MET:HE1	2.30	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
3:C:1046:MET:HE1	3:C:1086:TYR:HB2	1.98	0.43
1:I:94:THR:OG1	3:K:589:GLU:OE2	2.27	0.43
3:C:856:ILE:CD1	3:C:927:MET:HE1	2.48	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:C:1271:PHE:CD2	3:C:1271:PHE:C	2.97	0.43
3:K:911:PHE:O	3:K:912:ARG:C	2.62	0.43
3:K:1091:TYR:O	3:K:1095:GLN:HG2	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:I:143:PHE:HB3	3:K:1232:PHE:CD1	2.55	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:1286:THR:C	10:K:1516:HOH:O	2.61	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
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
3:C:1203:LEU:C	3:C:1203:LEU:HD12	2.45	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:464:ILE:HD13	2:B:464:ILE:HG21	1.82	0.42
3:C:1145:ASN:CG	3:C:1145:ASN:O	2.62	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
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
3:K:1284:GLN:O	3:K:1284:GLN:HG3	2.18	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: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:1143:GLU:C	3:C:1144:THR:HG23	2.45	0.41
3:C:1183:GLY:HA2	3:C:1247:CYS:O	2.21	0.41
3:K:1046:MET:HE1	3:K:1087:GLY:HA2	2.01	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
2:J:337:PHE:O	2:J:338:ALA:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:722:GLY:HA2	3:C:857:VAL:HG12	2.03	0.41
3:C:1216:GLU:CD	3:C:1216:GLU:N	2.79	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: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: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
1:A:104:ARG:NH1	10:A:646:HOH:O	2.54	0.40
3:C:1046:MET:HE1	3:C:1086:TYR:CB	2.48	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%)	9 10
1	I	160/219 (73%)	150 (94%)	7 (4%)	3 (2%)	6 5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	303/350 (87%)	286 (94%)	16 (5%)	1 (0%)	36	46
2	J	303/350 (87%)	286 (94%)	12 (4%)	5 (2%)	7	7
3	C	756/763 (99%)	710 (94%)	30 (4%)	16 (2%)	5	4
3	K	743/763 (97%)	704 (95%)	29 (4%)	10 (1%)	9	10
All	All	2425/2664 (91%)	2287 (94%)	101 (4%)	37 (2%)	8	8

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 ⓘ

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%)	130 (96%)	5 (4%)	30	45
1	I	130/187 (70%)	124 (95%)	6 (5%)	24	36
2	B	259/302 (86%)	245 (95%)	14 (5%)	20	29
2	J	254/302 (84%)	237 (93%)	17 (7%)	15	21
3	C	630/639 (99%)	588 (93%)	42 (7%)	15	21
3	K	623/639 (98%)	586 (94%)	37 (6%)	18	26
All	All	2031/2256 (90%)	1910 (94%)	121 (6%)	17	25

All (121) 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	89	GLU
2	B	241	THR
2	B	243	LYS
2	B	256	LYS
2	B	257	LEU
2	B	277	MET
2	B	286	GLU
2	B	348	LEU
2	B	370	THR

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Mol	Chain	Res	Type
2	B	371	LYS
2	B	397	LEU
2	B	427	ARG
2	B	472	LYS
2	B	476	LYS
2	B	484	GLN
3	C	598	ARG
3	C	609	THR
3	C	616	LYS
3	C	627	LYS
3	C	657	LYS
3	C	670	VAL
3	C	684	VAL
3	C	705	ASN
3	C	715	GLU
3	C	719	LEU
3	C	743	TYR
3	C	764	VAL
3	C	774	SER
3	C	779	MET
3	C	782	VAL
3	C	848	VAL
3	C	871	ARG
3	C	890	LYS
3	C	900	LEU
3	C	939	GLU
3	C	940	GLU
3	C	960	GLU
3	C	969	ASP
3	C	1001	ILE
3	C	1003	THR
3	C	1013	PHE
3	C	1046	MET
3	C	1061	ILE
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

