Full wwPDB X-ray Structure Validation Report (i)

Mar 8, 2026 – 03:28 PM UTC

PDB ID	:	3EUB / pdb_00003eub
Title	:	Crystal Structure of Desulfo-Xanthine Oxidase with Xanthine
Authors	:	Pauff, J.M.; Cao, H.; Hille, R.
Deposited on	:	2008-10-09
Resolution	:	2.60 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
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:

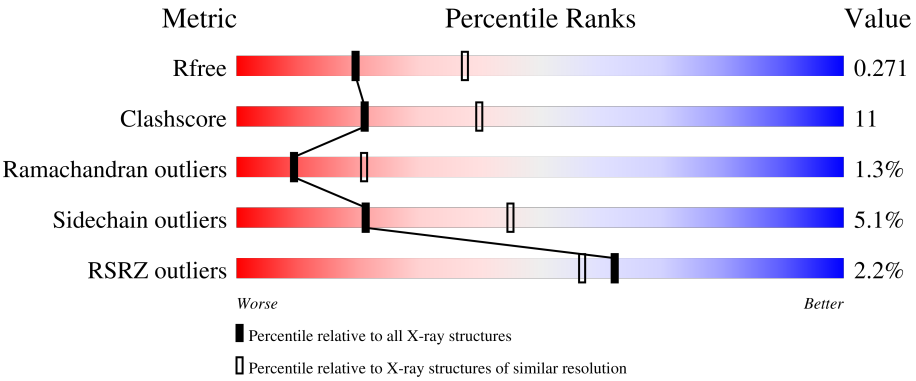
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

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

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	2	165	5% 79% 16%
1	A	165	5% 78% 18%
1	J	165	% 79% 16%
1	S	165	3% 79% 14%
2	3	305	2% 77% 19%

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Mol	Chain	Length	Quality of chain
2	B	305	3% 76% 20%
2	K	305	2% 77% 20%
2	T	305	3% 81% 16%
3	4	762	2% 76% 20%
3	C	762	2% 74% 22%
3	L	762	% 73% 23%
3	U	762	% 75% 20%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	MOM	4	1334	-	-	X	-
7	MOM	C	1334	-	-	X	-
7	MOM	L	1334	-	-	X	-
7	MOM	U	1334	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 38070 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	0	0	0
			1243	781	223	227	12			
1	J	162	Total	C	N	O	S	0	0	0
			1243	781	223	227	12			
1	S	161	Total	C	N	O	S	0	0	0
			1234	775	221	226	12			
1	2	164	Total	C	N	O	S	0	0	0
			1255	788	225	230	12			

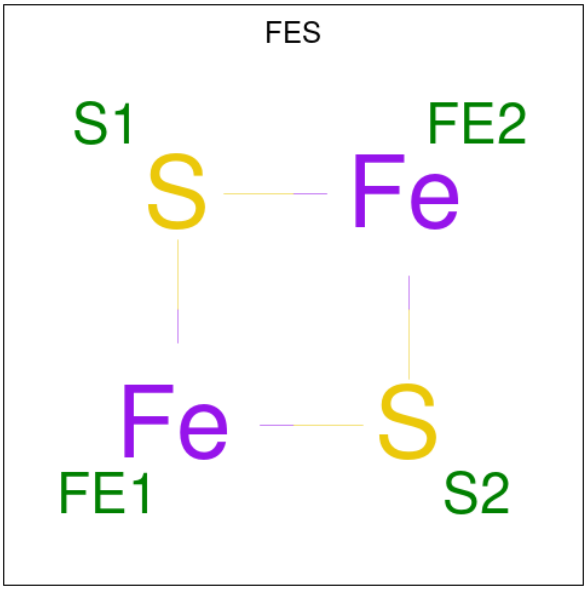
- Molecule 2 is a protein called Xanthine dehydrogenase/oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	304	Total	C	N	O	S	0	0	0
			2385	1537	401	434	13			
2	K	302	Total	C	N	O	S	0	0	0
			2369	1526	398	432	13			
2	T	305	Total	C	N	O	S	0	0	0
			2389	1539	402	435	13			
2	3	305	Total	C	N	O	S	0	0	0
			2389	1539	402	435	13			

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

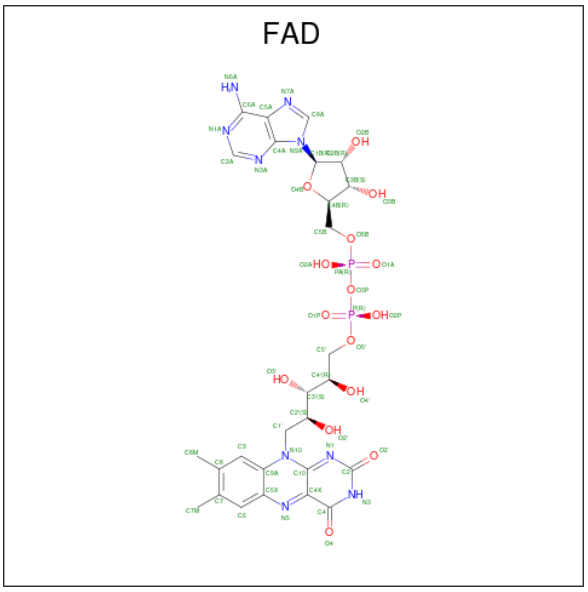
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	753	Total	C	N	O	S	0	0	0
			5809	3673	1001	1101	34			
3	L	745	Total	C	N	O	S	0	0	0
			5761	3643	992	1093	33			
3	U	745	Total	C	N	O	S	0	0	0
			5761	3643	992	1093	33			
3	4	756	Total	C	N	O	S	0	0	0
			5832	3686	1005	1106	35			

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



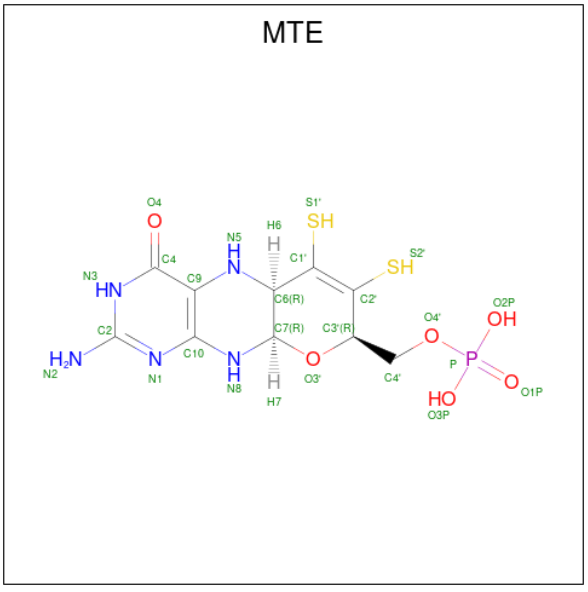
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Fe S 4 2 2	0	0
4	A	1	Total Fe S 4 2 2	0	0
4	J	1	Total Fe S 4 2 2	0	0
4	J	1	Total Fe S 4 2 2	0	0
4	S	1	Total Fe S 4 2 2	0	0
4	S	1	Total Fe S 4 2 2	0	0
4	2	1	Total Fe S 4 2 2	0	0
4	2	1	Total Fe S 4 2 2	0	0

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



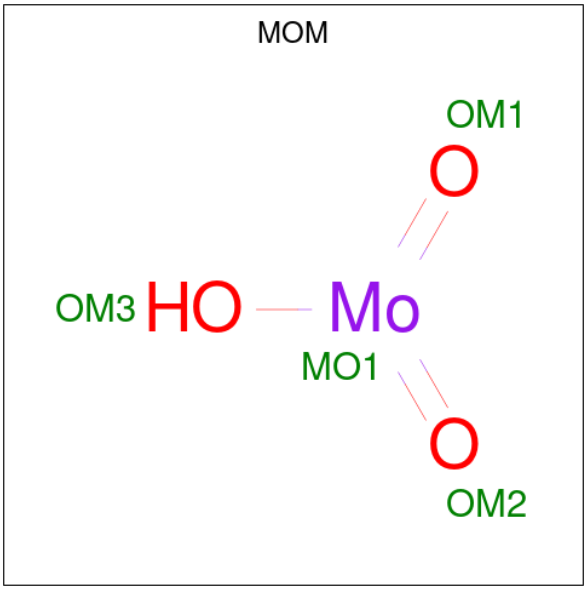
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	K	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	T	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	3	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 6 is PHOSPHONIC ACIDMONO-(2-AMINO-5,6-DIMERCAPTO-4-OXO-3,7,8A, 9,10,10A-HEXAHYDRO-4H-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-7-YLMETHYL) ESTER (CCD ID: MTE) (formula: $C_{10}H_{14}N_5O_6PS_2$).



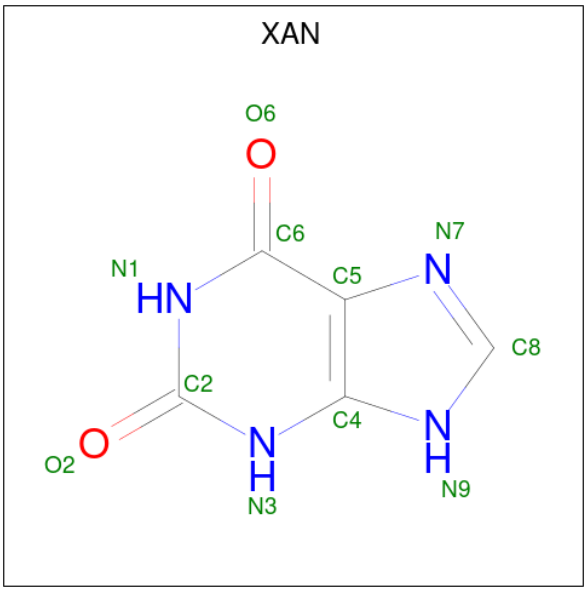
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	C	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
6	L	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
6	U	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
6	4	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		

- Molecule 7 is HYDROXY(DIOXO)MOLYBDENUM (CCD ID: MOM) (formula: $HMoO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	Mo	O		0	0
			4	1	3			
7	L	1	Total	Mo	O		0	0
			4	1	3			
7	U	1	Total	Mo	O		0	0
			4	1	3			
7	4	1	Total	Mo	O		0	0
			4	1	3			

- Molecule 8 is XANTHINE (CCD ID: XAN) (formula: $C_5H_4N_4O_2$).



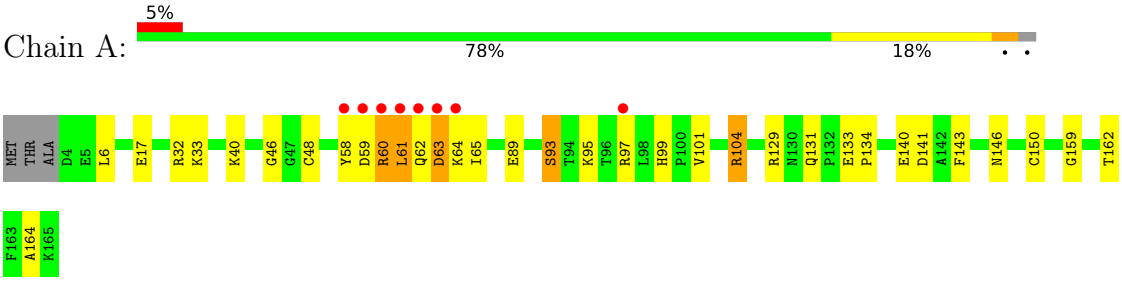
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total C N O 11 5 4 2	0	0
8	L	1	Total C N O 11 5 4 2	0	0
8	U	1	Total C N O 11 5 4 2	0	0
8	4	1	Total C N O 11 5 4 2	0	0

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.

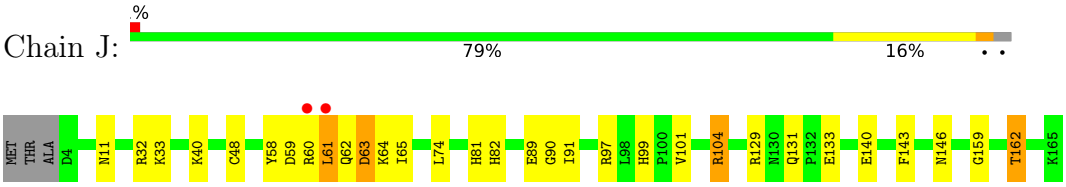
• Molecule 1: Xanthine dehydrogenase/oxidase

Chain A:



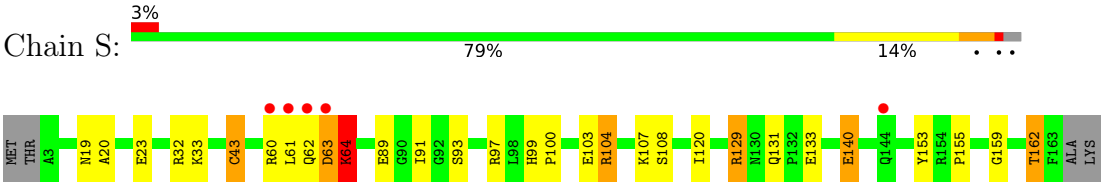
• Molecule 1: Xanthine dehydrogenase/oxidase

Chain J:



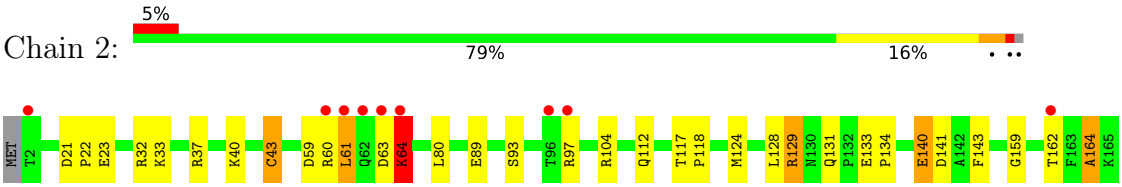
• Molecule 1: Xanthine dehydrogenase/oxidase

Chain S:



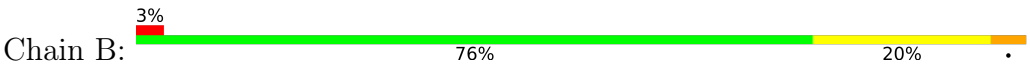
• Molecule 1: Xanthine dehydrogenase/oxidase

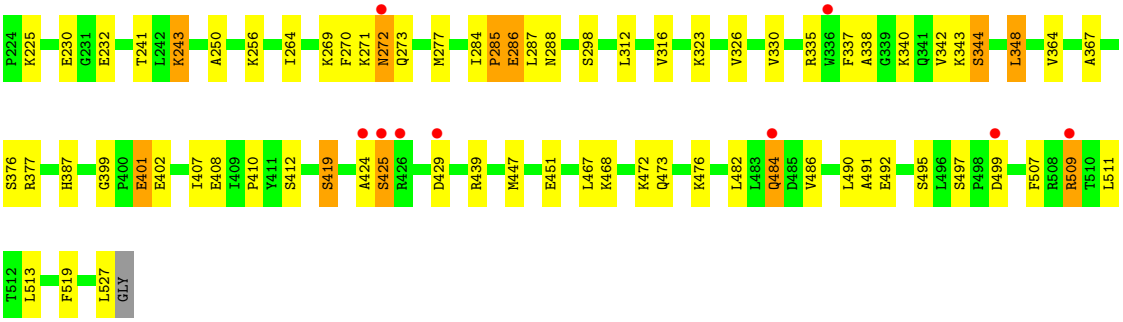
Chain 2:



• Molecule 2: Xanthine dehydrogenase/oxidase

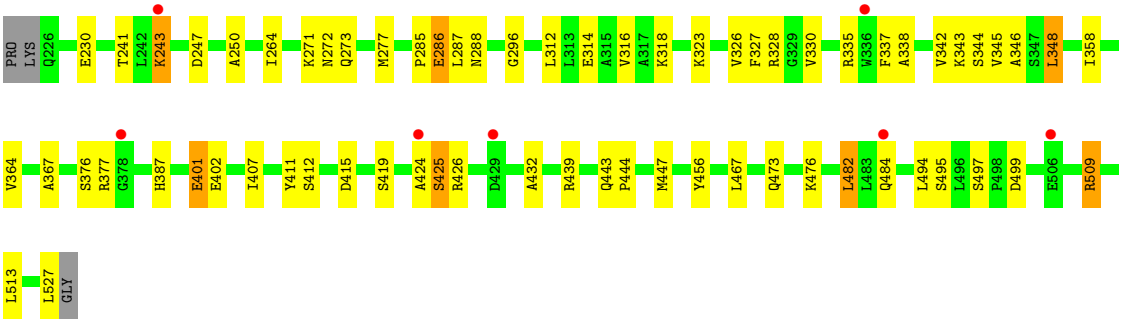
Chain B:





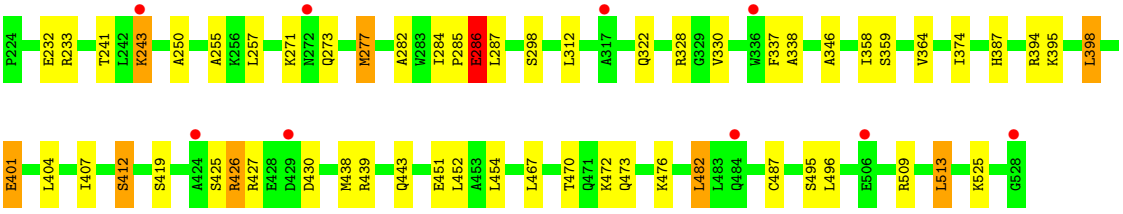
• Molecule 2: Xanthine dehydrogenase/oxidase

Chain K:



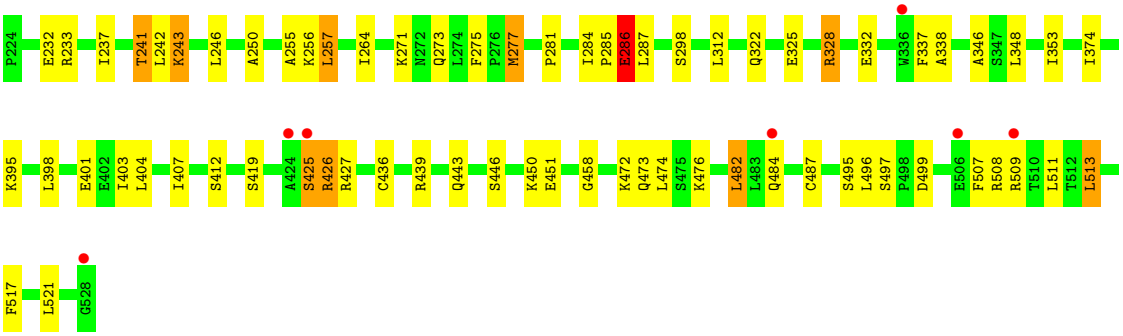
• Molecule 2: Xanthine dehydrogenase/oxidase

Chain T:



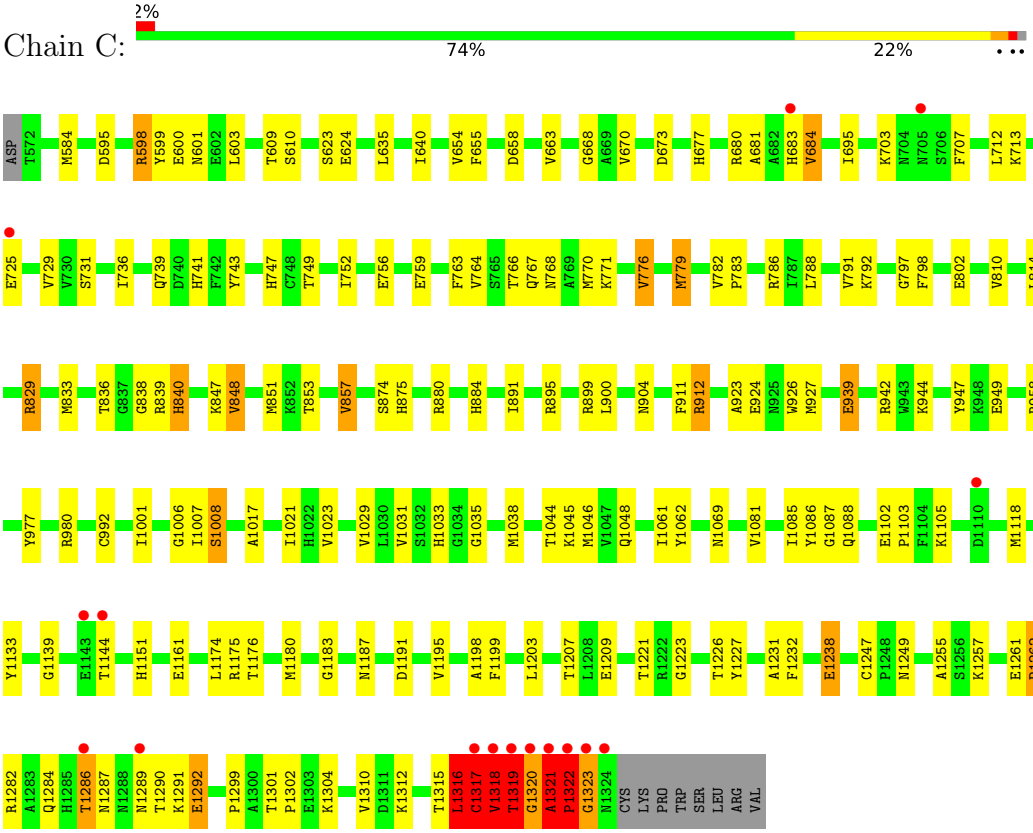
• Molecule 2: Xanthine dehydrogenase/oxidase

Chain 3:



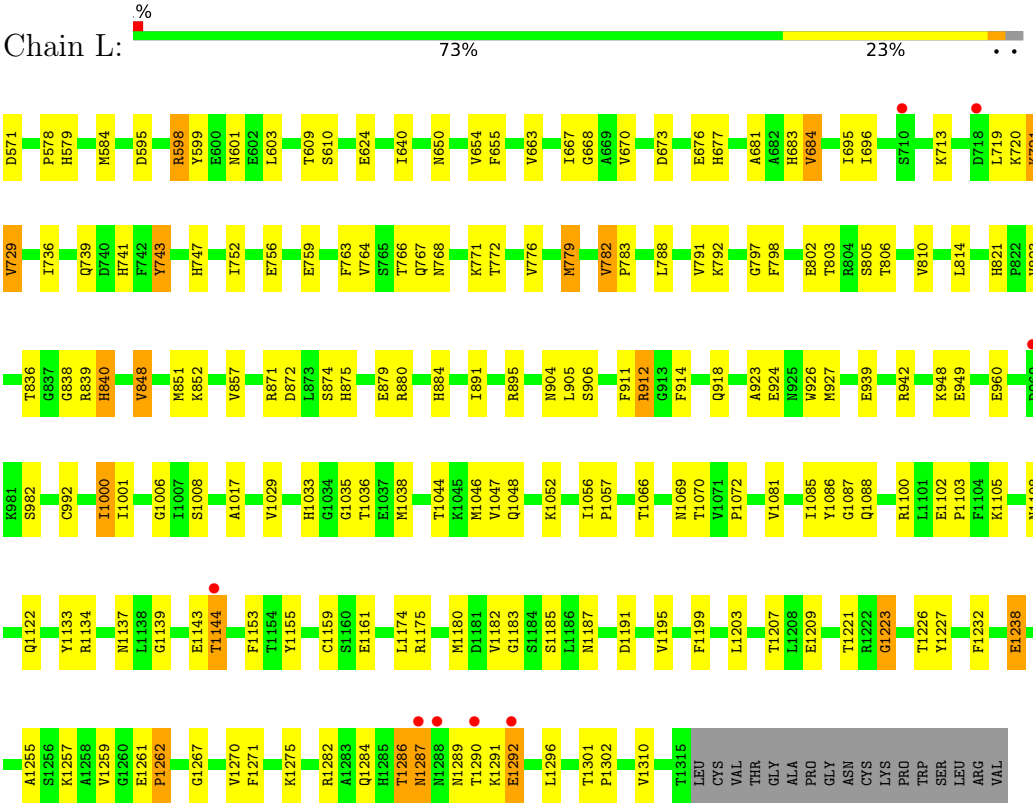
• Molecule 3: Xanthine dehydrogenase/oxidase

