



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:55 AM UTC

PDB ID : 2W3S / pdb_00002w3s
Title : Crystal Structure of Xanthine Dehydrogenase (desulfo form) from Rhodobacter capsulatus in Complex with Xanthine
Authors : Dietzel, U.; Kuper, J.; Leimkuhler, S.; Kisker, C.
Deposited on : 2008-11-14
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

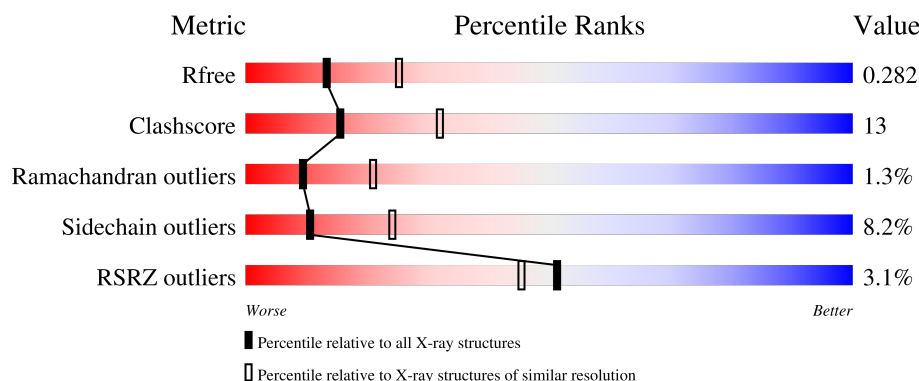
1 Overall quality at a glance

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.



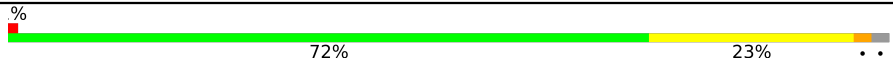
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	462	7% 58% 35% • •
1	C	462	8% 77% 18% • •
1	E	462	6% 63% 30% • •
1	G	462	7% 57% 35% 5% •
2	B	777	70% 24% • •

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Mol	Chain	Length	Quality of chain
2	D	777	
2	F	777	
2	H	777	

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
5	MTE	B	1778	X	-	-	-
5	MTE	D	1778	X	-	-	-
5	MTE	F	1778	X	-	-	-
5	MTE	H	1778	X	-	-	-
8	MOM	B	1781	-	-	X	-
8	MOM	D	1781	-	-	X	-
8	MOM	F	1781	-	-	X	-
8	MOM	H	1781	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 36858 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	450	Total	C	N	O	S	0	0	0
			3376	2115	608	628	25			
1	C	450	Total	C	N	O	S	0	0	0
			3376	2115	608	628	25			
1	E	450	Total	C	N	O	S	0	0	0
			3376	2115	608	628	25			
1	G	450	Total	C	N	O	S	0	0	0
			3376	2115	608	628	25			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	TRP	LEU	conflict	UNP O54050
C	26	TRP	LEU	conflict	UNP O54050
E	26	TRP	LEU	conflict	UNP O54050
G	26	TRP	LEU	conflict	UNP O54050

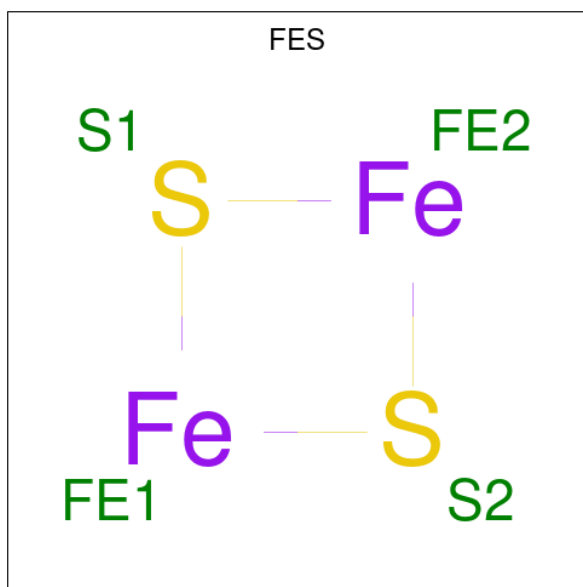
- Molecule 2 is a protein called XANTHINE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	760	Total	C	N	O	S	0	0	0
			5717	3581	1056	1054	26			
2	D	760	Total	C	N	O	S	0	0	0
			5717	3581	1056	1054	26			
2	F	760	Total	C	N	O	S	0	0	0
			5717	3581	1056	1054	26			
2	H	760	Total	C	N	O	S	0	0	0
			5717	3581	1056	1054	26			

There are 4 discrepancies between the modelled and reference sequences:

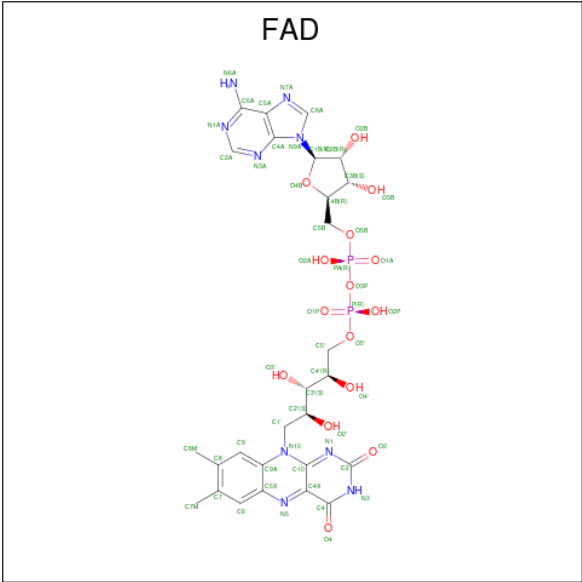
Chain	Residue	Modelled	Actual	Comment	Reference
B	772	ARG	GLY	conflict	UNP O54051
D	772	ARG	GLY	conflict	UNP O54051
F	772	ARG	GLY	conflict	UNP O54051
H	772	ARG	GLY	conflict	UNP O54051

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



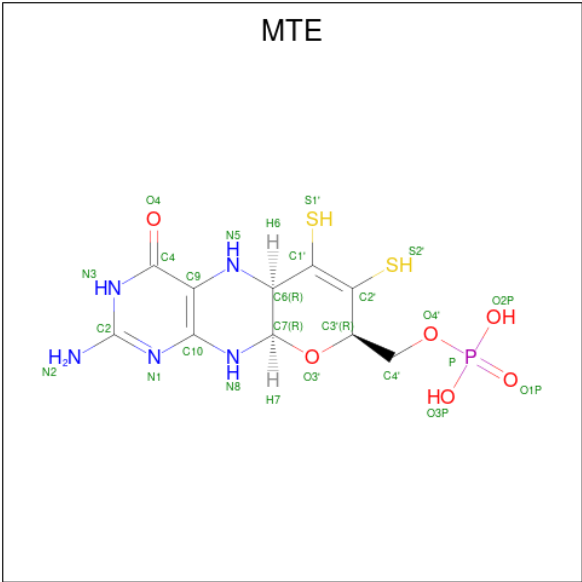
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	C	1	Total	Fe	S	0	0
			4	2	2		
3	C	1	Total	Fe	S	0	0
			4	2	2		
3	E	1	Total	Fe	S	0	0
			4	2	2		
3	E	1	Total	Fe	S	0	0
			4	2	2		
3	G	1	Total	Fe	S	0	0
			4	2	2		
3	G	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	G	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 5 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).

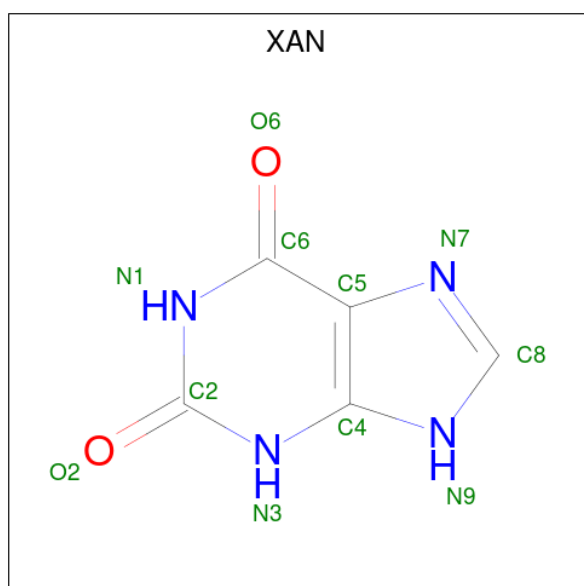


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	S	
			24	10	5	6	1	2	0
5	D	1	Total	C	N	O	P	S	
			24	10	5	6	1	2	0
5	F	1	Total	C	N	O	P	S	
			24	10	5	6	1	2	0
5	H	1	Total	C	N	O	P	S	
			24	10	5	6	1	2	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Ca	0	0
			1	1		
6	D	1	Total	Ca	0	0
			1	1		
6	F	1	Total	Ca	0	0
			1	1		
6	H	1	Total	Ca	0	0
			1	1		

- Molecule 7 is XANTHINE (CCD ID: XAN) (formula: C₅H₄N₄O₂).



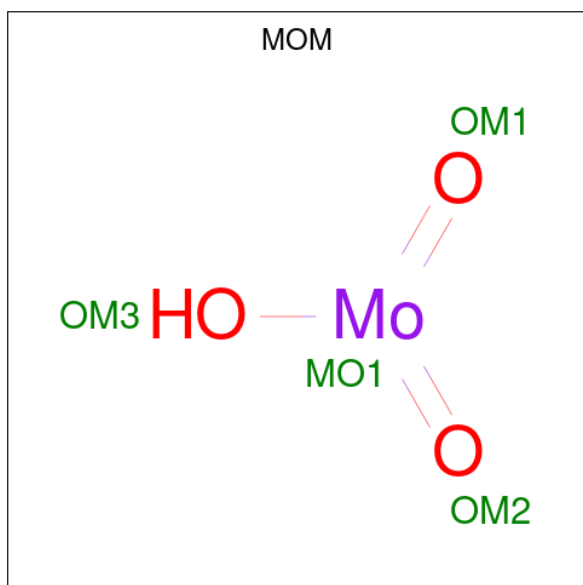
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O		
			22	10	8	4	0	1
7	D	1	Total	C	N	O		
			22	10	8	4	0	1

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	F	1	Total	C	N	O	0	1
			22	10	8	4		
7	H	1	Total	C	N	O	0	1
			22	10	8	4		

- Molecule 8 is HYDROXY(DIOXO)MOLYBDENUM (CCD ID: MOM) (formula: HMoO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Mo	O	0	0
			4	1	3		
8	D	1	Total	Mo	O	0	0
			4	1	3		
8	F	1	Total	Mo	O	0	0
			4	1	3		
8	H	1	Total	Mo	O	0	0
			4	1	3		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	3	Total	O	0	0
			3	3		
9	B	9	Total	O	0	0
			9	9		
9	C	4	Total	O	0	0
			4	4		

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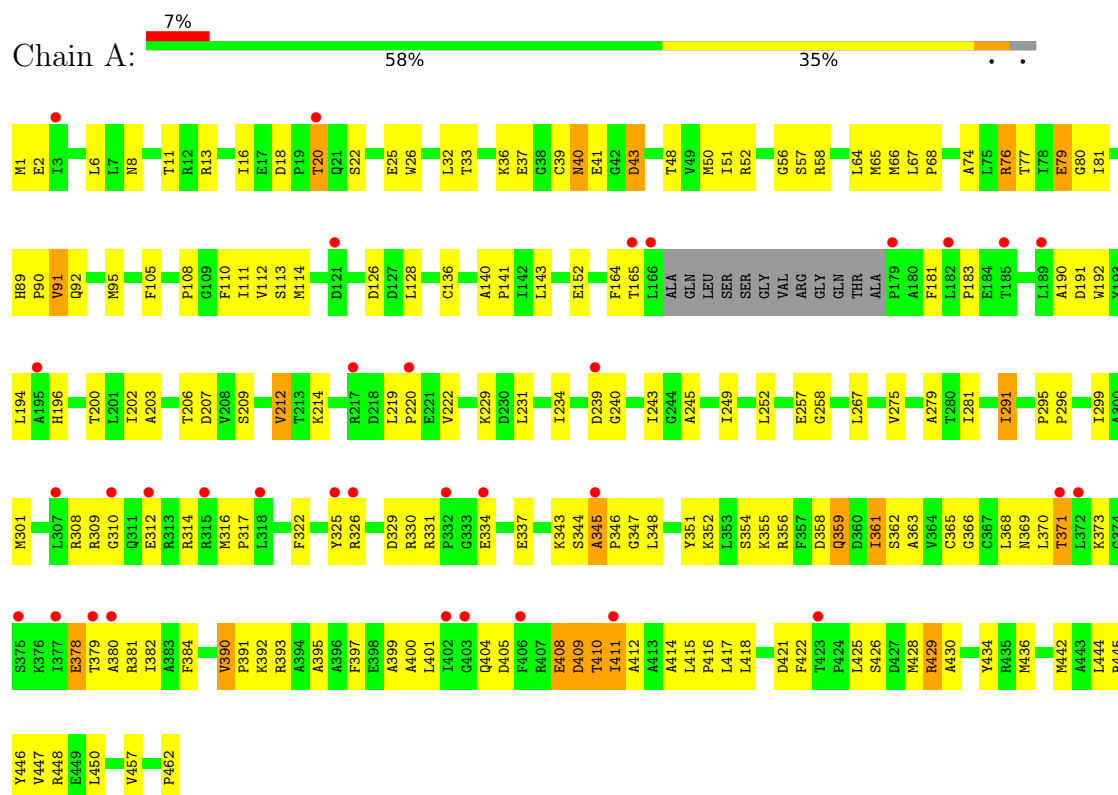
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	7	Total 7	O 7	0	0
9	E	2	Total 2	O 2	0	0
9	F	6	Total 6	O 6	0	0
9	H	7	Total 7	O 7	0	0

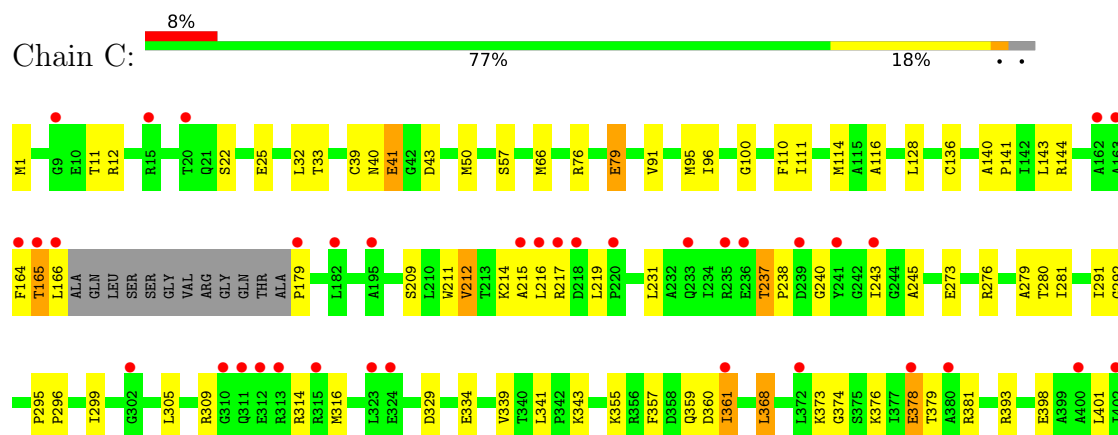
3 Residue-property plots

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

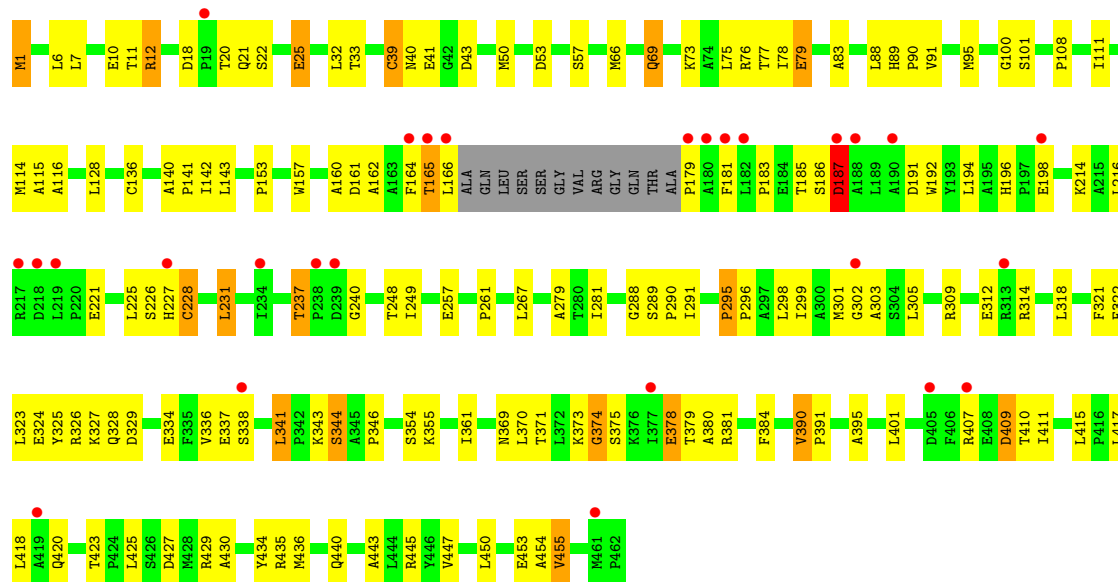


• Molecule 1: XANTHINE DEHYDROGENASE

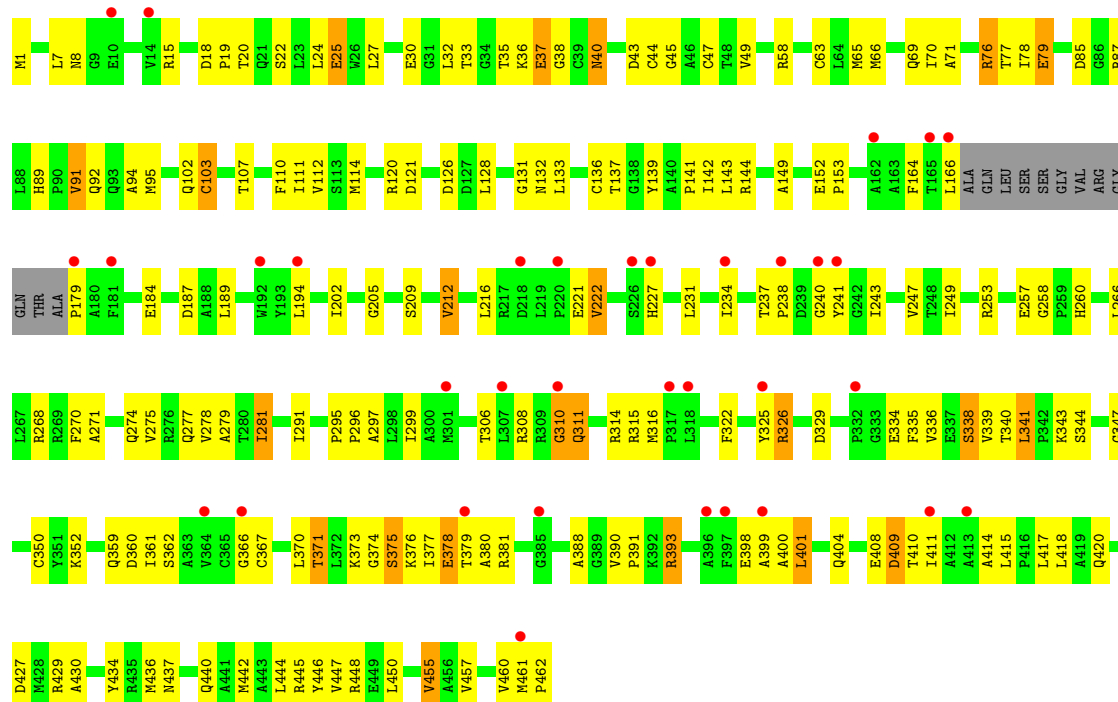




• Molecule 1: XANTHINE DEHYDROGENASE

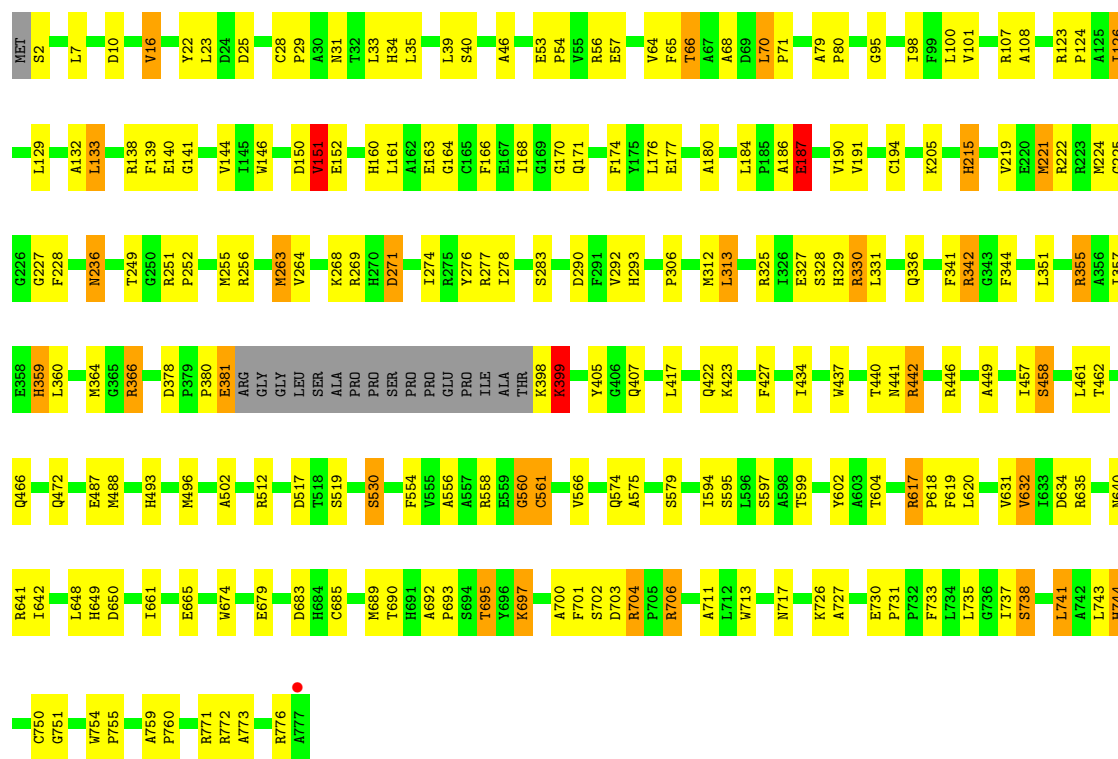


• Molecule 1: XANTHINE DEHYDROGENASE



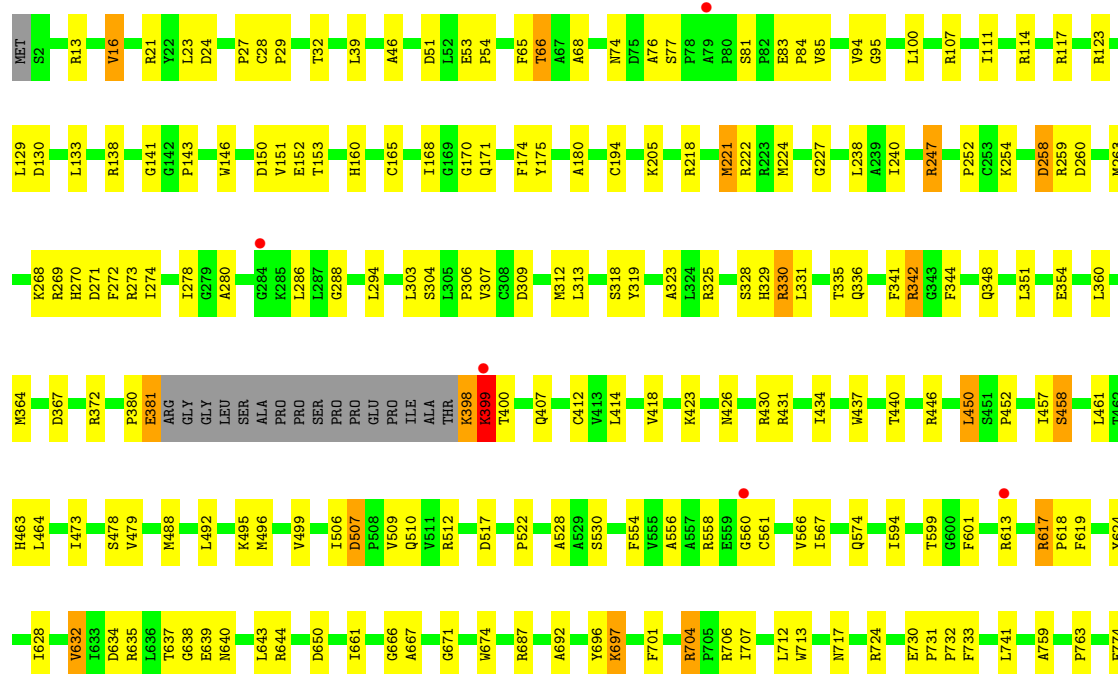
• Molecule 2: XANTHINE DEHYDROGENASE

Chain B: 