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Mol	Chain	Res	Type
3	C	1287	ASN
3	C	1289	ASN
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	65	ILE
1	I	66	ILE
1	I	89	GLU
1	I	104	ARG
2	J	241	THR
2	J	243	LYS
2	J	257	LEU
2	J	286	GLU
2	J	295	GLU
2	J	298	SER
2	J	312	LEU
2	J	348	LEU
2	J	377	ARG
2	J	379	THR
2	J	406	SER
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	598	ARG
3	K	609	THR
3	K	616	LYS
3	K	670	VAL
3	K	684	VAL
3	K	686	LYS
3	K	688	THR
3	K	706	SER
3	K	720	LYS
3	K	743	TYR
3	K	764	VAL
3	K	779	MET
3	K	782	VAL

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Mol	Chain	Res	Type
3	K	818	LYS
3	K	848	VAL
3	K	852	LYS
3	K	899	ARG
3	K	939	GLU
3	K	952	LEU
3	K	960	GLU
3	K	983	GLU
3	K	1001	ILE
3	K	1003	THR
3	K	1013	PHE
3	K	1051	SER
3	K	1099	LYS
3	K	1122	GLN
3	K	1134	ARG
3	K	1172	LYS
3	K	1190	ILE
3	K	1203	LEU
3	K	1208	LEU
3	K	1237	THR
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 (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	131	GLN
1	A	144	GLN
2	B	251	GLN
2	B	272	ASN
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	884	HIS

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Mol	Chain	Res	Type
3	C	893	ASN
3	C	904	ASN
3	C	925	ASN
3	C	1016	GLN
3	C	1033	HIS
3	C	1048	GLN
3	C	1137	ASN
3	C	1212	HIS
3	C	1284	GLN
3	C	1287	ASN
3	C	1289	ASN
1	I	71	ASN
1	I	82	HIS
1	I	131	GLN
1	I	146	ASN
2	J	226	GLN
2	J	252	HIS
2	J	272	ASN
2	J	333	GLN
2	J	448	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	1088	GLN
3	K	1108	ASN
3	K	1220	HIS
3	K	1284	GLN
3	K	1307	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
5	FAD	J	606	-	58,58,58	1.18	4 (6%)	85,89,89	1.75	17 (20%)
7	MTE	K	1333	8	21,26,26	1.48	1 (4%)	19,40,40	2.17	8 (42%)
9	290	C	1335	-	11,12,12	1.21	1 (9%)	10,17,17	2.29	3 (30%)
7	MTE	C	1333	8	21,26,26	1.81	4 (19%)	19,40,40	2.34	9 (47%)
9	290	K	1335	-	11,12,12	1.25	1 (9%)	10,17,17	2.15	2 (20%)
4	FES	I	602	1	0,4,4	-	-	-	-	-
4	FES	A	601	1	0,4,4	-	-	-	-	-
8	MOS	C	1334	7	0,3,3	-	-	-	-	-
5	FAD	B	606	-	58,58,58	1.14	3 (5%)	85,89,89	1.83	23 (27%)
4	FES	I	601	1	0,4,4	-	-	-	-	-
8	MOS	K	1334	7	0,3,3	-	-	-	-	-
4	FES	A	602	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
5	FAD	J	606	-	-	5/34/50/50	0/6/6/6

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

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	1333	MTE	C9-C10	5.21	1.47	1.38
7	K	1333	MTE	C9-C10	4.95	1.47	1.38
7	C	1333	MTE	C7-C6	-3.90	1.50	1.53
5	J	606	FAD	C4X-N5	3.87	1.39	1.30
5	J	606	FAD	C2A-N1A	3.59	1.40	1.33
5	B	606	FAD	C4X-N5	3.34	1.38	1.30
5	J	606	FAD	C10-N1	3.29	1.39	1.33
7	C	1333	MTE	C4-N3	-3.18	1.32	1.38
5	B	606	FAD	P-O3P	2.89	1.62	1.59
5	B	606	FAD	C2A-N1A	2.66	1.38	1.33
7	C	1333	MTE	C9-C4	2.60	1.49	1.41
5	J	606	FAD	C8A-N7A	2.33	1.36	1.31
9	C	1335	290	C6-N1	2.30	1.35	1.32
9	K	1335	290	C8-N9	2.25	1.38	1.35

