



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 12:37 PM UTC

PDB ID : 2E1Q / pdb_00002e1q
Title : Crystal Structure of Human Xanthine Oxidoreductase mutant, Glu803Val
Authors : Yamaguchi, Y.; Matsumura, T.; Ichida, K.; Okamoto, K.; Nishino, T.
Deposited on : 2006-10-27
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 ⓘ symbol.

The types of validation reports are described at

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

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

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

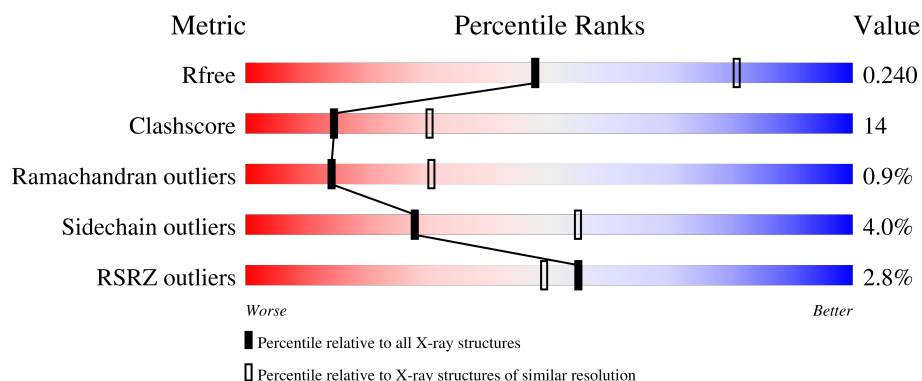
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1333	3% 67% 28% ..
1	B	1333	3% 67% 27% ..
1	C	1333	3% 69% 26% ..
1	D	1333	3% 69% 25% ..

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	A	2005	-	-	X	-
7	MOM	B	3005	-	-	X	-
7	MOM	C	4005	-	-	X	-
7	MOM	D	5005	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 41721 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	1307	Total	C	N	O	S	0	0	0
			10088	6394	1737	1891	66			
1	B	1307	Total	C	N	O	S	0	0	0
			10088	6394	1737	1891	66			
1	C	1307	Total	C	N	O	S	0	0	0
			10088	6394	1737	1891	66			
1	D	1307	Total	C	N	O	S	0	0	0
			10088	6394	1737	1891	66			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P47989
A	803	VAL	GLU	engineered mutation	UNP P47989
B	1	MET	-	initiating methionine	UNP P47989
B	803	VAL	GLU	engineered mutation	UNP P47989
C	1	MET	-	initiating methionine	UNP P47989
C	803	VAL	GLU	engineered mutation	UNP P47989
D	1	MET	-	initiating methionine	UNP P47989
D	803	VAL	GLU	engineered mutation	UNP P47989

- Molecule 2 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 1 3	0	0
2	B	1	Total C O 4 1 3	0	0
2	C	1	Total C O 4 1 3	0	0
2	D	1	Total C O 4 1 3	0	0

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

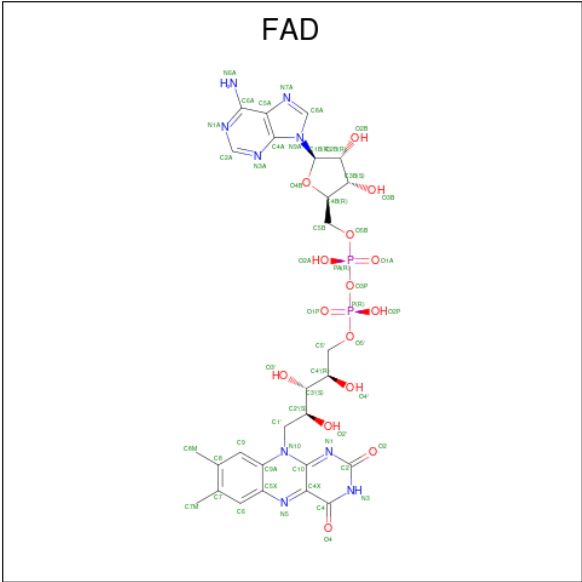
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Ca 2 2	0	0
3	B	2	Total Ca 2 2	0	0
3	C	2	Total Ca 2 2	0	0
3	D	2	Total Ca 2 2	0	0

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



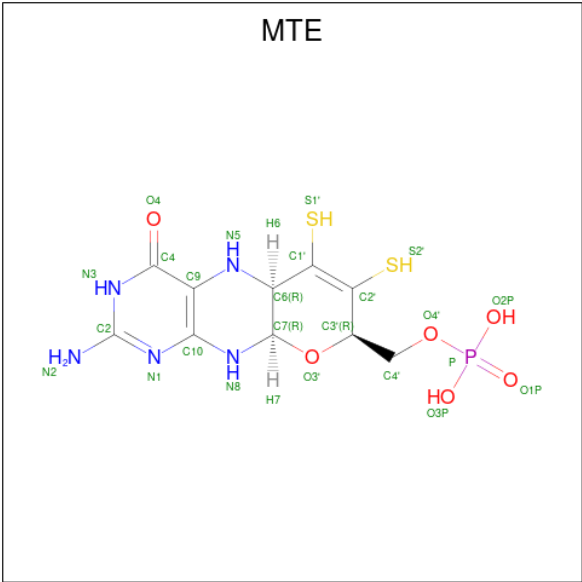
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			4	2	2		
4	A	1	Total	Fe	S	0	0
			4	2	2		
4	B	1	Total	Fe	S	0	0
			4	2	2		
4	B	1	Total	Fe	S	0	0
			4	2	2		
4	C	1	Total	Fe	S	0	0
			4	2	2		
4	C	1	Total	Fe	S	0	0
			4	2	2		
4	D	1	Total	Fe	S	0	0
			4	2	2		
4	D	1	Total	Fe	S	0	0
			4	2	2		

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



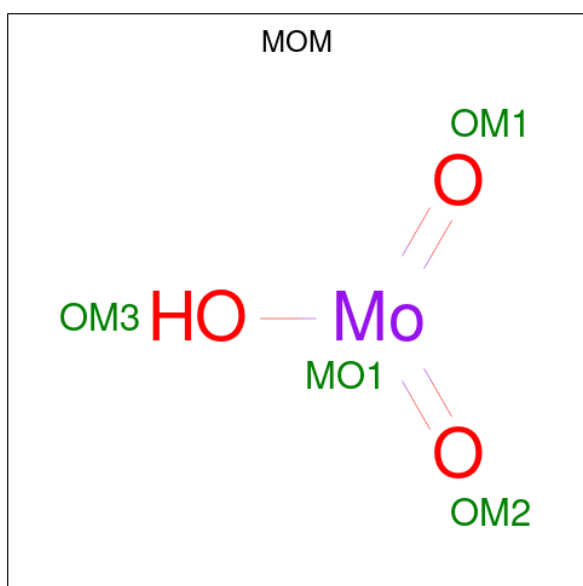
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- 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: C₁₀H₁₄N₅O₆PS₂).



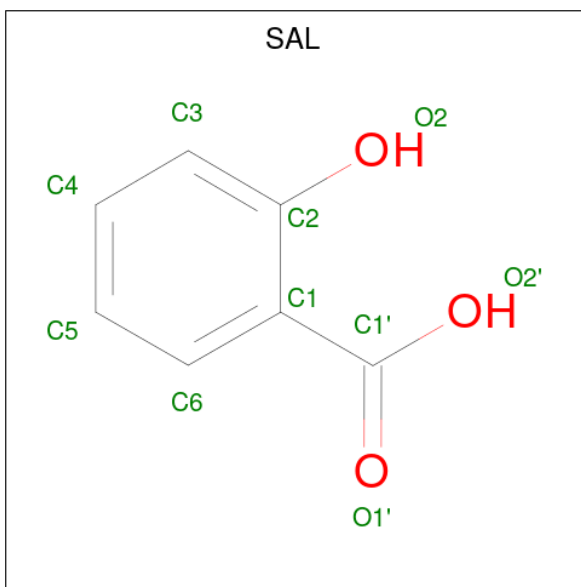
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	S	
			24	10	5	6	1	2	
6	B	1	Total	C	N	O	P	S	
			24	10	5	6	1	2	
6	C	1	Total	C	N	O	P	S	
			24	10	5	6	1	2	
6	D	1	Total	C	N	O	P	S	
			24	10	5	6	1	2	

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	Mo	O		
			4	1	3	0	0
7	B	1	Total	Mo	O		
			4	1	3	0	0
7	C	1	Total	Mo	O		
			4	1	3	0	0
7	D	1	Total	Mo	O		
			4	1	3	0	0

- Molecule 8 is 2-HYDROXYBENZOIC ACID (CCD ID: SAL) (formula: $\text{C}_7\text{H}_6\text{O}_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			10	7	3		
8	B	1	Total	C	O	0	0
			10	7	3		
8	C	1	Total	C	O	0	0
			10	7	3		
8	D	1	Total	C	O	0	0
			10	7	3		

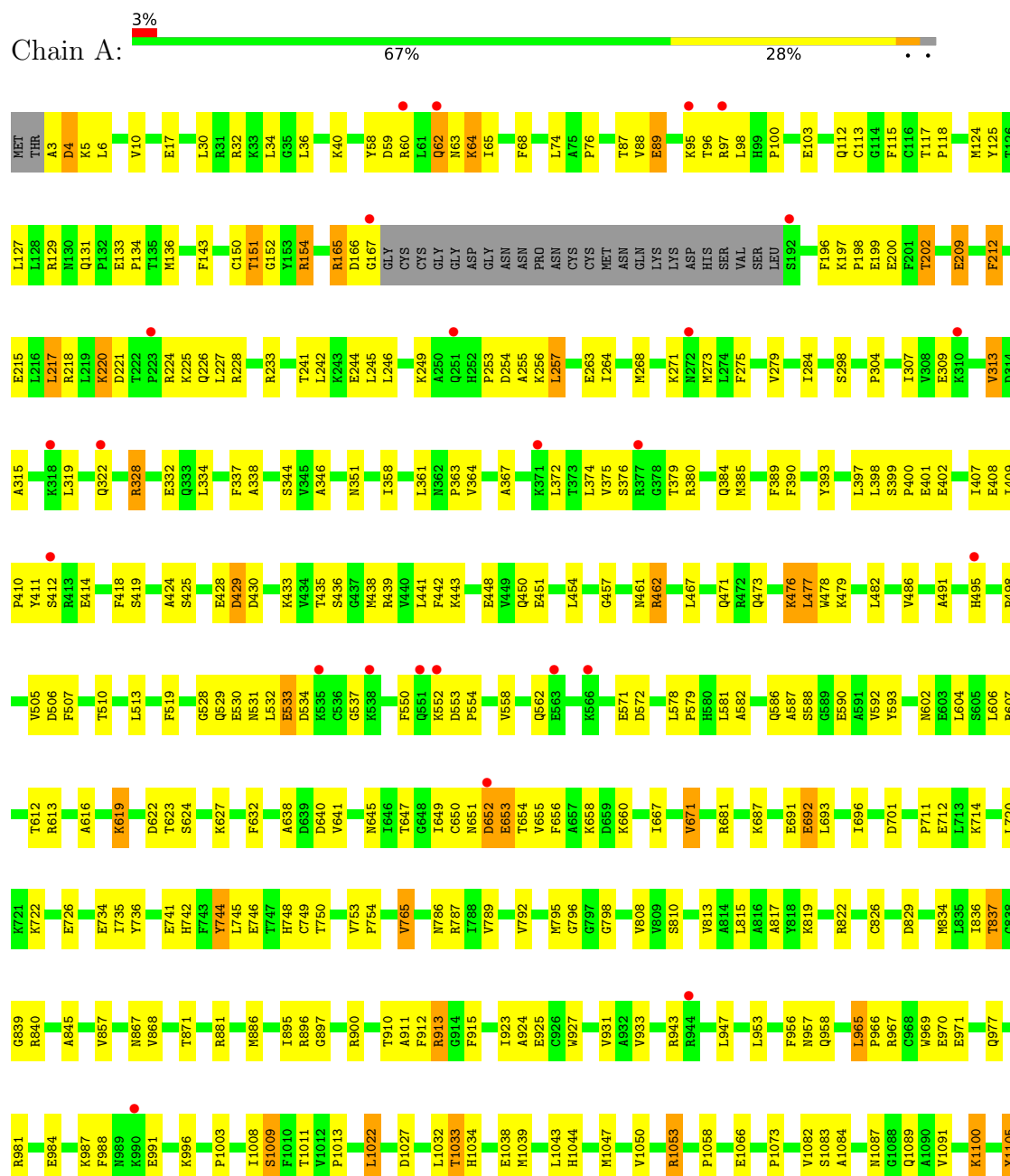
- Molecule 9 is water.

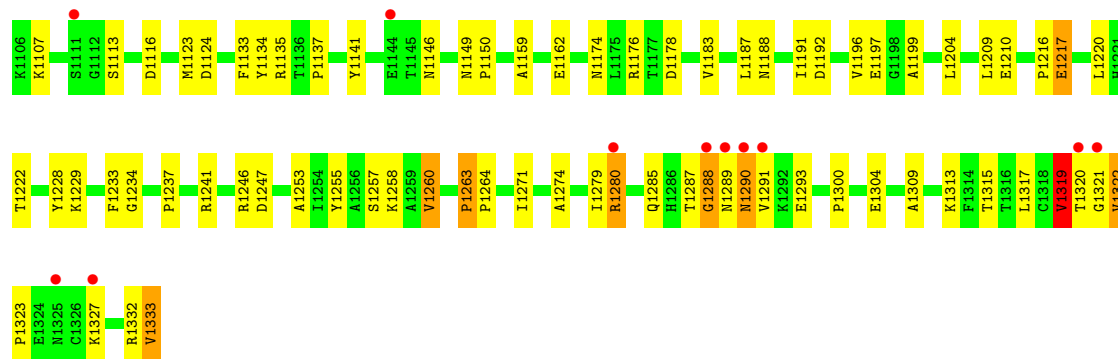
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	234	Total	O	0	0
			234	234		
9	B	245	Total	O	0	0
			245	245		
9	C	237	Total	O	0	0
			237	237		
9	D	233	Total	O	0	0
			233	233		

3 Residue-property plots

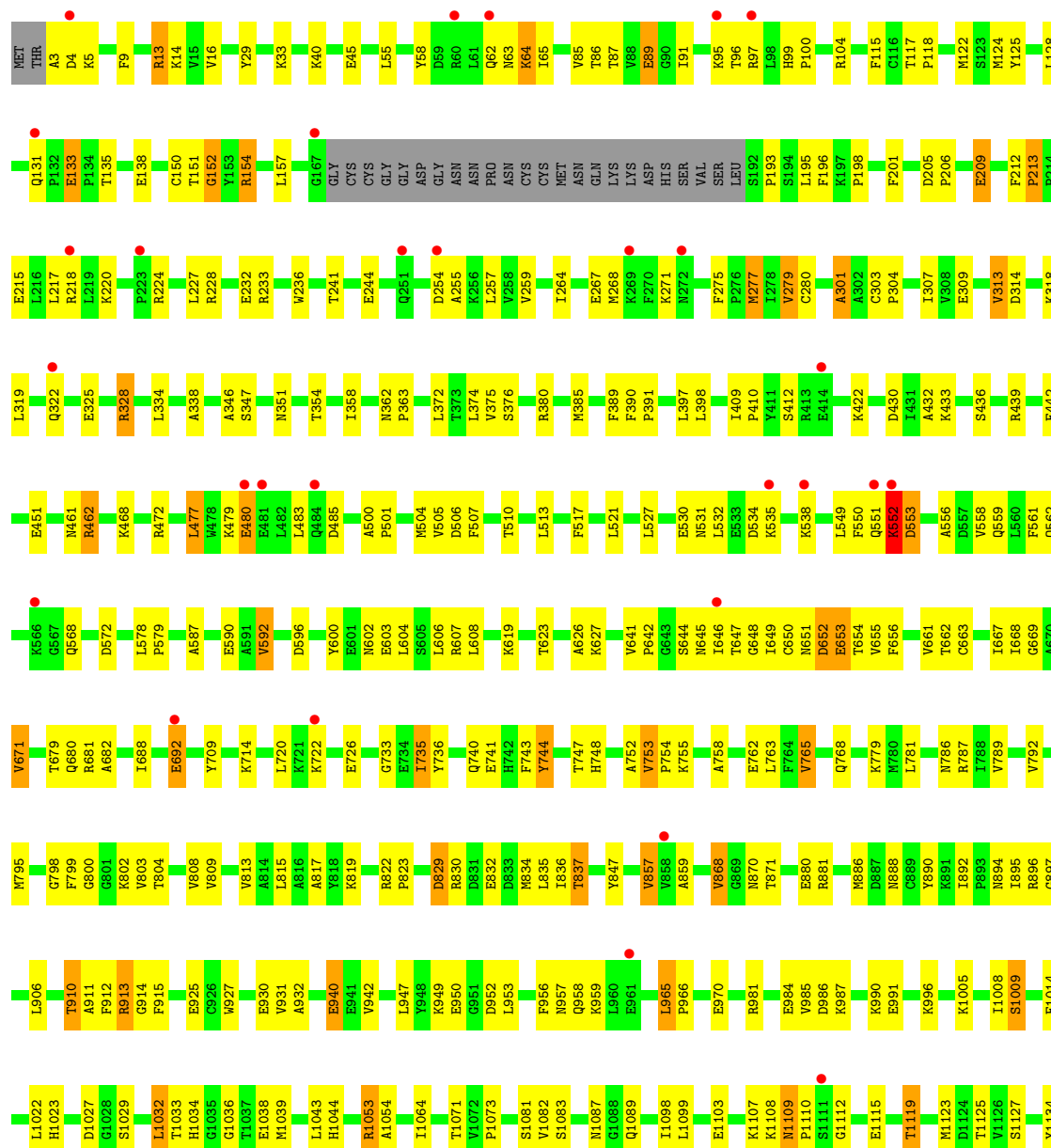
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

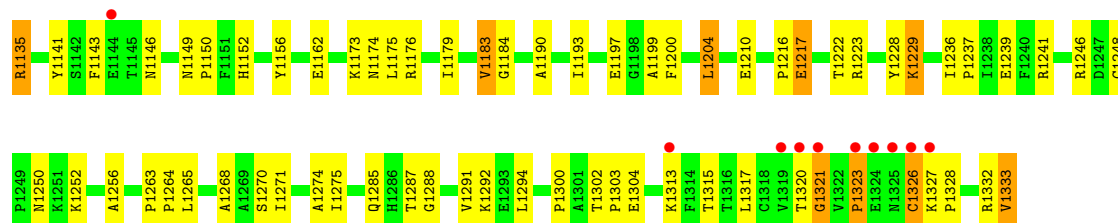
• Molecule 1: Xanthine dehydrogenase/oxidase



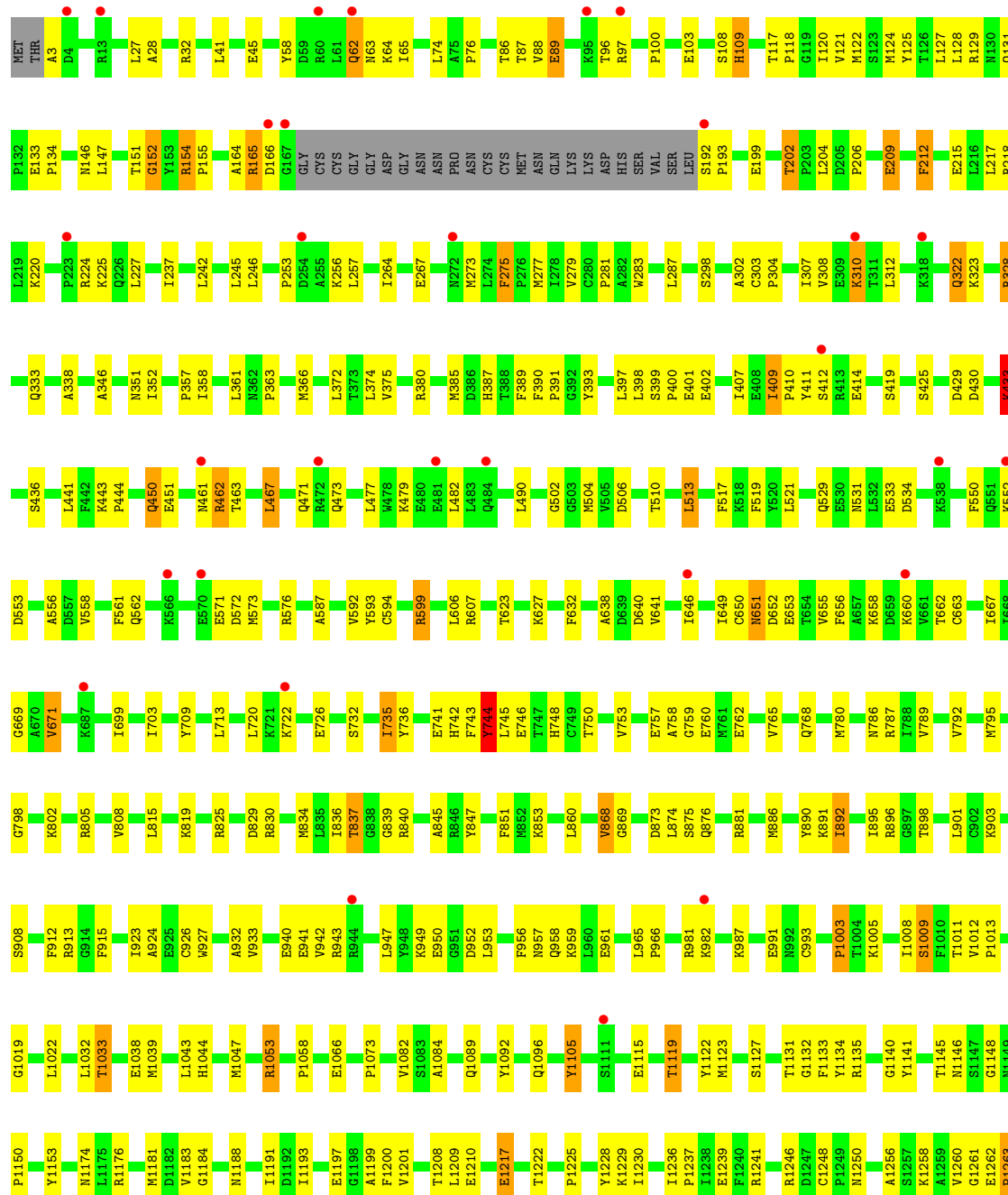


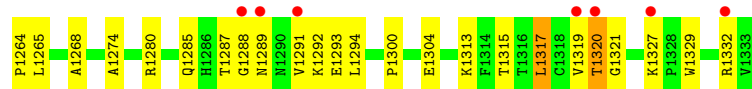
• Molecule 1: Xanthine dehydrogenase/oxidase



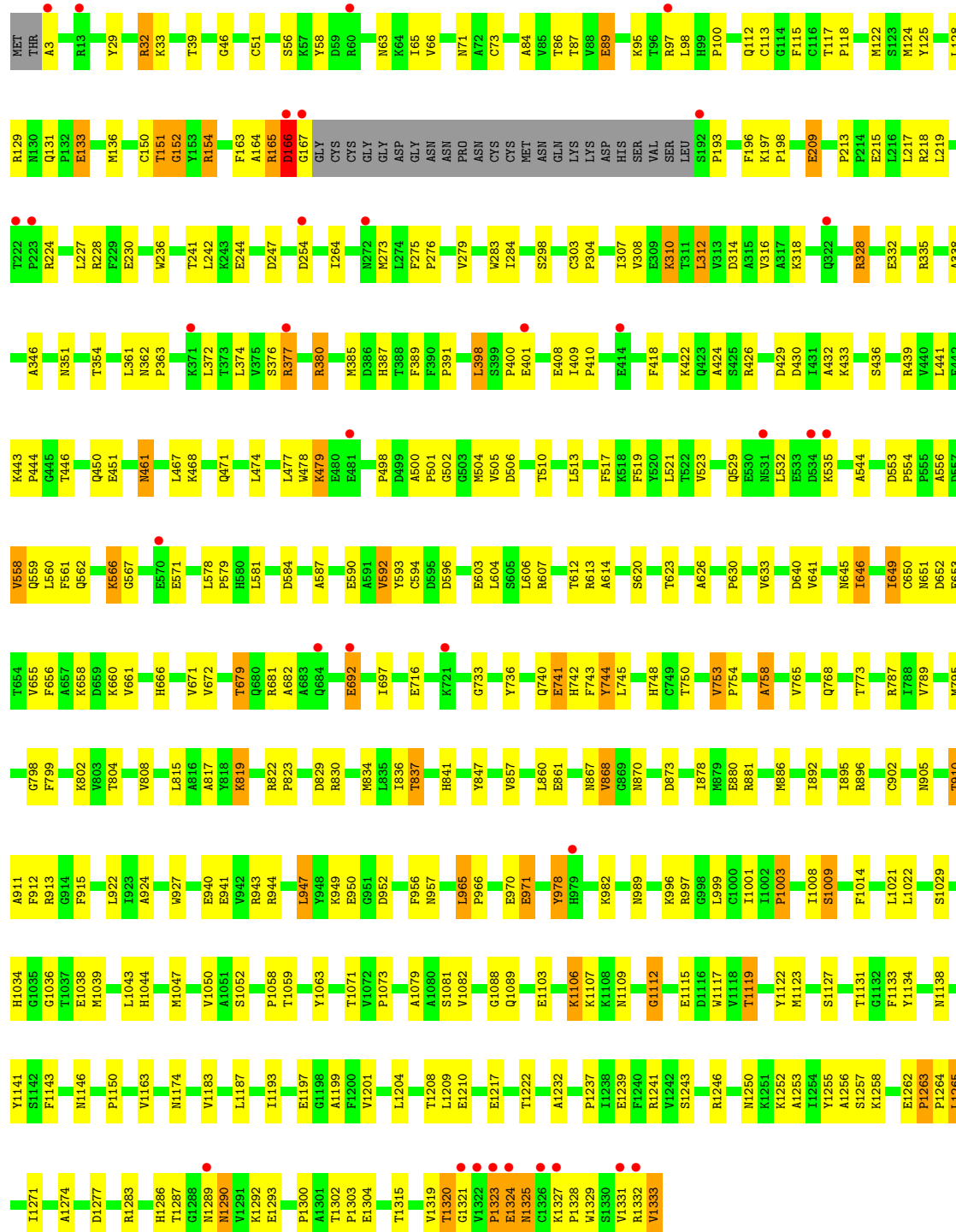


• Molecule 1: Xanthine dehydrogenase/oxidase





● Molecule 1: Xanthine dehydrogenase/oxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	134.57Å 140.94Å 176.48Å 90.00° 91.49° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 50.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.0 (50.00-2.60) 95.0 (50.00-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.27 (at 2.58Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.192 , 0.246 0.186 , 0.240	Depositor DCC
R_{free} test set	3840 reflections (1.91%)	wwPDB-VP
Wilson B-factor (Å ²)	26.4	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.014 for -k,-h,-l 0.014 for k,h,-l 0.146 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	41721	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.42	0/10303	0.96	32/13950 (0.2%)
1	B	0.42	0/10303	0.98	47/13950 (0.3%)
1	C	0.42	0/10303	0.96	34/13950 (0.2%)
1	D	0.43	1/10303 (0.0%)	0.97	43/13950 (0.3%)
All	All	0.42	1/41212 (0.0%)	0.97	156/55800 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	753	VAL	CA-CB	5.84	1.59	1.54