Chain C:



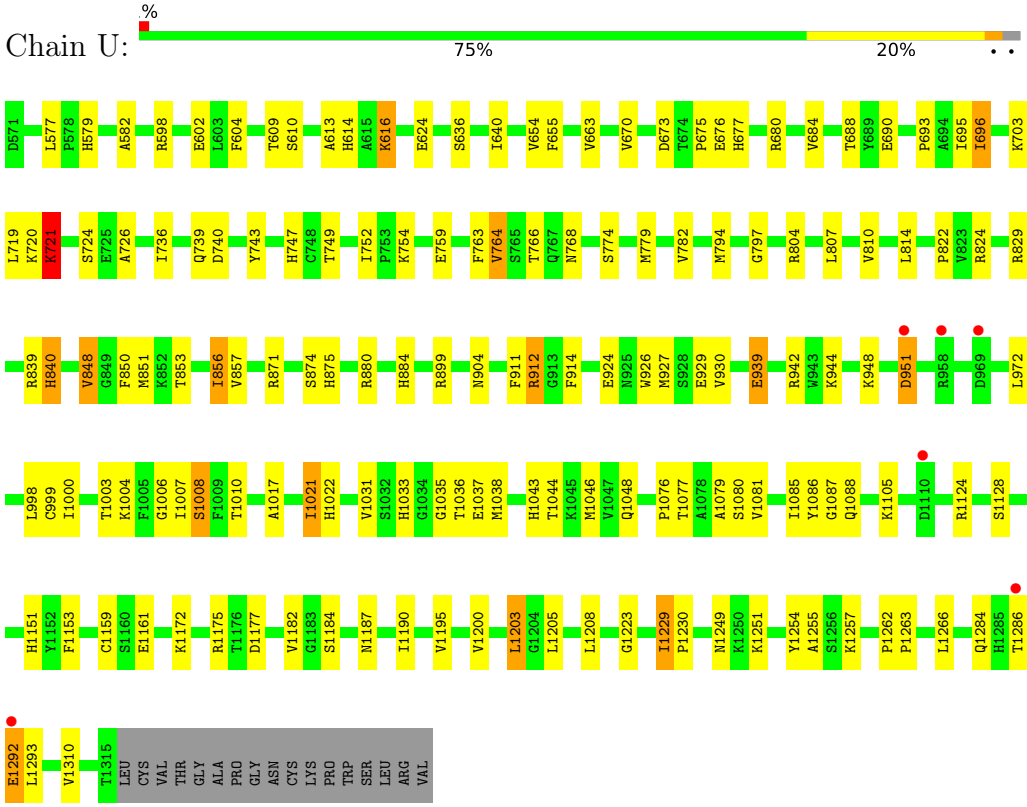
• Molecule 3: Xanthine dehydrogenase/oxidase

Chain L:



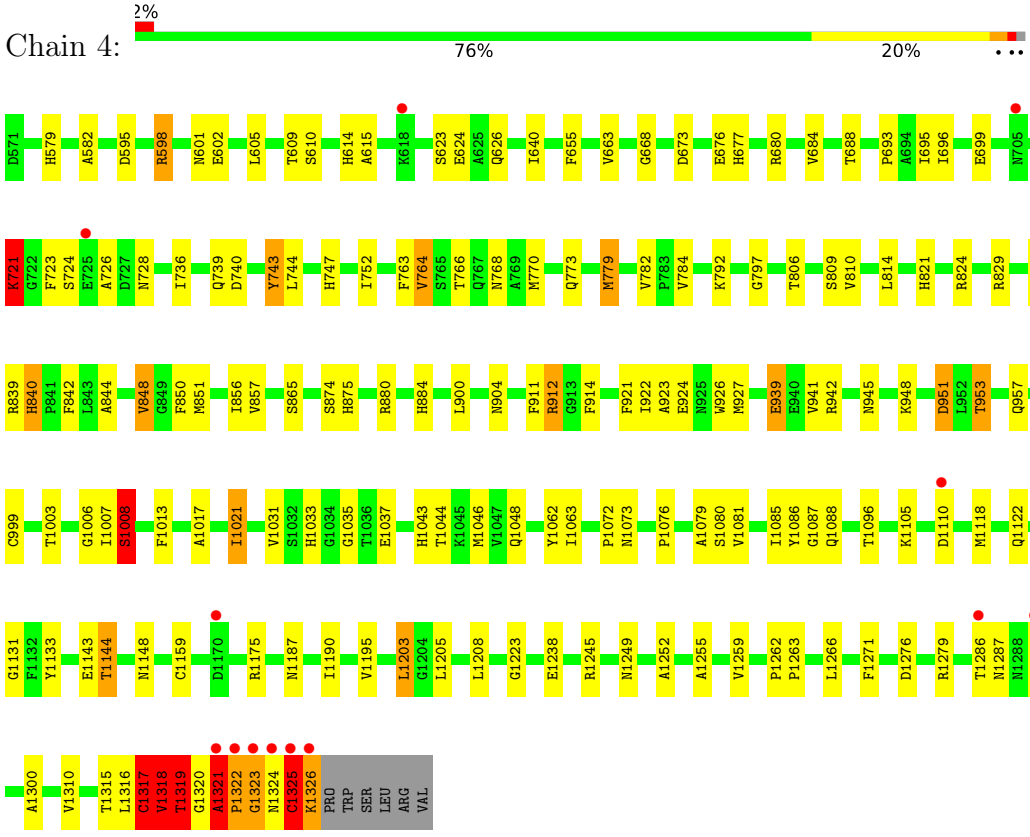
• Molecule 3: Xanthine dehydrogenase/oxidase

Chain U:



• Molecule 3: Xanthine dehydrogenase/oxidase

Chain 4:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	73.30Å 133.18Å 142.63Å 96.88° 93.11° 90.02°	Depositor
Resolution (Å)	33.08 – 2.60 33.08 – 2.60	Depositor EDS
% Data completeness (in resolution range)	72.7 (33.08-2.60) 72.7 (33.08-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.03 (at 2.61Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.214 , 0.268 0.218 , 0.271	Depositor DCC
R_{free} test set	6008 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	19.7	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 25.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	38070	wwPDB-VP
Average B, all atoms (Å^2)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.64% 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: MOM, FES, MTE, XAN, 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	2	0.93	1/1277 (0.1%)	1.04	1/1723 (0.1%)
1	A	0.93	0/1265	1.04	1/1706 (0.1%)
1	J	0.89	0/1265	1.00	0/1706
1	S	0.88	0/1256	1.01	0/1695
2	3	0.85	0/2438	1.03	2/3290 (0.1%)
2	B	0.88	0/2434	1.05	4/3285 (0.1%)
2	K	0.85	1/2417 (0.0%)	1.01	2/3263 (0.1%)
2	T	0.85	0/2438	1.04	1/3290 (0.0%)
3	4	0.94	1/5960 (0.0%)	1.09	17/8072 (0.2%)
3	C	0.92	2/5937 (0.0%)	1.11	20/8042 (0.2%)
3	L	0.92	2/5888 (0.0%)	1.09	17/7974 (0.2%)
3	U	0.91	0/5888	1.08	11/7974 (0.1%)
All	All	0.91	7/38463 (0.0%)	1.07	76/52020 (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
2	B	0	1
3	4	0	4
3	C	0	2
All	All	0	7

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	112	GLN	CA-C	6.72	1.56	1.52
3	C	1319	THR	CA-CB	6.58	1.64	1.53
3	4	1144	THR	CA-CB	6.01	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1322	PRO	N-CA	5.86	1.54	1.47
3	L	1144	THR	CA-CB	5.32	1.62	1.53
3	L	1070	THR	CA-CB	5.20	1.62	1.53
2	K	345	VAL	CA-CB	5.14	1.61	1.55

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1315	THR	CA-C-N	-9.52	104.66	122.27
3	C	1315	THR	C-N-CA	-9.52	104.66	122.27
3	C	1317	CYS	CA-C-N	9.18	138.22	121.70
3	C	1317	CYS	C-N-CA	9.18	138.22	121.70
3	4	1323	GLY	N-CA-C	-8.46	93.13	113.18
3	L	654	VAL	N-CA-C	-8.24	102.82	110.82
3	U	1262	PRO	N-CA-C	8.17	120.67	110.70
2	K	286	GLU	N-CA-C	-7.85	94.07	110.80
3	C	1318	VAL	N-CA-C	-7.80	89.17	111.00
3	4	1262	PRO	N-CA-C	7.47	119.81	110.70
2	B	286	GLU	N-CA-C	-7.42	94.99	110.80
3	C	1315	THR	O-C-N	-6.53	115.63	122.94
3	C	776	VAL	N-CA-C	-6.49	104.43	110.53
3	L	667	ILE	N-CA-C	-6.29	106.67	112.96
3	4	840	HIS	CA-C-N	-6.29	113.30	119.78
3	4	840	HIS	C-N-CA	-6.29	113.30	119.78
2	T	286	GLU	N-CA-C	-6.26	97.47	110.80
2	B	399	GLY	N-CA-C	-6.25	104.41	112.10
3	L	650	ASN	N-CA-C	6.15	120.10	112.47
3	4	1318	VAL	CA-C-N	6.09	132.66	121.70
3	4	1318	VAL	C-N-CA	6.09	132.66	121.70
3	4	1317	CYS	N-CA-CB	6.06	120.73	110.49
3	L	840	HIS	CA-C-N	-6.05	113.53	119.76
3	L	840	HIS	C-N-CA	-6.05	113.53	119.76
3	L	1137	ASN	N-CA-C	5.99	119.66	111.39
3	C	1319	THR	CB-CA-C	5.93	122.23	110.42
2	3	286	GLU	N-CA-C	-5.92	98.18	110.80
2	B	272	ASN	N-CA-C	5.78	119.54	111.74
3	U	840	HIS	CA-C-N	-5.77	113.84	119.78
3	U	840	HIS	C-N-CA	-5.77	113.84	119.78
3	U	577	LEU	CA-C-N	-5.59	114.49	120.03
3	U	577	LEU	C-N-CA	-5.59	114.49	120.03
3	4	1252	ALA	N-CA-C	5.58	118.17	109.52
3	U	696	ILE	N-CA-C	5.55	116.34	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	891	ILE	CA-C-N	5.54	125.38	119.28
3	C	891	ILE	C-N-CA	5.54	125.38	119.28
2	K	432	ALA	N-CA-C	5.54	119.33	112.24
3	L	791	VAL	CB-CA-C	-5.53	104.95	111.09
3	4	1021	ILE	N-CA-C	5.52	115.90	108.17
3	U	654	VAL	N-CA-C	-5.51	105.48	110.82
1	A	64	LYS	N-CA-C	5.50	117.64	110.43
3	4	1262	PRO	CA-C-N	-5.49	114.35	120.45
3	4	1262	PRO	C-N-CA	-5.49	114.35	120.45
3	C	1316	LEU	N-CA-C	5.39	119.57	111.81
3	C	1321	ALA	N-CA-C	5.39	121.71	109.81
3	C	857	VAL	CB-CA-C	5.38	116.18	110.91
3	L	1223	GLY	CA-C-N	5.35	125.17	119.28
3	L	1223	GLY	C-N-CA	5.35	125.17	119.28
3	L	722	GLY	N-CA-C	-5.31	106.06	112.49
3	L	1262	PRO	N-CA-C	5.26	117.12	110.70
3	L	782	VAL	CA-C-N	-5.26	114.36	119.78
3	L	782	VAL	C-N-CA	-5.26	114.36	119.78
3	4	1317	CYS	CB-CA-C	5.26	120.89	110.42
3	4	1131	GLY	N-CA-C	-5.25	103.10	111.18
2	3	436	CYS	N-CA-C	5.24	117.16	109.24
3	U	1010	THR	CA-C-N	-5.22	119.05	122.60
3	U	1010	THR	C-N-CA	-5.22	119.05	122.60
3	C	1262	PRO	N-CA-C	5.22	117.07	110.70
3	4	1318	VAL	CA-C-O	-5.17	114.31	120.78
3	4	1148	ASN	N-CA-C	5.16	117.79	110.10
3	C	654	VAL	N-CA-C	-5.13	105.70	110.53
3	L	891	ILE	CA-C-N	5.12	124.73	119.05
3	L	891	ILE	C-N-CA	5.12	124.73	119.05
3	C	840	HIS	CA-C-N	-5.11	114.51	119.78
3	C	840	HIS	C-N-CA	-5.11	114.51	119.78
2	B	429	ASP	N-CA-C	5.10	117.24	111.02
3	4	1319	THR	N-CA-C	5.10	125.27	111.00
3	C	791	VAL	CB-CA-C	-5.09	102.94	111.29
3	L	1029	VAL	N-CA-C	5.07	115.21	108.11
3	4	615	ALA	N-CA-C	5.07	116.23	108.42
1	2	64	LYS	N-CA-C	5.07	121.60	110.80
3	C	1151	HIS	N-CA-C	-5.06	106.27	112.90
3	U	1229	ILE	CA-C-N	-5.05	114.75	119.90
3	U	1229	ILE	C-N-CA	-5.05	114.75	119.90
3	C	658	ASP	N-CA-C	-5.04	107.20	113.55
3	L	1144	THR	N-CA-CB	5.04	119.00	110.49

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	4	1317	CYS	Peptide
3	4	1318	VAL	Peptide
3	4	1321	ALA	Peptide
3	4	1322	PRO	Peptide
2	B	285	PRO	Peptide
3	C	1317	CYS	Peptide
3	C	1318	VAL	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	2	1255	0	1265	25	0
1	A	1243	0	1253	19	0
1	J	1243	0	1253	21	0
1	S	1234	0	1240	22	0
2	3	2389	0	2459	47	0
2	B	2385	0	2456	50	0
2	K	2369	0	2435	45	0
2	T	2389	0	2459	35	0
3	4	5832	0	5759	175	0
3	C	5809	0	5737	166	0
3	L	5761	0	5685	138	0
3	U	5761	0	5685	138	0
4	2	8	0	0	0	0
4	A	8	0	0	2	0
4	J	8	0	0	0	0
4	S	8	0	0	0	0
5	3	53	0	31	2	0
5	B	53	0	31	1	0
5	K	53	0	31	3	0
5	T	53	0	31	2	0
6	4	24	0	10	0	0
6	C	24	0	10	0	0
6	L	24	0	10	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	U	24	0	10	0	0
7	4	4	0	0	2	0
7	C	4	0	0	2	0
7	L	4	0	0	2	0
7	U	4	0	0	3	0
8	4	11	0	4	1	0
8	C	11	0	4	1	0
8	L	11	0	4	1	0
8	U	11	0	4	2	0
All	All	38070	0	37866	834	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 11.