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	606	FAD	N3A-C2A-N1A	-7.58	117.10	128.58
5	J	606	FAD	N3A-C2A-N1A	-6.78	118.32	128.58
7	K	1333	MTE	C2-N1-C10	4.95	122.10	113.36
9	K	1335	290	C61-C6-N1	4.73	122.83	116.77
5	B	606	FAD	N9A-C8A-N7A	-4.33	107.79	113.94
7	C	1333	MTE	C7-C6-N5	4.33	112.12	107.87
9	C	1335	290	C61-C6-N1	4.29	122.27	116.77
9	C	1335	290	C2-N1-C6	4.07	122.62	118.86
7	C	1333	MTE	O3'-C7-N8	3.79	112.05	108.61
5	B	606	FAD	C4X-C10-N10	3.71	121.79	116.48
7	C	1333	MTE	C2-N1-C10	3.70	119.88	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	606	FAD	O2A-PA-O3P	3.65	117.14	107.27
9	K	1335	290	C2-N1-C6	3.62	122.21	118.86
5	J	606	FAD	C2A-N3A-C4A	3.52	120.44	111.83
5	J	606	FAD	C5A-C4A-N3A	-3.49	121.90	126.72
7	C	1333	MTE	C4-C9-N5	3.48	125.75	116.27
5	J	606	FAD	N9A-C8A-N7A	-3.47	109.01	113.94
5	B	606	FAD	C2A-N3A-C4A	3.35	120.02	111.83
7	K	1333	MTE	C4-C9-N5	3.32	125.31	116.27
5	B	606	FAD	C2A-N1A-C6A	3.20	123.99	118.73
5	B	606	FAD	O5'-C5'-C4'	-3.17	100.89	109.36
7	C	1333	MTE	O4'-P-O1P	-3.17	97.89	106.44
7	K	1333	MTE	O4-C4-C9	-3.15	119.68	127.26
5	J	606	FAD	C5A-C6A-N6A	-3.14	115.52	123.29
5	B	606	FAD	O2A-PA-O3P	3.06	115.55	107.27
5	J	606	FAD	O3'-C3'-C2'	-3.04	102.01	108.93
5	B	606	FAD	C5A-N7A-C8A	2.99	108.14	103.45
5	J	606	FAD	C4'-C3'-C2'	-2.98	108.62	113.57
5	J	606	FAD	C5A-N7A-C8A	2.75	107.77	103.45
5	B	606	FAD	C10-C4X-N5	-2.74	119.21	124.81
5	B	606	FAD	C2B-C1B-N9A	2.69	119.98	113.30
7	K	1333	MTE	C9-C4-N3	2.66	119.44	112.13
5	B	606	FAD	C4A-N9A-C1B	-2.65	120.44	126.63
5	J	606	FAD	C9A-C5X-N5	-2.64	119.65	122.45
7	K	1333	MTE	N2-C2-N3	2.62	122.29	116.76
5	J	606	FAD	O4'-C4'-C3'	2.62	115.37	109.25
5	J	606	FAD	O3P-PA-O1A	-2.61	102.87	110.70
5	B	606	FAD	C4A-N9A-C8A	2.60	108.47	105.74
5	B	606	FAD	C4-C4X-N5	2.60	121.80	118.21
7	K	1333	MTE	O2P-P-O4'	-2.43	100.34	106.67
5	B	606	FAD	O2P-P-O3P	2.40	113.77	107.27
5	B	606	FAD	O4'-C4'-C3'	2.39	114.85	109.25
5	J	606	FAD	C4X-C4-N3	2.37	119.29	113.25
7	C	1333	MTE	O4'-C4'-C3'	2.33	114.34	108.58
7	C	1333	MTE	O2P-P-O1P	2.31	119.85	110.83
5	J	606	FAD	N3A-C4A-N9A	2.30	131.07	127.17
7	K	1333	MTE	O3P-P-O4'	-2.26	100.77	106.67
5	B	606	FAD	C5A-C4A-N3A	-2.26	123.60	126.72
7	K	1333	MTE	O2P-P-O1P	2.26	119.64	110.83
5	B	606	FAD	C10-N1-C2	2.25	121.73	116.85
9	C	1335	290	C4-C5-N7	-2.24	106.40	109.28
5	J	606	FAD	O4-C4-C4X	-2.23	120.64	126.53
7	C	1333	MTE	C9-C4-N3	2.23	118.26	112.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	606	FAD	C4X-C4-N3	2.22	118.91	113.25
5	B	606	FAD	O3'-C3'-C2'	-2.17	103.99	108.93
5	J	606	FAD	C10-C4X-N5	-2.17	120.37	124.81
5	B	606	FAD	O4B-C1B-N9A	-2.12	104.01	108.09
5	B	606	FAD	O2-C2-N3	2.10	122.62	118.58
7	C	1333	MTE	O2P-P-O4'	-2.08	101.26	106.67
5	B	606	FAD	C4-N3-C2	-2.07	121.96	125.64
5	B	606	FAD	O4-C4-C4X	-2.05	121.13	126.53
5	J	606	FAD	C4-N3-C2	-2.02	122.05	125.64