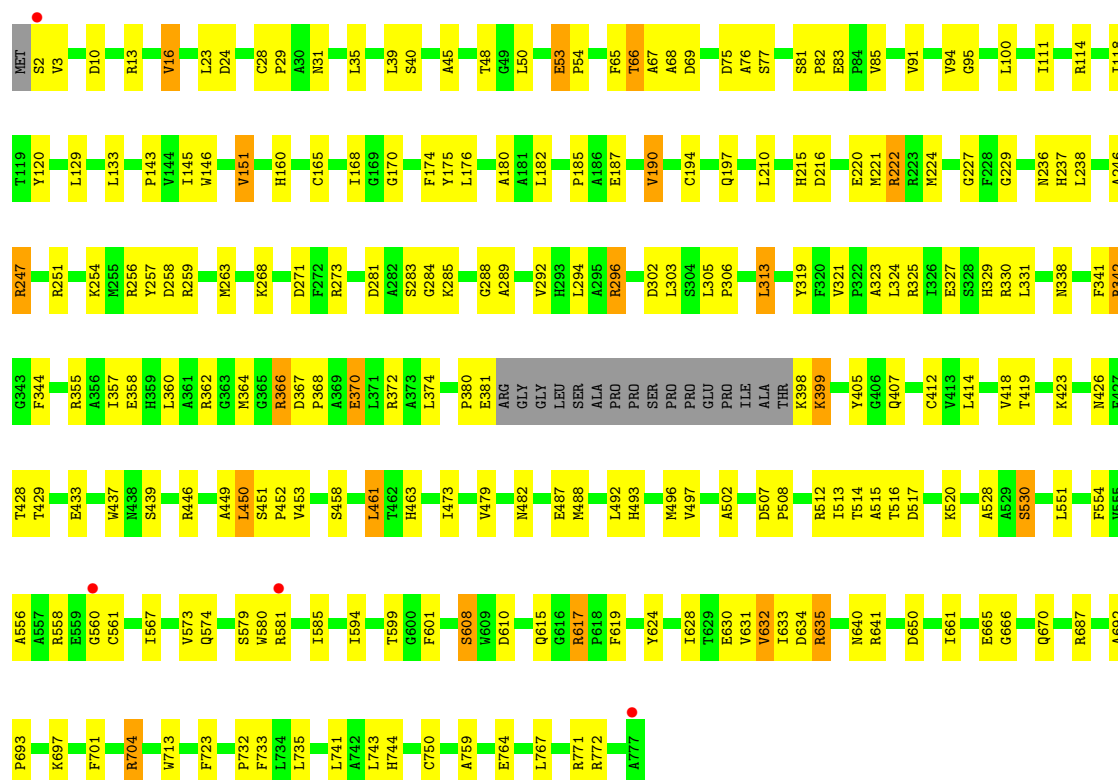
• Molecule 2: XANTHINE DEHYDROGENASE

Chain D: 

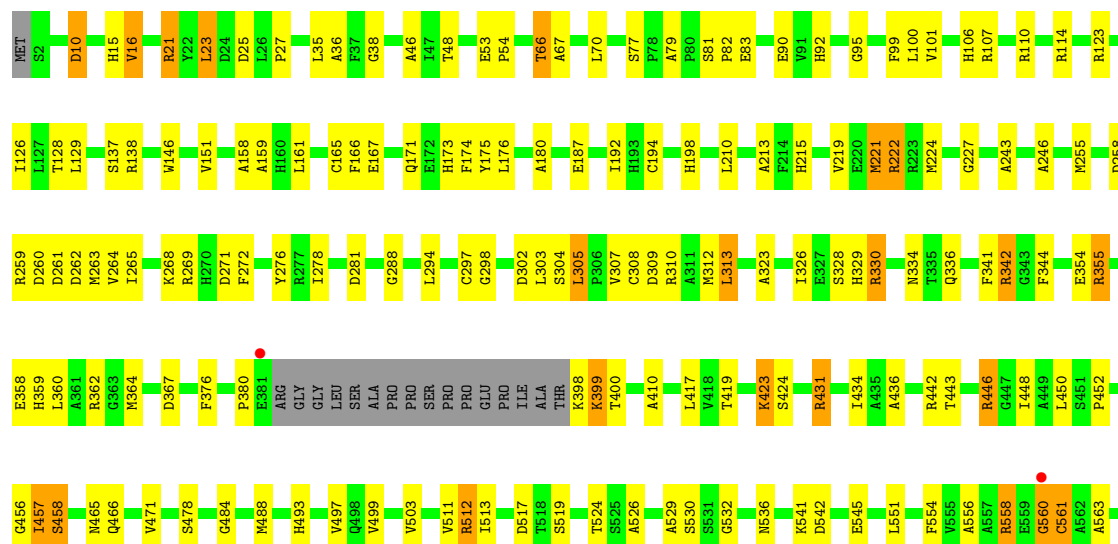


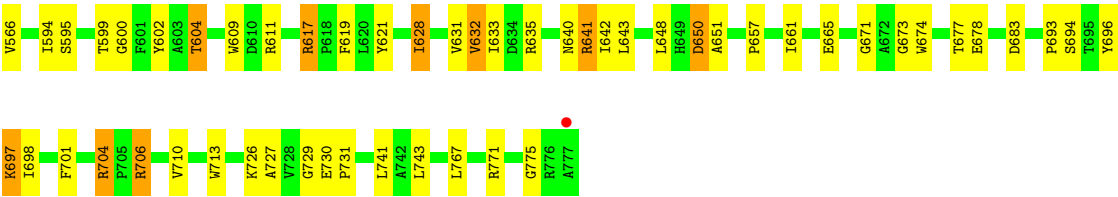


- Molecule 2: XANTHINE DEHYDROGENASE



- Molecule 2: XANTHINE DEHYDROGENASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	92.83Å 140.56Å 158.17Å 109.60° 105.89° 101.18°	Depositor
Resolution (Å)	50.12 – 2.60 50.12 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.7 (50.12-2.60) 97.7 (50.12-2.60)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0055	Depositor
R, R_{free}	0.232 , 0.284 0.234 , 0.282	Depositor DCC
R_{free} test set	10343 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	41.5	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 55.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	36858	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.63	0/3439	0.96	5/4659 (0.1%)
1	C	0.66	0/3439	0.92	1/4659 (0.0%)
1	E	0.63	0/3439	0.94	4/4659 (0.1%)
1	G	0.69	0/3439	1.01	8/4659 (0.2%)
2	B	0.71	0/5845	0.98	10/7942 (0.1%)
2	D	0.74	0/5845	0.97	2/7942 (0.0%)
2	F	0.75	0/5845	1.01	7/7942 (0.1%)
2	H	0.71	0/5845	0.96	7/7942 (0.1%)
All	All	0.70	0/37136	0.97	44/50404 (0.1%)

There are no bond length outliers.