All (834) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:1318:VAL:HG13	3:4:1319:THR:CG2	1.55	1.34
3:C:1316:LEU:O	3:C:1318:VAL:HB	1.41	1.20
3:L:924:GLU:OE1	3:L:942:ARG:NH1	1.78	1.14
3:L:1046:MET:HE1	3:L:1087:GLY:HA2	1.17	1.12
2:K:241:THR:HG22	2:K:243:LYS:HE2	1.28	1.11
1:S:129:ARG:HG3	1:S:129:ARG:HH11	0.98	1.11
1:S:129:ARG:HH11	1:S:129:ARG:CG	1.64	1.11
3:C:1046:MET:HE1	3:C:1087:GLY:HA2	1.33	1.10
3:4:1318:VAL:HG13	3:4:1319:THR:HG22	1.28	1.08
3:4:1318:VAL:HG13	3:4:1319:THR:HG23	1.28	1.06
3:C:1317:CYS:HB3	3:C:1318:VAL:HG23	1.35	1.06
1:2:129:ARG:HH11	1:2:129:ARG:CG	1.69	1.05
3:4:924:GLU:OE1	3:4:942:ARG:NH1	1.89	1.04
3:4:1046:MET:HE1	3:4:1087:GLY:HA2	1.35	1.04
3:L:1100:ARG:HG2	3:4:1110:ASP:OD2	1.58	1.04
3:U:924:GLU:OE1	3:U:942:ARG:NH1	1.89	1.03
3:C:924:GLU:OE1	3:C:942:ARG:NH1	1.91	1.02
2:K:241:THR:CG2	2:K:243:LYS:HE2	1.89	1.01
3:U:1046:MET:HE1	3:U:1087:GLY:HA2	1.38	1.01
1:2:129:ARG:HH11	1:2:129:ARG:HG3	0.88	1.01
3:4:1318:VAL:CG1	3:4:1319:THR:HG22	1.90	1.00
2:B:241:THR:CG2	2:B:243:LYS:HE2	1.92	0.99
3:4:764:VAL:HG23	3:4:766:THR:HG22	1.44	0.97
2:B:241:THR:HG22	2:B:243:LYS:HE2	1.46	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:856:ILE:HD13	3:4:927:MET:HE1	1.47	0.96
3:U:726:ALA:HA	3:U:851:MET:HE1	1.48	0.96
3:4:1318:VAL:CG1	3:4:1319:THR:CG2	2.42	0.96
3:C:1286:THR:HG22	3:C:1310:VAL:O	1.68	0.93
3:4:726:ALA:HA	3:4:851:MET:HE1	1.52	0.92
7:U:1334:MOM:OM1	8:U:7319:XAN:H8	1.70	0.92
1:2:129:ARG:HG3	1:2:129:ARG:NH1	1.69	0.91
3:U:720:LYS:O	3:U:721:LYS:HB3	1.70	0.90
3:4:764:VAL:CG2	3:4:766:THR:HG22	2.03	0.89
3:L:1046:MET:HE1	3:L:1087:GLY:CA	2.01	0.89
2:B:495:SER:HB2	2:B:509:ARG:HH22	1.38	0.89
3:L:764:VAL:HG23	3:L:766:THR:HG22	1.54	0.89
1:S:129:ARG:HG3	1:S:129:ARG:NH1	1.81	0.89
2:B:484:GLN:HE22	3:C:1318:VAL:HG22	1.35	0.88
2:T:286:GLU:O	2:T:287:LEU:HB2	1.73	0.88
3:4:1317:CYS:HB2	3:4:1321:ALA:HA	1.56	0.87
7:4:1334:MOM:OM1	8:4:7319:XAN:H8	1.73	0.87
3:U:1046:MET:HE1	3:U:1087:GLY:CA	2.04	0.87
3:4:720:LYS:O	3:4:721:LYS:HB3	1.71	0.86
3:C:764:VAL:HG23	3:C:766:THR:HG22	1.55	0.85
3:C:1048:GLN:HE22	3:C:1187:ASN:HD22	1.21	0.85
3:C:1088:GLN:HG2	3:C:1133:TYR:CD1	2.12	0.85
3:C:1046:MET:HE1	3:C:1087:GLY:CA	2.07	0.85
2:B:424:ALA:O	2:B:425:SER:HB3	1.75	0.84
1:2:129:ARG:CG	1:2:129:ARG:NH1	2.35	0.84
2:T:495:SER:HB2	2:T:509:ARG:HH22	1.41	0.84
2:K:495:SER:HB2	2:K:509:ARG:HH22	1.43	0.83
3:U:726:ALA:HA	3:U:851:MET:CE	2.09	0.82
3:L:851:MET:HE2	3:L:857:VAL:HG21	1.59	0.82
3:C:958:ARG:NH2	3:U:711:GLU:HB3	1.95	0.82
3:4:779:MET:HG2	3:4:810:VAL:HG13	1.62	0.82
3:4:880:ARG:O	3:4:884:HIS:HD2	1.63	0.82
3:4:1320:GLY:O	3:4:1321:ALA:O	1.98	0.82
3:4:829:ARG:HG3	3:4:833:MET:HE2	1.62	0.81
2:K:424:ALA:O	2:K:425:SER:HB3	1.79	0.81
7:C:1334:MOM:OM1	8:C:7319:XAN:H8	1.81	0.81
3:C:829:ARG:HG3	3:C:833:MET:HE2	1.63	0.80
3:C:1048:GLN:NE2	3:C:1187:ASN:HD22	1.78	0.80
3:4:1325:CYS:SG	3:4:1326:LYS:N	2.52	0.80
3:U:851:MET:HE3	3:U:857:VAL:HG21	1.65	0.79
3:C:739:GLN:OE1	3:C:839:ARG:NH1	2.15	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:1046:MET:HE1	3:4:1087:GLY:CA	2.13	0.79
2:T:496:LEU:H	2:T:509:ARG:NH2	1.81	0.79
3:U:695:ILE:H	3:U:904:ASN:HD22	1.27	0.79
3:L:720:LYS:O	3:L:721:LYS:HB2	1.80	0.79
3:U:1048:GLN:HE22	3:U:1187:ASN:HD22	1.30	0.79
1:S:129:ARG:CG	1:S:129:ARG:NH1	2.33	0.79
3:C:747:HIS:CD2	3:C:836:THR:HG21	2.17	0.78
7:L:1334:MOM:OM1	8:L:7319:XAN:H8	1.84	0.77
3:U:720:LYS:O	3:U:721:LYS:CB	2.32	0.77
3:L:739:GLN:OE1	3:L:839:ARG:NH1	2.16	0.77
3:C:851:MET:HE2	3:C:857:VAL:HG21	1.65	0.77
1:2:159:GLY:O	1:2:162:THR:HG22	1.84	0.77
3:4:695:ILE:H	3:4:904:ASN:HD22	1.33	0.77
3:C:720:LYS:O	3:C:721:LYS:HB2	1.85	0.76
3:U:739:GLN:OE1	3:U:839:ARG:NH1	2.18	0.76
3:4:764:VAL:HG23	3:4:766:THR:CG2	2.16	0.76
3:C:884:HIS:HE1	3:C:1006:GLY:H	1.32	0.76
3:L:1286:THR:HG22	3:L:1310:VAL:O	1.85	0.76
3:4:739:GLN:OE1	3:4:839:ARG:NH1	2.18	0.76
3:U:1287:ASN:HD22	3:U:1289:ASN:H	1.33	0.76
2:K:447:MET:HG2	2:K:527:LEU:HD13	1.69	0.75
3:4:764:VAL:CG2	3:4:766:THR:CG2	2.64	0.75
1:A:159:GLY:O	1:A:162:THR:HG22	1.87	0.75
3:C:840:HIS:HE1	3:C:874:SER:OG	1.70	0.75
3:L:1046:MET:CE	3:L:1087:GLY:HA2	2.09	0.74
3:4:624:GLU:HB2	3:4:684:VAL:CG1	2.17	0.74
3:L:1088:GLN:HG2	3:L:1133:TYR:CD1	2.22	0.74
2:T:241:THR:HG22	2:T:243:LYS:HE2	1.68	0.74
2:3:496:LEU:H	2:3:509:ARG:NH2	1.86	0.74
3:C:958:ARG:HH22	3:U:711:GLU:HB3	1.52	0.74
1:2:32:ARG:NH1	3:4:676:GLU:OE2	2.21	0.73
3:4:726:ALA:HA	3:4:851:MET:CE	2.18	0.73
3:U:624:GLU:HB2	3:U:684:VAL:HG12	1.70	0.72
1:S:61:LEU:C	1:S:63:ASP:H	1.97	0.72
3:L:884:HIS:HE1	3:L:1006:GLY:H	1.38	0.72
3:4:1317:CYS:CB	3:4:1321:ALA:HA	2.20	0.72
3:L:848:VAL:HG21	3:L:926:TRP:HB2	1.72	0.72
3:4:747:HIS:CD2	3:4:836:THR:HG21	2.23	0.72
3:4:720:LYS:O	3:4:721:LYS:CB	2.38	0.72
3:L:1301:THR:HB	3:L:1302:PRO:HD2	1.71	0.71
3:U:624:GLU:HB2	3:U:684:VAL:CG1	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1318:VAL:H	3:C:1319:THR:HA	1.56	0.71
3:4:1286:THR:C	3:4:1326:LYS:O	2.33	0.71
3:C:764:VAL:CG2	3:C:766:THR:HG22	2.21	0.71
2:3:404:LEU:HD21	2:3:407:ILE:HD11	1.73	0.71
3:C:1175:ARG:HG3	3:C:1238:GLU:HB3	1.71	0.71
2:3:495:SER:HB2	2:3:509:ARG:HH22	1.54	0.71
3:C:1033:HIS:HD2	3:C:1035:GLY:H	1.37	0.71
1:S:140:GLU:HG3	1:S:140:GLU:O	1.89	0.71
3:4:833:MET:HE1	3:4:1223:GLY:HA2	1.74	0.70
2:T:496:LEU:H	2:T:509:ARG:HH21	1.40	0.70
2:3:241:THR:HG22	2:3:243:LYS:HE2	1.74	0.70
3:4:1316:LEU:O	3:4:1318:VAL:N	2.25	0.70
1:J:131:GLN:HE21	1:J:133:GLU:H	1.38	0.70
3:U:948:LYS:HB2	3:U:951:ASP:OD1	1.92	0.70
1:S:159:GLY:O	1:S:162:THR:HG22	1.92	0.70
3:C:1318:VAL:O	3:C:1320:GLY:N	2.25	0.69
1:S:32:ARG:NH1	3:U:676:GLU:OE2	2.25	0.69
3:C:640:ILE:HG12	3:C:779:MET:HE1	1.75	0.69
3:C:720:LYS:O	3:C:721:LYS:CB	2.38	0.69
3:C:829:ARG:CG	3:C:833:MET:HE2	2.21	0.69
3:L:640:ILE:HG12	3:L:779:MET:HE1	1.74	0.69
1:S:131:GLN:HE21	1:S:133:GLU:H	1.39	0.69
3:4:1318:VAL:CG1	3:4:1319:THR:HG23	2.14	0.69
2:K:241:THR:CG2	2:K:243:LYS:CE	2.70	0.69
2:T:495:SER:HB2	2:T:509:ARG:NH2	2.07	0.69
3:4:1287:ASN:HD22	3:4:1289:ASN:H	1.41	0.69
3:4:624:GLU:HB2	3:4:684:VAL:HG12	1.75	0.69
3:4:884:HIS:HE1	3:4:1006:GLY:H	1.39	0.68
3:C:695:ILE:H	3:C:904:ASN:HD22	1.41	0.68
3:L:673:ASP:OD2	3:L:677:HIS:HD2	1.76	0.68
3:C:1320:GLY:O	3:C:1321:ALA:HB2	1.92	0.68
3:4:1321:ALA:HB1	3:4:1322:PRO:HA	1.74	0.68
3:L:720:LYS:O	3:L:721:LYS:CB	2.41	0.68
2:3:286:GLU:O	2:3:287:LEU:HB2	1.94	0.68
3:4:1037:GLU:HB2	3:4:1043:HIS:CD2	2.29	0.68
2:T:286:GLU:O	2:T:287:LEU:CB	2.42	0.68
3:U:768:ASN:ND2	3:U:1076:PRO:HG3	2.09	0.67
3:C:1118:MET:O	3:C:1122:GLN:HG2	1.94	0.67
3:C:848:VAL:HG21	3:C:926:TRP:HB2	1.74	0.67
3:U:602:GLU:OE2	3:U:824:ARG:NE	2.22	0.67
3:C:884:HIS:CE1	3:C:1006:GLY:H	2.13	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:495:SER:HB2	2:B:509:ARG:NH2	2.10	0.67
3:U:747:HIS:CD2	3:U:836:THR:HG21	2.30	0.67
3:C:1249:ASN:O	3:C:1255:ALA:HA	1.95	0.67
1:J:11:ASN:OD1	1:J:90:GLY:HA3	1.95	0.66
2:K:338:ALA:HB1	2:K:342:VAL:HB	1.76	0.66
3:4:1319:THR:OG1	3:4:1320:GLY:N	2.22	0.66
3:U:695:ILE:H	3:U:904:ASN:ND2	1.93	0.66
3:4:839:ARG:NH2	3:4:912:ARG:O	2.29	0.66
3:L:1033:HIS:HD2	3:L:1035:GLY:H	1.42	0.66
1:2:23:GLU:OE1	2:3:233:ARG:NH2	2.26	0.66
3:4:1249:ASN:O	3:4:1255:ALA:HA	1.95	0.66
3:L:1048:GLN:NE2	3:L:1187:ASN:HD22	1.94	0.66
3:U:1048:GLN:NE2	3:U:1187:ASN:HD22	1.93	0.66
2:3:322:GLN:O	2:3:412:SER:HB3	1.96	0.66
2:T:271:LYS:O	2:T:271:LYS:HG3	1.96	0.66
3:U:839:ARG:NH2	3:U:912:ARG:O	2.28	0.66
3:U:779:MET:HG2	3:U:810:VAL:HG13	1.78	0.66
3:U:764:VAL:CG2	3:U:766:THR:HG22	2.26	0.66
3:4:948:LYS:HB2	3:4:951:ASP:OD1	1.96	0.66
2:T:285:PRO:O	2:T:286:GLU:HB2	1.94	0.65
3:4:856:ILE:CD1	3:4:927:MET:HE1	2.24	0.65
3:4:1286:THR:HG22	3:4:1310:VAL:O	1.96	0.65
3:4:1048:GLN:HE22	3:4:1187:ASN:HD22	1.44	0.65
3:4:1317:CYS:HB3	3:4:1323:GLY:O	1.95	0.65
3:L:1175:ARG:HG3	3:L:1238:GLU:HB3	1.77	0.65
3:L:747:HIS:CD2	3:L:836:THR:HG21	2.31	0.65
3:C:1322:PRO:O	3:C:1323:GLY:O	2.15	0.65
2:B:338:ALA:HB1	2:B:342:VAL:HB	1.79	0.64
1:2:61:LEU:C	1:2:63:ASP:H	2.05	0.64
3:U:833:MET:HE1	3:U:1223:GLY:HA2	1.79	0.64
2:3:271:LYS:HG3	2:3:273:GLN:HE21	1.63	0.64
3:U:614:HIS:HD2	3:U:693:PRO:O	1.80	0.64
1:2:131:GLN:HE21	1:2:133:GLU:H	1.44	0.64
2:3:425:SER:O	2:3:426:ARG:HB2	1.98	0.64
2:3:487:CYS:HB3	2:3:513:LEU:HD13	1.79	0.64
3:C:1033:HIS:CD2	3:C:1035:GLY:H	2.16	0.64
3:L:1048:GLN:HE22	3:L:1187:ASN:HD22	1.44	0.64
2:B:271:LYS:HG3	2:B:273:GLN:HE21	1.63	0.64
3:U:1033:HIS:HD2	3:U:1035:GLY:H	1.44	0.64
3:L:1118:MET:O	3:L:1122:GLN:HG2	1.98	0.64
3:U:1003:THR:HG22	3:U:1266:LEU:HD21	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:1033:HIS:CD2	3:U:1035:GLY:H	2.16	0.64
3:C:713:LYS:HD2	3:C:895:ARG:NH1	2.13	0.63
3:C:1088:GLN:HG2	3:C:1133:TYR:CE1	2.33	0.63
3:L:1100:ARG:HG2	3:4:1110:ASP:CG	2.23	0.63
2:3:255:ALA:HB2	2:3:277:MET:HG2	1.81	0.63
2:B:484:GLN:CD	3:C:1318:VAL:HA	2.24	0.63
3:L:1301:THR:HB	3:L:1302:PRO:CD	2.28	0.63
3:4:848:VAL:HG21	3:4:926:TRP:HB2	1.81	0.63
3:4:610:SER:O	3:4:663:VAL:O	2.16	0.63
2:T:404:LEU:HD21	2:T:407:ILE:HD11	1.81	0.63
3:4:1316:LEU:O	3:4:1318:VAL:HG12	1.98	0.63
3:U:752:ILE:HD12	3:U:763:PHE:HE1	1.64	0.63
7:4:1334:MOM:MO1	7:4:1334:MOM:OM2	1.69	0.63
3:U:1044:THR:O	3:U:1048:GLN:HG3	1.99	0.62
3:U:673:ASP:OD2	3:U:677:HIS:HD2	1.82	0.62
2:B:272:ASN:ND2	3:C:683:HIS:CE1	2.67	0.62
2:B:484:GLN:NE2	3:C:1318:VAL:HA	2.14	0.62
2:T:473:GLN:HE21	2:T:482:LEU:HD12	1.63	0.62
3:U:829:ARG:HG3	3:U:833:MET:HE2	1.80	0.62
3:4:1315:THR:HB	3:4:1324:ASN:H	1.63	0.62
3:C:949:GLU:HG2	3:U:899:ARG:HH12	1.63	0.62
2:K:241:THR:HG22	2:K:243:LYS:CE	2.16	0.62
3:U:740:ASP:OD2	3:U:833:MET:HG2	2.00	0.62
1:2:140:GLU:O	1:2:140:GLU:HG3	2.00	0.62
3:L:840:HIS:HE1	3:L:874:SER:OG	1.83	0.62
3:L:1249:ASN:O	3:L:1255:ALA:HA	2.00	0.62
2:T:255:ALA:HB2	2:T:277:MET:HG2	1.82	0.61
3:L:764:VAL:CG2	3:L:766:THR:HG22	2.29	0.61
3:C:1317:CYS:HB3	3:C:1318:VAL:CG2	2.22	0.61
3:U:1046:MET:HE1	3:U:1087:GLY:N	2.15	0.61
2:3:439:ARG:NH2	2:3:451:GLU:OE1	2.34	0.61
2:B:447:MET:HG2	2:B:527:LEU:HD13	1.81	0.61
7:C:1334:MOM:OM2	7:C:1334:MOM:MO1	1.71	0.61
7:U:1334:MOM:OM2	7:U:1334:MOM:MO1	1.70	0.61
3:C:880:ARG:O	3:C:884:HIS:HD2	1.83	0.61
3:U:764:VAL:HG23	3:U:766:THR:HG22	1.83	0.61
3:C:759:GLU:OE2	3:L:792:LYS:NZ	2.34	0.61
7:L:1334:MOM:OM2	7:L:1334:MOM:MO1	1.70	0.61
3:4:1321:ALA:CB	3:4:1322:PRO:HA	2.31	0.61
1:A:59:ASP:OD2	1:A:62:GLN:HG2	2.01	0.61
3:L:1289:ASN:HB2	3:L:1292:GLU:HB3	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:1292:GLU:HG2	3:U:1293:LEU:N	2.16	0.60
3:4:740:ASP:OD2	3:4:833:MET:HG2	2.01	0.60
2:3:496:LEU:H	2:3:509:ARG:HH21	1.48	0.60
3:C:1318:VAL:C	3:C:1320:GLY:H	2.09	0.60
2:T:250:ALA:HA	2:T:401:GLU:HG2	1.83	0.60
2:K:484:GLN:HA	2:K:484:GLN:NE2	2.16	0.60
3:U:972:LEU:HD23	3:U:1000:ILE:HD13	1.84	0.60
2:T:330:VAL:HG22	2:T:364:VAL:HG11	1.83	0.60
3:4:839:ARG:NH1	3:4:1205:LEU:HD22	2.16	0.60
2:B:285:PRO:C	2:B:286:GLU:O	2.38	0.60
3:C:1322:PRO:O	3:C:1323:GLY:C	2.44	0.60
3:U:721:LYS:HA	3:U:724:SER:HB2	1.83	0.60
3:C:747:HIS:HD2	3:C:836:THR:HG21	1.63	0.59
3:4:1323:GLY:HA3	3:4:1324:ASN:C	2.27	0.59
3:C:1048:GLN:HE22	3:C:1187:ASN:ND2	1.97	0.59
2:B:285:PRO:O	2:B:286:GLU:HB2	2.01	0.59
3:C:1312:LYS:O	3:C:1317:CYS:HA	2.03	0.59
3:L:1088:GLN:HG2	3:L:1133:TYR:CE1	2.37	0.59
3:C:673:ASP:OD2	3:C:677:HIS:HD2	1.85	0.59
5:T:606:FAD:H51A	5:T:606:FAD:H8A	1.85	0.59
3:U:939:GLU:HG2	3:U:977:TYR:CE2	2.37	0.59
3:4:880:ARG:O	3:4:884:HIS:CD2	2.50	0.59
3:U:764:VAL:CG2	3:U:766:THR:CG2	2.80	0.59
3:U:779:MET:HE1	3:U:814:LEU:HD13	1.85	0.59
3:4:851:MET:HE3	3:4:857:VAL:HG21	1.82	0.59
3:C:731:SER:HB3	3:C:847:LYS:HG3	1.83	0.59
3:C:1286:THR:OG1	3:C:1287:ASN:N	2.35	0.59
2:3:285:PRO:O	2:3:286:GLU:CB	2.51	0.59
3:C:782:VAL:HG13	3:C:783:PRO:HD2	1.84	0.58
3:L:695:ILE:H	3:L:904:ASN:HD22	1.51	0.58
3:U:856:ILE:HD13	3:U:927:MET:HE1	1.83	0.58
3:C:926:TRP:CZ3	3:C:927:MET:HE2	2.38	0.58
3:C:1161:GLU:HG2	3:C:1174:LEU:HD12	1.84	0.58
3:C:1316:LEU:O	3:C:1318:VAL:CB	2.34	0.58
2:T:285:PRO:O	2:T:286:GLU:CB	2.50	0.58
2:3:271:LYS:HG3	2:3:271:LYS:O	2.04	0.58
3:U:848:VAL:HG21	3:U:926:TRP:HB2	1.84	0.58
3:L:884:HIS:CE1	3:L:1006:GLY:H	2.21	0.58
3:4:884:HIS:CE1	3:4:1006:GLY:H	2.21	0.58
2:B:285:PRO:O	2:B:286:GLU:CB	2.52	0.58
2:K:424:ALA:O	2:K:425:SER:CB	2.48	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:250:ALA:HA	2:3:401:GLU:HG2	1.85	0.58
3:L:571:ASP:OD2	3:L:1052:LYS:HE3	2.04	0.58
3:4:673:ASP:OD2	3:4:677:HIS:HD2	1.85	0.58
3:C:1318:VAL:O	3:C:1318:VAL:HG12	2.04	0.58
2:B:241:THR:CG2	2:B:243:LYS:HG2	2.34	0.57
3:L:980:ARG:CZ	3:L:1175:ARG:HD3	2.33	0.57
3:U:1088:GLN:HG2	3:U:1133:TYR:CD1	2.39	0.57
3:U:1132:PHE:CD1	3:4:1126:SER:HB2	2.39	0.57
3:4:941:VAL:O	3:4:945:ASN:ND2	2.31	0.57
3:4:1316:LEU:O	3:4:1318:VAL:CB	2.51	0.57
2:K:387:HIS:CE1	2:K:467:LEU:HD11	2.38	0.57
2:3:285:PRO:O	2:3:286:GLU:HB2	2.04	0.57
3:4:1286:THR:CG2	3:4:1310:VAL:HB	2.34	0.57
3:U:1124:ARG:HD3	3:4:1013:PHE:HA	1.85	0.57
3:C:788:LEU:HD13	3:C:1069:ASN:HB3	1.86	0.57
3:4:579:HIS:HB3	3:4:582:ALA:HB2	1.86	0.57
3:4:1088:GLN:HG2	3:4:1133:TYR:CE1	2.40	0.57
3:4:1315:THR:HG21	3:4:1325:CYS:HA	1.87	0.57
2:K:367:ALA:O	2:K:439:ARG:HD3	2.05	0.57
2:K:285:PRO:C	2:K:286:GLU:O	2.42	0.57
3:U:624:GLU:CB	3:U:684:VAL:CG1	2.83	0.57
3:U:884:HIS:HE1	3:U:1006:GLY:H	1.52	0.57
3:4:1088:GLN:HG2	3:4:1133:TYR:CD1	2.39	0.57
1:A:143:PHE:HB3	3:C:1232:PHE:CE1	2.39	0.57
2:B:424:ALA:O	2:B:425:SER:CB	2.48	0.57
1:J:58:TYR:CE1	1:J:63:ASP:O	2.58	0.57
1:2:124:MET:HE3	1:2:128:LEU:HG	1.87	0.57
1:J:59:ASP:OD2	1:J:62:GLN:HG2	2.05	0.56
2:K:285:PRO:O	2:K:286:GLU:HB2	2.04	0.56
2:T:322:GLN:O	2:T:412:SER:HB3	2.04	0.56
3:4:829:ARG:CG	3:4:833:MET:HE2	2.34	0.56
3:L:839:ARG:NH2	3:L:912:ARG:O	2.38	0.56
3:C:655:PHE:CD2	3:C:668:GLY:HA2	2.41	0.56
3:C:670:VAL:HG11	3:C:681:ALA:HB3	1.88	0.56
3:L:713:LYS:HD2	3:L:895:ARG:NH1	2.19	0.56
3:L:880:ARG:O	3:L:884:HIS:HD2	1.88	0.56
2:T:271:LYS:HG3	2:T:273:GLN:HE21	1.70	0.56
3:C:949:GLU:CG	3:U:899:ARG:HH12	2.19	0.56
3:L:1000:ILE:HG13	3:L:1159:CYS:HB2	1.87	0.56
3:U:880:ARG:O	3:U:884:HIS:HD2	1.88	0.56
1:J:159:GLY:O	1:J:162:THR:HG22	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:346:ALA:HB1	5:T:606:FAD:H4'	1.87	0.56
3:C:1118:MET:SD	3:C:1122:GLN:NE2	2.79	0.56
3:L:1033:HIS:CD2	3:L:1035:GLY:H	2.24	0.56
3:C:1081:VAL:O	3:C:1085:ILE:HG12	2.06	0.56
2:K:346:ALA:HB1	5:K:606:FAD:H4'	1.86	0.56
3:L:829:ARG:CG	3:L:833:MET:HE2	2.36	0.56
3:U:880:ARG:HD2	3:U:914:PHE:HB3	1.88	0.56
3:4:1003:THR:HG22	3:4:1266:LEU:HD21	1.87	0.56
3:4:1048:GLN:NE2	3:4:1187:ASN:HD22	2.04	0.56
2:K:247:ASP:OD1	2:K:377:ARG:HD3	2.06	0.55
2:K:271:LYS:HG3	2:K:273:GLN:HE21	1.71	0.55
3:4:926:TRP:CZ3	3:4:927:MET:HE2	2.42	0.55
3:U:853:THR:HG22	3:U:944:LYS:HZ2	1.71	0.55
3:U:995:LYS:NZ	3:U:1284:GLN:HE21	2.04	0.55
3:C:749:THR:OG1	3:C:764:VAL:HG12	2.06	0.55
3:C:1207:THR:HG21	3:C:1270:VAL:HG12	1.89	0.55
3:C:958:ARG:NH2	3:U:711:GLU:O	2.40	0.55
3:U:853:THR:CG2	3:U:944:LYS:NZ	2.70	0.55
2:B:484:GLN:OE1	3:C:1318:VAL:HA	2.07	0.55
3:U:853:THR:HG22	3:U:944:LYS:NZ	2.21	0.55
3:L:684:VAL:O	3:L:684:VAL:HG13	2.06	0.55
3:L:829:ARG:HG3	3:L:833:MET:HE2	1.87	0.55
3:L:1207:THR:HG21	3:L:1270:VAL:HG12	1.89	0.55
3:U:1046:MET:HE1	3:U:1086:TYR:C	2.32	0.55
3:C:600:GLU:HG2	3:L:598:ARG:O	2.06	0.55
3:C:640:ILE:HG12	3:C:779:MET:CE	2.37	0.54
3:C:1318:VAL:H	3:C:1319:THR:CA	2.17	0.54
3:U:995:LYS:NZ	3:U:1284:GLN:NE2	2.55	0.54
3:4:773:GLN:HG2	3:4:784:VAL:HG13	1.89	0.54
2:T:425:SER:O	2:T:426:ARG:HB2	2.07	0.54
2:B:232:GLU:OE2	3:C:680:ARG:NH1	2.34	0.54
2:B:484:GLN:OE1	3:C:1317:CYS:SG	2.49	0.54
3:C:725:GLU:HG3	3:C:851:MET:HE1	1.89	0.54
3:C:839:ARG:NH2	3:C:912:ARG:O	2.41	0.54
2:T:337:PHE:O	2:T:338:ALA:C	2.49	0.54
3:U:1046:MET:CE	3:U:1086:TYR:C	2.80	0.54
3:C:911:PHE:O	3:C:912:ARG:C	2.48	0.54
3:L:782:VAL:HG13	3:L:783:PRO:HD2	1.89	0.54
1:A:131:GLN:HE21	1:A:133:GLU:H	1.56	0.54
3:C:764:VAL:CG2	3:C:766:THR:CG2	2.86	0.54
3:C:833:MET:HE1	3:C:1223:GLY:HA2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1282:ARG:HA	3:C:1286:THR:HG23	1.90	0.54
2:3:495:SER:HB2	2:3:509:ARG:NH2	2.19	0.54
2:K:264:ILE:HD11	5:K:606:FAD:H3B	1.88	0.54
3:4:939:GLU:HG2	3:4:977:TYR:CE2	2.43	0.54
3:4:1259:VAL:O	3:4:1263:PRO:HD3	2.07	0.54
3:U:794:MET:HE3	3:U:1038:MET:HB3	1.90	0.54
3:4:695:ILE:H	3:4:904:ASN:ND2	2.03	0.54
3:4:1033:HIS:CD2	3:4:1035:GLY:H	2.26	0.54
2:K:272:ASN:ND2	3:L:683:HIS:CE1	2.76	0.54
1:S:61:LEU:C	1:S:63:ASP:N	2.65	0.54
3:U:1037:GLU:HB2	3:U:1043:HIS:CD2	2.43	0.54
3:4:779:MET:CE	3:4:814:LEU:HB2	2.38	0.54
3:L:1048:GLN:HE22	3:L:1187:ASN:HB2	1.72	0.54
1:2:40:LYS:NZ	3:4:595:ASP:OD2	2.41	0.54
1:A:40:LYS:NZ	3:C:595:ASP:OD2	2.40	0.54
2:K:285:PRO:O	2:K:286:GLU:CB	2.56	0.54
2:T:284:ILE:HB	2:T:287:LEU:HD12	1.90	0.54
3:U:972:LEU:CD2	3:U:1000:ILE:HD13	2.38	0.54
2:3:458:GLY:O	2:3:508:ARG:NH1	2.41	0.53
3:U:1286:THR:HG22	3:U:1310:VAL:O	2.08	0.53
3:4:602:GLU:OE2	3:4:824:ARG:NE	2.33	0.53
3:4:1286:THR:HG22	3:4:1310:VAL:HB	1.89	0.53
1:A:58:TYR:HE2	1:A:60:ARG:HG2	1.72	0.53
3:L:603:LEU:HB2	3:L:823:VAL:HG22	1.91	0.53
3:U:1128:SER:HB2	3:4:1072:PRO:HG3	1.90	0.53
3:L:923:ALA:HA	3:L:926:TRP:NE1	2.23	0.53
3:L:926:TRP:CZ3	3:L:927:MET:HE2	2.44	0.53
3:C:874:SER:HB3	3:C:900:LEU:HD22	1.91	0.53
3:C:923:ALA:HA	3:C:926:TRP:NE1	2.24	0.53
3:4:1316:LEU:O	3:4:1318:VAL:HB	2.09	0.53
3:4:1317:CYS:HB2	3:4:1321:ALA:CA	2.34	0.53
3:C:1318:VAL:C	3:C:1320:GLY:N	2.67	0.53
3:L:695:ILE:H	3:L:904:ASN:ND2	2.07	0.53
3:4:1203:LEU:HD12	3:4:1203:LEU:C	2.33	0.53
1:A:32:ARG:HG2	3:C:598:ARG:CZ	2.39	0.53
2:B:250:ALA:HA	2:B:401:GLU:HG2	1.91	0.53
2:3:286:GLU:O	2:3:287:LEU:CB	2.57	0.53
2:3:484:GLN:NE2	3:4:1318:VAL:O	2.41	0.53
2:B:264:ILE:HD11	5:B:606:FAD:H3B	1.91	0.52
3:C:1289:ASN:HB2	3:C:1292:GLU:HB3	1.90	0.52
2:3:374:ILE:HD13	2:3:398:LEU:CD2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:326:VAL:O	2:K:327:PHE:C	2.51	0.52
3:4:721:LYS:HA	3:4:724:SER:HB2	1.91	0.52
1:J:99:HIS:CE1	1:J:101:VAL:HG23	2.45	0.52
3:C:764:VAL:HG23	3:C:766:THR:CG2	2.35	0.52
1:J:131:GLN:NE2	1:J:133:GLU:H	2.04	0.52
2:K:473:GLN:O	2:K:476:LYS:HB2	2.10	0.52
3:U:655:PHE:HE1	3:U:814:LEU:CD2	2.23	0.52
3:L:772:THR:O	3:L:776:VAL:HG23	2.10	0.52
2:3:284:ILE:HB	2:3:287:LEU:HD12	1.92	0.52
3:C:601:ASN:HB2	3:C:821:HIS:CD2	2.45	0.52
2:K:241:THR:CG2	2:K:243:LYS:HG2	2.40	0.52
3:4:1033:HIS:HD2	3:4:1035:GLY:H	1.58	0.52
3:4:1096:THR:HB	3:4:1129:THR:HG21	1.91	0.52
3:4:1320:GLY:O	3:4:1321:ALA:C	2.53	0.51
3:4:833:MET:HE1	3:4:1223:GLY:CA	2.39	0.51
2:K:495:SER:HB2	2:K:509:ARG:NH2	2.18	0.51
3:L:992:CYS:HA	3:L:1284:GLN:NE2	2.26	0.51
2:T:241:THR:CG2	2:T:243:LYS:HE2	2.38	0.51
3:C:599:TYR:HA	3:L:599:TYR:HA	1.92	0.51
3:L:741:HIS:CE1	3:L:838:GLY:HA2	2.46	0.51
2:B:439:ARG:NH2	2:B:451:GLU:OE1	2.44	0.51
3:C:980:ARG:CZ	3:C:1175:ARG:HD3	2.41	0.51
3:4:614:HIS:HD2	3:4:693:PRO:O	1.93	0.51
3:4:1203:LEU:HD12	3:4:1203:LEU:O	2.11	0.51
3:C:584:MET:SD	3:L:756:GLU:HB3	2.50	0.51
3:C:853:THR:HG22	3:C:944:LYS:HZ2	1.75	0.51
3:4:624:GLU:CB	3:4:684:VAL:CG1	2.87	0.51
3:L:788:LEU:HD13	3:L:1069:ASN:HB3	1.92	0.51
3:4:911:PHE:O	3:4:912:ARG:C	2.53	0.51