There are no chirality outliers.

All (9) 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
5	J	606	FAD	P-O3P-PA-O1A

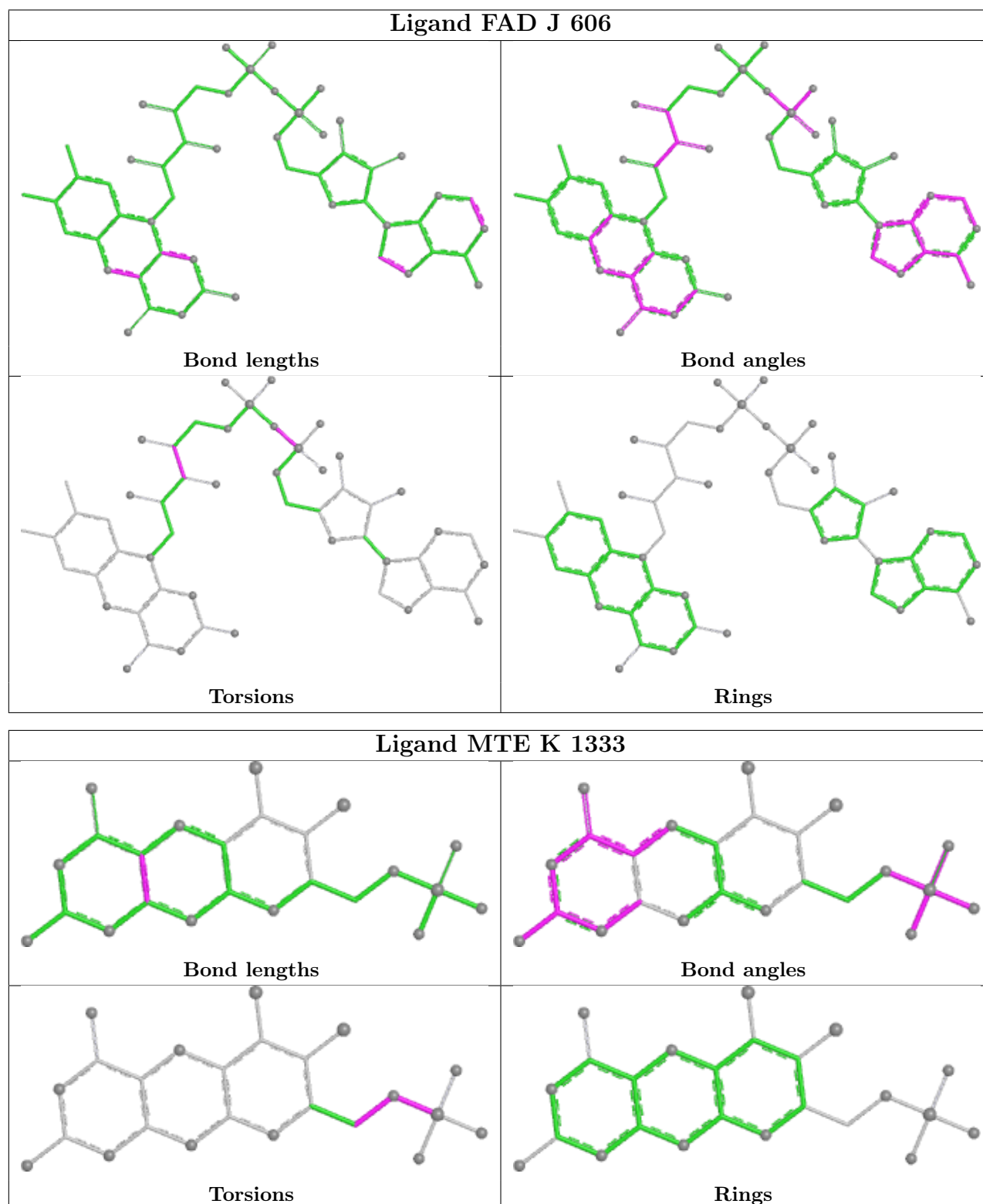
There are no ring outliers.