All (156) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	836	ILE	N-CA-C	11.36	121.21	110.53
1	C	165	ARG	N-CA-C	-11.24	99.60	113.20
1	D	409	ILE	CA-C-N	10.76	130.84	119.76
1	D	409	ILE	C-N-CA	10.76	130.84	119.76
1	B	655	VAL	N-CA-C	-10.73	100.41	110.82
1	A	836	ILE	N-CA-C	10.41	120.31	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	836	ILE	N-CA-C	10.31	120.22	110.53
1	D	151	THR	N-CA-C	10.19	123.64	111.82
1	C	151	THR	N-CA-C	9.74	123.12	111.82
1	D	655	VAL	N-CA-C	-9.32	101.78	110.82
1	B	151	THR	N-CA-C	9.32	122.63	111.82
1	D	957	ASN	N-CA-C	8.93	123.75	112.86
1	A	655	VAL	N-CA-C	-8.79	101.42	111.00
1	A	151	THR	N-CA-C	8.65	121.66	111.71
1	B	1263	PRO	N-CA-C	8.51	121.08	110.70
1	C	1261	GLY	N-CA-C	8.28	122.65	112.64
1	C	433	LYS	N-CA-C	-8.23	101.02	112.45
1	A	409	ILE	CA-C-N	8.16	128.19	119.78
1	A	409	ILE	C-N-CA	8.16	128.19	119.78
1	D	433	LYS	N-CA-C	-8.05	100.86	111.24
1	D	836	ILE	N-CA-C	7.95	118.84	111.45
1	B	957	ASN	N-CA-C	7.85	122.16	112.58
1	A	1263	PRO	N-CA-C	7.80	120.22	110.70
1	A	433	LYS	N-CA-C	-7.66	101.02	112.04
1	A	1124	ASP	N-CA-C	-7.57	103.35	112.59
1	C	957	ASN	N-CA-C	7.46	122.33	113.23
1	A	1274	ALA	N-CA-C	-7.44	103.25	111.36
1	C	409	ILE	CA-C-N	7.36	127.34	119.76
1	C	409	ILE	C-N-CA	7.36	127.34	119.76
1	B	390	PHE	CA-C-N	7.32	127.17	119.05
1	B	390	PHE	C-N-CA	7.32	127.17	119.05
1	D	1263	PRO	N-CA-C	7.29	119.59	110.70
1	A	957	ASN	N-CA-C	7.18	121.62	112.86
1	C	892	ILE	CA-C-N	7.11	126.64	119.24
1	C	892	ILE	C-N-CA	7.11	126.64	119.24
1	B	653	GLU	N-CA-C	7.07	120.62	109.81
1	C	655	VAL	N-CA-C	-7.03	103.62	110.72
1	B	1326	CYS	N-CA-C	-7.02	101.23	110.43
1	D	653	GLU	N-CA-C	7.00	120.52	109.81
1	B	600	TYR	N-CA-C	-6.95	101.57	110.53
1	B	1274	ALA	N-CA-C	-6.77	103.36	111.69
1	A	653	GLU	N-CA-C	6.70	119.34	109.69
1	B	837	THR	N-CA-C	6.65	121.23	113.18
1	D	837	THR	N-CA-C	6.60	121.19	113.20
1	A	165	ARG	N-CA-C	-6.57	105.26	113.28
1	A	212	PHE	N-CA-C	-6.55	101.40	109.65
1	A	436	SER	N-CA-C	6.53	118.99	109.07
1	B	433	LYS	N-CA-C	-6.46	102.74	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1274	ALA	N-CA-C	-6.45	104.33	111.82
1	D	150	CYS	N-CA-C	6.45	121.33	112.04
1	D	744	TYR	N-CA-C	-6.45	100.28	109.96
1	D	1265	LEU	N-CA-C	6.45	118.85	111.11
1	D	436	SER	N-CA-C	6.43	118.84	109.07
1	C	1265	LEU	N-CA-C	6.39	118.78	111.11
1	B	436	SER	N-CA-C	6.35	118.50	108.79
1	B	914	GLY	N-CA-C	-6.33	106.81	113.58
1	D	697	ILE	N-CA-C	6.28	117.64	111.67
1	C	467	LEU	N-CA-C	6.28	117.79	111.07
1	C	411	TYR	N-CA-C	-6.22	102.76	110.41
1	B	133	GLU	CA-C-N	6.20	126.16	120.21
1	B	133	GLU	C-N-CA	6.20	126.16	120.21
1	B	1027	ASP	N-CA-C	-6.20	105.29	112.92
1	D	829	ASP	N-CA-C	-6.17	102.23	110.55
1	A	829	ASP	N-CA-C	-6.12	102.29	110.55
1	B	744	TYR	N-CA-C	-6.08	100.84	109.96
1	D	692	GLU	N-CA-C	6.08	118.14	110.24
1	C	436	SER	N-CA-C	6.06	118.06	108.79
1	B	661	VAL	N-CA-C	-6.06	99.76	108.48
1	A	411	TYR	N-CA-C	-6.05	102.72	110.53
1	B	890	TYR	N-CA-C	6.04	119.24	109.40
1	D	1112	GLY	N-CA-C	6.03	118.97	112.33
1	B	410	PRO	N-CA-C	6.01	120.43	111.41
1	D	354	THR	N-CA-C	-5.97	104.84	111.71
1	A	152	GLY	N-CA-C	-5.94	107.05	115.43
1	C	152	GLY	N-CA-C	-5.93	107.06	115.30
1	C	653	GLU	N-CA-C	5.91	118.83	110.14
1	D	773	THR	N-CA-C	-5.91	104.75	111.07
1	C	837	THR	N-CA-C	5.90	119.74	112.54
1	B	152	GLY	N-CA-C	-5.87	107.15	115.43
1	C	390	PHE	CA-C-N	5.85	125.54	119.05
1	C	390	PHE	C-N-CA	5.85	125.54	119.05
1	B	338	ALA	CB-CA-C	-5.83	109.84	116.54
1	B	1210	GLU	N-CA-C	5.83	117.70	108.67
1	A	338	ALA	CB-CA-C	-5.83	109.84	116.54
1	B	150	CYS	N-CA-C	5.82	120.42	112.68
1	C	592	VAL	N-CA-C	5.80	116.65	108.36
1	B	829	ASP	N-CA-C	-5.78	102.74	110.55
1	C	308	VAL	N-CA-C	-5.78	104.88	110.72
1	D	1071	THR	N-CA-C	-5.78	106.27	113.55
1	A	765	VAL	N-CA-C	5.78	117.07	108.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1027	ASP	N-CA-C	-5.76	105.91	113.17
1	D	197	LYS	CA-C-N	5.76	125.62	119.28
1	D	197	LYS	C-N-CA	5.76	125.62	119.28
1	D	152	GLY	N-CA-C	-5.75	107.33	115.43
1	D	338	ALA	CB-CA-C	-5.75	109.93	116.54
1	C	1263	PRO	N-CA-C	5.71	117.67	110.70
1	A	744	TYR	N-CA-C	-5.70	101.41	109.96
1	B	870	ASN	N-CA-C	5.68	119.95	113.19
1	B	1109	ASN	CA-C-N	5.67	125.52	119.28
1	B	1109	ASN	C-N-CA	5.67	125.52	119.28
1	C	275	PHE	CA-C-N	5.65	125.76	119.32
1	C	275	PHE	C-N-CA	5.65	125.76	119.32
1	A	5	LYS	N-CA-C	5.62	117.85	109.59
1	A	837	THR	N-CA-C	5.62	119.97	113.18
1	B	319	LEU	CA-C-N	5.61	125.78	119.90
1	B	319	LEU	C-N-CA	5.61	125.78	119.90
1	B	592	VAL	N-CA-C	5.60	116.37	108.36
1	C	450	GLN	N-CA-C	-5.60	106.50	113.55
1	D	1138	ASN	N-CA-C	5.58	119.27	111.74
1	D	1082	VAL	N-CA-C	5.57	117.53	112.29
1	A	692	GLU	N-CA-C	5.55	118.33	110.50
1	A	390	PHE	CA-C-N	5.54	126.77	119.84
1	A	390	PHE	C-N-CA	5.54	126.77	119.84
1	D	922	LEU	N-CA-C	-5.54	105.32	111.36
1	D	581	LEU	N-CA-C	5.54	118.03	111.33
1	B	910	THR	N-CA-C	5.50	115.29	108.19
1	D	1274	ALA	N-CA-C	-5.50	105.20	111.14
1	B	1071	THR	N-CA-C	-5.46	106.55	113.43
1	B	301	ALA	N-CA-C	5.44	117.21	111.28
1	B	1229	LYS	N-CA-C	5.44	117.57	107.99
1	C	212	PHE	N-CA-C	-5.36	101.62	109.50
1	C	768	GLN	N-CA-C	-5.35	106.80	113.38
1	C	744	TYR	N-CA-C	-5.34	102.37	110.28
1	D	410	PRO	N-CA-C	5.33	119.46	111.14
1	D	679	THR	N-CA-C	-5.31	105.67	111.82
1	B	354	THR	N-CA-C	-5.30	105.50	111.28
1	A	592	VAL	N-CA-C	5.26	115.67	107.99
1	D	892	ILE	CA-C-N	5.25	124.43	118.97
1	D	892	ILE	C-N-CA	5.25	124.43	118.97
1	D	529	GLN	N-CA-C	-5.25	105.73	111.82
1	D	870	ASN	N-CA-C	5.22	119.40	113.19
1	B	409	ILE	CA-C-N	5.20	125.18	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	409	ILE	C-N-CA	5.20	125.18	120.03
1	B	376	SER	N-CA-C	-5.16	101.06	108.60
1	D	1187	LEU	N-CA-C	-5.14	106.86	113.23
1	D	544	ALA	N-CA-C	5.14	117.27	111.11
1	A	1187	LEU	N-CA-C	-5.12	105.78	112.23
1	C	109	HIS	N-CA-C	-5.12	106.34	112.58
1	B	275	PHE	CA-C-N	5.11	124.77	119.56
1	B	275	PHE	C-N-CA	5.11	124.77	119.56
1	D	1106	LYS	N-CA-C	-5.11	105.89	111.82
1	A	457	GLY	N-CA-C	-5.11	103.06	111.38
1	B	1082	VAL	N-CA-C	5.08	117.07	112.29
1	D	1210	GLU	N-CA-C	5.08	117.58	109.96
1	C	1012	VAL	CA-C-N	5.07	126.18	119.84
1	C	1012	VAL	C-N-CA	5.07	126.18	119.84
1	C	982	LYS	N-CA-C	-5.06	105.76	111.28
1	B	1183	VAL	N-CA-C	-5.06	106.52	111.88
1	A	410	PRO	N-CA-C	5.05	119.24	111.21
1	D	592	VAL	N-CA-C	5.05	115.85	108.58
1	D	113	CYS	N-CA-C	-5.04	106.39	112.54
1	B	765	VAL	N-CA-C	5.03	115.96	108.46
1	D	910	THR	N-CA-C	5.03	115.17	108.23
1	B	692	GLU	N-CA-C	5.02	117.51	110.23
1	A	581	LEU	N-CA-C	5.01	117.40	111.33
1	A	1091	VAL	N-CA-C	-5.00	105.62	110.42

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1105	TYR	Sidechain
1	C	1105	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10088	0	10112	299	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	10088	0	10111	292	0
1	C	10088	0	10110	291	0
1	D	10088	0	10112	259	0
2	A	4	0	0	1	0
2	B	4	0	0	1	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	8	0	0	0	0
4	B	8	0	0	0	0
4	C	8	0	0	0	0
4	D	8	0	0	1	0
5	A	53	0	31	2	0
5	B	53	0	31	3	0
5	C	53	0	31	2	0
5	D	53	0	31	3	0
6	A	24	0	10	4	0
6	B	24	0	8	3	0
6	C	24	0	10	2	0
6	D	24	0	10	2	0
7	A	4	0	0	2	0
7	B	4	0	0	2	0
7	C	4	0	0	2	0
7	D	4	0	0	3	0
8	A	10	0	4	0	0
8	B	10	0	4	0	0
8	C	10	0	4	0	0
8	D	10	0	4	0	0
9	A	234	0	0	7	0
9	B	245	0	0	3	0
9	C	237	0	0	2	0
9	D	233	0	0	6	0
All	All	41721	0	40623	1142	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 14.