1:S:104:ARG:O	1:S:108:SER:HB2	2.10	0.50
3:U:616:LYS:HB3	3:U:690:GLU:HB3	1.93	0.50
2:B:241:THR:HG21	2:B:243:LYS:HG2	1.94	0.50
3:C:779:MET:HG2	3:C:810:VAL:HG13	1.92	0.50
2:T:439:ARG:NH2	2:T:451:GLU:OE1	2.44	0.50
3:4:806:THR:HA	3:4:809:SER:HB2	1.93	0.50
3:4:848:VAL:CG2	3:4:926:TRP:HB2	2.41	0.50
3:L:1108:ASN:ND2	3:L:1111:GLY:HA3	2.26	0.50
3:4:842:PHE:CE2	3:4:865:SER:HB3	2.47	0.50
3:4:844:ALA:HB2	3:4:922:ILE:HD13	1.93	0.50
2:K:241:THR:HG21	2:K:243:LYS:HG2	1.94	0.50
2:B:271:LYS:HG3	2:B:271:LYS:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:673:ASP:OD2	3:L:677:HIS:CD2	2.60	0.50
3:U:610:SER:O	3:U:663:VAL:O	2.30	0.50
3:U:884:HIS:CE1	3:U:1006:GLY:H	2.29	0.50
3:U:1249:ASN:O	3:U:1255:ALA:HA	2.12	0.50
1:2:61:LEU:C	1:2:63:ASP:N	2.70	0.50
3:L:624:GLU:HB2	3:L:684:VAL:HG13	1.94	0.50
3:L:655:PHE:CD2	3:L:668:GLY:HA2	2.47	0.50
3:U:911:PHE:O	3:U:912:ARG:C	2.55	0.50
3:U:1079:ALA:O	3:U:1080:SER:HB2	2.12	0.50
3:U:1289:ASN:HB3	3:U:1292:GLU:HB3	1.93	0.50
3:4:699:GLU:CD	3:4:699:GLU:H	2.20	0.50
3:L:880:ARG:HD2	3:L:914:PHE:HB3	1.93	0.50
3:C:603:LEU:HB2	3:C:823:VAL:HG22	1.94	0.49
3:U:1007:ILE:O	3:U:1008:SER:CB	2.60	0.49
3:4:840:HIS:HE1	3:4:874:SER:OG	1.95	0.49
3:4:926:TRP:HZ3	3:4:927:MET:HE2	1.77	0.49
3:C:829:ARG:CG	3:C:833:MET:CE	2.90	0.49
1:J:143:PHE:HB3	3:L:1232:PHE:CE1	2.47	0.49
3:L:725:GLU:O	3:L:851:MET:HE1	2.12	0.49
3:C:601:ASN:HB2	3:C:821:HIS:HD2	1.77	0.49
3:U:1088:GLN:HG2	3:U:1133:TYR:CE1	2.48	0.49
1:S:61:LEU:O	1:S:63:ASP:N	2.44	0.49
3:U:604:PHE:CD2	3:U:675:PRO:HG3	2.47	0.49
3:4:1318:VAL:CG2	3:4:1319:THR:HG22	2.42	0.49
3:L:960:GLU:OE2	3:4:1245:ARG:NH2	2.45	0.49
1:S:153:TYR:C	1:S:155:PRO:HD2	2.38	0.49
3:4:779:MET:HE1	3:4:814:LEU:HD13	1.95	0.49
3:C:695:ILE:H	3:C:904:ASN:ND2	2.10	0.49
3:L:1036:THR:HG22	3:L:1066:THR:HG21	1.95	0.49
2:3:241:THR:CG2	2:3:243:LYS:HE2	2.42	0.49
3:4:779:MET:HE1	3:4:814:LEU:HB2	1.95	0.49
3:C:1021:ILE:HD12	3:C:1031:VAL:HG22	1.95	0.49
3:L:640:ILE:HG12	3:L:779:MET:CE	2.41	0.49
3:4:1187:ASN:CG	3:4:1190:ILE:HG12	2.38	0.48
3:4:1286:THR:C	3:4:1326:LYS:C	2.81	0.48
3:4:1321:ALA:CB	3:4:1322:PRO:CA	2.91	0.48
1:S:129:ARG:NH1	1:S:129:ARG:HG2	2.26	0.48
3:4:640:ILE:HG12	3:4:779:MET:CE	2.42	0.48
3:C:624:GLU:HB2	3:C:684:VAL:HG13	1.94	0.48
3:U:759:GLU:OE2	3:4:792:LYS:NZ	2.46	0.48
3:U:1290:THR:HB	3:U:1291:LYS:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:1044:THR:O	3:4:1048:GLN:HG3	2.12	0.48
3:4:1118:MET:O	3:4:1122:GLN:HG2	2.13	0.48
3:C:926:TRP:HZ3	3:C:927:MET:HE2	1.76	0.48
3:4:923:ALA:HA	3:4:926:TRP:NE1	2.28	0.48
3:C:1301:THR:HB	3:C:1302:PRO:HD2	1.96	0.48
2:K:286:GLU:O	2:K:288:ASN:N	2.44	0.48
3:4:655:PHE:CD2	3:4:668:GLY:HA2	2.48	0.48
3:C:756:GLU:HB3	3:L:584:MET:SD	2.53	0.48
3:C:840:HIS:CE1	3:C:874:SER:OG	2.59	0.48
3:L:695:ILE:N	3:L:904:ASN:HD22	2.11	0.48
1:S:103:GLU:O	1:S:107:LYS:HG3	2.14	0.48
3:4:953:THR:HG23	3:4:957:GLN:O	2.13	0.48
3:C:673:ASP:OD2	3:C:677:HIS:CD2	2.65	0.48
3:L:610:SER:O	3:L:663:VAL:O	2.32	0.48
3:4:1048:GLN:HE22	3:4:1187:ASN:HB2	1.79	0.48
2:B:340:LYS:O	2:B:344:SER:HB2	2.14	0.48
3:C:1180:MET:HG3	3:C:1195:VAL:HG22	1.95	0.48
3:L:767:GLN:HG2	3:L:1038:MET:CE	2.43	0.48
3:U:1286:THR:CG2	3:U:1310:VAL:HB	2.44	0.48
2:3:450:LYS:O	2:3:474:LEU:HD22	2.13	0.48
3:L:1081:VAL:O	3:L:1085:ILE:HG12	2.14	0.48
2:T:232:GLU:OE2	3:U:680:ARG:NH1	2.46	0.48
2:T:387:HIS:CE1	2:T:467:LEU:HD11	2.48	0.48
3:U:749:THR:HG23	3:U:764:VAL:HG12	1.94	0.48
3:4:719:LEU:HD13	3:4:723:PHE:HE1	1.79	0.48
3:4:1316:LEU:O	3:4:1318:VAL:CG1	2.60	0.48
2:B:419:SER:HB2	2:B:519:PHE:CD1	2.49	0.47
3:C:782:VAL:CG1	3:C:783:PRO:HD2	2.44	0.47
1:2:43:CYS:HA	3:4:829:ARG:HB2	1.96	0.47
2:B:286:GLU:C	2:B:288:ASN:H	2.22	0.47
3:L:741:HIS:HB2	3:L:743:TYR:CE2	2.49	0.47
3:U:764:VAL:HG23	3:U:766:THR:CG2	2.43	0.47
3:4:1319:THR:O	3:4:1320:GLY:C	2.56	0.47
2:B:387:HIS:CE1	2:B:467:LEU:HD11	2.50	0.47
2:B:491:ALA:CB	3:C:1316:LEU:HD21	2.44	0.47
3:C:1023:VAL:HG22	3:C:1029:VAL:HG22	1.96	0.47
2:K:243:LYS:HD3	2:K:243:LYS:N	2.30	0.47
3:L:752:ILE:HD12	3:L:763:PHE:HE1	1.79	0.47
2:3:353:ILE:HG13	5:3:606:FAD:C2A	2.44	0.47
1:A:58:TYR:CE1	1:A:63:ASP:O	2.67	0.47
3:L:1261:GLU:N	3:L:1262:PRO:CD	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:1017:ALA:HB1	3:U:1086:TYR:CD2	2.48	0.47
3:C:1046:MET:CE	3:C:1087:GLY:HA2	2.24	0.47
3:4:605:LEU:C	3:4:605:LEU:HD23	2.40	0.47
3:4:911:PHE:HD2	3:4:912:ARG:N	2.11	0.47
1:A:99:HIS:CE1	1:A:101:VAL:HG23	2.49	0.47
3:4:1195:VAL:HA	3:4:1263:PRO:HG2	1.96	0.47
3:4:1315:THR:O	3:4:1316:LEU:HB2	2.13	0.47
1:A:104:ARG:HD2	1:A:104:ARG:HA	1.34	0.47
3:L:768:ASN:HB2	3:L:802:GLU:O	2.15	0.47
3:U:579:HIS:HB3	3:U:582:ALA:HB2	1.96	0.47
3:U:840:HIS:HE1	3:U:874:SER:OG	1.97	0.47
1:2:63:ASP:O	1:2:64:LYS:O	2.33	0.47
3:C:1183:GLY:HA2	3:C:1247:CYS:O	2.15	0.47
3:U:1128:SER:HB2	3:4:1072:PRO:CG	2.45	0.47
3:C:829:ARG:HG2	3:C:833:MET:CE	2.45	0.47
2:K:250:ALA:HA	2:K:401:GLU:HG2	1.97	0.47
1:A:131:GLN:NE2	1:A:133:GLU:H	2.12	0.47
2:B:367:ALA:O	2:B:439:ARG:HD3	2.15	0.47
3:L:571:ASP:CG	3:L:1052:LYS:HG3	2.40	0.47
3:L:721:LYS:O	3:L:725:GLU:HB3	2.15	0.47
3:4:752:ILE:HD12	3:4:763:PHE:HE1	1.80	0.47
3:4:1286:THR:CA	3:4:1326:LYS:O	2.63	0.47
3:L:725:GLU:HG3	3:L:851:MET:HE1	1.97	0.46
3:U:712:LEU:HD21	3:U:875:HIS:CE1	2.50	0.46
3:4:747:HIS:HD2	3:4:836:THR:HG21	1.78	0.46
3:C:721:LYS:O	3:C:725:GLU:HB3	2.15	0.46
3:L:1259:VAL:HG22	3:L:1259:VAL:O	2.15	0.46
3:L:1287:ASN:HD22	3:L:1289:ASN:H	1.62	0.46
1:S:100:PRO:O	1:S:104:ARG:HB2	2.16	0.46
3:4:1292:GLU:HG2	3:4:1293:LEU:N	2.29	0.46
2:K:376:SER:HB3	2:K:402:GLU:HG2	1.97	0.46
3:L:601:ASN:HB2	3:L:821:HIS:CD2	2.51	0.46
3:C:719:LEU:HD11	3:C:895:ARG:HB3	1.96	0.46
1:J:32:ARG:NH1	3:L:676:GLU:OE2	2.43	0.46
2:K:497:SER:C	2:K:499:ASP:H	2.24	0.46
3:U:640:ILE:HG12	3:U:779:MET:CE	2.45	0.46
3:U:663:VAL:HG12	3:U:834:LEU:HD11	1.97	0.46
3:4:684:VAL:HG12	3:4:684:VAL:O	2.14	0.46
3:C:610:SER:O	3:C:663:VAL:O	2.34	0.46
3:C:949:GLU:HG2	3:U:899:ARG:NH1	2.28	0.46
3:C:1048:GLN:HE22	3:C:1187:ASN:HB2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1316:LEU:H	3:C:1322:PRO:HG2	1.80	0.46
2:K:286:GLU:C	2:K:288:ASN:H	2.23	0.46
3:4:624:GLU:CB	3:4:684:VAL:HG11	2.46	0.46
2:B:241:THR:HG22	2:B:243:LYS:H	1.79	0.46
2:3:484:GLN:CD	3:4:1318:VAL:O	2.59	0.46
3:C:1088:GLN:CG	3:C:1133:TYR:CD1	2.92	0.46
3:4:1319:THR:HG1	3:4:1320:GLY:H	1.57	0.46
1:A:6:LEU:HB3	1:A:17:GLU:HB3	1.98	0.46
3:U:640:ILE:HG12	3:U:779:MET:HE2	1.98	0.46
3:U:1081:VAL:O	3:U:1085:ILE:HG12	2.16	0.46
3:4:1013:PHE:CD1	3:4:1013:PHE:C	2.94	0.46
3:L:684:VAL:O	3:L:684:VAL:CG1	2.64	0.45
3:L:1221:THR:HA	3:L:1226:THR:OG1	2.16	0.45
2:T:452:LEU:HD23	2:T:470:THR:HA	1.98	0.45
3:U:853:THR:CG2	3:U:944:LYS:HZ3	2.28	0.45
3:4:1175:ARG:HG3	3:4:1238:GLU:HB3	1.97	0.45
3:L:875:HIS:CD2	3:L:879:GLU:OE2	2.69	0.45
3:L:1182:VAL:C	3:L:1257:LYS:HB2	2.42	0.45
3:U:1187:ASN:CG	3:U:1190:ILE:HG12	2.42	0.45
1:A:134:PRO:O	1:A:164:ALA:HA	2.16	0.45
2:B:376:SER:HB3	2:B:402:GLU:HG2	1.97	0.45
3:L:976:GLN:O	3:L:980:ARG:HG3	2.16	0.45
2:3:517:PHE:CZ	2:3:521:LEU:HD11	2.52	0.45
3:4:874:SER:HB3	3:4:900:LEU:HD22	1.99	0.45
3:4:1317:CYS:HB2	3:4:1321:ALA:CB	2.46	0.45
3:C:792:LYS:NZ	3:L:759:GLU:OE2	2.50	0.45
3:C:947:TYR:HB2	3:C:962:PHE:CZ	2.51	0.45
3:L:747:HIS:ND1	3:L:805:SER:HA	2.32	0.45
3:U:684:VAL:HG12	3:U:684:VAL:O	2.17	0.45
3:4:880:ARG:HD2	3:4:914:PHE:HB3	1.98	0.45
2:B:468:LYS:NZ	2:B:492:GLU:OE1	2.50	0.45
2:B:484:GLN:HE22	3:C:1318:VAL:CG2	2.18	0.45
3:C:1231:ALA:O	3:C:1232:PHE:C	2.59	0.45
3:L:670:VAL:HG11	3:L:681:ALA:HB3	1.98	0.45
2:3:255:ALA:CB	2:3:277:MET:HG2	2.46	0.45
2:K:330:VAL:HG22	2:K:364:VAL:HG11	1.99	0.45
3:U:1286:THR:CG2	3:U:1310:VAL:O	2.65	0.45
3:C:712:LEU:HD21	3:C:875:HIS:CE1	2.52	0.45
3:C:1209:GLU:HB3	3:C:1227:TYR:CZ	2.52	0.45
3:L:1282:ARG:HA	3:L:1286:THR:HG23	1.99	0.45
2:3:473:GLN:HE21	2:3:482:LEU:HD12	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:1286:THR:OG1	3:L:1287:ASN:N	2.45	0.44
3:U:1182:VAL:C	3:U:1257:LYS:HB2	2.42	0.44
3:4:1017:ALA:HB2	3:4:1085:ILE:HD12	1.98	0.44
3:4:1286:THR:CG2	3:4:1310:VAL:O	2.64	0.44
2:B:348:LEU:HD13	2:B:407:ILE:HD13	1.98	0.44
3:C:1320:GLY:O	3:C:1321:ALA:CB	2.59	0.44
1:J:40:LYS:NZ	3:L:595:ASP:OD2	2.47	0.44
3:L:1017:ALA:HB1	3:L:1086:TYR:CD2	2.52	0.44
3:C:752:ILE:HD12	3:C:763:PHE:HE1	1.82	0.44
3:C:980:ARG:NH1	3:C:1161:GLU:OE1	2.49	0.44
3:C:1102:GLU:HB3	3:C:1103:PRO:HD3	1.99	0.44
1:J:104:ARG:HA	1:J:104:ARG:HD2	1.38	0.44
5:K:606:FAD:H8A	5:K:606:FAD:H51A	1.98	0.44
3:U:1048:GLN:HE22	3:U:1187:ASN:HB2	1.83	0.44
3:L:1102:GLU:HB3	3:L:1103:PRO:HD3	1.99	0.44
2:3:425:SER:O	2:3:426:ARG:CB	2.65	0.44
2:B:284:ILE:O	2:B:286:GLU:O	2.35	0.44
3:4:640:ILE:HG12	3:4:779:MET:HE2	1.99	0.44
3:C:684:VAL:HG13	3:C:684:VAL:O	2.18	0.44
1:J:91:ILE:O	1:J:99:HIS:HB2	2.17	0.44
3:L:1289:ASN:HB3	3:L:1292:GLU:H	1.81	0.44
2:K:443:GLN:OE1	2:K:443:GLN:HA	2.16	0.44
3:L:752:ILE:CD1	3:L:763:PHE:HE1	2.30	0.44
3:L:833:MET:HE1	3:L:1223:GLY:HA2	2.00	0.44
3:C:741:HIS:CE1	3:C:838:GLY:HA2	2.53	0.44
3:L:1182:VAL:O	3:L:1257:LYS:HB2	2.17	0.44
3:U:655:PHE:HE1	3:U:814:LEU:HD23	1.81	0.44
3:U:740:ASP:CG	3:U:833:MET:HG2	2.42	0.44
3:U:929:GLU:HG2	3:U:1293:LEU:HD13	2.00	0.44
3:U:1036:THR:O	3:U:1077:THR:HG21	2.18	0.44
1:A:93:SER:C	1:A:95:LYS:H	2.25	0.44
3:C:1045:LYS:NZ	3:C:1191:ASP:OD1	2.39	0.44
3:C:1318:VAL:O	3:C:1318:VAL:CG1	2.65	0.44
3:L:767:GLN:HG2	3:L:1038:MET:HE1	2.00	0.44
3:L:1180:MET:HG3	3:L:1195:VAL:HG22	2.00	0.44
3:4:1007:ILE:O	3:4:1008:SER:CB	2.66	0.44
2:K:424:ALA:O	3:L:1302:PRO:HG2	2.18	0.43
3:L:1275:LYS:HG3	3:L:1296:LEU:HD23	1.99	0.43
3:U:995:LYS:HZ1	3:U:1284:GLN:NE2	2.15	0.43
2:3:337:PHE:O	2:3:338:ALA:C	2.59	0.43
3:4:921:PHE:O	3:4:922:ILE:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:707:PHE:CD2	3:C:899:ARG:HG3	2.54	0.43
3:L:1289:ASN:HB3	3:L:1292:GLU:N	2.33	0.43
3:L:1289:ASN:C	3:L:1291:LYS:H	2.25	0.43
1:S:63:ASP:O	1:S:64:LYS:O	2.36	0.43
2:3:497:SER:C	2:3:499:ASP:H	2.27	0.43
3:4:768:ASN:ND2	3:4:1076:PRO:HG3	2.33	0.43
1:A:99:HIS:HE1	1:A:101:VAL:HG23	1.83	0.43
1:J:48:CYS:O	1:J:146:ASN:HA	2.18	0.43
3:L:1044:THR:O	3:L:1048:GLN:HG3	2.17	0.43
3:U:833:MET:HE1	3:U:1223:GLY:CA	2.45	0.43
1:2:32:ARG:HG2	3:4:598:ARG:CZ	2.47	0.43
1:2:117:THR:O	1:2:118:PRO:C	2.61	0.43
2:3:443:GLN:HB2	2:3:446:SER:OG	2.19	0.43
2:B:298:SER:HA	2:B:408:GLU:HA	2.00	0.43
3:L:829:ARG:HG2	3:L:833:MET:CE	2.49	0.43
2:T:358:ILE:O	2:T:359:SER:C	2.60	0.43
2:T:374:ILE:HD13	2:T:398:LEU:CD2	2.48	0.43
3:U:759:GLU:OE2	3:4:1062:TYR:OH	2.26	0.43
1:2:63:ASP:OD1	1:2:64:LYS:N	2.52	0.43
3:C:770:MET:HE2	3:C:771:LYS:HE2	2.01	0.43
3:C:779:MET:SD	3:C:779:MET:C	3.01	0.43
3:C:1198:ALA:HB3	3:C:1263:PRO:HB2	2.01	0.43
2:K:296:GLY:HA2	2:K:411:TYR:CD1	2.53	0.43
3:U:613:ALA:O	3:U:904:ASN:HB3	2.19	0.43
2:3:484:GLN:OE1	3:4:1319:THR:N	2.51	0.43
3:4:1286:THR:HG21	3:4:1310:VAL:HB	2.01	0.43
2:T:496:LEU:N	2:T:509:ARG:NH2	2.60	0.43
3:U:1175:ARG:NE	3:U:1177:ASP:OD2	2.51	0.43
3:4:1017:ALA:HB1	3:4:1086:TYR:CD2	2.54	0.43
2:K:348:LEU:HD13	2:K:407:ILE:HD13	2.01	0.43
3:L:779:MET:HG2	3:L:810:VAL:HG13	2.01	0.43
3:L:1183:GLY:HA2	3:L:1247:CYS:O	2.18	0.43
2:3:325:GLU:HB2	2:3:412:SER:OG	2.18	0.43
2:3:403:ILE:HD12	2:3:403:ILE:C	2.44	0.43
2:T:255:ALA:CB	2:T:277:MET:HG2	2.47	0.43
2:3:232:GLU:OE2	3:4:680:ARG:NH1	2.46	0.43
3:C:1249:ASN:HD22	3:C:1257:LYS:HG2	1.84	0.43
1:J:81:HIS:CD2	1:J:82:HIS:CD2	3.07	0.43
2:K:484:GLN:HA	2:K:484:GLN:HE21	1.81	0.43
3:L:918:GLN:OE1	3:L:918:GLN:N	2.39	0.43
3:U:829:ARG:CG	3:U:833:MET:HE2	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:328:ARG:O	2:3:332:GLU:HG2	2.19	0.43
1:A:48:CYS:O	1:A:146:ASN:HA	2.19	0.43
2:B:330:VAL:HG22	2:B:364:VAL:HG11	2.01	0.43
3:C:725:GLU:O	3:C:851:MET:HE1	2.19	0.43
3:L:578:PRO:O	3:L:579:HIS:C	2.62	0.43
3:L:1153:PHE:HB2	3:L:1155:TYR:CZ	2.54	0.43
3:L:1289:ASN:C	3:L:1291:LYS:N	2.76	0.43
1:S:104:ARG:HA	1:S:104:ARG:HD2	1.85	0.43
3:U:624:GLU:CB	3:U:684:VAL:HG11	2.49	0.43
3:U:1195:VAL:HA	3:U:1263:PRO:HG2	2.01	0.43
3:4:770:MET:SD	3:4:1073:ASN:HA	2.58	0.43
3:L:655:PHE:HE1	3:L:814:LEU:CD2	2.32	0.42
3:U:804:ARG:NH2	3:U:807:LEU:HD11	2.34	0.42
3:U:1229:ILE:O	3:U:1230:PRO:C	2.61	0.42
3:U:1254:TYR:O	3:U:1255:ALA:HB3	2.19	0.42
2:B:241:THR:HG22	2:B:243:LYS:HG2	2.01	0.42
2:B:497:SER:C	2:B:499:ASP:H	2.26	0.42
1:J:74:LEU:HD23	1:J:74:LEU:HA	1.90	0.42
2:K:323:LYS:HA	2:K:412:SER:O	2.19	0.42
3:L:771:LYS:HD3	3:L:771:LYS:HA	1.75	0.42
2:T:438:MET:HE2	2:T:454:LEU:HD22	2.01	0.42
1:2:141:ASP:C	1:2:143:PHE:H	2.27	0.42
3:C:853:THR:HG22	3:C:944:LYS:NZ	2.34	0.42
3:L:798:PHE:HA	6:L:1333:MTE:S1'	2.58	0.42
3:L:1161:GLU:HG2	3:L:1174:LEU:HD12	2.01	0.42
2:T:443:GLN:OE1	2:T:443:GLN:HA	2.19	0.42
3:U:998:LEU:CD1	3:U:1161:GLU:HB2	2.49	0.42
2:3:256:LYS:HG3	2:3:275:PHE:CG	2.55	0.42
2:B:486:VAL:O	2:B:490:LEU:HG	2.20	0.42
3:C:767:GLN:HG2	3:C:1038:MET:CE	2.50	0.42
1:J:62:GLN:O	1:J:63:ASP:HB3	2.20	0.42
7:U:1334:MOM:OM1	8:U:7319:XAN:C8	2.55	0.42
1:2:32:ARG:HG2	3:4:598:ARG:NH2	2.33	0.42
2:B:507:PHE:CZ	2:B:511:LEU:HD11	2.54	0.42
3:C:992:CYS:HA	3:C:1284:GLN:NE2	2.34	0.42
2:K:314:GLU:HG2	2:K:318:LYS:NZ	2.34	0.42
3:L:655:PHE:CE2	3:L:668:GLY:HA2	2.54	0.42
3:L:1209:GLU:HB3	3:L:1227:TYR:CZ	2.54	0.42
1:2:134:PRO:O	1:2:164:ALA:HA	2.20	0.42
3:C:939:GLU:HG2	3:C:977:TYR:CE2	2.54	0.42
3:C:1176:THR:HG21	3:C:1199:PHE:CZ	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:719:LEU:HD11	3:L:895:ARG:HB3	2.02	0.42
3:L:980:ARG:NH1	3:L:1161:GLU:OE1	2.52	0.42
3:4:739:GLN:HB2	3:4:1205:LEU:HD13	2.02	0.42
3:4:1276:ASP:O	3:4:1279:ARG:HB2	2.20	0.42
3:4:740:ASP:CG	3:4:833:MET:HG2	2.45	0.42
3:4:1007:ILE:HG23	3:4:1081:VAL:HG12	2.02	0.42
2:B:484:GLN:HE22	3:C:1318:VAL:HA	1.85	0.42
1:J:61:LEU:C	1:J:63:ASP:H	2.28	0.42
1:J:63:ASP:OD1	1:J:63:ASP:C	2.63	0.42
2:K:323:LYS:C	2:K:412:SER:HB3	2.45	0.42
3:4:712:LEU:HD21	3:4:875:HIS:CE1	2.55	0.42
2:B:473:GLN:O	2:B:476:LYS:HB2	2.20	0.42
3:C:1046:MET:HE1	3:C:1087:GLY:N	2.34	0.42
1:2:59:ASP:C	1:2:61:LEU:H	2.27	0.42
3:4:999:CYS:O	3:4:1159:CYS:HA	2.19	0.42
3:C:1017:ALA:HB1	3:C:1086:TYR:CD2	2.55	0.42
2:K:415:ASP:OD2	2:K:444:PRO:HA	2.20	0.42
3:L:948:LYS:O	3:L:949:GLU:C	2.62	0.42
1:S:43:CYS:HA	3:U:829:ARG:HB2	2.00	0.42
3:U:850:PHE:CD1	3:U:930:VAL:HG13	2.55	0.42
3:4:1079:ALA:O	3:4:1080:SER:HB2	2.20	0.42
2:K:473:GLN:HE21	2:K:482:LEU:HD12	1.85	0.41
3:U:1203:LEU:C	3:U:1203:LEU:HD12	2.45	0.41
3:4:1318:VAL:HG22	3:4:1319:THR:HG22	2.01	0.41
3:C:853:THR:CG2	3:C:944:LYS:NZ	2.84	0.41
3:C:1299:PRO:O	3:C:1304:LYS:HD2	2.20	0.41
1:A:62:GLN:O	1:A:63:ASP:HB3	2.18	0.41
1:J:104:ARG:HE	1:J:162:THR:HG21	1.85	0.41
3:L:1199:PHE:CE1	3:L:1267:GLY:HA2	2.54	0.41
3:4:743:TYR:HD1	3:4:743:TYR:O	2.04	0.41
3:4:1007:ILE:CG2	3:4:1081:VAL:HG12	2.51	0.41
3:C:635:LEU:HD13	3:C:814:LEU:HD23	2.03	0.41
3:C:1287:ASN:HD22	3:C:1289:ASN:H	1.67	0.41
3:L:729:VAL:O	3:L:729:VAL:HG12	2.20	0.41
3:L:803:THR:O	3:L:806:THR:HG23	2.21	0.41
3:L:905:LEU:O	3:L:906:SER:C	2.63	0.41
3:U:1151:HIS:NE2	3:U:1251:LYS:HB3	2.36	0.41
2:3:346:ALA:HB1	5:3:606:FAD:H4'	2.02	0.41
3:4:663:VAL:HG12	3:4:834:LEU:HD11	2.02	0.41
3:4:1031:VAL:HB	3:4:1063:ILE:HG12	2.02	0.41
3:L:840:HIS:CE1	3:L:874:SER:OG	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:23:GLU:OE1	2:T:233:ARG:NH2	2.29	0.41
3:U:624:GLU:HB3	3:U:684:VAL:HG11	2.02	0.41
3:4:1318:VAL:CB	3:4:1319:THR:HG22	2.49	0.41
3:C:670:VAL:HG11	3:C:681:ALA:CB	2.50	0.41
3:C:1261:GLU:N	3:C:1262:PRO:CD	2.83	0.41
3:U:853:THR:HG23	3:U:944:LYS:NZ	2.36	0.41
3:U:1021:ILE:HD13	3:U:1031:VAL:HG13	2.03	0.41
3:C:1318:VAL:N	3:C:1319:THR:HA	2.30	0.41
2:K:456:TYR:CE1	2:K:494:LEU:HD11	2.55	0.41
2:T:487:CYS:HB3	2:T:513:LEU:HD13	2.03	0.41
3:U:703:LYS:HG2	3:U:704:ASN:ND2	2.36	0.41
3:U:779:MET:CE	3:U:814:LEU:HB2	2.51	0.41
3:U:848:VAL:CG2	3:U:926:TRP:HB2	2.50	0.41
3:C:768:ASN:HB2	3:C:802:GLU:O	2.21	0.41
3:C:1044:THR:O	3:C:1048:GLN:HG3	2.20	0.41
3:C:1221:THR:HA	3:C:1226:THR:OG1	2.20	0.41
3:L:871:ARG:O	3:L:872:ASP:C	2.64	0.41
2:T:394:ARG:NH2	2:T:430:ASP:OD2	2.42	0.41
3:U:1143:GLU:O	3:U:1144:THR:HG23	2.21	0.41
1:2:37:ARG:HG2	3:4:595:ASP:HA	2.01	0.41
1:2:80:LEU:HD23	1:2:80:LEU:HA	1.77	0.41
3:4:728:ASN:HB2	3:4:850:PHE:CZ	2.56	0.41
3:4:1271:PHE:CE1	3:4:1300:ALA:HB2	2.56	0.41
3:4:1323:GLY:C	3:4:1325:CYS:HB2	2.45	0.41
2:B:424:ALA:O	3:C:1302:PRO:HG2	2.21	0.41
3:C:1128:SER:HB2	3:L:1072:PRO:HG3	2.03	0.41
3:C:1289:ASN:C	3:C:1291:LYS:N	2.77	0.41
1:J:62:GLN:C	1:J:64:LYS:H	2.28	0.41
2:K:286:GLU:O	2:K:287:LEU:HB2	2.20	0.41
3:L:829:ARG:HG2	3:L:833:MET:HE2	2.02	0.41
3:L:1185:SER:OG	3:L:1191:ASP:OD2	2.25	0.41
3:U:1004:LYS:HE2	3:U:1153:PHE:CE2	2.56	0.41
3:U:1286:THR:HG22	3:U:1310:VAL:HB	2.03	0.41
2:3:507:PHE:CZ	2:3:511:LEU:HD11	2.56	0.41
2:B:323:LYS:HA	2:B:412:SER:O	2.20	0.41
3:C:782:VAL:CG1	3:C:786:ARG:HG3	2.50	0.41
3:C:880:ARG:O	3:C:884:HIS:CD2	2.70	0.41
2:K:314:GLU:O	2:K:318:LYS:HD3	2.20	0.41
3:L:1270:VAL:O	3:L:1271:PHE:C	2.64	0.41
1:S:91:ILE:O	1:S:99:HIS:HB2	2.21	0.41
3:4:601:ASN:HB2	3:4:821:HIS:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:1316:LEU:O	3:4:1318:VAL:CA	2.68	0.41
1:A:46:GLY:HA2	4:A:602:FES:S1	2.60	0.40
2:B:326:VAL:HG11	2:B:410:PRO:HD2	2.02	0.40
1:S:19:ASN:O	1:S:20:ALA:C	2.61	0.40
3:U:1132:PHE:CG	3:4:1126:SER:HB2	2.56	0.40
2:3:242:LEU:O	2:3:246:LEU:HG	2.21	0.40
2:B:286:GLU:O	2:B:288:ASN:N	2.54	0.40
3:L:911:PHE:O	3:L:912:ARG:C	2.63	0.40
3:L:1056:ILE:HB	3:L:1057:PRO:HD2	2.03	0.40
3:U:839:ARG:NH1	3:U:1205:LEU:HD22	2.36	0.40
3:U:999:CYS:O	3:U:1159:CYS:HA	2.21	0.40
3:U:1000:ILE:HD12	3:U:1159:CYS:HB2	2.04	0.40
3:U:1046:MET:CE	3:U:1086:TYR:O	2.68	0.40
2:3:257:LEU:HD13	2:3:281:PRO:HG3	2.02	0.40
1:A:150:CYS:HB2	4:A:601:FES:S1	2.60	0.40
3:C:1289:ASN:C	3:C:1291:LYS:H	2.29	0.40
1:J:99:HIS:HE1	1:J:101:VAL:HG23	1.82	0.40
3:L:601:ASN:HB2	3:L:821:HIS:HD2	1.86	0.40
1:2:21:ASP:HA	1:2:22:PRO:HD3	1.97	0.40
2:3:285:PRO:O	2:3:286:GLU:CD	2.64	0.40
2:B:269:LYS:HG2	2:B:270:PHE:CE1	2.57	0.40
3:C:853:THR:CG2	3:C:944:LYS:HZ2	2.34	0.40
3:C:1007:ILE:O	3:C:1008:SER:CB	2.69	0.40
3:L:1118:MET:SD	3:L:1122:GLN:NE2	2.91	0.40
3:U:1022:HIS:ND1	3:4:1072:PRO:HG3	2.35	0.40
3:U:1046:MET:HE2	3:U:1086:TYR:C	2.46	0.40
2:3:508:ARG:O	2:3:509:ARG:C	2.63	0.40
3:C:776:VAL:O	3:C:779:MET:HG3	2.22	0.40
3:C:1061:ILE:HG22	3:C:1062:TYR:N	2.36	0.40
3:U:602:GLU:HG3	3:U:822:PRO:HB2	2.04	0.40
2:3:264:ILE:HD13	2:3:264:ILE:HA	1.93	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	2	162/165 (98%)	149 (92%)	9 (6%)	4 (2%)	4 8
1	A	160/165 (97%)	150 (94%)	8 (5%)	2 (1%)	9 21
1	J	160/165 (97%)	151 (94%)	6 (4%)	3 (2%)	6 13
1	S	159/165 (96%)	146 (92%)	7 (4%)	6 (4%)	2 3
2	3	303/305 (99%)	283 (93%)	17 (6%)	3 (1%)	12 28
2	B	302/305 (99%)	282 (93%)	17 (6%)	3 (1%)	12 28
2	K	300/305 (98%)	276 (92%)	22 (7%)	2 (1%)	18 38
2	T	303/305 (99%)	284 (94%)	16 (5%)	3 (1%)	12 28
3	4	754/762 (99%)	702 (93%)	42 (6%)	10 (1%)	9 21
3	C	751/762 (99%)	714 (95%)	23 (3%)	14 (2%)	6 13
3	L	743/762 (98%)	707 (95%)	30 (4%)	6 (1%)	16 34
3	U	743/762 (98%)	701 (94%)	37 (5%)	5 (1%)	18 38
All	All	4840/4928 (98%)	4545 (94%)	234 (5%)	61 (1%)	9 21