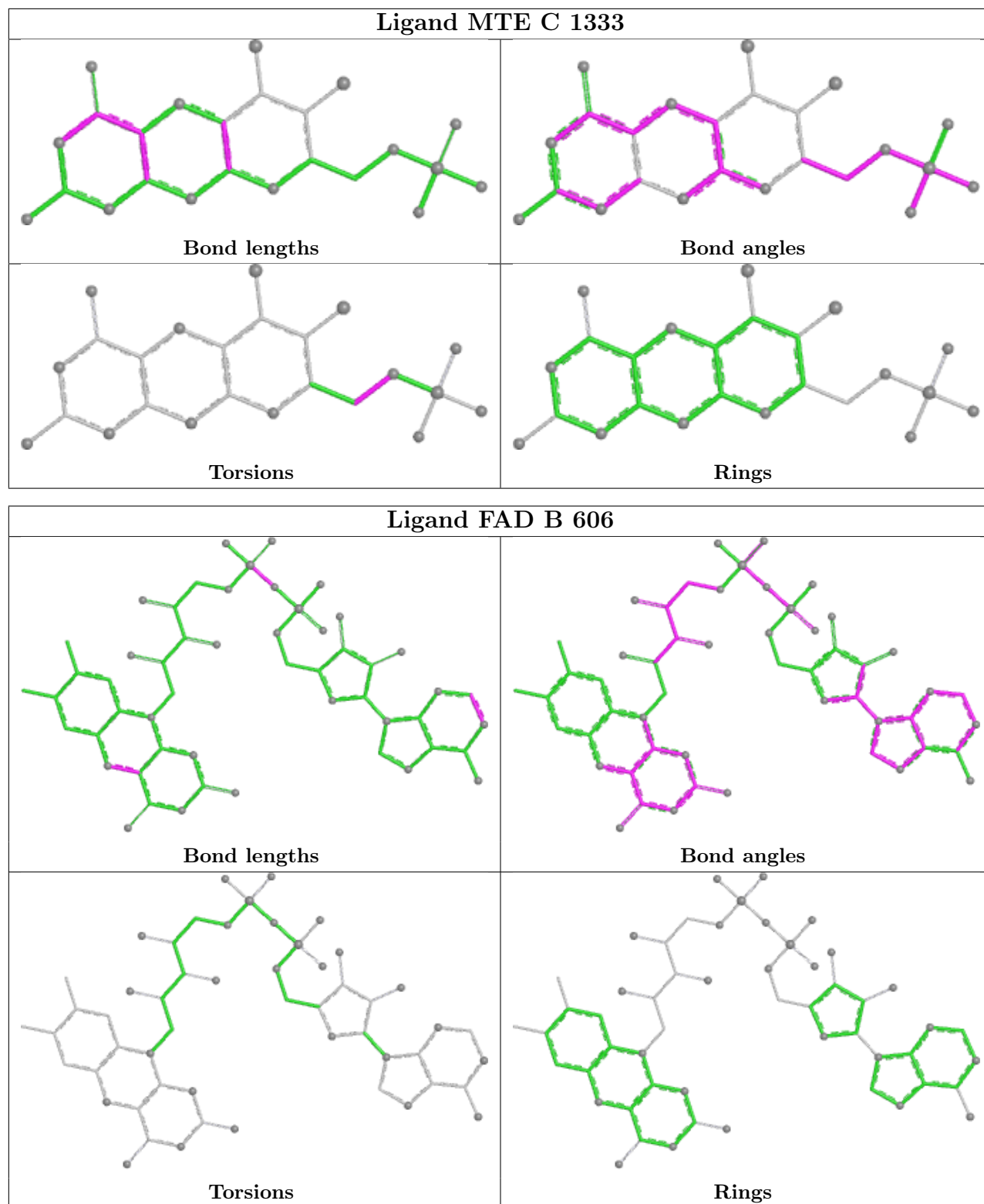
7 monomers are involved in 24 short contacts:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	162/219 (73%)	-0.26	2 (1%) 76 77	13, 21, 37, 50	0
1	I	162/219 (73%)	-0.10	3 (1%) 66 68	17, 27, 44, 54	0
2	B	305/350 (87%)	-0.03	3 (0%) 79 80	15, 28, 39, 43	0
2	J	305/350 (87%)	0.14	3 (0%) 79 80	22, 34, 44, 47	0
3	C	758/763 (99%)	-0.09	13 (1%) 69 70	13, 25, 39, 51	0
3	K	747/763 (97%)	-0.15	7 (0%) 81 82	12, 25, 40, 55	0
All	All	2439/2664 (91%)	-0.08	31 (1%) 75 76	12, 26, 41, 55	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	1325	CYS	6.9
3	C	1323	GLY	4.3
3	K	1316	LEU	4.2
3	C	1328	TRP	3.9
3	C	1321	ALA	3.5
3	C	1319	THR	3.4
2	B	425	SER	3.4
3	K	725	GLU	3.4
2	J	429	ASP	3.3
3	C	1326	LYS	3.3
1	I	61	LEU	3.1
3	K	1248	PRO	3.0
3	C	1316	LEU	2.8
2	J	506	GLU	2.8
3	C	1318	VAL	2.8
1	I	60	ARG	2.7
3	C	1317	CYS	2.7
3	C	717	GLY	2.6
3	K	1290	THR	2.6