All (1142) 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)
6:A:2004:MTE:C9	6:A:2004:MTE:N5	1.68	1.52
6:C:4004:MTE:C9	6:C:4004:MTE:N5	1.68	1.51
1:A:133:GLU:HG2	1:A:165:ARG:HB3	1.40	1.03
1:D:1320:THR:HG23	1:D:1321:GLY:H	1.26	1.00
1:A:3:ALA:HB1	1:A:228:ARG:H	1.28	0.99
1:C:1287:THR:HG22	1:C:1288:GLY:H	1.31	0.95
1:D:372:LEU:HD11	1:D:385:MET:HE3	1.48	0.95
1:C:154:ARG:HD3	1:C:1197:GLU:OE2	1.67	0.93
1:C:956:PHE:HA	1:C:1146:ASN:HD21	1.31	0.93
1:C:131:GLN:HE21	1:C:133:GLU:H	1.15	0.92
1:B:558:VAL:HG22	1:B:1241:ARG:HG2	1.53	0.90
1:B:1141:TYR:HB2	1:B:1150:PRO:HG3	1.51	0.90
1:B:538:LYS:H	1:B:538:LYS:HD2	1.36	0.89
1:D:314:ASP:O	1:D:318:LYS:HD3	1.72	0.88
1:B:64:LYS:HD2	1:B:65:ILE:H	1.38	0.88
1:D:264:ILE:HD11	5:D:5003:FAD:H3B	1.56	0.87
1:B:3:ALA:HB1	1:B:228:ARG:H	1.39	0.86
1:B:64:LYS:HD2	1:B:65:ILE:N	1.91	0.86
1:B:372:LEU:HD11	1:B:385:MET:HE3	1.59	0.85
1:B:741:GLU:HG2	1:B:834:MET:HE3	1.58	0.85
1:C:558:VAL:HG22	1:C:1241:ARG:HG2	1.59	0.85
1:B:1313:LYS:O	1:B:1317:LEU:HD23	1.77	0.84
1:B:264:ILE:HG22	1:B:268:MET:HE2	1.61	0.83
1:B:480:GLU:CD	1:B:480:GLU:H	1.85	0.82
1:B:1323:PRO:HG2	1:B:1326:CYS:HB3	1.62	0.82
1:D:741:GLU:HG3	1:D:834:MET:HG2	1.62	0.82
1:D:380:ARG:HH11	1:D:380:ARG:HB2	1.45	0.81
1:B:461:ASN:OD1	1:B:462:ARG:HD3	1.81	0.81
1:D:649:ILE:HD12	1:D:649:ILE:H	1.45	0.80
1:A:558:VAL:HG22	1:A:1241:ARG:HG2	1.64	0.79
1:D:671:VAL:HG11	1:D:682:ALA:HB3	1.63	0.79
1:D:646:ILE:HD11	1:D:651:ASN:CG	2.06	0.79
1:A:309:GLU:O	1:A:313:VAL:HG12	1.82	0.79
1:C:133:GLU:HG2	1:C:165:ARG:HB2	1.64	0.79
1:C:736:TYR:CE2	1:C:1332:ARG:HD2	2.19	0.78
1:C:556:ALA:HB3	1:C:1239:GLU:HG2	1.65	0.78
1:D:154:ARG:HD3	1:D:1197:GLU:OE2	1.83	0.78
1:D:646:ILE:HD11	1:D:651:ASN:ND2	1.98	0.78
1:B:538:LYS:HD2	1:B:538:LYS:N	1.99	0.78
1:C:667:ILE:HD12	1:C:808:VAL:HG22	1.65	0.78
1:B:193:PRO:HG2	1:B:561:PHE:CE2	2.20	0.77
1:D:124:MET:HE3	1:D:128:LEU:HG	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:125:TYR:OH	1:D:209:GLU:HG3	1.85	0.75
1:C:215:GLU:HG3	1:C:218:ARG:HH22	1.51	0.75
1:D:164:ALA:C	1:D:166:ASP:H	1.95	0.75
1:D:424:ALA:HB1	1:D:430:ASP:OD2	1.87	0.75
1:A:741:GLU:HG3	1:A:834:MET:HG2	1.68	0.74
1:A:956:PHE:HA	1:A:1146:ASN:HD21	1.51	0.74
1:A:376:SER:HB3	1:A:379:THR:OG1	1.87	0.74
1:D:649:ILE:HD12	1:D:649:ILE:N	2.03	0.74
1:D:506:ASP:OD1	1:D:1320:THR:HG22	1.87	0.74
1:C:748:HIS:CD2	1:C:837:THR:HG21	2.23	0.74
1:D:504:MET:HE2	1:D:1304:GLU:OE1	1.88	0.74
1:C:987:LYS:O	1:C:991:GLU:HG3	1.88	0.73
1:A:36:LEU:HD22	1:A:89:GLU:HG3	1.71	0.73
1:C:374:LEU:HD13	1:C:398:LEU:HD13	1.71	0.73
1:C:1115:GLU:O	1:C:1119:THR:HG23	1.88	0.72
1:C:125:TYR:OH	1:C:209:GLU:HG3	1.90	0.72
1:A:264:ILE:HG22	1:A:268:MET:HE2	1.72	0.72
1:C:374:LEU:HD22	1:C:398:LEU:HD11	1.72	0.72
1:B:374:LEU:HD22	1:B:398:LEU:HD21	1.71	0.72
1:D:736:TYR:CE2	1:D:1332:ARG:HD2	2.24	0.72
1:C:477:LEU:HD23	1:C:479:LYS:HE3	1.71	0.71
1:A:1204:LEU:HD13	1:A:1271:ILE:HD12	1.70	0.71
1:B:241:THR:OG1	1:B:244:GLU:HG3	1.91	0.71
1:C:433:LYS:HE2	1:C:504:MET:SD	2.30	0.71
1:D:1036:GLY:HA3	1:D:1043:LEU:HD21	1.72	0.71
1:D:867:ASN:ND2	1:D:1333:VAL:HG13	2.06	0.71
1:C:164:ALA:C	1:C:166:ASP:H	1.99	0.71
1:D:310:LYS:HE2	1:D:310:LYS:HA	1.71	0.71
1:D:374:LEU:HD13	1:D:398:LEU:HD22	1.72	0.71
1:B:1115:GLU:O	1:B:1119:THR:HG23	1.90	0.70
1:C:981:ARG:NH1	1:C:1176:ARG:HD3	2.06	0.70
1:B:215:GLU:HA	1:B:218:ARG:NH1	2.06	0.70
1:A:97:ARG:NH1	1:A:97:ARG:HB2	2.07	0.70
1:C:1123:MET:HE2	1:C:1123:MET:HA	1.73	0.70
1:B:953:LEU:HD23	1:B:959:LYS:HA	1.73	0.70
1:C:97:ARG:HB2	1:C:97:ARG:NH1	2.07	0.70
1:D:623:THR:O	1:D:623:THR:HG22	1.92	0.69
1:D:886:MET:HE2	1:D:895:ILE:HD11	1.75	0.69
1:B:649:ILE:HD11	1:B:804:THR:HG21	1.75	0.69
1:B:765:VAL:O	1:B:792:VAL:HG22	1.93	0.69
1:D:312:LEU:O	1:D:316:VAL:HG23	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:MET:HE2	1:D:167:GLY:HA2	1.74	0.69
1:B:125:TYR:OH	1:B:209:GLU:HG3	1.93	0.69
1:B:886:MET:HE2	1:B:895:ILE:HD11	1.75	0.68
6:C:4004:MTE:C9	6:C:4004:MTE:C6	2.69	0.68
1:D:559:GLN:HB3	1:D:1193:ILE:HD13	1.76	0.68
1:B:753:VAL:HG13	1:B:762:GLU:HB3	1.74	0.68
1:D:193:PRO:HG2	1:D:561:PHE:CE2	2.28	0.68
1:C:765:VAL:O	1:C:792:VAL:HG22	1.93	0.68
1:B:956:PHE:HA	1:B:1146:ASN:HD21	1.58	0.68
1:B:736:TYR:CD2	1:B:1332:ARG:HD2	2.28	0.68
1:C:1250:ASN:O	1:C:1256:ALA:HA	1.94	0.68
1:A:154:ARG:HD3	1:A:1197:GLU:OE2	1.93	0.68
1:D:1320:THR:HG23	1:D:1321:GLY:N	2.05	0.67
1:A:1135:ARG:HD3	1:B:1125:THR:OG1	1.94	0.67
1:B:3:ALA:HA	1:B:227:LEU:HD22	1.77	0.67
6:A:2004:MTE:C9	6:A:2004:MTE:C6	2.73	0.67
1:C:215:GLU:HG3	1:C:218:ARG:NH2	2.08	0.67
1:C:322:GLN:HA	1:C:322:GLN:HE21	1.60	0.67
1:D:1141:TYR:HB2	1:D:1150:PRO:HG3	1.76	0.67
1:D:956:PHE:HA	1:D:1146:ASN:HD21	1.59	0.67
1:A:103:GLU:OE2	1:A:202:THR:HG23	1.95	0.67
1:A:351:ASN:ND2	1:A:361:LEU:HB2	2.11	0.67
1:B:552:LYS:O	1:B:553:ASP:HB2	1.95	0.67
1:B:623:THR:HG22	1:B:623:THR:O	1.94	0.66
1:C:741:GLU:HG3	1:C:834:MET:HG2	1.77	0.66
1:A:441:LEU:HB3	1:A:451:GLU:HB2	1.77	0.66
1:B:656:PHE:HE2	1:B:815:LEU:HD23	1.60	0.66
1:D:1204:LEU:HD13	1:D:1271:ILE:HD12	1.78	0.66
1:C:993:CYS:HA	1:C:1285:GLN:HE22	1.60	0.66
1:B:472:ARG:HD2	1:B:485:ASP:OD1	1.95	0.66
1:A:604:LEU:HD21	1:A:822:ARG:NH2	2.10	0.66
1:B:1089:GLN:HG2	1:B:1134:TYR:CD1	2.31	0.65
1:A:748:HIS:CD2	1:A:837:THR:HG21	2.31	0.65
1:C:1320:THR:HG23	1:C:1321:GLY:H	1.61	0.65
1:B:309:GLU:O	1:B:313:VAL:HG13	1.96	0.65
1:B:748:HIS:CD2	1:B:837:THR:HG21	2.31	0.65
1:C:881:ARG:HD2	1:C:915:PHE:HB3	1.77	0.65
1:D:578:LEU:HD12	1:D:579:PRO:HD2	1.79	0.65
1:A:400:PRO:HG2	1:A:401:GLU:OE2	1.97	0.65
1:A:473:GLN:HA	1:A:476:LYS:HD3	1.79	0.65
1:D:328:ARG:HG2	1:D:328:ARG:HH11	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:604:LEU:HD21	1:D:822:ARG:NH2	2.12	0.65
1:B:95:LYS:HG3	1:B:590:GLU:OE2	1.97	0.64
1:D:32:ARG:HG3	1:D:32:ARG:HH11	1.62	0.64
1:D:446:THR:HB	1:D:535:LYS:NZ	2.12	0.64
1:D:944:ARG:O	1:D:947:LEU:HB2	1.97	0.64
1:B:64:LYS:CD	1:B:65:ILE:H	2.08	0.64
1:B:255:ALA:HB2	1:B:277:MET:HG2	1.79	0.64
1:A:3:ALA:CB	1:A:228:ARG:H	2.06	0.64
1:A:1135:ARG:HH12	1:A:1137:PRO:HB3	1.63	0.64
1:A:124:MET:HE1	1:A:127:LEU:HD23	1.80	0.64
1:B:531:ASN:O	1:B:532:LEU:HD12	1.97	0.64
1:C:372:LEU:HD11	1:C:385:MET:HE3	1.78	0.64
1:D:1174:ASN:O	1:D:1237:PRO:HA	1.97	0.64
1:A:64:LYS:HE2	1:A:65:ILE:H	1.62	0.64
1:A:372:LEU:HD11	1:A:385:MET:HE3	1.78	0.64
1:D:649:ILE:H	1:D:649:ILE:CD1	2.11	0.64
1:B:218:ARG:CB	1:B:218:ARG:HH11	2.11	0.64
1:B:1141:TYR:CB	1:B:1150:PRO:HG3	2.26	0.64
1:C:933:VAL:HG11	1:C:1280:ARG:HH21	1.63	0.64
1:D:193:PRO:HG2	1:D:561:PHE:CZ	2.33	0.64
1:D:241:THR:OG1	1:D:244:GLU:HG3	1.97	0.63
1:C:1287:THR:HG22	1:C:1288:GLY:N	2.09	0.63
1:D:1115:GLU:O	1:D:1119:THR:HG22	1.98	0.63
1:D:1324:GLU:CD	1:D:1325:ASN:H	2.06	0.63
1:C:667:ILE:HD12	1:C:808:VAL:CG2	2.28	0.63
1:B:389:PHE:HA	1:B:397:LEU:HG	1.80	0.63
1:C:389:PHE:HA	1:C:397:LEU:HG	1.81	0.63
1:A:987:LYS:O	1:A:991:GLU:HG3	1.99	0.63
1:C:1293:GLU:HG2	1:C:1294:LEU:N	2.14	0.62
1:D:748:HIS:CD2	1:D:837:THR:HG21	2.34	0.62
1:A:1008:ILE:O	1:A:1009:SER:HB2	1.98	0.62
1:A:131:GLN:HE21	1:A:133:GLU:H	1.48	0.62
1:D:607:ARG:NH1	1:D:679:THR:OG1	2.32	0.62
1:A:125:TYR:OH	1:A:209:GLU:HG3	2.00	0.62
1:A:1089:GLN:HG2	1:A:1134:TYR:CD1	2.35	0.62
1:C:1011:THR:O	1:C:1013:PRO:HD3	1.99	0.62
1:A:722:LYS:O	1:A:726:GLU:HG3	1.99	0.62
7:D:5005:MOM:OM2	7:D:5005:MOM:MO1	1.71	0.62
1:C:103:GLU:OE2	1:C:202:THR:HG23	2.00	0.62
1:C:933:VAL:HG11	1:C:1280:ARG:NH2	2.15	0.62
1:A:981:ARG:HH11	1:A:981:ARG:HB3	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1216:PRO:HG2	1:B:1327:LYS:CD	2.29	0.61
1:B:949:LYS:HG2	1:B:952:ASP:OD2	2.00	0.61
1:C:958:GLN:OE1	1:C:1150:PRO:HD2	2.01	0.61
1:D:303:CYS:SG	1:D:307:ILE:HD11	2.40	0.61
1:A:606:LEU:C	1:A:606:LEU:HD23	2.26	0.61
1:C:1313:LYS:O	1:C:1317:LEU:HD23	2.01	0.61
7:C:4005:MOM:OM2	7:C:4005:MOM:MO1	1.72	0.61
1:A:1313:LYS:O	1:A:1317:LEU:HD23	2.01	0.61
7:A:2005:MOM:OM2	7:A:2005:MOM:MO1	1.72	0.61
1:A:1280:ARG:HG2	1:A:1280:ARG:HH11	1.66	0.61
1:D:754:PRO:HD3	1:D:817:ALA:HB1	1.83	0.61
1:A:443:LYS:HG3	1:A:448:GLU:HG3	1.82	0.61
1:D:131:GLN:HE21	1:D:133:GLU:H	1.49	0.61
1:A:528:GLY:HA2	1:A:533:GLU:HB3	1.82	0.61
1:B:722:LYS:O	1:B:726:GLU:HG3	2.01	0.61
1:D:971:GLU:HG2	9:D:7225:HOH:O	2.00	0.61
1:C:868:VAL:HB	1:C:875:SER:OG	2.01	0.60
1:A:735:ILE:HD12	1:A:735:ILE:O	2.01	0.60
7:A:2005:MOM:MO1	7:A:2005:MOM:OM3	1.72	0.60
1:A:3:ALA:HA	1:A:227:LEU:HD22	1.82	0.60
1:C:753:VAL:CG2	1:C:762:GLU:HB3	2.31	0.60
7:C:4005:MOM:MO1	7:C:4005:MOM:OM3	1.72	0.60
1:D:982:LYS:HG2	1:D:999:LEU:HD23	1.83	0.60
7:B:3005:MOM:OM2	7:B:3005:MOM:MO1	1.72	0.60
1:C:623:THR:O	1:C:627:LYS:HG3	2.01	0.60
7:D:5005:MOM:MO1	7:D:5005:MOM:OM3	1.72	0.60
1:A:304:PRO:HD2	1:A:307:ILE:HD12	1.83	0.60
1:C:638:ALA:O	1:C:641:VAL:HG22	2.02	0.60
1:A:1332:ARG:HG2	1:A:1332:ARG:HH11	1.67	0.60
1:D:671:VAL:HG11	1:D:682:ALA:CB	2.30	0.60
1:C:310:LYS:HE2	1:C:310:LYS:HA	1.84	0.59
7:B:3005:MOM:MO1	7:B:3005:MOM:OM3	1.73	0.59
1:D:1324:GLU:O	1:D:1325:ASN:HB2	2.02	0.59
1:A:562:GLN:HG3	1:A:1246:ARG:CZ	2.32	0.59
1:A:1100:LYS:HE3	1:A:1100:LYS:O	2.01	0.59
1:A:3:ALA:HB1	1:A:228:ARG:N	2.10	0.59
1:A:30:LEU:HD23	1:A:34:LEU:HD12	1.84	0.59
1:A:322:GLN:O	1:A:412:SER:HB3	2.02	0.59
1:B:328:ARG:HG2	1:B:328:ARG:HH11	1.67	0.59
1:D:566:LYS:HD3	1:D:567:GLY:N	2.17	0.59
1:C:131:GLN:HE21	1:C:133:GLU:N	1.95	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1008:ILE:O	1:C:1009:SER:HB2	2.01	0.59
1:A:720:LEU:HD11	1:A:896:ARG:CB	2.33	0.59
1:B:259:VAL:HG11	1:B:347:SER:HB3	1.84	0.59
1:B:649:ILE:HD11	1:B:804:THR:CG2	2.31	0.59
1:C:1141:TYR:HB2	1:C:1150:PRO:HG3	1.83	0.59
1:A:389:PHE:HA	1:A:397:LEU:HG	1.85	0.59
1:A:613:ARG:HH11	1:A:692:GLU:HG3	1.66	0.59
1:A:638:ALA:O	1:A:641:VAL:HG22	2.02	0.59
1:D:136:MET:HE2	1:D:167:GLY:CA	2.33	0.59
1:D:242:LEU:HA	1:D:284:ILE:HD13	1.83	0.59
1:A:613:ARG:NH1	1:A:692:GLU:HG3	2.18	0.59
1:C:1043:LEU:O	1:C:1047:MET:HG2	2.03	0.59
1:A:197:LYS:HD2	1:A:200:GLU:OE2	2.03	0.58
1:B:267:GLU:HA	1:B:271:LYS:HG2	1.83	0.58
1:C:400:PRO:HG2	1:C:401:GLU:OE2	2.03	0.58
1:C:1089:GLN:HG2	1:C:1134:TYR:CD1	2.38	0.58
1:C:1280:ARG:NH2	1:C:1293:GLU:O	2.36	0.58
1:D:471:GLN:NE2	1:D:474:LEU:HD11	2.18	0.58
1:A:881:ARG:HD2	1:A:915:PHE:HB3	1.86	0.58
1:B:131:GLN:HE21	1:B:133:GLU:H	1.51	0.58
1:D:656:PHE:HE2	1:D:815:LEU:HD23	1.66	0.58
1:D:860:LEU:HD12	1:D:861:GLU:H	1.68	0.58
1:B:558:VAL:CG2	1:B:1241:ARG:HG2	2.30	0.58
1:C:1217:GLU:CD	1:C:1217:GLU:H	2.10	0.58
1:C:407:ILE:N	1:C:407:ILE:HD12	2.19	0.58
1:A:443:LYS:HG3	1:A:448:GLU:CG	2.33	0.58
1:D:215:GLU:O	1:D:219:LEU:HG	2.03	0.58
1:D:418:PHE:CD1	1:D:439:ARG:HB2	2.38	0.58
1:A:1011:THR:O	1:A:1013:PRO:HD3	2.04	0.58
1:B:562:GLN:HG3	1:B:1246:ARG:HG2	1.86	0.58
1:C:965:LEU:HB3	1:C:966:PRO:HD3	1.85	0.58
1:D:1250:ASN:O	1:D:1256:ALA:HA	2.04	0.58
1:C:1332:ARG:HG2	1:C:1332:ARG:HH11	1.69	0.58
1:D:351:ASN:ND2	1:D:361:LEU:HB2	2.19	0.58
1:A:245:LEU:HD11	1:A:257:LEU:HD11	1.86	0.58
1:B:304:PRO:HA	1:B:346:ALA:O	2.02	0.58
1:B:1034:HIS:HB2	1:B:1087:ASN:HD22	1.69	0.58
1:C:1153:TYR:CE1	1:C:1258:LYS:HG2	2.39	0.58
1:D:1286:HIS:O	1:D:1287:THR:HG23	2.03	0.58
1:B:880:GLU:HG2	1:B:1143:PHE:CZ	2.39	0.58
1:C:1222:THR:HG22	1:C:1228:TYR:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1324:GLU:CD	1:D:1325:ASN:N	2.62	0.58
1:D:504:MET:HE2	1:D:1304:GLU:CD	2.29	0.57
1:D:641:VAL:HG21	1:D:645:ASN:HB2	1.85	0.57
1:A:786:ASN:ND2	1:B:1029:SER:HB2	2.19	0.57
1:B:559:GLN:HB3	1:B:1193:ILE:HD13	1.86	0.57
1:B:649:ILE:CD1	1:B:804:THR:HG21	2.34	0.57
1:D:868:VAL:HG13	1:D:902:CYS:O	2.04	0.57
1:B:996:LYS:HZ3	1:B:1285:GLN:HE22	1.52	0.57
1:B:1287:THR:HG22	1:B:1288:GLY:N	2.19	0.57
1:D:510:THR:HG21	1:D:1315:THR:HG22	1.86	0.57
1:D:125:TYR:HH	1:D:209:GLU:HG3	1.67	0.57
1:B:374:LEU:HD22	1:B:398:LEU:CD2	2.35	0.57
1:C:713:LEU:HD21	1:C:876:GLN:HE21	1.70	0.57
1:B:152:GLY:O	1:B:1236:ILE:HG21	2.05	0.57
1:A:645:ASN:O	1:A:654:THR:HA	2.05	0.57
1:B:996:LYS:NZ	1:B:1285:GLN:HE22	2.03	0.57
1:A:215:GLU:HG3	1:A:218:ARG:HH22	1.70	0.56
1:A:1280:ARG:NH2	1:A:1293:GLU:O	2.32	0.56
1:B:375:VAL:HG12	1:B:380:ARG:HG3	1.86	0.56
1:C:164:ALA:C	1:C:166:ASP:N	2.59	0.56
1:A:720:LEU:HD11	1:A:896:ARG:HB3	1.87	0.56
1:C:124:MET:HE1	1:C:127:LEU:HD23	1.86	0.56
1:D:553:ASP:HB3	1:D:554:PRO:HD2	1.85	0.56
1:A:367:ALA:O	1:A:439:ARG:HD3	2.05	0.56
1:B:743:PHE:HA	1:B:830:ARG:HH21	1.70	0.56
1:B:795:MET:HE3	1:B:1039:MET:HB3	1.86	0.56
1:C:504:MET:HG2	1:C:1304:GLU:OE2	2.04	0.56
1:C:795:MET:HE3	1:C:1039:MET:HB3	1.87	0.56
1:A:479:LYS:HG2	1:A:537:GLY:N	2.21	0.56
1:C:32:ARG:HD2	9:C:7058:HOH:O	2.04	0.56
1:C:328:ARG:HH11	1:C:328:ARG:HG2	1.70	0.56
1:C:606:LEU:HD23	1:C:606:LEU:C	2.31	0.56
1:C:735:ILE:HD12	1:C:735:ILE:O	2.06	0.56
1:C:131:GLN:NE2	1:C:133:GLU:H	1.95	0.56
1:D:881:ARG:HD2	1:D:915:PHE:HB3	1.86	0.56
1:B:1174:ASN:O	1:B:1237:PRO:HA	2.06	0.56
1:C:662:THR:O	1:C:663:CYS:HB3	2.05	0.56
1:A:650:CYS:HB2	1:A:652:ASP:OD2	2.05	0.56
1:B:809:VAL:O	1:B:813:VAL:HG23	2.05	0.56
1:B:1216:PRO:HG2	1:B:1327:LYS:HD2	1.88	0.56
1:A:505:VAL:HG21	1:A:1320:THR:HG21	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:GLU:HA	1:B:218:ARG:HH11	1.69	0.56
1:B:1216:PRO:HG2	1:B:1327:LYS:HD3	1.88	0.56
1:C:193:PRO:HG2	1:C:561:PHE:CE2	2.41	0.56
1:C:322:GLN:HG2	1:C:414:GLU:CD	2.31	0.56
1:A:510:THR:HG21	1:A:1315:THR:HG22	1.86	0.56
1:A:622:ASP:HB3	1:A:687:LYS:HB3	1.87	0.56
1:C:1291:VAL:HG13	1:C:1292:LYS:HG3	1.88	0.56
1:D:86:THR:O	1:D:122:MET:HE2	2.05	0.56
1:B:218:ARG:HH11	1:B:218:ARG:HB3	1.70	0.55
1:B:218:ARG:NH1	1:B:218:ARG:HB2	2.22	0.55
1:B:720:LEU:HD11	1:B:896:ARG:HB3	1.89	0.55
1:C:217:LEU:O	1:C:220:LYS:HG2	2.07	0.55
1:A:374:LEU:HD13	1:A:398:LEU:CD2	2.37	0.55
1:B:1332:ARG:HG2	1:B:1332:ARG:HH11	1.71	0.55
1:C:886:MET:HE2	1:C:895:ILE:HD11	1.87	0.55
1:A:477:LEU:HD23	1:A:479:LYS:HE2	1.87	0.55
1:A:667:ILE:HD12	1:A:808:VAL:HG13	1.89	0.55
1:A:712:GLU:N	1:A:900:ARG:HH11	2.04	0.55
1:C:372:LEU:CD2	1:C:407:ILE:HG23	2.36	0.55
1:C:1127:SER:HB2	1:D:1133:PHE:CG	2.42	0.55
1:D:623:THR:HG23	1:D:626:ALA:HB3	1.88	0.55
1:B:1204:LEU:HD12	1:B:1204:LEU:O	2.06	0.55
1:C:1008:ILE:O	1:C:1009:SER:CB	2.55	0.55
1:D:498:PRO:HG2	1:D:1323:PRO:CD	2.37	0.55
1:D:880:GLU:HG2	1:D:1143:PHE:CZ	2.41	0.55
1:A:507:PHE:HB2	1:A:1304:GLU:HG3	1.89	0.55
1:C:744:TYR:O	1:C:830:ARG:NH2	2.31	0.55
1:C:558:VAL:CG2	1:C:1241:ARG:HG2	2.34	0.55
1:B:799:PHE:HA	6:B:3004:MTE:S1'	2.48	0.54
1:C:281:PRO:HB2	1:C:287:LEU:CD1	2.37	0.54
1:A:1199:ALA:HB3	1:A:1264:PRO:HB2	1.89	0.54
1:B:603:GLU:HG3	1:B:823:PRO:HB2	1.88	0.54
1:D:196:PHE:CE2	1:D:198:PRO:HG3	2.42	0.54
1:D:1290:ASN:ND2	1:D:1292:LYS:H	2.05	0.54
1:A:473:GLN:HA	1:A:476:LYS:CD	2.36	0.54
1:A:656:PHE:HE2	1:A:815:LEU:HD23	1.71	0.54
1:A:136:MET:HE2	1:A:166:ASP:HB3	1.88	0.54
1:D:535:LYS:O	1:D:535:LYS:HG2	2.07	0.54
1:A:133:GLU:CG	1:A:165:ARG:HB3	2.25	0.54
1:B:224:ARG:HH11	1:B:224:ARG:HG2	1.72	0.54
1:C:709:TYR:CZ	1:C:903:LYS:HG3	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:GLN:HA	1:B:322:GLN:OE1	2.07	0.54
1:C:430:ASP:CG	1:C:1229:LYS:HE2	2.32	0.54
1:B:538:LYS:H	1:B:538:LYS:CD	2.16	0.54
1:C:3:ALA:HB2	1:C:225:LYS:NZ	2.23	0.54
1:C:667:ILE:CD1	1:C:808:VAL:HG22	2.36	0.54
1:D:95:LYS:HG3	1:D:590:GLU:OE2	2.07	0.54
1:A:241:THR:OG1	1:A:244:GLU:HG3	2.08	0.54
1:A:249:LYS:HD3	1:A:257:LEU:HD21	1.88	0.54
1:C:940:GLU:HG2	1:C:941:GLU:N	2.22	0.54
1:D:376:SER:O	1:D:377:ARG:C	2.50	0.54
1:D:164:ALA:C	1:D:166:ASP:N	2.65	0.54
1:A:550:PHE:CE2	1:A:552:LYS:HD2	2.42	0.53
1:B:714:LYS:HD2	1:B:896:ARG:NH1	2.23	0.53
1:C:473:GLN:NE2	1:C:482:LEU:HG	2.23	0.53
1:C:891:LYS:HD2	1:C:952:ASP:OD2	2.09	0.53
1:D:940:GLU:HG2	1:D:941:GLU:N	2.22	0.53
1:D:1265:LEU:HD23	1:D:1265:LEU:C	2.33	0.53
1:A:1123:MET:HE3	1:B:1014:PHE:CE2	2.42	0.53
1:B:996:LYS:NZ	1:B:1285:GLN:NE2	2.56	0.53
1:B:1109:ASN:ND2	1:B:1112:GLY:HA3	2.23	0.53
1:D:1283:ARG:HH21	1:D:1293:GLU:CD	2.16	0.53
1:A:87:THR:OG1	1:A:89:GLU:HG2	2.08	0.53
1:A:150:CYS:HB3	6:A:2004:MTE:N2	2.24	0.53
1:C:1188:ASN:CG	1:C:1191:ILE:HG12	2.33	0.53
1:D:758:ALA:HB1	1:D:787:ARG:HE	1.72	0.53
1:A:616:ALA:HA	1:A:693:LEU:HG	1.90	0.53
1:A:886:MET:HE2	1:A:895:ILE:HD11	1.91	0.53
1:A:958:GLN:OE1	1:A:1150:PRO:HD2	2.08	0.53
1:B:196:PHE:CE2	1:B:198:PRO:HG3	2.43	0.53
1:D:444:PRO:O	1:D:446:THR:HG23	2.08	0.53
1:A:742:HIS:HA	1:A:912:PHE:CE2	2.44	0.53
1:B:578:LEU:HD12	1:B:579:PRO:HD2	1.89	0.53
1:B:888:ASN:O	1:B:1005:LYS:HE2	2.07	0.53
1:C:322:GLN:HA	1:C:322:GLN:NE2	2.21	0.53
1:D:136:MET:HE2	1:D:167:GLY:H	1.74	0.53
1:D:1263:PRO:HB2	1:D:1264:PRO:HD3	1.90	0.53
1:A:212:PHE:CE2	1:A:217:LEU:HD13	2.44	0.53
1:A:910:THR:OG1	1:A:911:ALA:N	2.42	0.53
1:B:910:THR:OG1	1:B:911:ALA:N	2.41	0.53
1:C:245:LEU:HD22	1:C:281:PRO:HB3	1.90	0.53
1:B:753:VAL:CG1	1:B:762:GLU:HB3	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:441:LEU:HB3	1:C:451:GLU:HB2	1.90	0.53
1:D:517:PHE:CZ	1:D:521:LEU:HD11	2.43	0.53
1:B:881:ARG:HD2	1:B:915:PHE:O	2.09	0.53
1:D:912:PHE:O	1:D:913:ARG:C	2.51	0.53
1:D:1008:ILE:O	1:D:1009:SER:CB	2.56	0.53
1:A:124:MET:CE	1:A:127:LEU:HD23	2.38	0.53
1:A:242:LEU:HA	1:A:284:ILE:HD13	1.90	0.53
1:A:253:PRO:HB3	1:A:400:PRO:HB2	1.91	0.53
1:B:372:LEU:HD11	1:B:385:MET:CE	2.35	0.53
1:C:805:ARG:O	1:C:808:VAL:HG12	2.07	0.53
1:A:787:ARG:HG2	1:A:787:ARG:HH11	1.75	0.52
1:C:1332:ARG:HG2	1:C:1332:ARG:NH1	2.23	0.52
1:A:438:MET:HG2	1:A:454:LEU:HD22	1.90	0.52
1:A:1008:ILE:O	1:A:1009:SER:CB	2.57	0.52
1:A:1135:ARG:O	1:A:1135:ARG:HG3	2.09	0.52
1:B:754:PRO:HD3	1:B:817:ALA:HB1	1.92	0.52
1:C:192:SER:N	1:C:193:PRO:CD	2.71	0.52
1:D:65:ILE:HD11	1:D:217:LEU:HD11	1.92	0.52
1:D:228:ARG:HE	1:D:230:GLU:CD	2.17	0.52
1:D:881:ARG:HD2	1:D:915:PHE:O	2.09	0.52
1:A:364:VAL:HG13	1:A:418:PHE:CZ	2.45	0.52
1:C:120:ILE:HD13	1:C:146:ASN:HB3	1.91	0.52
1:D:646:ILE:HD12	1:D:646:ILE:C	2.34	0.52
1:A:220:LYS:HE2	1:A:221:ASP:OD1	2.09	0.52
1:B:800:GLY:HA2	1:B:803:VAL:HG23	1.91	0.52
1:A:462:ARG:HB3	9:A:7121:HOH:O	2.09	0.52
1:C:389:PHE:O	1:C:391:PRO:HD3	2.09	0.52
1:D:1332:ARG:HG2	1:D:1332:ARG:HH11	1.74	0.52
1:A:3:ALA:HA	1:A:227:LEU:CD2	2.39	0.52
1:B:505:VAL:HG23	1:B:506:ASP:N	2.23	0.52
1:D:949:LYS:HG2	1:D:952:ASP:OD2	2.09	0.52
1:D:1300:PRO:HG2	1:D:1302:THR:HG23	1.90	0.52
1:D:372:LEU:HD11	1:D:385:MET:CE	2.32	0.52
1:B:422:LYS:HE3	1:B:432:ALA:HB2	1.92	0.52
1:C:375:VAL:HG12	1:C:380:ARG:HG3	1.92	0.52
1:A:881:ARG:HD2	1:A:915:PHE:O	2.10	0.52
1:A:1089:GLN:HG2	1:A:1134:TYR:CE1	2.45	0.52
1:B:154:ARG:HD3	1:B:1197:GLU:OE2	2.10	0.52
1:B:218:ARG:NH1	1:B:218:ARG:CB	2.72	0.52
1:B:743:PHE:HA	1:B:830:ARG:NH2	2.24	0.52
1:B:912:PHE:O	1:B:913:ARG:C	2.52	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:857:VAL:CG2	1:B:892:ILE:HG12	2.40	0.52
1:C:607:ARG:NH2	1:C:829:ASP:OD2	2.43	0.52
1:C:713:LEU:HD21	1:C:876:GLN:NE2	2.24	0.52
1:D:467:LEU:O	1:D:471:GLN:HB2	2.10	0.52
1:D:1038:GLU:HB2	1:D:1044:HIS:CD2	2.44	0.52
1:D:1208:THR:O	1:D:1209:LEU:HD12	2.09	0.52
1:D:571:GLU:CD	1:D:1058:PRO:HG3	2.35	0.51
1:B:389:PHE:O	1:B:391:PRO:HD3	2.10	0.51
1:C:303:CYS:HB3	1:C:307:ILE:HD11	1.92	0.51
1:C:571:GLU:CD	1:C:1058:PRO:HG3	2.35	0.51
1:C:736:TYR:CZ	1:C:1332:ARG:HD2	2.45	0.51
1:B:135:THR:OG1	1:B:138:GLU:HG3	2.11	0.51
1:C:517:PHE:CZ	1:C:521:LEU:HD11	2.45	0.51
1:A:1260:VAL:O	1:A:1260:VAL:HG22	2.10	0.51
1:D:385:MET:HE2	1:D:389:PHE:CD2	2.45	0.51
1:D:443:LYS:HD2	1:D:450:GLN:NE2	2.24	0.51
1:D:633:VAL:HB	1:D:672:VAL:O	2.11	0.51
1:B:720:LEU:HD11	1:B:896:ARG:CB	2.41	0.51
1:D:606:LEU:C	1:D:606:LEU:HD23	2.36	0.51
1:A:117:THR:CG2	1:A:587:ALA:HA	2.40	0.51
1:D:32:ARG:HG3	1:D:32:ARG:NH1	2.24	0.51
1:A:531:ASN:HA	1:A:533:GLU:OE1	2.11	0.51
1:B:1179:ILE:HD11	1:B:1200:PHE:CD1	2.46	0.51
1:C:224:ARG:HG2	1:C:224:ARG:HH11	1.75	0.51
1:C:646:ILE:HG13	1:C:646:ILE:O	2.10	0.51
1:A:88:VAL:HG13	1:A:89:GLU:N	2.26	0.51
1:A:912:PHE:O	1:A:913:ARG:C	2.54	0.51
1:A:981:ARG:HB3	1:A:981:ARG:NH1	2.26	0.51
1:A:233:ARG:CZ	1:A:681:ARG:HD3	2.41	0.51
1:A:389:PHE:HA	1:A:397:LEU:CD1	2.41	0.51
1:B:608:LEU:HD13	1:B:667:ILE:CD1	2.40	0.51
1:B:762:GLU:C	1:B:763:LEU:HD12	2.35	0.51
1:C:490:LEU:HB2	1:C:513:LEU:HD22	1.93	0.51
1:C:510:THR:HG21	1:C:1315:THR:HG22	1.92	0.51
1:A:166:ASP:O	1:A:167:GLY:C	2.53	0.51
1:A:965:LEU:N	1:A:966:PRO:CD	2.74	0.51
1:B:1038:GLU:HB2	1:B:1044:HIS:CD2	2.46	0.51
1:C:787:ARG:HG2	1:C:787:ARG:HH11	1.76	0.51
1:C:956:PHE:CA	1:C:1146:ASN:HD21	2.15	0.51
1:C:1320:THR:HG23	1:C:1321:GLY:N	2.26	0.51
1:A:653:GLU:HB3	1:A:871:THR:CG2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:750:THR:HG21	1:A:810:SER:HA	1.93	0.50
1:A:953:LEU:HA	1:A:958:GLN:O	2.11	0.50
1:A:1038:GLU:HB2	1:A:1044:HIS:CD2	2.46	0.50
1:B:1022:LEU:HD22	1:B:1098:ILE:HG13	1.93	0.50
1:A:553:ASP:HB3	1:A:554:PRO:HD2	1.93	0.50
1:D:556:ALA:HB3	1:D:1239:GLU:HG2	1.93	0.50
1:D:1081:SER:OG	1:D:1262:GLU:HG3	2.11	0.50
1:D:1332:ARG:HG2	1:D:1332:ARG:NH1	2.26	0.50
1:A:1280:ARG:HH11	1:A:1280:ARG:CG	2.24	0.50
1:B:374:LEU:CD2	1:B:398:LEU:HD21	2.41	0.50
1:B:1039:MET:HE3	6:B:3004:MTE:H4'1	1.92	0.50
1:D:136:MET:HE2	1:D:167:GLY:N	2.26	0.50
1:D:1021:LEU:HD13	1:D:1131:THR:HG22	1.93	0.50
1:B:915:PHE:HA	2:B:6002:BCT:O3	2.12	0.50
1:D:400:PRO:HG2	1:D:401:GLU:OE2	2.11	0.50
1:A:491:ALA:O	1:A:495:HIS:HB2	2.11	0.50
1:B:607:ARG:HH11	1:B:680:GLN:N	2.09	0.50
1:C:531:ASN:HA	1:C:533:GLU:OE1	2.11	0.50
1:C:699:ILE:O	1:C:703:ILE:HG13	2.11	0.50
1:D:716:GLU:HB2	1:D:896:ARG:HG3	1.93	0.50
1:D:1320:THR:CG2	1:D:1321:GLY:H	2.09	0.50
1:A:696:ILE:HG23	1:A:701:ASP:CB	2.41	0.50
1:A:867:ASN:ND2	1:A:1333:VAL:HG13	2.26	0.50
1:A:1084:ALA:HB3	9:A:7178:HOH:O	2.11	0.50
1:C:562:GLN:HG3	1:C:1246:ARG:CZ	2.42	0.50
1:C:753:VAL:HG23	1:C:753:VAL:O	2.12	0.50
1:A:736:TYR:CD2	1:A:1332:ARG:HD2	2.46	0.50
1:B:104:ARG:HD3	1:B:201:PHE:CD2	2.47	0.50
1:B:881:ARG:HD2	1:B:915:PHE:HB3	1.93	0.50
1:B:932:ALA:HA	1:B:942:VAL:HG21	1.93	0.50
1:C:323:LYS:HA	1:C:412:SER:O	2.12	0.50
1:A:65:ILE:HD12	1:A:212:PHE:CD2	2.46	0.50
1:A:1141:TYR:OH	1:A:1146:ASN:ND2	2.45	0.50
1:A:1327:LYS:HD2	1:A:1327:LYS:C	2.37	0.50
1:B:3:ALA:O	1:B:5:LYS:N	2.41	0.50
1:D:58:TYR:OH	1:D:63:ASN:ND2	2.45	0.50
1:B:1271:ILE:O	1:B:1275:ILE:HG13	2.12	0.50
1:D:124:MET:HE2	1:D:163:PHE:CD2	2.46	0.50
1:A:399:SER:HB2	1:A:400:PRO:HD2	1.93	0.49
1:A:399:SER:OG	1:A:402:GLU:HG3	2.11	0.49
1:D:1327:LYS:HD2	1:D:1327:LYS:C	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:PHE:HE2	1:A:217:LEU:HD13	1.75	0.49
1:B:958:GLN:OE1	1:B:1150:PRO:HD2	2.12	0.49
1:B:986:ASP:O	1:B:990:LYS:HG3	2.12	0.49
1:C:264:ILE:HD11	5:C:4003:FAD:H3B	1.92	0.49
1:D:380:ARG:HH11	1:D:380:ARG:CB	2.22	0.49
1:D:640:ASP:HB3	1:D:819:LYS:HE3	1.93	0.49
1:A:131:GLN:O	1:A:134:PRO:HD3	2.12	0.49
1:A:572:ASP:OD1	1:A:1053:ARG:HD3	2.12	0.49
1:B:325:GLU:HB2	1:B:412:SER:OG	2.11	0.49
1:B:374:LEU:HD13	1:B:398:LEU:CD2	2.41	0.49
1:B:623:THR:HG22	1:B:627:LYS:HG3	1.95	0.49
1:A:1073:PRO:HD3	1:B:1023:HIS:CE1	2.47	0.49
1:B:958:GLN:HG3	1:B:1149:ASN:OD1	2.12	0.49
1:B:1184:GLY:HA2	1:B:1248:CYS:O	2.13	0.49
1:C:322:GLN:HG2	1:C:414:GLU:OE1	2.12	0.49
1:D:224:ARG:HD3	1:D:283:TRP:CE3	2.47	0.49
1:D:1008:ILE:O	1:D:1009:SER:HB2	2.11	0.49
1:D:1022:LEU:HD23	1:D:1022:LEU:C	2.37	0.49
1:D:1047:MET:HE2	1:D:1047:MET:HA	1.93	0.49
1:D:1324:GLU:OE2	1:D:1325:ASN:N	2.45	0.49
1:A:1033:THR:CG2	1:A:1066:GLU:O	2.60	0.49
1:A:1050:VAL:HG13	1:A:1255:TYR:HE2	1.78	0.49
1:B:117:THR:HB	1:B:118:PRO:HD3	1.94	0.49
1:B:1083:SER:HB2	6:B:3004:MTE:O3P	2.13	0.49
1:B:1152:HIS:CE1	1:B:1252:LYS:HD2	2.47	0.49
1:C:742:HIS:HA	1:C:912:PHE:CZ	2.48	0.49
1:D:736:TYR:CZ	1:D:1332:ARG:HD2	2.47	0.49
1:A:696:ILE:HG23	1:A:701:ASP:HB3	1.94	0.49
1:D:1001:ILE:HG23	1:D:1001:ILE:O	2.12	0.49
1:A:712:GLU:N	1:A:900:ARG:NH1	2.60	0.49
1:B:307:ILE:C	1:B:307:ILE:HD12	2.38	0.49
1:B:374:LEU:HD13	1:B:398:LEU:HD23	1.93	0.49
1:B:602:ASN:ND2	1:B:823:PRO:HD2	2.27	0.49
1:B:5:LYS:HE3	1:B:16:VAL:HG13	1.93	0.49
1:B:1326:CYS:O	1:B:1328:PRO:HD3	2.13	0.49
1:C:419:SER:HB2	1:C:519:PHE:CD1	2.47	0.49
1:A:473:GLN:O	1:A:476:LYS:HB2	2.13	0.49
1:A:1089:GLN:HG3	9:A:7061:HOH:O	2.12	0.49
1:A:58:TYR:OH	1:A:63:ASN:ND2	2.45	0.49
1:C:742:HIS:CE1	1:C:839:GLY:HA2	2.48	0.49
1:D:519:PHE:O	1:D:523:VAL:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1323:PRO:O	1:D:1324:GLU:C	2.56	0.49
1:B:87:THR:OG1	1:B:89:GLU:HG2	2.13	0.48
1:B:193:PRO:HG2	1:B:561:PHE:CZ	2.48	0.48
1:A:393:TYR:N	1:A:461:ASN:HD21	2.11	0.48
1:B:530:GLU:O	1:B:531:ASN:HB2	2.12	0.48
1:B:556:ALA:HB3	1:B:1239:GLU:HG2	1.94	0.48
1:B:1204:LEU:HD12	1:B:1204:LEU:C	2.38	0.48
1:D:742:HIS:HA	1:D:912:PHE:CZ	2.48	0.48
1:A:1174:ASN:O	1:A:1237:PRO:HA	2.14	0.48
1:A:1321:GLY:O	1:A:1322:VAL:HB	2.14	0.48
1:B:58:TYR:HE1	1:B:63:ASN:HD22	1.59	0.48
1:B:505:VAL:HG23	1:B:506:ASP:H	1.77	0.48
1:B:646:ILE:HG13	1:B:646:ILE:O	2.12	0.48
1:C:351:ASN:ND2	1:C:361:LEU:HB2	2.28	0.48
1:D:748:HIS:CE1	1:D:802:LYS:HG2	2.48	0.48
1:D:965:LEU:HB3	1:D:966:PRO:HD3	1.95	0.48
1:D:1089:GLN:HG2	1:D:1134:TYR:CD1	2.47	0.48
1:A:1263:PRO:HB2	1:A:1264:PRO:HD3	1.96	0.48
1:B:40:LYS:HB3	1:B:115:PHE:CZ	2.48	0.48
1:B:1250:ASN:O	1:B:1256:ALA:HA	2.12	0.48
1:C:419:SER:HB2	1:C:519:PHE:HD1	1.79	0.48
1:C:868:VAL:O	1:C:868:VAL:HG23	2.11	0.48
1:A:131:GLN:NE2	1:A:133:GLU:H	2.11	0.48
1:A:346:ALA:HB1	5:A:2003:FAD:H4'	1.94	0.48
1:A:1188:ASN:CG	1:A:1191:ILE:HG12	2.38	0.48
1:C:62:GLN:HB3	1:C:64:LYS:HG2	1.95	0.48
1:D:471:GLN:HE22	1:D:474:LEU:HD11	1.78	0.48
1:A:653:GLU:HB3	1:A:871:THR:HG21	1.95	0.48
1:B:735:ILE:H	1:B:735:ILE:HD12	1.79	0.48
1:D:743:PHE:HA	1:D:830:ARG:NH2	2.27	0.48
1:D:1331:VAL:HG22	1:D:1332:ARG:N	2.28	0.48
1:A:1033:THR:HG21	9:A:7095:HOH:O	2.13	0.48
1:C:1131:THR:HG23	1:D:1131:THR:HG23	1.94	0.48
1:C:1320:THR:OG1	1:C:1321:GLY:N	2.45	0.48
1:A:623:THR:HG22	1:A:627:LYS:HG3	1.94	0.48
1:B:606:LEU:C	1:B:606:LEU:HD23	2.38	0.48
1:C:338:ALA:HA	1:C:429:ASP:OD1	2.14	0.48