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	107	THR	CA-C-N	-6.97	111.31	119.05
1	G	107	THR	C-N-CA	-6.97	111.31	119.05
2	B	462	THR	N-CA-C	6.88	118.44	111.07
1	A	258	GLY	CA-C-N	6.27	125.76	119.24
1	A	258	GLY	C-N-CA	6.27	125.76	119.24
2	F	81	SER	CA-C-N	6.20	127.59	119.84
2	F	81	SER	C-N-CA	6.20	127.59	119.84
2	H	457	ILE	N-CA-C	5.94	116.48	108.17
1	A	363	ALA	N-CA-C	-5.92	104.91	111.36
2	H	305	LEU	CA-C-N	-5.75	113.09	119.19
2	H	305	LEU	C-N-CA	-5.75	113.09	119.19
1	A	344	SER	N-CA-C	5.71	117.20	108.52
1	G	153	PRO	CA-C-N	5.67	126.93	119.84
1	G	153	PRO	C-N-CA	5.67	126.93	119.84
1	C	43	ASP	N-CA-C	5.63	118.61	111.69
2	B	70	LEU	CA-C-N	5.61	125.07	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	70	LEU	C-N-CA	5.61	125.07	119.24
1	G	260	HIS	N-CA-C	5.51	116.70	108.76
1	A	229	LYS	N-CA-C	5.50	117.98	111.33
2	D	507	ASP	CA-C-N	5.46	125.81	119.47
2	D	507	ASP	C-N-CA	5.46	125.81	119.47
2	F	632	VAL	CB-CA-C	-5.43	102.55	110.81
1	G	258	GLY	CA-C-N	5.39	125.72	119.47
1	G	258	GLY	C-N-CA	5.39	125.72	119.47
2	H	10	ASP	N-CA-C	5.38	118.63	111.75
2	B	378	ASP	CA-C-N	5.35	125.89	120.38
2	B	378	ASP	C-N-CA	5.35	125.89	120.38
2	F	190	VAL	CB-CA-C	-5.35	102.58	110.82
2	B	640	ASN	N-CA-C	5.35	116.66	108.42
1	E	384	PHE	N-CA-C	5.33	117.77	108.76
2	H	246	ALA	N-CA-C	-5.28	105.43	111.07
2	F	229	GLY	N-CA-C	-5.21	108.49	114.69
2	F	237	HIS	N-CA-C	5.17	116.60	111.07
2	B	236	ASN	N-CA-C	5.16	117.30	111.11
2	B	151	VAL	CB-CA-C	-5.16	105.28	111.88
2	H	79	ALA	CA-C-N	5.13	126.25	119.84
2	H	79	ALA	C-N-CA	5.13	126.25	119.84
1	E	153	PRO	CA-C-N	5.11	125.05	119.78
1	E	153	PRO	C-N-CA	5.11	125.05	119.78
1	G	344	SER	N-CA-C	5.08	116.79	109.07
2	B	7	LEU	CA-C-N	5.06	125.07	120.21
2	B	7	LEU	C-N-CA	5.06	125.07	120.21
2	F	75	ASP	N-CA-C	5.02	116.23	107.49
1	E	295	PRO	N-CA-C	5.02	116.82	110.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3376	0	3367	140	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3376	0	3367	61	0
1	E	3376	0	3367	107	0
1	G	3376	0	3367	132	0
2	B	5717	0	5631	168	0
2	D	5717	0	5631	135	0
2	F	5717	0	5631	148	0
2	H	5717	0	5630	150	0
3	A	8	0	0	1	0
3	C	8	0	0	0	0
3	E	8	0	0	0	0
3	G	8	0	0	1	0
4	A	53	0	31	6	0
4	C	53	0	31	4	0
4	E	53	0	31	3	0
4	G	53	0	31	3	0
5	B	24	0	8	0	0
5	D	24	0	9	1	0
5	F	24	0	8	2	0
5	H	24	0	8	3	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
6	H	1	0	0	0	0
7	B	22	0	8	0	0
7	D	22	0	8	3	0
7	F	22	0	8	0	0
7	H	22	0	8	0	0
8	B	4	0	0	2	0
8	D	4	0	0	5	0
8	F	4	0	0	2	0
8	H	4	0	0	2	0
9	A	3	0	0	0	0
9	B	9	0	0	0	0
9	C	4	0	0	0	0
9	D	7	0	0	0	0
9	E	2	0	0	0	0
9	F	6	0	0	0	0
9	H	7	0	0	0	0
All	All	36858	0	36180	978	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (978) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:247:ARG:HG2	2:F:247:ARG:HH11	1.11	1.07
1:G:240:GLY:HA2	1:G:343:LYS:HG2	1.34	1.04
1:A:240:GLY:HA2	1:A:343:LYS:HG2	1.41	1.03
1:G:361:ILE:HD11	1:G:429:ARG:NH2	1.75	1.01
2:D:247:ARG:HG2	2:D:247:ARG:HH11	1.27	1.00
2:D:446:ARG:HD3	2:D:632:VAL:HG13	1.44	0.99
1:G:24:LEU:HD21	1:G:37:GLU:HG3	1.42	0.97
1:C:291:ILE:HD13	1:C:361:ILE:HD12	1.45	0.97
1:A:426:SER:H	2:F:574:GLN:HE22	1.15	0.94
1:G:18:ASP:OD2	1:G:20:THR:HG22	1.67	0.94
2:H:701:PHE:O	2:H:704:ARG:HG2	1.73	0.89
1:G:58:ARG:HD3	1:G:277:GLN:OE1	1.72	0.88
1:C:240:GLY:HA2	1:C:343:LYS:HG2	1.55	0.88
2:F:221:MET:HE2	2:F:224:MET:HE2	1.56	0.88
2:D:280:ALA:HB3	2:D:364:MET:HE1	1.55	0.87
2:F:247:ARG:HG2	2:F:247:ARG:NH1	1.89	0.87
1:C:216:LEU:HD12	2:D:114:ARG:NH1	1.90	0.86
2:B:690:THR:HA	2:B:695:THR:OG1	1.76	0.86
2:B:126:ILE:HD12	2:B:126:ILE:N	1.89	0.86
1:A:345:ALA:HB3	1:A:346:PRO:HA	1.57	0.86
1:A:361:ILE:HG12	1:A:429:ARG:CZ	2.06	0.85
2:F:221:MET:HE1	2:F:224:MET:HG3	1.61	0.83
7:D:1780[A]:XAN:H8	8:D:1781:MOM:OM2	1.79	0.82
2:D:247:ARG:HG2	2:D:247:ARG:NH1	1.83	0.82
2:F:174:PHE:HZ	2:F:693:PRO:HG3	1.44	0.82
1:E:370:LEU:HD22	1:E:380:ALA:HA	1.63	0.81
2:H:259:ARG:HG3	2:H:263:MET:HE2	1.63	0.81
2:D:360:LEU:HG	2:D:364:MET:HE3	1.64	0.80
1:G:444:LEU:O	1:G:448:ARG:HG3	1.80	0.80
2:H:360:LEU:HG	2:H:364:MET:HE2	1.64	0.79
1:E:12:ARG:HH11	1:E:12:ARG:HG2	1.46	0.79
2:F:66:THR:HG22	2:F:68:ALA:H	1.48	0.79
1:C:279:ALA:HB1	4:C:1465:FAD:H4'	1.65	0.78
2:F:23:LEU:HD13	2:F:194:CYS:HA	1.66	0.78
1:A:190:ALA:HB1	1:A:310:GLY:HA2	1.66	0.78
2:D:380:PRO:O	2:D:381:GLU:HB2	1.83	0.78
2:F:305:LEU:HB3	2:F:306:PRO:HD3	1.65	0.78
1:G:361:ILE:HD11	1:G:429:ARG:HH21	1.47	0.78
1:A:279:ALA:HB1	4:A:1465:FAD:H4'	1.67	0.77
2:F:77:SER:HB2	2:F:83:GLU:HB3	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:MET:HE2	1:C:114:MET:HE1	1.67	0.76
1:E:7:LEU:HD12	1:E:75:LEU:HD23	1.66	0.76
2:F:341:PHE:HD2	2:F:342:ARG:N	1.82	0.76
2:B:263:MET:HE3	2:B:692:ALA:HA	1.67	0.75
2:D:247:ARG:HH11	2:D:247:ARG:CG	1.99	0.75
2:D:66:THR:HG22	2:D:68:ALA:H	1.49	0.75
2:H:276:TYR:OH	2:H:359:HIS:HD2	1.69	0.75
2:D:221:MET:HE2	2:D:224:MET:HE2	1.68	0.75
1:C:32:LEU:HD22	1:C:79:GLU:HG3	1.69	0.74
2:B:138:ARG:NH2	2:B:329:HIS:ND1	2.32	0.74
1:E:95:MET:HE2	1:E:114:MET:HE1	1.69	0.74
1:A:347:GLY:O	1:A:446:TYR:OH	2.05	0.74
1:G:279:ALA:HB1	4:G:1465:FAD:H4'	1.70	0.74
2:H:450:LEU:HD12	2:H:628:ILE:HD11	1.69	0.74
1:C:216:LEU:HD12	2:D:114:ARG:HH11	1.53	0.74
1:E:7:LEU:CD1	1:E:75:LEU:HD23	2.18	0.73
1:G:110:PHE:O	1:G:114:MET:HG3	1.88	0.73
2:B:560:GLY:O	2:B:561:CYS:HB3	1.86	0.73
1:G:266:LEU:HD13	1:G:350:CYS:HB3	1.71	0.73
2:F:701:PHE:O	2:F:704:ARG:HG2	1.88	0.73
1:A:371:THR:OG1	1:A:379:THR:HB	1.89	0.72
1:C:462:PRO:HA	2:D:643:LEU:HD22	1.72	0.72
1:A:330:ARG:HH21	4:A:1465:FAD:H2A	1.54	0.72
2:F:473:ILE:HG12	2:F:479:VAL:HG22	1.71	0.72
1:G:352:LYS:HG3	1:G:362:SER:HB3	1.72	0.72
1:E:323:LEU:HD21	1:E:329:ASP:HB2	1.71	0.71
2:F:599:THR:HG23	2:H:599:THR:HG23	1.71	0.71
2:B:35:LEU:HB2	2:B:255:MET:HB2	1.71	0.71
1:C:41:GLU:HG3	1:C:214:LYS:HE3	1.72	0.71
1:A:202:ILE:HD13	1:A:222:VAL:HG13	1.72	0.71
2:F:341:PHE:HD2	2:F:342:ARG:H	1.37	0.71
1:G:445:ARG:HG3	1:G:455:VAL:HG11	1.71	0.71
1:G:143:LEU:C	1:G:143:LEU:HD23	2.15	0.71
2:B:221:MET:HE2	2:B:224:MET:HE2	1.73	0.71
2:H:221:MET:HE2	2:H:224:MET:HE2	1.72	0.71
1:G:65:MET:HE1	1:G:278:VAL:HG11	1.73	0.71
4:A:1465:FAD:N1	4:A:1465:FAD:H2'	2.06	0.70
2:B:351:LEU:HD13	2:B:737:ILE:HG12	1.74	0.70
1:E:279:ALA:HB1	4:E:1465:FAD:H4'	1.72	0.70
2:F:174:PHE:CZ	2:F:693:PRO:HG3	2.26	0.70
2:D:53:GLU:HB3	2:D:54:PRO:HD3	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:174:PHE:HZ	2:H:693:PRO:HG3	1.56	0.70
1:E:95:MET:HE2	1:E:114:MET:CE	2.21	0.70
1:A:322:PHE:HB3	1:A:390:VAL:CG2	2.21	0.69
1:G:1:MET:HB2	1:G:179:PRO:HG3	1.71	0.69
1:E:445:ARG:NH2	2:F:634:ASP:OD2	2.25	0.69
1:C:50:MET:HE3	1:C:116:ALA:HA	1.75	0.69
1:G:216:LEU:HD12	2:H:114:ARG:NH1	2.08	0.68
1:C:110:PHE:HB3	1:C:114:MET:HE2	1.74	0.68
1:G:322:PHE:HB3	1:G:390:VAL:HG23	1.76	0.68
2:H:354:GLU:HA	2:H:354:GLU:OE1	1.93	0.68
2:B:23:LEU:HD13	2:B:194:CYS:HA	1.76	0.68
2:B:126:ILE:N	2:B:126:ILE:CD1	2.57	0.68
2:B:292:VAL:HG22	2:B:327:GLU:HB3	1.75	0.68
1:G:347:GLY:O	1:G:446:TYR:OH	2.10	0.68
2:H:23:LEU:HD22	2:H:180:ALA:HB1	1.76	0.68
2:D:168:ILE:HD13	2:D:351:LEU:HD23	1.75	0.68
1:A:345:ALA:CB	1:A:346:PRO:HA	2.24	0.67
2:B:66:THR:HG22	2:B:68:ALA:H	1.59	0.67
2:D:701:PHE:O	2:D:704:ARG:HG2	1.94	0.67
2:D:138:ARG:NH2	2:D:329:HIS:ND1	2.41	0.67
1:E:95:MET:HE1	1:E:142:ILE:HG12	1.77	0.67
2:F:360:LEU:HG	2:F:364:MET:HE3	1.77	0.67
1:G:253:ARG:NH2	1:G:268:ARG:HG3	2.10	0.67
2:H:541:LYS:O	2:H:545:GLU:HG3	1.95	0.67
1:A:202:ILE:CD1	1:A:222:VAL:HG13	2.25	0.67
2:H:259:ARG:HG3	2:H:263:MET:CE	2.23	0.67
1:G:322:PHE:HB3	1:G:390:VAL:CG2	2.25	0.66
1:A:41:GLU:HG3	1:A:214:LYS:HE3	1.76	0.66
2:B:751:GLY:HA3	2:B:773:ALA:O	1.95	0.66
2:B:39:LEU:HD22	2:B:95:GLY:O	1.96	0.66
1:C:360:ASP:OD1	2:D:697:LYS:HE3	1.96	0.66
1:C:445:ARG:NH2	2:D:634:ASP:OD2	2.28	0.66
2:D:218:ARG:NH2	2:D:517:ASP:OD1	2.29	0.66
2:D:288:GLY:HA2	2:D:323:ALA:O	1.96	0.66
2:H:665:GLU:HG2	2:H:710:VAL:HG21	1.78	0.65
1:C:291:ILE:CD1	1:C:361:ILE:HD12	2.25	0.65
2:F:263:MET:HE3	2:F:692:ALA:HA	1.78	0.65
2:H:138:ARG:NH2	2:H:329:HIS:ND1	2.44	0.65
1:A:390:VAL:HG22	1:A:391:PRO:HD2	1.78	0.65
1:G:390:VAL:HG22	1:G:391:PRO:HD2	1.78	0.65
1:A:181:PHE:CZ	1:A:183:PRO:HB3	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:LEU:O	1:A:231:LEU:HD23	1.96	0.65
2:D:556:ALA:HB1	2:D:561:CYS:O	1.96	0.65
2:D:635:ARG:NH1	2:D:774:GLU:OE2	2.26	0.65
2:B:599:THR:HG23	2:D:599:THR:HG23	1.79	0.65
2:D:77:SER:HB2	2:D:83:GLU:HB3	1.77	0.65
2:F:281:ASP:HB2	2:F:285:LYS:H	1.61	0.65
1:G:360:ASP:OD1	2:H:697:LYS:HE3	1.96	0.65
1:A:206:THR:HG21	1:A:275:VAL:HG13	1.79	0.65
1:A:428:MET:HE3	1:A:428:MET:H	1.60	0.65
2:F:617:ARG:HD3	2:F:619:PHE:O	1.96	0.65
2:H:450:LEU:HD12	2:H:628:ILE:CD1	2.27	0.64
1:G:89:HIS:ND1	1:G:91:VAL:HB	2.12	0.64
2:D:76:ALA:HB2	2:D:85:VAL:HG22	1.79	0.64
2:D:205:LYS:HB3	2:D:240:ILE:HD11	1.80	0.64
2:H:23:LEU:HD13	2:H:194:CYS:HA	1.80	0.64
2:H:560:GLY:O	2:H:561:CYS:HB3	1.96	0.64
1:C:407:ARG:HD2	1:C:409:ASP:OD2	1.98	0.64
1:A:2:GLU:OE1	1:A:13:ARG:HG2	1.98	0.64
2:F:507:ASP:OD1	2:F:508:PRO:HD2	1.98	0.64
2:B:129:LEU:HD12	2:B:129:LEU:H	1.63	0.63
2:D:146:TRP:O	2:D:325:ARG:HG3	1.99	0.63
2:D:270:HIS:NE2	2:D:304:SER:OG	2.31	0.63
1:E:111:ILE:HD11	2:F:16:VAL:CG2	2.29	0.63
1:C:50:MET:HE2	1:C:57:SER:HB2	1.80	0.63
2:H:556:ALA:HB2	2:H:563:ALA:HA	1.81	0.63
2:D:496:MET:HA	2:D:496:MET:HE2	1.81	0.63
1:G:297:ALA:HA	1:G:367:CYS:SG	2.38	0.63
2:H:360:LEU:HG	2:H:364:MET:CE	2.27	0.63
1:E:228:CYS:SG	1:E:231:LEU:HB2	2.39	0.63
1:A:252:LEU:HD22	1:A:281:ILE:HG21	1.81	0.63
8:F:1781:MOM:OM1	8:F:1781:MOM:MO1	1.70	0.63
2:D:617:ARG:HD3	2:D:619:PHE:O	1.99	0.62
2:B:556:ALA:HB1	2:B:561:CYS:O	2.00	0.62
1:E:361:ILE:HD11	1:E:429:ARG:NH1	2.14	0.62
1:G:299:ILE:O	1:G:381:ARG:NH1	2.33	0.62
2:D:554:PHE:HB2	2:D:594:ILE:HD13	1.80	0.62
1:A:426:SER:H	2:F:574:GLN:NE2	1.92	0.62
2:B:126:ILE:HD12	2:B:126:ILE:H	1.65	0.62
7:D:1780[A]:XAN:C8	8:D:1781:MOM:OM2	2.46	0.62
1:G:326:ARG:HG2	1:G:326:ARG:HH11	1.63	0.62
2:H:46:ALA:HB2	2:H:123:ARG:NH2	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:CYS:HB2	3:A:1463:FES:S2	2.40	0.61
8:D:1781:MOM:OM1	8:D:1781:MOM:MO1	1.70	0.61
2:F:633:ILE:HG22	2:F:640:ASN:HB3	1.82	0.61
2:H:77:SER:HB2	2:H:83:GLU:HB3	1.82	0.61
1:A:352:LYS:HG3	1:A:362:SER:OG	2.00	0.61
2:F:160:HIS:HB3	2:F:364:MET:HE2	1.82	0.61
8:F:1781:MOM:MO1	8:F:1781:MOM:OM3	1.71	0.61
1:A:66:MET:HE3	1:A:209:SER:HB3	1.82	0.61
1:C:373:LYS:HB2	1:C:378:GLU:CG	2.31	0.61
2:B:755:PRO:O	2:B:772:ARG:HD2	2.01	0.61
8:B:1781:MOM:MO1	8:B:1781:MOM:OM3	1.71	0.61
2:H:146:TRP:CZ3	2:H:313:LEU:HD13	2.35	0.61
1:A:8:ASN:HA	1:A:76:ARG:HD2	1.81	0.60
1:E:88:LEU:HD21	2:F:13:ARG:NH1	2.16	0.60
1:A:445:ARG:NH2	2:B:634:ASP:OD1	2.34	0.60
2:B:380:PRO:O	2:B:381:GLU:HB2	2.01	0.60
2:B:160:HIS:HB3	2:B:364:MET:CE	2.30	0.60
8:D:1781:MOM:MO1	8:D:1781:MOM:OM3	1.72	0.60
2:H:192:ILE:HB	2:H:219:VAL:HG22	1.84	0.60
2:B:46:ALA:HB2	2:B:123:ARG:NH2	2.17	0.60
2:D:407:GLN:OE1	2:D:618:PRO:HD2	2.01	0.60
1:A:32:LEU:HD22	1:A:79:GLU:HG3	1.84	0.60
1:G:24:LEU:CD2	1:G:37:GLU:HG3	2.23	0.60
1:E:370:LEU:HD22	1:E:380:ALA:CA	2.31	0.60
8:H:1781:MOM:MO1	8:H:1781:MOM:OM3	1.71	0.60
2:B:560:GLY:O	2:B:561:CYS:CB	2.50	0.59
1:G:43:ASP:HB3	2:H:693:PRO:HB2	1.84	0.59
8:H:1781:MOM:MO1	8:H:1781:MOM:OM1	1.72	0.59
2:H:198:HIS:ND1	2:H:526:ALA:HB2	2.17	0.59
2:D:23:LEU:HD22	2:D:180:ALA:HB1	1.82	0.59
2:H:657:PRO:O	2:H:661:ILE:HG12	2.00	0.59
2:B:53:GLU:HG3	2:B:57:GLU:OE2	2.02	0.59
2:B:635:ARG:HD3	2:B:750:CYS:SG	2.42	0.59
1:E:355:LYS:NZ	1:E:429:ARG:HA	2.18	0.59
2:D:446:ARG:HD3	2:D:632:VAL:CG1	2.24	0.59
2:D:507:ASP:OD1	2:D:509:VAL:HG23	2.02	0.59
1:A:11:THR:HG22	1:A:164:PHE:HE1	1.67	0.59
2:B:617:ARG:HD3	2:B:619:PHE:O	2.03	0.59
8:B:1781:MOM:MO1	8:B:1781:MOM:OM1	1.73	0.59
1:A:347:GLY:O	1:A:369:ASN:HA	2.03	0.59
1:E:1:MET:HB3	1:E:179:PRO:HG2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:SER:OG	1:A:25:GLU:OE1	2.20	0.58
1:E:50:MET:HE2	1:E:57:SER:HB2	1.85	0.58
2:F:170:GLY:N	2:F:271:ASP:HB3	2.18	0.58
2:F:221:MET:CE	2:F:224:MET:HG3	2.32	0.58
1:A:1:MET:HE2	1:A:16:ILE:HD12	1.86	0.58
1:A:330:ARG:NH2	4:A:1465:FAD:H2A	2.18	0.58
1:G:359:GLN:HE22	4:G:1465:FAD:H6	1.67	0.58
1:E:291:ILE:HD13	1:E:361:ILE:HD12	1.85	0.58
1:E:355:LYS:HZ2	1:E:429:ARG:HA	1.68	0.58
2:F:210:LEU:HD22	2:F:247:ARG:HD3	1.86	0.58
1:G:326:ARG:HG2	1:G:326:ARG:NH1	2.16	0.58
2:H:530:SER:HA	5:H:1778:MTE:C4'	2.33	0.58
1:A:18:ASP:OD2	1:A:20:THR:HG22	2.04	0.58
2:D:171:GLN:NE2	2:D:674:TRP:HB2	2.18	0.58
2:B:224:MET:HE3	2:B:488:MET:HB3	1.85	0.58
1:C:216:LEU:HD13	2:D:111:ILE:HG13	1.85	0.58
2:D:528:ALA:HA	5:D:1778:MTE:S2'	2.43	0.58
2:F:224:MET:HE3	2:F:488:MET:HB3	1.86	0.58
1:C:314:ARG:HD3	1:C:334:GLU:OE1	2.04	0.58
2:D:66:THR:HG22	2:D:68:ALA:N	2.17	0.58
1:G:388:ALA:C	1:G:390:VAL:H	2.12	0.58
2:H:767:LEU:O	2:H:771:ARG:HG3	2.02	0.58
1:A:401:LEU:HD11	1:A:411:ILE:HD13	1.86	0.58
2:B:274:ILE:HG12	2:B:293:HIS:CD2	2.39	0.58
2:F:24:ASP:OD2	2:F:254:LYS:NZ	2.36	0.58
1:A:408:GLU:OE1	2:B:442:ARG:NH2	2.36	0.58
2:B:166:PHE:CZ	2:B:355:ARG:HG3	2.38	0.58
1:C:373:LYS:HB2	1:C:378:GLU:HG2	1.86	0.57
1:A:314:ARG:NH1	1:A:331:ARG:HG2	2.19	0.57
2:F:65:PHE:HB2	2:F:100:LEU:HB3	1.85	0.57
2:D:74:ASN:O	2:D:84:PRO:HA	2.04	0.57
2:F:288:GLY:HA2	2:F:323:ALA:O	2.03	0.57
1:A:89:HIS:ND1	1:A:91:VAL:HB	2.20	0.57
1:A:405:ASP:O	1:A:410:THR:HG21	2.05	0.57
2:B:434:ILE:HG23	2:B:446:ARG:HB2	1.86	0.57
1:E:32:LEU:HD22	1:E:79:GLU:HG3	1.84	0.57
1:G:314:ARG:NH1	1:G:334:GLU:OE2	2.38	0.57
2:H:651:ALA:C	2:H:726:LYS:HB2	2.30	0.57
2:B:163:GLU:HG2	2:B:277:ARG:HG2	1.87	0.57
2:F:487:GLU:HB2	2:F:493:HIS:CD2	2.40	0.57
2:H:92:HIS:O	2:H:334:ASN:HB3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:274:ILE:HG12	2:B:293:HIS:HD2	1.68	0.57
2:H:560:GLY:O	2:H:561:CYS:CB	2.52	0.57
2:H:643:LEU:O	2:H:706:ARG:HB2	2.05	0.57
2:F:28:CYS:HB2	2:F:29:PRO:CD	2.34	0.56
1:A:231:LEU:HD21	1:A:245:ALA:HB3	1.87	0.56
2:F:281:ASP:HB3	2:F:283:SER:H	1.69	0.56
2:F:492:LEU:O	2:F:496:MET:HG2	2.05	0.56
1:G:401:LEU:HD11	1:G:411:ILE:HD13	1.87	0.56
2:B:126:ILE:CD1	2:B:126:ILE:H	2.17	0.56
1:E:374:GLY:O	1:E:375:SER:HB3	2.04	0.56
2:F:530:SER:HA	5:F:1778:MTE:H4'2	1.87	0.56
1:A:322:PHE:HB3	1:A:390:VAL:HG22	1.87	0.56
2:D:273:ARG:HD2	2:D:294:LEU:HD12	1.87	0.56
2:H:650:ASP:HA	2:H:713:TRP:HB3	1.87	0.56
1:A:309:ARG:HB3	1:A:312:GLU:HG3	1.88	0.56
1:A:428:MET:HE2	2:B:689:MET:HB3	1.88	0.56
2:D:160:HIS:HB2	2:D:364:MET:HE2	1.87	0.56
2:B:174:PHE:HZ	2:B:693:PRO:HG3	1.70	0.56
2:F:407:GLN:OE1	2:F:617:ARG:HG2	2.05	0.56
2:F:573:VAL:HG21	2:F:585:ILE:HG13	1.87	0.56
2:F:160:HIS:HB3	2:F:364:MET:CE	2.36	0.56
2:B:163:GLU:CG	2:B:277:ARG:HG2	2.36	0.56
2:F:94:VAL:HG11	2:F:687:ARG:HG2	1.86	0.56
2:F:693:PRO:O	2:F:697:LYS:HE2	2.07	0.56
2:H:530:SER:O	2:H:727:ALA:HB1	2.06	0.56
1:A:325:TYR:O	1:A:326:ARG:HB2	2.06	0.55
2:B:648:LEU:HD12	2:B:711:ALA:O	2.06	0.55
2:D:661:ILE:HD11	2:D:712:LEU:HG	1.87	0.55
1:G:361:ILE:CD1	1:G:429:ARG:NH2	2.60	0.55
1:C:141:PRO:HA	1:C:144:ARG:HH11	1.71	0.55
1:A:351:TYR:CE2	1:A:445:ARG:HD3	2.41	0.55
1:E:53:ASP:HB3	1:E:73:LYS:HD3	1.89	0.55
1:G:247:VAL:HB	1:G:281:ILE:HD11	1.88	0.55
2:H:493:HIS:CG	2:H:513:ILE:HG12	2.42	0.55
1:E:91:VAL:CG1	1:E:114:MET:HE3	2.37	0.55
1:A:322:PHE:CB	1:A:390:VAL:HG22	2.37	0.55
2:B:641:ARG:NH2	2:B:706:ARG:HH12	2.05	0.55
1:E:434:TYR:CD1	2:F:764:GLU:HG3	2.41	0.55
2:F:3:VAL:HG21	2:F:723:PHE:CE1	2.41	0.55
1:G:216:LEU:HD23	2:H:107:ARG:NH1	2.22	0.55
2:H:457:ILE:O	2:H:458:SER:CB	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:LEU:HB2	1:A:446:TYR:CD1	2.41	0.55
1:A:409:ASP:HA	1:A:412:ALA:HB3	1.88	0.55
1:A:418:LEU:HA	1:A:421:ASP:HB2	1.87	0.55
1:A:356:ARG:NH2	1:A:359:GLN:O	2.35	0.55
2:B:150:ASP:OD2	2:F:423:LYS:HE2	2.06	0.55
2:F:581:ARG:HB2	2:F:581:ARG:NH1	2.22	0.55
2:D:205:LYS:HA	2:D:205:LYS:HE2	1.88	0.55
2:D:434:ILE:HG23	2:D:446:ARG:HB2	1.89	0.55
1:E:12:ARG:HH11	1:E:12:ARG:CG	2.19	0.55
2:F:247:ARG:NH1	2:F:247:ARG:CG	2.64	0.55
1:G:85:ASP:OD2	1:G:87:ARG:NH1	2.40	0.55
2:H:303:LEU:O	2:H:307:VAL:HG23	2.07	0.55
1:A:314:ARG:HH12	1:A:331:ARG:HG2	1.71	0.55
2:B:79:ALA:HB1	2:B:80:PRO:HD2	1.88	0.55
2:D:224:MET:HE3	2:D:488:MET:HB3	1.89	0.55
2:F:453:VAL:CG2	2:F:735:LEU:HD23	2.36	0.54
1:A:52:ARG:HA	1:A:56:GLY:O	2.07	0.54
2:D:74:ASN:OD1	2:D:85:VAL:N	2.35	0.54
2:F:496:MET:HE2	2:F:496:MET:HA	1.88	0.54
2:H:633:ILE:HG22	2:H:640:ASN:HB3	1.89	0.54
2:B:23:LEU:HD22	2:B:180:ALA:HB1	1.88	0.54
2:D:263:MET:HE3	2:D:692:ALA:HA	1.89	0.54
1:A:400:ALA:CB	1:A:417:LEU:HD13	2.37	0.54
2:B:701:PHE:O	2:B:704:ARG:HG2	2.07	0.54
2:F:66:THR:H	2:F:69:ASP:HB2	1.72	0.54
2:F:185:PRO:HD3	2:F:246:ALA:HB1	1.89	0.54
1:G:44:CYS:O	1:G:132:ASN:HA	2.07	0.54
1:G:411:ILE:O	1:G:415:LEU:HG	2.08	0.54
2:B:66:THR:HG22	2:B:68:ALA:N	2.22	0.54
1:G:408:GLU:OE1	2:H:442:ARG:NH2	2.41	0.54
1:C:1:MET:HB3	1:C:179:PRO:HG2	1.90	0.54
1:C:111:ILE:HD11	2:D:16:VAL:CG2	2.38	0.54
2:H:173:HIS:HA	2:H:341:PHE:CE1	2.43	0.54
2:H:530:SER:HA	5:H:1778:MTE:H4'2	1.90	0.54
2:B:407:GLN:OE1	2:B:618:PRO:HD2	2.07	0.53
2:D:644:ARG:HG3	2:D:707:ILE:HB	1.88	0.53
1:A:373:LYS:HB2	1:A:378:GLU:HG3	1.90	0.53
2:B:23:LEU:CD1	2:B:194:CYS:HA	2.38	0.53
4:E:1465:FAD:H2'	4:E:1465:FAD:N1	2.23	0.53
1:G:66:MET:HE3	1:G:209:SER:HB3	1.89	0.53
1:G:445:ARG:HG3	1:G:455:VAL:CG1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:160:HIS:HB3	2:B:364:MET:HE2	1.91	0.53
1:C:50:MET:HE2	1:C:57:SER:CB	2.37	0.53
2:H:609:TRP:CZ3	2:H:611:ARG:HA	2.43	0.53
1:A:110:PHE:HB3	1:A:114:MET:HE2	1.90	0.53
2:B:56:ARG:HG2	2:B:64:VAL:HG21	1.91	0.53
2:F:40:SER:HB2	2:F:91:VAL:HG11	1.90	0.53
1:A:426:SER:N	2:F:574:GLN:HE22	1.96	0.53
2:B:466:GLN:HA	2:B:602:TYR:O	2.09	0.53
1:E:305:LEU:HD11	1:E:336:VAL:HG13	1.90	0.53
2:F:306:PRO:HB2	2:F:344:PHE:CZ	2.44	0.53
1:G:32:LEU:HD22	1:G:79:GLU:HG3	1.91	0.53
1:G:45:GLY:HA3	1:G:131:GLY:O	2.08	0.53
2:H:380:PRO:HB3	2:H:410:ALA:O	2.08	0.53
2:B:123:ARG:HB3	2:B:124:PRO:HD2	1.91	0.53
1:G:411:ILE:HG13	1:G:447:VAL:CG2	2.39	0.53
1:A:50:MET:HE2	1:A:57:SER:HB2	1.91	0.53
1:E:290:PRO:HA	1:E:391:PRO:HD3	1.91	0.53
2:D:150:ASP:OD2	2:D:153:THR:OG1	2.27	0.53
2:H:77:SER:HB2	2:H:83:GLU:CB	2.38	0.53
2:H:457:ILE:O	2:H:458:SER:HB2	2.07	0.53
2:D:426:ASN:O	2:D:430:ARG:HG3	2.10	0.52
1:E:344:SER:OG	1:E:346:PRO:HD3	2.10	0.52
2:H:341:PHE:O	2:H:342:ARG:C	2.51	0.52
1:A:354:SER:OG	1:A:356:ARG:O	2.27	0.52
1:G:95:MET:HG3	1:G:114:MET:HE1	1.92	0.52
2:H:213:ALA:HB3	2:H:215:HIS:CD2	2.44	0.52
1:A:345:ALA:CB	1:A:346:PRO:CA	2.87	0.52
2:H:174:PHE:HA	2:H:259:ARG:HH21	1.75	0.52
2:B:329:HIS:HB3	2:B:331:LEU:HD21	1.91	0.52
2:B:457:ILE:O	2:B:458:SER:CB	2.58	0.52
1:E:77:THR:OG1	1:E:79:GLU:HG2	2.10	0.52
1:A:425:LEU:HD12	2:F:579:SER:HB2	1.92	0.52
2:D:39:LEU:HD22	2:D:95:GLY:O	2.08	0.52
2:F:635:ARG:HD3	2:F:750:CYS:SG	2.50	0.52
1:A:418:LEU:HB3	1:A:436:MET:HE1	1.92	0.52
2:B:33:LEU:HD12	2:B:249:THR:HG21	1.90	0.52
2:B:730:GLU:H	2:B:731:PRO:HD2	1.74	0.52
2:F:23:LEU:CD1	2:F:194:CYS:HA	2.37	0.52
1:G:409:ASP:OD2	1:G:409:ASP:N	2.43	0.52
2:H:173:HIS:HA	2:H:341:PHE:CZ	2.45	0.52
2:D:23:LEU:HD13	2:D:194:CYS:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:426:ASN:HD21	2:F:429:THR:HB	1.75	0.52
2:B:631:VAL:HG12	2:B:642:ILE:HA	1.91	0.52
2:D:418:VAL:HG13	2:D:450:LEU:HD11	1.90	0.52
1:E:7:LEU:HD21	1:E:32:LEU:HD11	1.92	0.52
1:E:430:ALA:HB1	1:E:434:TYR:HD2	1.74	0.52
2:H:632:VAL:O	2:H:640:ASN:HA	2.10	0.52
2:D:94:VAL:HG11	2:D:687:ARG:HG2	1.92	0.52
1:G:102:GLN:O	2:H:15:HIS:HE1	1.93	0.52
2:H:297:CYS:HB3	2:H:304:SER:OG	2.10	0.52
2:B:28:CYS:HB2	2:B:29:PRO:CD	2.40	0.52
2:B:95:GLY:HA3	2:B:264:VAL:HG12	1.92	0.52
2:B:160:HIS:HB3	2:B:364:MET:HE1	1.92	0.52
1:C:237:THR:OG1	1:C:238:PRO:HD2	2.10	0.52
1:E:22:SER:OG	1:E:25:GLU:HG2	2.10	0.52
1:E:164:PHE:C	1:E:166:LEU:H	2.18	0.52
1:G:209:SER:HA	1:G:212:VAL:HG13	1.92	0.52
1:G:393:ARG:NH1	1:G:398:GLU:OE1	2.43	0.52
2:D:21:ARG:HH21	2:D:27:PRO:CD	2.23	0.51
2:D:457:ILE:O	2:D:458:SER:CB	2.59	0.51
4:G:1465:FAD:N1	4:G:1465:FAD:H2'	2.25	0.51
2:H:673:GLY:O	2:H:678:GLU:HB2	2.10	0.51
2:B:617:ARG:NH1	2:B:620:LEU:HA	2.26	0.51
1:E:192:TRP:O	1:E:196:HIS:HD2	1.93	0.51
1:E:298:LEU:HB3	1:E:303:ALA:HB3	1.92	0.51
1:E:370:LEU:HD22	1:E:380:ALA:CB	2.39	0.51
1:E:453:GLU:HG2	1:E:454:ALA:N	2.25	0.51
2:F:151:VAL:HG21	2:F:325:ARG:HB3	1.93	0.51
1:G:38:GLY:O	2:H:259:ARG:HD3	2.10	0.51
2:H:298:GLY:HA3	2:H:336:GLN:O	2.10	0.51
2:B:278:ILE:HG12	2:B:360:LEU:HD22	1.93	0.51
2:F:601:PHE:CG	2:H:595:SER:HB2	2.45	0.51
1:A:51:ILE:HD11	1:A:58:ARG:NH1	2.25	0.51
2:D:160:HIS:CB	2:D:364:MET:HE2	2.39	0.51
1:E:249:ILE:HG23	1:E:267:LEU:HD22	1.93	0.51
1:G:94:ALA:HB2	1:G:149:ALA:HB2	1.93	0.51
2:H:67:ALA:HA	2:H:70:LEU:HD12	1.93	0.51
1:A:322:PHE:CB	1:A:390:VAL:CG2	2.86	0.51
1:A:430:ALA:HB1	1:A:434:TYR:HD2	1.76	0.51
1:C:215:ALA:CB	1:C:217:ARG:HH21	2.23	0.51
1:A:110:PHE:O	1:A:114:MET:HG3	2.10	0.51
1:A:140:ALA:HB3	1:A:141:PRO:CD	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:283:SER:O	2:B:366:ARG:NH1	2.42	0.51
1:A:252:LEU:HD22	1:A:281:ILE:CG2	2.41	0.51
1:G:27:LEU:O	1:G:30:GLU:HB2	2.11	0.51
1:G:371:THR:HB	1:G:378:GLU:HB2	1.93	0.51
1:G:418:LEU:HD12	1:G:440:GLN:HG2	1.92	0.51
2:D:129:LEU:HD22	2:D:331:LEU:HD12	1.93	0.51
2:H:694:SER:O	2:H:697:LYS:HE2	2.10	0.51
2:B:228:PHE:O	2:B:341:PHE:HA	2.11	0.51
1:C:316:MET:HE1	1:C:329:ASP:OD2	2.11	0.51
1:E:91:VAL:HG13	1:E:114:MET:HE3	1.92	0.51
2:F:380:PRO:HD3	2:F:412:CYS:O	2.10	0.50
1:G:187:ASP:HA	1:G:308:ARG:NH2	2.25	0.50
1:G:377:ILE:N	1:G:404:GLN:O	2.43	0.50
1:A:409:ASP:OD2	1:A:409:ASP:N	2.44	0.50
2:D:730:GLU:N	2:D:731:PRO:CD	2.74	0.50
2:F:168:ILE:HA	2:F:759:ALA:HB3	1.92	0.50
2:D:28:CYS:HB2	2:D:29:PRO:CD	2.41	0.50
2:D:412:CYS:HA	2:D:624:TYR:CZ	2.46	0.50
2:D:730:GLU:H	2:D:731:PRO:CD	2.24	0.50
1:A:314:ARG:HD3	1:A:334:GLU:OE1	2.12	0.50
2:F:220:GLU:HG2	2:F:517:ASP:OD1	2.11	0.50
2:F:358:GLU:O	2:F:362:ARG:HG2	2.11	0.50
2:H:35:LEU:HB3	2:H:100:LEU:HD11	1.94	0.50
2:B:190:VAL:HG22	2:B:191:VAL:N	2.26	0.50
2:B:735:LEU:O	2:B:738:SER:HB3	2.12	0.50
2:F:305:LEU:HB3	2:F:306:PRO:CD	2.40	0.50
1:C:361:ILE:HG12	1:C:429:ARG:CZ	2.41	0.50
1:E:78:ILE:HG23	1:E:79:GLU:N	2.26	0.50
1:E:111:ILE:HD11	2:F:16:VAL:HG23	1.92	0.50
2:F:482:ASN:ND2	2:F:514:THR:OG1	2.43	0.50
2:H:146:TRP:HZ3	2:H:313:LEU:HD13	1.76	0.50
2:H:166:PHE:CE2	2:H:355:ARG:HG3	2.46	0.50
1:A:200:THR:HG21	1:A:219:LEU:HD13	1.93	0.50
1:A:361:ILE:HG12	1:A:429:ARG:NE	2.27	0.50
2:B:168:ILE:HD13	2:B:351:LEU:HD23	1.92	0.50
2:B:221:MET:CE	2:B:224:MET:HE2	2.41	0.50
1:C:212:VAL:O	1:C:216:LEU:HA	2.12	0.50
1:E:299:ILE:HG13	1:E:318:LEU:HD23	1.93	0.50
1:G:111:ILE:HD11	2:H:16:VAL:HG22	1.94	0.50
2:H:53:GLU:HB3	2:H:54:PRO:HD3	1.92	0.50
1:C:214:LYS:NZ	2:D:258:ASP:OD1	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:77:SER:HB2	2:F:83:GLU:CB	2.38	0.50
1:G:430:ALA:HB1	1:G:434:TYR:HD2	1.77	0.50
1:A:392:LYS:HG3	1:A:422:PHE:HE2	1.77	0.49
2:B:341:PHE:O	2:B:342:ARG:C	2.55	0.49
1:C:462:PRO:HB3	2:D:706:ARG:HB2	1.94	0.49
2:F:216:ASP:OD1	2:H:512:ARG:HD2	2.11	0.49
2:H:450:LEU:HD23	2:H:450:LEU:C	2.36	0.49
2:D:32:THR:HG23	2:D:252:PRO:HB2	1.93	0.49
2:F:146:TRP:CZ3	2:F:313:LEU:HD13	2.47	0.49
1:A:411:ILE:HG13	1:A:447:VAL:HG21	1.94	0.49
2:B:641:ARG:HH21	2:B:706:ARG:HH12	1.60	0.49