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Mol	Chain	Res	Type	RSRZ
2	J	528	GLY	2.6
3	C	1320	GLY	2.5
3	K	1320	GLY	2.5
3	K	1292	GLU	2.5
2	B	336	TRP	2.4
3	C	1324	ASN	2.2
2	B	429	ASP	2.2
3	C	1102	GLU	2.2
1	I	159	GLY	2.1
3	K	992	CYS	2.1
1	A	63	ASP	2.1
1	A	62	GLN	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	CA	C	1	1/1	0.84	0.15	49,49,49,49	0
9	290	C	1335	11/11	0.84	0.14	30,31,32,32	0
9	290	K	1335	11/11	0.93	0.09	19,21,22,23	0
5	FAD	J	606	53/53	0.95	0.07	19,25,30,37	0
7	MTE	K	1333	24/24	0.96	0.07	27,29,32,35	0
8	MOS	K	1334	4/4	0.96	0.18	40,44,45,46	0
5	FAD	B	606	53/53	0.96	0.06	13,22,25,27	0
7	MTE	C	1333	24/24	0.96	0.06	20,24,29,32	0
8	MOS	C	1334	4/4	0.98	0.16	42,45,48,49	0
4	FES	A	601	4/4	0.99	0.03	13,16,18,18	0
4	FES	A	602	4/4	0.99	0.03	13,14,16,18	0

