



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 04:59 pm BST

PDB ID : 2W3S
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

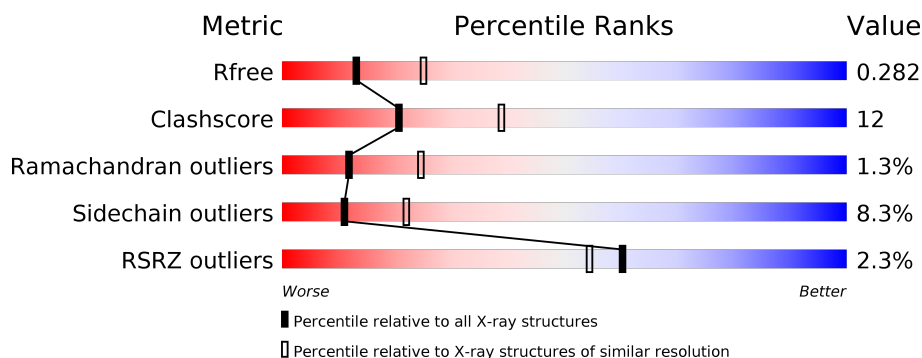
1 Overall quality at a glance

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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 on 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	<div> <div>6%</div> <div> <div></div> <div>62%</div> <div>31%</div> <div>• •</div> </div> </div>
1	C	462	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>16%</div> <div>• •</div> </div> </div>
1	E	462	<div> <div>5%</div> <div> <div></div> <div>66%</div> <div>28%</div> <div>• •</div> </div> </div>
1	G	462	<div> <div>8%</div> <div> <div></div> <div>60%</div> <div>33%</div> <div>• •</div> </div> </div>
2	B	777	<div> <div></div> <div> <div></div> <div>71%</div> <div>23%</div> <div>• •</div> </div> </div>
2	D	777	<div> <div></div> <div> <div></div> <div>73%</div> <div>23%</div> <div>• •</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	F	777	 70% 26% . .
2	H	777	 % 71% 24% . .

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

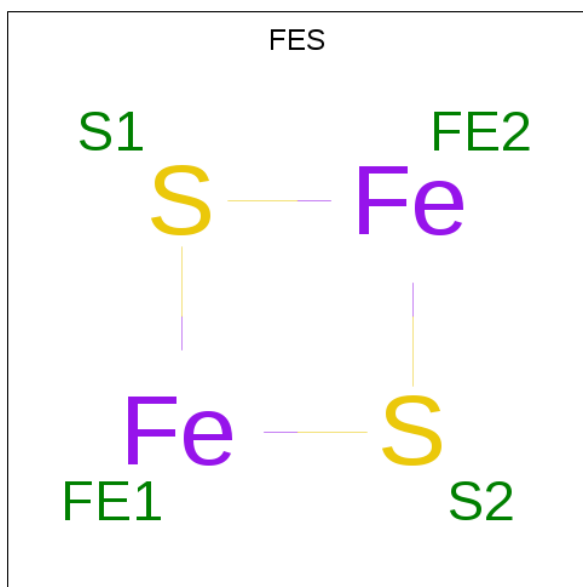
- Molecule 2 is a protein called XANTHINE DEHYDROGENASE.

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:

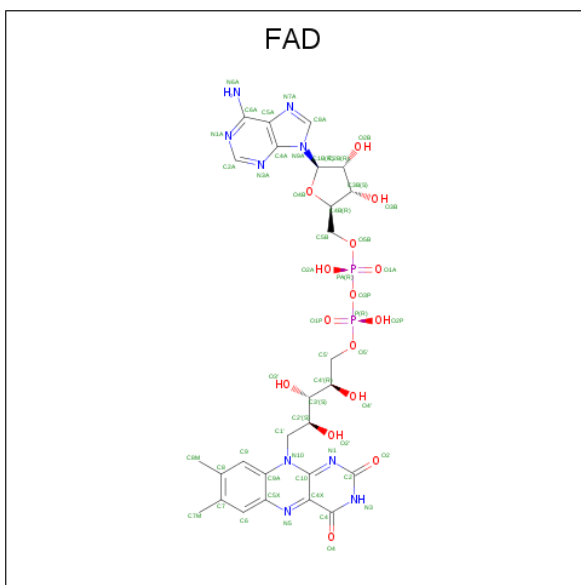
Chain	Residue	Modelled	Actual	Comment	Reference
B	772	ARG	GLY	conflict	UNP O54051
D	772	ARG	GLY	conflict	UNP O54051
F	772	ARG	GLY	conflict	UNP O54051
H	772	ARG	GLY	conflict	UNP O54051

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



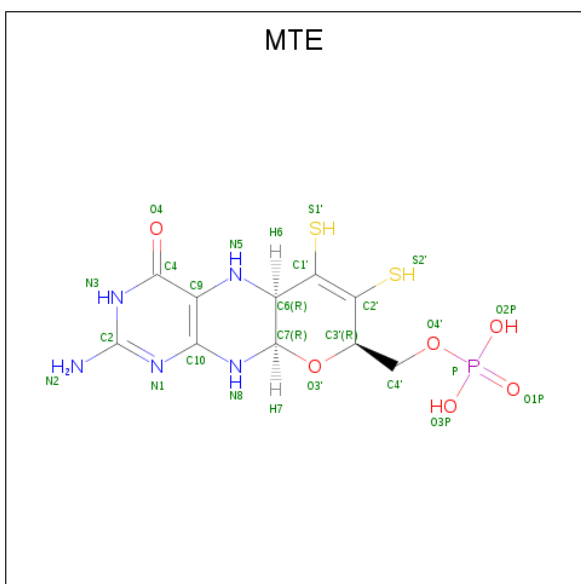
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	C	1	Total	Fe	S	0	0
			4	2	2		
3	C	1	Total	Fe	S	0	0
			4	2	2		
3	E	1	Total	Fe	S	0	0
			4	2	2		
3	E	1	Total	Fe	S	0	0
			4	2	2		
3	G	1	Total	Fe	S	0	0
			4	2	2		
3	G	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: 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 53	C 27	N 9	O 15	P 2	0	0
4	C	1	Total 53	C 27	N 9	O 15	P 2	0	0
4	E	1	Total 53	C 27	N 9	O 15	P 2	0	0
4	G	1	Total 53	C 27	N 9	O 15	P 2	0	0

- 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 (three-letter code: MTE) (formula: $C_{10}H_{14}N_5O_6PS_2$).

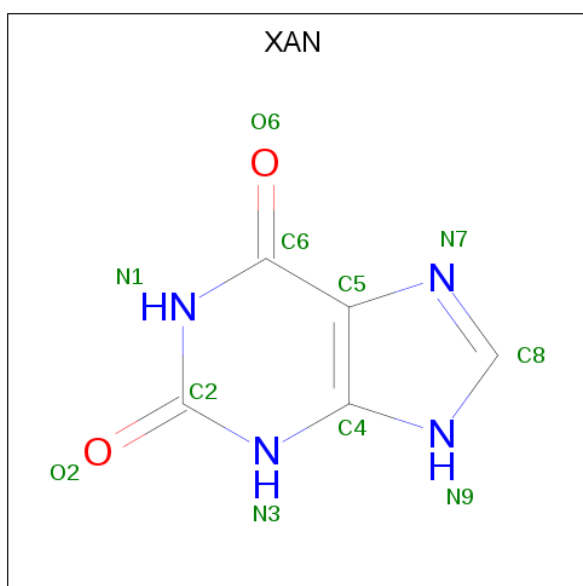


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	S	
			24	10	5	6	1	2	
5	D	1	Total	C	N	O	P	S	
			24	10	5	6	1	2	
5	F	1	Total	C	N	O	P	S	
			24	10	5	6	1	2	
5	H	1	Total	C	N	O	P	S	
			24	10	5	6	1	2	

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

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

- Molecule 7 is XANTHINE (three-letter code: XAN) (formula: C₅H₄N₄O₂).



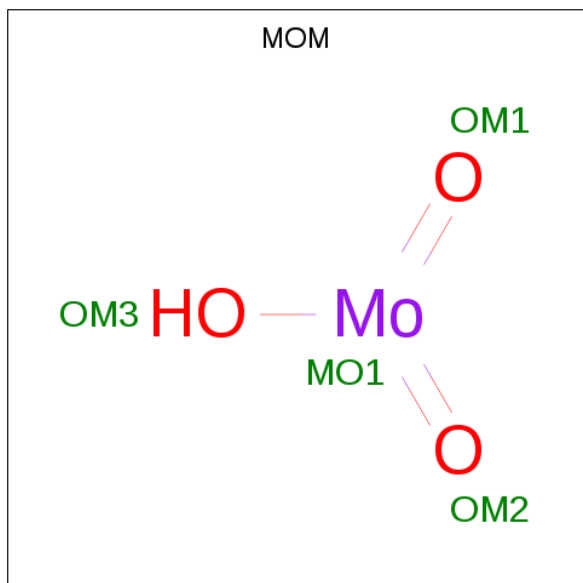
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O		
			22	10	8	4	0	1
7	D	1	Total	C	N	O		
			22	10	8	4	0	1

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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 (three-letter code: 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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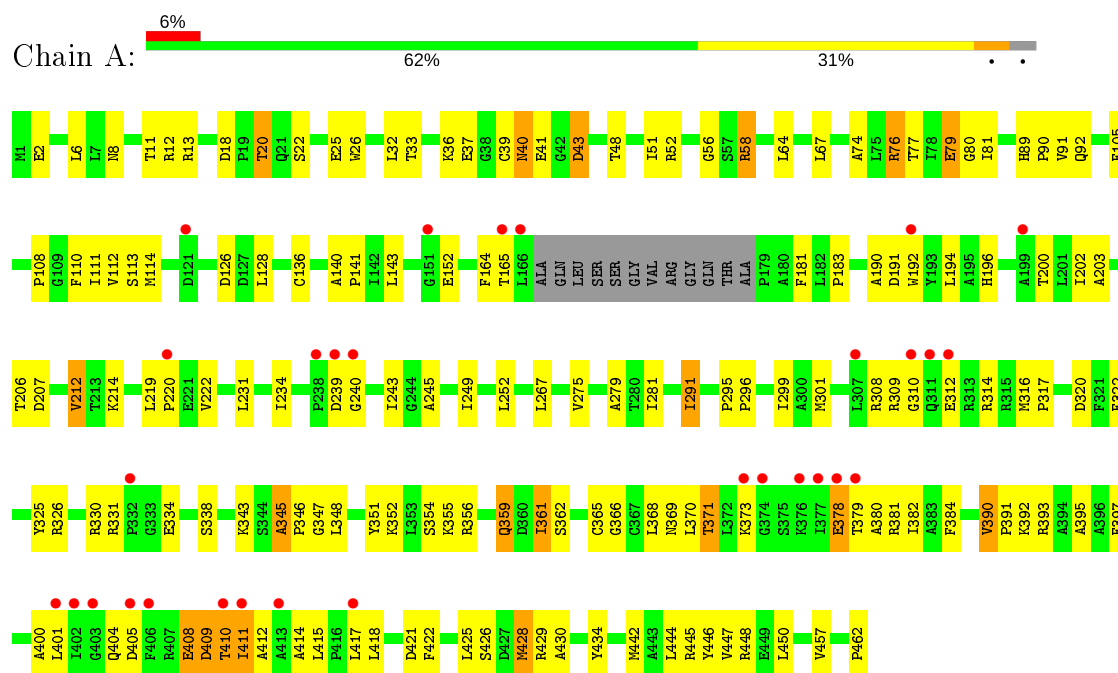
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	7	Total 7	O 7	0	0
9	E	2	Total 2	O 2	0	0
9	F	6	Total 6	O 6	0	0
9	H	7	Total 7	O 7	0	0

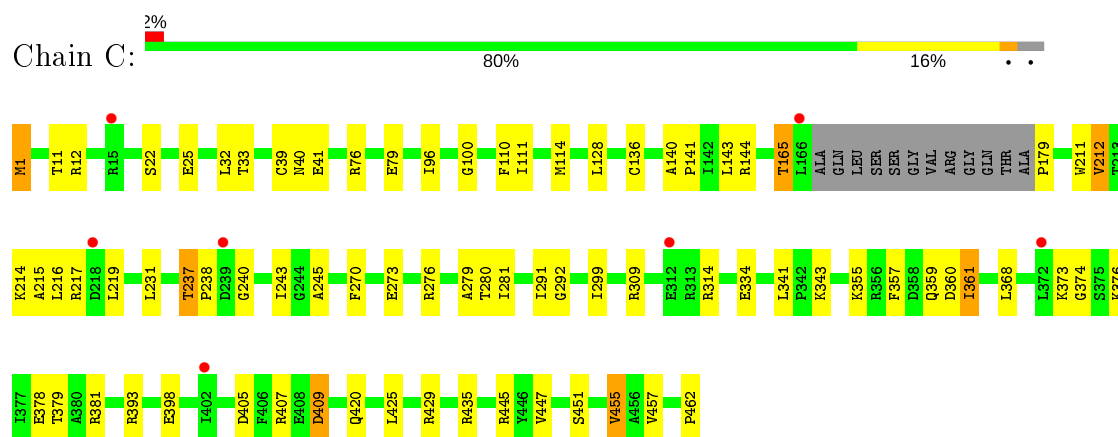
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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