2:D:238:LEU:HD12	2:D:238:LEU:H	1.77	0.49
1:E:411:ILE:CG2	1:E:443:ALA:HB1	2.43	0.49
2:F:23:LEU:HD22	2:F:180:ALA:HB1	1.93	0.49
2:H:38:GLY:HA3	2:H:99:PHE:CE2	2.48	0.49
2:B:65:PHE:HB2	2:B:100:LEU:HB3	1.93	0.49
2:B:702:SER:O	2:B:706:ARG:NH2	2.44	0.49
1:E:136:CYS:O	2:F:666:GLY:HA3	2.11	0.49
2:F:556:ALA:HB1	2:F:561:CYS:O	2.13	0.49
1:G:194:LEU:HD22	1:G:310:GLY:HA3	1.95	0.49
1:G:460:VAL:HG11	2:H:632:VAL:HG11	1.93	0.49
2:F:31:ASN:O	2:F:251:ARG:HD3	2.12	0.49
2:F:284:GLY:O	2:F:374:LEU:HD23	2.13	0.49
2:D:638:GLY:HA3	2:D:763:PRO:O	2.13	0.49
2:H:443:THR:O	2:H:635:ARG:HB2	2.12	0.49
1:A:111:ILE:HD11	2:B:16:VAL:HG22	1.94	0.49
1:C:140:ALA:N	1:C:141:PRO:HD2	2.27	0.49
1:A:190:ALA:HB1	1:A:310:GLY:CA	2.40	0.49
2:B:146:TRP:CZ3	2:B:313:LEU:HD13	2.48	0.49
2:B:554:PHE:HB2	2:B:594:ILE:CD1	2.42	0.49
2:D:309:ASP:OD1	2:D:330:ARG:NH2	2.44	0.49
1:G:1:MET:HB2	1:G:179:PRO:CG	2.40	0.49
2:B:595:SER:HB2	2:D:601:PHE:CG	2.47	0.49
4:C:1465:FAD:H2'	4:C:1465:FAD:N1	2.28	0.49
1:E:89:HIS:O	1:E:90:PRO:C	2.56	0.49
2:H:354:GLU:OE2	2:H:452:PRO:HD2	2.13	0.49
1:E:66:MET:O	1:E:69:GLN:HB2	2.13	0.49
2:H:261:ASP:HB3	2:H:265:ILE:HD12	1.95	0.49
1:A:361:ILE:HG12	1:A:429:ARG:NH2	2.28	0.48
2:B:517:ASP:OD2	2:B:519:SER:OG	2.25	0.48
1:C:457:VAL:HG23	2:D:634:ASP:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:95:MET:HE2	1:E:114:MET:SD	2.52	0.48
1:A:444:LEU:O	1:A:448:ARG:HG3	2.12	0.48
1:C:216:LEU:HD22	2:D:107:ARG:HD3	1.94	0.48
2:D:495:LYS:O	2:D:499:VAL:HG23	2.13	0.48
2:F:39:LEU:HD22	2:F:95:GLY:O	2.13	0.48
1:G:411:ILE:HG13	1:G:447:VAL:HG21	1.95	0.48
2:D:319:TYR:OH	2:D:372:ARG:HD3	2.13	0.48
1:E:407:ARG:HB2	1:E:407:ARG:NH1	2.28	0.48
2:F:661:ILE:O	2:F:665:GLU:HG3	2.13	0.48
1:G:436:MET:HE3	1:G:436:MET:HA	1.95	0.48
2:D:473:ILE:HG12	2:D:479:VAL:HG22	1.96	0.48
1:E:111:ILE:HD11	2:F:16:VAL:HG22	1.95	0.48
2:B:186:ALA:O	2:B:187:GLU:C	2.57	0.48
2:D:637:THR:OG1	2:D:639:GLU:HG3	2.13	0.48
1:G:22:SER:OG	1:G:25:GLU:HG2	2.12	0.48
1:G:240:GLY:O	1:G:343:LYS:HE3	2.14	0.48
2:B:328:SER:OG	2:B:330:ARG:NH1	2.46	0.48
2:D:65:PHE:HB2	2:D:100:LEU:HB3	1.93	0.48
1:E:415:LEU:HD22	1:E:440:GLN:HB3	1.95	0.48
1:G:164:PHE:O	1:G:166:LEU:HG	2.14	0.48
1:A:355:LYS:HE2	2:B:679:GLU:OE1	2.14	0.48
1:A:414:ALA:O	1:A:417:LEU:HD12	2.14	0.48
1:E:50:MET:HE2	1:E:57:SER:CB	2.42	0.48
1:G:126:ASP:OD1	2:H:704:ARG:NH1	2.38	0.48
2:H:36:ALA:HA	2:H:255:MET:HE3	1.95	0.48
2:B:398:LYS:HB3	2:B:399:LYS:NZ	2.29	0.48
1:E:21:GLN:HG2	1:E:22:SER:N	2.29	0.48
1:G:7:LEU:O	1:G:8:ASN:C	2.56	0.48
2:H:276:TYR:OH	2:H:359:HIS:CD2	2.59	0.48
2:H:278:ILE:HG23	2:H:360:LEU:HD13	1.96	0.48
2:B:446:ARG:HD3	2:B:632:VAL:HG13	1.95	0.48
1:E:6:LEU:HD12	1:E:10:GLU:C	2.38	0.48
1:E:237:THR:HG23	1:E:240:GLY:O	2.14	0.48
1:E:371:THR:O	1:E:378:GLU:HB2	2.14	0.48
1:G:241:TYR:O	1:G:341:LEU:N	2.43	0.48
1:A:37:GLU:OE1	2:B:256:ARG:NH2	2.47	0.48
1:E:43:ASP:CB	2:F:693:PRO:HB2	2.44	0.48
2:F:697:LYS:HA	2:F:697:LYS:HD3	1.56	0.48
1:G:408:GLU:OE2	1:G:444:LEU:HD22	2.14	0.48
1:A:243:ILE:HG21	1:A:252:LEU:HD13	1.96	0.47
2:B:641:ARG:NH2	2:B:706:ARG:NH1	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:LEU:HD13	1:A:206:THR:HG22	1.97	0.47
1:A:26:TRP:CD1	1:A:67:LEU:HD11	2.50	0.47
2:B:595:SER:HB2	2:D:601:PHE:CD1	2.48	0.47
2:H:21:ARG:HH21	2:H:27:PRO:HD3	1.80	0.47
1:A:126:ASP:OD1	2:B:704:ARG:NH1	2.39	0.47
2:D:506:ILE:HD12	2:D:510:GLN:HB2	1.96	0.47
1:E:160:ALA:O	1:E:162:ALA:N	2.47	0.47
2:H:641:ARG:HH12	2:H:706:ARG:NH1	2.13	0.47
2:H:683:ASP:OD1	2:H:683:ASP:C	2.58	0.47
2:D:51:ASP:HB3	2:D:117:ARG:HB2	1.96	0.47
1:G:216:LEU:HD12	2:H:114:ARG:HH11	1.79	0.47
1:G:271:ALA:HB1	1:G:275:VAL:HB	1.96	0.47
2:H:617:ARG:HD3	2:H:619:PHE:O	2.15	0.47
1:A:111:ILE:HA	1:A:114:MET:HE3	1.95	0.47
1:A:368:LEU:HD23	1:A:382:ILE:HG12	1.97	0.47
1:C:445:ARG:HG3	1:C:455:VAL:HG13	1.95	0.47
1:E:18:ASP:OD2	1:E:20:THR:HG22	2.15	0.47
1:G:136:CYS:HB2	3:G:1463:FES:S2	2.54	0.47
1:A:309:ARG:HB3	1:A:312:GLU:CG	2.44	0.47
2:D:280:ALA:CB	2:D:364:MET:HE1	2.38	0.47
1:E:240:GLY:HA2	1:E:343:LYS:HG2	1.96	0.47
1:E:289:SER:OG	1:E:291:ILE:HG13	2.15	0.47
1:G:240:GLY:CA	1:G:343:LYS:HG2	2.25	0.47
1:G:295:PRO:O	1:G:296:PRO:C	2.58	0.47
1:G:376:LYS:HA	1:G:404:GLN:O	2.15	0.47
2:B:215:HIS:ND1	2:D:478:SER:HB2	2.30	0.47
1:C:243:ILE:HD12	1:C:341:LEU:HG	1.97	0.47
1:C:299:ILE:O	1:C:381:ARG:NH1	2.46	0.47
1:C:66:MET:HE3	1:C:209:SER:HB3	1.97	0.47
2:D:697:LYS:HD2	2:D:697:LYS:N	2.30	0.47
1:E:83:ALA:HB2	1:E:157:TRP:CZ3	2.49	0.47
1:G:141:PRO:HA	1:G:144:ARG:HH11	1.80	0.47
1:G:359:GLN:O	1:G:359:GLN:HG3	2.15	0.47
1:G:399:ALA:C	1:G:401:LEU:H	2.23	0.47
2:B:174:PHE:CZ	2:B:693:PRO:HG3	2.50	0.47
2:F:449:ALA:O	2:F:628:ILE:HA	2.15	0.47
1:G:187:ASP:HA	1:G:308:ARG:HH22	1.80	0.47
2:H:158:ALA:O	2:H:159:ALA:C	2.57	0.47
2:B:22:TYR:CD1	2:B:22:TYR:N	2.84	0.46
1:E:418:LEU:HB3	1:E:436:MET:HE1	1.97	0.46
2:F:66:THR:CG2	2:F:67:ALA:N	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:453:VAL:HG21	2:F:735:LEU:HD23	1.96	0.46
2:H:456:GLY:HA3	2:H:619:PHE:CD1	2.50	0.46
1:E:111:ILE:CD1	2:F:16:VAL:HG22	2.46	0.46
2:F:341:PHE:CD2	2:F:342:ARG:N	2.73	0.46
2:F:507:ASP:OD1	2:F:508:PRO:CD	2.63	0.46
1:G:306:THR:HB	1:G:338:SER:HB2	1.98	0.46
2:H:35:LEU:HA	2:H:101:VAL:O	2.15	0.46
2:H:466:GLN:HA	2:H:602:TYR:O	2.15	0.46
2:H:517:ASP:OD2	2:H:519:SER:N	2.48	0.46
1:C:373:LYS:HB2	1:C:378:GLU:HG3	1.97	0.46
2:D:168:ILE:HA	2:D:759:ALA:HB3	1.97	0.46
1:G:390:VAL:CG2	1:G:391:PRO:HD2	2.44	0.46
1:A:190:ALA:O	1:A:194:LEU:HB2	2.15	0.46
1:E:298:LEU:HB2	1:E:318:LEU:CD2	2.45	0.46
1:G:77:THR:OG1	1:G:79:GLU:HG2	2.15	0.46
1:G:371:THR:OG1	1:G:379:THR:HB	2.16	0.46
1:G:373:LYS:HB2	1:G:378:GLU:CG	2.45	0.46
1:A:43:ASP:CB	2:B:693:PRO:HB2	2.45	0.46
1:A:90:PRO:HB3	1:A:152:GLU:HG3	1.96	0.46
2:B:661:ILE:O	2:B:665:GLU:HG3	2.15	0.46
2:D:461:LEU:HG	2:D:463:HIS:CE1	2.51	0.46
2:D:717:ASN:O	2:D:724:ARG:HD2	2.16	0.46
2:F:143:PRO:HG3	2:F:329:HIS:CE1	2.50	0.46
2:F:197:GLN:HG2	2:F:488:MET:CE	2.45	0.46
2:F:238:LEU:HD11	2:F:257:TYR:CZ	2.50	0.46
1:A:105:PHE:CD1	2:B:177:GLU:HB2	2.50	0.46
2:B:129:LEU:O	2:B:133:LEU:HD22	2.15	0.46
1:C:100:GLY:HA2	1:C:141:PRO:HB2	1.96	0.46
1:E:427:ASP:OD1	1:E:435:ARG:NH2	2.48	0.46
2:F:50:LEU:CD1	2:F:118:ILE:HG12	2.45	0.46
2:F:319:TYR:OH	2:F:372:ARG:HG2	2.15	0.46
1:G:325:TYR:CE2	1:G:326:ARG:HG3	2.49	0.46
2:H:174:PHE:CZ	2:H:693:PRO:HG3	2.42	0.46
1:G:133:LEU:HD13	2:H:698:ILE:HD11	1.97	0.46
1:E:50:MET:HE3	1:E:116:ALA:HA	1.97	0.46
1:G:314:ARG:HH22	1:G:329:ASP:CG	2.24	0.46
2:H:310:ARG:HD2	2:H:344:PHE:O	2.16	0.46
2:H:771:ARG:O	2:H:775:GLY:N	2.43	0.46
1:E:370:LEU:CD2	1:E:380:ALA:HA	2.40	0.46
2:F:292:VAL:HG22	2:F:327:GLU:HB3	1.97	0.46
2:H:53:GLU:OE1	2:H:53:GLU:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:210:LEU:HD11	2:H:243:ALA:HB1	1.98	0.46
2:H:532:GLY:O	2:H:536:ASN:HB2	2.16	0.46
1:A:48:THR:HG21	1:A:113:SER:OG	2.15	0.46
2:B:2:SER:N	2:B:502:ALA:HB2	2.31	0.46
2:D:437:TRP:CE3	2:D:446:ARG:HG2	2.52	0.46
1:E:302:GLY:HA2	1:E:381:ARG:CZ	2.45	0.46
1:E:409:ASP:OD2	1:E:409:ASP:N	2.49	0.46
1:G:366:GLY:HA3	1:G:442:MET:SD	2.56	0.46
2:H:175:TYR:OH	2:H:262:ASP:OD2	2.31	0.46
1:A:418:LEU:CB	1:A:436:MET:HE1	2.45	0.45
2:B:717:ASN:HD22	2:B:726:LYS:HG2	1.81	0.45
7:D:1780[B]:XAN:O2	8:D:1781:MOM:OM2	2.33	0.45
1:E:140:ALA:N	1:E:141:PRO:HD2	2.31	0.45
2:F:294:LEU:HD23	2:F:329:HIS:CD2	2.51	0.45
2:F:414:LEU:O	2:F:418:VAL:HG23	2.15	0.45
2:F:426:ASN:ND2	2:F:429:THR:HB	2.30	0.45
2:H:730:GLU:N	2:H:731:PRO:CD	2.80	0.45
1:A:40:ASN:HD22	1:A:40:ASN:HA	1.61	0.45
2:B:151:VAL:HG21	2:B:325:ARG:HB3	1.99	0.45
1:G:373:LYS:HB2	1:G:378:GLU:HG2	1.97	0.45
2:H:465:ASN:HB3	2:H:604:THR:OG1	2.16	0.45
1:A:295:PRO:O	1:A:296:PRO:C	2.59	0.45
2:B:276:TYR:OH	2:B:359:HIS:CD2	2.70	0.45
1:C:111:ILE:CD1	2:D:16:VAL:HG22	2.46	0.45
1:C:368:LEU:HD12	1:C:368:LEU:N	2.31	0.45
1:E:288:GLY:HA2	1:E:322:PHE:HE2	1.80	0.45
2:F:129:LEU:HD21	2:F:296:ARG:HB2	1.99	0.45
2:B:139:PHE:O	2:B:140:GLU:HB2	2.17	0.45
2:B:151:VAL:HG11	2:B:290:ASP:HB2	1.97	0.45
2:B:457:ILE:O	2:B:458:SER:HB2	2.17	0.45
2:F:554:PHE:HB2	2:F:594:ILE:CD1	2.46	0.45
1:G:95:MET:CG	1:G:114:MET:HE1	2.46	0.45
2:H:621:TYR:CE1	2:H:726:LYS:HG2	2.51	0.45
1:A:8:ASN:OD1	1:A:80:GLY:HA3	2.15	0.45
1:A:95:MET:SD	1:A:114:MET:HE1	2.57	0.45
2:D:146:TRP:CZ3	2:D:312:MET:HB3	2.51	0.45
1:E:225:LEU:O	1:E:227:HIS:N	2.50	0.45
2:F:215:HIS:ND1	2:H:478:SER:HB2	2.31	0.45
2:F:554:PHE:HB2	2:F:594:ILE:HD13	1.98	0.45
2:F:573:VAL:CG2	2:F:585:ILE:HG13	2.46	0.45
1:A:140:ALA:N	1:A:141:PRO:HD2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:166:PHE:HB3	2:B:355:ARG:NH2	2.31	0.45
2:B:407:GLN:HG3	2:B:617:ARG:HG2	1.98	0.45
2:B:530:SER:HB2	2:B:727:ALA:HB1	1.99	0.45
2:D:566:VAL:HA	2:D:574:GLN:O	2.17	0.45
1:G:89:HIS:HB3	1:G:92:GLN:HG3	1.99	0.45
1:G:370:LEU:HD22	1:G:380:ALA:HA	1.97	0.45
1:A:77:THR:OG1	1:A:79:GLU:HG2	2.17	0.45
2:B:150:ASP:OD2	2:F:423:LYS:CE	2.65	0.45
2:F:296:ARG:O	2:F:338:ASN:ND2	2.44	0.45
1:G:325:TYR:O	1:G:326:ARG:HB2	2.17	0.45
2:H:302:ASP:OD1	2:H:303:LEU:N	2.50	0.45
1:A:299:ILE:O	1:A:381:ARG:NH1	2.50	0.45
2:B:184:LEU:HD23	2:B:252:PRO:HB3	1.99	0.45
2:B:187:GLU:HG2	2:D:21:ARG:HD2	1.99	0.45
1:C:273:GLU:HA	1:C:276:ARG:NH1	2.31	0.45
1:E:373:LYS:HB2	1:E:378:GLU:HG3	1.99	0.45
2:H:529:ALA:O	2:H:530:SER:C	2.60	0.45
2:H:556:ALA:HB1	2:H:561:CYS:O	2.17	0.45
2:B:566:VAL:HG13	2:B:575:ALA:HB2	1.98	0.45
1:G:253:ARG:HH21	1:G:268:ARG:HG3	1.77	0.45
2:H:542:ASP:OD2	2:H:600:GLY:HA2	2.17	0.45
1:C:216:LEU:CD2	2:D:107:ARG:HD3	2.47	0.44
1:E:337:GLU:O	1:E:338:SER:HB3	2.17	0.44
2:F:273:ARG:HD2	2:F:294:LEU:HD12	1.98	0.44
2:F:283:SER:O	2:F:366:ARG:NH1	2.45	0.44
2:F:321:VAL:HG12	2:F:323:ALA:O	2.17	0.44
2:B:276:TYR:OH	2:B:359:HIS:HD2	2.00	0.44
2:D:175:TYR:O	2:D:259:ARG:NH2	2.37	0.44
2:H:484:GLY:HA3	2:H:524:THR:HG21	2.00	0.44
2:B:129:LEU:O	2:B:132:ALA:HB3	2.16	0.44
2:B:144:VAL:HG12	2:B:312:MET:HE1	1.99	0.44
1:C:216:LEU:HD22	2:D:107:ARG:CD	2.47	0.44
2:D:398:LYS:HB3	2:D:399:LYS:HD2	1.99	0.44
1:E:240:GLY:HA3	1:E:341:LEU:O	2.18	0.44
2:F:222:ARG:HD2	2:F:515:ALA:HB2	1.99	0.44
2:F:580:TRP:HB2	2:F:585:ILE:HD11	1.98	0.44
1:G:92:GLN:HB3	2:H:16:VAL:HG13	1.98	0.44
1:G:139:TYR:HA	1:G:142:ILE:HD12	1.98	0.44
2:B:236:ASN:N	2:B:236:ASN:HD22	2.15	0.44
2:B:269:ARG:NH2	2:B:733:PHE:CZ	2.85	0.44
2:D:24:ASP:OD2	2:D:254:LYS:NZ	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:450:LEU:HB2	2:D:628:ILE:HG12	1.99	0.44
1:E:228:CYS:SG	1:E:228:CYS:O	2.75	0.44
1:C:216:LEU:CD1	2:D:114:ARG:NH1	2.71	0.44
1:E:186:SER:O	1:E:187:ASP:C	2.61	0.44
1:E:322:PHE:CB	1:E:390:VAL:HG23	2.48	0.44
2:H:434:ILE:HD13	2:H:448:ILE:HB	1.99	0.44
1:A:400:ALA:HB3	1:A:417:LEU:HD13	1.99	0.44
2:B:263:MET:HE3	2:B:692:ALA:CA	2.42	0.44
2:D:133:LEU:HD12	2:D:133:LEU:HA	1.87	0.44
1:G:131:GLY:HA3	1:G:274:GLN:OE1	2.18	0.44
2:H:171:GLN:NE2	2:H:674:TRP:HB2	2.33	0.44
2:H:446:ARG:HD3	2:H:632:VAL:HG13	1.99	0.44
2:H:499:VAL:O	2:H:503:VAL:HG23	2.18	0.44
1:A:92:GLN:HB3	2:B:16:VAL:HG13	1.99	0.44
2:B:35:LEU:HA	2:B:101:VAL:O	2.17	0.44
1:C:393:ARG:HD2	1:C:398:GLU:OE1	2.17	0.44
2:F:767:LEU:O	2:F:771:ARG:HG3	2.18	0.44
1:G:24:LEU:HD13	1:G:47:CYS:HB2	1.99	0.44
1:G:460:VAL:HG21	2:H:632:VAL:HG11	1.99	0.44
2:H:272:PHE:HA	2:H:294:LEU:O	2.17	0.44
2:H:729:GLY:HA3	5:H:1778:MTE:H4'2	1.99	0.44
2:D:46:ALA:HB2	2:D:123:ARG:NH2	2.33	0.44
2:D:306:PRO:HB2	2:D:344:PHE:HE2	1.83	0.44
1:G:322:PHE:CB	1:G:390:VAL:CG2	2.95	0.44
2:H:224:MET:HE1	2:H:488:MET:HE2	2.00	0.44
1:A:52:ARG:HB3	1:A:74:ALA:HB3	1.99	0.44
1:A:365:CYS:O	1:A:384:PHE:HA	2.17	0.44
1:E:7:LEU:HD13	1:E:75:LEU:HD23	1.99	0.44
2:F:631:VAL:HG21	2:F:743:LEU:HA	2.00	0.44
2:H:423:LYS:HE2	2:H:423:LYS:HB3	1.65	0.44
2:D:650:ASP:HA	2:D:713:TRP:HB3	2.00	0.43
1:E:181:PHE:CZ	1:E:183:PRO:HB3	2.53	0.43
2:F:133:LEU:HD12	2:F:133:LEU:HA	1.76	0.43
1:A:397:PHE:HE1	1:A:415:LEU:HA	1.84	0.43
2:D:269:ARG:NH2	2:D:341:PHE:CD2	2.86	0.43
1:E:12:ARG:HG2	1:E:12:ARG:NH1	2.22	0.43
2:F:418:VAL:HG13	2:F:450:LEU:HD11	2.00	0.43
1:G:205:GLY:O	1:G:209:SER:OG	2.28	0.43
2:H:419:THR:O	2:H:423:LYS:HD2	2.19	0.43
1:C:95:MET:CE	1:C:114:MET:HE1	2.42	0.43
1:C:211:TRP:O	1:C:215:ALA:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:GLU:OE1	1:C:276:ARG:NH1	2.51	0.43
2:D:76:ALA:HB2	2:D:85:VAL:CG2	2.47	0.43
1:E:295:PRO:HB2	1:E:296:PRO:HD3	2.00	0.43
2:F:236:ASN:HD22	2:F:236:ASN:HA	1.69	0.43
2:F:528:ALA:HA	5:F:1778:MTE:S2'	2.59	0.43
2:F:670:GLN:HG2	2:F:733:PHE:HE1	1.83	0.43
1:G:202:ILE:HD12	1:G:222:VAL:HG11	2.00	0.43
2:H:106:HIS:CE1	2:H:110:ARG:HD3	2.53	0.43
2:H:310:ARG:HA	2:H:313:LEU:HB2	1.99	0.43
1:A:366:GLY:HA3	1:A:442:MET:SD	2.57	0.43
2:B:107:ARG:O	2:B:108:ALA:C	2.60	0.43
2:H:671:GLY:O	2:H:674:TRP:HB3	2.19	0.43
1:A:291:ILE:H	1:A:291:ILE:HG12	1.74	0.43
2:B:700:ALA:O	2:B:703:ASP:HB2	2.18	0.43
1:C:164:PHE:C	1:C:166:LEU:H	2.27	0.43
2:D:335:THR:O	2:D:336:GLN:C	2.61	0.43
2:D:354:GLU:OE1	2:D:372:ARG:NE	2.50	0.43
1:E:325:TYR:O	1:E:326:ARG:HB2	2.18	0.43
1:G:414:ALA:O	1:G:417:LEU:HD12	2.18	0.43
2:H:328:SER:OG	2:H:330:ARG:NH1	2.47	0.43
2:H:376:PHE:HE2	2:H:452:PRO:HG3	1.84	0.43
1:A:207:ASP:OD2	4:A:1465:FAD:O2'	2.27	0.43
2:B:171:GLN:NE2	2:B:674:TRP:HB2	2.33	0.43
2:B:597:SER:HB2	2:D:522:PRO:HG3	1.99	0.43
2:D:174:PHE:HE1	2:D:263:MET:HE1	1.83	0.43
1:E:214:LYS:HD3	1:E:214:LYS:HA	1.85	0.43
2:F:221:MET:CE	2:F:224:MET:HE2	2.38	0.43
1:G:15:ARG:HH11	1:G:15:ARG:HG2	1.83	0.43
1:A:212:VAL:O	2:B:107:ARG:NH1	2.51	0.43
1:A:370:LEU:HD22	1:A:380:ALA:HA	1.99	0.43
2:B:422:GLN:HG2	2:B:427:PHE:CD2	2.53	0.43
2:D:278:ILE:HD11	2:D:286:LEU:HD22	2.00	0.43
1:E:445:ARG:HG3	1:E:455:VAL:HG11	1.99	0.43
1:G:70:ILE:O	1:G:71:ALA:C	2.61	0.43
2:H:81:SER:HA	2:H:82:PRO:HD3	1.92	0.43
1:A:351:TYR:CZ	1:A:445:ARG:HD3	2.53	0.43
2:B:360:LEU:O	2:B:364:MET:HE3	2.19	0.43
1:C:357:PHE:HE1	2:D:640:ASN:O	2.01	0.43
2:D:318:SER:HB3	2:D:414:LEU:HD13	2.00	0.43
2:D:437:TRP:CZ3	2:D:446:ARG:HG2	2.53	0.43
1:G:237:THR:O	1:G:238:PRO:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:631:VAL:HG12	2:H:642:ILE:HA	1.99	0.43
2:B:683:ASP:OD1	2:B:685:CYS:N	2.49	0.43
2:F:306:PRO:HB2	2:F:344:PHE:HZ	1.84	0.43
1:G:316:MET:HE1	1:G:329:ASP:OD2	2.19	0.43
2:H:221:MET:HE1	2:H:224:MET:HG3	2.00	0.43
1:A:36:LYS:NZ	2:B:25:ASP:OD2	2.51	0.43
1:A:308:ARG:O	1:A:334:GLU:HA	2.19	0.43
1:E:198:GLU:H	1:E:198:GLU:CD	2.26	0.43
2:F:451:SER:HA	2:F:452:PRO:HD3	1.83	0.43
1:G:40:ASN:HD22	1:G:40:ASN:HA	1.54	0.43
1:G:120:ARG:O	1:G:121:ASP:C	2.62	0.43
1:G:427:ASP:OD1	1:G:427:ASP:C	2.62	0.43
2:B:306:PRO:HB2	2:B:344:PHE:HE2	1.84	0.42
2:B:313:LEU:HD12	2:B:405:TYR:CD2	2.54	0.42
2:B:449:ALA:CB	2:B:741:LEU:HB3	2.49	0.42
1:C:245:ALA:O	1:C:280:THR:HB	2.18	0.42
2:D:272:PHE:CD2	2:D:348:GLN:HG2	2.54	0.42
1:E:248:THR:HA	1:E:279:ALA:O	2.19	0.42
1:E:369:ASN:C	1:E:370:LEU:HD23	2.44	0.42
2:F:289:ALA:O	2:F:324:LEU:HA	2.19	0.42
1:G:8:ASN:HA	1:G:76:ARG:HD3	2.00	0.42
2:H:224:MET:HE3	2:H:488:MET:HB3	2.01	0.42
2:H:554:PHE:HB2	2:H:594:ILE:CD1	2.48	0.42
2:B:558:ARG:HE	2:B:558:ARG:HB3	1.70	0.42
1:C:292:GLY:HA2	4:C:1465:FAD:O2	2.19	0.42
2:D:407:GLN:CD	2:D:617:ARG:HG2	2.43	0.42
2:D:440:THR:HG22	2:D:440:THR:O	2.18	0.42
1:E:12:ARG:CG	1:E:12:ARG:NH1	2.79	0.42
2:F:461:LEU:HD11	2:F:463:HIS:CE1	2.54	0.42
2:F:482:ASN:ND2	2:F:520:LYS:HD3	2.34	0.42
2:H:288:GLY:HA2	2:H:323:ALA:O	2.19	0.42
2:H:308:CYS:O	2:H:312:MET:HG3	2.19	0.42
2:H:497:VAL:HG13	2:H:511:VAL:HB	2.01	0.42
2:B:70:LEU:HA	2:B:71:PRO:HD3	1.95	0.42
2:B:487:GLU:HB2	2:B:493:HIS:CD2	2.53	0.42
1:E:321:PHE:CE1	1:E:328:GLN:HB3	2.55	0.42
1:E:324:GLU:HB2	1:E:327:LYS:HD3	2.01	0.42
2:F:2:SER:N	2:F:502:ALA:HB2	2.34	0.42
1:G:102:GLN:HG3	1:G:137:THR:HG22	2.01	0.42
1:G:335:PHE:HD1	1:G:336:VAL:O	2.01	0.42
2:H:417:LEU:HG	2:H:648:LEU:HD23	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:496:MET:N	2:B:496:MET:HE2	2.35	0.42
2:B:683:ASP:OD1	2:B:683:ASP:C	2.62	0.42
1:E:39:CYS:O	1:E:41:GLU:HB2	2.19	0.42
1:E:415:LEU:HD22	1:E:440:GLN:CB	2.49	0.42
2:H:146:TRP:CH2	2:H:313:LEU:HD13	2.54	0.42
2:H:696:TYR:C	2:H:697:LYS:HD2	2.44	0.42
1:A:356:ARG:CZ	2:B:697:LYS:HZ3	2.32	0.42
1:A:442:MET:O	1:A:445:ARG:HB3	2.19	0.42
1:A:462:PRO:HG3	2:B:706:ARG:HB3	2.02	0.42
2:B:31:ASN:O	2:B:251:ARG:HD3	2.20	0.42
2:F:412:CYS:HA	2:F:624:TYR:CZ	2.55	0.42
1:A:392:LYS:CG	1:A:422:PHE:HE2	2.32	0.42
1:C:96:ILE:HD11	2:D:13:ARG:HA	2.01	0.42
1:C:111:ILE:HD11	2:D:16:VAL:HG22	2.02	0.42
2:D:53:GLU:HB3	2:D:54:PRO:CD	2.48	0.42
2:D:143:PRO:HB3	2:D:329:HIS:CE1	2.55	0.42
2:F:437:TRP:CE3	2:F:446:ARG:HG3	2.54	0.42
2:H:269:ARG:HG3	2:H:269:ARG:HH11	1.85	0.42
1:A:81:ILE:HD13	1:A:81:ILE:HA	1.95	0.42
1:A:192:TRP:O	1:A:196:HIS:HD2	2.01	0.42
2:B:771:ARG:HD2	2:B:776:ARG:HD2	2.01	0.42
2:D:303:LEU:O	2:D:307:VAL:HG23	2.19	0.42
1:E:114:MET:O	1:E:115:ALA:C	2.63	0.42
2:F:238:LEU:HD11	2:F:257:TYR:CE1	2.55	0.42
2:F:461:LEU:CD1	2:F:463:HIS:CE1	3.02	0.42
1:G:126:ASP:OD2	2:H:706:ARG:NH2	2.53	0.42
2:H:21:ARG:HB3	2:H:25:ASP:HB2	2.00	0.42
1:A:108:PRO:O	1:A:112:VAL:HG23	2.20	0.42
1:A:316:MET:HE1	1:A:329:ASP:OD2	2.19	0.42
2:B:160:HIS:CB	2:B:364:MET:CE	2.97	0.42
2:B:186:ALA:O	2:B:187:GLU:O	2.38	0.42
2:B:407:GLN:HE22	2:B:619:PHE:HB2	1.85	0.42
2:B:744:HIS:CD2	2:B:744:HIS:C	2.94	0.42
2:F:302:ASP:OD1	2:F:303:LEU:N	2.48	0.42
2:F:419:THR:O	2:F:423:LYS:HG2	2.18	0.42
1:G:103:CYS:HB3	1:G:136:CYS:SG	2.60	0.42
1:G:373:LYS:O	1:G:375:SER:N	2.45	0.42
1:A:234:ILE:HG12	1:A:243:ILE:HG23	2.02	0.42
2:B:730:GLU:N	2:B:731:PRO:HD2	2.34	0.42
1:E:100:GLY:HA2	1:E:141:PRO:HB2	2.02	0.42
1:E:312:GLU:H	1:E:312:GLU:HG3	1.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:322:PHE:HB3	1:E:390:VAL:HG23	2.02	0.42
2:F:732:PRO:HA	2:F:735:LEU:HG	2.02	0.42
1:G:43:ASP:CB	2:H:693:PRO:HB2	2.48	0.42
1:G:78:ILE:CD1	1:G:111:ILE:HG21	2.50	0.42
2:H:23:LEU:CD1	2:H:194:CYS:HA	2.47	0.42
2:H:95:GLY:HA3	2:H:264:VAL:HG12	2.02	0.42
2:H:530:SER:O	2:H:727:ALA:CB	2.68	0.42
2:H:551:LEU:HD23	2:H:551:LEU:HA	1.73	0.42
2:B:381:GLU:OE2	2:B:381:GLU:HA	2.20	0.42
1:A:301:MET:HB3	1:A:348:LEU:HD22	2.01	0.41
1:A:345:ALA:HB3	1:A:346:PRO:CA	2.38	0.41
1:A:399:ALA:C	1:A:401:LEU:H	2.28	0.41
1:C:295:PRO:O	1:C:296:PRO:C	2.63	0.41
2:F:53:GLU:N	2:F:54:PRO:CD	2.83	0.41
2:F:175:TYR:O	2:F:259:ARG:NH2	2.51	0.41
1:G:184:GLU:HA	1:G:227:HIS:O	2.20	0.41
1:G:311:GLN:CD	1:G:311:GLN:O	2.62	0.41
1:A:249:ILE:HG23	1:A:267:LEU:HD22	2.03	0.41
1:A:356:ARG:NH2	2:B:697:LYS:NZ	2.68	0.41
2:B:417:LEU:HG	2:B:648:LEU:HD23	2.02	0.41
1:E:417:LEU:O	1:E:420:GLN:HB2	2.19	0.41
2:F:129:LEU:HD22	2:F:331:LEU:HD12	2.02	0.41
2:F:358:GLU:HB2	2:F:372:ARG:HH22	1.85	0.41
2:F:551:LEU:HD23	2:F:551:LEU:HA	1.92	0.41
1:A:65:MET:HE3	1:A:65:MET:HB2	1.94	0.41
1:A:192:TRP:O	1:A:196:HIS:CD2	2.74	0.41
1:A:314:ARG:NH1	1:A:334:GLU:OE2	2.53	0.41
1:A:370:LEU:CD2	1:A:380:ALA:HA	2.50	0.41
2:B:53:GLU:HB3	2:B:54:PRO:HD3	2.01	0.41
1:E:216:LEU:HD13	2:F:111:ILE:HG13	2.02	0.41
2:F:271:ASP:OD1	2:F:296:ARG:HD2	2.20	0.41
1:G:47:CYS:SG	1:G:63:CYS:HB3	2.59	0.41
1:G:149:ALA:O	1:G:152:GLU:HB2	2.20	0.41
1:A:316:MET:HG3	1:A:317:PRO:O	2.21	0.41
2:B:34:HIS:C	2:B:35:LEU:HD23	2.45	0.41
2:B:170:GLY:N	2:B:271:ASP:HB3	2.35	0.41
2:B:177:GLU:OE1	2:B:225:GLY:N	2.50	0.41
2:B:597:SER:HB2	2:D:522:PRO:CG	2.51	0.41
2:B:649:HIS:O	2:B:713:TRP:N	2.52	0.41
1:C:136:CYS:O	2:D:666:GLY:HA3	2.20	0.41
2:F:174:PHE:HE1	2:F:263:MET:HE1	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:305:LEU:C	2:H:305:LEU:HD23	2.45	0.41
2:B:215:HIS:CG	2:D:478:SER:HB2	2.55	0.41
2:F:367:ASP:HA	2:F:368:PRO:HD3	1.85	0.41
1:G:461:MET:HA	1:G:462:PRO:HD2	1.78	0.41
2:H:309:ASP:OD1	2:H:330:ARG:NH2	2.44	0.41
1:A:6:LEU:HD13	1:A:164:PHE:CD1	2.56	0.41
1:A:8:ASN:HA	1:A:76:ARG:CD	2.50	0.41
2:B:40:SER:HB2	2:B:98:ILE:HD11	2.03	0.41
2:B:364:MET:HE2	2:B:364:MET:HB3	1.68	0.41
2:D:696:TYR:C	2:D:697:LYS:HD2	2.46	0.41
2:F:493:HIS:CG	2:F:513:ILE:HG12	2.55	0.41
2:F:650:ASP:HA	2:F:713:TRP:HB3	2.03	0.41
2:H:126:ILE:HD12	2:H:137:SER:CB	2.50	0.41
2:H:222:ARG:NH2	2:H:493:HIS:HD2	2.19	0.41
2:H:367:ASP:OD2	2:H:431:ARG:NH1	2.52	0.41
2:B:164:GLY:HA3	2:B:276:TYR:CZ	2.56	0.41
2:B:706:ARG:HA	2:B:706:ARG:HD3	1.36	0.41
2:D:328:SER:OG	2:D:330:ARG:NH1	2.48	0.41
2:D:341:PHE:O	2:D:342:ARG:C	2.64	0.41
2:D:492:LEU:O	2:D:496:MET:HG2	2.20	0.41
2:F:45:ALA:HB1	2:F:120:TYR:HB3	2.03	0.41
1:A:358:ASP:O	1:A:359:GLN:C	2.63	0.41
1:A:404:GLN:HB3	1:A:410:THR:CG2	2.50	0.41
2:B:150:ASP:OD1	2:B:150:ASP:C	2.63	0.41
2:B:574:GLN:HG2	2:B:579:SER:HB3	2.02	0.41
1:E:78:ILE:HD13	1:E:108:PRO:HA	2.02	0.41
1:E:160:ALA:C	1:E:162:ALA:H	2.29	0.41
1:E:191:ASP:O	1:E:194:LEU:HB3	2.20	0.41
1:G:8:ASN:HA	1:G:76:ARG:CD	2.51	0.41
1:G:36:LYS:HA	1:G:36:LYS:HD3	1.82	0.41
2:H:358:GLU:O	2:H:362:ARG:HG2	2.20	0.41
1:A:231:LEU:CD2	1:A:245:ALA:HB3	2.51	0.41
2:B:437:TRP:CE3	2:B:446:ARG:HG3	2.55	0.41
1:C:361:ILE:HG12	1:C:429:ARG:NE	2.35	0.41
4:C:1465:FAD:HM81	4:C:1465:FAD:HM73	1.84	0.41
2:D:170:GLY:N	2:D:271:ASP:HB3	2.36	0.41
2:D:461:LEU:HD23	2:D:464:LEU:HD11	2.03	0.41
2:D:671:GLY:HA2	2:D:733:PHE:CZ	2.56	0.41
1:E:314:ARG:NH1	1:E:334:GLU:OE2	2.54	0.41
4:E:1465:FAD:N1	4:E:1465:FAD:C2'	2.84	0.41
1:G:249:ILE:HG21	1:G:270:PHE:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:563:ALA:O	2:H:566:VAL:HG23	2.21	0.41
2:H:694:SER:C	2:H:697:LYS:HE2	2.45	0.41
1:A:415:LEU:O	1:A:416:PRO:C	2.64	0.41
2:B:205:LYS:HG3	2:B:236:ASN:OD1	2.21	0.41
2:B:325:ARG:HG2	2:B:325:ARG:HH11	1.85	0.41
2:B:446:ARG:HG2	2:B:632:VAL:HG12	2.02	0.41
1:C:445:ARG:HG3	1:C:455:VAL:CG1	2.51	0.41
2:D:21:ARG:HH21	2:D:27:PRO:HD2	1.85	0.41
2:D:632:VAL:HG22	2:D:643:LEU:HD11	2.03	0.41
1:E:289:SER:C	1:E:291:ILE:N	2.79	0.41
1:G:143:LEU:HD23	1:G:143:LEU:O	2.18	0.41
2:B:160:HIS:CB	2:B:364:MET:HE1	2.50	0.40
2:B:754:TRP:HA	2:B:755:PRO:HD3	1.94	0.40
2:F:76:ALA:HB2	2:F:85:VAL:HG22	2.03	0.40
1:G:65:MET:HE3	1:G:65:MET:HB2	1.68	0.40
2:H:66:THR:O	2:H:67:ALA:C	2.63	0.40
2:H:730:GLU:H	2:H:731:PRO:CD	2.35	0.40
2:B:35:LEU:HB3	2:B:100:LEU:HD11	2.02	0.40
2:B:66:THR:CG2	2:B:68:ALA:H	2.29	0.40
2:B:152:GLU:HG2	2:F:423:LYS:HB2	2.02	0.40
1:C:22:SER:OG	1:C:25:GLU:HG2	2.20	0.40
1:E:295:PRO:O	1:E:296:PRO:C	2.60	0.40
1:A:67:LEU:O	1:A:68:PRO:C	2.64	0.40
2:D:165:CYS:HA	2:D:274:ILE:O	2.21	0.40
2:F:366:ARG:NE	2:F:370:GLU:OE1	2.47	0.40
2:F:610:ASP:N	2:F:615:GLN:O	2.45	0.40
2:H:281:ASP:OD1	2:H:281:ASP:C	2.64	0.40
2:B:219:VAL:O	2:B:517:ASP:HA	2.21	0.40
2:B:759:ALA:HA	2:B:760:PRO:C	2.46	0.40
2:D:667:ALA:HB3	2:D:732:PRO:HB2	2.04	0.40
2:F:437:TRP:CZ3	2:F:446:ARG:HG3	2.56	0.40
1:G:49:VAL:HA	1:G:112:VAL:HG11	2.03	0.40
1:A:203:ALA:HB3	4:A:1465:FAD:O1P	2.21	0.40
2:B:697:LYS:HZ2	2:B:697:LYS:HG3	1.70	0.40
1:E:216:LEU:HD12	2:F:114:ARG:NH1	2.36	0.40
1:G:18:ASP:HA	1:G:19:PRO:HD3	1.94	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	446/462 (96%)	402 (90%)	38 (8%)	6 (1%)	9	21
1	C	446/462 (96%)	422 (95%)	20 (4%)	4 (1%)	14	30
1	E	446/462 (96%)	389 (87%)	46 (10%)	11 (2%)	4	8
1	G	446/462 (96%)	383 (86%)	56 (13%)	7 (2%)	7	16
2	B	756/777 (97%)	706 (93%)	39 (5%)	11 (2%)	8	18
2	D	756/777 (97%)	713 (94%)	36 (5%)	7 (1%)	14	30
2	F	756/777 (97%)	707 (94%)	41 (5%)	8 (1%)	11	25
2	H	756/777 (97%)	689 (91%)	58 (8%)	9 (1%)	10	23
All	All	4808/4956 (97%)	4411 (92%)	334 (7%)	63 (1%)	9	21