1:C:709:TYR:HB2	1:C:901:LEU:HB2	1.95	0.48
1:C:1199:ALA:HB3	1:C:1264:PRO:HB2	1.96	0.48
1:C:372:LEU:HD11	1:C:385:MET:CE	2.44	0.48
1:C:389:PHE:HD1	1:C:397:LEU:HD12	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:603:GLU:HA	1:D:823:PRO:HG2	1.95	0.48
1:B:736:TYR:CE2	1:B:1332:ARG:HD2	2.48	0.48
1:B:748:HIS:CE1	1:B:802:LYS:HG2	2.49	0.48
1:C:786:ASN:OD1	1:C:787:ARG:NH1	2.47	0.48
1:C:1009:SER:HA	1:C:1082:VAL:HG11	1.94	0.48
1:D:351:ASN:HB2	5:D:5003:FAD:O4'	2.14	0.48
1:B:124:MET:HE3	1:B:128:LEU:HG	1.95	0.47
1:C:97:ARG:HB2	1:C:97:ARG:CZ	2.43	0.47
1:C:1089:GLN:HB3	1:C:1134:TYR:CG	2.49	0.47
1:D:623:THR:O	1:D:623:THR:CG2	2.61	0.47
1:C:27:LEU:HD21	1:C:41:LEU:HB2	1.96	0.47
1:C:287:LEU:O	1:C:302:ALA:HB3	2.15	0.47
1:C:346:ALA:HB1	5:C:4003:FAD:H4'	1.96	0.47
1:C:606:LEU:HD23	1:C:607:ARG:N	2.29	0.47
1:D:117:THR:HB	1:D:118:PRO:HD3	1.95	0.47
1:D:799:PHE:HA	6:D:5004:MTE:S1'	2.54	0.47
1:D:943:ARG:HD2	9:D:7129:HOH:O	2.13	0.47
1:A:1192:ASP:O	1:A:1196:VAL:HG23	2.15	0.47
1:B:592:VAL:HG13	1:B:596:ASP:HB2	1.96	0.47
1:B:1162:GLU:HG2	1:B:1175:LEU:HD12	1.96	0.47
1:C:88:VAL:HG13	1:C:89:GLU:N	2.29	0.47
1:C:96:THR:OG1	1:C:97:ARG:N	2.44	0.47
1:C:736:TYR:CD2	1:C:1332:ARG:HD2	2.49	0.47
1:C:912:PHE:O	1:C:913:ARG:C	2.57	0.47
1:C:1181:MET:HE2	1:C:1264:PRO:HG3	1.96	0.47
1:D:1122:TYR:CD2	1:D:1123:MET:HE2	2.49	0.47
1:A:1288:GLY:O	1:A:1289:ASN:HB3	2.13	0.47
1:B:517:PHE:CZ	1:B:521:LEU:HD11	2.49	0.47
1:B:741:GLU:HB3	1:B:1228:TYR:CE2	2.50	0.47
1:B:786:ASN:OD1	1:B:787:ARG:NH1	2.46	0.47
1:C:571:GLU:OE2	1:C:1058:PRO:HG3	2.14	0.47
1:D:129:ARG:NE	1:D:209:GLU:HG2	2.30	0.47
1:A:363:PRO:HG2	1:A:435:THR:HG23	1.96	0.47
1:A:428:GLU:O	1:A:429:ASP:C	2.57	0.47
1:B:1119:THR:O	1:B:1123:MET:HG2	2.14	0.47
1:D:115:PHE:HD2	1:D:745:LEU:HB3	1.80	0.47
1:D:247:ASP:OD1	1:D:377:ARG:HD3	2.15	0.47
1:D:346:ALA:HB1	5:D:5003:FAD:H4'	1.96	0.47
1:A:845:ALA:CB	1:A:923:ILE:HD13	2.44	0.47
1:B:510:THR:HG21	1:B:1315:THR:HG22	1.96	0.47
1:B:709:TYR:CE2	1:B:868:VAL:HG22	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:741:GLU:OE1	1:C:743:PHE:N	2.46	0.47
1:D:3:ALA:HA	1:D:227:LEU:CD2	2.44	0.47
1:A:217:LEU:O	1:A:220:LYS:HG2	2.15	0.47
1:A:224:ARG:HG2	1:A:224:ARG:HH11	1.80	0.47
1:A:795:MET:HE3	1:A:1039:MET:HB3	1.97	0.47
1:A:1033:THR:HG23	1:A:1066:GLU:O	2.14	0.47
1:B:91:ILE:O	1:B:99:HIS:HB2	2.15	0.47
1:B:535:LYS:HG2	1:B:535:LYS:O	2.15	0.47
1:B:607:ARG:NH1	1:B:680:GLN:HB2	2.30	0.47
1:B:733:GLY:HA3	1:B:847:TYR:CZ	2.50	0.47
1:B:930:GLU:OE2	1:B:1294:LEU:HB3	2.15	0.47
1:B:1287:THR:HG22	1:B:1288:GLY:H	1.80	0.47
1:C:253:PRO:HB3	1:C:400:PRO:HB2	1.97	0.47
1:C:1033:THR:HG23	1:C:1066:GLU:O	2.14	0.47
1:D:716:GLU:OE2	1:D:896:ARG:HD3	2.14	0.47
1:D:741:GLU:HG2	9:D:7119:HOH:O	2.14	0.47
1:A:532:LEU:C	1:A:534:ASP:H	2.23	0.47
1:A:925:GLU:OE1	1:A:943:ARG:NE	2.47	0.47
1:A:1141:TYR:HB2	1:A:1150:PRO:HG3	1.97	0.47
1:B:644:SER:OG	1:B:646:ILE:HG12	2.15	0.47
1:C:322:GLN:O	1:C:412:SER:HB3	2.15	0.47
1:C:352:ILE:CD1	1:C:407:ILE:HG12	2.44	0.47
1:C:1208:THR:C	1:C:1209:LEU:HD12	2.39	0.47
1:A:1222:THR:HG22	1:A:1228:TYR:HB2	1.97	0.47
1:B:647:THR:HG23	1:B:648:GLY:N	2.29	0.47
1:D:426:ARG:HD2	1:D:1232:ALA:HB2	1.96	0.47
1:D:1327:LYS:HD2	1:D:1328:PRO:O	2.14	0.47
1:A:328:ARG:HG2	1:A:328:ARG:HH11	1.80	0.47
1:A:714:LYS:HD2	1:A:896:ARG:NH1	2.30	0.47
1:B:668:ILE:HD13	1:B:688:ILE:HD13	1.96	0.47
1:B:1222:THR:HG22	1:B:1228:TYR:HB2	1.95	0.47
1:C:599:ARG:HH21	1:C:825:ARG:HD2	1.79	0.47
1:D:461:ASN:N	1:D:461:ASN:HD22	2.11	0.47
1:A:351:ASN:HD22	1:A:361:LEU:HB2	1.79	0.46
1:B:735:ILE:HD12	1:B:735:ILE:N	2.29	0.46
1:C:3:ALA:HA	1:C:227:LEU:HD22	1.96	0.46
1:C:656:PHE:HE2	1:C:815:LEU:HD23	1.79	0.46
1:D:740:GLN:HG2	1:D:912:PHE:CE2	2.50	0.46
1:D:1250:ASN:OD1	1:D:1252:LYS:HB2	2.15	0.46
1:A:115:PHE:HD2	1:A:745:LEU:HB3	1.81	0.46
1:B:623:THR:O	1:B:623:THR:CG2	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:MET:CE	1:C:127:LEU:HD23	2.44	0.46
1:C:467:LEU:O	1:C:471:GLN:HG2	2.15	0.46
1:C:746:GLU:O	1:C:802:LYS:NZ	2.48	0.46
1:C:1119:THR:O	1:C:1123:MET:HG2	2.15	0.46
1:A:505:VAL:HG23	1:A:506:ASP:N	2.30	0.46
1:B:257:LEU:O	5:B:3003:FAD:H2B	2.15	0.46
1:A:374:LEU:HD22	1:A:398:LEU:HD21	1.98	0.46
1:A:765:VAL:O	1:A:792:VAL:HG22	2.15	0.46
1:A:933:VAL:HG11	1:A:1280:ARG:NH2	2.30	0.46
1:B:314:ASP:O	1:B:318:LYS:HE2	2.15	0.46
1:B:987:LYS:O	1:B:991:GLU:HG3	2.16	0.46
1:B:1054:ALA:O	1:B:1099:LEU:HD11	2.14	0.46
1:C:881:ARG:HD2	1:C:915:PHE:O	2.16	0.46
1:C:1174:ASN:O	1:C:1237:PRO:HA	2.16	0.46
1:D:566:LYS:HD3	1:D:566:LYS:C	2.41	0.46
1:D:910:THR:OG1	1:D:911:ALA:N	2.43	0.46
1:A:969:TRP:HZ3	1:A:1003:PRO:HD3	1.79	0.46
1:C:409:ILE:HA	1:C:410:PRO:HD3	1.74	0.46
1:D:498:PRO:HG2	1:D:1323:PRO:HD3	1.97	0.46
1:A:650:CYS:O	1:A:651:ASN:C	2.57	0.46
1:B:45:GLU:O	1:B:45:GLU:HG2	2.16	0.46
1:B:653:GLU:HB3	1:B:871:THR:HG21	1.97	0.46
1:C:304:PRO:O	1:C:307:ILE:HG13	2.16	0.46
1:C:735:ILE:CD1	1:C:845:ALA:HB3	2.45	0.46
1:D:304:PRO:HG2	1:D:307:ILE:HG23	1.96	0.46
1:A:97:ARG:HB2	1:A:97:ARG:HH11	1.81	0.46
1:A:552:LYS:HD3	1:A:552:LYS:N	2.31	0.46
1:A:641:VAL:O	1:A:641:VAL:HG23	2.14	0.46
1:A:1043:LEU:O	1:A:1047:MET:HG2	2.16	0.46
1:B:506:ASP:OD2	1:B:1320:THR:HG22	2.16	0.46
1:B:1300:PRO:HG2	1:B:1302:THR:HG23	1.96	0.46
1:C:117:THR:CG2	1:C:587:ALA:HA	2.45	0.46
1:C:218:ARG:HH11	1:C:218:ARG:CB	2.29	0.46
1:C:393:TYR:N	1:C:461:ASN:ND2	2.64	0.46
1:C:709:TYR:CE2	1:C:868:VAL:HG22	2.51	0.46
1:A:374:LEU:HD22	1:A:398:LEU:CD2	2.46	0.46
1:A:746:GLU:HB3	1:A:796:GLY:HA3	1.97	0.46
1:B:3:ALA:HB1	1:B:228:ARG:N	2.20	0.46
1:B:606:LEU:HD23	1:B:607:ARG:N	2.31	0.46
1:B:1089:GLN:HG2	1:B:1134:TYR:CE1	2.51	0.46
1:C:152:GLY:HA2	1:C:1201:VAL:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:650:CYS:O	1:C:651:ASN:C	2.58	0.46
1:D:924:ALA:HA	1:D:927:TRP:NE1	2.30	0.46
1:D:989:ASN:OD1	1:D:996:LYS:HA	2.15	0.46
1:D:1050:VAL:HG13	1:D:1255:TYR:HE2	1.80	0.46
1:D:1262:GLU:N	1:D:1263:PRO:CD	2.79	0.46
1:A:254:ASP:O	1:A:255:ALA:C	2.59	0.46
1:A:754:PRO:HD3	1:A:817:ALA:HB1	1.98	0.46
1:B:236:TRP:CD1	1:B:236:TRP:C	2.94	0.46
1:B:829:ASP:HB2	1:B:832:GLU:HG3	1.97	0.46
1:B:1005:LYS:HG3	1:B:1156:TYR:CE1	2.50	0.46
1:C:393:TYR:N	1:C:461:ASN:HD21	2.12	0.46
1:C:829:ASP:O	1:C:830:ARG:C	2.59	0.46
1:C:890:TYR:OH	1:C:943:ARG:HD3	2.16	0.46
1:D:768:GLN:HG3	1:D:802:LYS:HB2	1.98	0.46
1:A:298:SER:HA	1:A:408:GLU:HA	1.97	0.46
1:A:482:LEU:O	1:A:486:VAL:HG23	2.15	0.46
1:A:506:ASP:OD2	1:A:1319:VAL:HA	2.16	0.46
1:B:309:GLU:HB2	1:B:334:LEU:HD13	1.97	0.46
1:B:1320:THR:HG23	1:B:1321:GLY:N	2.31	0.46
1:C:147:LEU:HD13	1:C:1230:ILE:HD11	1.98	0.46
1:C:757:GLU:O	1:C:759:GLY:N	2.49	0.46
1:C:1263:PRO:HB2	1:C:1264:PRO:HD3	1.98	0.46
1:D:1109:ASN:ND2	1:D:1112:GLY:HA3	2.31	0.46
1:B:13:ARG:CB	1:B:13:ARG:HH11	2.29	0.45
1:B:857:VAL:HG21	1:B:892:ILE:HG12	1.99	0.45
1:C:3:ALA:HA	1:C:227:LEU:CD2	2.46	0.45
1:D:387:HIS:ND1	1:D:467:LEU:HD11	2.32	0.45
1:A:424:ALA:HB1	1:A:430:ASP:OD2	2.16	0.45
1:A:735:ILE:HD11	1:A:923:ILE:HG12	1.99	0.45
1:C:840:ARG:HB2	1:C:912:PHE:CD2	2.51	0.45
1:D:318:LYS:HD2	1:D:318:LYS:N	2.30	0.45
1:D:612:THR:O	1:D:613:ARG:HD3	2.16	0.45
1:A:375:VAL:HG12	1:A:380:ARG:HG3	1.97	0.45
1:A:550:PHE:HE2	1:A:552:LYS:HD2	1.80	0.45
1:B:236:TRP:CZ2	1:B:280:CYS:HB2	2.51	0.45
1:B:755:LYS:HE2	1:B:762:GLU:HB2	1.98	0.45
1:C:237:ILE:HD11	1:C:277:MET:HE2	1.98	0.45
1:C:256:LYS:HG3	1:C:275:PHE:CD1	2.50	0.45
1:D:217:LEU:HD12	1:D:217:LEU:HA	1.77	0.45
1:D:649:ILE:HD11	1:D:804:THR:HB	1.99	0.45
1:A:62:GLN:HG3	1:A:64:LYS:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:ILE:CG2	1:A:268:MET:HE2	2.43	0.45
1:A:372:LEU:HD23	1:A:407:ILE:HG13	1.97	0.45
1:C:780:MET:SD	1:C:780:MET:C	3.00	0.45
1:C:1319:VAL:O	1:C:1319:VAL:HG23	2.15	0.45
1:D:997:ARG:HA	1:D:1163:VAL:O	2.16	0.45
1:D:1115:GLU:O	1:D:1119:THR:CG2	2.64	0.45
1:A:196:PHE:CE2	1:A:198:PRO:HG3	2.51	0.45
1:A:571:GLU:OE2	1:A:1058:PRO:HG3	2.17	0.45
1:A:1332:ARG:HG2	1:A:1332:ARG:NH1	2.30	0.45
1:B:768:GLN:HG3	1:B:802:LYS:HB2	1.97	0.45
1:C:399:SER:HB2	1:C:400:PRO:HD2	1.98	0.45
1:D:112:GLN:NE2	1:D:151:THR:HA	2.31	0.45
1:D:630:PRO:HD2	1:D:681:ARG:NH2	2.32	0.45
1:A:95:LYS:HG3	1:A:590:GLU:OE2	2.16	0.45
1:A:154:ARG:NH1	1:A:1197:GLU:OE1	2.50	0.45
1:A:442:PHE:HE1	1:A:478:TRP:HB2	1.82	0.45
1:B:195:LEU:HD22	1:B:1190:ALA:HA	1.99	0.45
1:C:97:ARG:CB	1:C:97:ARG:HH11	2.29	0.45
1:C:304:PRO:HG2	1:C:307:ILE:HG23	1.98	0.45
1:C:851:PHE:N	1:C:851:PHE:CD1	2.84	0.45
1:D:275:PHE:HA	1:D:276:PRO:HD2	1.82	0.45
1:D:422:LYS:HE3	1:D:432:ALA:HB2	1.99	0.45
1:D:1050:VAL:HG13	1:D:1255:TYR:CE2	2.52	0.45
1:A:98:LEU:HD21	1:A:588:SER:HB3	1.97	0.45
1:A:400:PRO:HG2	1:A:401:GLU:CD	2.42	0.45
1:B:257:LEU:HD22	1:B:279:VAL:HG13	1.98	0.45
1:B:604:LEU:HD21	1:B:822:ARG:NH2	2.32	0.45
1:B:662:THR:O	1:B:663:CYS:HB3	2.16	0.45
1:B:709:TYR:HE2	1:B:868:VAL:HG22	1.81	0.45
1:C:224:ARG:HD3	1:C:283:TRP:CE3	2.52	0.45
1:C:257:LEU:CD2	1:C:279:VAL:HG13	2.47	0.45
1:C:713:LEU:O	1:C:898:THR:HA	2.17	0.45
1:A:1216:PRO:HD2	1:A:1217:GLU:OE2	2.17	0.45
1:B:656:PHE:CD1	1:B:669:GLY:HA2	2.51	0.45
1:B:1199:ALA:HB3	1:B:1264:PRO:HB2	1.99	0.45
1:C:1327:LYS:HD2	1:C:1327:LYS:C	2.42	0.45
1:D:215:GLU:HG3	1:D:218:ARG:HH12	1.82	0.45
1:D:742:HIS:HA	1:D:912:PHE:CE2	2.52	0.45
1:D:949:LYS:O	1:D:950:GLU:C	2.59	0.45
1:A:530:GLU:O	1:A:531:ASN:HB2	2.16	0.45
1:A:578:LEU:HD12	1:A:579:PRO:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:927:TRP:O	1:A:931:VAL:HG23	2.17	0.45
1:A:981:ARG:NH1	1:A:1162:GLU:OE1	2.49	0.45
1:A:1289:ASN:O	1:A:1290:ASN:HB2	2.17	0.45
1:B:58:TYR:CZ	1:B:220:LYS:HD2	2.52	0.45
1:B:430:ASP:CG	1:B:1229:LYS:HE2	2.41	0.45
1:C:1184:GLY:HA2	1:C:1248:CYS:O	2.16	0.45
1:B:96:THR:OG1	1:B:97:ARG:N	2.49	0.45
1:B:906:LEU:HD11	1:B:1333:VAL:HG22	1.99	0.45
1:C:640:ASP:HB3	1:C:819:LYS:HE3	1.99	0.45
1:D:1119:THR:O	1:D:1123:MET:HG2	2.17	0.45
1:A:924:ALA:HA	1:A:927:TRP:NE1	2.31	0.44
1:B:97:ARG:HB3	1:B:97:ARG:NH1	2.31	0.44
1:C:533:GLU:HG2	1:C:534:ASP:OD1	2.17	0.44
1:A:64:LYS:CE	1:A:65:ILE:H	2.28	0.44
1:B:439:ARG:NH2	1:B:451:GLU:OE1	2.50	0.44
1:B:607:ARG:HB3	1:B:679:THR:HB	1.99	0.44
1:B:949:LYS:O	1:B:950:GLU:C	2.59	0.44
1:C:257:LEU:HD23	1:C:279:VAL:HG13	1.98	0.44
1:D:224:ARG:HG2	1:D:224:ARG:HH11	1.83	0.44
1:D:1052:SER:HB2	1:D:1059:THR:HG22	1.98	0.44
1:D:1287:THR:OG1	1:D:1289:ASN:ND2	2.51	0.44
1:A:616:ALA:HB2	1:A:692:GLU:HA	1.99	0.44
1:B:1089:GLN:HG2	1:B:1134:TYR:CG	2.53	0.44
1:B:1302:THR:HB	1:B:1303:PRO:HD2	1.99	0.44
1:B:1332:ARG:HG2	1:B:1332:ARG:NH1	2.31	0.44
1:C:117:THR:HB	1:C:118:PRO:HD3	1.99	0.44
1:C:124:MET:HE2	1:C:128:LEU:HG	1.98	0.44
1:C:502:GLY:H	1:C:1329:TRP:CG	2.35	0.44
1:C:651:ASN:HD22	1:C:651:ASN:HA	1.59	0.44
1:C:760:GLU:OE2	1:D:1063:TYR:OH	2.34	0.44
1:C:1320:THR:CG2	1:C:1321:GLY:H	2.22	0.44
1:D:978:TYR:CE2	1:D:982:LYS:HD2	2.52	0.44
1:A:358:ILE:HD12	1:A:358:ILE:C	2.42	0.44
1:B:667:ILE:HD12	1:B:808:VAL:HG13	2.00	0.44
1:B:940:GLU:C	1:B:940:GLU:OE1	2.60	0.44
1:C:425:SER:HB2	1:C:1229:LYS:HG3	1.98	0.44
1:C:473:GLN:HE21	1:C:482:LEU:HG	1.82	0.44
1:D:97:ARG:CZ	1:D:98:LEU:H	2.30	0.44
1:D:273:MET:HE2	1:D:273:MET:HA	1.98	0.44
1:D:623:THR:CG2	1:D:626:ALA:HB3	2.47	0.44
1:A:40:LYS:HB3	1:A:115:PHE:CZ	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:LYS:HE2	1:A:65:ILE:N	2.30	0.44
1:A:65:ILE:HD12	1:A:212:PHE:CE2	2.52	0.44
1:C:1123:MET:HE1	1:D:1014:PHE:CZ	2.53	0.44
1:A:271:LYS:O	1:A:273:MET:HE3	2.18	0.44
1:A:448:GLU:HG3	1:A:448:GLU:O	2.18	0.44
1:A:467:LEU:O	1:A:471:GLN:HG2	2.18	0.44
1:B:125:TYR:HH	1:B:209:GLU:HG3	1.79	0.44
1:C:97:ARG:NH1	1:C:97:ARG:CB	2.78	0.44
1:C:1287:THR:CG2	1:C:1288:GLY:H	2.14	0.44
1:A:131:GLN:HE21	1:A:133:GLU:N	2.13	0.44
1:A:606:LEU:HD13	1:A:813:VAL:HA	1.98	0.44
1:A:996:LYS:NZ	1:A:1285:GLN:NE2	2.66	0.44
1:A:1287:THR:O	1:A:1288:GLY:C	2.60	0.44
1:B:358:ILE:C	1:B:358:ILE:HD12	2.43	0.44
1:C:1262:GLU:N	1:C:1263:PRO:CD	2.80	0.44
1:D:39:THR:HG22	1:D:51:CYS:HA	2.00	0.44
1:D:152:GLY:HA2	1:D:1201:VAL:HG21	2.00	0.44
1:A:117:THR:HG21	1:A:587:ALA:HA	1.99	0.44
1:A:1287:THR:O	1:A:1289:ASN:N	2.50	0.44
1:B:232:GLU:OE2	1:B:681:ARG:NH2	2.44	0.44
1:C:443:LYS:HD3	1:C:444:PRO:HD2	1.99	0.44
1:C:1200:PHE:CE1	1:C:1268:ALA:HA	2.53	0.44
1:D:1283:ARG:NH2	1:D:1293:GLU:OE2	2.50	0.44
1:A:117:THR:HB	1:A:118:PRO:HD3	1.99	0.44
1:A:256:LYS:HG3	1:A:275:PHE:CG	2.53	0.44
1:C:63:ASN:CG	1:C:63:ASN:O	2.59	0.44
1:D:46:GLY:HA2	4:D:2002:FES:S1	2.58	0.44
1:D:795:MET:HE3	1:D:1039:MET:HB3	1.99	0.44
1:A:443:LYS:HG2	1:A:450:GLN:HB2	2.00	0.43
1:B:507:PHE:HB2	1:B:1304:GLU:HG3	1.99	0.43
1:C:58:TYR:OH	1:C:63:ASN:ND2	2.46	0.43
1:C:65:ILE:HD12	1:C:212:PHE:CD2	2.53	0.43
1:C:720:LEU:HD11	1:C:896:ARG:CB	2.48	0.43
1:C:1038:GLU:HB2	1:C:1044:HIS:CD2	2.53	0.43
1:A:97:ARG:HH11	1:A:97:ARG:CB	2.31	0.43
1:B:58:TYR:OH	1:B:63:ASN:ND2	2.52	0.43
1:C:310:LYS:HE2	1:C:310:LYS:CA	2.47	0.43
1:C:873:ASP:CG	1:C:874:LEU:H	2.26	0.43
1:C:932:ALA:HA	1:C:942:VAL:HG21	2.00	0.43
1:D:196:PHE:O	1:D:198:PRO:HD3	2.19	0.43
1:A:298:SER:HA	1:A:407:ILE:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:602:ASN:O	1:A:822:ARG:HD2	2.17	0.43
1:B:3:ALA:HA	1:B:227:LEU:CD2	2.46	0.43
1:B:667:ILE:HD12	1:B:808:VAL:CG1	2.48	0.43
1:C:257:LEU:HD23	1:C:279:VAL:CG1	2.48	0.43
1:C:550:PHE:CE2	1:C:552:LYS:HG3	2.53	0.43
1:D:1302:THR:HB	1:D:1303:PRO:HD2	2.00	0.43
1:A:113:CYS:O	1:A:593:TYR:OH	2.34	0.43
1:A:322:GLN:HG2	1:A:414:GLU:CD	2.43	0.43
1:B:58:TYR:CE1	1:B:63:ASN:ND2	2.86	0.43
1:B:1183:VAL:HG22	9:B:7068:HOH:O	2.18	0.43
1:C:117:THR:O	1:C:121:VAL:HG23	2.19	0.43
1:C:267:GLU:HB3	1:C:273:MET:HG3	2.00	0.43
1:D:733:GLY:HA3	1:D:847:TYR:CZ	2.54	0.43
1:D:1047:MET:SD	1:D:1088:GLY:HA2	2.59	0.43
1:A:616:ALA:CB	1:A:692:GLU:HA	2.48	0.43
1:A:1220:LEU:HD21	1:A:1222:THR:O	2.18	0.43
1:B:58:TYR:HE1	1:B:63:ASN:ND2	2.16	0.43
1:B:1320:THR:OG1	1:B:1321:GLY:N	2.49	0.43
1:C:154:ARG:N	1:C:155:PRO:HD2	2.33	0.43
1:D:298:SER:HA	1:D:408:GLU:HA	1.99	0.43
1:A:1009:SER:HA	1:A:1082:VAL:HG11	2.01	0.43
1:A:1083:SER:HB2	6:A:2004:MTE:O3P	2.19	0.43
1:A:1133:PHE:CG	1:B:1127:SER:HB2	2.53	0.43
1:B:888:ASN:ND2	1:B:925:GLU:OE2	2.51	0.43
1:B:1008:ILE:O	1:B:1009:SER:CB	2.66	0.43
1:A:197:LYS:HB2	1:A:200:GLU:HG3	2.01	0.43
1:A:1217:GLU:CD	1:A:1217:GLU:H	2.26	0.43
1:C:131:GLN:O	1:C:134:PRO:HD3	2.19	0.43
1:C:490:LEU:HB2	1:C:513:LEU:CD2	2.49	0.43
1:D:87:THR:OG1	1:D:89:GLU:HG2	2.18	0.43
1:D:1323:PRO:O	1:D:1325:ASN:N	2.51	0.43
1:A:967:ARG:O	1:A:971:GLU:HB2	2.19	0.43
1:B:362:ASN:N	1:B:363:PRO:CD	2.82	0.43
1:B:1291:VAL:HG13	1:B:1292:LYS:HG3	2.00	0.43
1:C:506:ASP:OD1	1:C:1320:THR:N	2.52	0.43
1:C:1133:PHE:CG	1:D:1127:SER:HB2	2.54	0.43
1:C:1217:GLU:CD	1:C:1217:GLU:N	2.75	0.43
1:A:443:LYS:HA	1:A:450:GLN:NE2	2.33	0.43
1:A:1222:THR:CG2	1:A:1228:TYR:HB2	2.49	0.43
1:C:333:GLN:OE1	1:C:333:GLN:HA	2.18	0.43
1:C:656:PHE:CD1	1:C:669:GLY:HA2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:374:LEU:HD13	1:D:398:LEU:CD2	2.45	0.43
1:D:1089:GLN:HG2	1:D:1134:TYR:CE1	2.53	0.43
1:A:256:LYS:HG3	1:A:275:PHE:CD1	2.54	0.43
1:A:389:PHE:HA	1:A:397:LEU:CG	2.47	0.43
1:A:1034:HIS:HB2	1:A:1087:ASN:HD22	1.83	0.43
1:B:623:THR:HG23	1:B:626:ALA:HB3	2.01	0.43
1:C:28:ALA:CB	1:C:32:ARG:HH12	2.32	0.43
1:C:204:LEU:HG	1:C:206:PRO:HD3	2.01	0.43
1:C:1141:TYR:OH	1:C:1146:ASN:ND2	2.52	0.43
1:A:32:ARG:HD2	9:A:7112:HOH:O	2.18	0.42
1:A:582:ALA:O	1:A:586:GLN:HG3	2.19	0.42
1:A:734:GLU:O	1:A:735:ILE:HG23	2.19	0.42
1:B:758:ALA:O	1:B:787:ARG:HD2	2.19	0.42
1:D:646:ILE:O	1:D:646:ILE:HG13	2.19	0.42
1:A:96:THR:OG1	1:A:97:ARG:N	2.51	0.42
1:A:632:PHE:HE1	1:A:671:VAL:HG22	1.83	0.42
1:A:1279:ILE:HG21	1:A:1309:ALA:HB1	2.01	0.42
1:B:552:LYS:O	1:B:553:ASP:CB	2.65	0.42
1:B:859:ALA:HA	1:B:894:ASN:O	2.19	0.42
1:C:572:ASP:OD1	1:C:1053:ARG:HD3	2.19	0.42
1:C:869:GLY:HA3	1:C:908:SER:HA	2.01	0.42
1:A:428:GLU:OE2	1:A:1234:GLY:HA3	2.20	0.42
1:B:550:PHE:CE1	1:B:1173:LYS:HD3	2.53	0.42
1:B:558:VAL:HG21	1:B:1241:ARG:NH1	2.34	0.42
1:B:652:ASP:HB3	1:B:871:THR:HB	2.01	0.42
1:C:74:LEU:O	1:C:76:PRO:HD3	2.19	0.42
1:C:108:SER:O	1:C:109:HIS:HB2	2.20	0.42
1:C:357:PRO:HG3	1:C:461:ASN:O	2.18	0.42
1:C:550:PHE:HE2	1:C:552:LYS:HG3	1.83	0.42
1:C:1183:VAL:C	1:C:1258:LYS:HB2	2.43	0.42
1:A:97:ARG:HB2	1:A:97:ARG:CZ	2.49	0.42
1:A:419:SER:HB2	1:A:519:PHE:CD1	2.54	0.42
1:D:661:VAL:HA	1:D:666:HIS:ND1	2.34	0.42
1:A:425:SER:HB2	1:A:1229:LYS:HG3	2.02	0.42
1:A:562:GLN:HG3	1:A:1246:ARG:NH2	2.35	0.42
1:A:977:GLN:O	1:A:981:ARG:HG3	2.18	0.42
1:B:55:LEU:CD2	1:B:85:VAL:HG22	2.50	0.42
1:B:346:ALA:HB1	5:B:3003:FAD:H4'	2.00	0.42
1:B:835:LEU:HD22	1:B:1223:ARG:NH1	2.35	0.42
1:B:1265:LEU:HD23	1:B:1265:LEU:C	2.45	0.42
1:C:363:PRO:HG3	1:C:463:THR:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:735:ILE:HG21	1:C:926:CYS:SG	2.59	0.42
1:D:117:THR:CG2	1:D:587:ALA:HA	2.50	0.42
1:D:446:THR:HB	1:D:535:LYS:HZ2	1.83	0.42
1:D:592:VAL:HG13	1:D:596:ASP:HB2	2.02	0.42
1:D:641:VAL:O	1:D:641:VAL:HG23	2.19	0.42
1:D:1034:HIS:NE2	1:D:1047:MET:HG3	2.35	0.42
1:A:498:PRO:HG3	1:A:1320:THR:OG1	2.20	0.42
1:A:711:PRO:C	1:A:900:ARG:NH1	2.78	0.42
1:B:642:PRO:HG2	1:B:781:LEU:HA	2.00	0.42
1:B:1109:ASN:N	1:B:1110:PRO:HD3	2.35	0.42
1:D:1079:ALA:HB1	7:D:5005:MOM:OM1	2.19	0.42
1:A:112:GLN:NE2	1:A:151:THR:HA	2.34	0.42
1:A:742:HIS:HA	1:A:912:PHE:CZ	2.55	0.42
1:A:1183:VAL:C	1:A:1258:LYS:HB2	2.45	0.42
1:B:29:TYR:CE1	1:B:33:LYS:HG2	2.54	0.42
1:B:886:MET:SD	1:B:897:GLY:HA3	2.59	0.42
1:B:1141:TYR:HE1	1:B:1146:ASN:HD22	1.68	0.42
1:C:217:LEU:HD12	1:C:217:LEU:HA	1.92	0.42
1:C:593:TYR:O	1:C:594:CYS:C	2.63	0.42
1:C:949:LYS:O	1:C:950:GLU:C	2.61	0.42
1:C:950:GLU:OE2	1:C:961:GLU:HA	2.19	0.42
1:C:1019:GLY:HA2	1:C:1132:GLY:O	2.20	0.42
1:D:71:ASN:C	1:D:73:CYS:N	2.76	0.42
1:D:613:ARG:NH1	1:D:692:GLU:HG3	2.34	0.42
1:D:649:ILE:HD13	1:D:873:ASP:OD1	2.19	0.42
1:A:68:PHE:HD2	1:A:344:SER:HB3	1.84	0.42
1:B:735:ILE:HD11	1:B:847:TYR:HD1	1.85	0.42
1:B:787:ARG:HG2	1:B:787:ARG:HH11	1.85	0.42
1:B:1022:LEU:HD23	1:B:1022:LEU:C	2.45	0.42
1:C:86:THR:O	1:C:122:MET:HE2	2.19	0.42
1:C:399:SER:OG	1:C:402:GLU:HG3	2.19	0.42
1:D:307:ILE:HG13	1:D:308:VAL:N	2.35	0.42
1:D:841:HIS:CE1	1:D:878:ILE:HD12	2.55	0.42
1:A:749:CYS:HA	1:A:826:CYS:O	2.20	0.42
1:A:1113:SER:O	1:A:1116:ASP:HB2	2.20	0.42
1:A:1149:ASN:HA	1:A:1150:PRO:HD3	1.85	0.42
1:B:500:ALA:HA	1:B:501:PRO:HD3	1.93	0.42
1:C:1105:TYR:CD1	1:C:1105:TYR:N	2.88	0.42
1:D:478:TRP:C	1:D:479:LYS:HG2	2.43	0.42
1:D:558:VAL:HG13	1:D:1241:ARG:HG2	2.01	0.42
1:D:650:CYS:HB2	1:D:652:ASP:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:860:LEU:HD22	1:D:927:TRP:CZ2	2.54	0.42
1:A:640:ASP:OD1	1:A:819:LYS:HE3	2.20	0.42
1:A:1105:TYR:CD1	1:A:1105:TYR:N	2.88	0.42
1:B:572:ASP:OD2	1:B:1053:ARG:HD2	2.20	0.42
1:B:1217:GLU:CD	1:B:1217:GLU:N	2.78	0.42
1:B:1268:ALA:C	1:B:1270:SER:N	2.77	0.42
1:C:45:GLU:CD	1:C:1225:PRO:HD2	2.44	0.42
1:C:786:ASN:ND2	1:D:1029:SER:HB2	2.35	0.42
1:A:257:LEU:HD13	1:A:279:VAL:HG13	2.02	0.41
1:A:443:LYS:HA	1:A:450:GLN:HE21	1.85	0.41
1:A:1210:GLU:O	1:A:1300:PRO:HG3	2.19	0.41
1:B:233:ARG:HD3	1:B:681:ARG:CZ	2.50	0.41
1:B:504:MET:HG2	1:B:1304:GLU:CD	2.44	0.41
1:B:1135:ARG:HD2	1:B:1135:ARG:C	2.45	0.41
1:C:1089:GLN:HG2	1:C:1134:TYR:CE1	2.55	0.41
1:C:1145:THR:O	1:C:1146:ASN:C	2.62	0.41
1:A:10:VAL:HG21	1:A:34:LEU:HD11	2.01	0.41
1:B:212:PHE:CD1	1:B:213:PRO:HD2	2.54	0.41
1:B:233:ARG:HD3	1:B:681:ARG:NH1	2.35	0.41
1:C:242:LEU:O	1:C:246:LEU:HG	2.20	0.41
1:C:658:LYS:C	1:C:660:LYS:H	2.28	0.41
1:C:924:ALA:HA	1:C:927:TRP:NE1	2.35	0.41
1:C:933:VAL:CG1	1:C:1280:ARG:HH21	2.29	0.41
1:C:953:LEU:HD23	1:C:959:LYS:HA	2.03	0.41
1:C:1122:TYR:CD2	1:C:1123:MET:HE3	2.55	0.41
1:D:502:GLY:H	1:D:1329:TRP:CG	2.38	0.41
1:D:561:PHE:HB2	9:D:7144:HOH:O	2.20	0.41
1:A:225:LYS:HE2	1:A:226:GLN:O	2.19	0.41
1:A:658:LYS:C	1:A:660:LYS:H	2.28	0.41
1:B:552:LYS:H	1:B:552:LYS:HG2	1.44	0.41
1:B:752:ALA:HB3	1:B:813:VAL:HG12	2.03	0.41
1:B:927:TRP:O	1:B:931:VAL:HG23	2.20	0.41
1:C:87:THR:OG1	1:C:89:GLU:HG2	2.21	0.41
1:C:152:GLY:O	1:C:1236:ILE:HG21	2.20	0.41
1:C:1135:ARG:HD2	1:C:1135:ARG:O	2.21	0.41
1:D:741:GLU:CG	1:D:834:MET:HG2	2.40	0.41
1:A:143:PHE:HB3	1:A:1233:PHE:CE1	2.55	0.41
1:A:1176:ARG:HH21	1:A:1241:ARG:CD	2.33	0.41
1:B:671:VAL:HG11	1:B:682:ALA:HB3	2.03	0.41
1:C:573:MET:HA	1:C:576:ARG:HD2	2.02	0.41
1:D:3:ALA:HA	1:D:227:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:236:TRP:CD1	1:D:236:TRP:C	2.98	0.41
1:D:441:LEU:HB3	1:D:451:GLU:HB2	2.02	0.41
1:D:1107:LYS:HB3	1:D:1107:LYS:HE2	1.85	0.41
1:A:117:THR:O	1:A:118:PRO:C	2.63	0.41
1:B:549:LEU:O	1:B:551:GLN:HG2	2.20	0.41
1:B:1103:GLU:O	1:B:1107:LYS:HG3	2.20	0.41
1:C:218:ARG:HB2	1:C:218:ARG:NH1	2.35	0.41
1:C:303:CYS:SG	1:C:307:ILE:HD11	2.60	0.41
1:C:607:ARG:HB3	1:C:671:VAL:HG12	2.03	0.41
1:C:632:PHE:HE1	1:C:671:VAL:HG22	1.86	0.41
1:C:722:LYS:C	1:C:722:LYS:HD2	2.46	0.41
1:C:722:LYS:HD3	1:C:726:GLU:OE2	2.19	0.41
1:D:584:ASP:HB2	9:D:7063:HOH:O	2.21	0.41
1:D:750:THR:HG23	1:D:765:VAL:HG22	2.01	0.41
1:D:860:LEU:HD12	1:D:861:GLU:N	2.34	0.41
1:A:154:ARG:CD	1:A:1197:GLU:OE2	2.67	0.41
1:A:619:LYS:HD2	1:A:691:GLU:HB2	2.01	0.41
1:C:1084:ALA:HB3	9:C:7132:HOH:O	2.21	0.41
1:C:1115:GLU:H	1:C:1115:GLU:CD	2.29	0.41
1:D:560:LEU:O	1:D:1243:SER:HA	2.20	0.41
1:D:614:ALA:O	1:D:905:ASN:HB3	2.21	0.41
1:D:1106:LYS:HE3	1:D:1117:TRP:CH2	2.56	0.41
1:A:1317:LEU:N	1:A:1317:LEU:HD22	2.35	0.41
1:B:224:ARG:HG2	1:B:224:ARG:NH1	2.36	0.41
1:B:303:CYS:HA	1:B:304:PRO:HD2	1.96	0.41
1:B:747:THR:HG23	9:B:7032:HOH:O	2.20	0.41
1:C:1092:TYR:O	1:C:1096:GLN:HG2	2.21	0.41
1:C:1236:ILE:HB	1:C:1237:PRO:HD2	2.02	0.41
1:D:56:SER:HA	1:D:66:VAL:O	2.20	0.41
1:D:562:GLN:HG3	1:D:1246:ARG:NH1	2.36	0.41
1:D:593:TYR:O	1:D:594:CYS:C	2.64	0.41
1:D:658:LYS:C	1:D:660:LYS:H	2.29	0.41
1:D:1253:ALA:HB3	1:D:1257:SER:O	2.21	0.41
1:A:59:ASP:OD1	1:A:62:GLN:HB3	2.21	0.41
1:A:68:PHE:CD2	1:A:344:SER:HB3	2.56	0.41
1:A:315:ALA:O	1:A:319:LEU:HG	2.20	0.41
1:A:1253:ALA:HB3	1:A:1257:SER:O	2.21	0.41
1:B:351:ASN:HB2	5:B:3003:FAD:O4'	2.21	0.41
1:B:504:MET:HG2	1:B:1304:GLU:OE2	2.20	0.41
1:B:568:GLN:HG2	1:B:572:ASP:HB3	2.03	0.41
1:B:650:CYS:O	1:B:651:ASN:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:ALA:HB2	1:C:225:LYS:HE3	2.01	0.41
1:C:357:PRO:HA	1:C:462:ARG:HA	2.02	0.41
1:C:732:SER:HA	1:C:847:TYR:O	2.20	0.41
1:C:1210:GLU:O	1:C:1300:PRO:HG3	2.21	0.41
1:D:303:CYS:HB3	1:D:307:ILE:HD11	2.03	0.41
1:D:1039:MET:HG3	6:D:5004:MTE:C4	2.50	0.41
1:A:334:LEU:HA	1:A:337:PHE:HB2	2.02	0.41
1:A:606:LEU:HD23	1:A:607:ARG:N	2.35	0.41
1:A:1174:ASN:HB3	9:A:7076:HOH:O	2.19	0.41
1:B:215:GLU:O	1:B:218:ARG:HB3	2.20	0.41
1:B:758:ALA:HB1	1:B:787:ARG:HE	1.86	0.41
1:C:192:SER:N	1:C:193:PRO:HD3	2.35	0.41
1:C:358:ILE:HD12	1:C:358:ILE:C	2.45	0.41
1:C:482:LEU:HD23	1:C:482:LEU:C	2.46	0.41
1:C:1140:GLY:O	1:C:1148:GLY:HA3	2.21	0.41
1:C:1193:ILE:O	1:C:1197:GLU:HG3	2.20	0.41
1:C:1260:VAL:O	1:C:1260:VAL:HG22	2.19	0.41
1:D:97:ARG:HA	1:D:97:ARG:NH1	2.36	0.41
1:D:165:ARG:O	1:D:166:ASP:O	2.39	0.41
1:A:418:PHE:HD1	1:A:439:ARG:HB2	1.86	0.41
1:A:742:HIS:CE1	1:A:839:GLY:HA2	2.56	0.41
1:A:1022:LEU:HD23	1:A:1032:LEU:HD13	2.03	0.41
1:B:9:PHE:CE2	1:B:14:LYS:HB2	2.55	0.41
1:B:86:THR:O	1:B:122:MET:HE2	2.20	0.41
1:B:117:THR:CG2	1:B:587:ALA:HA	2.51	0.41
1:B:154:ARG:HD2	9:B:7076:HOH:O	2.21	0.41
1:B:205:ASP:HA	1:B:206:PRO:HD2	1.91	0.41
1:B:477:LEU:HB3	1:B:479:LYS:HG2	2.03	0.41
1:B:645:ASN:O	1:B:654:THR:HA	2.21	0.41
1:B:646:ILE:HG13	1:B:779:LYS:NZ	2.36	0.41
1:B:740:GLN:HG2	1:B:912:PHE:CE2	2.56	0.41
1:B:981:ARG:O	1:B:985:VAL:HG23	2.20	0.41
1:B:1036:GLY:HA3	1:B:1043:LEU:HD21	2.03	0.41
1:C:298:SER:HA	1:C:407:ILE:O	2.21	0.41
1:C:366:MET:HE2	1:C:387:HIS:HA	2.03	0.41
1:C:1022:LEU:C	1:C:1022:LEU:HD23	2.46	0.41
1:A:647:THR:HG21	9:A:7205:HOH:O	2.20	0.40
1:A:886:MET:SD	1:A:897:GLY:HA3	2.61	0.40
1:A:988:PHE:CD1	1:A:988:PHE:C	2.99	0.40
1:A:1159:ALA:HA	1:A:1178:ASP:O	2.21	0.40
1:B:301:ALA:O	1:B:347:SER:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:981:ARG:CZ	1:B:1176:ARG:HD3	2.52	0.40
1:C:443:LYS:HD3	1:C:450:GLN:NE2	2.37	0.40
1:D:56:SER:HB2	1:D:84:ALA:HB3	2.03	0.40
1:D:1183:VAL:C	1:D:1258:LYS:HB2	2.47	0.40
1:A:6:LEU:HB3	1:A:17:GLU:HB3	2.03	0.40
1:A:384:GLN:O	1:A:384:GLN:HG3	2.21	0.40
1:B:157:LEU:HD23	1:B:157:LEU:HA	1.92	0.40
1:C:735:ILE:CD1	1:C:923:ILE:HG12	2.52	0.40
1:A:74:LEU:O	1:A:76:PRO:HD3	2.21	0.40
1:B:154:ARG:CD	1:B:1197:GLU:OE2	2.69	0.40
1:B:709:TYR:CE2	1:B:868:VAL:CG2	3.04	0.40
1:C:328:ARG:HH11	1:C:328:ARG:CG	2.35	0.40
1:D:29:TYR:O	1:D:33:LYS:HB3	2.21	0.40
1:D:362:ASN:N	1:D:363:PRO:CD	2.85	0.40
1:D:418:PHE:HD1	1:D:439:ARG:HB2	1.85	0.40
1:D:1199:ALA:HB3	1:D:1264:PRO:HB2	2.03	0.40
1:A:218:ARG:HB2	1:A:218:ARG:NH1	2.37	0.40
1:A:263:GLU:HB3	5:A:2003:FAD:H52A	2.03	0.40
1:A:840:ARG:HG3	2:A:6001:BCT:O1	2.21	0.40
1:A:1107:LYS:HE2	1:A:1107:LYS:HB3	1.90	0.40
1:B:442:PHE:CE2	1:B:527:LEU:HD21	2.56	0.40
1:B:480:GLU:O	1:B:483:LEU:HB3	2.21	0.40
1:B:1032:LEU:O	1:B:1064:ILE:HG12	2.22	0.40
1:B:1200:PHE:CE1	1:B:1268:ALA:HA	2.56	0.40
1:C:750:THR:HG23	1:C:765:VAL:HG22	2.04	0.40
1:C:860:LEU:HD22	1:C:892:ILE:HD13	2.03	0.40
1:A:242:LEU:O	1:A:246:LEU:HG	2.21	0.40
1:A:1022:LEU:C	1:A:1022:LEU:HD13	2.45	0.40
1:B:217:LEU:HD12	1:B:217:LEU:HA	1.79	0.40
1:B:965:LEU:N	1:B:966:PRO:CD	2.84	0.40
1:C:1122:TYR:HD1	9:D:7164:HOH:O	2.04	0.40
1:D:332:GLU:O	1:D:335:ARG:HB3	2.22	0.40
1:D:500:ALA:HA	1:D:501:PRO:HD3	1.96	0.40
1:D:505:VAL:HG23	1:D:506:ASP:N	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1303/1333 (98%)	1225 (94%)	64 (5%)	14 (1%)	11	25
1	B	1303/1333 (98%)	1228 (94%)	65 (5%)	10 (1%)	16	34
1	C	1303/1333 (98%)	1228 (94%)	69 (5%)	6 (0%)	24	46
1	D	1303/1333 (98%)	1223 (94%)	64 (5%)	16 (1%)	10	23
All	All	5212/5332 (98%)	4904 (94%)	262 (5%)	46 (1%)	14	30