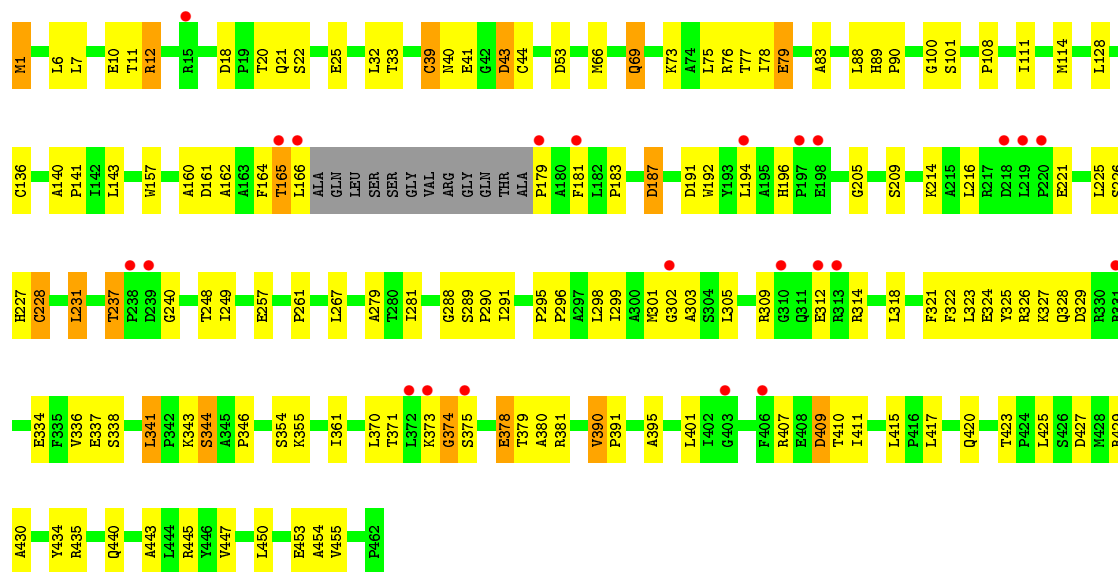


• Molecule 1: XANTHINE DEHYDROGENASE

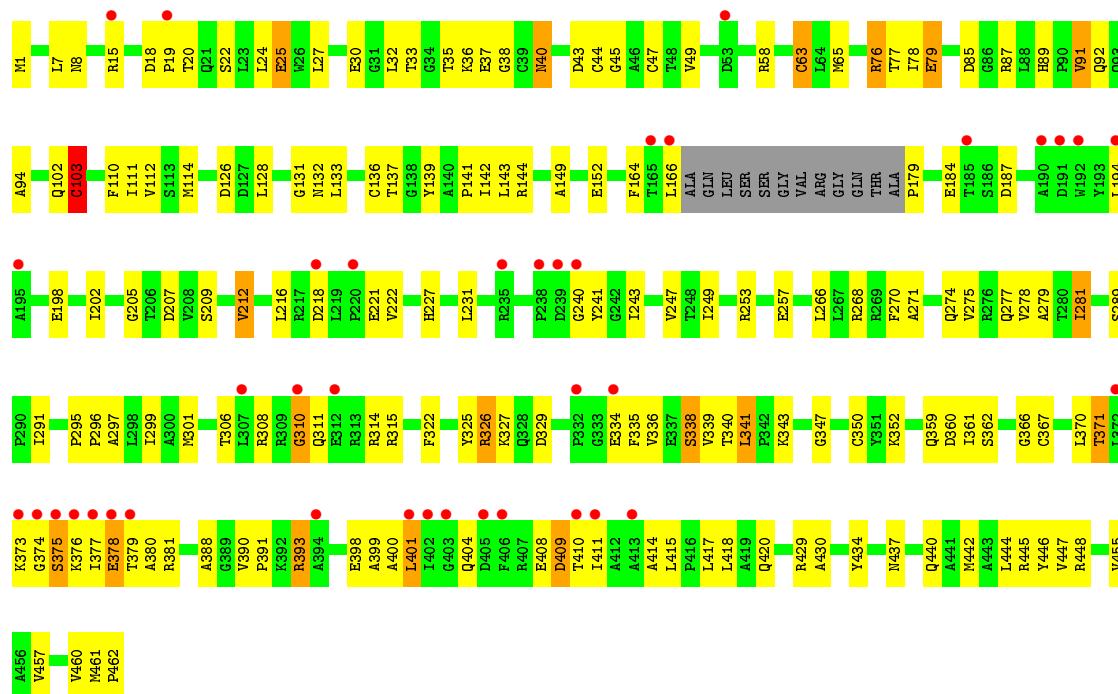


• Molecule 1: XANTHINE DEHYDROGENASE



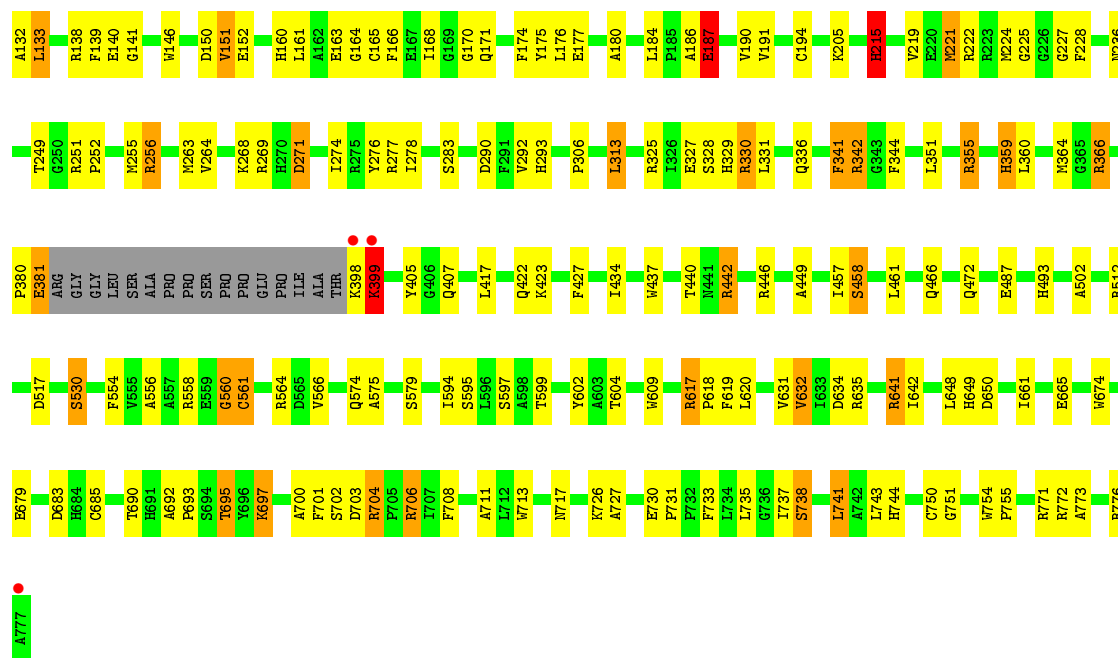


• Molecule 1: XANTHINE DEHYDROGENASE



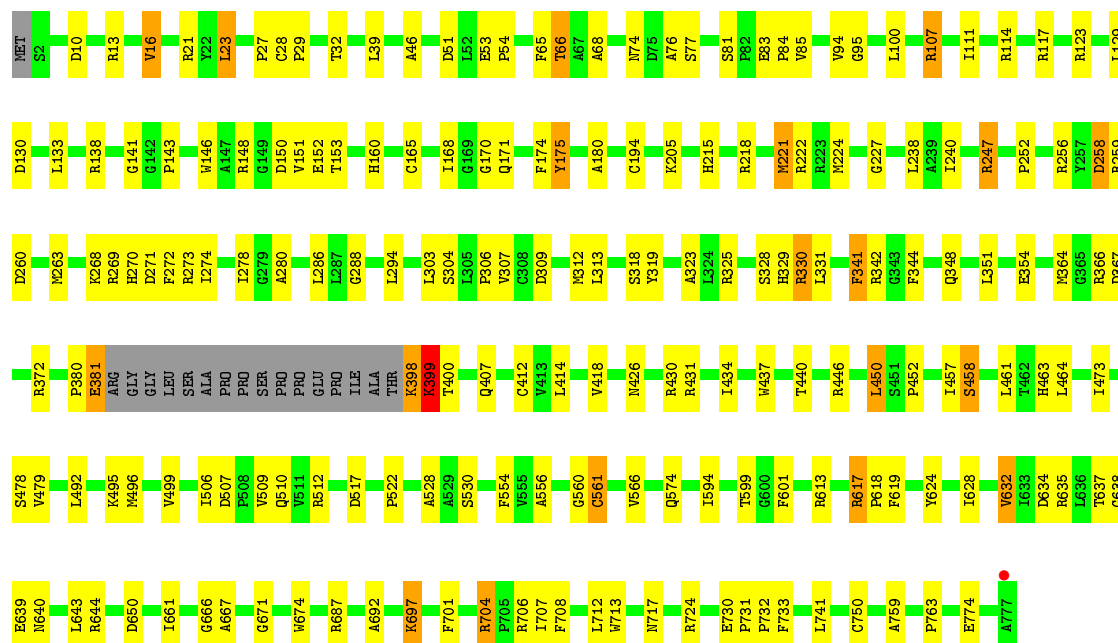
• Molecule 2: XANTHINE DEHYDROGENASE





• Molecule 2: XANTHINE DEHYDROGENASE

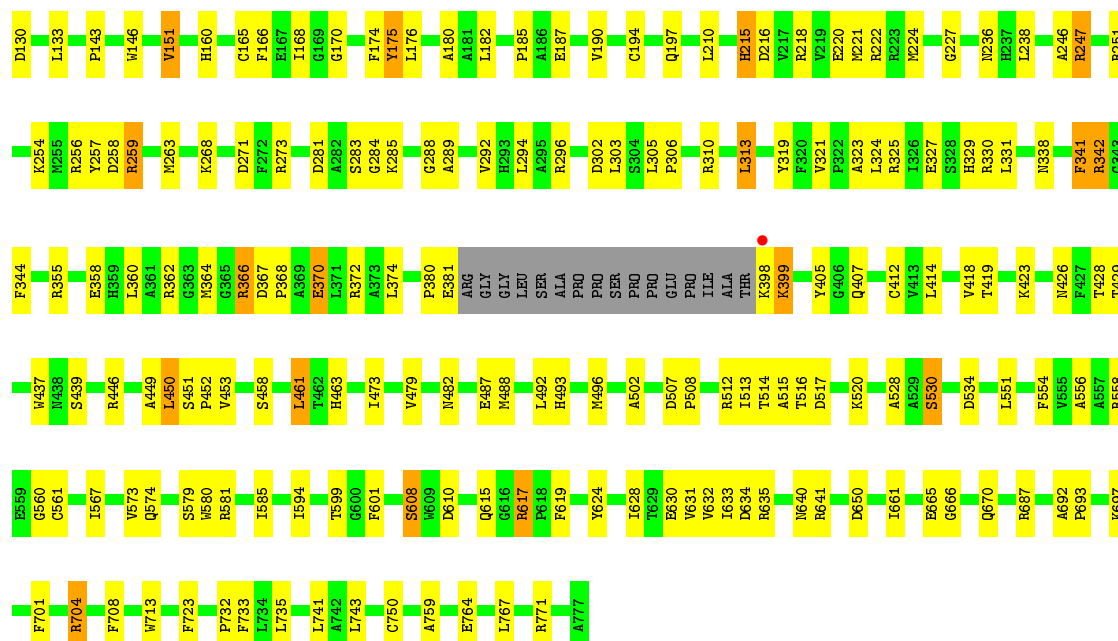
Chain D: 73% 23% ..



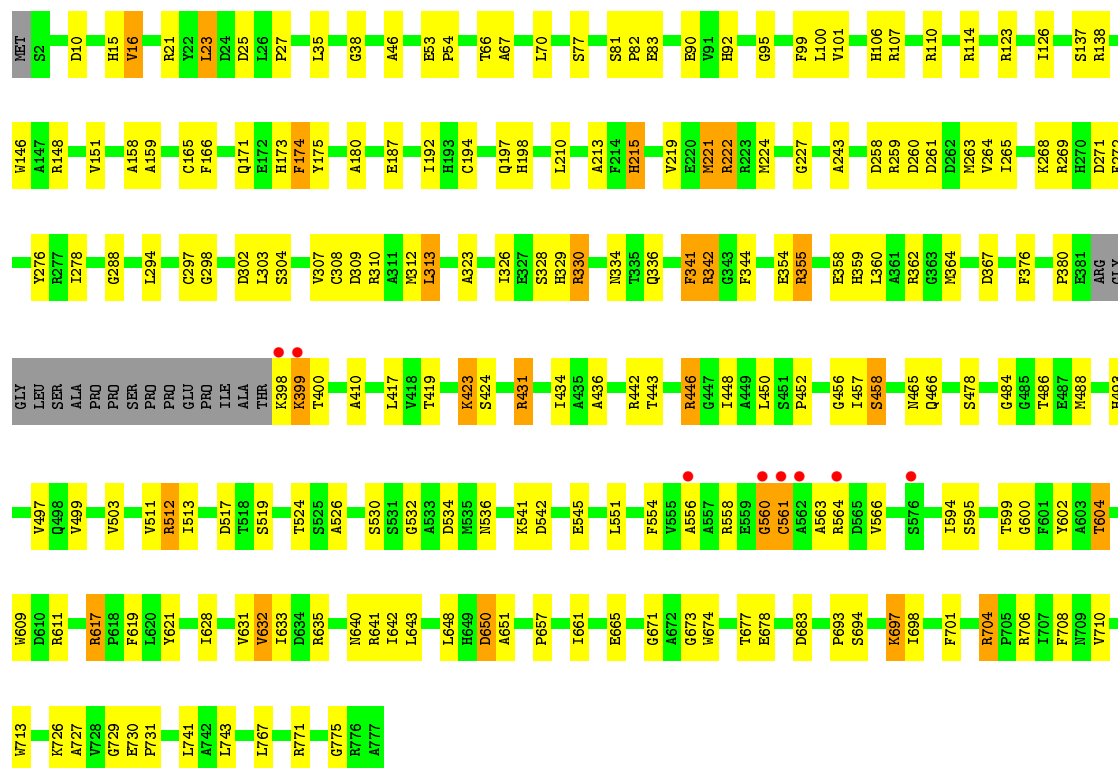
• Molecule 2: XANTHINE DEHYDROGENASE

Chain F: 70% 26% ..





• 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 50.01 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.7 (50.12-2.60) 97.7 (50.01-2.60)	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 (5.01%)	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)	0.36 , 55.8	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: XAN, CA, FES, MOM, FAD, 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	0.50	0/3439	0.67	0/4659
1	C	0.50	0/3439	0.64	0/4659
1	E	0.51	0/3439	0.66	0/4659
1	G	0.54	1/3439 (0.0%)	0.69	0/4659
2	B	0.56	0/5845	0.70	0/7942
2	D	0.57	1/5845 (0.0%)	0.70	0/7942
2	F	0.58	0/5845	0.71	0/7942
2	H	0.57	0/5845	0.69	0/7942
All	All	0.55	2/37136 (0.0%)	0.69	0/50404