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	165	THR
1	A	345	ALA
2	B	187	GLU
2	B	458	SER
2	D	458	SER
1	E	374	GLY
2	F	458	SER
1	G	375	SER
2	H	187	GLU
2	H	458	SER
2	H	561	CYS
1	A	359	GLN
2	B	560	GLY
2	B	561	CYS
1	C	165	THR
1	C	374	GLY
2	D	141	GLY

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Mol	Chain	Res	Type
2	D	560	GLY
1	E	161	ASP
1	E	226	SER
2	F	187	GLU
2	F	399	LYS
2	F	560	GLY
2	F	608	SER
1	G	221	GLU
1	G	378	GLU
2	H	227	GLY
2	H	342	ARG
2	H	399	LYS
2	H	560	GLY
1	A	395	ALA
2	B	141	GLY
2	B	227	GLY
2	B	342	ARG
2	B	738	SER
2	D	342	ARG
2	D	399	LYS
1	E	39	CYS
1	E	221	GLU
1	E	395	ALA
1	E	410	THR
2	F	82	PRO
2	F	342	ARG
1	G	400	ALA
2	H	436	ALA
2	H	558	ARG
1	A	39	CYS
1	C	39	CYS
1	C	359	GLN
1	E	165	THR
1	E	187	ASP
1	E	378	GLU
1	G	310	GLY
1	G	437	ASN
2	B	215	HIS
2	B	336	GLN
2	B	399	LYS
1	G	374	GLY
2	D	227	GLY

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Mol	Chain	Res	Type
2	F	227	GLY
1	A	220	PRO
2	D	452	PRO
1	E	261	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	339/347 (98%)	312 (92%)	27 (8%)	11	25
1	C	339/347 (98%)	306 (90%)	33 (10%)	8	17
1	E	339/347 (98%)	305 (90%)	34 (10%)	7	16
1	G	339/347 (98%)	303 (89%)	36 (11%)	6	14
2	B	571/584 (98%)	530 (93%)	41 (7%)	13	30
2	D	571/584 (98%)	539 (94%)	32 (6%)	19	40
2	F	571/584 (98%)	522 (91%)	49 (9%)	10	22
2	H	571/584 (98%)	525 (92%)	46 (8%)	11	24
All	All	3640/3724 (98%)	3342 (92%)	298 (8%)	10	24

All (298) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	THR
1	A	33	THR
1	A	40	ASN
1	A	43	ASP
1	A	76	ARG
1	A	79	GLU
1	A	91	VAL
1	A	128	LEU
1	A	143	LEU
1	A	191	ASP
1	A	212	VAL

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Mol	Chain	Res	Type
1	A	239	ASP
1	A	257	GLU
1	A	291	ILE
1	A	337	GLU
1	A	361	ILE
1	A	371	THR
1	A	378	GLU
1	A	390	VAL
1	A	393	ARG
1	A	408	GLU
1	A	409	ASP
1	A	410	THR
1	A	411	ILE
1	A	429	ARG
1	A	450	LEU
1	A	457	VAL
2	B	10	ASP
2	B	16	VAL
2	B	66	THR
2	B	126	ILE
2	B	133	LEU
2	B	151	VAL
2	B	161	LEU
2	B	176	LEU
2	B	187	GLU
2	B	221	MET
2	B	222	ARG
2	B	263	MET
2	B	268	LYS
2	B	271	ASP
2	B	313	LEU
2	B	330	ARG
2	B	355	ARG
2	B	357	ILE
2	B	359	HIS
2	B	366	ARG
2	B	381	GLU
2	B	399	LYS
2	B	423	LYS
2	B	440	THR
2	B	441	ASN
2	B	442	ARG

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Mol	Chain	Res	Type
2	B	461	LEU
2	B	472	GLN
2	B	512	ARG
2	B	530	SER
2	B	604	THR
2	B	617	ARG
2	B	632	VAL
2	B	650	ASP
2	B	695	THR
2	B	697	LYS
2	B	704	ARG
2	B	706	ARG
2	B	741	LEU
2	B	743	LEU
2	B	744	HIS
1	C	11	THR
1	C	12	ARG
1	C	33	THR
1	C	40	ASN
1	C	41	GLU
1	C	76	ARG
1	C	79	GLU
1	C	91	VAL
1	C	128	LEU
1	C	143	LEU
1	C	165	THR
1	C	212	VAL
1	C	219	LEU
1	C	231	LEU
1	C	237	THR
1	C	281	ILE
1	C	305	LEU
1	C	309	ARG
1	C	339	VAL
1	C	355	LYS
1	C	361	ILE
1	C	368	LEU
1	C	376	LYS
1	C	378	GLU
1	C	379	THR
1	C	401	LEU
1	C	409	ASP

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Mol	Chain	Res	Type
1	C	420	GLN
1	C	425	LEU
1	C	435	ARG
1	C	447	VAL
1	C	451	SER
1	C	455	VAL
2	D	16	VAL
2	D	66	THR
2	D	81	SER
2	D	130	ASP
2	D	151	VAL
2	D	152	GLU
2	D	221	MET
2	D	222	ARG
2	D	247	ARG
2	D	258	ASP
2	D	260	ASP
2	D	268	LYS
2	D	313	LEU
2	D	330	ARG
2	D	367	ASP
2	D	381	GLU
2	D	398	LYS
2	D	399	LYS
2	D	400	THR
2	D	423	LYS
2	D	431	ARG
2	D	450	LEU
2	D	512	ARG
2	D	530	SER
2	D	558	ARG
2	D	567	ILE
2	D	613	ARG
2	D	617	ARG
2	D	632	VAL
2	D	697	LYS
2	D	704	ARG
2	D	741	LEU
1	E	1	MET
1	E	11	THR
1	E	12	ARG
1	E	25	GLU

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Mol	Chain	Res	Type
1	E	33	THR
1	E	40	ASN
1	E	69	GLN
1	E	76	ARG
1	E	79	GLU
1	E	101	SER
1	E	128	LEU
1	E	143	LEU
1	E	165	THR
1	E	185	THR
1	E	187	ASP
1	E	228	CYS
1	E	231	LEU
1	E	237	THR
1	E	257	GLU
1	E	281	ILE
1	E	301	MET
1	E	309	ARG
1	E	341	LEU
1	E	344	SER
1	E	354	SER
1	E	379	THR
1	E	390	VAL
1	E	401	LEU
1	E	409	ASP
1	E	423	THR
1	E	425	LEU
1	E	447	VAL
1	E	450	LEU
1	E	455	VAL
2	F	10	ASP
2	F	16	VAL
2	F	35	LEU
2	F	48	THR
2	F	53	GLU
2	F	66	THR
2	F	145	ILE
2	F	151	VAL
2	F	165	CYS
2	F	176	LEU
2	F	182	LEU
2	F	190	VAL

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Mol	Chain	Res	Type
2	F	222	ARG
2	F	247	ARG
2	F	256	ARG
2	F	258	ASP
2	F	268	LYS
2	F	296	ARG
2	F	313	LEU
2	F	330	ARG
2	F	355	ARG
2	F	357	ILE
2	F	366	ARG
2	F	370	GLU
2	F	381	GLU
2	F	398	LYS
2	F	399	LYS
2	F	405	TYR
2	F	428	THR
2	F	433	GLU
2	F	439	SER
2	F	450	LEU
2	F	461	LEU
2	F	497	VAL
2	F	512	ARG
2	F	516	THR
2	F	530	SER
2	F	558	ARG
2	F	567	ILE
2	F	608	SER
2	F	617	ARG
2	F	630	GLU
2	F	632	VAL
2	F	635	ARG
2	F	641	ARG
2	F	704	ARG
2	F	741	LEU
2	F	744	HIS
2	F	772	ARG
1	G	25	GLU
1	G	33	THR
1	G	35	THR
1	G	37	GLU
1	G	40	ASN

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Mol	Chain	Res	Type
1	G	69	GLN
1	G	76	ARG
1	G	79	GLU
1	G	91	VAL
1	G	103	CYS
1	G	128	LEU
1	G	189	LEU
1	G	212	VAL
1	G	222	VAL
1	G	231	LEU
1	G	234	ILE
1	G	243	ILE
1	G	257	GLU
1	G	281	ILE
1	G	291	ILE
1	G	311	GLN
1	G	315	ARG
1	G	326	ARG
1	G	338	SER
1	G	339	VAL
1	G	340	THR
1	G	341	LEU
1	G	371	THR
1	G	393	ARG
1	G	401	LEU
1	G	409	ASP
1	G	410	THR
1	G	420	GLN
1	G	450	LEU
1	G	455	VAL
1	G	457	VAL
2	H	10	ASP
2	H	16	VAL
2	H	21	ARG
2	H	23	LEU
2	H	48	THR
2	H	66	THR
2	H	90	GLU
2	H	128	THR
2	H	129	LEU
2	H	151	VAL
2	H	161	LEU

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Mol	Chain	Res	Type
2	H	165	CYS
2	H	167	GLU
2	H	176	LEU
2	H	221	MET
2	H	222	ARG
2	H	258	ASP
2	H	260	ASP
2	H	268	LYS
2	H	271	ASP
2	H	313	LEU
2	H	326	ILE
2	H	330	ARG
2	H	355	ARG
2	H	398	LYS
2	H	399	LYS
2	H	400	THR
2	H	423	LYS
2	H	424	SER
2	H	431	ARG
2	H	446	ARG
2	H	471	VAL
2	H	512	ARG
2	H	558	ARG
2	H	604	THR
2	H	617	ARG
2	H	628	ILE
2	H	632	VAL
2	H	641	ARG
2	H	650	ASP
2	H	677	THR
2	H	697	LYS
2	H	704	ARG
2	H	706	ARG
2	H	741	LEU
2	H	743	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	196	HIS
1	A	359	GLN

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Mol	Chain	Res	Type
2	B	106	HIS
2	B	193	HIS
2	B	204	HIS
2	B	208	HIS
2	B	236	ASN
2	B	293	HIS
2	B	359	HIS
2	B	466	GLN
2	B	574	GLN
2	B	640	ASN
1	C	40	ASN
1	C	98	HIS
1	C	233	GLN
1	C	359	GLN
1	C	369	ASN
1	C	420	GLN
2	D	198	HIS
2	D	208	HIS
2	D	234	GLN
2	D	236	ASN
2	D	293	HIS
2	D	359	HIS
2	D	426	ASN
2	D	441	ASN
2	D	463	HIS
2	D	715	GLN
2	D	744	HIS
1	E	40	ASN
1	E	61	ASN
1	E	196	HIS
1	E	359	GLN
2	F	19	GLN
2	F	193	HIS
2	F	204	HIS
2	F	236	ASN
2	F	359	HIS
2	F	426	ASN
2	F	441	ASN
2	F	463	HIS
2	F	482	ASN
2	F	574	GLN
2	F	715	GLN