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1009	SER
1	A	1290	ASN
1	B	553	ASP
1	B	1009	SER
1	C	758	ALA
1	C	1009	SER
1	C	1320	THR
1	D	166	ASP
1	D	1009	SER
1	D	1324	GLU
1	D	1325	ASN
1	D	377	ARG
1	D	391	PRO
1	D	758	ALA
1	D	798	GLY
1	D	1319	VAL
1	D	1320	THR
1	A	429	ASP
1	A	1288	GLY
1	B	552	LYS
1	B	798	GLY
1	D	1290	ASN

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Mol	Chain	Res	Type
1	A	4	ASP
1	A	533	GLU
1	A	624	SER
1	A	798	GLY
1	A	913	ARG
1	B	4	ASP
1	B	913	ARG
1	D	429	ASP
1	D	1323	PRO
1	B	1323	PRO
1	C	798	GLY
1	C	1289	ASN
1	D	978	TYR
1	A	1247	ASP
1	A	1319	VAL
1	B	213	PRO
1	B	1081	SER
1	A	1260	VAL
1	A	1322	VAL
1	A	1323	PRO
1	B	1321	GLY
1	C	1003	PRO
1	D	1003	PRO
1	D	213	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1104/1126 (98%)	1058 (96%)	46 (4%)	26	52
1	B	1104/1126 (98%)	1058 (96%)	46 (4%)	26	52
1	C	1104/1126 (98%)	1066 (97%)	38 (3%)	32	60
1	D	1104/1126 (98%)	1058 (96%)	46 (4%)	26	52
All	All	4416/4504 (98%)	4240 (96%)	176 (4%)	28	55

All (176) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	60	ARG
1	A	62	GLN
1	A	64	LYS
1	A	89	GLU
1	A	100	PRO
1	A	129	ARG
1	A	154	ARG
1	A	199	GLU
1	A	202	THR
1	A	209	GLU
1	A	217	LEU
1	A	220	LYS
1	A	257	LEU
1	A	313	VAL
1	A	328	ARG
1	A	332	GLU
1	A	462	ARG
1	A	476	LYS
1	A	477	LEU
1	A	513	LEU
1	A	529	GLN
1	A	612	THR
1	A	619	LYS
1	A	649	ILE
1	A	652	ASP
1	A	671	VAL
1	A	744	TYR
1	A	753	VAL
1	A	789	VAL
1	A	857	VAL
1	A	868	VAL
1	A	947	LEU
1	A	965	LEU
1	A	970	GLU
1	A	984	GLU
1	A	1022	LEU
1	A	1033	THR
1	A	1053	ARG
1	A	1100	LYS
1	A	1209	LEU
1	A	1217	GLU