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	103	CYS	CB-SG	-5.70	1.72	1.81
2	D	750	CYS	CB-SG	-5.15	1.73	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3376	0	3367	127	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3376	0	3367	52	0
1	E	3376	0	3367	94	0
1	G	3376	0	3367	123	0
2	B	5717	0	5631	154	0
2	D	5717	0	5631	125	0
2	F	5717	0	5631	143	0
2	H	5717	0	5630	141	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	3	0
4	E	53	0	31	3	0
4	G	53	0	31	4	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	896	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (896) 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:HH11	2:F:247:ARG:HG2	1.11	1.07
1:G:240:GLY:HA2	1:G:343:LYS:HG2	1.34	1.04
2:F:221:MET:HE1	2:F:224:MET:HG3	1.40	1.03
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:HH11	2:D:247:ARG:HG2	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:247:ARG:NH1	2:F:247:ARG:HG2	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:H:360:LEU:HG	2:H:364:MET:HE2	1.59	0.83
2:H:259:ARG:HG3	2:H:263:MET:HE2	1.61	0.82
7:D:1780[A]:XAN:H8	8:D:1781:MOM:OM2	1.79	0.82
2:D:247:ARG:NH1	2:D:247:ARG:HG2	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
1:G:444:LEU:O	1:G:448:ARG:HG3	1.80	0.80
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
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:D:247:ARG:HH11	2:D:247:ARG:CG	1.99	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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
2:H:174:PHE:HZ	2:H:693:PRO:HG3	1.56	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:G:216:LEU:HD12	2:H:114:ARG:NH1	2.08	0.68
1:G:322:PHE:HB3	1:G:390:VAL:HG23	1.76	0.68
2:H:354:GLU:OE1	2:H:354:GLU:HA	1.93	0.68
2:B:23:LEU:HD13	2:B:194:CYS:HA	1.76	0.68
2:B:126:ILE:CD1	2:B:126:ILE:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:143:LEU:C	1:G:143:LEU:HD23	2.15	0.66
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:160:HIS:HB3	2:F:364:MET:HE2	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
1:A:231:LEU:HD23	1:A:231:LEU:O	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
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:65:MET:HE1	1:G:278:VAL:HG11	1.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	2:B:129:LEU:HD12	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
2:H:556:ALA:HB2	2:H:563:ALA:HA	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
2:F:360:LEU:HG	2:F:364:MET:HE3	1.81	0.63
1:A:252:LEU:HD22	1:A:281:ILE:HG21	1.81	0.63
8:F:1781:MOM:MO1	8:F:1781:MOM:OM1	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:HH11	1:G:326:ARG:HG2	1.63	0.62
2:H:46:ALA:HB2	2:H:123:ARG:NH2	2.15	0.62
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
8:F:1781:MOM:MO1	8:F:1781:MOM:OM3	1.71	0.61
1:C:373:LYS:HB2	1:C:378:GLU:CG	2.31	0.61
8:B:1781:MOM:OM3	8:B:1781:MOM:MO1	1.71	0.61
2:B:755:PRO:O	2:B:772:ARG:HD2	2.01	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:111:ILE:HA	1:A:114:MET:HE2	1.83	0.60
2:B:380:PRO:O	2:B:381:GLU:HB2	2.01	0.60
1:A:445:ARG:NH2	2:B:634:ASP:OD1	2.34	0.60
2:B:160:HIS:HB3	2:B:364:MET:CE	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:1781:MOM:OM3	8:D:1781:MOM:MO1	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:OM3	8:H:1781:MOM:MO1	1.71	0.60
2:B:560:GLY:O	2:B:561:CYS:CB	2.50	0.59
8:H:1781:MOM:OM1	8:H:1781:MOM:MO1	1.72	0.59
1:G:43:ASP:HB3	2:H:693:PRO:HB2	1.84	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
8:B:1781:MOM:OM1	8:B:1781:MOM:MO1	1.73	0.59
2:B:617:ARG:HD3	2:B:619:PHE:O	2.03	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
2:F:170:GLY:N	2:F:271:ASP:HB3	2.18	0.58
1:A:330:ARG:NH2	4:A:1465:FAD:H2A	2.18	0.58
1:G:111:ILE:HA	1:G:114:MET:HE2	1.86	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
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:160:HIS:HB3	2:B:364:MET:HE2	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:166:PHE:CZ	2:B:355:ARG:HG3	2.38	0.58
1:A:408:GLU:OE1	2:B:442:ARG:NH2	2.36	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:405:ASP:O	1:A:410:THR:HG21	2.05	0.57
1:A:89:HIS:ND1	1:A:91:VAL:HB	2.20	0.57
2:B:434:ILE:HG23	2:B:446:ARG:HB2	1.86	0.57
2:D:280:ALA:HB3	2:D:364:MET:HE1	1.85	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: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
2:B:274:ILE:HG12	2:B:293:HIS:HD2	1.68	0.57
1:C:110:PHE:HB3	1:C:114:MET:HE1	1.85	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:263:MET:HE3	2:B:692:ALA:HA	1.89	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: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
2:F:3:VAL:HG21	2:F:723:PHE:CE1	2.41	0.55
1:E:434:TYR:CD1	2:F:764:GLU:HG3	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
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:368:LEU:HB2	1:A:446:TYR:CD1	2.41	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:NH1	2:F:581:ARG:HB2	2.22	0.55
2:D:205:LYS:HE2	2:D:205:LYS:HA	1.88	0.55
2:D:434:ILE:HG23	2:D:446:ARG:HB2	1.89	0.55
1:E:12:ARG:CG	1:E:12:ARG:HH11	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
1:A:22:SER:OG	1:A:25:GLU:OE1	2.20	0.54
2:F:160:HIS:HB3	2:F:364:MET:CE	2.36	0.54
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:H:457:ILE:O	2:H:458:SER:HB2	2.07	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:428:MET:H	1:A:428:MET:HE3	1.72	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:221:MET:HE1	2:H:224:MET:HG3	1.90	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:388:ALA:C	1:G:390:VAL:H	2.12	0.53
1:G:445:ARG:HG3	1:G:455:VAL:CG1	2.38	0.53
2:H:609:TRP:CZ3	2:H:611:ARG:HA	2.43	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
2:B:466:GLN:HA	2:B:602:TYR:O	2.09	0.53
1:A:426:SER:N	2:F:574:GLN:HE22	1.96	0.53
1:E:111:ILE:HA	1:E:114:MET:HE3	1.91	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: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: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
1:A:354:SER:OG	1:A:356:ARG:O	2.27	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:H:651:ALA:C	2:H:726:LYS:HB2	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:39:LEU:HD22	2:D:95:GLY:O	2.08	0.52
1:A:425:LEU:HD12	2:F:579:SER:HB2	1.92	0.52
2:F:635:ARG:HD3	2:F:750:CYS:SG	2.50	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:N	1:G:409:ASP:OD2	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
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:ILE:HD11	1:A:58:ARG:NH1	2.25	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
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
2:F:263:MET:HE3	2:F:692:ALA:HA	1.92	0.50
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:N	1:A:409:ASP:OD2	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:358:GLU:O	2:F:362:ARG:HG2	2.11	0.50
2:F:220:GLU:HG2	2:F:517:ASP:OD1	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:111:ILE:HD11	2:F:16:VAL:HG23	1.92	0.50
1:E:78:ILE:HG23	1:E:79:GLU:N	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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: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:H	2:D:238:LEU:HD12	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
2:D:221:MET:HE1	2:D:224:MET:HG3	1.92	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:N1	4:C:1465:FAD:H2'	2.28	0.49
2:H:354:GLU:OE2	2:H:452:PRO:HD2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:457:VAL:HG23	2:D:634:ASP:HB2	1.94	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:NH1	1:E:407:ARG:HB2	2.28	0.48
2:F:661:ILE:O	2:F:665:GLU:HG3	2.13	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: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:G:126:ASP:OD1	2:H:704:ARG:NH1	2.38	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
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: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
2:H:341:PHE:O	2:H:342:ARG:C	2.51	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:HD3	2:F:697:LYS:HA	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
1:E:289:SER:OG	1:E:291:ILE:HG13	2.15	0.47
1:E:240:GLY:HA2	1:E:343:LYS:HG2	1.96	0.47
1:G:240:GLY:CA	1:G:343:LYS:HG2	2.25	0.47
1:E:164:PHE:C	1:E:166:LEU:H	2.18	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:299:ILE:O	1:C:381:ARG:NH1	2.46	0.47
1:C:243:ILE:HD12	1:C:341:LEU:HG	1.97	0.47
2:D:697:LYS:N	2:D:697:LYS:HD2	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
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:B:22:TYR:N	2:B:22:TYR:CD1	2.84	0.46
2:F:453:VAL:HG21	2:F:735:LEU:HD23	1.96	0.46
2:F:66:THR:CG2	2:F:67:ALA:N	2.78	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:517:ASP:OD2	2:H:519:SER:N	2.48	0.46
2:H:466:GLN:HA	2:H:602:TYR:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:G:77:THR:OG1	1:G:79:GLU:HG2	2.15	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:160:HIS:HB3	2:B:364:MET:HE1	1.97	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: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
2:F:143:PRO:HG3	2:F:329:HIS:CE1	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:319:TYR:OH	2:F:372:ARG:HG2	2.15	0.46
2:F:50:LEU:CD1	2:F:118:ILE:HG12	2.45	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
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: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
2:H:53:GLU:HA	2:H:53:GLU:OE1	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	1:A:40:ASN:HD22	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
2:B:276:TYR:OH	2:B:359:HIS:CD2	2.70	0.45
1:C:368:LEU:N	1:C:368:LEU:HD12	2.31	0.45
1:C:111:ILE:CD1	2:D:16:VAL:HG22	2.46	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
2:H:450:LEU:C	2:H:450:LEU:HD23	2.36	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
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:573:VAL:CG2	2:F:585:ILE:HG13	2.46	0.45
2:F:554:PHE:HB2	2:F:594:ILE:HD13	1.98	0.45
2:F:215:HIS:ND1	2:H:478:SER:HB2	2.31	0.45
1:A:140:ALA:N	1:A:141:PRO:HD2	2.32	0.45
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:263:MET:CE	2:B:692:ALA:HA	2.47	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
2:B:341:PHE:O	2:B:342:ARG:C	2.55	0.45
2:D:263:MET:HE3	2:D:692:ALA:HA	1.98	0.45
1:E:337:GLU:O	1:E:338:SER:HB3	2.17	0.45
1:G:370:LEU:HD22	1:G:380:ALA:HA	1.97	0.45
1:G:89:HIS:HB3	1:G:92:GLN:HG3	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:273:GLU:HA	1:C:276:ARG:NH1	2.31	0.45
2:B:187:GLU:HG2	2:D:21:ARG:HD2	1.99	0.45
1:E:205:GLY:O	1:E:209:SER:OG	2.24	0.45
1:E:373:LYS:HB2	1:E:378:GLU:HG3	1.99	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:A:428:MET:H	1:A:428:MET:CE	2.30	0.44
1:C:216:LEU:CD2	2:D:107:ARG:HD3	2.47	0.44
2:F:283:SER:O	2:F:366:ARG:NH1	2.45	0.44
2:F:273:ARG:HD2	2:F:294:LEU:HD12	1.98	0.44
2:F:321:VAL:HG12	2:F:323:ALA:O	2.17	0.44
2:H:197:GLN:HG2	2:H:488:MET:HE1	1.99	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
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:139:TYR:HA	1:G:142:ILE:HD12	1.98	0.44
1:G:92:GLN:HB3	2:H:16:VAL:HG13	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: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: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:D:133:LEU:HD12	2:D:133:LEU:HA	1.87	0.44
1:E:89:HIS:O	1:E:90:PRO:C	2.56	0.44
1:G:131:GLY:HA3	1:G:274:GLN:OE1	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:171:GLN:NE2	2:H:674:TRP:HB2	2.33	0.44
2:B:35:LEU:HA	2:B:101:VAL:O	2.17	0.44
1:A:92:GLN:HB3	2:B:16:VAL:HG13	1.99	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
2:H:729:GLY:HA3	5:H:1778:MTE:H4'2	1.99	0.44
2:H:272:PHE:HA	2:H:294:LEU:O	2.17	0.44
1:G:460:VAL:HG21	2:H:632:VAL:HG11	1.99	0.44
2:B:360:LEU:O	2:B:364:MET:HE3	2.18	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
1:A:365:CYS:O	1:A:384:PHE:HA	2.17	0.44
1:A:52:ARG:HB3	1:A:74:ALA:HB3	1.99	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
2:F:160:HIS:CB	2:F:364:MET:HE2	2.48	0.43
1:A:397:PHE:HE1	1:A:415:LEU:HA	1.84	0.43
2:B:186:ALA:O	2:B:187:GLU:C	2.57	0.43
2:D:269:ARG:NH2	2:D:341:PHE:CD2	2.86	0.43
1:E:12:ARG:NH1	1:E:12:ARG:HG2	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:211:TRP:O	1:C:215:ALA:HB3	2.18	0.43
1:C:273:GLU:OE1	1:C:276:ARG:NH1	2.51	0.43
2:D:280:ALA:HB3	2:D:364:MET:CE	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:671:GLY:O	2:H:674:TRP:HB3	2.19	0.43
1:A:291:ILE:HG12	1:A:291:ILE:H	1.74	0.43
2:B:700:ALA:O	2:B:703:ASP:HB2	2.18	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
1:G:7:LEU:O	1:G:8:ASN:C	2.56	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:597:SER:HB2	2:D:522:PRO:HG3	1.99	0.43
2:B:171:GLN:NE2	2:B:674:TRP:HB2	2.33	0.43
1:E:214:LYS:HA	1:E:214:LYS:HD3	1.85	0.43
1:E:6:LEU:HD12	1:E:10:GLU:C	2.38	0.43
1:G:15:ARG:HG2	1:G:15:ARG:HH11	1.83	0.43
2:H:221:MET:HE2	2:H:486:THR:HB	2.01	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
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: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:C:357:PHE:HE1	2:D:640:ASN:O	2.01	0.43
1:E:355:LYS:HZ2	1:E:429:ARG:HA	1.84	0.43
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
1:E:114:MET:HE3	1:E:114:MET:HB2	1.88	0.43
2:F:306:PRO:HB2	2:F:344:PHE:HZ	1.84	0.43
1:G:143:LEU:O	1:G:143:LEU:HD23	2.18	0.43
1:A:308:ARG:O	1:A:334:GLU:HA	2.19	0.43
1:A:36:LYS:NZ	2:B:25:ASP:OD2	2.51	0.43
2:F:451:SER:HA	2:F:452:PRO:HD3	1.83	0.43
1:G:40:ASN:HA	1:G:40:ASN:HD22	1.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:248:THR:HA	1:E:279:ALA:O	2.19	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:554:PHE:HB2	2:H:594:ILE:CD1	2.48	0.42
2:H:683:ASP:C	2:H:683:ASP:OD1	2.58	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:440:THR:O	2:D:440:THR:HG22	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:487:GLU:HB2	2:B:493:HIS:CD2	2.53	0.42
2:B:70:LEU:HA	2:B:71:PRO:HD3	1.95	0.42
1:E:324:GLU:HB2	1:E:327:LYS:HD3	2.01	0.42
1:E:321:PHE:CE1	1:E:328:GLN:HB3	2.55	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
1:E:415:LEU:HD22	1:E:440:GLN:CB	2.49	0.42
1:E:39:CYS:O	1:E:41:GLU:HB2	2.19	0.42
1:G:295:PRO:O	1:G:296:PRO:C	2.58	0.42
2:H:146:TRP:CH2	2:H:313:LEU:HD13	2.54	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
1:A:356:ARG:CZ	2:B:697:LYS:HZ3	2.32	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:111:ILE:HD11	2:D:16:VAL:HG22	2.02	0.42
1:C:96:ILE:HD11	2:D:13:ARG:HA	2.01	0.42
2:D:143:PRO:HB3	2:D:329:HIS:CE1	2.55	0.42
2:D:53:GLU:HB3	2:D:54:PRO:CD	2.48	0.42
2:F:437:TRP:CE3	2:F:446:ARG:HG3	2.54	0.42
2:H:269:ARG:HH11	2:H:269:ARG:HG3	1.85	0.42
1:A:192:TRP:O	1:A:196:HIS:HD2	2.01	0.42
1:A:81:ILE:HD13	1:A:81:ILE:HA	1.95	0.42
2:B:771:ARG:HD2	2:B:776:ARG:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:303:LEU:O	2:D:307:VAL:HG23	2.19	0.42
1:E:355:LYS:HZ1	1:E:429:ARG:HA	1.84	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
2:B:186:ALA:O	2:B:187:GLU:O	2.38	0.42
2:B:160:HIS:CB	2:B:364:MET:CE	2.97	0.42
2:B:407:GLN:HE22	2:B:619:PHE:HB2	1.85	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
2:H:158:ALA:O	2:H:159:ALA:C	2.57	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:HG3	1:E:312:GLU:H	1.54	0.42
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: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: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
1:G:43:ASP:CB	2:H:693:PRO:HB2	2.48	0.42
2:H:95:GLY:HA3	2:H:264:VAL:HG12	2.02	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
2:F:175:TYR:O	2:F:259:ARG:NH2	2.51	0.41
2:F:53:GLU:N	2:F:54:PRO:CD	2.83	0.41
1:G:184:GLU:HA	1:G:227:HIS:O	2.20	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:192:TRP:O	1:A:196:HIS:CD2	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:149:ALA:O	1:G:152:GLU:HB2	2.20	0.41
1:G:47:CYS:SG	1:G:63:CYS:HB3	2.59	0.41
1:A:316:MET:HG3	1:A:317:PRO:O	2.21	0.41
2:B:177:GLU:OE1	2:B:225:GLY:N	2.50	0.41
2:B:170:GLY:N	2:B:271:ASP:HB3	2.35	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: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:221:MET:HE1	2:B:224:MET:HG3	2.02	0.41
2:B:40:SER:HB2	2:B:98:ILE:HD11	2.03	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
1:G:314:ARG:HH22	1:G:329:ASP:CG	2.24	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:HD3	2:B:706:ARG:HA	1.36	0.41
2:D:328:SER:OG	2:D:330:ARG:NH1	2.48	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:404:GLN:HB3	1:A:410:THR:CG2	2.50	0.41
2:B:574:GLN:HG2	2:B:579:SER:HB3	2.02	0.41
1:E:191:ASP:O	1:E:194:LEU:HB3	2.20	0.41
1:E:78:ILE:HD13	1:E:108:PRO:HA	2.02	0.41
1:G:36:LYS:HA	1:G:36:LYS:HD3	1.82	0.41
1:G:8:ASN:HA	1:G:76:ARG:CD	2.51	0.41
2:H:358:GLU:O	2:H:362:ARG:HG2	2.20	0.41
1:C:361:ILE:HG12	1:C:429:ARG:NE	2.35	0.41
2:D:671:GLY:HA2	2:D:733:PHE:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:249:ILE:HG21	1:G:270:PHE:CD2	2.56	0.41
2:H:563:ALA:O	2:H:566:VAL:HG23	2.21	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
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
4:E:1465:FAD:N1	4:E:1465:FAD:C2'	2.84	0.41
1:E:314:ARG:NH1	1:E:334:GLU:OE2	2.54	0.41
1:G:399:ALA:C	1:G:401:LEU:H	2.23	0.41
1:A:295:PRO:O	1:A:296:PRO:C	2.59	0.41
2:B:205:LYS:HG3	2:B:236:ASN:OD1	2.21	0.41
2:B:325:ARG:HH11	2:B:325:ARG:HG2	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:160:HIS:HB2	2:D:364:MET:HE1	2.03	0.41
2:D:632:VAL:HG22	2:D:643:LEU:HD11	2.03	0.41
1:G:207:ASP:OD2	4:G:1465:FAD:O2'	2.35	0.41
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
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:152:GLU:HG2	2:F:423:LYS:HB2	2.02	0.40
2:B:66:THR:CG2	2:B:68:ALA:H	2.29	0.40
1:C:22:SER:OG	1:C:25:GLU:HG2	2.20	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:B:219:VAL:O	2:B:517:ASP:HA	2.21	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:HG3	2:B:697:LYS:HZ2	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%)	12	24
1	C	446/462 (96%)	422 (95%)	20 (4%)	4 (1%)	17	35
1	E	446/462 (96%)	389 (87%)	46 (10%)	11 (2%)	5	9
1	G	446/462 (96%)	383 (86%)	56 (13%)	7 (2%)	9	19
2	B	756/777 (97%)	706 (93%)	39 (5%)	11 (2%)	10	21
2	D	756/777 (97%)	713 (94%)	36 (5%)	7 (1%)	17	35
2	F	756/777 (97%)	707 (94%)	41 (5%)	8 (1%)	14	30
2	H	756/777 (97%)	689 (91%)	58 (8%)	9 (1%)	13	27
All	All	4808/4956 (97%)	4411 (92%)	334 (7%)	63 (1%)	12	24