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Mol	Chain	Res	Type
2	F	744	HIS
1	G	40	ASN
1	G	98	HIS
1	G	196	HIS
1	G	359	GLN
2	H	106	HIS
2	H	208	HIS
2	H	236	ASN
2	H	293	HIS
2	H	359	HIS
2	H	536	ASN
2	H	572	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 4 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	$\# Z > 2$
3	FES	A	1464	1	0,4,4	-	-	-		
3	FES	G	1463	1	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	XAN	D	1780[B]	-	12,12,12	1.96	2 (16%)	14,17,17	2.43	8 (57%)
7	XAN	F	1780[A]	-	12,12,12	1.94	1 (8%)	14,17,17	2.30	6 (42%)
8	MOM	H	1781	5	0,3,3	-	-	-	-	-
7	XAN	H	1780[A]	-	12,12,12	1.94	2 (16%)	14,17,17	2.23	5 (35%)
7	XAN	B	1780[B]	-	12,12,12	2.06	2 (16%)	14,17,17	2.34	6 (42%)
8	MOM	F	1781	5	0,3,3	-	-	-	-	-
5	MTE	F	1778	8	21,26,26	4.26	6 (28%)	19,40,40	3.17	9 (47%)
3	FES	C	1463	1	0,4,4	-	-	-	-	-
7	XAN	F	1780[B]	-	12,12,12	1.95	2 (16%)	14,17,17	2.34	6 (42%)
7	XAN	H	1780[B]	-	12,12,12	2.03	2 (16%)	14,17,17	2.38	6 (42%)
5	MTE	D	1778	8	21,26,26	4.16	6 (28%)	19,40,40	3.45	7 (36%)
8	MOM	D	1781	5	0,3,3	-	-	-	-	-
5	MTE	B	1778	8	21,26,26	4.12	5 (23%)	19,40,40	3.58	8 (42%)
3	FES	A	1463	1	0,4,4	-	-	-	-	-
4	FAD	G	1465	-	58,58,58	1.39	8 (13%)	85,89,89	1.78	18 (21%)
8	MOM	B	1781	5	0,3,3	-	-	-	-	-
3	FES	G	1464	1	0,4,4	-	-	-	-	-
5	MTE	H	1778	8	21,26,26	3.95	6 (28%)	19,40,40	3.16	6 (31%)
3	FES	E	1464	1	0,4,4	-	-	-	-	-
4	FAD	E	1465	-	58,58,58	1.46	9 (15%)	85,89,89	1.70	21 (24%)
4	FAD	A	1465	-	58,58,58	1.43	7 (12%)	85,89,89	1.71	19 (22%)
7	XAN	D	1780[A]	-	12,12,12	1.95	2 (16%)	14,17,17	2.19	5 (35%)
3	FES	E	1463	1	0,4,4	-	-	-	-	-
7	XAN	B	1780[A]	-	12,12,12	1.96	2 (16%)	14,17,17	2.30	6 (42%)
3	FES	C	1464	1	0,4,4	-	-	-	-	-
4	FAD	C	1465	-	58,58,58	1.64	10 (17%)	85,89,89	1.83	21 (24%)

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
3	FES	A	1464	1	-	-	0/1/1/1
3	FES	G	1463	1	-	-	0/1/1/1
7	XAN	D	1780[B]	-	-	-	0/2/2/2
7	XAN	F	1780[A]	-	-	-	0/2/2/2
7	XAN	H	1780[A]	-	-	-	0/2/2/2
7	XAN	B	1780[B]	-	-	-	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MTE	F	1778	8	1/1/6/8	1/6/34/34	0/3/3/3
3	FES	C	1463	1	-	-	0/1/1/1
7	XAN	F	1780[B]	-	-	-	0/2/2/2
7	XAN	H	1780[B]	-	-	-	0/2/2/2
5	MTE	D	1778	8	1/1/6/8	2/6/34/34	0/3/3/3
5	MTE	B	1778	8	1/1/6/8	1/6/34/34	0/3/3/3
3	FES	A	1463	1	-	-	0/1/1/1
4	FAD	G	1465	-	-	8/34/50/50	0/6/6/6
3	FES	G	1464	1	-	-	0/1/1/1
5	MTE	H	1778	8	1/1/6/8	2/6/34/34	0/3/3/3
3	FES	E	1464	1	-	-	0/1/1/1
4	FAD	E	1465	-	-	16/34/50/50	0/6/6/6
4	FAD	A	1465	-	-	11/34/50/50	0/6/6/6
7	XAN	D	1780[A]	-	-	-	0/2/2/2
3	FES	E	1463	1	-	-	0/1/1/1
7	XAN	B	1780[A]	-	-	-	0/2/2/2
3	FES	C	1464	1	-	-	0/1/1/1
4	FAD	C	1465	-	-	9/34/50/50	0/6/6/6

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	1778	MTE	C4'-C3'	-14.24	1.32	1.51
5	B	1778	MTE	C4'-C3'	-13.59	1.33	1.51
5	D	1778	MTE	C4'-C3'	-13.42	1.33	1.51
5	H	1778	MTE	C4'-C3'	-11.87	1.35	1.51
5	D	1778	MTE	C6-N5	-11.30	1.33	1.46
5	F	1778	MTE	C6-N5	-11.00	1.34	1.46
5	H	1778	MTE	C6-N5	-10.99	1.34	1.46
5	B	1778	MTE	C6-N5	-10.81	1.34	1.46
5	H	1778	MTE	C9-C10	5.48	1.48	1.38
7	B	1780[B]	XAN	C5-C4	5.39	1.48	1.38
5	B	1778	MTE	C9-C10	5.29	1.47	1.38
7	H	1780[B]	XAN	C5-C4	5.28	1.48	1.38
4	A	1465	FAD	C4X-N5	5.16	1.41	1.30
7	B	1780[A]	XAN	C5-C4	5.13	1.48	1.38
7	H	1780[A]	XAN	C5-C4	5.08	1.48	1.38
7	D	1780[A]	XAN	C5-C4	5.07	1.47	1.38
7	F	1780[B]	XAN	C5-C4	5.05	1.47	1.38
7	F	1780[A]	XAN	C5-C4	5.03	1.47	1.38
5	D	1778	MTE	C9-C10	5.01	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	1780[B]	XAN	C5-C4	4.90	1.47	1.38
4	E	1465	FAD	C4X-N5	4.84	1.41	1.30
5	F	1778	MTE	C9-C10	4.79	1.46	1.38
4	C	1465	FAD	C10-N1	4.45	1.42	1.33
4	C	1465	FAD	C4X-N5	4.43	1.40	1.30
4	C	1465	FAD	P-O3P	4.41	1.64	1.59
4	G	1465	FAD	C4X-N5	4.14	1.39	1.30
4	E	1465	FAD	C10-N1	4.07	1.41	1.33
4	G	1465	FAD	C10-N1	4.03	1.41	1.33
4	C	1465	FAD	C2'-C3'	-3.76	1.46	1.53
4	A	1465	FAD	C10-N1	3.75	1.40	1.33
4	G	1465	FAD	O4B-C1B	3.49	1.50	1.42
5	H	1778	MTE	C9-N5	3.30	1.45	1.37
4	G	1465	FAD	PA-O3P	3.26	1.63	1.59
5	F	1778	MTE	C7-C6	-3.18	1.51	1.53
4	A	1465	FAD	C5A-N7A	-3.18	1.33	1.39
5	B	1778	MTE	C9-N5	3.15	1.45	1.37
4	E	1465	FAD	O4B-C1B	3.12	1.49	1.42
4	A	1465	FAD	C1'-C2'	3.08	1.56	1.52
4	C	1465	FAD	PA-O3P	3.05	1.62	1.59
5	F	1778	MTE	C9-N5	3.00	1.44	1.37
5	D	1778	MTE	C9-N5	2.96	1.44	1.37
4	G	1465	FAD	C5A-N7A	-2.84	1.33	1.39
5	H	1778	MTE	C7-C6	-2.80	1.51	1.53
4	E	1465	FAD	C5A-N7A	-2.79	1.34	1.39
4	E	1465	FAD	P-O3P	2.78	1.62	1.59
4	C	1465	FAD	C5A-N7A	-2.59	1.34	1.39
4	E	1465	FAD	PA-O3P	2.59	1.62	1.59
4	A	1465	FAD	O4B-C1B	2.57	1.47	1.42
7	D	1780[B]	XAN	C6-N1	-2.55	1.34	1.38
5	D	1778	MTE	C9-C4	2.52	1.49	1.41
4	C	1465	FAD	C2-N1	2.43	1.42	1.36
4	E	1465	FAD	C5B-C4B	2.39	1.58	1.51
7	B	1780[B]	XAN	C6-N1	-2.34	1.34	1.38
7	H	1780[B]	XAN	C6-N1	-2.33	1.34	1.38
5	H	1778	MTE	C9-C4	2.31	1.48	1.41
4	A	1465	FAD	C8A-N9A	-2.29	1.33	1.37
4	A	1465	FAD	C10-N10	2.26	1.42	1.37
5	B	1778	MTE	C9-C4	2.22	1.48	1.41
5	F	1778	MTE	C9-C4	2.22	1.48	1.41
4	E	1465	FAD	C10-N10	2.22	1.42	1.37
4	C	1465	FAD	C4A-N9A	-2.21	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1465	FAD	C10-N10	2.18	1.42	1.37
4	G	1465	FAD	C8A-N9A	-2.13	1.33	1.37
7	B	1780[A]	XAN	C6-N1	-2.13	1.34	1.38
5	D	1778	MTE	C7-C6	-2.13	1.52	1.53
7	F	1780[B]	XAN	C6-N1	-2.11	1.34	1.38
7	H	1780[A]	XAN	C6-N1	-2.09	1.34	1.38
4	C	1465	FAD	O5'-C5'	-2.07	1.36	1.44
4	G	1465	FAD	C2-N1	2.07	1.41	1.36
4	G	1465	FAD	C10-N10	2.06	1.41	1.37
7	D	1780[A]	XAN	C6-N1	-2.05	1.35	1.38
4	E	1465	FAD	C4A-N9A	-2.02	1.33	1.37

All (157) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1778	MTE	C7-C6-N5	11.04	118.72	107.87
5	D	1778	MTE	C7-C6-N5	10.49	118.17	107.87
5	H	1778	MTE	C7-C6-N5	10.28	117.97	107.87
5	F	1778	MTE	C7-C6-N5	9.08	116.79	107.87
4	C	1465	FAD	O4B-C1B-N9A	-5.85	96.85	108.09
4	A	1465	FAD	C5A-C4A-N3A	-5.58	119.04	126.72
4	C	1465	FAD	C5A-C4A-N3A	-5.54	119.08	126.72
5	H	1778	MTE	O4'-C4'-C3'	5.51	122.18	108.58
5	D	1778	MTE	O4'-C4'-C3'	5.40	121.92	108.58
5	F	1778	MTE	C2-N1-C10	5.39	122.88	113.36
4	E	1465	FAD	C5A-C4A-N3A	-5.33	119.38	126.72
5	D	1778	MTE	O3'-C7-C6	5.31	112.51	108.96
4	G	1465	FAD	O4B-C1B-N9A	-5.25	98.01	108.09
4	G	1465	FAD	C5A-C4A-N3A	-5.21	119.54	126.72
4	G	1465	FAD	N3A-C2A-N1A	-5.05	120.93	128.58
5	F	1778	MTE	O4'-C4'-C3'	4.87	120.61	108.58
5	B	1778	MTE	O4'-C4'-C3'	4.87	120.59	108.58
4	E	1465	FAD	N3A-C2A-N1A	-4.81	121.30	128.58
5	B	1778	MTE	O3'-C7-C6	4.77	112.15	108.96
7	B	1780[B]	XAN	N1-C2-N3	4.75	123.21	115.74
7	H	1780[B]	XAN	N1-C2-N3	4.75	123.20	115.74
7	D	1780[B]	XAN	N1-C2-N3	4.61	122.99	115.74
4	A	1465	FAD	N3A-C2A-N1A	-4.60	121.62	128.58
7	B	1780[A]	XAN	N1-C2-N3	4.58	122.94	115.74
5	B	1778	MTE	C2-N1-C10	4.46	121.23	113.36
5	D	1778	MTE	C2-N1-C10	4.38	121.09	113.36
7	F	1780[B]	XAN	N1-C2-N3	4.36	122.59	115.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	1780[A]	XAN	N1-C2-N3	4.35	122.58	115.74
7	H	1780[A]	XAN	N1-C2-N3	4.33	122.55	115.74
7	D	1780[A]	XAN	N1-C2-N3	4.27	122.45	115.74
4	A	1465	FAD	N3A-C4A-N9A	4.21	134.32	127.17
4	G	1465	FAD	C2B-C1B-N9A	4.21	123.75	113.30
5	H	1778	MTE	C2-N1-C10	4.10	120.60	113.36
4	C	1465	FAD	N3A-C2A-N1A	-3.99	122.54	128.58
4	C	1465	FAD	C4'-C3'-C2'	-3.99	106.94	113.57
4	G	1465	FAD	C2A-N3A-C4A	3.82	121.17	111.83
4	E	1465	FAD	N3A-C4A-N9A	3.81	133.64	127.17
4	E	1465	FAD	C2A-N3A-C4A	3.80	121.12	111.83
4	C	1465	FAD	C2A-N3A-C4A	3.77	121.04	111.83
4	C	1465	FAD	N3A-C4A-N9A	3.72	133.50	127.17
4	G	1465	FAD	N3A-C4A-N9A	3.70	133.46	127.17
4	G	1465	FAD	N9A-C8A-N7A	-3.66	108.74	113.94
5	B	1778	MTE	O3P-P-O4'	-3.65	97.16	106.67
4	A	1465	FAD	C2A-N3A-C4A	3.52	120.42	111.83
5	B	1778	MTE	O3'-C7-N8	-3.47	105.46	108.61
4	A	1465	FAD	N9A-C8A-N7A	-3.45	109.04	113.94
7	D	1780[B]	XAN	C6-C5-N7	3.45	136.56	130.29
7	F	1780[B]	XAN	C6-C5-N7	3.36	136.40	130.29
4	E	1465	FAD	O4B-C1B-N9A	3.36	114.54	108.09
5	D	1778	MTE	C4-C9-N5	3.36	125.42	116.27
4	C	1465	FAD	N9A-C8A-N7A	-3.34	109.20	113.94
4	G	1465	FAD	C4-N3-C2	-3.33	119.73	125.64
7	H	1780[B]	XAN	C6-C5-N7	3.30	136.30	130.29
4	G	1465	FAD	C5A-N7A-C8A	3.27	108.58	103.45
4	E	1465	FAD	C4-N3-C2	-3.27	119.84	125.64
5	F	1778	MTE	O3P-P-O4'	-3.26	98.18	106.67
7	F	1780[A]	XAN	N9-C4-N3	3.24	135.25	128.34
7	F	1780[B]	XAN	N9-C4-N3	3.22	135.21	128.34
7	B	1780[B]	XAN	C6-C5-N7	3.20	136.12	130.29
4	E	1465	FAD	C9A-C5X-N5	-3.19	119.06	122.45
5	H	1778	MTE	C4-C9-N5	3.19	124.97	116.27
4	A	1465	FAD	C5A-N7A-C8A	3.19	108.47	103.45
7	H	1780[A]	XAN	N9-C4-N3	3.19	135.14	128.34
4	A	1465	FAD	C4-N3-C2	-3.16	120.02	125.64
7	H	1780[B]	XAN	N9-C4-N3	3.16	135.09	128.34
7	D	1780[A]	XAN	N9-C4-N3	3.16	135.08	128.34
7	B	1780[A]	XAN	N9-C4-N3	3.14	135.04	128.34
5	B	1778	MTE	C4-C9-N5	3.14	124.83	116.27
7	D	1780[B]	XAN	N9-C4-N3	3.14	135.03	128.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	1778	MTE	C4-C9-N5	3.13	124.80	116.27
4	A	1465	FAD	O4B-C1B-N9A	-3.12	102.09	108.09
7	F	1780[A]	XAN	C6-C5-N7	3.12	135.97	130.29
7	H	1780[B]	XAN	C6-N1-C2	-3.11	122.09	126.37
4	C	1465	FAD	C4A-C5A-N7A	-3.10	107.03	110.58
7	B	1780[B]	XAN	N9-C4-N3	3.10	134.95	128.34
7	D	1780[B]	XAN	C6-N1-C2	-3.10	122.11	126.37
7	B	1780[A]	XAN	C6-N1-C2	-3.08	122.12	126.37
4	G	1465	FAD	C4A-C5A-N7A	-3.08	107.06	110.58
4	A	1465	FAD	C5X-C9A-N10	3.06	120.73	117.97
7	F	1780[A]	XAN	C6-N1-C2	-3.04	122.19	126.37
4	A	1465	FAD	C4X-C10-N10	3.01	120.79	116.48
4	C	1465	FAD	O2'-C2'-C3'	-3.01	102.21	109.25
7	F	1780[B]	XAN	C6-N1-C2	-2.99	122.25	126.37
7	B	1780[B]	XAN	C6-N1-C2	-2.98	122.26	126.37
4	C	1465	FAD	C5A-N7A-C8A	2.97	108.12	103.45
4	A	1465	FAD	C2B-C1B-N9A	2.97	120.68	113.30
7	H	1780[A]	XAN	C6-C5-N7	2.97	135.69	130.29
4	C	1465	FAD	C2B-C1B-N9A	2.94	120.61	113.30
7	B	1780[A]	XAN	C6-C5-N7	2.92	135.60	130.29
5	D	1778	MTE	O3P-P-O4'	-2.87	99.18	106.67
7	H	1780[A]	XAN	C6-N1-C2	-2.87	122.42	126.37
4	C	1465	FAD	C4-N3-C2	-2.86	120.56	125.64
7	D	1780[A]	XAN	C6-C5-N7	2.84	135.46	130.29
4	E	1465	FAD	N9A-C8A-N7A	-2.82	109.93	113.94
4	E	1465	FAD	C4X-C4-N3	2.82	120.42	113.25
4	C	1465	FAD	C9A-C5X-N5	-2.80	119.48	122.45
5	F	1778	MTE	O4-C4-C9	-2.75	120.64	127.26
4	G	1465	FAD	C4A-N9A-C8A	2.73	108.61	105.74
4	E	1465	FAD	C10-C4X-N5	-2.73	119.24	124.81
4	A	1465	FAD	C4A-C5A-N7A	-2.72	107.47	110.58
4	G	1465	FAD	C4X-C4-N3	2.71	120.15	113.25
7	D	1780[A]	XAN	C6-N1-C2	-2.69	122.67	126.37
5	H	1778	MTE	O3'-C7-C6	-2.68	107.17	108.96
7	D	1780[B]	XAN	C8-N7-C5	2.63	107.94	104.38
4	G	1465	FAD	C10-C4X-N5	-2.59	119.52	124.81
4	A	1465	FAD	C4X-C4-N3	2.57	119.80	113.25
4	E	1465	FAD	C4X-C10-N1	-2.55	118.33	124.59
4	E	1465	FAD	C5X-C9A-N10	2.52	120.25	117.97
5	F	1778	MTE	C9-C4-N3	2.52	119.05	112.13
4	A	1465	FAD	C4A-N9A-C8A	2.51	108.38	105.74
4	C	1465	FAD	C5X-N5-C4X	2.50	122.13	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1465	FAD	C4X-C10-N10	2.48	120.03	116.48
4	C	1465	FAD	C4X-C4-N3	2.45	119.50	113.25
4	C	1465	FAD	O3'-C3'-C4'	2.45	114.49	108.93
7	D	1780[B]	XAN	O2-C2-N1	-2.44	117.52	121.86
4	C	1465	FAD	C10-C4X-N5	-2.43	119.84	124.81
4	A	1465	FAD	O4-C4-C4X	-2.41	120.17	126.53
4	E	1465	FAD	C5A-N7A-C8A	2.41	107.23	103.45
7	F	1780[B]	XAN	C8-N7-C5	2.40	107.62	104.38
7	D	1780[A]	XAN	O6-C6-C5	-2.39	120.21	126.53
4	C	1465	FAD	O4-C4-C4X	-2.38	120.24	126.53
4	G	1465	FAD	C4X-C10-N10	2.38	119.89	116.48
7	B	1780[B]	XAN	O2-C2-N1	-2.38	117.64	121.86
4	C	1465	FAD	C4A-N9A-C8A	2.36	108.22	105.74
5	F	1778	MTE	O3P-P-O1P	2.32	119.86	110.83
7	H	1780[B]	XAN	O2-C2-N1	-2.30	117.78	121.86
4	C	1465	FAD	C4-C4X-C10	2.29	120.86	116.93
7	F	1780[B]	XAN	O2-C2-N1	-2.29	117.79	121.86
4	A	1465	FAD	C4X-C10-N1	-2.29	118.98	124.59
4	A	1465	FAD	C10-C4X-N5	-2.27	120.17	124.81
7	H	1780[B]	XAN	C8-N7-C5	2.26	107.43	104.38
4	E	1465	FAD	C5X-N5-C4X	2.26	121.74	118.09
4	G	1465	FAD	C9A-C5X-N5	-2.26	120.06	122.45
7	B	1780[B]	XAN	C8-N7-C5	2.25	107.42	104.38
5	B	1778	MTE	C9-C4-N3	2.25	118.30	112.13
4	E	1465	FAD	O3'-C3'-C4'	2.25	114.04	108.93
4	E	1465	FAD	C4A-C5A-N7A	-2.24	108.02	110.58
7	B	1780[A]	XAN	O6-C6-C5	-2.23	120.66	126.53
7	H	1780[A]	XAN	O6-C6-C5	-2.21	120.71	126.53
7	F	1780[A]	XAN	C8-N7-C5	2.20	107.36	104.38
7	F	1780[A]	XAN	O6-C6-C5	-2.19	120.75	126.53
4	G	1465	FAD	O3B-C3B-C4B	-2.18	104.83	111.08
4	G	1465	FAD	C4X-C10-N1	-2.17	119.28	124.59
7	D	1780[B]	XAN	C4-C5-N7	-2.15	106.52	109.28
4	A	1465	FAD	C4-C4X-C10	2.14	120.60	116.93
4	C	1465	FAD	O5'-C5'-C4'	-2.14	103.66	109.36
4	G	1465	FAD	C4-C4X-C10	2.12	120.56	116.93
4	E	1465	FAD	C6-C5X-C9A	2.11	121.95	119.05
5	D	1778	MTE	C9-C4-N3	2.10	117.91	112.13
7	D	1780[B]	XAN	N9-C8-N7	-2.09	110.55	112.98
5	F	1778	MTE	C2-N3-C4	-2.08	121.34	125.11
4	E	1465	FAD	C4-C4X-C10	2.07	120.48	116.93
4	E	1465	FAD	O4-C4-C4X	-2.06	121.08	126.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	1778	MTE	C9-C4-N3	2.06	117.78	112.13
4	A	1465	FAD	O4'-C4'-C3'	2.05	114.05	109.25
4	E	1465	FAD	C5'-C4'-C3'	-2.05	108.34	112.22
7	B	1780[A]	XAN	C8-N7-C5	2.04	107.13	104.38

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	1778	MTE	C3'
5	D	1778	MTE	C3'
5	F	1778	MTE	C3'
5	H	1778	MTE	C3'

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1465	FAD	C2'-C1'-N10-C10
4	A	1465	FAD	N10-C1'-C2'-O2'
4	A	1465	FAD	N10-C1'-C2'-C3'
4	A	1465	FAD	C2'-C3'-C4'-O4'
4	A	1465	FAD	C2'-C3'-C4'-C5'
4	A	1465	FAD	O3'-C3'-C4'-O4'
4	A	1465	FAD	O3'-C3'-C4'-C5'
4	A	1465	FAD	C3'-C4'-C5'-O5'
4	A	1465	FAD	O4'-C4'-C5'-O5'
4	A	1465	FAD	C5'-O5'-P-O3P
4	C	1465	FAD	N10-C1'-C2'-O2'
4	C	1465	FAD	N10-C1'-C2'-C3'
4	C	1465	FAD	C2'-C3'-C4'-O4'
4	C	1465	FAD	C2'-C3'-C4'-C5'
4	C	1465	FAD	O3'-C3'-C4'-O4'
4	C	1465	FAD	O3'-C3'-C4'-C5'
4	C	1465	FAD	C3'-C4'-C5'-O5'
4	C	1465	FAD	O4'-C4'-C5'-O5'
4	E	1465	FAD	O4B-C4B-C5B-O5B
4	E	1465	FAD	C2'-C1'-N10-C10
4	E	1465	FAD	N10-C1'-C2'-O2'
4	E	1465	FAD	N10-C1'-C2'-C3'
4	E	1465	FAD	C2'-C3'-C4'-O4'
4	E	1465	FAD	C2'-C3'-C4'-C5'
4	E	1465	FAD	O3'-C3'-C4'-O4'
4	E	1465	FAD	O3'-C3'-C4'-C5'

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Mol	Chain	Res	Type	Atoms
4	E	1465	FAD	C3'-C4'-C5'-O5'
4	E	1465	FAD	O4'-C4'-C5'-O5'
4	G	1465	FAD	C2'-C3'-C4'-O4'
4	G	1465	FAD	C2'-C3'-C4'-C5'
4	G	1465	FAD	O3'-C3'-C4'-O4'
4	G	1465	FAD	O3'-C3'-C4'-C5'
5	B	1778	MTE	C2'-C3'-C4'-O4'
5	D	1778	MTE	O3'-C3'-C4'-O4'
5	F	1778	MTE	O3'-C3'-C4'-O4'
5	H	1778	MTE	O3'-C3'-C4'-O4'
4	E	1465	FAD	C3B-C4B-C5B-O5B
4	G	1465	FAD	C3'-C4'-C5'-O5'
4	G	1465	FAD	O4'-C4'-C5'-O5'
4	G	1465	FAD	N10-C1'-C2'-C3'
4	A	1465	FAD	C5'-O5'-P-O1P
4	C	1465	FAD	C2'-C1'-N10-C10
4	E	1465	FAD	C5B-O5B-PA-O1A
4	E	1465	FAD	C5B-O5B-PA-O2A
4	E	1465	FAD	C5B-O5B-PA-O3P
5	H	1778	MTE	C3'-C4'-O4'-P
4	E	1465	FAD	C4'-C5'-O5'-P
5	D	1778	MTE	C3'-C4'-O4'-P
4	G	1465	FAD	N10-C1'-C2'-O2'
4	E	1465	FAD	PA-O3P-P-O1P

There are no ring outliers.