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Mol	Chain	Res	Type
1	A	1280	ARG
1	A	1291	VAL
1	A	1319	VAL
1	A	1333	VAL
1	B	13	ARG
1	B	62	GLN
1	B	64	LYS
1	B	89	GLU
1	B	100	PRO
1	B	154	ARG
1	B	209	GLU
1	B	254	ASP
1	B	277	MET
1	B	279	VAL
1	B	313	VAL
1	B	328	ARG
1	B	462	ARG
1	B	468	LYS
1	B	477	LEU
1	B	480	GLU
1	B	513	LEU
1	B	534	ASP
1	B	552	LYS
1	B	619	LYS
1	B	641	VAL
1	B	652	ASP
1	B	671	VAL
1	B	692	GLU
1	B	735	ILE
1	B	744	TYR
1	B	753	VAL
1	B	789	VAL
1	B	819	LYS
1	B	857	VAL
1	B	868	VAL
1	B	940	GLU
1	B	947	LEU
1	B	965	LEU
1	B	970	GLU
1	B	984	GLU
1	B	1032	LEU
1	B	1033	THR

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Mol	Chain	Res	Type
1	B	1053	ARG
1	B	1073	PRO
1	B	1108	LYS
1	B	1119	THR
1	B	1135	ARG
1	B	1204	LEU
1	B	1217	GLU
1	B	1333	VAL
1	C	62	GLN
1	C	89	GLU
1	C	100	PRO
1	C	129	ARG
1	C	154	ARG
1	C	199	GLU
1	C	202	THR
1	C	209	GLU
1	C	310	LYS
1	C	312	LEU
1	C	322	GLN
1	C	328	ARG
1	C	433	LYS
1	C	462	ARG
1	C	513	LEU
1	C	529	GLN
1	C	553	ASP
1	C	599	ARG
1	C	649	ILE
1	C	651	ASN
1	C	652	ASP
1	C	671	VAL
1	C	735	ILE
1	C	744	TYR
1	C	745	LEU
1	C	789	VAL
1	C	853	LYS
1	C	868	VAL
1	C	947	LEU
1	C	1003	PRO
1	C	1005	LYS
1	C	1032	LEU
1	C	1033	THR
1	C	1053	ARG

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Mol	Chain	Res	Type
1	C	1073	PRO
1	C	1119	THR
1	C	1217	GLU
1	C	1317	LEU
1	D	32	ARG
1	D	89	GLU
1	D	100	PRO
1	D	133	GLU
1	D	154	ARG
1	D	165	ARG
1	D	166	ASP
1	D	209	GLU
1	D	254	ASP
1	D	279	VAL
1	D	310	LYS
1	D	312	LEU
1	D	328	ARG
1	D	380	ARG
1	D	398	LEU
1	D	461	ASN
1	D	468	LYS
1	D	477	LEU
1	D	479	LYS
1	D	513	LEU
1	D	532	LEU
1	D	558	VAL
1	D	566	LYS
1	D	620	SER
1	D	646	ILE
1	D	649	ILE
1	D	741	GLU
1	D	744	TYR
1	D	753	VAL
1	D	789	VAL
1	D	808	VAL
1	D	819	LYS
1	D	857	VAL
1	D	868	VAL
1	D	947	LEU
1	D	965	LEU
1	D	970	GLU
1	D	971	GLU

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Mol	Chain	Res	Type
1	D	1003	PRO
1	D	1073	PRO
1	D	1103	GLU
1	D	1119	THR
1	D	1217	GLU
1	D	1222	THR
1	D	1277	ASP
1	D	1333	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	63	ASN
1	A	131	GLN
1	A	208	GLN
1	A	252	HIS
1	A	261	ASN
1	A	351	ASN
1	A	450	GLN
1	A	473	GLN
1	A	484	GLN
1	A	531	ASN
1	A	551	GLN
1	A	748	HIS
1	A	1087	ASN
1	A	1089	GLN
1	A	1109	ASN
1	A	1146	ASN
1	A	1213	HIS
1	A	1285	GLN
1	B	63	ASN
1	B	71	ASN
1	B	131	GLN
1	B	226	GLN
1	B	261	ASN
1	B	351	ASN
1	B	450	GLN
1	B	471	GLN
1	B	473	GLN
1	B	484	GLN
1	B	531	ASN

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Mol	Chain	Res	Type
1	B	586	GLN
1	B	680	GLN
1	B	706	ASN
1	B	748	HIS
1	B	979	HIS
1	B	1087	ASN
1	B	1109	ASN
1	B	1146	ASN
1	B	1213	HIS
1	B	1285	GLN
1	B	1289	ASN
1	B	1325	ASN
1	C	63	ASN
1	C	131	GLN
1	C	158	GLN
1	C	208	GLN
1	C	272	ASN
1	C	322	GLN
1	C	384	GLN
1	C	423	GLN
1	C	450	GLN
1	C	461	ASN
1	C	473	GLN
1	C	484	GLN
1	C	529	GLN
1	C	559	GLN
1	C	586	GLN
1	C	651	ASN
1	C	684	GLN
1	C	876	GLN
1	C	979	HIS
1	C	1089	GLN
1	C	1109	ASN
1	C	1146	ASN
1	C	1174	ASN
1	C	1285	GLN
1	D	62	GLN
1	D	63	ASN
1	D	131	GLN
1	D	158	GLN
1	D	261	ASN
1	D	450	GLN

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Mol	Chain	Res	Type
1	D	461	ASN
1	D	471	GLN
1	D	473	GLN
1	D	529	GLN
1	D	586	GLN
1	D	651	ASN
1	D	680	GLN
1	D	706	ASN
1	D	841	HIS
1	D	957	ASN
1	D	1109	ASN
1	D	1146	ASN
1	D	1213	HIS
1	D	1285	GLN
1	D	1289	ASN
1	D	1290	ASN
1	D	1325	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](#)

Of 36 ligands modelled in this entry, 8 are monoatomic - leaving 28 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BCT	D	6004	-	3,3,3	0.61	0	2,3,3	1.89	0
8	SAL	C	4006	-	10,10,10	2.05	5 (50%)	13,13,13	2.13	4 (30%)
4	FES	C	2001	1	0,4,4	-	-	-	-	-
7	MOM	A	2005	6	0,3,3	-	-	-	-	-
4	FES	B	2002	1	0,4,4	-	-	-	-	-
5	FAD	C	4003	-	58,58,58	2.28	24 (41%)	85,89,89	2.11	31 (36%)
6	MTE	C	4004	7	21,26,26	7.20	12 (57%)	19,40,40	3.29	10 (52%)
5	FAD	D	5003	-	58,58,58	2.25	23 (39%)	85,89,89	2.10	28 (32%)
7	MOM	B	3005	6	0,3,3	-	-	-	-	-
4	FES	C	2002	1	0,4,4	-	-	-	-	-
7	MOM	D	5005	6	0,3,3	-	-	-	-	-
5	FAD	B	3003	-	58,58,58	2.34	24 (41%)	85,89,89	2.13	30 (35%)
7	MOM	C	4005	6	0,3,3	-	-	-	-	-
4	FES	D	2001	1	0,4,4	-	-	-	-	-
6	MTE	A	2004	7	21,26,26	7.34	11 (52%)	19,40,40	3.03	9 (47%)
2	BCT	A	6001	-	3,3,3	0.69	0	2,3,3	1.72	0
8	SAL	B	3006	-	10,10,10	1.98	5 (50%)	13,13,13	2.16	4 (30%)
8	SAL	A	2006	-	10,10,10	2.01	3 (30%)	13,13,13	2.23	5 (38%)
8	SAL	D	5006	-	10,10,10	2.12	5 (50%)	13,13,13	2.16	4 (30%)
6	MTE	D	5004	7	21,26,26	7.07	13 (61%)	19,40,40	3.17	10 (52%)
6	MTE	B	3004	7	21,26,26	6.79	11 (52%)	19,40,40	3.18	10 (52%)
4	FES	A	2001	1	0,4,4	-	-	-	-	-
2	BCT	C	6003	-	3,3,3	0.87	0	2,3,3	1.70	0
4	FES	A	2002	1	0,4,4	-	-	-	-	-
4	FES	D	2002	1	0,4,4	-	-	-	-	-
2	BCT	B	6002	-	3,3,3	0.86	0	2,3,3	1.63	0
5	FAD	A	2003	-	58,58,58	2.30	21 (36%)	85,89,89	2.11	31 (36%)
4	FES	B	2001	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
8	SAL	C	4006	-	-	0/4/4/4	0/1/1/1
4	FES	C	2001	1	-	-	0/1/1/1
4	FES	B	2002	1	-	-	0/1/1/1
5	FAD	C	4003	-	-	4/34/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MTE	C	4004	7	-	6/6/34/34	0/3/3/3
5	FAD	D	5003	-	-	4/34/50/50	0/6/6/6
4	FES	C	2002	1	-	-	0/1/1/1
5	FAD	B	3003	-	-	4/34/50/50	0/6/6/6
4	FES	D	2001	1	-	-	0/1/1/1
6	MTE	A	2004	7	-	3/6/34/34	0/3/3/3
8	SAL	B	3006	-	-	0/4/4/4	0/1/1/1
8	SAL	A	2006	-	-	0/4/4/4	0/1/1/1
8	SAL	D	5006	-	-	0/4/4/4	0/1/1/1
6	MTE	D	5004	7	-	2/6/34/34	0/3/3/3
6	MTE	B	3004	7	-	3/6/34/34	0/3/3/3
4	FES	A	2001	1	-	-	0/1/1/1
4	FES	A	2002	1	-	-	0/1/1/1
4	FES	D	2002	1	-	-	0/1/1/1
5	FAD	A	2003	-	-	4/34/50/50	0/6/6/6
4	FES	B	2001	1	-	-	0/1/1/1

All (157) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	5004	MTE	C7-C6	18.61	1.68	1.53
6	A	2004	MTE	C7-C6	18.49	1.68	1.53
6	B	3004	MTE	C7-C6	18.07	1.68	1.53
6	C	4004	MTE	C7-C6	17.81	1.67	1.53
6	A	2004	MTE	C6-N5	15.21	1.63	1.46
6	B	3004	MTE	C4'-C3'	-14.85	1.31	1.51
6	A	2004	MTE	C9-C10	14.33	1.63	1.38
6	C	4004	MTE	C9-C10	14.11	1.62	1.38
6	B	3004	MTE	C9-C10	14.10	1.62	1.38
6	D	5004	MTE	C9-C10	14.05	1.62	1.38
6	C	4004	MTE	C9-N5	13.15	1.68	1.37
6	A	2004	MTE	C9-N5	13.02	1.68	1.37
6	D	5004	MTE	C4'-C3'	-12.55	1.34	1.51
6	C	4004	MTE	C4'-C3'	-11.75	1.35	1.51
6	D	5004	MTE	C9-N5	9.99	1.61	1.37
6	C	4004	MTE	O4'-C4'	-8.63	1.11	1.44
6	D	5004	MTE	O4'-C4'	-8.41	1.12	1.44
6	B	3004	MTE	C6-N5	8.28	1.55	1.46
6	A	2004	MTE	C4'-C3'	-7.47	1.41	1.51
6	C	4004	MTE	C6-N5	-7.27	1.38	1.46
6	D	5004	MTE	C6-N5	7.10	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	3004	MTE	P-O4'	-6.95	1.38	1.60
6	C	4004	MTE	P-O4'	-6.81	1.38	1.60
6	D	5004	MTE	P-O4'	-6.67	1.39	1.60
6	A	2004	MTE	P-O4'	-6.60	1.39	1.60
5	B	3003	FAD	C10-N1	6.25	1.45	1.33
5	A	2003	FAD	C10-N1	5.90	1.45	1.33
5	C	4003	FAD	C10-N1	5.66	1.44	1.33
5	D	5003	FAD	C10-N1	5.52	1.44	1.33
5	B	3003	FAD	C10-N10	4.99	1.48	1.37
6	C	4004	MTE	C10-N8	4.90	1.40	1.35
6	C	4004	MTE	P-O3P	-4.89	1.36	1.54
5	C	4003	FAD	C10-N10	4.87	1.47	1.37
5	A	2003	FAD	C9A-C5X	4.81	1.48	1.41
6	A	2004	MTE	P-O3P	-4.79	1.37	1.54
6	D	5004	MTE	P-O3P	-4.79	1.37	1.54
5	B	3003	FAD	C9-C9A	4.75	1.47	1.39
5	C	4003	FAD	C9A-N10	4.69	1.49	1.41
5	C	4003	FAD	C9A-C5X	4.68	1.48	1.41
5	A	2003	FAD	C10-N10	4.67	1.47	1.37
5	D	5003	FAD	C10-N10	4.59	1.47	1.37
5	A	2003	FAD	C9-C9A	4.58	1.47	1.39
6	B	3004	MTE	P-O3P	-4.56	1.37	1.54
5	A	2003	FAD	C9A-N10	4.53	1.49	1.41
5	C	4003	FAD	C9-C9A	4.47	1.46	1.39
5	D	5003	FAD	C9A-C5X	4.47	1.48	1.41
5	B	3003	FAD	C9A-C5X	4.41	1.48	1.41
6	B	3004	MTE	C10-N8	4.41	1.40	1.35
6	B	3004	MTE	O4-C4	4.40	1.31	1.23
6	D	5004	MTE	O4-C4	4.37	1.31	1.23
5	D	5003	FAD	C9A-N10	4.34	1.48	1.41
5	B	3003	FAD	C9A-N10	4.33	1.48	1.41
5	D	5003	FAD	C9-C9A	4.30	1.46	1.39
6	A	2004	MTE	C10-N8	4.17	1.39	1.35
5	A	2003	FAD	C4X-N5	4.13	1.39	1.30
5	D	5003	FAD	C4X-N5	4.08	1.39	1.30
5	B	3003	FAD	C4X-N5	3.98	1.39	1.30
5	B	3003	FAD	C6-C7	3.94	1.45	1.39
6	A	2004	MTE	O4-C4	3.93	1.31	1.23
5	C	4003	FAD	C4X-N5	3.91	1.39	1.30
6	C	4004	MTE	O4-C4	3.88	1.30	1.23
5	D	5003	FAD	C6-C7	3.86	1.44	1.39
5	A	2003	FAD	C6-C7	3.84	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	5003	FAD	C1'-C2'	3.71	1.57	1.52
5	B	3003	FAD	C5A-N7A	-3.71	1.32	1.39
5	B	3003	FAD	C1'-C2'	3.69	1.57	1.52
5	C	4003	FAD	C1'-C2'	3.68	1.57	1.52
8	A	2006	SAL	C5-C6	3.60	1.45	1.38
5	A	2003	FAD	C1'-C2'	3.56	1.57	1.52
8	D	5006	SAL	C5-C6	3.54	1.45	1.38
6	D	5004	MTE	C10-N8	3.53	1.39	1.35
6	B	3004	MTE	C9-N5	3.50	1.46	1.37
5	A	2003	FAD	C6-C5X	3.49	1.45	1.40
5	D	5003	FAD	C5A-N7A	-3.44	1.32	1.39
8	B	3006	SAL	C5-C6	3.40	1.44	1.38
5	C	4003	FAD	C4A-N3A	3.39	1.40	1.34
5	C	4003	FAD	C5A-N7A	-3.39	1.32	1.39
6	A	2004	MTE	C2-N1	3.39	1.41	1.33
8	C	4006	SAL	C5-C6	3.34	1.44	1.38
5	D	5003	FAD	C4A-N3A	3.32	1.40	1.34
5	A	2003	FAD	C5A-N7A	-3.31	1.33	1.39
5	A	2003	FAD	C4A-N3A	3.29	1.40	1.34
5	B	3003	FAD	C4A-N3A	3.28	1.40	1.34
6	B	3004	MTE	C2-N1	3.27	1.41	1.33
5	B	3003	FAD	C6-C5X	3.26	1.44	1.40
5	C	4003	FAD	C6-C7	3.22	1.44	1.39
5	D	5003	FAD	C6-C5X	3.06	1.44	1.40
5	B	3003	FAD	C4-N3	3.04	1.44	1.38
5	C	4003	FAD	C5'-C4'	3.01	1.55	1.51
5	C	4003	FAD	C6-C5X	3.01	1.44	1.40
5	C	4003	FAD	C4-N3	2.99	1.44	1.38
5	A	2003	FAD	C5'-C4'	2.97	1.55	1.51
5	C	4003	FAD	C8-C7	2.96	1.48	1.40
6	C	4004	MTE	C2-N1	2.94	1.40	1.33
8	A	2006	SAL	C6-C1	2.92	1.44	1.39
5	A	2003	FAD	C4-N3	2.90	1.44	1.38
8	D	5006	SAL	C6-C1	2.89	1.44	1.39
5	A	2003	FAD	C8-C7	2.89	1.47	1.40
5	D	5003	FAD	C8-C7	2.86	1.47	1.40
5	B	3003	FAD	C2A-N1A	2.85	1.39	1.33
5	B	3003	FAD	C8-C7	2.81	1.47	1.40
6	D	5004	MTE	C2-N1	2.79	1.39	1.33
5	D	5003	FAD	C2A-N1A	2.75	1.38	1.33
5	D	5003	FAD	C4'-C3'	2.75	1.58	1.53
8	C	4006	SAL	C6-C1	2.74	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	4003	FAD	C4'-C3'	2.69	1.58	1.53
5	B	3003	FAD	C9-C8	2.66	1.43	1.39
5	B	3003	FAD	C4'-C3'	2.63	1.58	1.53
5	D	5003	FAD	C4-N3	2.60	1.43	1.38
5	C	4003	FAD	C2A-N1A	2.59	1.38	1.33
5	A	2003	FAD	C2A-N1A	2.57	1.38	1.33
8	C	4006	SAL	C1-C1'	-2.56	1.44	1.49
6	D	5004	MTE	P-O1P	2.55	1.58	1.50
8	B	3006	SAL	C6-C1	2.54	1.43	1.39
5	A	2003	FAD	P-O1P	2.54	1.59	1.50
8	A	2006	SAL	C3-C2	2.52	1.43	1.39
8	D	5006	SAL	C1-C1'	-2.51	1.44	1.49
6	D	5004	MTE	C9-C4	2.51	1.49	1.41
5	C	4003	FAD	C1'-N10	2.46	1.53	1.47
5	D	5003	FAD	C5'-C4'	2.45	1.55	1.51
5	D	5003	FAD	PA-O1A	2.45	1.59	1.50
5	C	4003	FAD	C9-C8	2.44	1.42	1.39
8	B	3006	SAL	C3-C2	2.44	1.43	1.39
8	D	5006	SAL	C3-C2	2.41	1.43	1.39
8	B	3006	SAL	C1-C1'	-2.41	1.44	1.49
5	B	3003	FAD	C5'-C4'	2.41	1.55	1.51
5	A	2003	FAD	PA-O1A	2.40	1.59	1.50
5	C	4003	FAD	P-O1P	2.40	1.59	1.50
5	B	3003	FAD	P-O1P	2.40	1.59	1.50
5	B	3003	FAD	C2-N1	2.40	1.42	1.36
8	C	4006	SAL	C3-C2	2.39	1.43	1.39
5	D	5003	FAD	P-O1P	2.36	1.59	1.50
5	D	5003	FAD	C1'-N10	2.36	1.53	1.47
5	B	3003	FAD	PA-O1A	2.35	1.59	1.50
6	B	3004	MTE	C9-C4	2.35	1.48	1.41
5	A	2003	FAD	C9-C8	2.34	1.42	1.39
6	A	2004	MTE	C9-C4	2.32	1.48	1.41
5	C	4003	FAD	C2'-C3'	2.32	1.57	1.53
5	C	4003	FAD	PA-O1A	2.31	1.58	1.50
5	B	3003	FAD	C1'-N10	2.30	1.53	1.47
5	D	5003	FAD	C5A-C4A	2.26	1.43	1.39
5	A	2003	FAD	C5A-C4A	2.23	1.43	1.39
5	A	2003	FAD	C1'-N10	2.22	1.53	1.47
8	B	3006	SAL	O2'-C1'	-2.18	1.24	1.30
5	B	3003	FAD	C2A-N3A	2.18	1.37	1.33
5	B	3003	FAD	C5A-C4A	2.18	1.43	1.39
8	D	5006	SAL	O2'-C1'	-2.17	1.24	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	4004	MTE	C9-C4	2.11	1.48	1.41
5	D	5003	FAD	C9-C8	2.10	1.42	1.39
5	A	2003	FAD	C8M-C8	2.09	1.54	1.51
5	B	3003	FAD	C2-N3	2.06	1.43	1.39
8	C	4006	SAL	O2'-C1'	-2.06	1.24	1.30
5	C	4003	FAD	C8M-C8	2.04	1.54	1.51
5	C	4003	FAD	C4A-N9A	-2.03	1.33	1.37
5	D	5003	FAD	C2A-N3A	2.02	1.37	1.33
5	D	5003	FAD	C4A-N9A	-2.01	1.33	1.37
5	C	4003	FAD	C5A-C4A	2.00	1.42	1.39

All (176) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	5004	MTE	C2-N1-C10	8.28	127.97	113.36
6	B	3004	MTE	C2-N1-C10	8.27	127.95	113.36
6	A	2004	MTE	C2-N1-C10	8.07	127.60	113.36
6	C	4004	MTE	C2-N1-C10	8.05	127.56	113.36
5	C	4003	FAD	N3A-C2A-N1A	-7.16	117.75	128.58
5	A	2003	FAD	N3A-C2A-N1A	-7.15	117.77	128.58
5	B	3003	FAD	N3A-C2A-N1A	-7.06	117.89	128.58
5	D	5003	FAD	N3A-C2A-N1A	-7.04	117.92	128.58
6	C	4004	MTE	C4-C9-N5	6.42	133.76	116.27
6	B	3004	MTE	C4-C9-N5	5.38	130.95	116.27
6	C	4004	MTE	O4-C4-C9	-5.34	114.38	127.26
6	A	2004	MTE	O4-C4-C9	-5.29	114.49	127.26
6	B	3004	MTE	O4-C4-C9	-5.26	114.58	127.26
5	A	2003	FAD	C2B-C1B-N9A	5.26	126.36	113.30
6	D	5004	MTE	O4-C4-C9	-5.23	114.65	127.26
5	D	5003	FAD	C2B-C1B-N9A	5.06	125.86	113.30
5	C	4003	FAD	C2B-C1B-N9A	5.04	125.83	113.30
5	B	3003	FAD	C2B-C1B-N9A	4.84	125.33	113.30
6	D	5004	MTE	C4-C9-N5	4.61	128.84	116.27
5	B	3003	FAD	O4'-C4'-C3'	4.46	119.68	109.25
5	B	3003	FAD	C5X-N5-C4X	4.40	125.21	118.09
5	C	4003	FAD	O4'-C4'-C3'	4.35	119.43	109.25
5	D	5003	FAD	O4'-C4'-C3'	4.32	119.36	109.25
5	C	4003	FAD	C5X-N5-C4X	4.31	125.05	118.09
5	B	3003	FAD	C5A-C4A-N3A	-4.23	120.90	126.72
8	A	2006	SAL	O2'-C1'-O1'	-4.21	114.31	123.35
5	C	4003	FAD	C2A-N3A-C4A	4.18	122.04	111.83
5	D	5003	FAD	C5A-C4A-N3A	-4.17	120.98	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	5003	FAD	C5X-N5-C4X	4.17	124.83	118.09
5	A	2003	FAD	C5A-C4A-N3A	-4.17	120.98	126.72
5	C	4003	FAD	C5A-C4A-N3A	-4.16	120.98	126.72
5	A	2003	FAD	O4'-C4'-C3'	4.16	118.97	109.25
5	A	2003	FAD	C2A-N3A-C4A	4.12	121.89	111.83
8	B	3006	SAL	O2'-C1'-O1'	-4.11	114.51	123.35
5	A	2003	FAD	C5X-N5-C4X	4.11	124.73	118.09
8	D	5006	SAL	O2'-C1'-O1'	-4.09	114.56	123.35
5	B	3003	FAD	C2A-N3A-C4A	4.08	121.80	111.83
5	D	5003	FAD	C2A-N3A-C4A	4.07	121.77	111.83
8	C	4006	SAL	O2'-C1'-O1'	-4.07	114.61	123.35
6	D	5004	MTE	O3'-C7-N8	-3.75	105.20	108.61
6	C	4004	MTE	O3'-C7-C6	-3.68	106.51	108.96
8	A	2006	SAL	C3-C2-C1	3.62	123.66	119.89
6	A	2004	MTE	C4-C9-N5	3.61	126.11	116.27
8	B	3006	SAL	C3-C2-C1	3.60	123.64	119.89
6	D	5004	MTE	N2-C2-N3	3.58	124.31	116.76
6	B	3004	MTE	O3'-C7-C6	-3.57	106.58	108.96
8	A	2006	SAL	C2-C1-C1'	3.56	123.65	120.00
5	A	2003	FAD	C1'-N10-C9A	3.54	127.52	120.63
6	D	5004	MTE	C7-C6-N5	3.52	111.33	107.87
8	D	5006	SAL	C2-C1-C1'	3.51	123.60	120.00
5	D	5003	FAD	C1'-N10-C9A	3.48	127.39	120.63
6	C	4004	MTE	N2-C2-N3	3.47	124.08	116.76
6	C	4004	MTE	O3'-C7-N8	-3.46	105.47	108.61
5	C	4003	FAD	C1'-N10-C9A	3.45	127.33	120.63
6	B	3004	MTE	N2-C2-N3	3.45	124.04	116.76
6	A	2004	MTE	N2-C2-N3	3.44	124.02	116.76
6	A	2004	MTE	O3'-C7-C6	-3.41	106.69	108.96
8	D	5006	SAL	C3-C2-C1	3.40	123.43	119.89
8	C	4006	SAL	C3-C2-C1	3.40	123.42	119.89
8	C	4006	SAL	C2-C1-C1'	3.39	123.48	120.00
5	A	2003	FAD	C5'-C4'-C3'	-3.38	105.84	112.22
5	B	3003	FAD	O3'-C3'-C4'	3.33	116.50	108.93
5	B	3003	FAD	C1'-N10-C9A	3.33	127.10	120.63
8	B	3006	SAL	C2-C1-C1'	3.28	123.36	120.00
6	C	4004	MTE	C9-C4-N3	3.27	121.12	112.13
5	D	5003	FAD	C5'-C4'-C3'	-3.26	106.06	112.22
5	B	3003	FAD	C9A-C5X-N5	-3.26	118.99	122.45
6	A	2004	MTE	C9-C4-N3	3.25	121.06	112.13
6	A	2004	MTE	O3'-C7-N8	-3.24	105.66	108.61
5	D	5003	FAD	C9A-C5X-N5	-3.24	119.02	122.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	3003	FAD	C5'-C4'-C3'	-3.19	106.19	112.22
5	A	2003	FAD	C9A-C5X-N5	-3.19	119.07	122.45
5	C	4003	FAD	C9A-C5X-N5	-3.17	119.09	122.45
6	D	5004	MTE	C9-C4-N3	3.17	120.84	112.13
6	B	3004	MTE	C9-C4-N3	3.14	120.76	112.13
5	C	4003	FAD	C5'-C4'-C3'	-3.10	106.37	112.22
5	D	5003	FAD	O3'-C3'-C4'	3.10	115.97	108.93
5	B	3003	FAD	N3A-C4A-N9A	3.08	132.40	127.17
5	C	4003	FAD	N3A-C4A-N9A	3.03	132.32	127.17
5	D	5003	FAD	N3A-C4A-N9A	3.02	132.30	127.17
5	A	2003	FAD	N3A-C4A-N9A	2.93	132.15	127.17
5	C	4003	FAD	O3'-C3'-C4'	2.93	115.59	108.93
5	A	2003	FAD	C4-C4X-N5	2.92	122.23	118.21
5	A	2003	FAD	O3'-C3'-C4'	2.87	115.45	108.93
5	C	4003	FAD	C4-C4X-N5	2.86	122.16	118.21
5	D	5003	FAD	C4-C4X-N5	2.86	122.15	118.21
5	B	3003	FAD	C3B-C2B-C1B	2.83	106.81	101.46
5	B	3003	FAD	O2B-C2B-C3B	2.80	120.78	111.82
5	D	5003	FAD	O2B-C2B-C3B	2.79	120.77	111.82
5	B	3003	FAD	O4B-C1B-N9A	-2.79	102.73	108.09
5	A	2003	FAD	C4'-C3'-C2'	-2.77	108.96	113.57
5	B	3003	FAD	C4-C4X-N5	2.75	122.01	118.21
5	A	2003	FAD	C4X-C4-N3	2.74	120.24	113.25
5	B	3003	FAD	C4X-C4-N3	2.74	120.22	113.25
5	D	5003	FAD	C4X-C4-N3	2.74	120.22	113.25
5	D	5003	FAD	C8M-C8-C9	-2.73	114.75	119.57
5	B	3003	FAD	C4'-C3'-C2'	-2.72	109.04	113.57
5	C	4003	FAD	O3B-C3B-C4B	-2.71	103.31	111.08
5	B	3003	FAD	C10-C4X-N5	-2.70	119.30	124.81
5	A	2003	FAD	O3B-C3B-C4B	-2.70	103.34	111.08
5	C	4003	FAD	C4X-C4-N3	2.67	120.04	113.25
5	B	3003	FAD	O3B-C3B-C4B	-2.66	103.43	111.08
5	A	2003	FAD	C2A-N1A-C6A	2.66	123.10	118.73
5	C	4003	FAD	C7M-C7-C6	-2.66	114.89	119.57
5	D	5003	FAD	C10-C4X-N5	-2.64	119.42	124.81
5	A	2003	FAD	C10-C4X-N5	-2.64	119.42	124.81
5	A	2003	FAD	C8M-C8-C9	-2.64	114.93	119.57
5	C	4003	FAD	C10-C4X-N5	-2.62	119.45	124.81
6	B	3004	MTE	O3'-C7-N8	-2.62	106.23	108.61
5	C	4003	FAD	C8M-C8-C9	-2.62	114.95	119.57
8	A	2006	SAL	O2'-C1'-C1	2.62	122.72	115.28
5	A	2003	FAD	O2B-C2B-C3B	2.58	120.09	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	4003	FAD	C4A-C5A-N7A	-2.58	107.64	110.58
5	C	4003	FAD	O2B-C2B-C3B	2.58	120.07	111.82
5	C	4003	FAD	C2A-N1A-C6A	2.57	122.96	118.73
5	B	3003	FAD	C4A-C5A-N7A	-2.57	107.64	110.58
5	A	2003	FAD	C7M-C7-C6	-2.57	115.05	119.57
8	B	3006	SAL	O2'-C1'-C1	2.57	122.57	115.28
5	D	5003	FAD	C2A-N1A-C6A	2.53	122.89	118.73
8	D	5006	SAL	O2'-C1'-C1	2.53	122.47	115.28
5	B	3003	FAD	C8M-C8-C9	-2.52	115.13	119.57
5	B	3003	FAD	C5A-N7A-C8A	2.52	107.41	103.45
5	D	5003	FAD	O3B-C3B-C4B	-2.51	103.87	111.08
5	A	2003	FAD	O5B-PA-O1A	2.50	118.86	108.94
5	A	2003	FAD	C4A-C5A-N7A	-2.50	107.72	110.58
8	C	4006	SAL	O2'-C1'-C1	2.48	122.33	115.28
5	D	5003	FAD	C4-N3-C2	-2.47	121.25	125.64
5	C	4003	FAD	C5A-N7A-C8A	2.47	107.33	103.45
5	D	5003	FAD	O5B-PA-O1A	2.47	118.72	108.94
5	D	5003	FAD	C4A-C5A-N7A	-2.46	107.76	110.58
5	C	4003	FAD	C4-N3-C2	-2.43	121.33	125.64
5	C	4003	FAD	O5B-PA-O1A	2.42	118.54	108.94
5	B	3003	FAD	C7M-C7-C6	-2.42	115.31	119.57
6	B	3004	MTE	O4-C4-N3	2.42	124.66	120.11
5	C	4003	FAD	C4'-C3'-C2'	-2.41	109.56	113.57
5	B	3003	FAD	C2A-N1A-C6A	2.40	122.68	118.73
5	D	5003	FAD	C7M-C7-C6	-2.39	115.36	119.57
5	D	5003	FAD	O4B-C1B-N9A	-2.39	103.50	108.09
5	D	5003	FAD	C8M-C8-C7	2.38	125.61	120.76
5	A	2003	FAD	C5A-N7A-C8A	2.37	107.17	103.45
5	B	3003	FAD	O5B-PA-O1A	2.36	118.28	108.94
6	D	5004	MTE	O4-C4-N3	2.34	124.51	120.11
5	D	5003	FAD	C5A-N7A-C8A	2.33	107.12	103.45
6	C	4004	MTE	O4-C4-N3	2.33	124.50	120.11
5	C	4003	FAD	C3B-C2B-C1B	2.33	105.87	101.46
5	B	3003	FAD	C4-N3-C2	-2.32	121.51	125.64
6	A	2004	MTE	O4-C4-N3	2.31	124.45	120.11
5	A	2003	FAD	C8M-C8-C7	2.29	125.44	120.76
6	B	3004	MTE	C7-C6-N5	-2.29	105.62	107.87
5	C	4003	FAD	C8M-C8-C7	2.29	125.43	120.76
5	A	2003	FAD	C3B-C2B-C1B	2.27	105.75	101.46
5	B	3003	FAD	C8M-C8-C7	2.27	125.39	120.76
5	A	2003	FAD	C4-N3-C2	-2.26	121.62	125.64
6	D	5004	MTE	O2P-P-O4'	2.25	112.54	106.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2003	FAD	O5'-P-O1P	2.22	117.72	108.94
6	B	3004	MTE	N3-C2-N1	-2.22	119.27	123.32
5	D	5003	FAD	C4'-C3'-C2'	-2.20	109.91	113.57
5	C	4003	FAD	C10-N1-C2	2.17	121.55	116.85
5	C	4003	FAD	C6A-C5A-N7A	2.15	136.23	132.09
5	A	2003	FAD	O4B-C1B-N9A	-2.14	103.98	108.09
6	C	4004	MTE	O2P-P-O4'	2.13	112.21	106.67
5	C	4003	FAD	O5'-P-O1P	2.12	117.35	108.94
5	D	5003	FAD	O5'-P-O1P	2.12	117.35	108.94
5	C	4003	FAD	O4B-C1B-N9A	-2.12	104.02	108.09
5	A	2003	FAD	C10-N1-C2	2.10	121.40	116.85
6	C	4004	MTE	N3-C2-N1	-2.09	119.49	123.32
5	A	2003	FAD	C6A-C5A-N7A	2.09	136.12	132.09
6	D	5004	MTE	N3-C2-N1	-2.09	119.50	123.32
5	B	3003	FAD	C10-N1-C2	2.07	121.34	116.85
6	A	2004	MTE	N3-C2-N1	-2.07	119.54	123.32
5	A	2003	FAD	C4X-C10-N1	-2.06	119.53	124.59
8	A	2006	SAL	C6-C1-C2	-2.06	115.56	118.15
5	B	3003	FAD	C4X-C10-N1	-2.06	119.55	124.59
5	C	4003	FAD	C4X-C10-N1	-2.04	119.59	124.59
5	B	3003	FAD	O5'-P-O1P	2.04	117.01	108.94
5	D	5003	FAD	C10-N1-C2	2.02	121.21	116.85