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%)	311 (92%)	28 (8%)	11	22
1	C	339/347 (98%)	311 (92%)	28 (8%)	11	22
1	E	339/347 (98%)	306 (90%)	33 (10%)	8	15
1	G	339/347 (98%)	304 (90%)	35 (10%)	7	13
2	B	571/584 (98%)	524 (92%)	47 (8%)	11	22
2	D	571/584 (98%)	530 (93%)	41 (7%)	14	29
2	F	571/584 (98%)	523 (92%)	48 (8%)	11	21
2	H	571/584 (98%)	529 (93%)	42 (7%)	13	28
All	All	3640/3724 (98%)	3338 (92%)	302 (8%)	11	22

All (302) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	20	THR
1	A	33	THR
1	A	40	ASN
1	A	43	ASP
1	A	58	ARG
1	A	76	ARG
1	A	79	GLU
1	A	128	LEU
1	A	143	LEU
1	A	191	ASP

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Mol	Chain	Res	Type
1	A	212	VAL
1	A	239	ASP
1	A	291	ILE
1	A	320	ASP
1	A	338	SER
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	428	MET
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	165	CYS
2	B	175	TYR
2	B	176	LEU
2	B	187	GLU
2	B	215	HIS
2	B	221	MET
2	B	222	ARG
2	B	256	ARG
2	B	268	LYS
2	B	271	ASP
2	B	313	LEU
2	B	330	ARG
2	B	341	PHE
2	B	355	ARG
2	B	359	HIS
2	B	366	ARG
2	B	381	GLU
2	B	399	LYS

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Mol	Chain	Res	Type
2	B	423	LYS
2	B	440	THR
2	B	442	ARG
2	B	461	LEU
2	B	472	GLN
2	B	512	ARG
2	B	530	SER
2	B	564	ARG
2	B	604	THR
2	B	609	TRP
2	B	617	ARG
2	B	632	VAL
2	B	641	ARG
2	B	650	ASP
2	B	695	THR
2	B	697	LYS
2	B	704	ARG
2	B	706	ARG
2	B	708	PHE
2	B	741	LEU
2	B	743	LEU
2	B	744	HIS
1	C	1	MET
1	C	11	THR
1	C	12	ARG
1	C	33	THR
1	C	40	ASN
1	C	76	ARG
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	270	PHE
1	C	281	ILE
1	C	309	ARG
1	C	355	LYS
1	C	361	ILE
1	C	376	LYS
1	C	379	THR

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Mol	Chain	Res	Type
1	C	405	ASP
1	C	409	ASP
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	10	ASP
2	D	16	VAL
2	D	23	LEU
2	D	66	THR
2	D	81	SER
2	D	107	ARG
2	D	130	ASP
2	D	148	ARG
2	D	151	VAL
2	D	152	GLU
2	D	174	PHE
2	D	175	TYR
2	D	215	HIS
2	D	221	MET
2	D	222	ARG
2	D	247	ARG
2	D	256	ARG
2	D	258	ASP
2	D	260	ASP
2	D	268	LYS
2	D	313	LEU
2	D	330	ARG
2	D	341	PHE
2	D	366	ARG
2	D	367	ASP
2	D	381	GLU
2	D	398	LYS
2	D	399	LYS
2	D	400	THR
2	D	431	ARG
2	D	450	LEU
2	D	512	ARG
2	D	530	SER
2	D	561	CYS

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Mol	Chain	Res	Type
2	D	613	ARG
2	D	617	ARG
2	D	632	VAL
2	D	697	LYS
2	D	704	ARG
2	D	708	PHE
2	D	741	LEU
1	E	1	MET
1	E	11	THR
1	E	12	ARG
1	E	33	THR
1	E	40	ASN
1	E	43	ASP
1	E	44	CYS
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	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
2	F	10	ASP
2	F	16	VAL

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Mol	Chain	Res	Type
2	F	48	THR
2	F	53	GLU
2	F	130	ASP
2	F	151	VAL
2	F	165	CYS
2	F	166	PHE
2	F	175	TYR
2	F	176	LEU
2	F	182	LEU
2	F	190	VAL
2	F	215	HIS
2	F	218	ARG
2	F	247	ARG
2	F	256	ARG
2	F	258	ASP
2	F	259	ARG
2	F	268	LYS
2	F	310	ARG
2	F	313	LEU
2	F	330	ARG
2	F	341	PHE
2	F	355	ARG
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	439	SER
2	F	450	LEU
2	F	461	LEU
2	F	512	ARG
2	F	516	THR
2	F	530	SER
2	F	534	ASP
2	F	558	ARG
2	F	567	ILE
2	F	608	SER
2	F	617	ARG
2	F	630	GLU
2	F	632	VAL

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Mol	Chain	Res	Type
2	F	641	ARG
2	F	704	ARG
2	F	708	PHE
2	F	741	LEU
1	G	25	GLU
1	G	33	THR
1	G	35	THR
1	G	40	ASN
1	G	63	CYS
1	G	76	ARG
1	G	79	GLU
1	G	91	VAL
1	G	103	CYS
1	G	128	LEU
1	G	198	GLU
1	G	212	VAL
1	G	218	ASP
1	G	231	LEU
1	G	243	ILE
1	G	257	GLU
1	G	281	ILE
1	G	289	SER
1	G	291	ILE
1	G	301	MET
1	G	311	GLN
1	G	315	ARG
1	G	326	ARG
1	G	327	LYS
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	457	VAL
2	H	10	ASP
2	H	16	VAL
2	H	23	LEU

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Mol	Chain	Res	Type
2	H	66	THR
2	H	90	GLU
2	H	148	ARG
2	H	151	VAL
2	H	165	CYS
2	H	174	PHE
2	H	175	TYR
2	H	215	HIS
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	341	PHE
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	512	ARG
2	H	534	ASP
2	H	564	ARG
2	H	604	THR
2	H	617	ARG
2	H	632	VAL
2	H	650	ASP
2	H	677	THR
2	H	697	LYS
2	H	704	ARG
2	H	708	PHE
2	H	741	LEU
2	H	743	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	196	HIS
1	A	359	GLN
2	B	204	HIS
2	B	208	HIS
2	B	236	ASN
2	B	293	HIS
2	B	359	HIS
2	B	426	ASN
2	B	463	HIS
2	B	574	GLN
1	C	40	ASN
1	C	233	GLN
1	C	359	GLN
1	C	420	GLN
2	D	198	HIS
2	D	208	HIS
2	D	236	ASN
2	D	293	HIS
2	D	359	HIS
2	D	426	ASN
2	D	463	HIS
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	204	HIS
2	F	236	ASN
2	F	359	HIS
2	F	426	ASN
2	F	463	HIS
2	F	482	ASN
2	F	574	GLN
2	F	744	HIS
1	G	40	ASN
1	G	196	HIS
1	G	328	GLN
1	G	359	GLN
2	H	106	HIS
2	H	208	HIS
2	H	236	ASN

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Mol	Chain	Res	Type
2	H	293	HIS
2	H	359	HIS
2	H	441	ASN
2	H	572	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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
7	XAN	D	1780[B]	-	8,12,12	2.05	2 (25%)	4,17,17	5.22	4 (100%)
7	XAN	H	1780[A]	-	8,12,12	1.94	2 (25%)	4,17,17	5.29	3 (75%)
7	XAN	H	1780[B]	-	8,12,12	2.09	2 (25%)	4,17,17	5.19	4 (100%)
3	FES	A	1463	1	0,4,4	0.00	-	-	-	-
4	FAD	E	1465	-	51,58,58	1.86	7 (13%)	60,89,89	1.74	11 (18%)
5	MTE	B	1778	8	21,26,26	3.89	5 (23%)	21,40,40	2.73	9 (42%)
4	FAD	A	1465	-	51,58,58	1.91	8 (15%)	60,89,89	1.69	10 (16%)
3	FES	G	1463	1	0,4,4	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FAD	C	1465	-	51,58,58	1.98	9 (17%)	60,89,89	1.89	15 (25%)
3	FES	C	1464	1	0,4,4	0.00	-	-		
8	MOM	D	1781	5	0,3,3	0.00	-	-		
3	FES	C	1463	1	0,4,4	0.00	-	-		
8	MOM	F	1781	5	0,3,3	0.00	-	-		
3	FES	E	1463	1	0,4,4	0.00	-	-		
3	FES	E	1464	1	0,4,4	0.00	-	-		
5	MTE	H	1778	8	21,26,26	3.68	6 (28%)	21,40,40	2.34	7 (33%)
3	FES	A	1464	1	0,4,4	0.00	-	-		
8	MOM	B	1781	5	0,3,3	0.00	-	-		
7	XAN	B	1780[B]	-	8,12,12	2.06	2 (25%)	4,17,17	5.27	4 (100%)
3	FES	G	1464	1	0,4,4	0.00	-	-		
7	XAN	F	1780[B]	-	8,12,12	2.06	2 (25%)	4,17,17	5.28	4 (100%)
7	XAN	B	1780[A]	-	8,12,12	1.96	2 (25%)	4,17,17	5.13	4 (100%)
4	FAD	G	1465	-	51,58,58	1.82	6 (11%)	60,89,89	1.59	11 (18%)
5	MTE	D	1778	8	21,26,26	3.96	6 (28%)	21,40,40	2.76	8 (38%)
7	XAN	F	1780[A]	-	8,12,12	2.03	2 (25%)	4,17,17	5.20	4 (100%)
5	MTE	F	1778	8	21,26,26	4.07	7 (33%)	21,40,40	2.55	9 (42%)
8	MOM	H	1781	5	0,3,3	0.00	-	-		
7	XAN	D	1780[A]	-	8,12,12	1.87	2 (25%)	4,17,17	5.43	3 (75%)

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
7	XAN	D	1780[B]	-	-	-	0/2/2/2
7	XAN	H	1780[A]	-	-	-	0/2/2/2
7	XAN	H	1780[B]	-	-	-	0/2/2/2
3	FES	A	1463	1	-	-	0/1/1/1
4	FAD	E	1465	-	-	16/30/50/50	0/6/6/6
5	MTE	B	1778	8	1/1/6/8	1/6/34/34	0/3/3/3
4	FAD	A	1465	-	-	12/30/50/50	0/6/6/6
3	FES	G	1463	1	-	-	0/1/1/1
4	FAD	C	1465	-	-	10/30/50/50	0/6/6/6
3	FES	C	1464	1	-	-	0/1/1/1
3	FES	C	1463	1	-	-	0/1/1/1
3	FES	E	1463	1	-	-	0/1/1/1
3	FES	E	1464	1	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MTE	H	1778	8	1/1/6/8	2/6/34/34	0/3/3/3
3	FES	A	1464	1	-	-	0/1/1/1
7	XAN	B	1780[B]	-	-	-	0/2/2/2
3	FES	G	1464	1	-	-	0/1/1/1
7	XAN	F	1780[B]	-	-	-	0/2/2/2
7	XAN	B	1780[A]	-	-	-	0/2/2/2
4	FAD	G	1465	-	-	9/30/50/50	0/6/6/6
5	MTE	D	1778	8	1/1/6/8	2/6/34/34	0/3/3/3
7	XAN	F	1780[A]	-	-	-	0/2/2/2
5	MTE	F	1778	8	1/1/6/8	1/6/34/34	0/3/3/3
7	XAN	D	1780[A]	-	-	-	0/2/2/2