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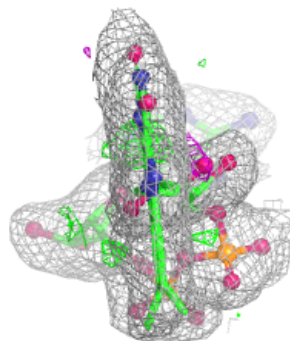
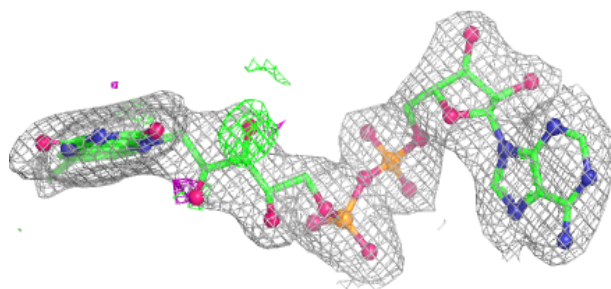
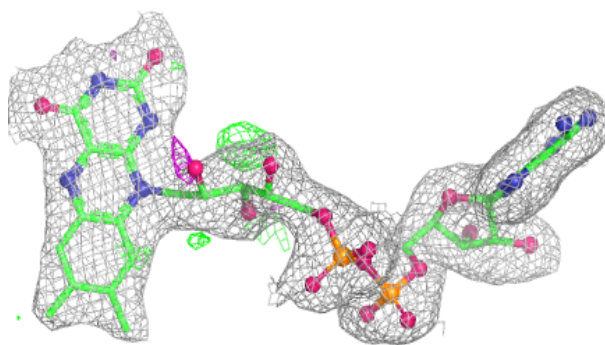
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	FES	I	601	4/4	0.99	0.03	19,19,20,21	0
4	FES	I	602	4/4	1.00	0.03	19,19,19,20	0

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.

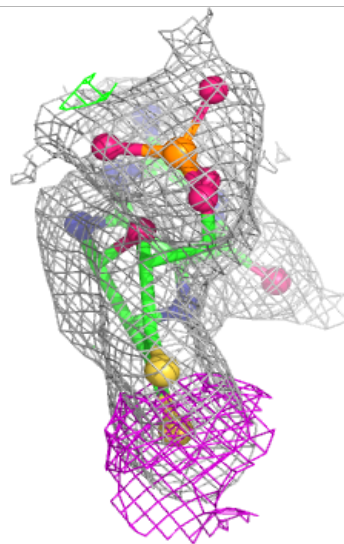
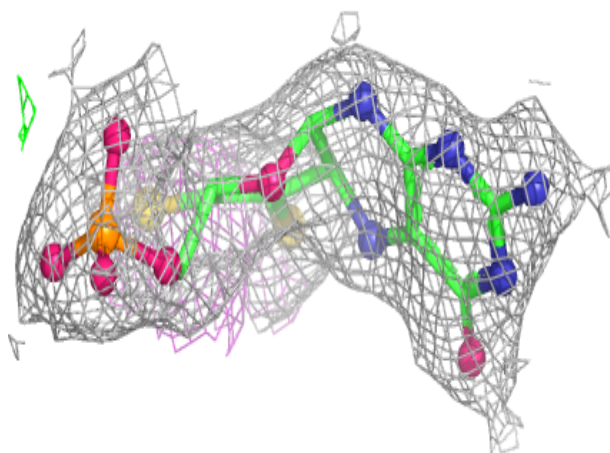
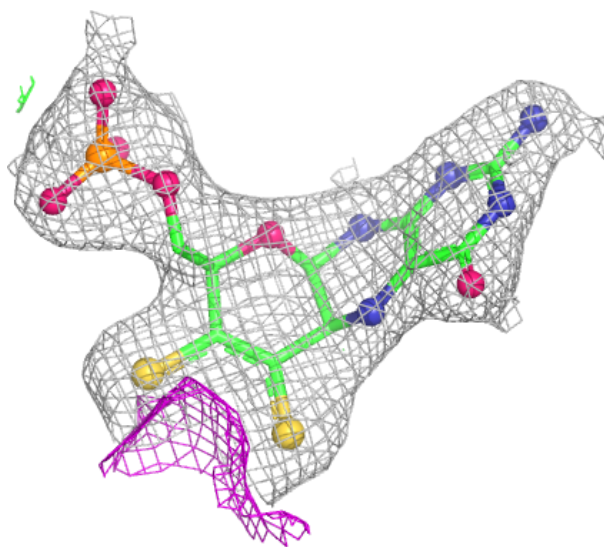
Electron density around FAD J 606:

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



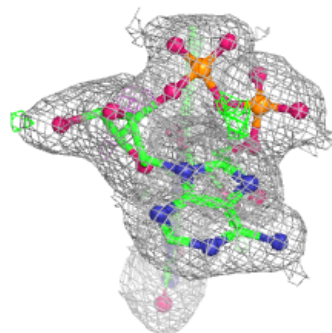
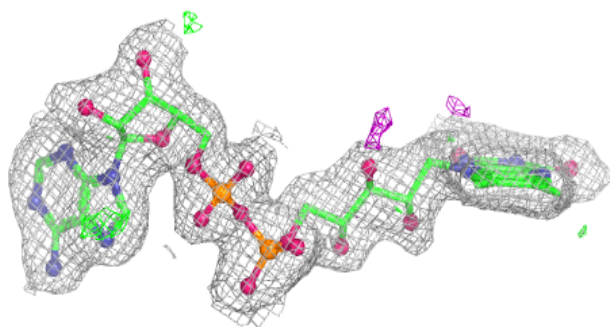
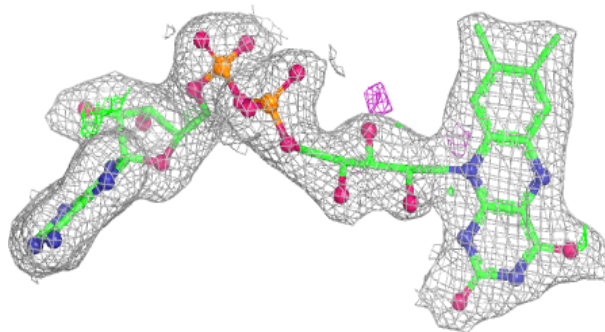
Electron density around MTE K 1333:

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



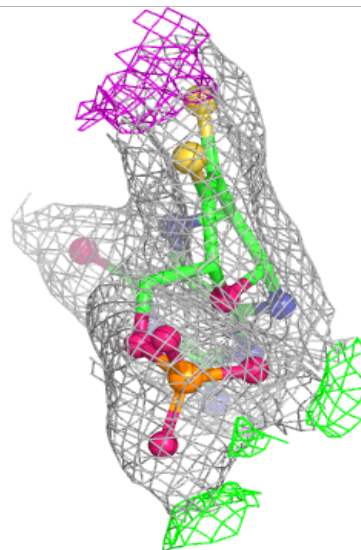
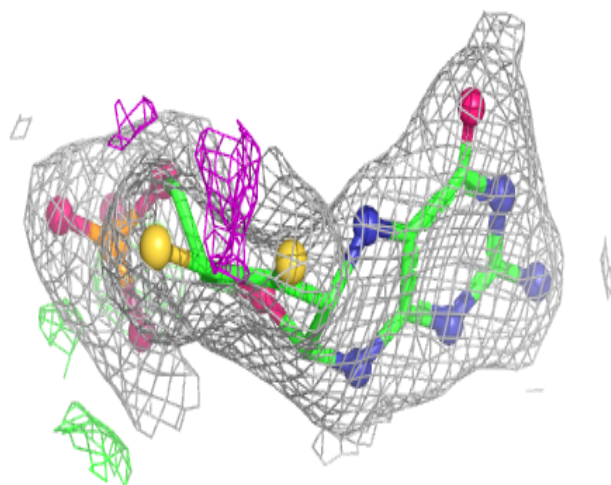
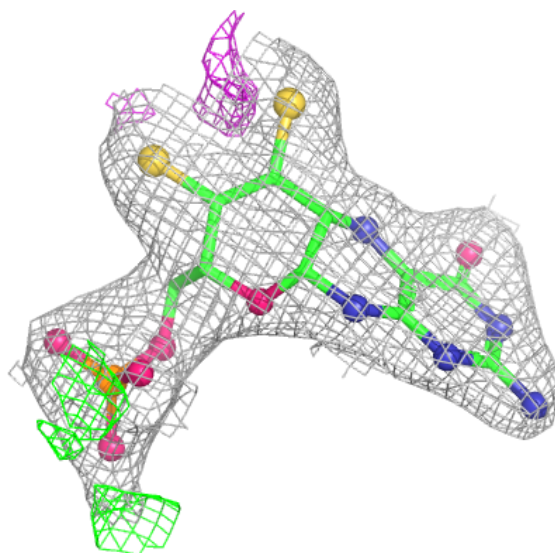
Electron density around FAD B 606:

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



Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.