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2003	FAD	N10-C1'-C2'-O2'
5	A	2003	FAD	N10-C1'-C2'-C3'
5	B	3003	FAD	N10-C1'-C2'-O2'
5	B	3003	FAD	N10-C1'-C2'-C3'
5	C	4003	FAD	N10-C1'-C2'-O2'
5	C	4003	FAD	N10-C1'-C2'-C3'
5	D	5003	FAD	N10-C1'-C2'-O2'
5	D	5003	FAD	N10-C1'-C2'-C3'
6	A	2004	MTE	C4'-O4'-P-O2P
6	A	2004	MTE	C4'-O4'-P-O3P
6	B	3004	MTE	C4'-O4'-P-O1P
6	B	3004	MTE	C4'-O4'-P-O2P
6	B	3004	MTE	C4'-O4'-P-O3P
6	C	4004	MTE	C4'-O4'-P-O1P
6	C	4004	MTE	C4'-O4'-P-O2P

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Mol	Chain	Res	Type	Atoms
6	C	4004	MTE	C4'-O4'-P-O3P
6	D	5004	MTE	C2'-C3'-C4'-O4'
5	B	3003	FAD	C2'-C3'-C4'-O4'
5	A	2003	FAD	C2'-C3'-C4'-O4'
5	C	4003	FAD	C2'-C3'-C4'-O4'
6	A	2004	MTE	C3'-C4'-O4'-P
6	C	4004	MTE	C2'-C3'-C4'-O4'
5	B	3003	FAD	O3'-C3'-C4'-O4'
6	C	4004	MTE	O3'-C3'-C4'-O4'
6	D	5004	MTE	O3'-C3'-C4'-O4'
5	D	5003	FAD	C2'-C3'-C4'-O4'
5	A	2003	FAD	O3'-C3'-C4'-O4'
5	C	4003	FAD	O3'-C3'-C4'-O4'
5	D	5003	FAD	O3'-C3'-C4'-O4'
6	C	4004	MTE	C3'-C4'-O4'-P

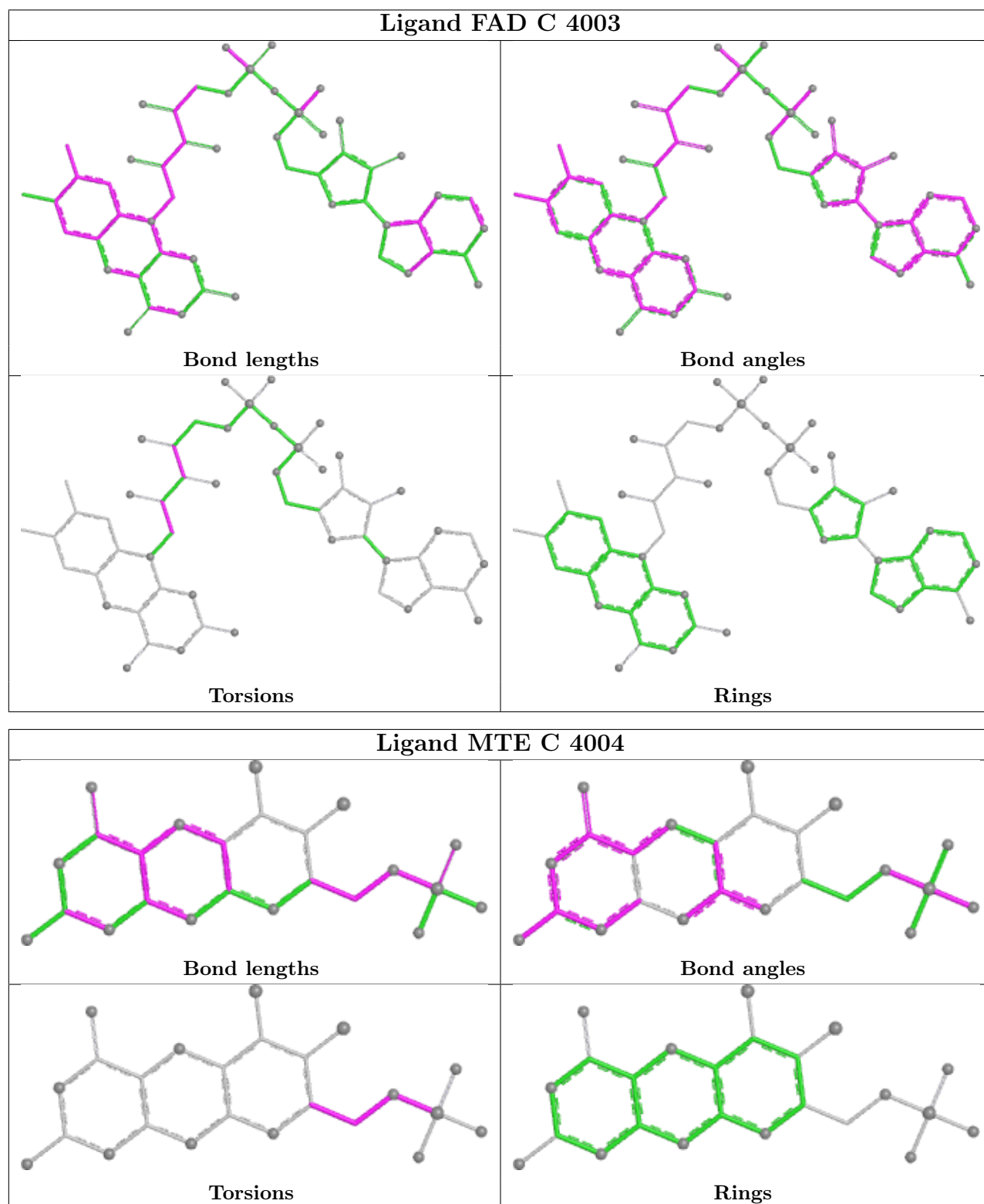
There are no ring outliers.

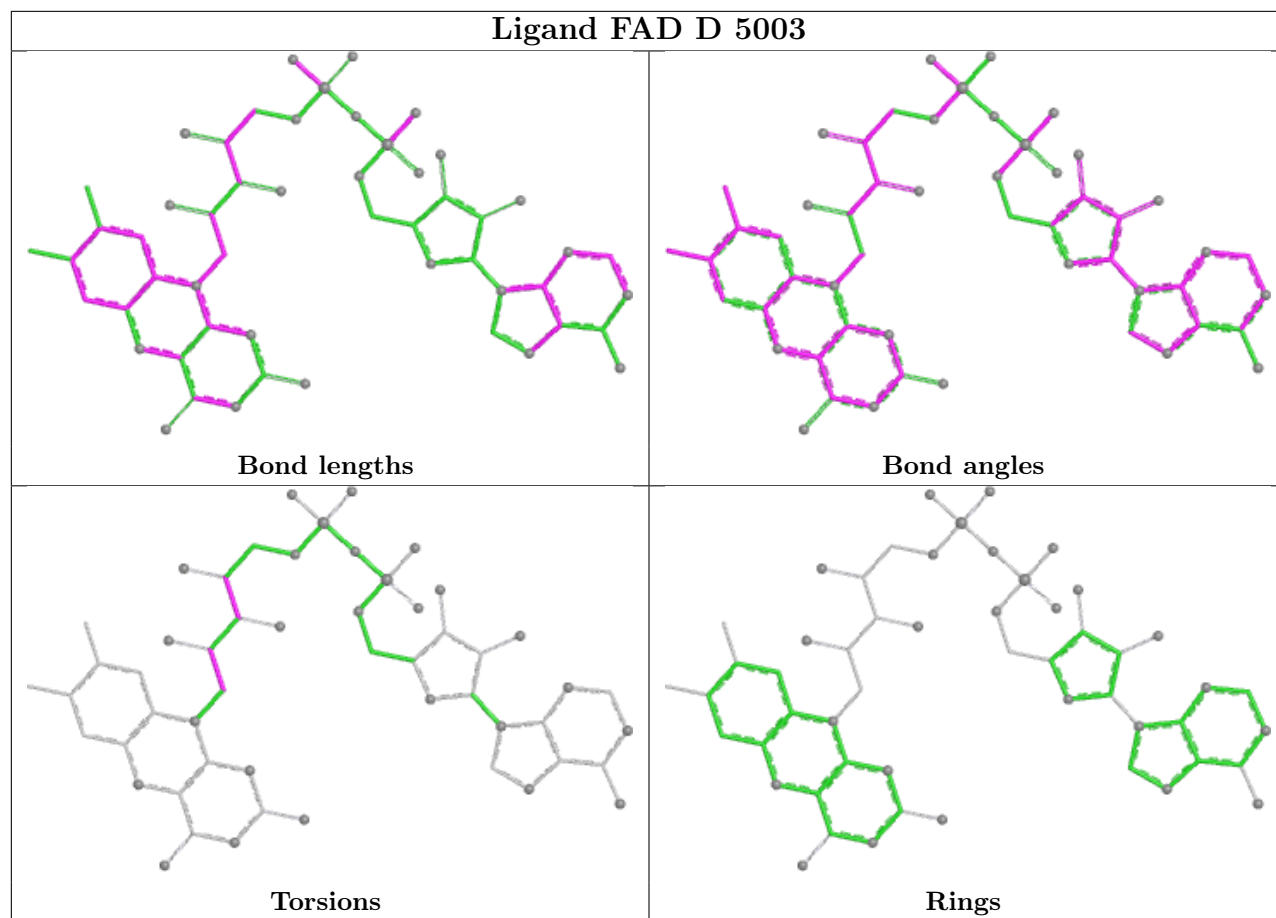
15 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	2005	MOM	2	0
5	C	4003	FAD	2	0
6	C	4004	MTE	2	0
5	D	5003	FAD	3	0
7	B	3005	MOM	2	0
7	D	5005	MOM	3	0
5	B	3003	FAD	3	0
7	C	4005	MOM	2	0
6	A	2004	MTE	4	0
2	A	6001	BCT	1	0
6	D	5004	MTE	2	0
6	B	3004	MTE	3	0
4	D	2002	FES	1	0
2	B	6002	BCT	1	0
5	A	2003	FAD	2	0

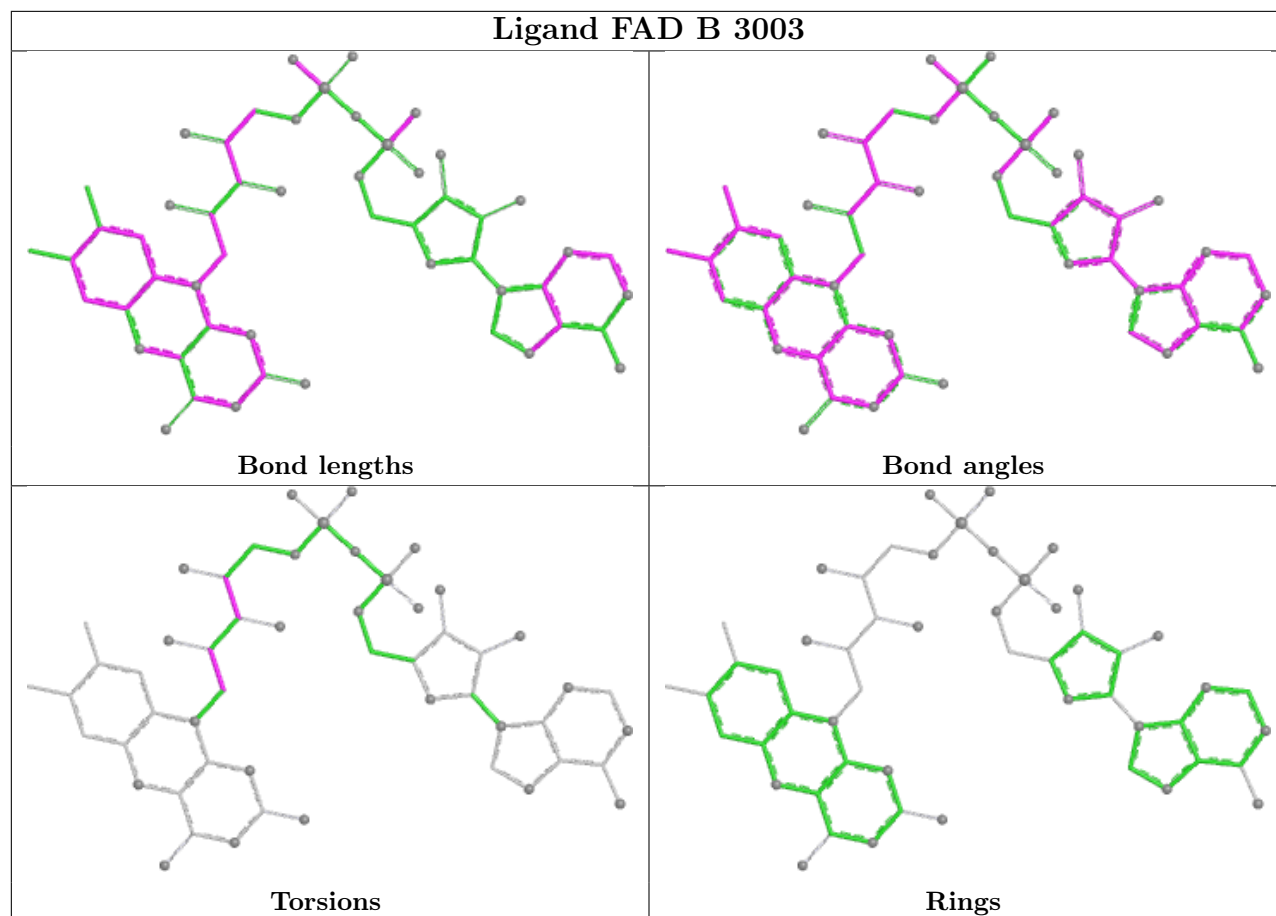
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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

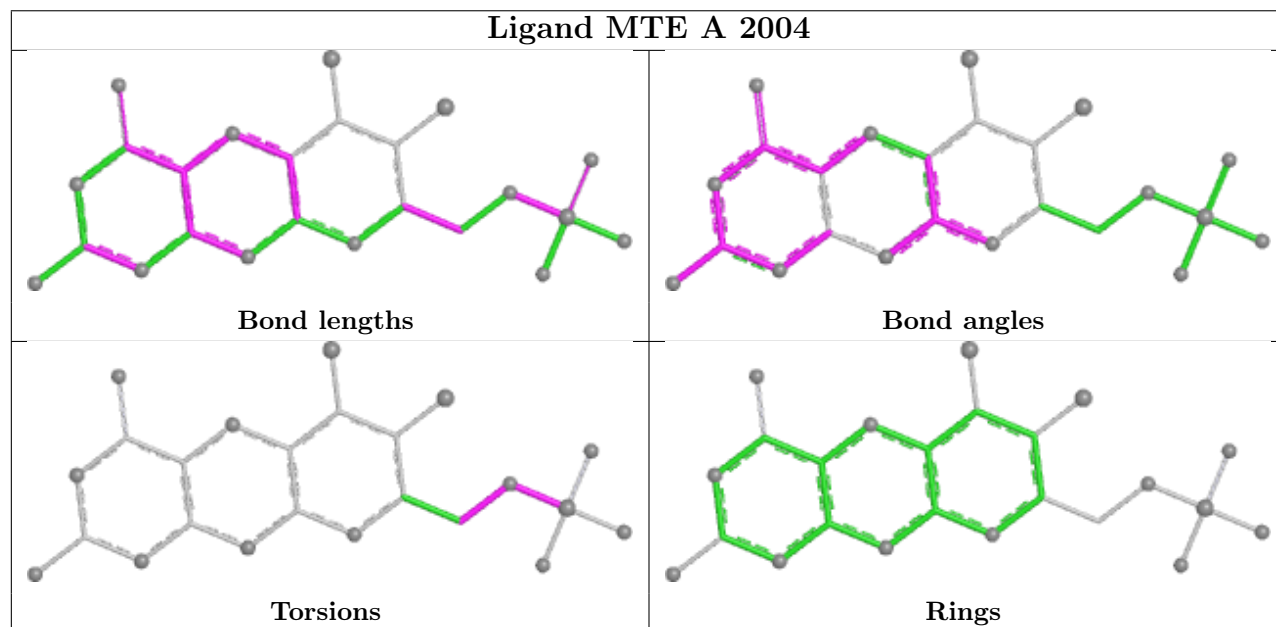




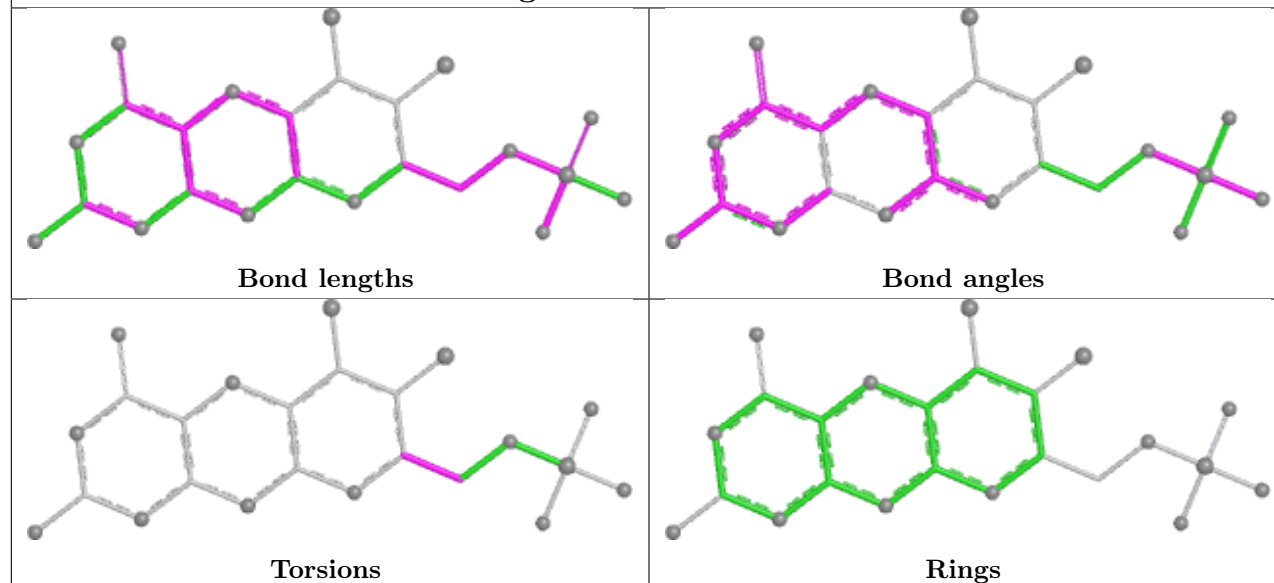
Ligand FAD B 3003



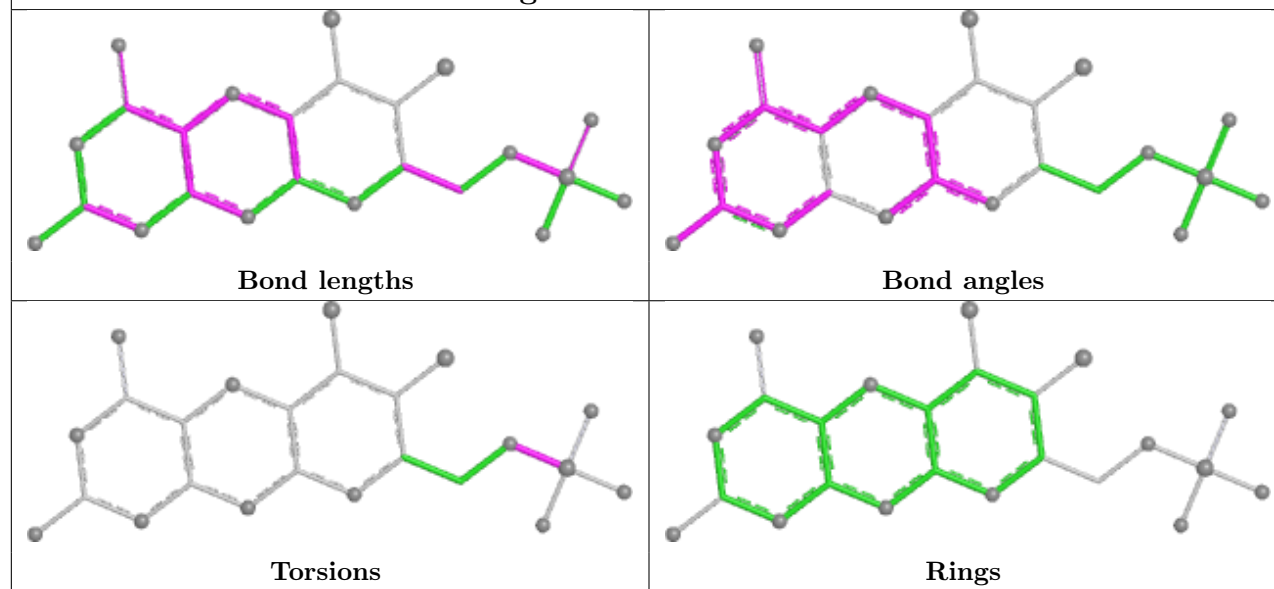
Ligand MTE A 2004

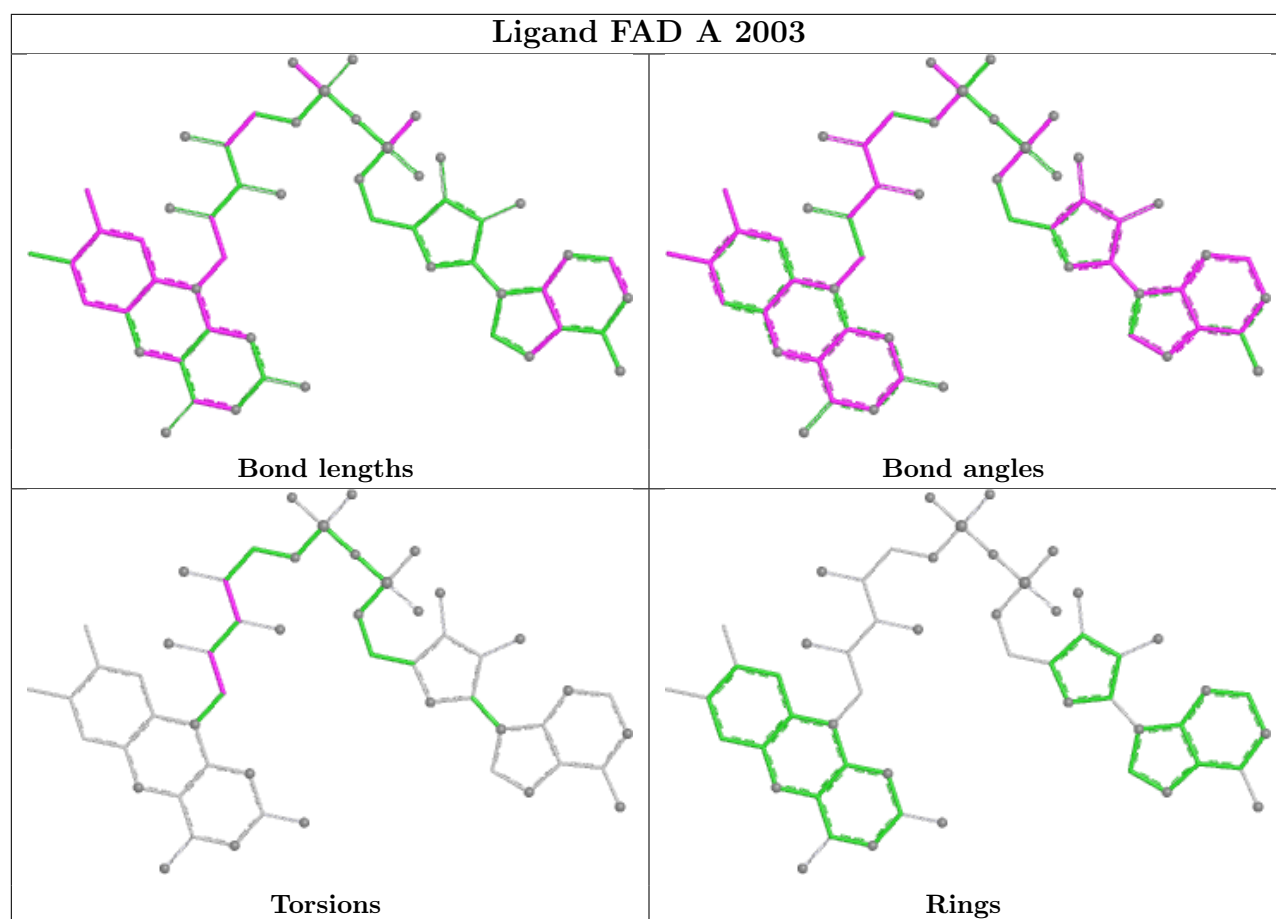


Ligand MTE D 5004



Ligand MTE B 3004





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	1307/1333 (98%)	-0.27	36 (2%)	55	49	10, 27, 56, 169	0
1	B	1307/1333 (98%)	-0.32	39 (2%)	52	47	10, 25, 52, 166	0
1	C	1307/1333 (98%)	-0.28	37 (2%)	55	49	9, 26, 54, 156	0
1	D	1307/1333 (98%)	-0.28	34 (2%)	57	51	8, 25, 55, 150	0
All	All	5228/5332 (98%)	-0.29	146 (2%)	55	49	8, 26, 55, 169	0