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	1778	MTE	C4'-C3'	-14.73	1.32	1.52
5	B	1778	MTE	C4'-C3'	-14.06	1.33	1.52
5	D	1778	MTE	C4'-C3'	-13.89	1.33	1.52
5	H	1778	MTE	C4'-C3'	-12.29	1.35	1.52
5	D	1778	MTE	C6-N5	-8.16	1.33	1.45
5	F	1778	MTE	C6-N5	-7.92	1.34	1.45
5	H	1778	MTE	C6-N5	-7.91	1.34	1.45
5	B	1778	MTE	C6-N5	-7.77	1.34	1.45
4	C	1465	FAD	C10-N1	6.98	1.42	1.33
4	G	1465	FAD	O4B-C1B	6.45	1.50	1.41
4	E	1465	FAD	C10-N1	6.38	1.41	1.33
4	G	1465	FAD	C10-N1	6.33	1.41	1.33
4	A	1465	FAD	C4X-N5	5.99	1.41	1.33
4	A	1465	FAD	C10-N1	5.89	1.40	1.33
4	E	1465	FAD	O4B-C1B	5.84	1.49	1.41
5	D	1778	MTE	C4-C9	5.81	1.49	1.41
4	E	1465	FAD	C4X-N5	5.51	1.41	1.33
5	H	1778	MTE	C4-C9	5.36	1.48	1.41
5	B	1778	MTE	C4-C9	5.17	1.48	1.41
5	F	1778	MTE	C4-C9	5.16	1.48	1.41
4	C	1465	FAD	C4-N3	5.13	1.42	1.33
4	A	1465	FAD	O4B-C1B	4.92	1.47	1.41
4	C	1465	FAD	C4X-N5	4.89	1.40	1.33
7	D	1780[B]	XAN	C6-C5	4.74	1.49	1.41
7	H	1780[B]	XAN	C6-C5	4.71	1.49	1.41
4	A	1465	FAD	C4-N3	4.69	1.41	1.33
7	F	1780[B]	XAN	C6-C5	4.67	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	1465	FAD	C4-N3	4.63	1.41	1.33
7	B	1780[B]	XAN	C6-C5	4.60	1.49	1.41
7	F	1780[A]	XAN	C6-C5	4.59	1.49	1.41
4	G	1465	FAD	C4X-N5	4.46	1.39	1.33
7	B	1780[A]	XAN	C6-C5	4.42	1.49	1.41
7	H	1780[A]	XAN	C6-C5	4.35	1.48	1.41
4	C	1465	FAD	C9A-N10	4.12	1.44	1.38
4	E	1465	FAD	C4-N3	4.05	1.40	1.33
7	D	1780[A]	XAN	C6-C5	3.97	1.48	1.41
4	C	1465	FAD	O4B-C1B	3.88	1.46	1.41
5	H	1778	MTE	C9-N5	3.71	1.45	1.38
5	B	1778	MTE	C9-N5	3.53	1.45	1.38
4	C	1465	FAD	C2'-C3'	-3.51	1.46	1.53
5	H	1778	MTE	C9-C10	3.48	1.48	1.41
5	F	1778	MTE	C9-N5	3.36	1.44	1.38
5	D	1778	MTE	C9-N5	3.31	1.44	1.38
5	B	1778	MTE	C9-C10	3.31	1.47	1.41
4	A	1465	FAD	C9A-N10	3.24	1.42	1.38
4	E	1465	FAD	C9A-N10	3.24	1.42	1.38
5	F	1778	MTE	C7-C6	-3.18	1.51	1.53
5	D	1778	MTE	C9-C10	3.06	1.47	1.41
4	A	1465	FAD	C1'-N10	3.03	1.51	1.48
4	E	1465	FAD	C5X-N5	3.00	1.40	1.35
4	A	1465	FAD	C5X-N5	2.93	1.40	1.35
7	B	1780[B]	XAN	C5-C4	2.88	1.48	1.40
5	F	1778	MTE	C9-C10	2.85	1.46	1.41
4	C	1465	FAD	C2B-C1B	-2.84	1.49	1.53
7	H	1780[B]	XAN	C5-C4	2.80	1.48	1.40
5	H	1778	MTE	C7-C6	-2.80	1.51	1.53
7	B	1780[A]	XAN	C5-C4	2.69	1.48	1.40
7	H	1780[A]	XAN	C5-C4	2.66	1.48	1.40
7	D	1780[A]	XAN	C5-C4	2.65	1.47	1.40
7	F	1780[B]	XAN	C5-C4	2.64	1.47	1.40
7	F	1780[A]	XAN	C5-C4	2.62	1.47	1.40
7	D	1780[B]	XAN	C5-C4	2.53	1.47	1.40
4	G	1465	FAD	C5X-N5	2.48	1.39	1.35
4	A	1465	FAD	C4X-C10	2.37	1.41	1.38
4	E	1465	FAD	C5B-C4B	2.29	1.58	1.51
4	C	1465	FAD	C5X-N5	2.26	1.39	1.35
4	G	1465	FAD	C9A-N10	2.14	1.41	1.38
5	D	1778	MTE	C7-C6	-2.13	1.52	1.53
4	C	1465	FAD	O5'-C5'	-2.08	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	1778	MTE	O3'-C3'	2.07	1.46	1.43

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	1780[A]	XAN	C6-N1-C2	8.91	122.67	115.14
7	H	1780[A]	XAN	C6-N1-C2	8.62	122.42	115.14
7	B	1780[B]	XAN	C6-N1-C2	8.44	122.26	115.14
7	F	1780[B]	XAN	C6-N1-C2	8.42	122.25	115.14
7	F	1780[A]	XAN	C6-N1-C2	8.35	122.19	115.14
7	B	1780[A]	XAN	C6-N1-C2	8.27	122.12	115.14
7	D	1780[B]	XAN	C6-N1-C2	8.25	122.11	115.14
7	H	1780[B]	XAN	C6-N1-C2	8.23	122.09	115.14
5	D	1778	MTE	C4-C9-N5	7.50	125.42	119.12
5	H	1778	MTE	C4-C9-N5	6.97	124.97	119.12
5	B	1778	MTE	C4-C9-N5	6.80	124.83	119.12
5	F	1778	MTE	C4-C9-N5	6.77	124.80	119.12
4	C	1465	FAD	C4-N3-C2	6.42	120.56	115.14
4	A	1465	FAD	C4-N3-C2	5.78	120.02	115.14
4	E	1465	FAD	C4-N3-C2	5.57	119.84	115.14
4	G	1465	FAD	C4-N3-C2	5.44	119.73	115.14
4	C	1465	FAD	C4X-N5-C5X	5.36	122.13	116.77
5	D	1778	MTE	O3'-C7-C6	5.31	112.51	108.96
4	E	1465	FAD	C4X-N5-C5X	4.97	121.74	116.77
4	G	1465	FAD	N3A-C2A-N1A	-4.96	120.93	128.68
4	C	1465	FAD	C1'-N10-C9A	4.80	122.07	118.29
5	B	1778	MTE	O3'-C7-C6	4.77	112.15	108.96
4	E	1465	FAD	N3A-C2A-N1A	-4.72	121.30	128.68
4	A	1465	FAD	N3A-C2A-N1A	-4.52	121.62	128.68
7	D	1780[A]	XAN	C5-C6-N1	-4.40	117.41	123.43
7	F	1780[B]	XAN	C6-C5-C4	-4.33	116.67	120.80
7	B	1780[B]	XAN	C5-C6-N1	-4.28	117.58	123.43
7	B	1780[A]	XAN	C5-C6-N1	-4.23	117.65	123.43
7	F	1780[A]	XAN	C6-C5-C4	-4.19	116.80	120.80
7	H	1780[A]	XAN	C5-C6-N1	-4.17	117.72	123.43
4	A	1465	FAD	C5X-C9A-N10	4.16	120.73	117.72
7	H	1780[B]	XAN	C6-C5-C4	-4.16	116.83	120.80
5	D	1778	MTE	C4-N3-C2	4.13	122.48	115.93
7	H	1780[A]	XAN	C6-C5-C4	-4.10	116.88	120.80
7	F	1780[A]	XAN	C5-C6-N1	-4.09	117.83	123.43
7	H	1780[B]	XAN	C5-C6-N1	-4.09	117.84	123.43
7	D	1780[B]	XAN	C5-C6-N1	-4.08	117.85	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	1780[B]	XAN	C6-C5-C4	-4.06	116.92	120.80
5	H	1778	MTE	C4-N3-C2	4.05	122.37	115.93
7	F	1780[B]	XAN	C5-C6-N1	-4.03	117.92	123.43
7	D	1780[A]	XAN	C6-C5-C4	-3.97	117.00	120.80
5	B	1778	MTE	C4-N3-C2	3.96	122.22	115.93
7	B	1780[B]	XAN	C6-C5-C4	-3.94	117.03	120.80
4	C	1465	FAD	N3A-C2A-N1A	-3.92	122.54	128.68
4	G	1465	FAD	C4X-N5-C5X	3.91	120.68	116.77
7	B	1780[A]	XAN	C6-C5-C4	-3.87	117.10	120.80
5	F	1778	MTE	C2-N1-C10	3.72	122.88	114.54
5	F	1778	MTE	C7-C6-C1'	3.66	118.74	110.53
4	A	1465	FAD	P-O3P-PA	-3.65	120.30	132.83
5	B	1778	MTE	C7-C6-C1'	3.60	118.60	110.53
5	B	1778	MTE	O3P-P-O4'	-3.60	97.16	106.73
5	D	1778	MTE	C7-C6-C1'	3.57	118.54	110.53
4	E	1465	FAD	C5X-C9A-N10	3.50	120.25	117.72
5	F	1778	MTE	C4-N3-C2	3.41	121.34	115.93
4	E	1465	FAD	C1'-N10-C9A	3.39	120.96	118.29
4	A	1465	FAD	C1'-N10-C10	3.31	121.37	118.41
5	F	1778	MTE	O3P-P-O4'	-3.21	98.18	106.73
4	C	1465	FAD	C4'-C3'-C2'	-3.09	106.94	113.36
4	E	1465	FAD	P-O3P-PA	-3.07	122.31	132.83
5	B	1778	MTE	O3'-C7-N8	-3.03	105.46	108.57
5	B	1778	MTE	C2-N1-C10	2.98	121.23	114.54
5	F	1778	MTE	C4-C9-C10	2.96	117.20	114.57
5	D	1778	MTE	C2-N1-C10	2.92	121.09	114.54
4	A	1465	FAD	C9A-N10-C10	-2.92	118.08	121.91
4	E	1465	FAD	C10-C4X-N5	-2.92	119.24	121.26
4	G	1465	FAD	P-O3P-PA	-2.90	122.86	132.83
4	C	1465	FAD	C4X-C4-N3	-2.88	119.50	123.43
5	D	1778	MTE	O3P-P-O4'	-2.84	99.18	106.73
5	H	1778	MTE	C7-C6-C1'	2.83	116.88	110.53
4	C	1465	FAD	O2'-C2'-C3'	-2.83	102.21	109.10
4	A	1465	FAD	C1'-N10-C9A	2.83	120.52	118.29
4	C	1465	FAD	P-O3P-PA	-2.78	123.27	132.83
4	A	1465	FAD	C4X-N5-C5X	2.77	119.54	116.77
7	D	1780[B]	XAN	C4-C5-N7	-2.76	106.52	109.40
5	H	1778	MTE	C2-N1-C10	2.70	120.60	114.54
5	H	1778	MTE	O3'-C7-C6	-2.68	107.17	108.96
4	A	1465	FAD	C4X-C4-N3	-2.65	119.80	123.43
4	C	1465	FAD	O4B-C1B-C2B	-2.63	103.09	106.93
4	G	1465	FAD	C10-C4X-N5	-2.51	119.52	121.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1778	MTE	C4-C9-C10	2.48	116.77	114.57
7	B	1780[B]	XAN	C4-C5-N7	-2.45	106.85	109.40
7	H	1780[B]	XAN	C4-C5-N7	-2.43	106.87	109.40
4	G	1465	FAD	C5X-C9A-N10	2.41	119.46	117.72
4	G	1465	FAD	C4X-C4-N3	-2.40	120.15	123.43
5	F	1778	MTE	N3-C2-N1	-2.38	121.68	125.42
7	F	1780[B]	XAN	C4-C5-N7	-2.36	106.94	109.40
4	C	1465	FAD	O3'-C3'-C4'	2.35	114.49	108.81
5	F	1778	MTE	O3P-P-O1P	2.34	119.86	110.68
4	C	1465	FAD	C4A-C5A-N7A	-2.27	107.03	109.40
4	G	1465	FAD	C4A-C5A-N7A	-2.25	107.06	109.40
4	C	1465	FAD	O2'-C2'-C1'	2.23	114.95	109.59
4	E	1465	FAD	C6-C5X-C9A	2.21	121.95	119.05
4	E	1465	FAD	C4X-C4-N3	-2.20	120.42	123.43
5	H	1778	MTE	C9-C4-N3	-2.19	117.78	124.01
5	F	1778	MTE	P-O4'-C4'	-2.17	112.31	118.30
4	E	1465	FAD	O3'-C3'-C4'	2.16	114.04	108.81
4	G	1465	FAD	O3B-C3B-C4B	-2.15	104.83	111.05
5	D	1778	MTE	C9-C4-N3	-2.15	117.91	124.01
4	C	1465	FAD	O5'-C5'-C4'	-2.14	103.66	109.36
4	E	1465	FAD	C9A-C5X-N5	-2.11	119.06	122.36
4	G	1465	FAD	C1'-N10-C9A	2.09	119.93	118.29
7	F	1780[A]	XAN	C4-C5-N7	-2.08	107.23	109.40
4	G	1465	FAD	C9A-N10-C10	-2.06	119.20	121.91
5	H	1778	MTE	C4-C9-C10	2.06	116.40	114.57
4	C	1465	FAD	C5X-C9A-N10	2.04	119.20	117.72
4	C	1465	FAD	C10-C4X-N5	-2.04	119.84	121.26
5	B	1778	MTE	N3-C2-N1	-2.04	122.22	125.42
4	A	1465	FAD	O4'-C4'-C3'	2.04	114.05	109.10
7	B	1780[A]	XAN	C4-C5-N7	-2.02	107.30	109.40
5	B	1778	MTE	C9-C4-N3	-2.01	118.30	124.01

All (4) chirality outliers are listed below:

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

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	1465	FAD	C5B-O5B-PA-O3P
4	E	1465	FAD	O4B-C4B-C5B-O5B
4	E	1465	FAD	C2'-C1'-N10-C9A
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'
4	E	1465	FAD	C3'-C4'-C5'-O5'
4	E	1465	FAD	O4'-C4'-C5'-O5'
4	A	1465	FAD	C2'-C1'-N10-C9A
4	A	1465	FAD	C2'-C1'-N10-C10
4	A	1465	FAD	N10-C1'-C2'-O2'
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	C2'-C1'-N10-C9A
4	C	1465	FAD	C2'-C1'-N10-C10
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'
5	B	1778	MTE	C2'-C3'-C4'-O4'
5	H	1778	MTE	O3'-C3'-C4'-O4'
4	G	1465	FAD	C2'-C1'-N10-C9A
4	G	1465	FAD	N10-C1'-C2'-C3'
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	D	1778	MTE	O3'-C3'-C4'-O4'
5	F	1778	MTE	O3'-C3'-C4'-O4'
4	E	1465	FAD	C3B-C4B-C5B-O5B