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	425	SER
3	C	1008	SER
3	C	1318	VAL
3	C	1319	THR
3	C	1321	ALA
2	K	425	SER
3	L	1008	SER
1	S	64	LYS
3	U	1008	SER
1	2	64	LYS
2	3	426	ARG
3	4	1008	SER
3	4	1319	THR
3	4	1321	ALA
1	A	61	LEU
3	C	721	LYS
3	C	798	PHE
3	C	912	ARG
3	C	1322	PRO

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Mol	Chain	Res	Type
3	C	1323	GLY
3	L	721	LYS
3	L	912	ARG
1	S	62	GLN
3	U	721	LYS
3	U	912	ARG
3	U	1144	THR
3	4	721	LYS
1	A	60	ARG
3	C	1139	GLY
3	C	1320	GLY
1	J	61	LEU
2	K	426	ARG
1	S	63	ASP
2	T	426	ARG
1	2	43	CYS
1	2	60	ARG
3	4	912	ARG
3	4	1144	THR
3	4	1317	CYS
1	S	60	ARG
1	S	162	THR
2	T	282	ALA
1	2	164	ALA
3	4	797	GLY
3	4	1325	CYS
2	B	287	LEU
2	B	377	ARG
3	C	797	GLY
1	J	60	ARG
1	J	162	THR
3	L	1287	ASN
1	S	43	CYS
2	3	286	GLU
2	3	425	SER
3	C	623	SER
3	C	1317	CYS
3	L	797	GLY
2	T	286	GLU
3	U	797	GLY
3	4	1318	VAL
3	L	1139	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	2	137/138 (99%)	129 (94%)	8 (6%)	18	39
1	A	136/138 (99%)	125 (92%)	11 (8%)	11	24
1	J	136/138 (99%)	128 (94%)	8 (6%)	18	38
1	S	135/138 (98%)	126 (93%)	9 (7%)	15	33
2	3	261/261 (100%)	245 (94%)	16 (6%)	17	37
2	B	261/261 (100%)	242 (93%)	19 (7%)	13	29
2	K	259/261 (99%)	242 (93%)	17 (7%)	15	34
2	T	261/261 (100%)	244 (94%)	17 (6%)	15	35
3	4	632/638 (99%)	604 (96%)	28 (4%)	25	50
3	C	629/638 (99%)	608 (97%)	21 (3%)	33	61
3	L	624/638 (98%)	599 (96%)	25 (4%)	28	55
3	U	624/638 (98%)	593 (95%)	31 (5%)	22	46
All	All	4095/4148 (99%)	3885 (95%)	210 (5%)	21	45

All (210) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LYS
1	A	61	LEU
1	A	63	ASP
1	A	65	ILE
1	A	89	GLU
1	A	93	SER
1	A	97	ARG
1	A	104	ARG
1	A	129	ARG
1	A	140	GLU
1	A	141	ASP
2	B	225	LYS
2	B	230	GLU
2	B	243	LYS

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Mol	Chain	Res	Type
2	B	256	LYS
2	B	277	MET
2	B	312	LEU
2	B	316	VAL
2	B	335	ARG
2	B	337	PHE
2	B	343	LYS
2	B	344	SER
2	B	348	LEU
2	B	401	GLU
2	B	419	SER
2	B	472	LYS
2	B	482	LEU
2	B	484	GLN
2	B	509	ARG
2	B	513	LEU
3	C	598	ARG
3	C	609	THR
3	C	684	VAL
3	C	703	LYS
3	C	729	VAL
3	C	736	ILE
3	C	743	TYR
3	C	779	MET
3	C	829	ARG
3	C	848	VAL
3	C	939	GLU
3	C	1001	ILE
3	C	1105	LYS
3	C	1144	THR
3	C	1203	LEU
3	C	1238	GLU
3	C	1286	THR
3	C	1290	THR
3	C	1292	GLU
3	C	1316	LEU
3	C	1318	VAL
1	J	33	LYS
1	J	63	ASP
1	J	65	ILE
1	J	89	GLU
1	J	97	ARG

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Mol	Chain	Res	Type
1	J	104	ARG
1	J	129	ARG
1	J	140	GLU
2	K	230	GLU
2	K	243	LYS
2	K	277	MET
2	K	312	LEU
2	K	316	VAL
2	K	328	ARG
2	K	335	ARG
2	K	337	PHE
2	K	343	LYS
2	K	344	SER
2	K	348	LEU
2	K	358	ILE
2	K	401	GLU
2	K	419	SER
2	K	482	LEU
2	K	509	ARG
2	K	513	LEU
3	L	598	ARG
3	L	609	THR
3	L	684	VAL
3	L	696	ILE
3	L	729	VAL
3	L	736	ILE
3	L	743	TYR
3	L	779	MET
3	L	829	ARG
3	L	848	VAL
3	L	852	LYS
3	L	939	GLU
3	L	982	SER
3	L	1000	ILE
3	L	1001	ILE
3	L	1047	VAL
3	L	1105	LYS
3	L	1134	ARG
3	L	1143	GLU
3	L	1144	THR
3	L	1203	LEU
3	L	1238	GLU

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Mol	Chain	Res	Type
3	L	1286	THR
3	L	1290	THR
3	L	1292	GLU
1	S	33	LYS
1	S	64	LYS
1	S	89	GLU
1	S	93	SER
1	S	97	ARG
1	S	104	ARG
1	S	120	ILE
1	S	129	ARG
1	S	140	GLU
2	T	243	LYS
2	T	257	LEU
2	T	277	MET
2	T	298	SER
2	T	312	LEU
2	T	328	ARG
2	T	395	LYS
2	T	398	LEU
2	T	401	GLU
2	T	412	SER
2	T	419	SER
2	T	427	ARG
2	T	472	LYS
2	T	476	LYS
2	T	482	LEU
2	T	513	LEU
2	T	525	LYS
3	U	598	ARG
3	U	609	THR
3	U	616	LYS
3	U	636	SER
3	U	670	VAL
3	U	688	THR
3	U	696	ILE
3	U	719	LEU
3	U	721	LYS
3	U	736	ILE
3	U	743	TYR
3	U	754	LYS
3	U	764	VAL

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Mol	Chain	Res	Type
3	U	774	SER
3	U	782	VAL
3	U	848	VAL
3	U	856	ILE
3	U	871	ARG
3	U	939	GLU
3	U	951	ASP
3	U	973	LYS
3	U	1021	ILE
3	U	1105	LYS
3	U	1143	GLU
3	U	1172	LYS
3	U	1184	SER
3	U	1200	VAL
3	U	1203	LEU
3	U	1208	LEU
3	U	1290	THR
3	U	1292	GLU
1	2	33	LYS
1	2	61	LEU
1	2	89	GLU
1	2	93	SER
1	2	97	ARG
1	2	104	ARG
1	2	129	ARG
1	2	140	GLU
2	3	237	ILE
2	3	241	THR
2	3	243	LYS
2	3	257	LEU
2	3	277	MET
2	3	298	SER
2	3	312	LEU
2	3	328	ARG
2	3	348	LEU
2	3	395	LYS
2	3	419	SER
2	3	427	ARG
2	3	472	LYS
2	3	476	LYS
2	3	482	LEU
2	3	513	LEU

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Mol	Chain	Res	Type
3	4	598	ARG
3	4	609	THR
3	4	623	SER
3	4	626	GLN
3	4	688	THR
3	4	696	ILE
3	4	719	LEU
3	4	721	LYS
3	4	736	ILE
3	4	743	TYR
3	4	744	LEU
3	4	764	VAL
3	4	779	MET
3	4	782	VAL
3	4	848	VAL
3	4	939	GLU
3	4	951	ASP
3	4	953	THR
3	4	1008	SER
3	4	1021	ILE
3	4	1105	LYS
3	4	1143	GLU
3	4	1203	LEU
3	4	1208	LEU
3	4	1290	THR
3	4	1318	VAL
3	4	1325	CYS
3	4	1326	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (103) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	HIS
1	A	131	GLN
2	B	261	ASN
2	B	272	ASN
2	B	273	GLN
2	B	351	ASN
2	B	473	GLN
3	C	614	HIS
3	C	626	GLN
3	C	677	HIS