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	167	GLY	5.6
1	C	1320	THR	5.5
1	B	552	LYS	5.2
1	D	167	GLY	5.2
1	C	552	LYS	4.7
1	D	481	GLU	4.5
1	C	60	ARG	4.4
1	D	1332	ARG	4.3
1	D	1322	VAL	4.3
1	B	322	GLN	4.2
1	D	377	ARG	4.2
1	A	1288	GLY	4.2
1	B	167	GLY	4.2
1	D	166	ASP	4.2
1	A	62	GLN	4.1
1	B	481	GLU	4.1
1	C	318	LYS	4.1
1	C	254	ASP	4.0
1	D	3	ALA	3.9
1	C	1289	ASN	3.8
1	B	60	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	1332	ARG	3.8
1	A	60	ARG	3.7
1	C	1291	VAL	3.7
1	C	1288	GLY	3.7
1	D	1327	LYS	3.7
1	A	1327	LYS	3.6
1	C	192	SER	3.6
1	C	167	GLY	3.6
1	C	1319	VAL	3.5
1	A	551	GLN	3.5
1	A	377	ARG	3.5
1	C	472	ARG	3.5
1	A	272	ASN	3.5
1	A	1289	ASN	3.5
1	A	535	LYS	3.4
1	B	538	LYS	3.4
1	A	1290	ASN	3.4
1	B	1323	PRO	3.4
1	A	322	GLN	3.4
1	D	1321	GLY	3.4
1	A	192	SER	3.4
1	B	62	GLN	3.4
1	A	552	LYS	3.3
1	B	1321	GLY	3.3
1	B	1326	CYS	3.3
1	B	223	PRO	3.3
1	B	480	GLU	3.3
1	B	1320	THR	3.2
1	B	566	LYS	3.2
1	D	272	ASN	3.1
1	A	538	LYS	3.1
1	A	495	HIS	3.1
1	A	251	GLN	3.1
1	C	223	PRO	3.1
1	D	254	ASP	3.0
1	D	97	ARG	3.0
1	D	223	PRO	3.0
1	D	1323	PRO	3.0
1	A	566	LYS	3.0
1	A	1321	GLY	3.0
1	C	461	ASN	3.0
1	A	1291	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	1325	ASN	3.0
1	D	322	GLN	3.0
1	C	272	ASN	2.9
1	B	722	LYS	2.8
1	C	982	LYS	2.8
1	C	687	LYS	2.8
1	A	1144	GLU	2.8
1	B	535	LYS	2.8
1	B	1111	SER	2.8
1	B	254	ASP	2.8
1	B	1144	GLU	2.8
1	C	566	LYS	2.8
1	B	646	ILE	2.8
1	B	272	ASN	2.8
1	B	414	GLU	2.7
1	C	538	LYS	2.7
1	B	961	GLU	2.7
1	A	652	ASP	2.7
1	A	95	LYS	2.7
1	D	535	LYS	2.7
1	C	13	ARG	2.6
1	B	1313	LYS	2.6
1	C	481	GLU	2.6
1	D	414	GLU	2.5
1	A	563	GLU	2.5
1	C	646	ILE	2.5
1	D	721	LYS	2.5
1	D	684	GLN	2.5
1	B	1327	LYS	2.5
1	D	570	GLU	2.5
1	D	692	GLU	2.5
1	A	310	LYS	2.4
1	A	1320	THR	2.4
1	A	318	LYS	2.4
1	D	534	ASP	2.4
1	B	1324	GLU	2.4
1	C	1327	LYS	2.4
1	B	251	GLN	2.4
1	C	97	ARG	2.4
1	A	412	SER	2.4
1	B	692	GLU	2.4
1	C	412	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	4	ASP	2.4
1	C	95	LYS	2.4
1	B	551	GLN	2.4
1	B	1319	VAL	2.3
1	D	60	ARG	2.3
1	B	1325	ASN	2.3
1	A	371	LYS	2.3
1	C	310	LYS	2.3
1	D	401	GLU	2.3
1	C	166	ASP	2.3
1	C	1111	SER	2.3
1	C	62	GLN	2.2
1	C	660	LYS	2.2
1	C	722	LYS	2.2
1	A	223	PRO	2.2
1	B	95	LYS	2.2
1	B	97	ARG	2.2
1	D	192	SER	2.2
1	D	13	ARG	2.1
1	D	222	THR	2.1
1	B	131	GLN	2.1
1	B	858	VAL	2.1
1	D	1324	GLU	2.1
1	C	484	GLN	2.1
1	D	1326	CYS	2.1
1	D	1331	VAL	2.1
1	B	484	GLN	2.1
1	A	1111	SER	2.1
1	A	1280	ARG	2.1
1	B	218	ARG	2.1
1	C	570	GLU	2.1
1	B	269	LYS	2.1
1	D	1289	ASN	2.1
1	A	944	ARG	2.0
1	B	4	ASP	2.0
1	A	990	LYS	2.0
1	D	371	LYS	2.0
1	A	97	ARG	2.0
1	D	979	HIS	2.0
1	D	531	ASN	2.0
1	C	944	ARG	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BCT	D	6004	4/4	0.89	0.18	17,18,19,19	0
8	SAL	A	2006	10/10	0.90	0.12	36,37,37,38	0
8	SAL	D	5006	10/10	0.90	0.15	41,42,42,43	0
2	BCT	C	6003	4/4	0.91	0.18	17,18,19,19	0
8	SAL	B	3006	10/10	0.91	0.13	41,42,42,43	0
8	SAL	C	4006	10/10	0.91	0.13	36,37,37,38	0
3	CA	D	7007	1/1	0.91	0.25	20,20,20,20	0
2	BCT	B	6002	4/4	0.92	0.17	17,18,19,19	0
2	BCT	A	6001	4/4	0.92	0.21	17,18,19,19	0
3	CA	B	7003	1/1	0.93	0.26	20,20,20,20	0
6	MTE	D	5004	24/24	0.93	0.10	19,23,28,30	0
6	MTE	C	4004	24/24	0.94	0.09	20,24,28,30	0
6	MTE	B	3004	24/24	0.94	0.09	19,23,28,30	0
5	FAD	C	4003	53/53	0.95	0.12	26,36,47,49	0
5	FAD	D	5003	53/53	0.95	0.11	26,35,45,47	0
6	MTE	A	2004	24/24	0.95	0.09	20,24,28,30	0
3	CA	C	7005	1/1	0.95	0.21	20,20,20,20	0
4	FES	A	2001	4/4	0.95	0.06	14,14,14,33	0
3	CA	C	7006	1/1	0.96	0.38	18,18,18,18	0
3	CA	B	7004	1/1	0.96	0.42	18,18,18,18	0
3	CA	A	7001	1/1	0.96	0.26	20,20,20,20	0
5	FAD	A	2003	53/53	0.96	0.10	26,36,46,48	0
5	FAD	B	3003	53/53	0.96	0.10	26,34,47,49	0
3	CA	A	7002	1/1	0.97	0.38	18,18,18,18	0
3	CA	D	7008	1/1	0.98	0.31	23,23,23,23	0
4	FES	B	2001	4/4	0.99	0.03	14,14,14,14	0
4	FES	B	2002	4/4	0.99	0.03	14,14,14,14	0

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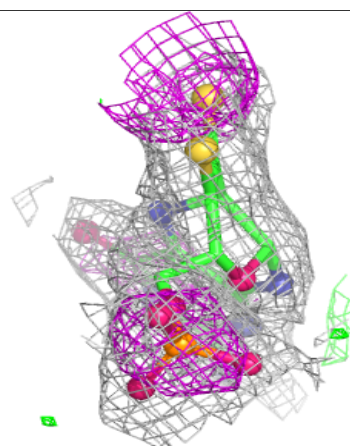
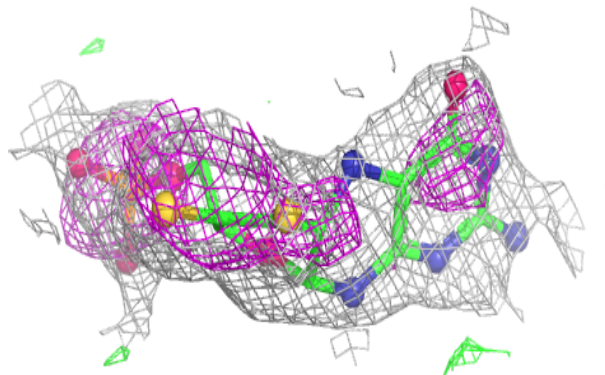
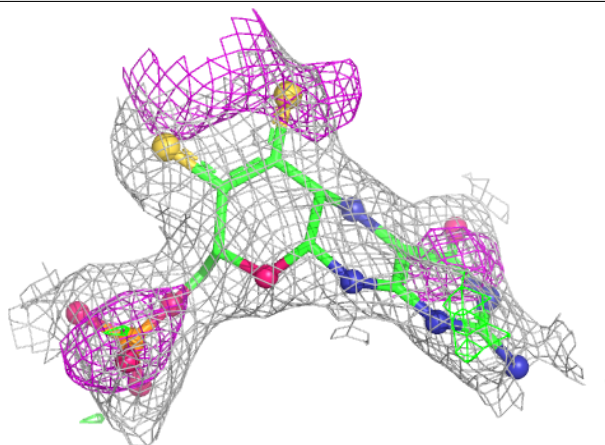
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	MOM	A	2005	4/4	0.99	0.21	28,29,30,31	0
7	MOM	B	3005	4/4	0.99	0.19	27,28,28,29	0
7	MOM	C	4005	4/4	0.99	0.19	28,29,30,31	0
7	MOM	D	5005	4/4	0.99	0.20	27,28,28,29	0
4	FES	C	2001	4/4	0.99	0.03	14,14,14,14	0
4	FES	C	2002	4/4	0.99	0.03	14,14,14,14	0
4	FES	D	2001	4/4	0.99	0.03	14,14,14,14	0
4	FES	D	2002	4/4	0.99	0.03	14,14,14,14	0
4	FES	A	2002	4/4	1.00	0.03	14,14,14,14	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.

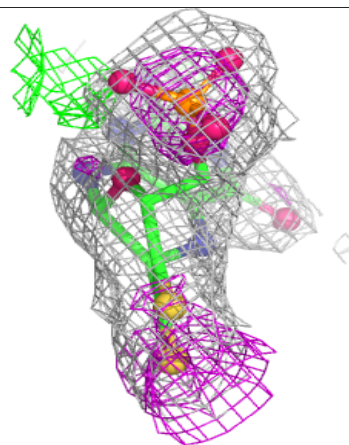
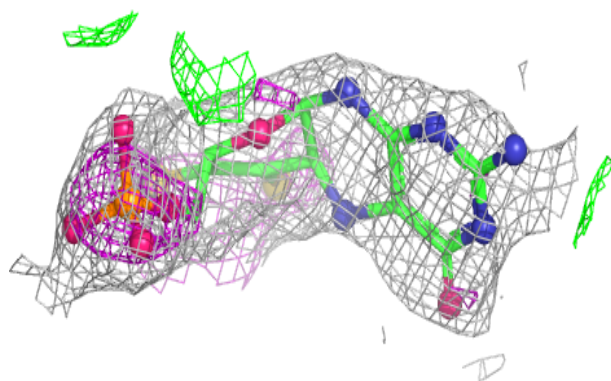
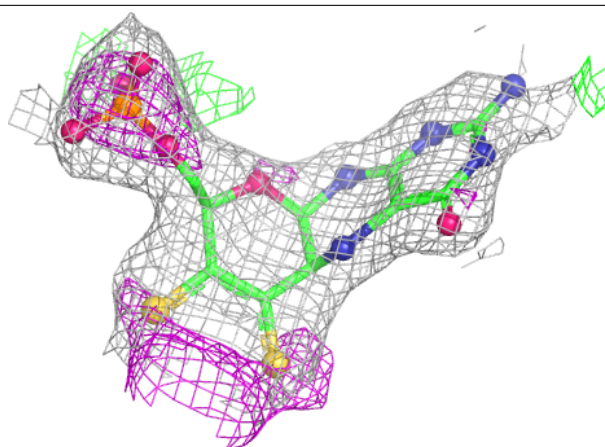
Electron density around MTE D 5004:

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



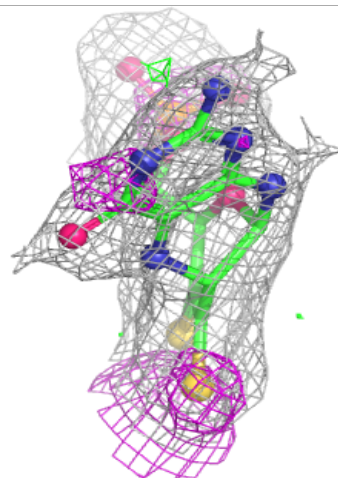
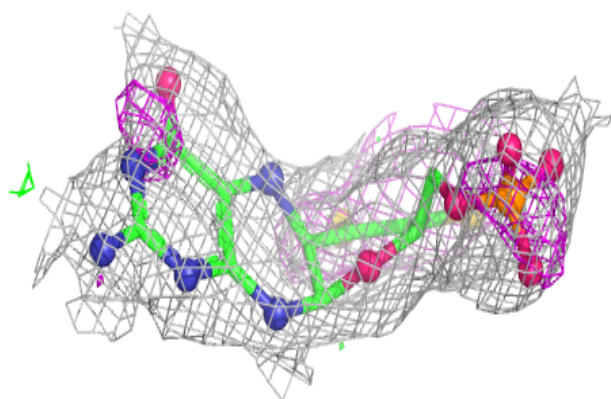
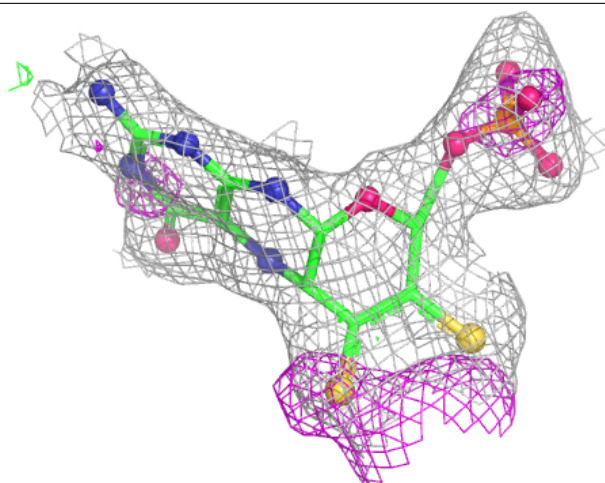
Electron density around MTE C 4004:

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



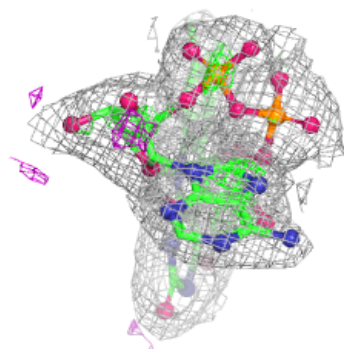
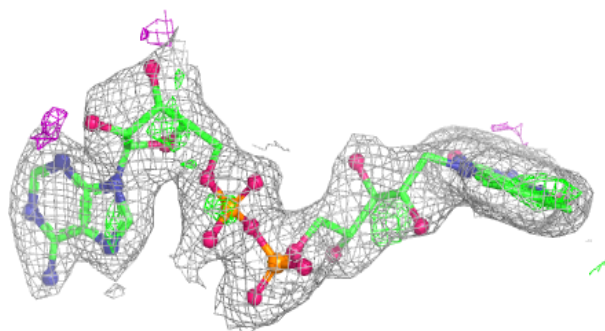
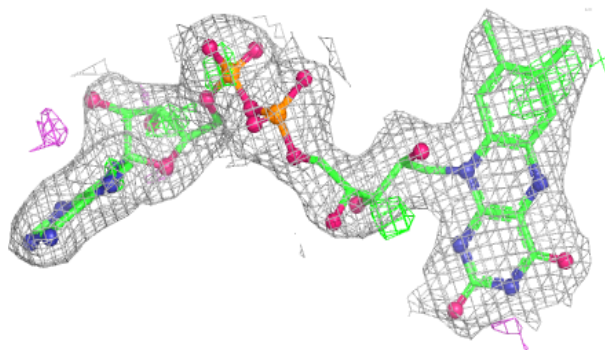
Electron density around MTE B 3004:

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

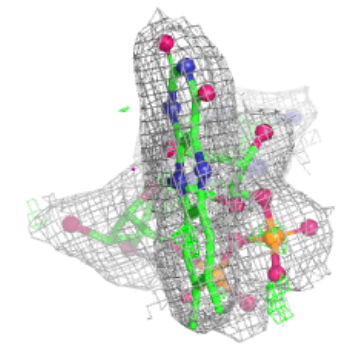
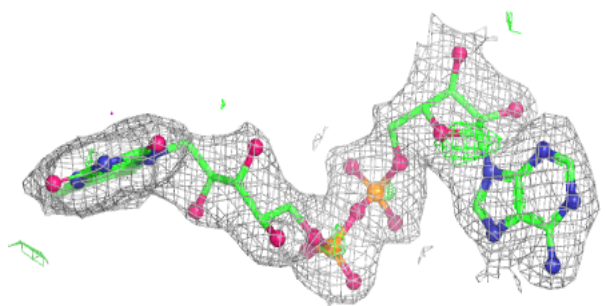
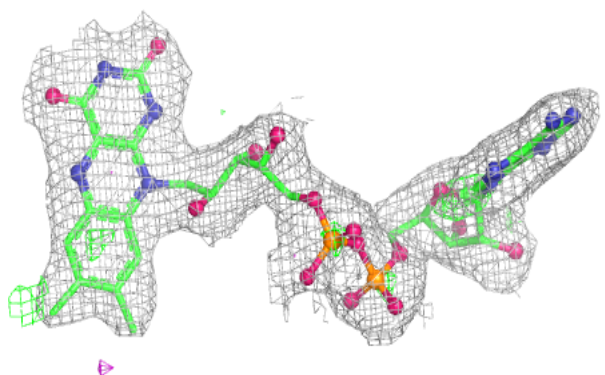


Electron density around FAD C 4003:

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

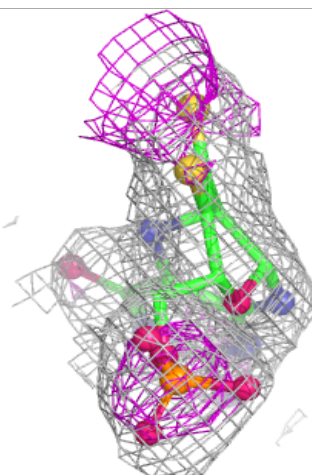
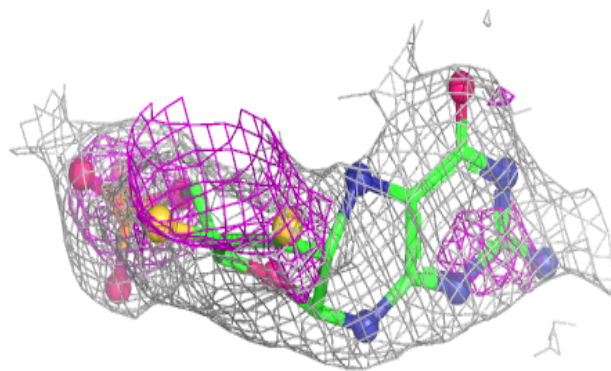
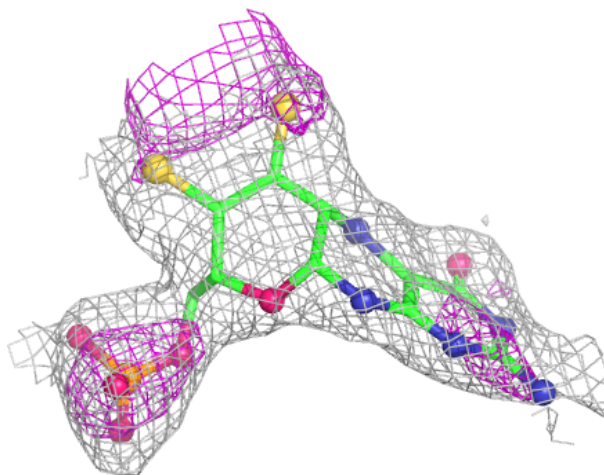
**Electron density around FAD D 5003:**

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



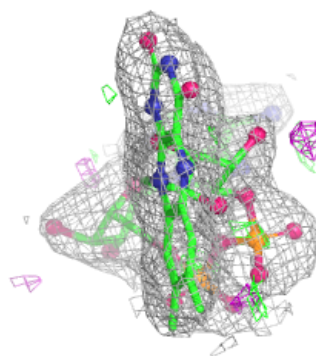
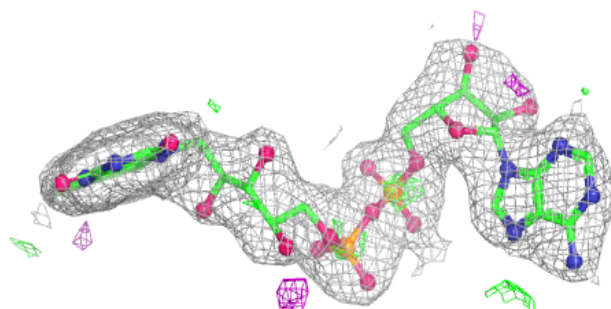
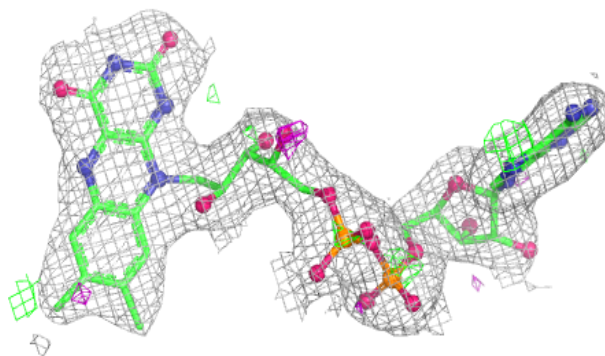
Electron density around MTE A 2004:

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

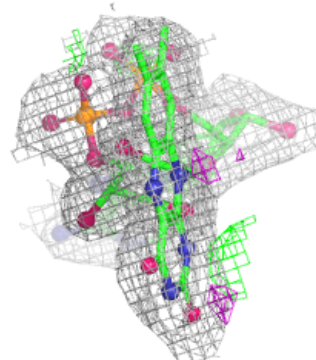
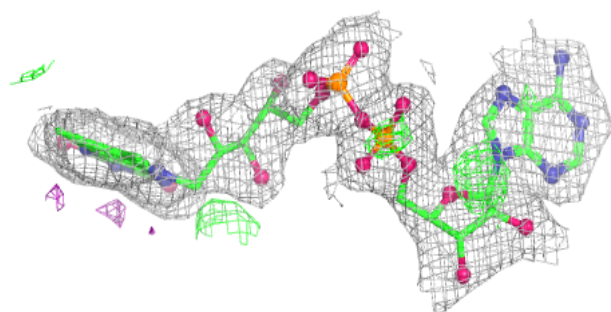
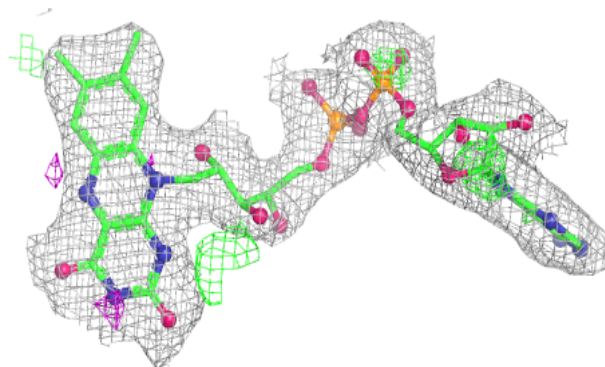


Electron density around FAD A 3003:

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

**Electron density around FAD B 3003:**

$2mF_o-DF_c$ (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.