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

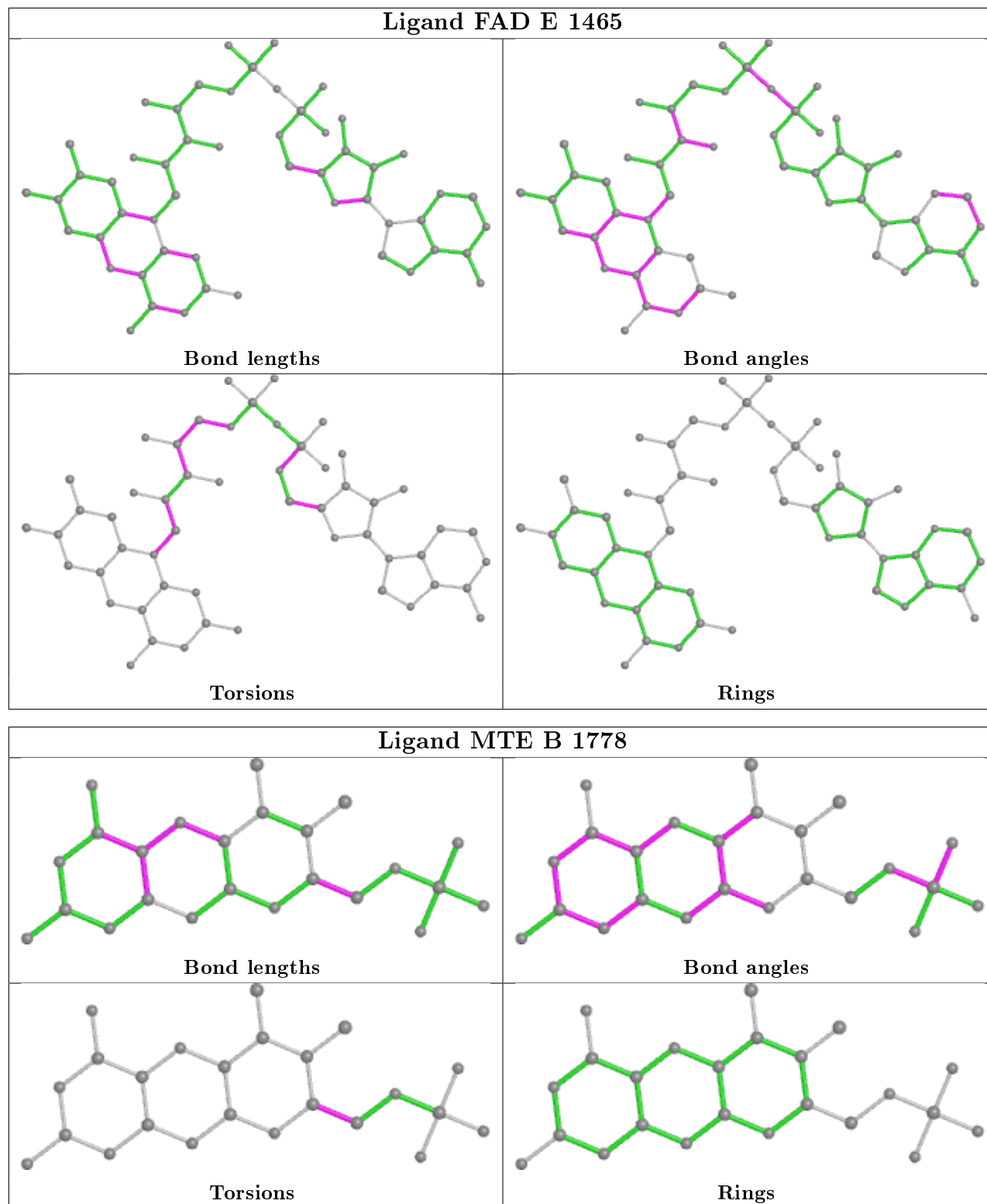
There are no ring outliers.

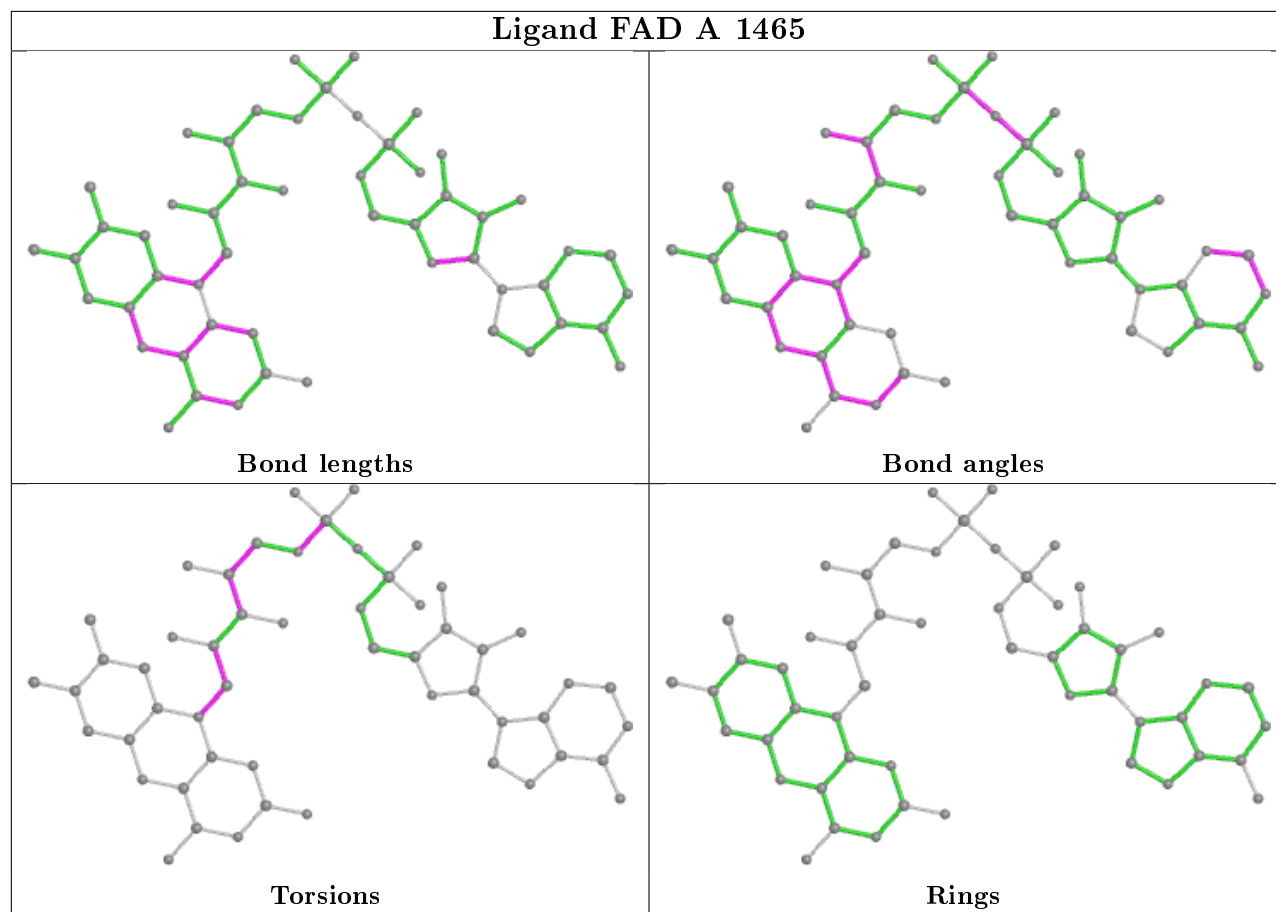
15 monomers are involved in 35 short contacts:

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

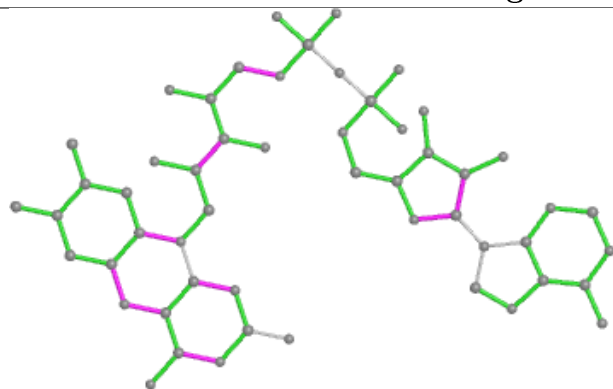
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

equivalents in the CSD to analyse the geometry.