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Mol	Chain	Res	Type
3	C	683	HIS
3	C	840	HIS
3	C	884	HIS
3	C	904	ASN
3	C	991	ASN
3	C	1016	GLN
3	C	1033	HIS
3	C	1048	GLN
3	C	1148	ASN
3	C	1173	ASN
3	C	1212	HIS
3	C	1220	HIS
3	C	1284	GLN
3	C	1285	HIS
3	C	1287	ASN
1	J	82	HIS
1	J	131	GLN
1	J	146	ASN
2	K	272	ASN
2	K	273	GLN
2	K	292	HIS
2	K	351	ASN
2	K	387	HIS
2	K	473	GLN
2	K	484	GLN
3	L	614	HIS
3	L	626	GLN
3	L	677	HIS
3	L	683	HIS
3	L	840	HIS
3	L	875	HIS
3	L	884	HIS
3	L	904	ASN
3	L	1016	GLN
3	L	1033	HIS
3	L	1048	GLN
3	L	1069	ASN
3	L	1108	ASN
3	L	1212	HIS
3	L	1284	GLN
3	L	1285	HIS
3	L	1287	ASN

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Mol	Chain	Res	Type
1	S	109	HIS
1	S	131	GLN
1	S	146	ASN
2	T	273	GLN
2	T	473	GLN
3	U	614	HIS
3	U	626	GLN
3	U	677	HIS
3	U	683	HIS
3	U	704	ASN
3	U	705	ASN
3	U	821	HIS
3	U	840	HIS
3	U	875	HIS
3	U	884	HIS
3	U	904	ASN
3	U	1016	GLN
3	U	1033	HIS
3	U	1048	GLN
3	U	1088	GLN
3	U	1095	GLN
3	U	1173	ASN
3	U	1284	GLN
3	U	1287	ASN
1	2	19	ASN
1	2	131	GLN
2	3	226	GLN
2	3	273	GLN
2	3	351	ASN
2	3	473	GLN
3	4	614	HIS
3	4	626	GLN
3	4	677	HIS
3	4	683	HIS
3	4	704	ASN
3	4	747	HIS
3	4	821	HIS
3	4	830	ASN
3	4	840	HIS
3	4	869	ASN
3	4	875	HIS
3	4	884	HIS

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Mol	Chain	Res	Type
3	4	904	ASN
3	4	1016	GLN
3	4	1033	HIS
3	4	1048	GLN
3	4	1148	ASN
3	4	1173	ASN
3	4	1284	GLN
3	4	1287	ASN
3	4	1307	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	FAD	T	606	-	58,58,58	1.21	6 (10%)	85,89,89	1.72	18 (21%)
8	XAN	C	7319	-	12,12,12	1.88	2 (16%)	14,17,17	2.31	6 (42%)
4	FES	A	602	1	0,4,4	-	-	-		
4	FES	S	602	1	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	FES	2	602	1	0,4,4	-	-	-		
4	FES	S	601	1	0,4,4	-	-	-		
6	MTE	U	1333	7	21,26,26	1.59	3 (14%)	19,40,40	2.42	9 (47%)
8	XAN	L	7319	-	12,12,12	1.86	1 (8%)	14,17,17	2.26	6 (42%)
7	MOM	4	1334	6	0,3,3	-	-	-		
5	FAD	K	606	-	58,58,58	1.05	5 (8%)	85,89,89	1.75	21 (24%)
8	XAN	4	7319	-	12,12,12	1.95	1 (8%)	14,17,17	2.41	7 (50%)
7	MOM	L	1334	6	0,3,3	-	-	-		
4	FES	J	602	1	0,4,4	-	-	-		
6	MTE	4	1333	7	21,26,26	1.82	3 (14%)	19,40,40	2.52	10 (52%)
8	XAN	U	7319	-	12,12,12	1.97	2 (16%)	14,17,17	2.19	6 (42%)
6	MTE	C	1333	7	21,26,26	1.70	2 (9%)	19,40,40	3.02	8 (42%)
4	FES	2	601	1	0,4,4	-	-	-		
5	FAD	3	606	-	58,58,58	1.27	5 (8%)	85,89,89	1.81	22 (25%)
5	FAD	B	606	-	58,58,58	1.18	5 (8%)	85,89,89	1.87	23 (27%)
7	MOM	U	1334	6	0,3,3	-	-	-		
6	MTE	L	1333	7	21,26,26	1.62	2 (9%)	19,40,40	2.55	8 (42%)
4	FES	A	601	1	0,4,4	-	-	-		
7	MOM	C	1334	6	0,3,3	-	-	-		
4	FES	J	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
5	FAD	T	606	-	-	4/34/50/50	0/6/6/6
8	XAN	C	7319	-	-	-	0/2/2/2
4	FES	A	602	1	-	-	0/1/1/1
4	FES	S	602	1	-	-	0/1/1/1
4	FES	2	602	1	-	-	0/1/1/1
4	FES	S	601	1	-	-	0/1/1/1
6	MTE	U	1333	7	-	3/6/34/34	0/3/3/3
8	XAN	L	7319	-	-	-	0/2/2/2
5	FAD	K	606	-	-	5/34/50/50	0/6/6/6
8	XAN	4	7319	-	-	-	0/2/2/2
4	FES	J	602	1	-	-	0/1/1/1
6	MTE	4	1333	7	-	1/6/34/34	0/3/3/3
8	XAN	U	7319	-	-	-	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MTE	C	1333	7	-	1/6/34/34	0/3/3/3
5	FAD	3	606	-	-	7/34/50/50	0/6/6/6
4	FES	2	601	1	-	-	0/1/1/1
5	FAD	B	606	-	-	3/34/50/50	0/6/6/6
6	MTE	L	1333	7	-	1/6/34/34	0/3/3/3
4	FES	A	601	1	-	-	0/1/1/1
4	FES	J	601	1	-	-	0/1/1/1

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	4	1333	MTE	C9-C10	6.69	1.50	1.38
6	L	1333	MTE	C9-C10	6.05	1.49	1.38
6	C	1333	MTE	C9-C10	6.03	1.48	1.38
6	U	1333	MTE	C9-C10	5.58	1.48	1.38
8	U	7319	XAN	C5-C4	5.41	1.48	1.38
8	L	7319	XAN	C5-C4	5.20	1.48	1.38
5	3	606	FAD	C4X-N5	5.01	1.41	1.30
8	4	7319	XAN	C5-C4	4.98	1.47	1.38
8	C	7319	XAN	C5-C4	4.79	1.47	1.38
5	B	606	FAD	C4X-N5	4.01	1.39	1.30
5	T	606	FAD	C4X-N5	3.44	1.38	1.30
5	K	606	FAD	C4X-N5	3.36	1.38	1.30
5	B	606	FAD	C2A-N1A	3.31	1.39	1.33
5	T	606	FAD	C2A-N1A	3.07	1.39	1.33
5	K	606	FAD	C8A-N7A	3.01	1.37	1.31
5	3	606	FAD	C2A-N1A	2.91	1.39	1.33
6	4	1333	MTE	C9-C4	2.73	1.50	1.41
5	3	606	FAD	C2A-N3A	2.69	1.38	1.33
5	3	606	FAD	C10-N1	2.68	1.38	1.33
5	K	606	FAD	C2A-N1A	2.63	1.38	1.33
5	K	606	FAD	C10-N1	2.58	1.38	1.33
6	C	1333	MTE	C9-C4	2.58	1.49	1.41
5	3	606	FAD	C5A-N7A	-2.55	1.34	1.39
5	T	606	FAD	C10-N1	2.52	1.38	1.33
5	T	606	FAD	C5A-N7A	-2.45	1.34	1.39
5	T	606	FAD	C8A-N7A	2.37	1.36	1.31
5	B	606	FAD	C10-N1	2.37	1.38	1.33
5	B	606	FAD	C8A-N7A	2.36	1.36	1.31
5	B	606	FAD	C2A-N3A	2.23	1.37	1.33
6	U	1333	MTE	C9-C4	2.22	1.48	1.41
5	T	606	FAD	C2A-N3A	2.15	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	7319	XAN	C4-N3	-2.10	1.33	1.37
8	U	7319	XAN	C6-N1	-2.09	1.34	1.38
6	U	1333	MTE	C4-N3	-2.08	1.35	1.38
6	L	1333	MTE	C4-N3	-2.05	1.35	1.38
6	4	1333	MTE	C4-N3	-2.05	1.35	1.38
5	K	606	FAD	O4B-C4B	-2.01	1.40	1.45

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	1333	MTE	O3'-C7-C6	7.57	114.01	108.96
6	4	1333	MTE	O3'-C7-N8	-6.26	102.92	108.61
5	B	606	FAD	N3A-C2A-N1A	-5.95	119.58	128.58
5	T	606	FAD	N3A-C2A-N1A	-5.86	119.70	128.58
6	C	1333	MTE	C7-C6-N5	5.81	113.58	107.87
5	3	606	FAD	N3A-C2A-N1A	-5.76	119.86	128.58
5	K	606	FAD	N3A-C2A-N1A	-5.76	119.87	128.58
6	C	1333	MTE	C2-N1-C10	5.10	122.36	113.36
6	L	1333	MTE	O3'-C7-N8	4.93	113.08	108.61
6	L	1333	MTE	C2-N1-C10	4.73	121.71	113.36
5	3	606	FAD	C5A-C4A-N3A	-4.73	120.21	126.72
5	K	606	FAD	N9A-C8A-N7A	-4.62	107.38	113.94
5	B	606	FAD	N9A-C8A-N7A	-4.53	107.51	113.94
6	U	1333	MTE	C2-N1-C10	4.52	121.34	113.36
8	U	7319	XAN	N1-C2-N3	4.49	122.80	115.74
8	C	7319	XAN	N1-C2-N3	4.42	122.69	115.74
8	4	7319	XAN	N1-C2-N3	4.33	122.55	115.74
5	B	606	FAD	C4-N3-C2	-4.11	118.34	125.64
6	L	1333	MTE	O3'-C7-C6	-4.11	106.22	108.96
5	T	606	FAD	N9A-C8A-N7A	-4.10	108.12	113.94
6	U	1333	MTE	O4'-P-O1P	-4.07	95.43	106.44
5	T	606	FAD	C5A-C4A-N3A	-4.06	121.12	126.72
6	L	1333	MTE	O4-C4-C9	-4.04	117.51	127.26
8	L	7319	XAN	N1-C2-N3	4.00	122.03	115.74
5	B	606	FAD	O3'-C3'-C2'	-4.00	99.85	108.93
5	K	606	FAD	C5A-C4A-N3A	-3.99	121.23	126.72
5	K	606	FAD	C5A-N7A-C8A	3.97	109.70	103.45
6	4	1333	MTE	O3'-C7-C6	3.96	111.61	108.96
6	U	1333	MTE	O3'-C7-N8	-3.90	105.07	108.61
5	K	606	FAD	C4-N3-C2	-3.87	118.77	125.64
6	C	1333	MTE	C4-C9-N5	3.77	126.55	116.27
6	U	1333	MTE	C7-C6-N5	3.73	111.53	107.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	606	FAD	C5A-N7A-C8A	3.71	109.28	103.45
5	B	606	FAD	C5A-C4A-N3A	-3.70	121.62	126.72
5	T	606	FAD	C5A-N7A-C8A	3.63	109.16	103.45
5	3	606	FAD	C2A-N3A-C4A	3.62	120.68	111.83
5	K	606	FAD	O2P-P-O3P	3.54	116.84	107.27
5	3	606	FAD	N9A-C8A-N7A	-3.48	108.99	113.94
8	L	7319	XAN	N9-C4-N3	3.48	135.76	128.34
5	T	606	FAD	C4-N3-C2	-3.46	119.50	125.64
5	T	606	FAD	O4-C4-C4X	-3.37	117.64	126.53
8	L	7319	XAN	O6-C6-C5	-3.34	117.71	126.53
8	4	7319	XAN	C6-N1-C2	-3.32	121.79	126.37
5	3	606	FAD	C5A-N7A-C8A	3.30	108.63	103.45
8	U	7319	XAN	N9-C4-N3	3.29	135.35	128.34
8	4	7319	XAN	C6-C5-N7	3.26	136.22	130.29
8	C	7319	XAN	C6-N1-C2	-3.23	121.92	126.37
6	4	1333	MTE	C4-C9-N5	3.23	125.07	116.27
5	K	606	FAD	C2A-N3A-C4A	3.22	119.70	111.83
5	B	606	FAD	C2A-N3A-C4A	3.21	119.67	111.83
8	4	7319	XAN	N9-C4-N3	3.21	135.19	128.34
5	B	606	FAD	C10-C4X-N5	-3.19	118.29	124.81
8	C	7319	XAN	N9-C4-N3	3.19	135.15	128.34
5	T	606	FAD	C2A-N3A-C4A	3.17	119.57	111.83
5	3	606	FAD	N3A-C4A-N9A	3.15	132.53	127.17
5	3	606	FAD	O3P-PA-O1A	3.11	120.07	110.70
6	L	1333	MTE	C9-C4-N3	3.03	120.46	112.13
5	3	606	FAD	C4-N3-C2	-3.01	120.30	125.64
5	B	606	FAD	C4X-C4-N3	2.98	120.84	113.25
6	4	1333	MTE	C2-N1-C10	2.97	118.59	113.36
8	L	7319	XAN	C6-N1-C2	-2.95	122.31	126.37
5	B	606	FAD	O4B-C1B-N9A	-2.94	102.44	108.09
8	C	7319	XAN	C6-C5-N7	2.92	135.61	130.29
6	L	1333	MTE	O4'-C4'-C3'	2.92	115.79	108.58
5	B	606	FAD	C5X-N5-C4X	2.84	122.68	118.09
5	3	606	FAD	C4X-C10-N10	2.84	120.54	116.48
6	4	1333	MTE	O2P-P-O1P	2.81	121.78	110.83
5	B	606	FAD	C9A-C5X-N5	-2.81	119.48	122.45
5	T	606	FAD	C9A-C5X-N5	-2.80	119.48	122.45
5	K	606	FAD	C10-C4X-N5	-2.80	119.10	124.81
5	3	606	FAD	O3B-C3B-C4B	-2.80	103.05	111.08
6	L	1333	MTE	C4-C9-N5	2.79	123.88	116.27
5	B	606	FAD	C4X-C10-N10	2.77	120.45	116.48
8	U	7319	XAN	O6-C6-C5	-2.77	119.23	126.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	4	1333	MTE	O4'-C4'-C3'	2.75	115.37	108.58
5	3	606	FAD	C4X-C4-N3	2.75	120.24	113.25
6	C	1333	MTE	O4'-P-O1P	-2.74	99.02	106.44
5	T	606	FAD	C4-C4X-C10	2.73	121.61	116.93
6	U	1333	MTE	N2-C2-N3	2.72	122.50	116.76
5	B	606	FAD	C6-C5X-C9A	2.72	122.78	119.05
5	B	606	FAD	O4'-C4'-C3'	2.70	115.57	109.25
8	U	7319	XAN	C6-N1-C2	-2.69	122.66	126.37
5	K	606	FAD	C4A-C5A-N7A	-2.69	107.51	110.58
5	B	606	FAD	N3A-C4A-N9A	2.68	131.72	127.17
6	U	1333	MTE	C4-C9-N5	2.67	123.56	116.27
5	K	606	FAD	O4-C4-C4X	-2.65	119.54	126.53
8	C	7319	XAN	O6-C6-C5	-2.62	119.62	126.53
5	3	606	FAD	O5'-C5'-C4'	-2.61	102.39	109.36
5	B	606	FAD	C4X-C10-N1	-2.61	118.19	124.59
6	C	1333	MTE	C9-C4-N3	2.58	119.21	112.13
6	4	1333	MTE	O4'-P-O1P	-2.57	99.51	106.44
5	B	606	FAD	C4A-N9A-C8A	2.56	108.43	105.74
6	U	1333	MTE	O4-C4-C9	-2.56	121.09	127.26
8	U	7319	XAN	O2-C2-N1	-2.55	117.34	121.86
5	T	606	FAD	N3A-C4A-N9A	2.53	131.47	127.17
5	K	606	FAD	N3A-C4A-N9A	2.53	131.47	127.17
5	B	606	FAD	C10-N1-C2	2.53	122.33	116.85
6	C	1333	MTE	O4'-C4'-C3'	2.53	114.82	108.58
5	3	606	FAD	C5'-C4'-C3'	-2.53	107.45	112.22
5	B	606	FAD	O5B-C5B-C4B	2.52	117.59	108.99
5	3	606	FAD	C10-C4X-N5	-2.52	119.66	124.81
5	K	606	FAD	O2-C2-N1	-2.51	117.63	121.80
8	4	7319	XAN	O6-C6-C5	-2.51	119.92	126.53
5	K	606	FAD	C5'-C4'-C3'	-2.48	107.54	112.22
5	T	606	FAD	C4A-C5A-N7A	-2.48	107.75	110.58
6	U	1333	MTE	N2-C2-N1	-2.47	114.85	119.67
6	C	1333	MTE	O2P-P-O1P	2.47	120.45	110.83
5	3	606	FAD	O3P-P-O1P	2.44	118.06	110.70
5	K	606	FAD	C9A-C5X-N5	-2.43	119.87	122.45
5	K	606	FAD	C4X-C4-N3	2.43	119.43	113.25
5	3	606	FAD	C3B-C2B-C1B	2.41	106.02	101.46
5	3	606	FAD	C4A-C5A-N7A	-2.40	107.84	110.58
5	K	606	FAD	C4X-C10-N10	2.40	119.91	116.48
5	B	606	FAD	C4-C4X-N5	2.38	121.49	118.21
5	3	606	FAD	C4X-C10-N1	-2.35	118.82	124.59
5	K	606	FAD	C4-C4X-C10	2.35	120.96	116.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	K	606	FAD	C5A-C6A-N6A	-2.33	117.50	123.29
6	U	1333	MTE	O2P-P-O1P	2.33	119.93	110.83
6	4	1333	MTE	O2P-P-O4'	-2.32	100.61	106.67
6	L	1333	MTE	C2-N3-C4	-2.31	120.92	125.11
8	L	7319	XAN	C6-C5-N7	2.30	134.48	130.29
8	4	7319	XAN	C8-N7-C5	2.30	107.48	104.38
5	T	606	FAD	O2'-C2'-C3'	2.29	114.60	109.25
5	3	606	FAD	C9A-C5X-N5	-2.29	120.03	122.45
5	K	606	FAD	C4A-N9A-C8A	2.26	108.11	105.74
8	4	7319	XAN	O2-C2-N3	-2.24	117.88	121.86
5	K	606	FAD	C5X-N5-C4X	2.24	121.71	118.09
5	T	606	FAD	C6A-C5A-C4A	2.23	120.23	117.18
5	3	606	FAD	O5'-P-O1P	-2.23	100.08	108.94
5	K	606	FAD	C4X-C10-N1	-2.22	119.14	124.59
5	3	606	FAD	C5X-C9A-N10	2.21	119.96	117.97
5	T	606	FAD	C10-C4X-N5	-2.20	120.31	124.81
8	U	7319	XAN	C6-C5-N7	2.20	134.29	130.29
6	4	1333	MTE	C9-C4-N3	2.17	118.08	112.13
5	B	606	FAD	C4A-C5A-N7A	-2.16	108.11	110.58
5	3	606	FAD	O2'-C2'-C3'	-2.16	104.19	109.25
5	T	606	FAD	O3'-C3'-C2'	-2.14	104.07	108.93
5	T	606	FAD	C5X-C9A-N10	2.13	119.90	117.97
5	T	606	FAD	C4X-C4-N3	2.13	118.68	113.25
6	4	1333	MTE	O4-C4-C9	-2.10	122.20	127.26
5	B	606	FAD	C2B-C3B-C4B	-2.06	98.63	102.61
8	L	7319	XAN	O6-C6-N1	2.04	123.96	120.11
8	C	7319	XAN	O2-C2-N1	-2.03	118.25	121.86
5	T	606	FAD	O5B-C5B-C4B	2.01	115.83	108.99

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	606	FAD	C5B-O5B-PA-O1A
5	K	606	FAD	C5B-O5B-PA-O1A
5	K	606	FAD	C5B-O5B-PA-O2A
5	K	606	FAD	C5B-O5B-PA-O3P
5	T	606	FAD	C5B-O5B-PA-O1A
5	T	606	FAD	C5B-O5B-PA-O2A
5	3	606	FAD	C5B-O5B-PA-O1A
5	3	606	FAD	C5B-O5B-PA-O2A
5	3	606	FAD	C5B-O5B-PA-O3P

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Mol	Chain	Res	Type	Atoms
6	U	1333	MTE	C2'-C3'-C4'-O4'
6	U	1333	MTE	O3'-C3'-C4'-O4'
5	3	606	FAD	O4B-C4B-C5B-O5B
6	C	1333	MTE	C3'-C4'-O4'-P
5	K	606	FAD	O4B-C4B-C5B-O5B
5	3	606	FAD	C3B-C4B-C5B-O5B
5	B	606	FAD	C3B-C4B-C5B-O5B
6	U	1333	MTE	C3'-C4'-O4'-P
5	B	606	FAD	O4B-C4B-C5B-O5B
5	K	606	FAD	C3B-C4B-C5B-O5B
6	L	1333	MTE	C3'-C4'-O4'-P
6	4	1333	MTE	C3'-C4'-O4'-P
5	T	606	FAD	O4B-C4B-C5B-O5B
5	T	606	FAD	C5B-O5B-PA-O3P
5	3	606	FAD	C4'-C5'-O5'-P
5	3	606	FAD	PA-O3P-P-O1P

There are no ring outliers.