15 monomers are involved in 35 short contacts:

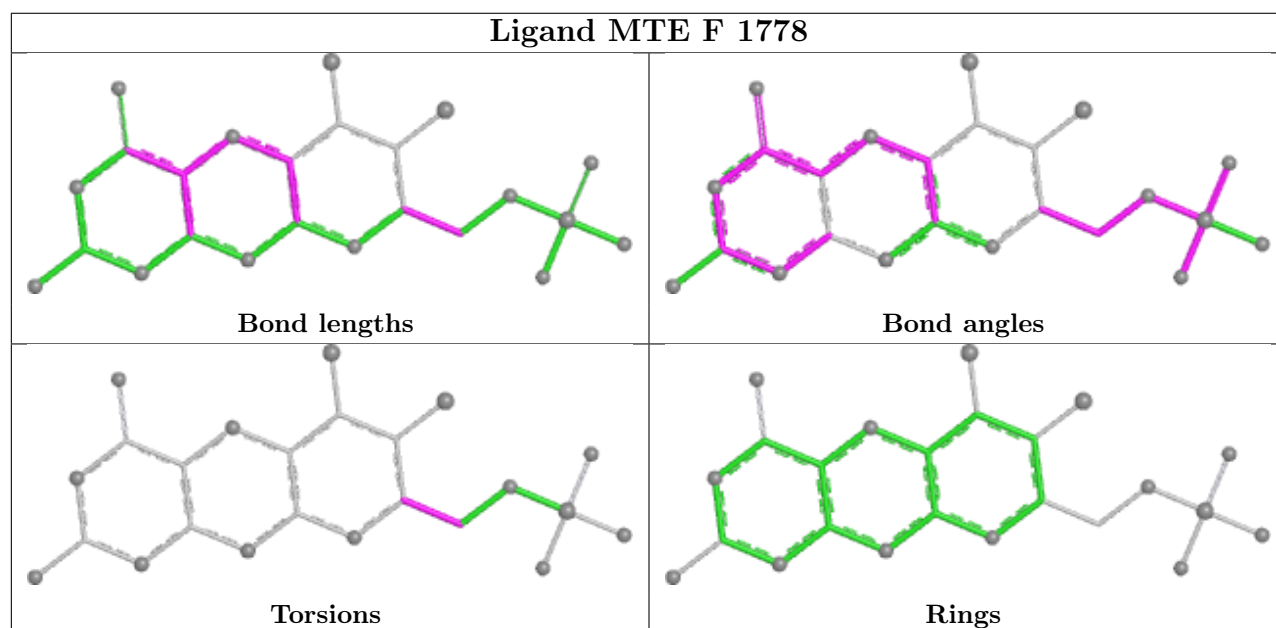
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1463	FES	1	0
7	D	1780[B]	XAN	1	0
8	H	1781	MOM	2	0
8	F	1781	MOM	2	0
5	F	1778	MTE	2	0
5	D	1778	MTE	1	0
8	D	1781	MOM	5	0
3	A	1463	FES	1	0
4	G	1465	FAD	3	0
8	B	1781	MOM	2	0
5	H	1778	MTE	3	0
4	E	1465	FAD	3	0
4	A	1465	FAD	6	0

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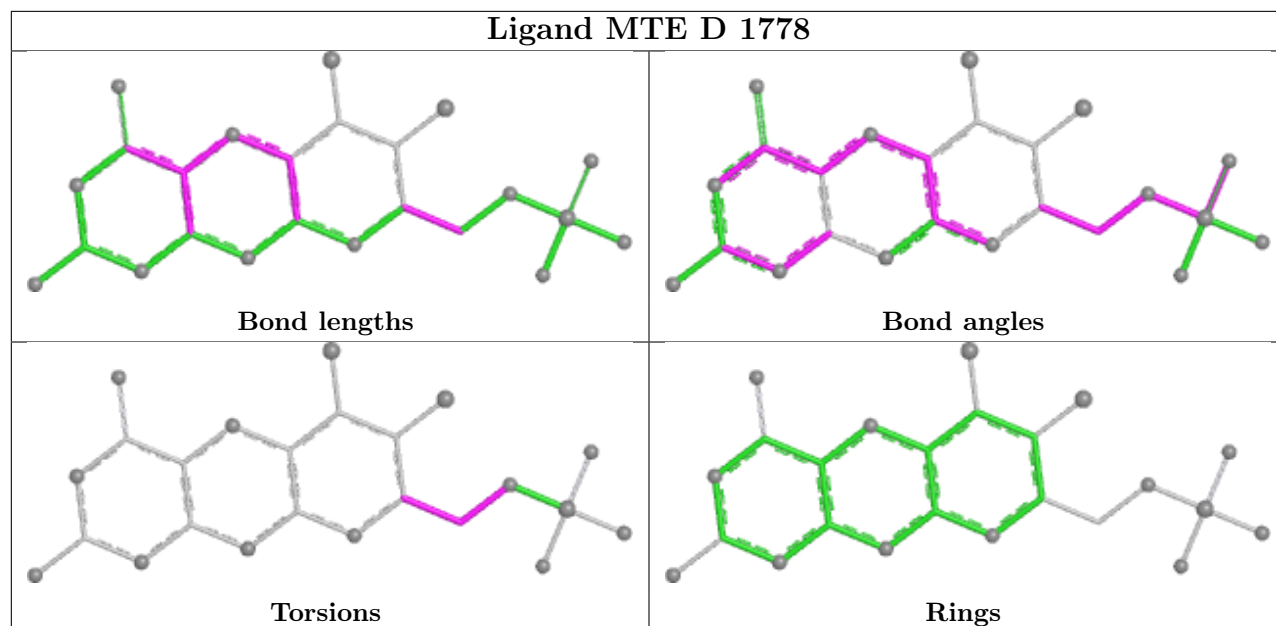
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	1780[A]	XAN	2	0
4	C	1465	FAD	4	0

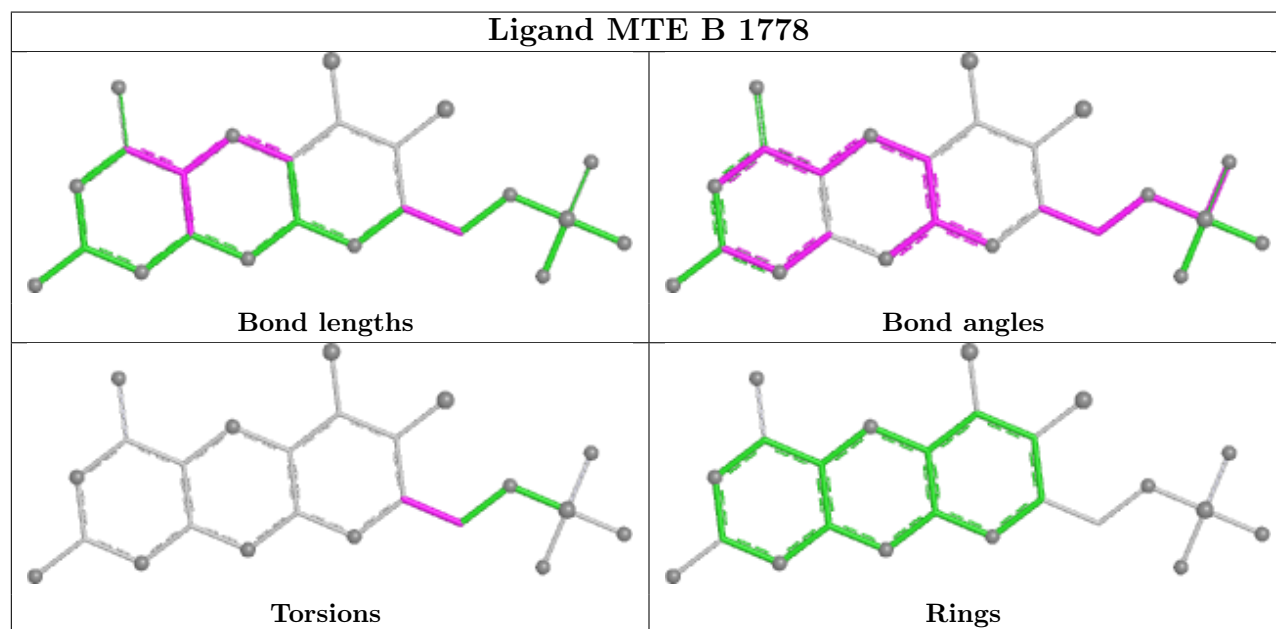
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



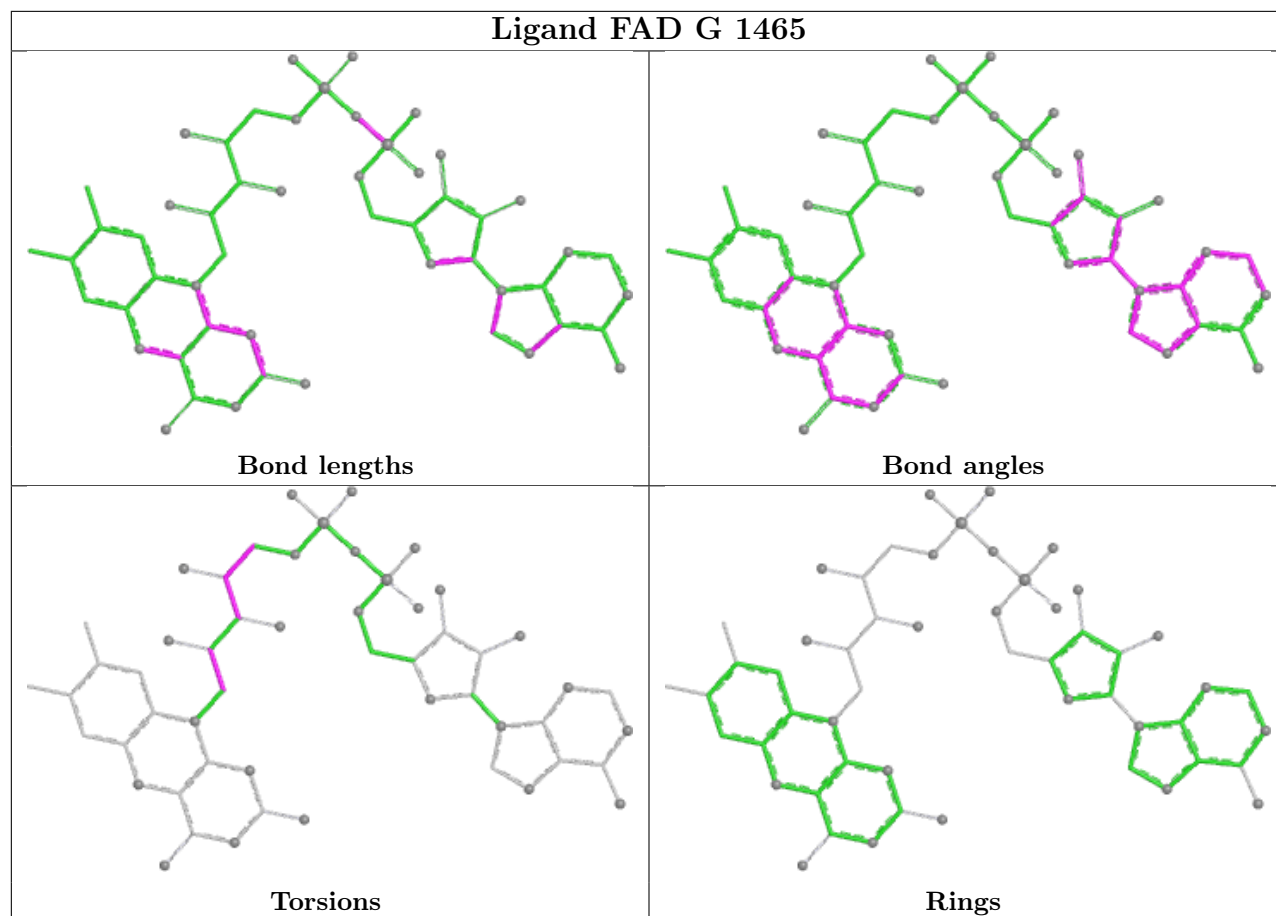
Ligand MTE D 1778



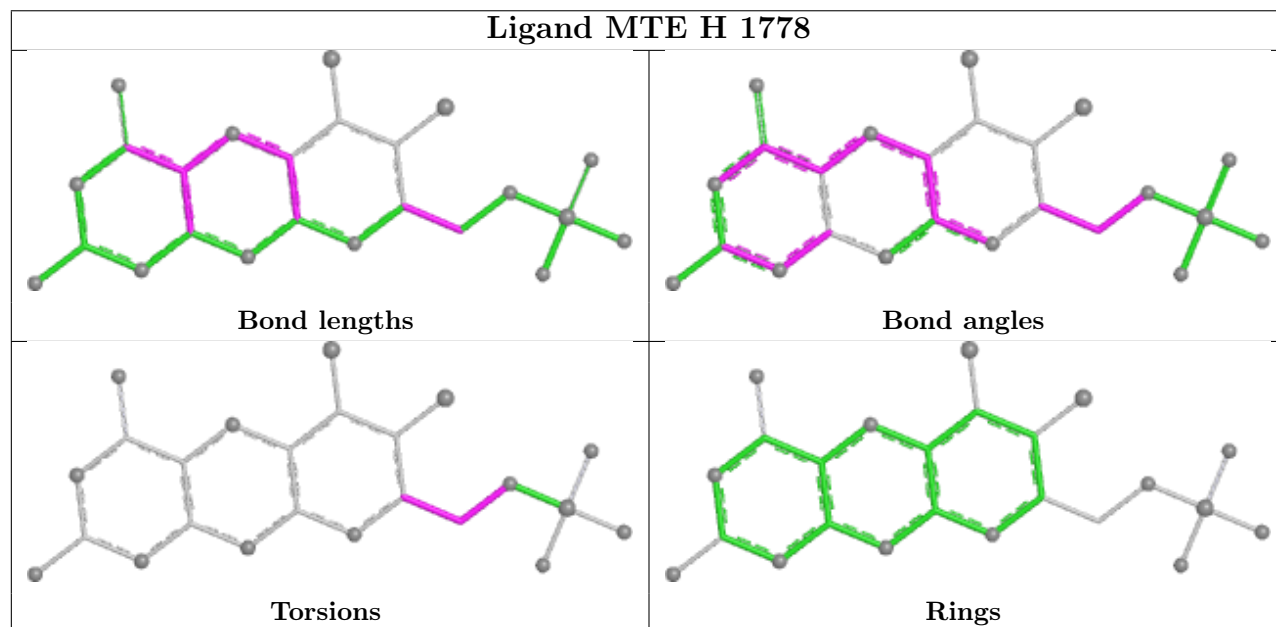
Ligand MTE B 1778

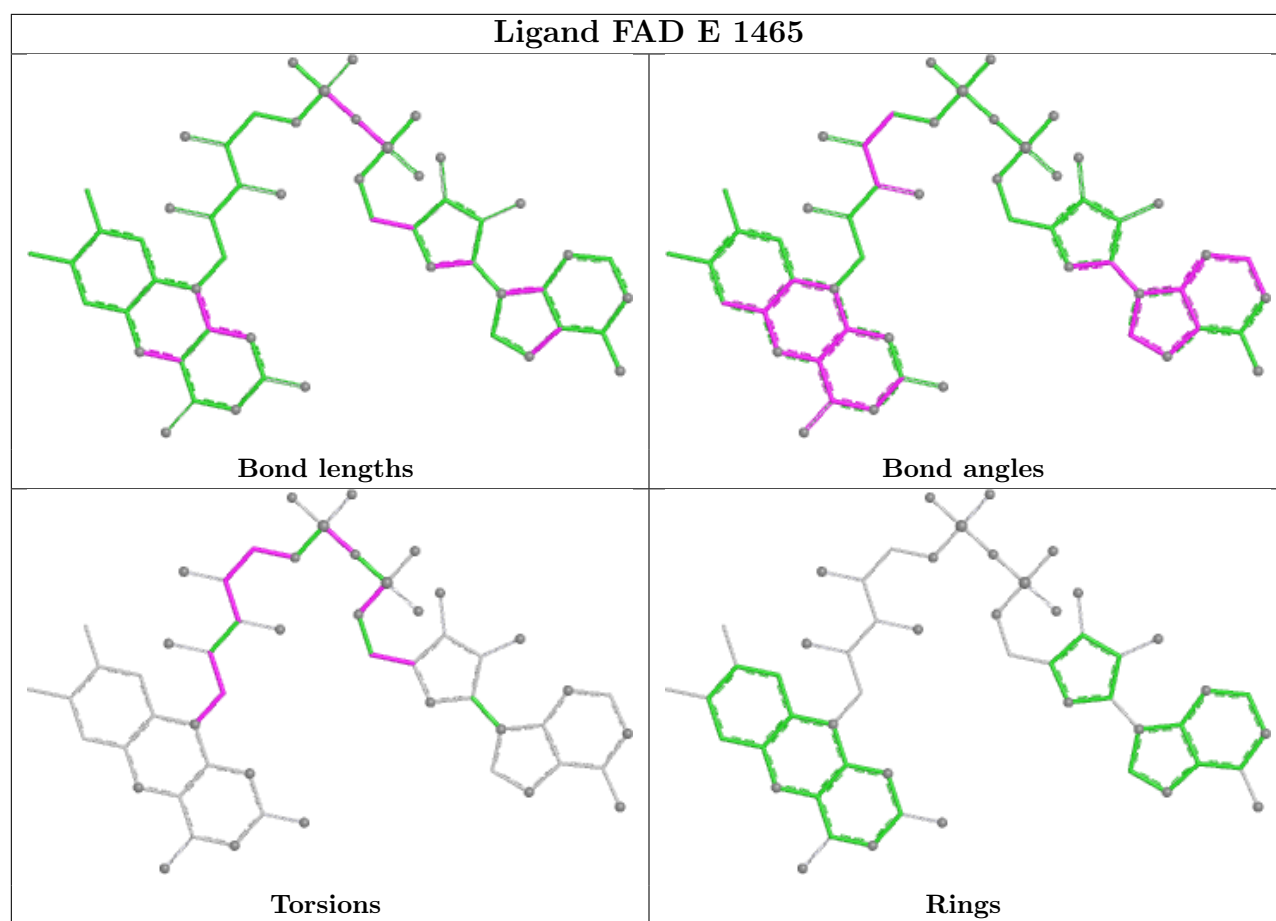


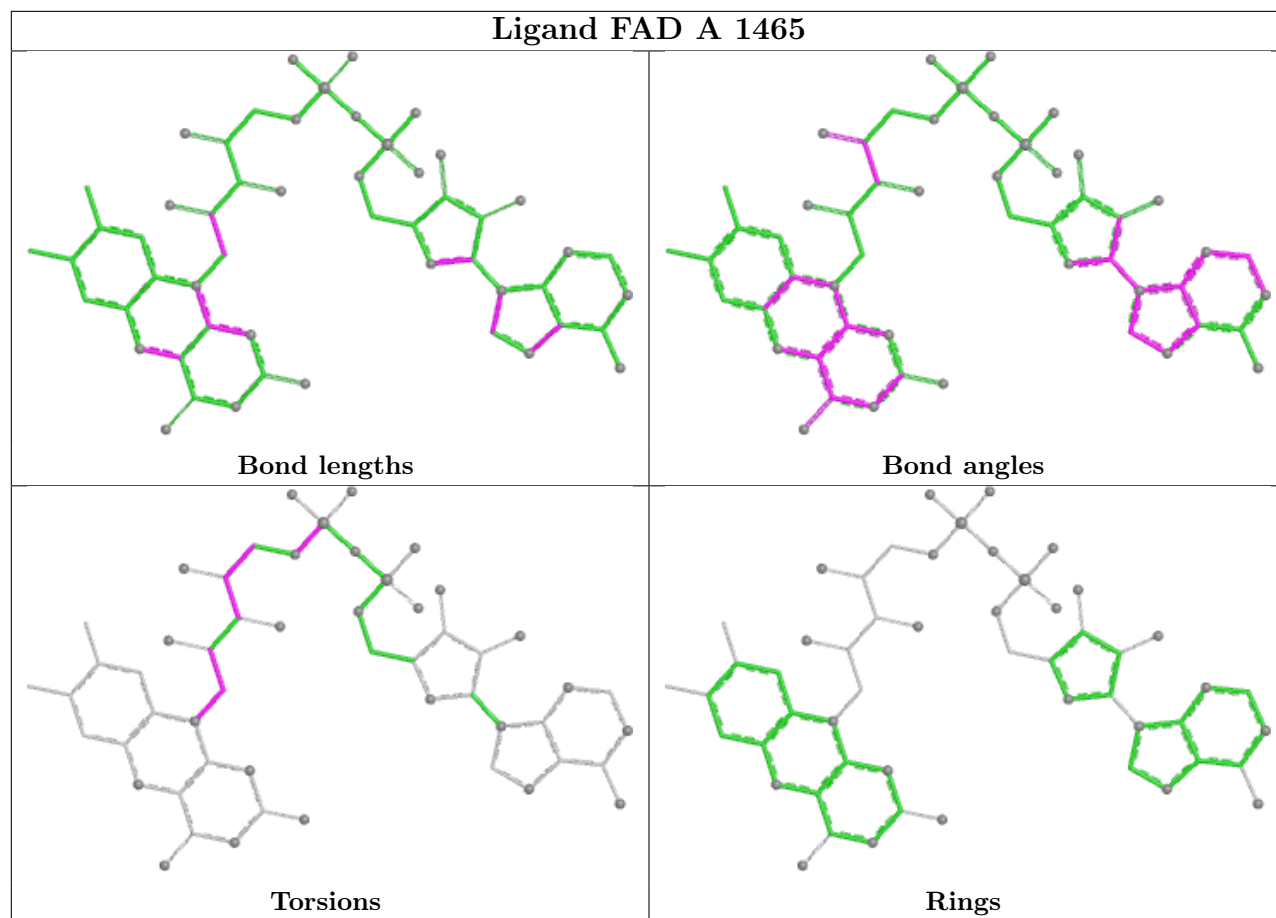
Ligand FAD G 1465

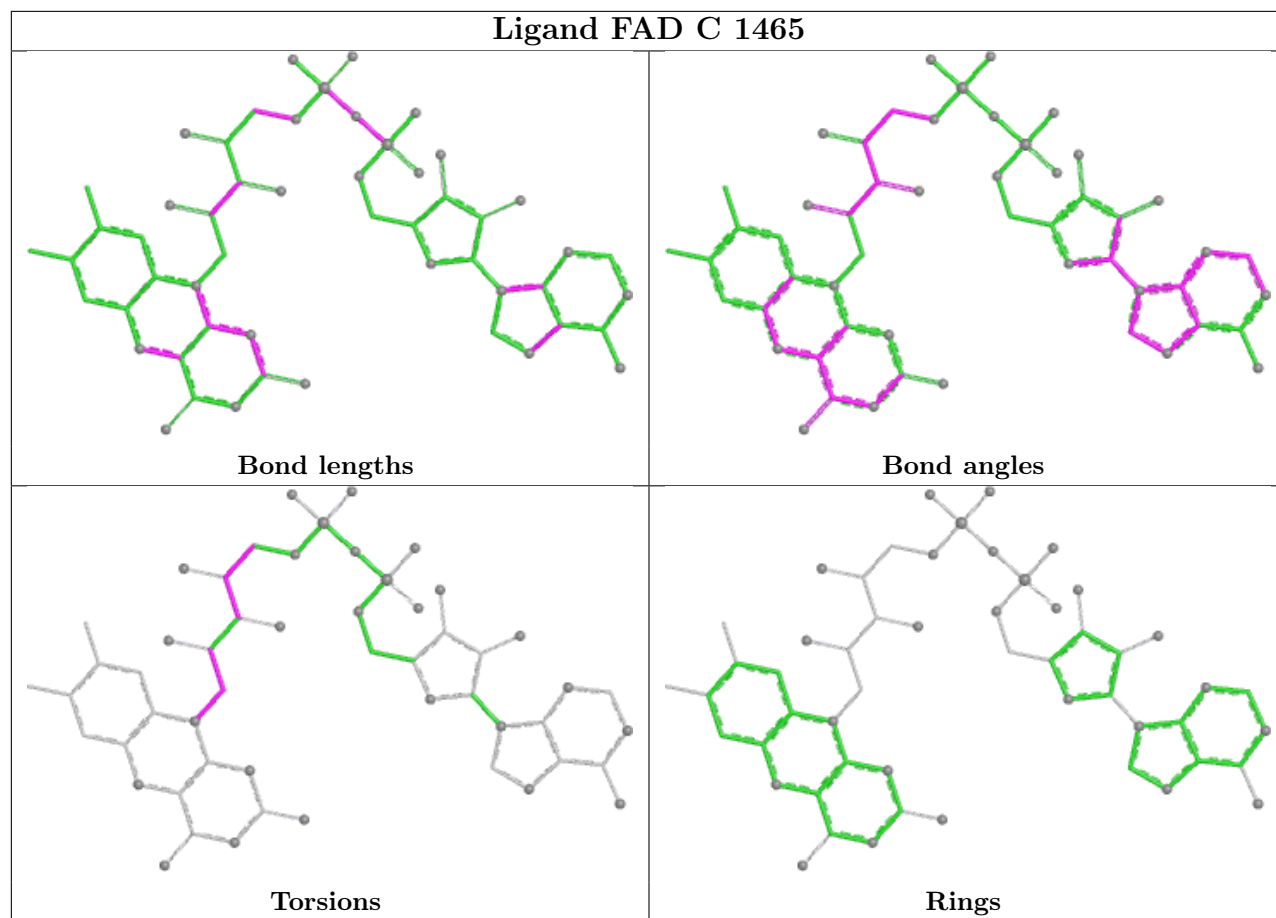


Ligand MTE H 1778









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	450/462 (97%)	0.76	34 (7%)	20	16	25, 49, 66, 70	0
1	C	450/462 (97%)	0.83	39 (8%)	16	12	22, 47, 66, 70	0
1	E	450/462 (97%)	0.81	27 (6%)	27	22	25, 48, 66, 71	0
1	G	450/462 (97%)	0.86	34 (7%)	20	16	26, 49, 66, 70	0
2	B	760/777 (97%)	0.08	1 (0%)	92	90	21, 35, 50, 59	0
2	D	760/777 (97%)	0.13	6 (0%)	82	80	20, 34, 49, 59	0
2	F	760/777 (97%)	0.16	4 (0%)	87	85	21, 34, 49, 59	0
2	H	760/777 (97%)	0.10	3 (0%)	88	86	22, 35, 50, 59	0
All	All	4840/4956 (97%)	0.38	148 (3%)	51	45	20, 39, 62, 71	0