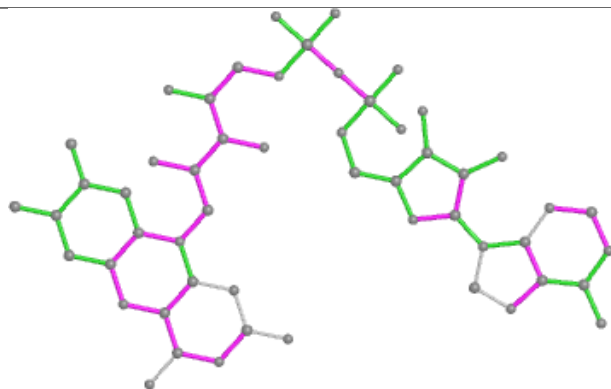




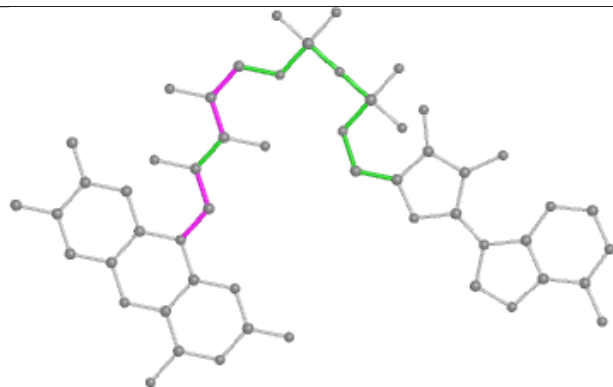
Ligand FAD C 1465



Bond lengths



Bond angles

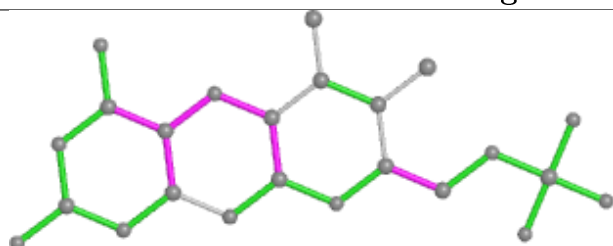


Torsions

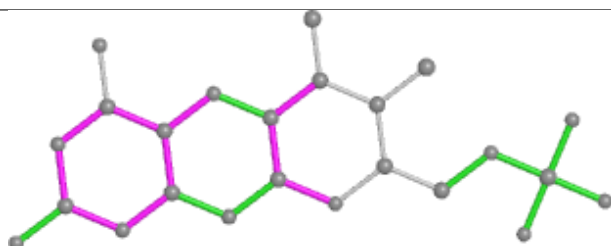


Rings

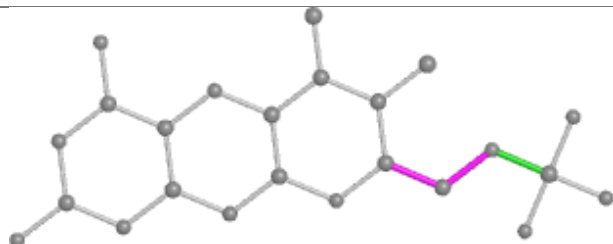
Ligand MTE H 1778



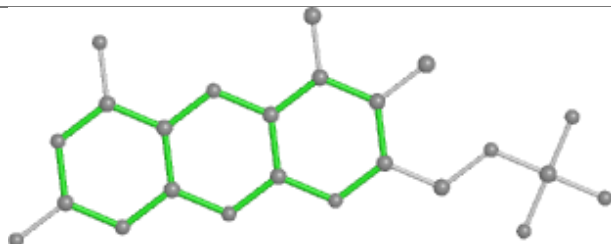
Bond lengths



Bond angles

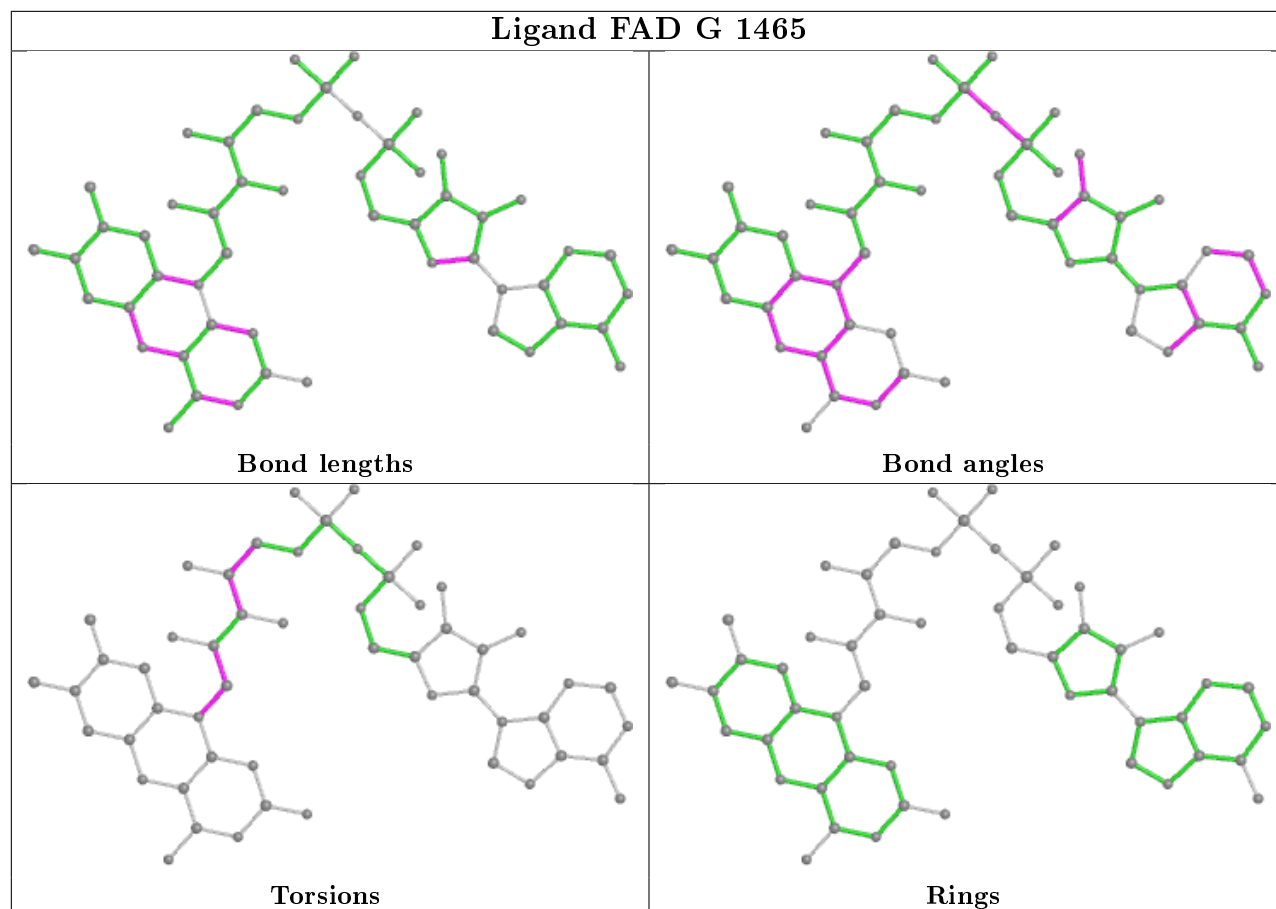


Torsions

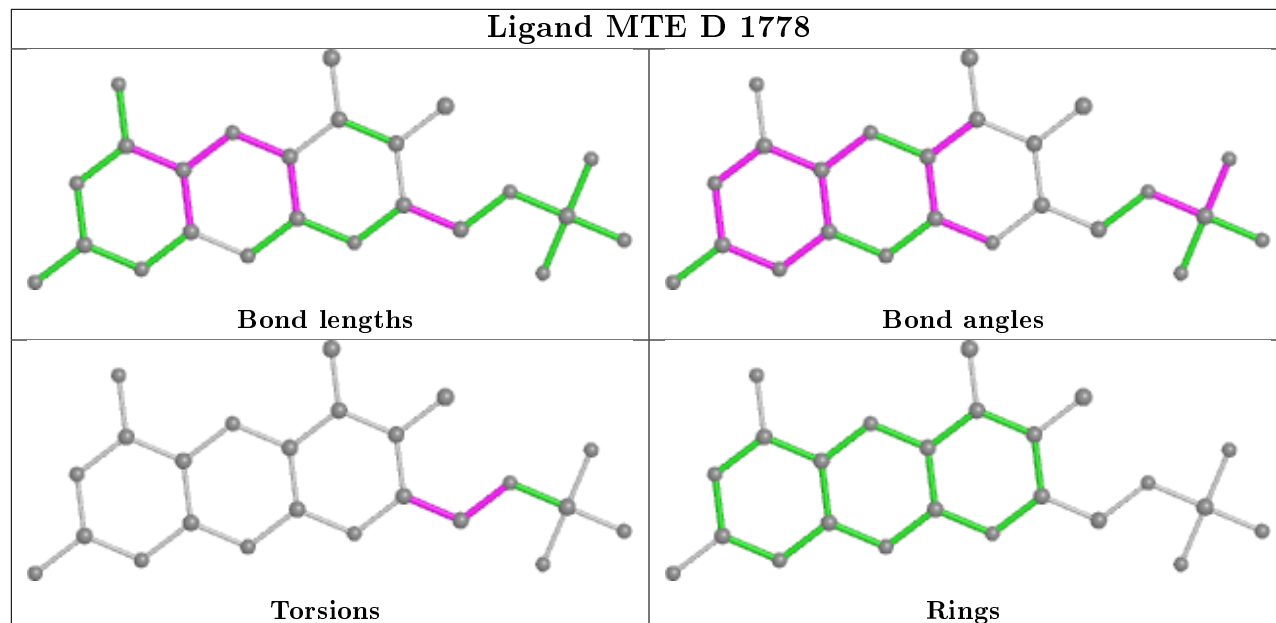


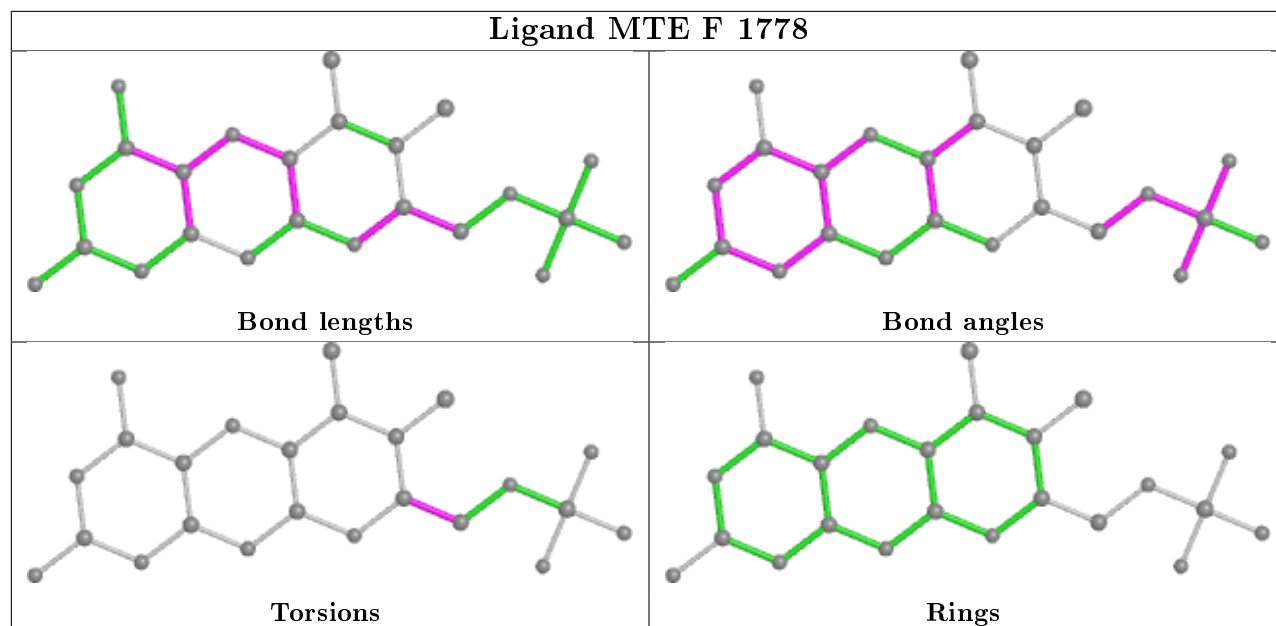
Rings

Ligand FAD G 1465



Ligand MTE D 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%)	0.22	30 (6%) 17 13	25, 49, 66, 70	0
1	C	450/462 (97%)	-0.04	7 (1%) 72 68	22, 47, 66, 70	0
1	E	450/462 (97%)	0.09	23 (5%) 28 22	25, 48, 66, 71	0
1	G	450/462 (97%)	0.25	39 (8%) 10 7	26, 49, 66, 70	0
2	B	760/777 (97%)	-0.27	3 (0%) 92 91	21, 35, 50, 59	0
2	D	760/777 (97%)	-0.28	1 (0%) 95 95	20, 34, 49, 59	0
2	F	760/777 (97%)	-0.36	1 (0%) 95 95	21, 34, 49, 59	0
2	H	760/777 (97%)	-0.35	8 (1%) 80 78	22, 35, 50, 59	0
All	All	4840/4956 (97%)	-0.15	112 (2%) 60 54	20, 39, 62, 71	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	374	GLY	4.4
1	A	411	ILE	4.2
1	A	376	LYS	4.0
1	E	166	LEU	4.0
1	A	377	ILE	3.9
1	G	239	ASP	3.9
1	A	413	ALA	3.9
2	B	777	ALA	3.8
1	A	310	GLY	3.6
1	G	240	GLY	3.6
1	G	410	THR	3.6
2	D	777	ALA	3.5
1	G	218	ASP	3.5
1	A	378	GLU	3.3
1	G	191	ASP	3.3
2	H	398	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	166	LEU	3.2
1	E	302	GLY	3.2
1	G	411	ILE	3.1
1	G	378	GLU	3.1
1	G	238	PRO	3.1
1	E	220	PRO	3.1
1	A	238	PRO	3.1
1	E	406	PHE	3.0
1	G	312	GLU	3.0
1	A	239	ASP	3.0
1	E	239	ASP	3.0
1	E	403	GLY	3.0
1	A	332	PRO	3.0
1	G	190	ALA	2.9
1	A	312	GLU	2.9
1	G	194	LEU	2.8
1	A	240	GLY	2.8
1	E	373	LYS	2.8
1	G	166	LEU	2.8
1	G	413	ALA	2.8
1	E	198	GLU	2.8
2	H	561	CYS	2.7
1	E	194	LEU	2.7
2	H	564	ARG	2.7
1	G	377	ILE	2.7
1	C	15	ARG	2.7
1	E	15	ARG	2.7
1	E	218	ASP	2.7
1	G	220	PRO	2.7
1	G	192	TRP	2.7
1	C	166	LEU	2.6
2	H	399	LYS	2.6
1	A	406	PHE	2.6
1	G	372	LEU	2.6
1	E	165	THR	2.6
2	H	560	GLY	2.6
1	A	417	LEU	2.5
1	G	402	ILE	2.5
1	G	15	ARG	2.5
1	G	165	THR	2.5
1	E	310	GLY	2.5
2	F	398	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	219	LEU	2.5
1	G	375	SER	2.5
2	B	399	LYS	2.5
1	A	403	GLY	2.5
1	A	379	THR	2.5
2	H	556	ALA	2.5
1	G	373	LYS	2.5
1	G	310	GLY	2.4
1	G	19	PRO	2.4
1	G	332	PRO	2.4
1	A	401	LEU	2.4
1	E	375	SER	2.4
1	A	405	ASP	2.4
1	C	218	ASP	2.4
2	B	398	LYS	2.4
1	E	238	PRO	2.4
1	G	185	THR	2.4
1	C	239	ASP	2.3
1	G	405	ASP	2.3
1	A	220	PRO	2.3
1	E	312	GLU	2.3
1	G	235	ARG	2.3
1	G	379	THR	2.3
1	E	181	PHE	2.3
1	A	307	LEU	2.2
1	E	197	PRO	2.2
1	E	372	LEU	2.2
1	G	376	LYS	2.2
1	G	307	LEU	2.2
1	A	165	THR	2.2
1	G	406	PHE	2.2
2	H	576	SER	2.2
1	C	402	ILE	2.2
1	A	151	GLY	2.2
1	A	373	LYS	2.2
1	C	372	LEU	2.2
1	G	195	ALA	2.2
1	C	312	GLU	2.1
1	G	401	LEU	2.1
1	A	121	ASP	2.1
1	G	403	GLY	2.1
1	A	402	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
2	H	562	ALA	2.1
1	A	374	GLY	2.1
1	A	199	ALA	2.1
1	G	53	ASP	2.1
1	A	410	THR	2.1
1	E	179	PRO	2.0
1	E	313	ARG	2.0
1	G	394	ALA	2.0
1	A	311	GLN	2.0
1	A	192	TRP	2.0
1	E	331	ARG	2.0
1	G	334	GLU	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 carbohydrates 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[B]	11/11	0.74	0.27	61,62,62,62	11
7	XAN	F	1780[A]	11/11	0.74	0.27	62,62,62,62	11
7	XAN	H	1780[A]	11/11	0.78	0.30	62,62,62,62	11
7	XAN	H	1780[B]	11/11	0.78	0.30	61,62,62,62	11
7	XAN	B	1780[A]	11/11	0.79	0.26	62,62,62,62	11
7	XAN	B	1780[B]	11/11	0.79	0.26	61,62,62,62	11
7	XAN	D	1780[B]	11/11	0.84	0.20	61,62,62,62	11
7	XAN	D	1780[A]	11/11	0.84	0.20	62,62,62,62	11
4	FAD	G	1465	53/53	0.91	0.17	41,50,63,64	0
5	MTE	H	1778	24/24	0.92	0.28	33,38,41,43	24
4	FAD	A	1465	53/53	0.93	0.15	38,48,56,56	0

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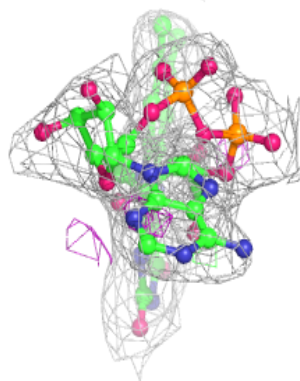
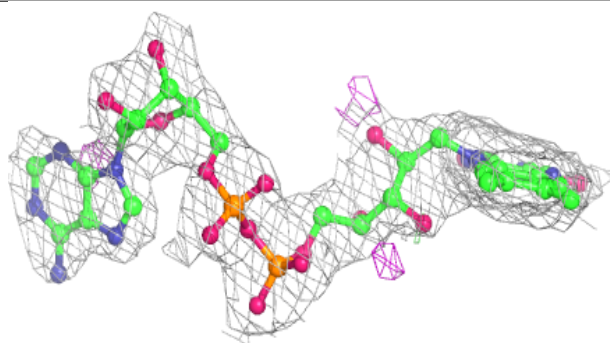
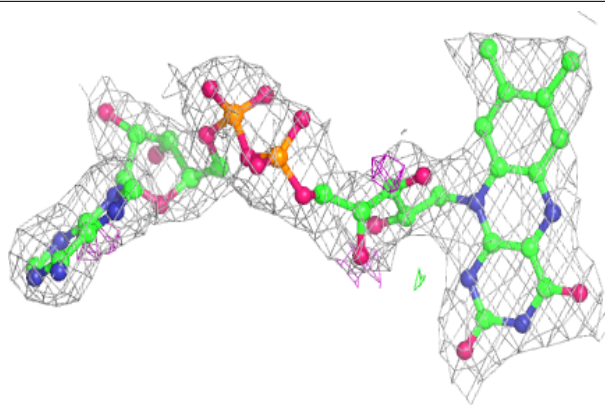
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	MTE	B	1778	24/24	0.93	0.34	27,36,42,43	24
4	FAD	E	1465	53/53	0.93	0.15	35,45,53,53	0
5	MTE	F	1778	24/24	0.94	0.27	22,29,34,36	24
5	MTE	D	1778	24/24	0.94	0.27	9,25,32,33	24
4	FAD	C	1465	53/53	0.96	0.14	16,27,35,37	0
6	CA	F	1779	1/1	0.97	0.26	56,56,56,56	0
3	FES	E	1464	4/4	0.97	0.17	38,38,40,42	0
3	FES	G	1464	4/4	0.97	0.19	39,40,42,42	0
6	CA	H	1779	1/1	0.97	0.22	58,58,58,58	0
3	FES	E	1463	4/4	0.97	0.15	26,27,30,31	0
8	MOM	B	1781	4/4	0.98	0.12	44,45,45,47	3
3	FES	C	1463	4/4	0.98	0.16	19,19,21,22	0
3	FES	G	1463	4/4	0.98	0.14	29,32,32,33	0
3	FES	A	1463	4/4	0.98	0.19	25,28,29,30	0
8	MOM	H	1781	4/4	0.98	0.12	44,44,44,45	3
6	CA	D	1779	1/1	0.98	0.18	49,49,49,49	0
3	FES	C	1464	4/4	0.99	0.17	33,35,35,37	0
8	MOM	F	1781	4/4	0.99	0.12	35,35,36,37	3
3	FES	A	1464	4/4	0.99	0.18	35,35,36,36	0
8	MOM	D	1781	4/4	0.99	0.10	34,34,34,37	3
6	CA	B	1779	1/1	0.99	0.22	48,48,48,48	0