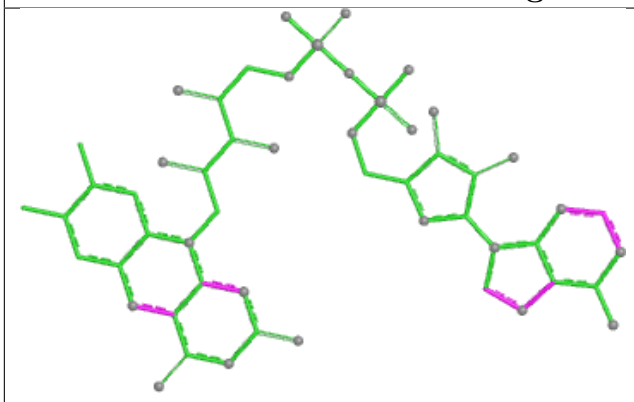
15 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	T	606	FAD	2	0
8	C	7319	XAN	1	0
4	A	602	FES	1	0
8	L	7319	XAN	1	0
7	4	1334	MOM	2	0
5	K	606	FAD	3	0
8	4	7319	XAN	1	0
7	L	1334	MOM	2	0
8	U	7319	XAN	2	0
5	3	606	FAD	2	0
5	B	606	FAD	1	0
7	U	1334	MOM	3	0
6	L	1333	MTE	1	0
4	A	601	FES	1	0
7	C	1334	MOM	2	0

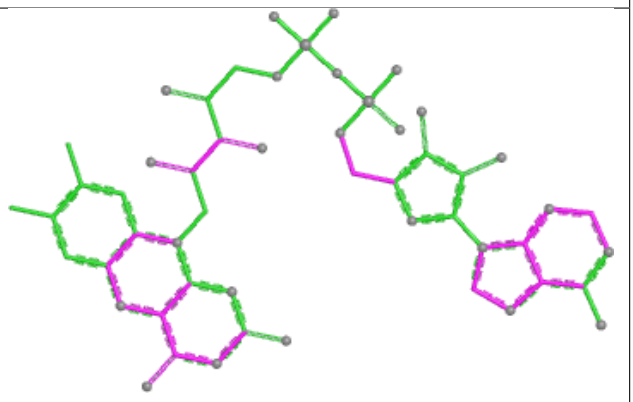
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

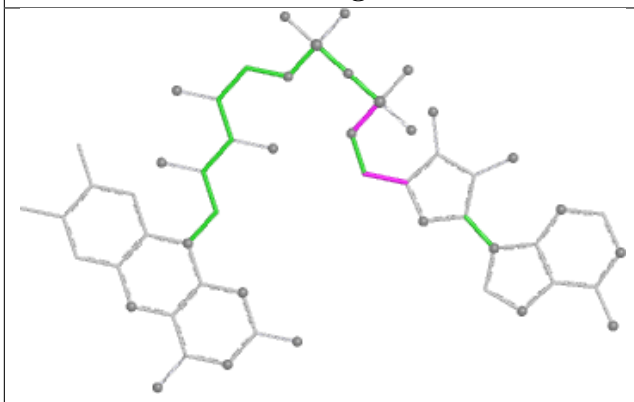
Ligand FAD T 606



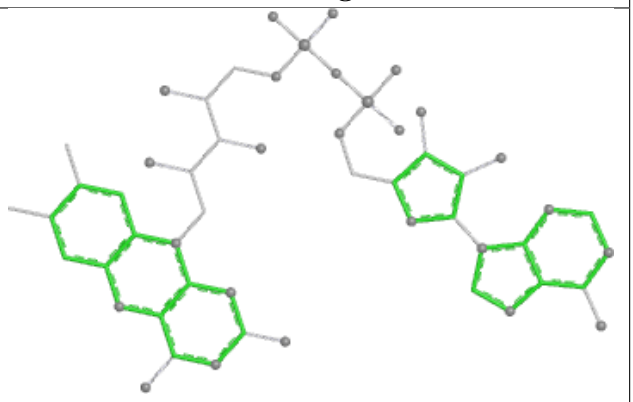
Bond lengths



Bond angles

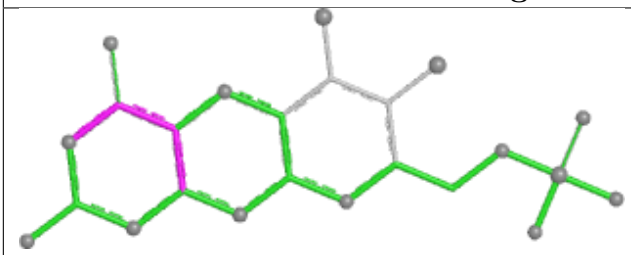


Torsions

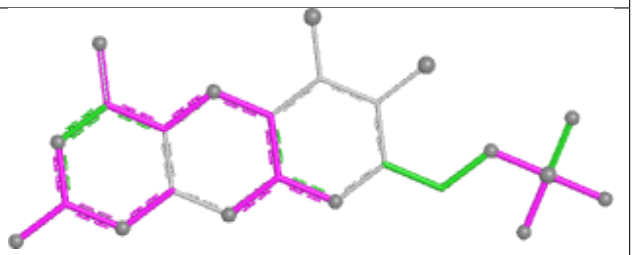


Rings

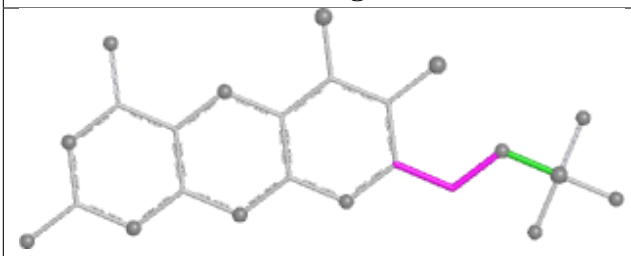
Ligand MTE U 1333



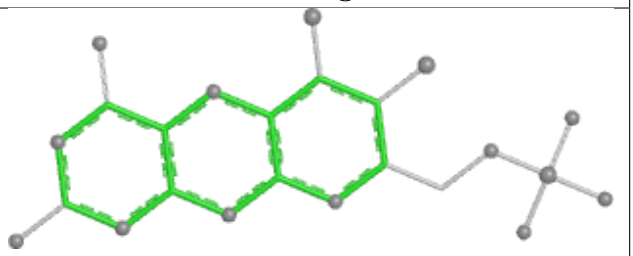
Bond lengths



Bond angles

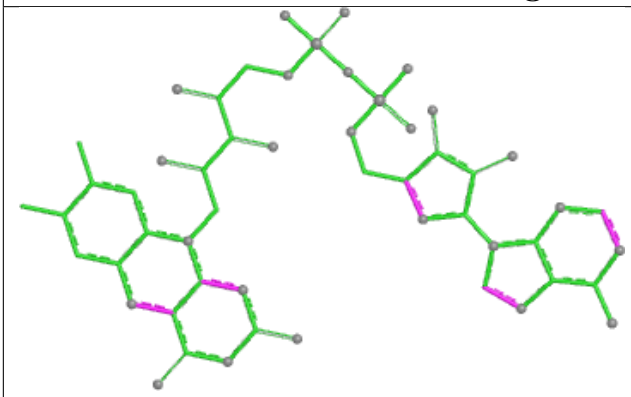


Torsions

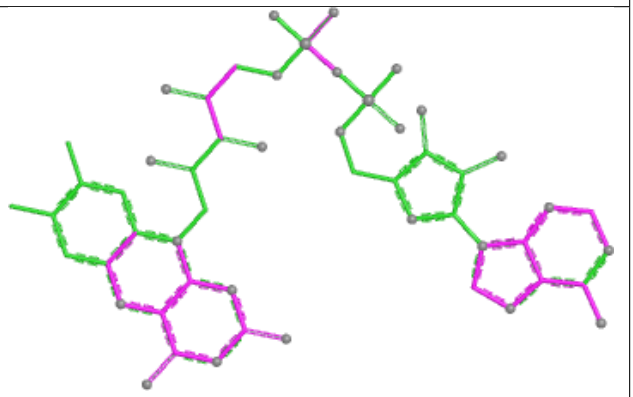


Rings

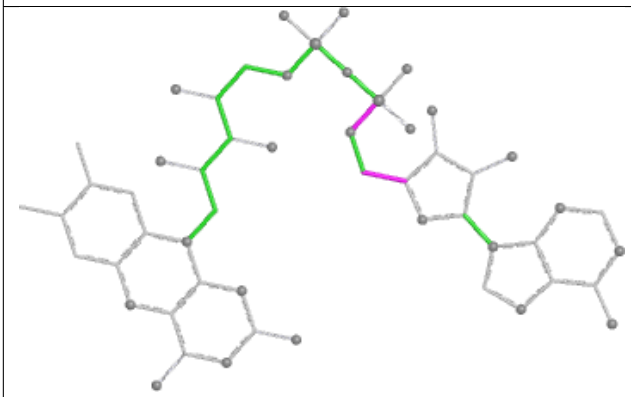
Ligand FAD K 606



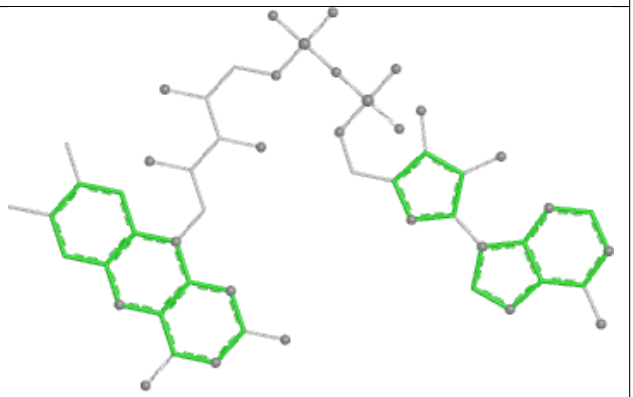
Bond lengths



Bond angles

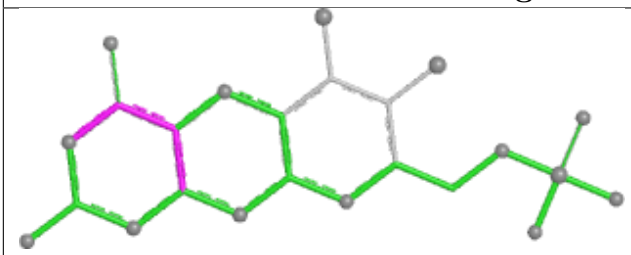


Torsions

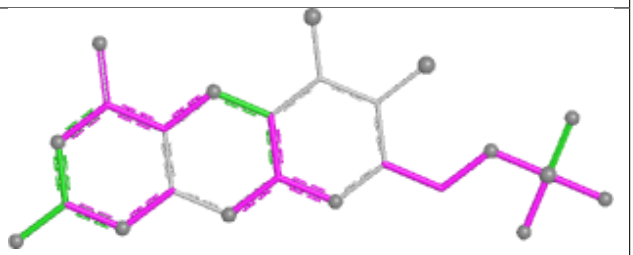


Rings

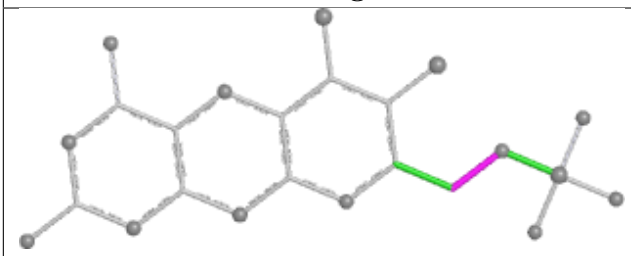
Ligand MTE 4 1333



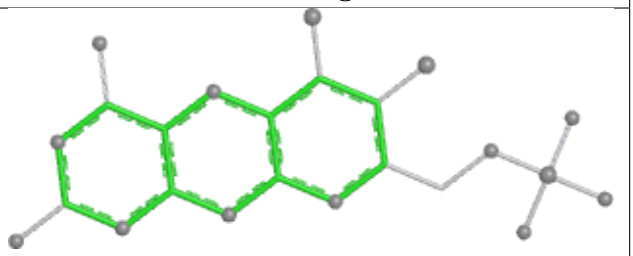
Bond lengths



Bond angles

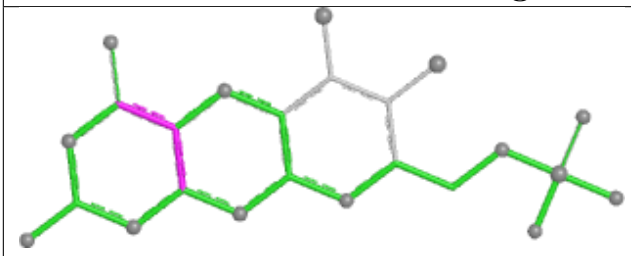


Torsions

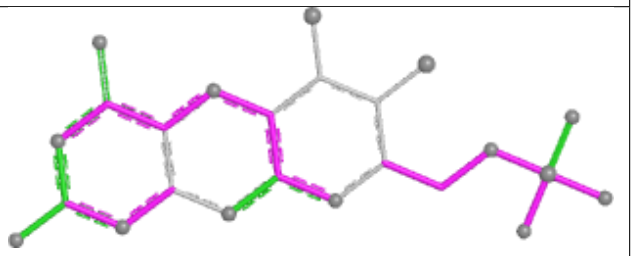


Rings

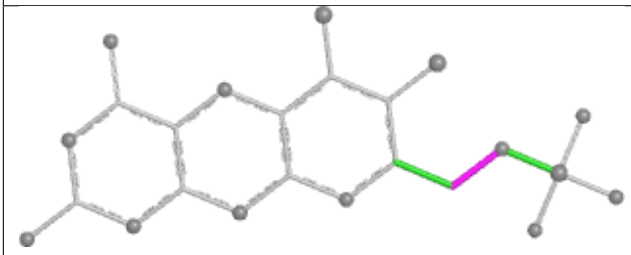
Ligand MTE C 1333



Bond lengths



Bond angles



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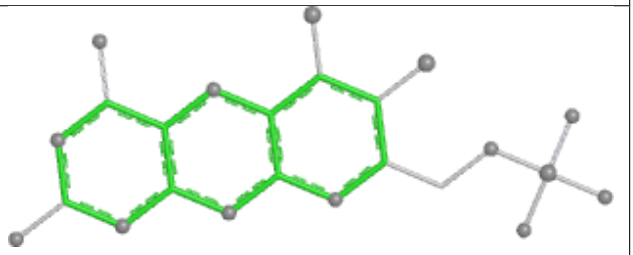
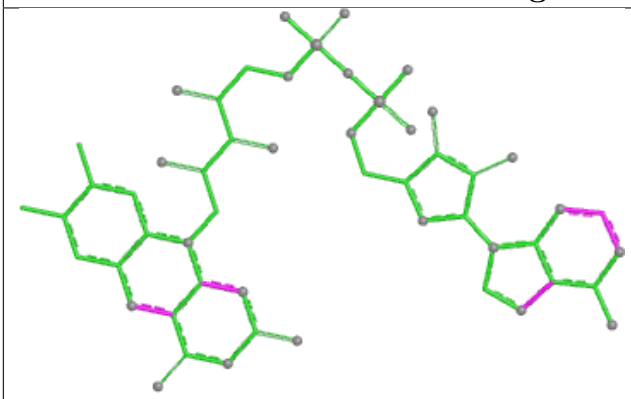
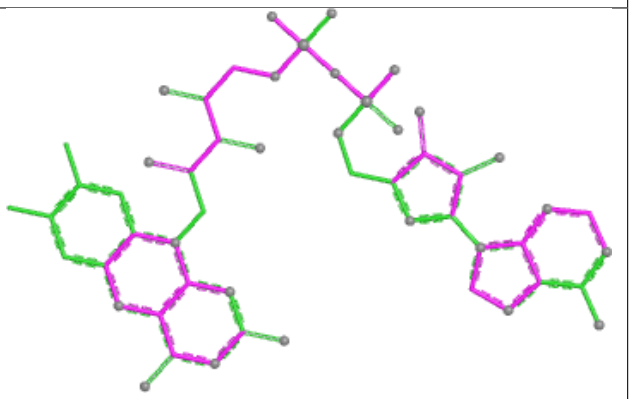


Rings

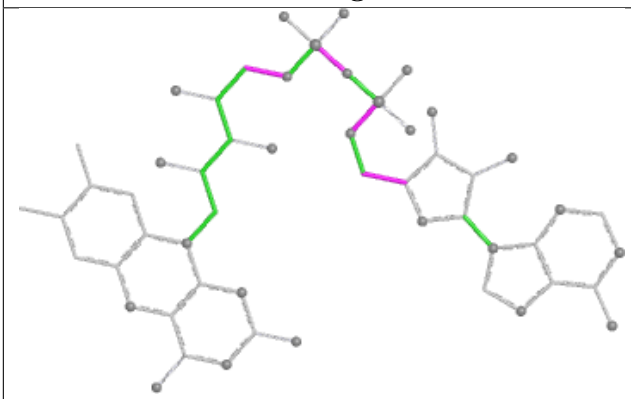
Ligand FAD 3 606



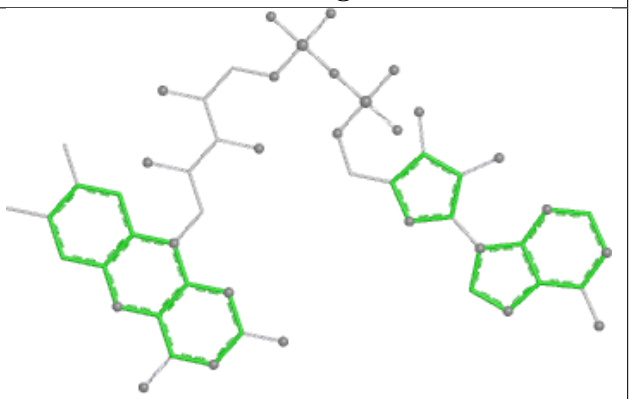
Bond lengths



Bond angles

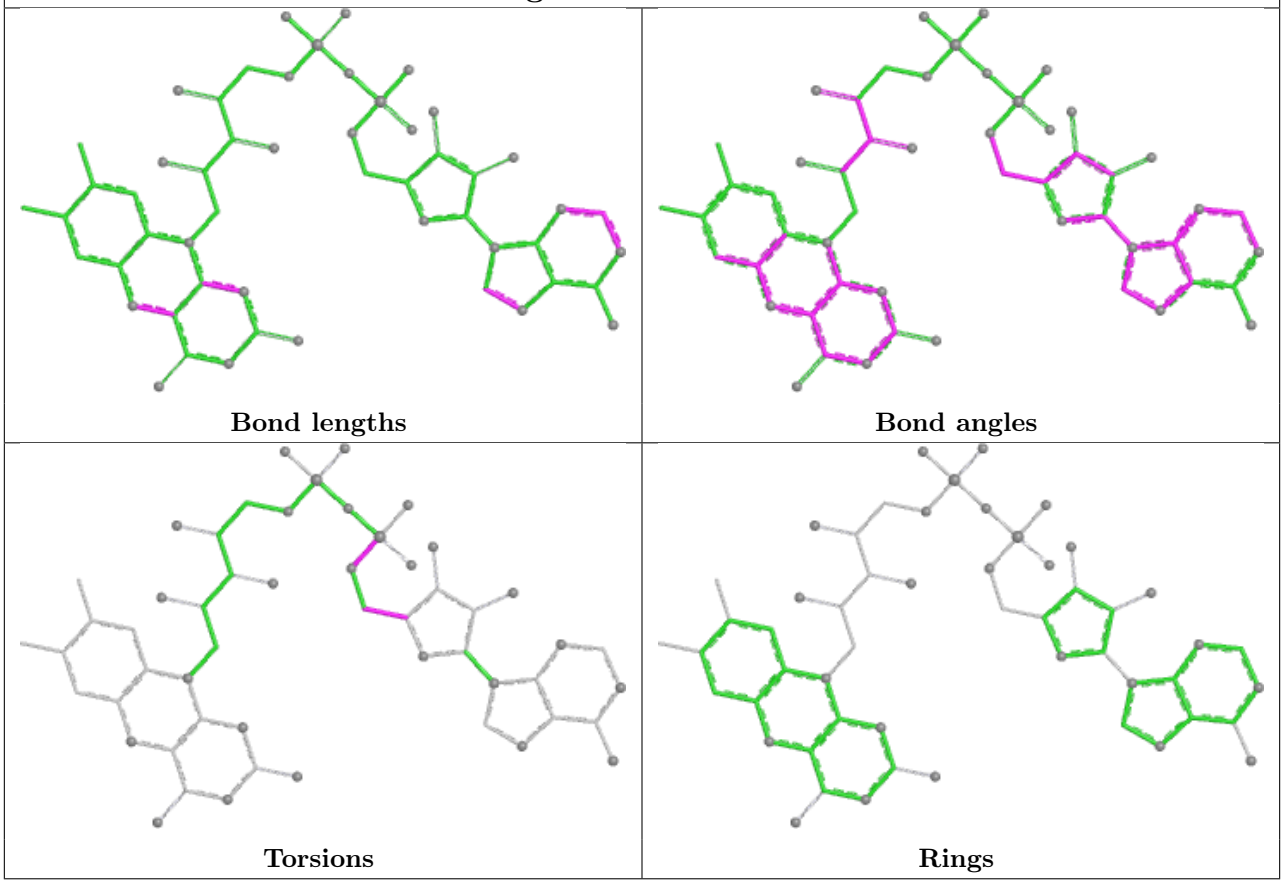


Torsions

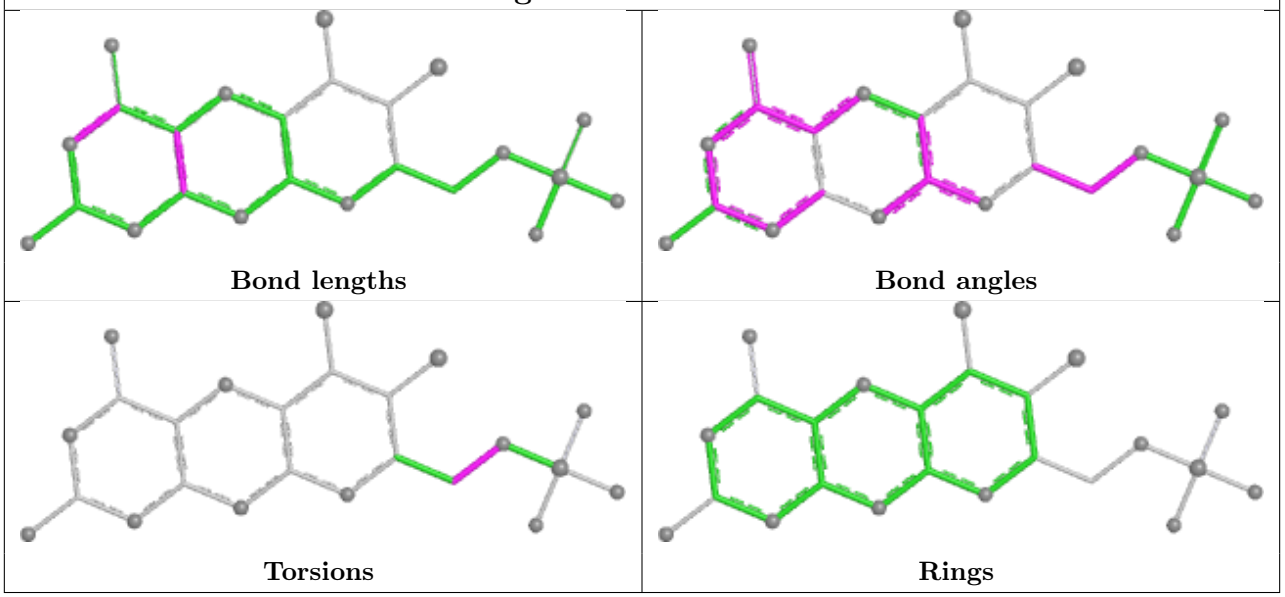


Rings

Ligand FAD B 606



Ligand MTE L 1333



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	2	164/165 (99%)	-0.05	9 (5%)	30	25	4, 10, 30, 43	0
1	A	162/165 (98%)	-0.01	8 (4%)	35	29	2, 9, 27, 41	0
1	J	162/165 (98%)	-0.18	2 (1%)	76	73	3, 9, 27, 41	0
1	S	161/165 (97%)	-0.08	5 (3%)	51	45	4, 10, 28, 43	0
2	3	305/305 (100%)	0.09	7 (2%)	61	55	5, 18, 28, 34	0
2	B	304/305 (99%)	0.10	9 (2%)	52	47	7, 17, 27, 35	0
2	K	302/305 (99%)	0.08	7 (2%)	61	55	7, 17, 27, 35	0
2	T	305/305 (100%)	0.07	9 (2%)	52	47	6, 18, 28, 34	0
3	4	756/762 (99%)	-0.08	14 (1%)	66	61	2, 12, 25, 39	0
3	C	753/762 (98%)	-0.14	18 (2%)	59	54	2, 10, 25, 42	0
3	L	745/762 (97%)	-0.18	10 (1%)	75	71	2, 10, 24, 40	0
3	U	745/762 (97%)	-0.14	9 (1%)	76	73	2, 11, 24, 37	0
All	All	4864/4928 (98%)	-0.07	107 (2%)	62	57	2, 12, 26, 43	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	61	LEU	5.0
3	U	1288	ASN	4.9
3	C	1322	PRO	4.7
3	C	1319	THR	4.6
3	C	1324	ASN	4.5
3	U	1290	THR	4.4
1	A	63	ASP	4.4
3	C	1143	GLU	4.3
3	L	1290	THR	4.3
3	4	1326	LYS	4.2
3	C	1289	ASN	4.2