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	166	LEU	7.9
2	B	777	ALA	5.9
1	G	166	LEU	5.2
1	C	166	LEU	4.7
1	A	166	LEU	4.7
1	A	345	ALA	4.1
1	A	179	PRO	3.6
1	A	332	PRO	3.5
1	C	15	ARG	3.5
1	C	235	ARG	3.4
2	F	777	ALA	3.4
1	C	239	ASP	3.4
1	E	238	PRO	3.3
2	H	777	ALA	3.3
1	A	312	GLU	3.2
1	E	302	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	165	THR	3.1
1	C	217	ARG	3.1
1	G	385	GLY	3.1
1	E	377	ILE	3.1
1	A	182	LEU	3.0
2	D	560	GLY	3.0
1	A	165	THR	3.0
1	C	218	ASP	2.9
2	F	560	GLY	2.9
1	A	318	LEU	2.9
1	A	310	GLY	2.9
1	A	372	LEU	2.9
1	E	179	PRO	2.9
2	D	777	ALA	2.9
1	C	215	ALA	2.8
1	G	318	LEU	2.8
1	G	179	PRO	2.8
1	G	317	PRO	2.8
1	C	302	GLY	2.8
1	A	375	SER	2.7
1	A	195	ALA	2.7
1	C	163	ALA	2.7
1	C	378	GLU	2.7
1	C	179	PRO	2.7
1	G	194	LEU	2.6
1	G	396	ALA	2.6
1	G	332	PRO	2.6
2	D	399	LYS	2.6
1	E	338	SER	2.6
1	G	240	GLY	2.6
2	D	284	GLY	2.6
1	G	397	PHE	2.6
1	E	234	ILE	2.5
1	A	189	LEU	2.5
1	E	190	ALA	2.5
1	E	165	THR	2.5
1	E	187	ASP	2.5
1	C	315	ARG	2.5
1	C	195	ALA	2.5
1	E	164	PHE	2.5
1	E	461	MET	2.5
1	A	326	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	372	LEU	2.5
1	C	324	GLU	2.5
1	A	406	PHE	2.5
1	C	361	ILE	2.5
1	C	402	ILE	2.5
1	C	311	GLN	2.5
1	C	162	ALA	2.5
2	D	79	ALA	2.5
1	A	239	ASP	2.4
1	C	400	ALA	2.4
2	D	613	ARG	2.4
1	G	181	PHE	2.4
1	G	310	GLY	2.4
1	A	217	ARG	2.4
1	E	407	ARG	2.4
1	A	380	ALA	2.4
1	C	380	ALA	2.4
1	C	216	LEU	2.3
1	A	411	ILE	2.3
1	A	379	THR	2.3
1	C	220	PRO	2.3
1	A	371	THR	2.3
1	A	334	GLU	2.3
1	G	218	ASP	2.3
1	G	238	PRO	2.3
1	E	239	ASP	2.3
1	C	9	GLY	2.3
1	C	403	GLY	2.3
1	E	219	LEU	2.3
1	C	243	ILE	2.3
1	G	162	ALA	2.3
1	A	20	THR	2.3
1	G	10	GLU	2.3
2	F	2	SER	2.3
1	G	192	TRP	2.3
1	E	181	PHE	2.3
1	G	165	THR	2.2
1	C	323	LEU	2.2
1	A	402	ILE	2.2
1	E	180	ALA	2.2
1	G	227	HIS	2.2
1	G	301	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	399	ALA	2.2
1	G	413	ALA	2.2
1	A	423	THR	2.2
1	E	198	GLU	2.2
1	G	307	LEU	2.2
1	C	241	TYR	2.2
1	A	307	LEU	2.2
1	G	14	VAL	2.2
1	A	3	ILE	2.2
1	A	315	ARG	2.2
1	E	313	ARG	2.2
1	E	188	ALA	2.1
1	C	312	GLU	2.1
1	C	20	THR	2.1
2	F	581	ARG	2.1
1	A	325	TYR	2.1
1	G	241	TYR	2.1
1	A	377	ILE	2.1
1	A	220	PRO	2.1
1	G	220	PRO	2.1
1	C	233	GLN	2.1
1	E	182	LEU	2.1
1	A	121	ASP	2.1
1	E	218	ASP	2.1
1	G	364	VAL	2.1
1	E	217	ARG	2.1
1	A	185	THR	2.1
1	A	403	GLY	2.1
1	G	366	GLY	2.1
1	G	411	ILE	2.1
1	E	405	ASP	2.1
1	C	236	GLU	2.1
1	C	313	ARG	2.1
1	E	419	ALA	2.1
2	H	381	GLU	2.1
1	C	310	GLY	2.1
2	H	560	GLY	2.1
1	G	226	SER	2.0
1	G	461	MET	2.0
1	C	182	LEU	2.0
1	G	234	ILE	2.0
1	C	164	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	406	PHE	2.0
1	C	407	ARG	2.0
1	E	19	PRO	2.0
1	G	379	THR	2.0
1	E	227	HIS	2.0
1	G	325	TYR	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(Å ²)	Q<0.9
7	XAN	F	1780[A]	11/11	0.64	0.29	62,62,62,62	11
7	XAN	F	1780[B]	11/11	0.64	0.29	61,62,62,62	11
7	XAN	H	1780[A]	11/11	0.74	0.26	62,62,62,62	11
7	XAN	H	1780[B]	11/11	0.74	0.26	61,62,62,62	11
7	XAN	B	1780[A]	11/11	0.76	0.24	62,62,62,62	11
7	XAN	B	1780[B]	11/11	0.76	0.24	61,62,62,62	11
7	XAN	D	1780[A]	11/11	0.76	0.21	62,62,62,62	11
7	XAN	D	1780[B]	11/11	0.76	0.21	61,62,62,62	11
5	MTE	F	1778	24/24	0.92	0.13	22,29,34,36	24
5	MTE	H	1778	24/24	0.92	0.13	33,38,41,43	24
4	FAD	A	1465	53/53	0.92	0.11	38,48,56,56	0
4	FAD	G	1465	53/53	0.92	0.12	41,50,63,64	0
5	MTE	B	1778	24/24	0.92	0.13	27,36,42,43	24
4	FAD	E	1465	53/53	0.93	0.11	35,45,53,53	0
5	MTE	D	1778	24/24	0.94	0.11	9,25,32,33	24
3	FES	G	1464	4/4	0.97	0.07	39,40,42,42	0
4	FAD	C	1465	53/53	0.97	0.07	16,27,35,37	0

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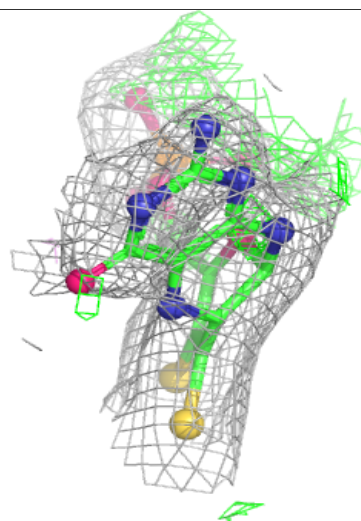
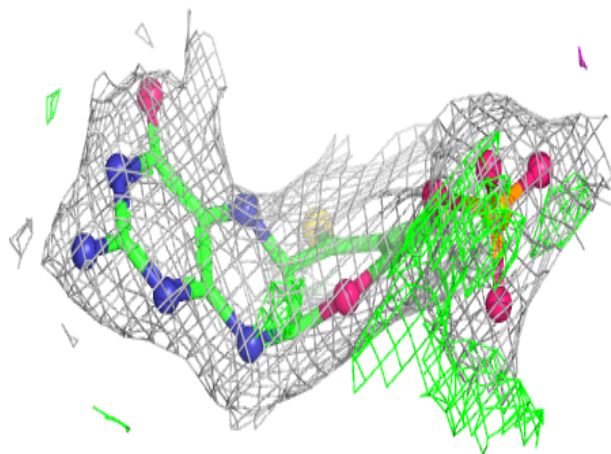
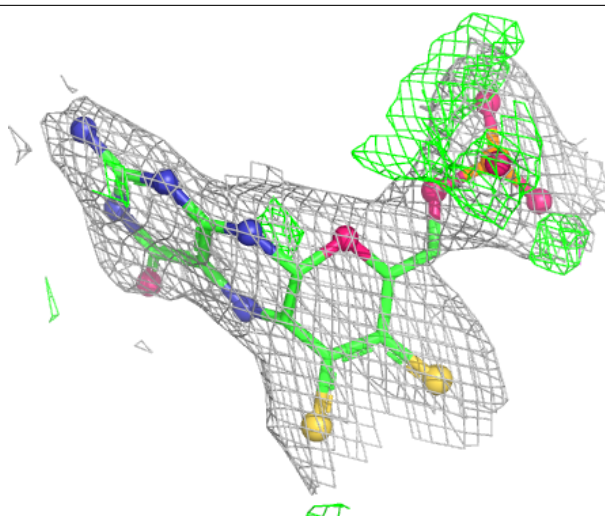
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	CA	F	1779	1/1	0.97	0.08	56,56,56,56	0
6	CA	H	1779	1/1	0.97	0.05	58,58,58,58	0
8	MOM	B	1781	4/4	0.97	0.11	44,45,45,47	3
6	CA	D	1779	1/1	0.98	0.05	49,49,49,49	0
3	FES	E	1463	4/4	0.98	0.05	26,27,30,31	0
3	FES	E	1464	4/4	0.98	0.06	38,38,40,42	0
3	FES	G	1463	4/4	0.98	0.04	29,32,32,33	0
3	FES	A	1463	4/4	0.98	0.04	25,28,29,30	0
6	CA	B	1779	1/1	0.98	0.04	48,48,48,48	0
8	MOM	F	1781	4/4	0.98	0.10	35,35,36,37	3
8	MOM	H	1781	4/4	0.98	0.11	44,44,44,45	3
3	FES	A	1464	4/4	0.99	0.05	35,35,36,36	0
8	MOM	D	1781	4/4	0.99	0.06	34,34,34,37	3
3	FES	C	1463	4/4	0.99	0.04	19,19,21,22	0
3	FES	C	1464	4/4	0.99	0.06	33,35,35,37	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.

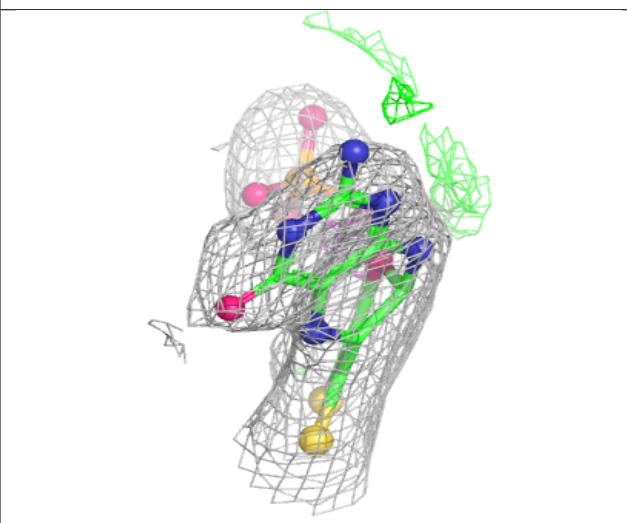
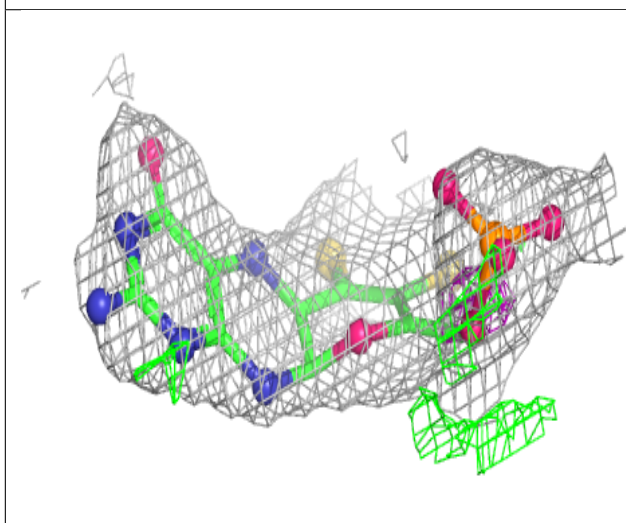
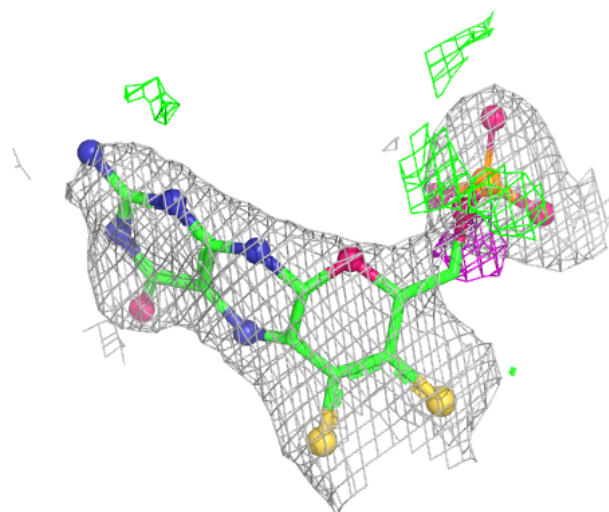
Electron density around MTE F 1778:

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



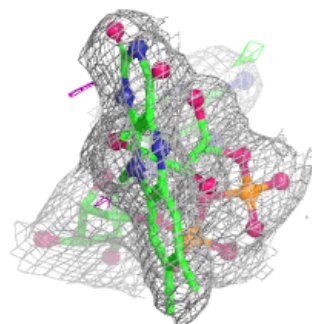
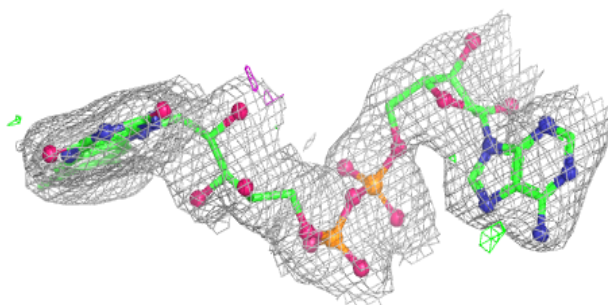
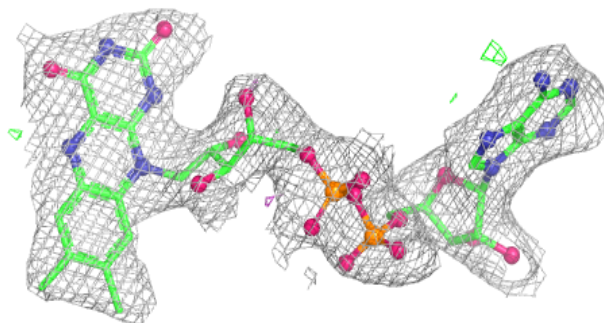
Electron density around MTE H 1778:

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

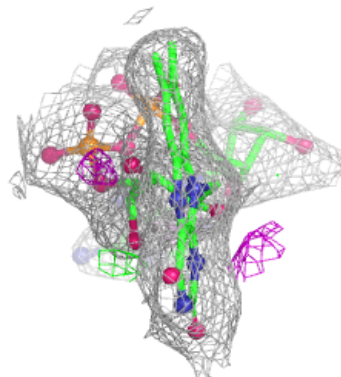
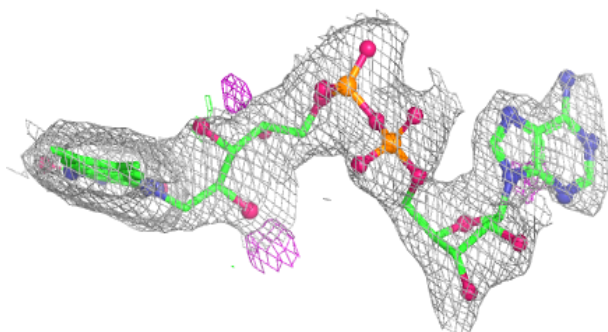
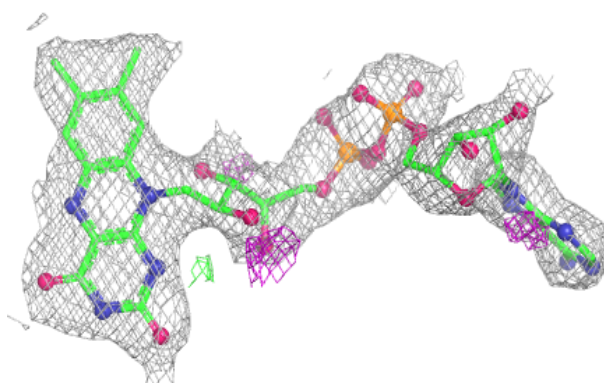


Electron density around FAD A 1465:

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

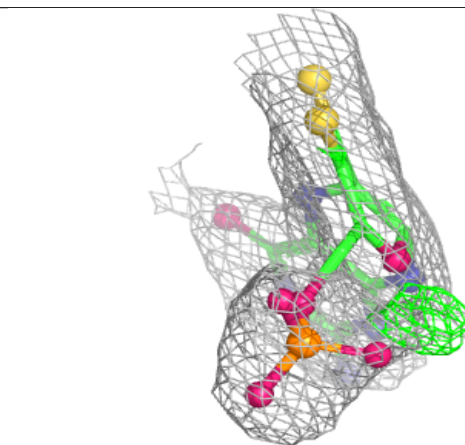
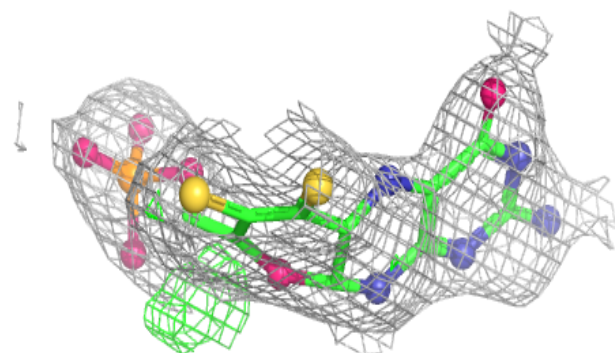
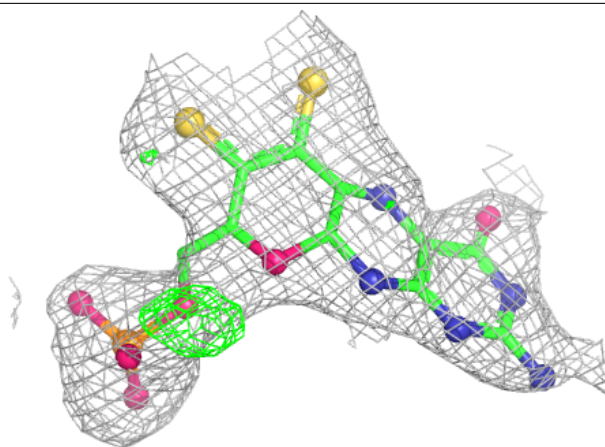
**Electron density around FAD G 1465:**

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

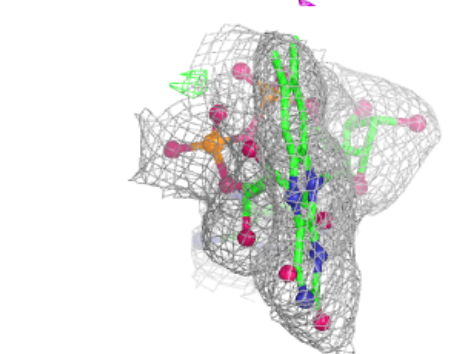
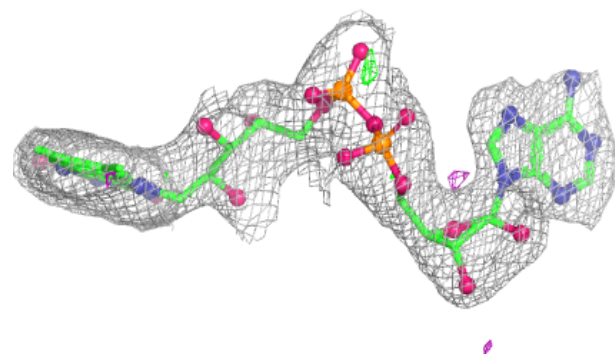
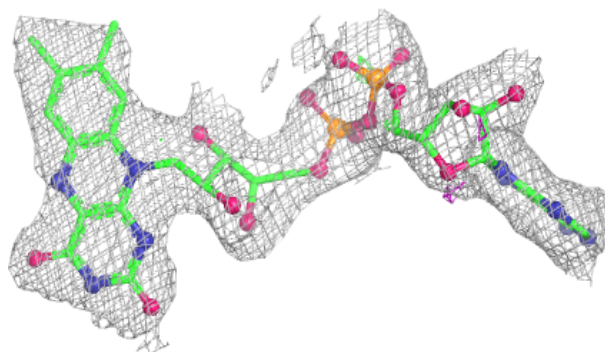


Electron density around MTE B 1778:

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

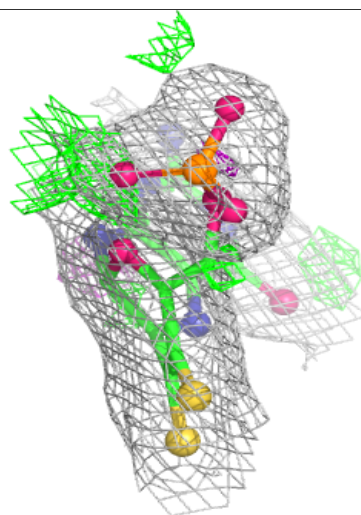
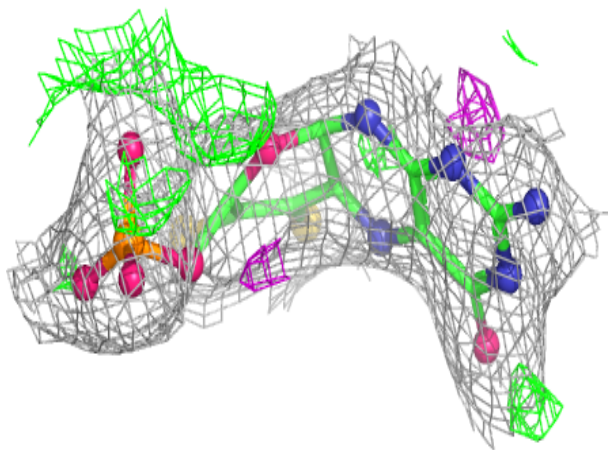
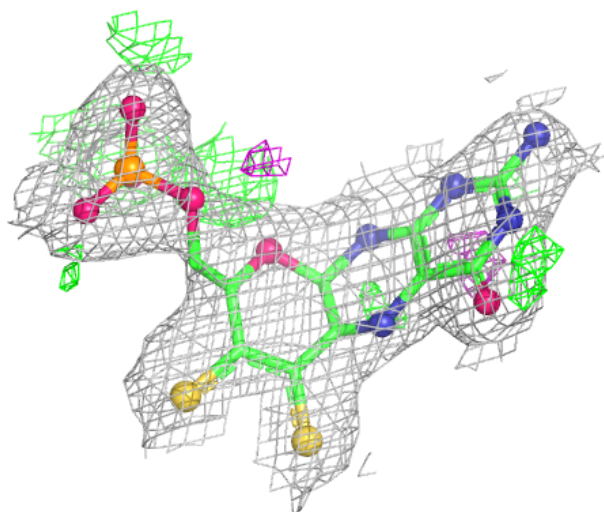
**Electron density around FAD E 1465:**

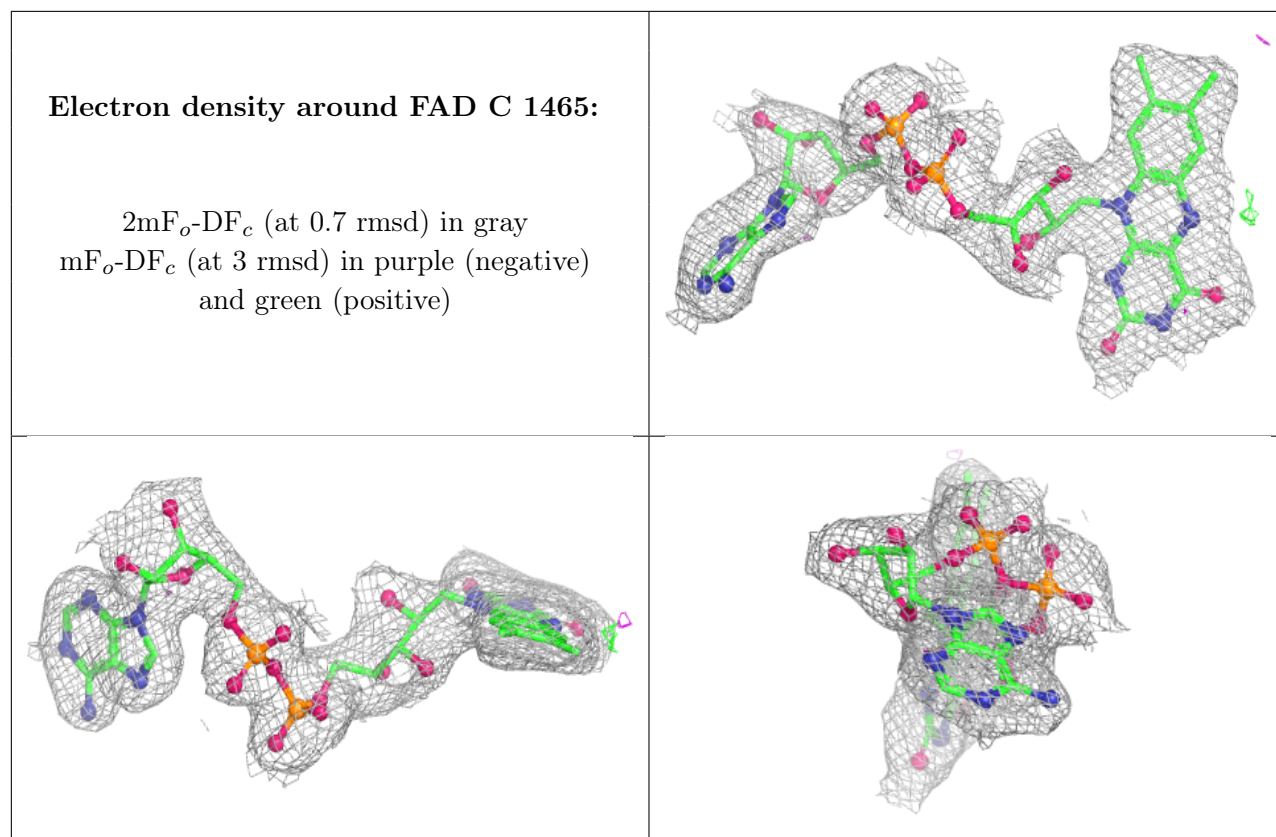
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MTE D 1778:

$2mF_o-DF_c$ (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.