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

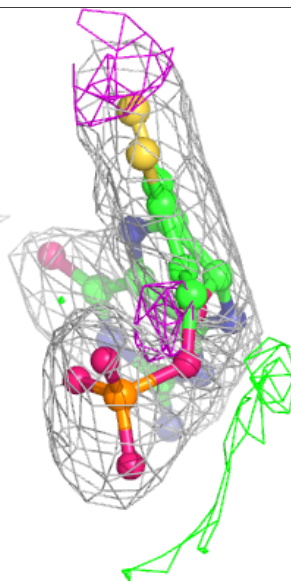
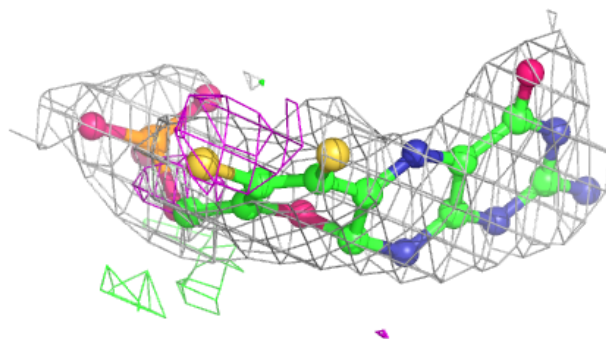
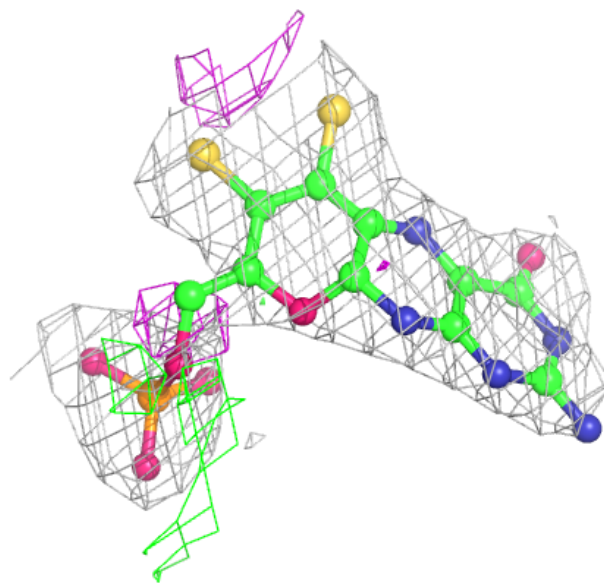
Electron density around FAD G 1465:

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



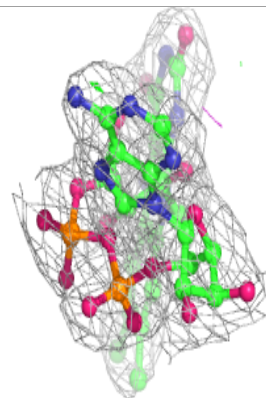
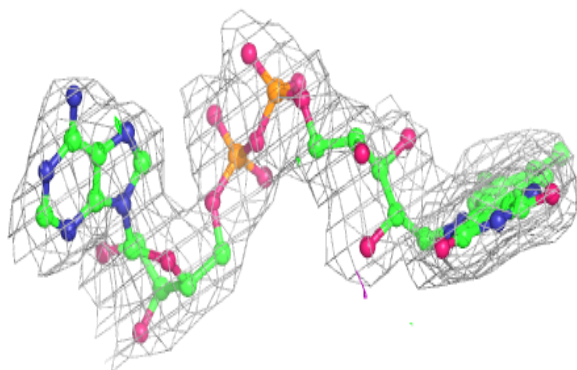
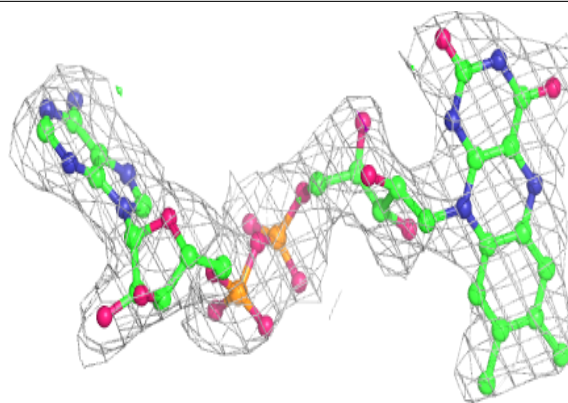
Electron density around MTE H 1778:

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



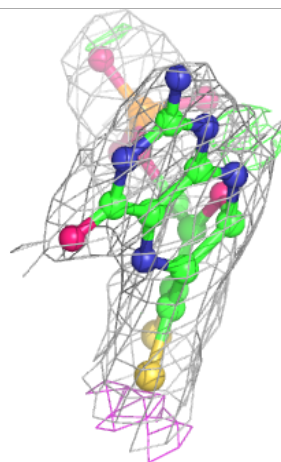
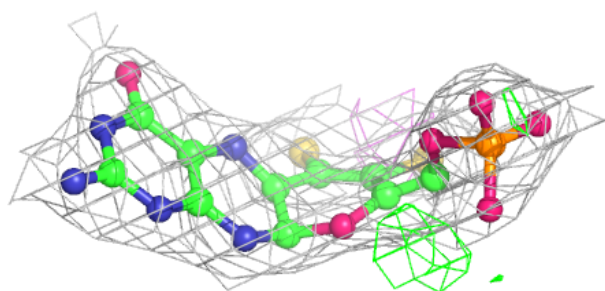
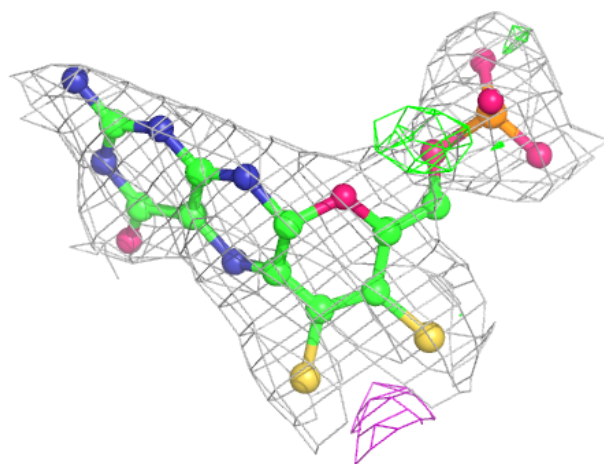
Electron density around FAD A 1465:

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



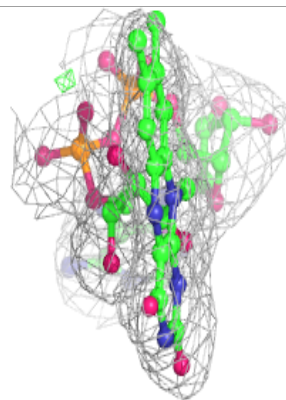
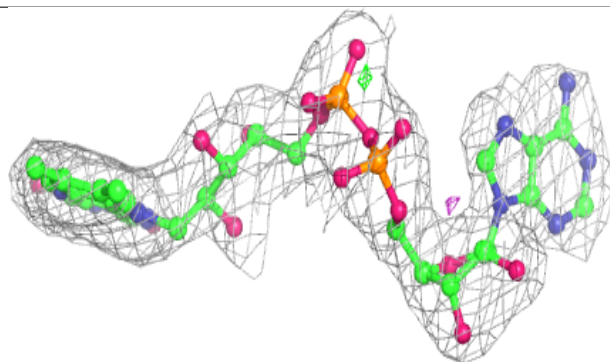
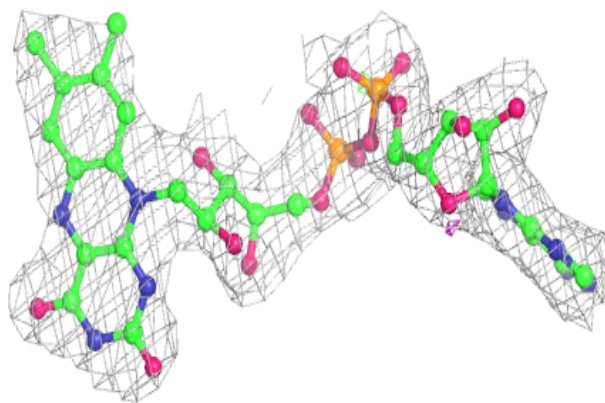
Electron density around MTE B 1778:

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



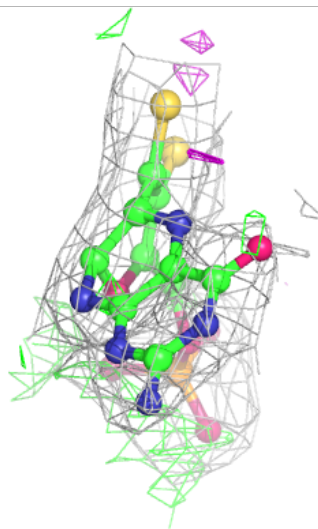
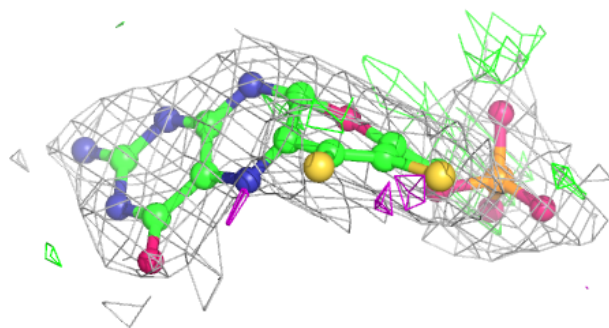
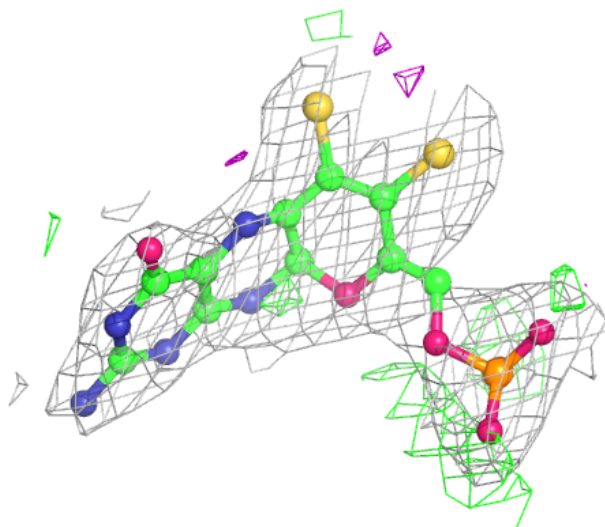
Electron density around FAD E 1465:

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



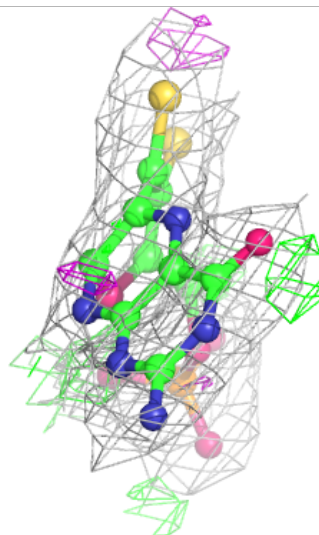
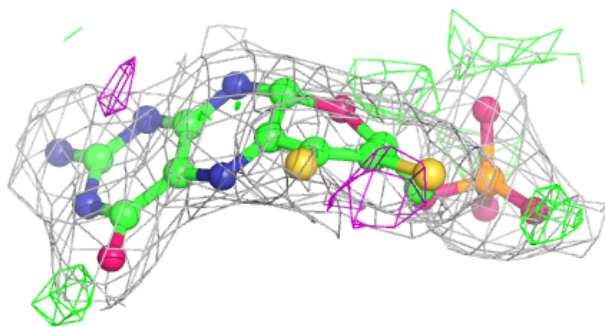
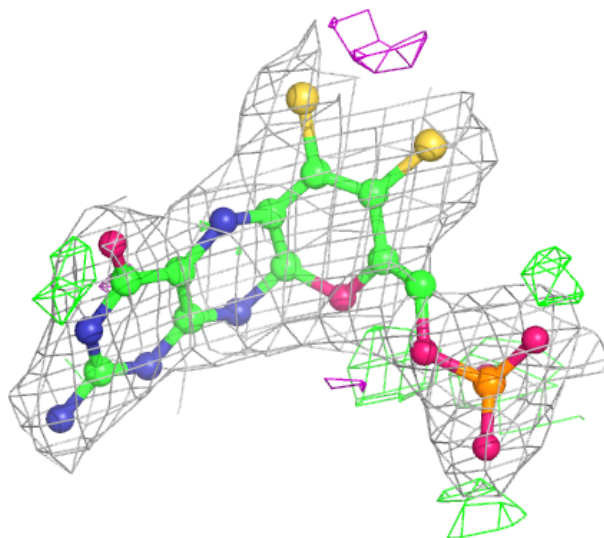
Electron density around MTE F 1778:

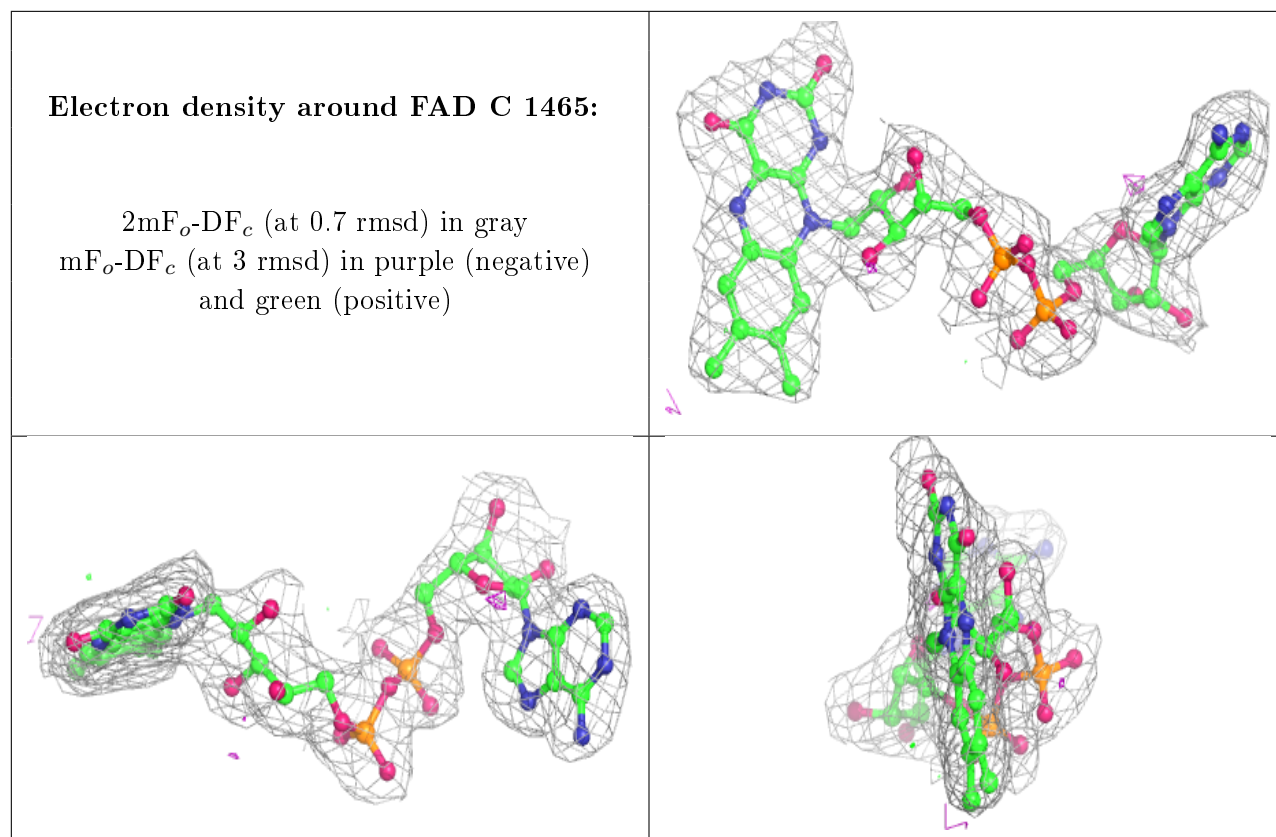
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MTE 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.