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Mol	Chain	Res	Type	RSRZ
3	4	1324	ASN	4.0
2	T	243	LYS	3.8
3	L	1288	ASN	3.7
3	C	1318	VAL	3.7
2	B	336	TRP	3.7
3	4	1321	ALA	3.7
2	T	424	ALA	3.6
3	C	969	ASP	3.6
1	A	62	GLN	3.6
3	L	1287	ASN	3.6
3	4	1323	GLY	3.6
2	3	336	TRP	3.5
2	T	528	GLY	3.4
3	C	1323	GLY	3.4
2	T	336	TRP	3.3
3	4	1110	ASP	3.3
1	2	61	LEU	3.3
1	S	61	LEU	3.2
2	K	506	GLU	3.2
1	2	63	ASP	3.2
1	A	60	ARG	3.2
2	T	484	GLN	3.0
3	L	969	ASP	3.0
3	U	969	ASP	3.0
2	3	425	SER	3.0
1	2	60	ARG	3.0
3	4	1325	CYS	2.9
2	K	424	ALA	2.9
3	C	1321	ALA	2.9
2	T	506	GLU	2.9
2	K	429	ASP	2.9
1	A	58	TYR	2.8
2	3	528	GLY	2.8
3	4	1322	PRO	2.8
2	K	484	GLN	2.8
2	K	336	TRP	2.8
1	2	96	THR	2.8
3	C	705	ASN	2.7
1	2	62	GLN	2.7
2	T	429	ASP	2.7
3	L	718	ASP	2.7
3	C	1317	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	S	62	GLN	2.7
2	B	425	SER	2.7
2	T	272	ASN	2.7
1	2	64	LYS	2.6
3	C	683	HIS	2.6
1	A	59	ASP	2.6
2	B	484	GLN	2.6
3	C	1144	THR	2.5
3	4	1286	THR	2.5
1	S	60	ARG	2.5
2	B	424	ALA	2.5
1	J	61	LEU	2.5
2	B	499	ASP	2.5
3	4	705	ASN	2.4
3	U	1286	THR	2.4
2	B	429	ASP	2.4
2	K	243	LYS	2.4
3	4	1289	ASN	2.4
2	K	378	GLY	2.4
3	4	725	GLU	2.3
2	3	484	GLN	2.3
3	U	1292	GLU	2.3
2	3	509	ARG	2.3
3	C	1320	GLY	2.3
1	2	162	THR	2.3
3	C	1286	THR	2.3
1	J	60	ARG	2.3
3	L	710	SER	2.3
3	4	969	ASP	2.3
3	L	1250	LYS	2.2
1	2	2	THR	2.2
3	C	725	GLU	2.2
2	B	272	ASN	2.2
3	U	958	ARG	2.2
3	C	1110	ASP	2.2
2	T	317	ALA	2.2
3	L	1292	GLU	2.2
1	S	144	GLN	2.2
1	S	63	ASP	2.2
1	2	97	ARG	2.2
2	3	424	ALA	2.2
2	3	506	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	97	ARG	2.2
3	U	951	ASP	2.1
2	B	509	ARG	2.1
1	A	64	LYS	2.1
3	U	1289	ASN	2.1
2	B	426	ARG	2.1
3	C	720	LYS	2.1
3	U	1110	ASP	2.1
3	L	725	GLU	2.1
3	4	618	LYS	2.1
3	4	1170	ASP	2.0
3	L	1144	THR	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 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, 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
8	XAN	U	7319	11/11	0.80	0.17	40,41,41,41	0
8	XAN	L	7319	11/11	0.83	0.14	31,32,33,33	0
8	XAN	C	7319	11/11	0.88	0.13	26,27,28,28	0
8	XAN	4	7319	11/11	0.88	0.12	33,34,34,35	0
6	MTE	4	1333	24/24	0.97	0.07	12,13,15,16	0
5	FAD	K	606	53/53	0.97	0.06	4,8,12,12	0
5	FAD	3	606	53/53	0.97	0.06	2,5,9,13	0
6	MTE	L	1333	24/24	0.97	0.06	6,8,13,14	0
6	MTE	U	1333	24/24	0.97	0.07	7,10,15,15	0
6	MTE	C	1333	24/24	0.98	0.06	7,11,15,17	0
4	FES	2	602	4/4	0.98	0.03	2,3,5,5	0

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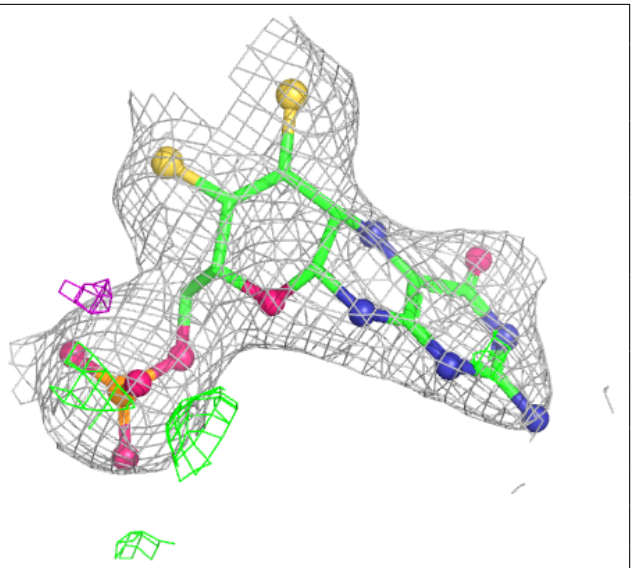
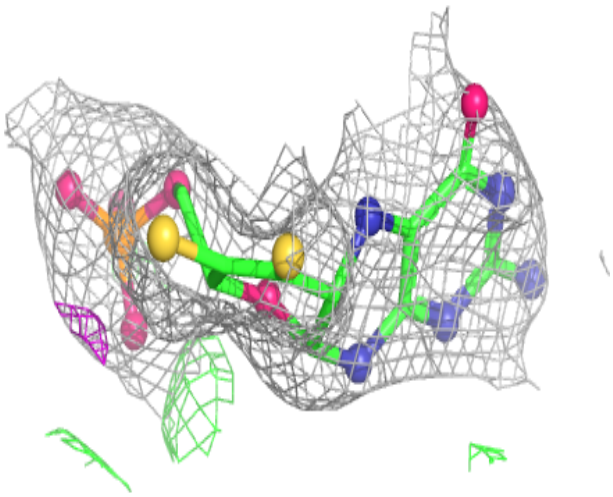
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	FAD	T	606	53/53	0.98	0.06	2,8,13,16	0
5	FAD	B	606	53/53	0.98	0.06	2,4,8,8	0
4	FES	2	601	4/4	0.99	0.03	2,2,3,5	0
4	FES	A	601	4/4	0.99	0.03	2,3,4,8	0
4	FES	A	602	4/4	0.99	0.03	2,2,3,4	0
4	FES	J	601	4/4	0.99	0.03	2,2,2,2	0
4	FES	J	602	4/4	0.99	0.04	2,3,3,4	0
4	FES	S	601	4/4	0.99	0.03	4,5,9,10	0
4	FES	S	602	4/4	0.99	0.04	4,4,6,9	0
7	MOM	C	1334	4/4	1.00	0.03	16,16,17,20	0
7	MOM	L	1334	4/4	1.00	0.03	12,15,15,16	0
7	MOM	U	1334	4/4	1.00	0.03	12,14,15,15	0
7	MOM	4	1334	4/4	1.00	0.04	12,12,14,18	0

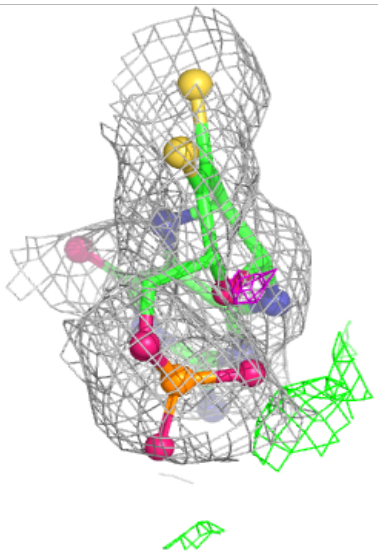
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MTE 4 1333:

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

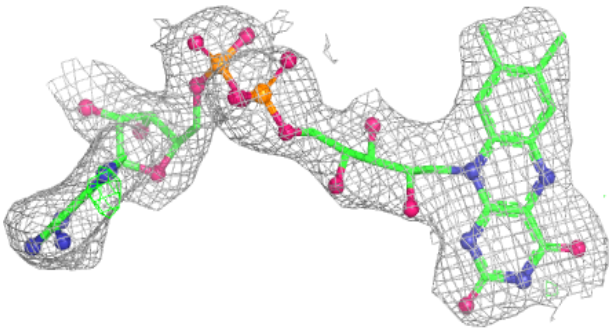


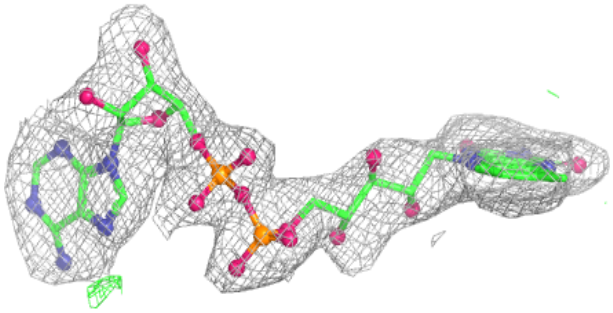


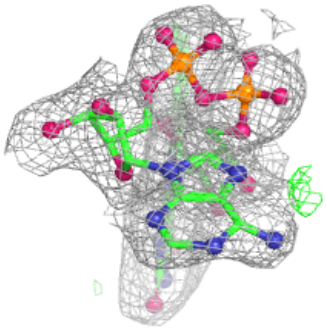


Electron density around FAD K 606:

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

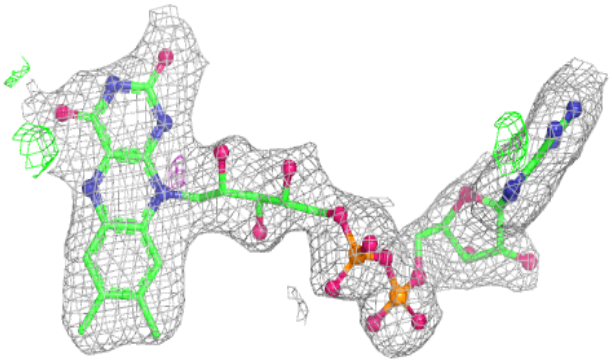


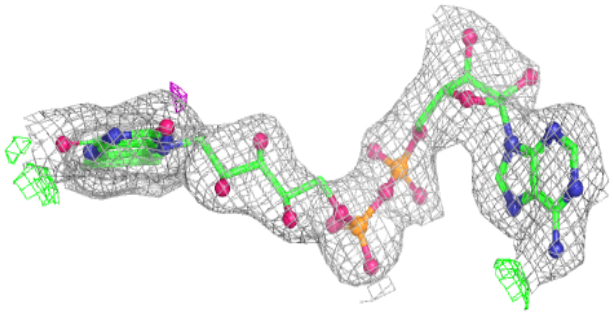


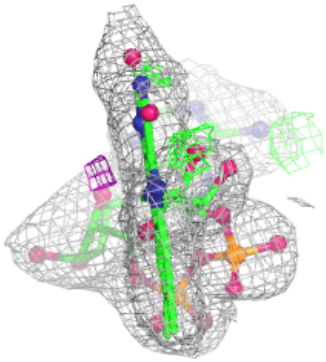


Electron density around FAD 3 606:

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

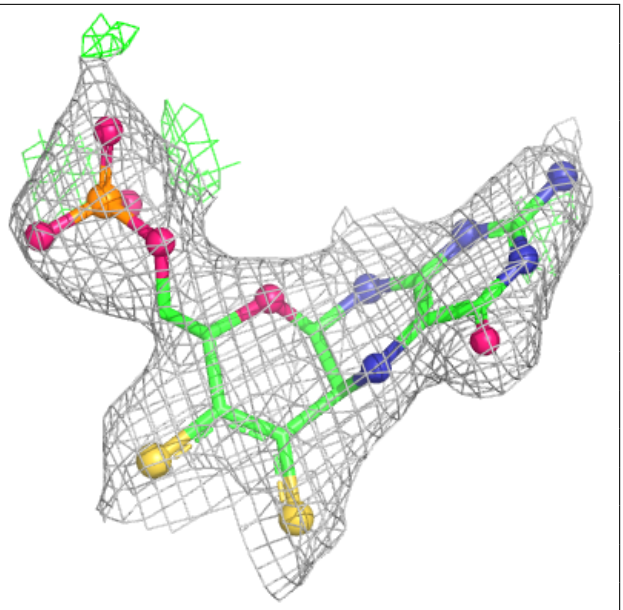


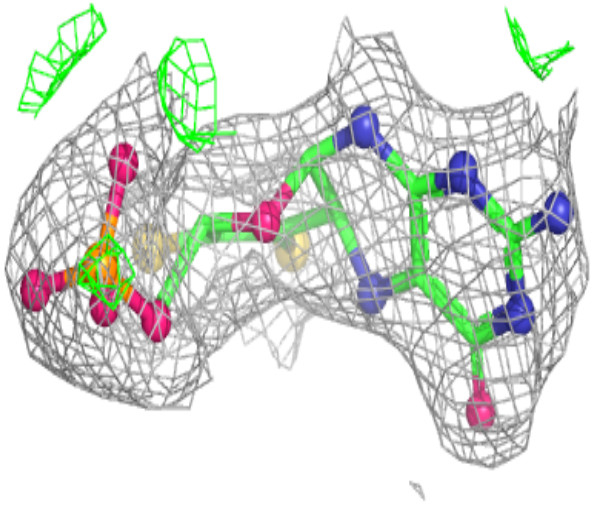


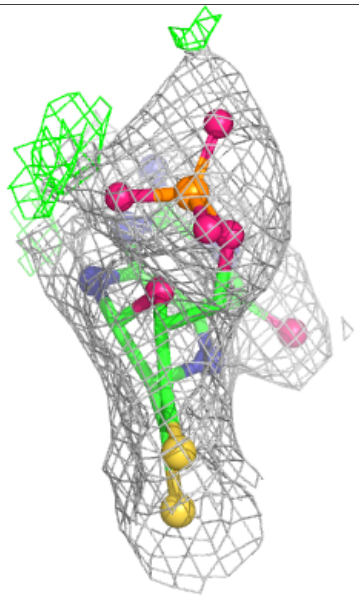


Electron density around MTE L 1333:

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

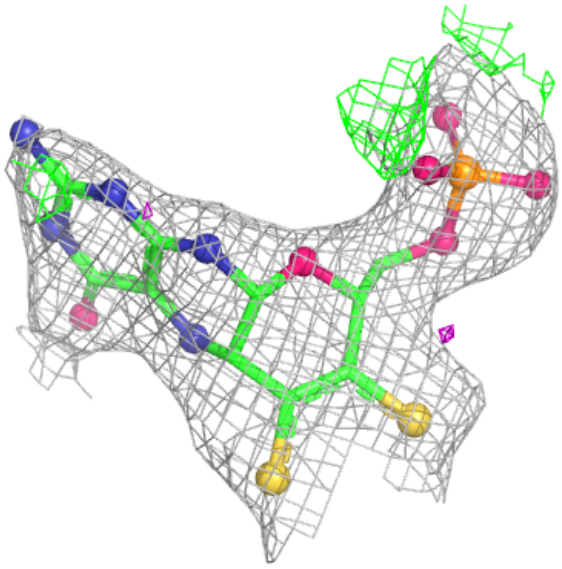


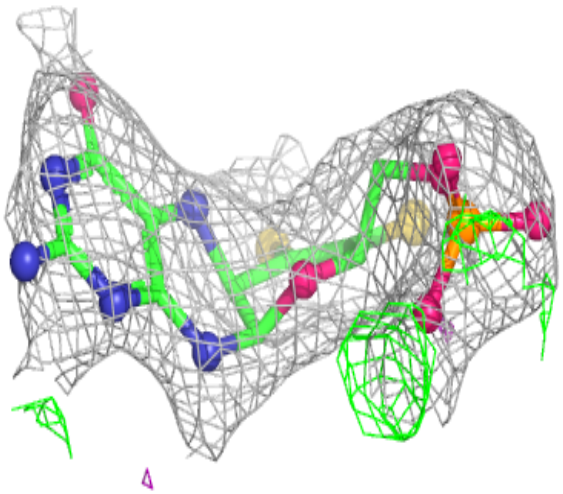


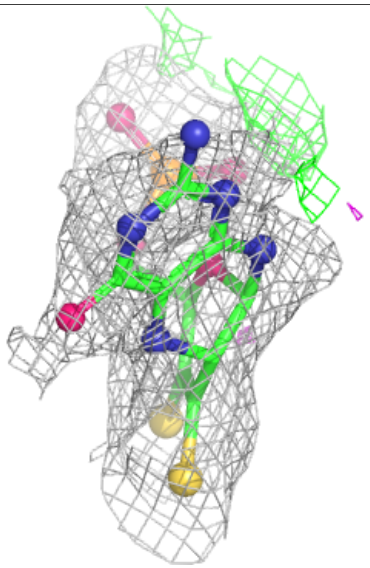


Electron density around MTE U 1333:

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

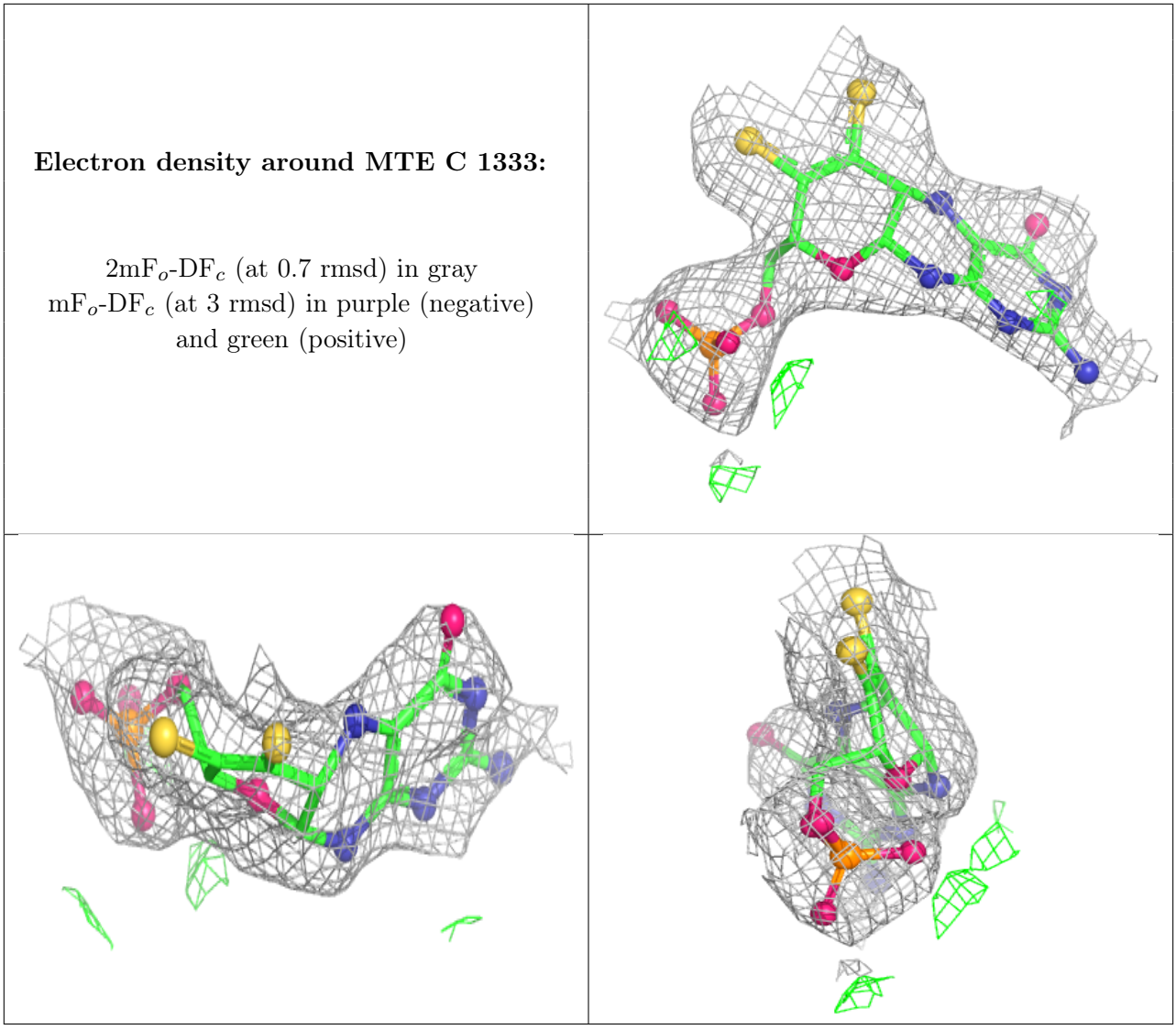






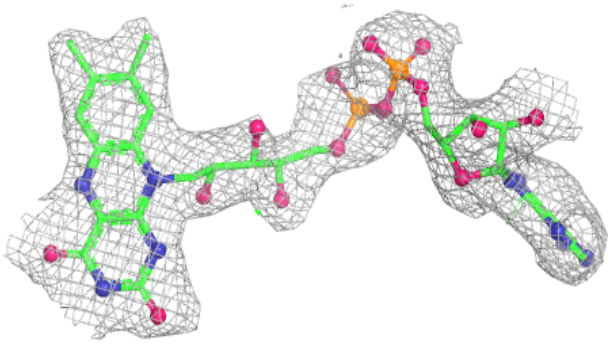
Electron density around MTE C 1333:

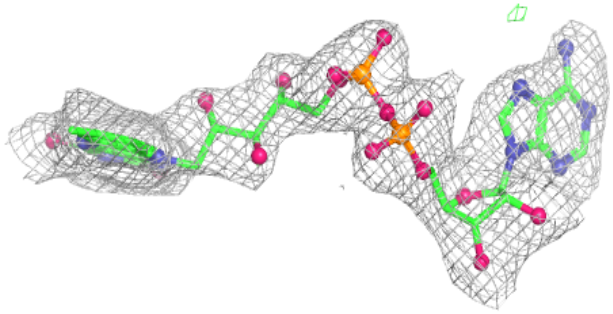
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

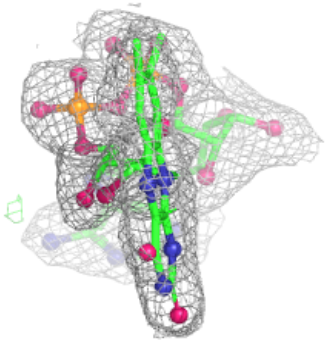


Electron density around FAD T 606:

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

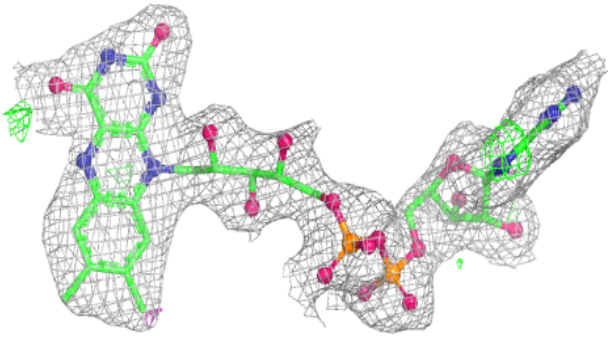


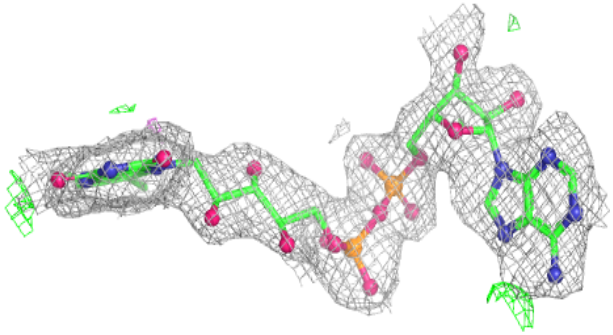


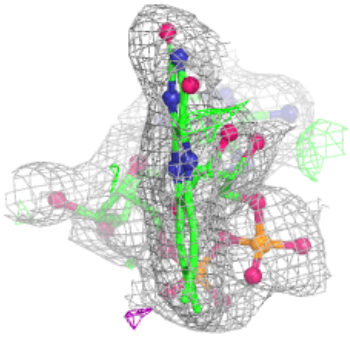


Electron density around FAD B 606:

$2mF_o$-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.