



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:07 AM UTC

PDB ID : 2F1O / pdb_00002f1o
Title : Crystal Structure of NQO1 with Dicoumarol
Authors : Shaul, Y.; Asher, G.; Dym, O.; Tsvetkov, P.; Adler, J.; Israel Structural Proteomics Center (ISPC)
Deposited on : 2005-11-15
Resolution : 2.75 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

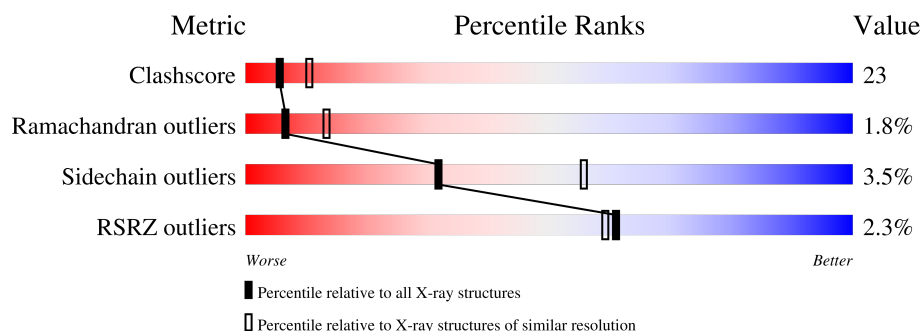
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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))
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	273	% 56% 41% .
1	B	273	% 51% 46% .
1	C	273	% 57% 38% 5%
1	D	273	3% 55% 40% 5%
1	E	273	% 60% 36% .
1	F	273	% 49% 48% .

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Mol	Chain	Length	Quality of chain
1	G	273	
1	H	273	

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
2	DTC	A	2280	X	-	-	-
2	DTC	B	3280	X	-	-	-
2	DTC	C	280	X	-	-	-
2	DTC	D	1280	X	-	-	-
2	DTC	E	4280	X	-	-	-
2	DTC	E	5280	X	-	-	-
2	DTC	G	7280	X	-	-	-
2	DTC	H	6280	X	-	-	-

2 Entry composition

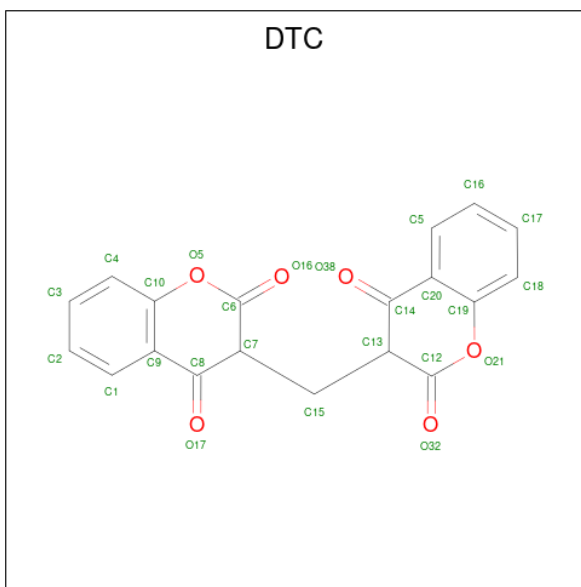
There are 4 unique types of molecules in this entry. The entry contains 18146 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NAD(P)H dehydrogenase [quinone] 1.

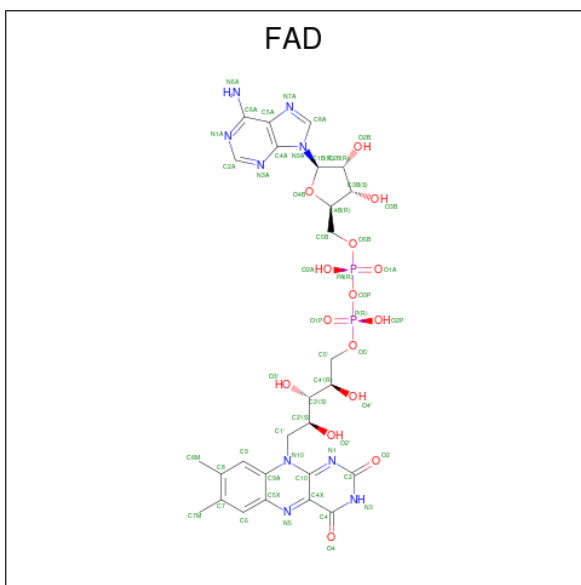
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2175	1414	365	389	7			
1	B	273	Total	C	N	O	S	0	0	0
			2175	1414	365	389	7			
1	C	273	Total	C	N	O	S	0	0	0
			2175	1414	365	389	7			
1	D	273	Total	C	N	O	S	0	0	0
			2175	1414	365	389	7			
1	E	273	Total	C	N	O	S	0	0	0
			2175	1414	365	389	7			
1	F	273	Total	C	N	O	S	0	0	0
			2175	1414	365	389	7			
1	G	273	Total	C	N	O	S	0	0	0
			2175	1414	365	389	7			
1	H	273	Total	C	N	O	S	0	0	0
			2175	1414	365	389	7			

- Molecule 2 is BISHYDROXY[2H-1-BENZOPYRAN-2-ONE,1,2-BENZOPYRONE] (CCD ID: DTC) (formula: C₁₉H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			25	19	6		
2	B	1	Total	C	O	0	0
			25	19	6		
2	C	1	Total	C	O	0	0
			25	19	6		
2	D	1	Total	C	O	0	0
			25	19	6		
2	E	1	Total	C	O	0	0
			25	19	6		
2	E	1	Total	C	O	0	0
			25	19	6		
2	G	1	Total	C	O	0	0
			25	19	6		
2	H	1	Total	C	O	0	0
			25	19	6		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	B	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	C	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	D	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	E	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	F	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	G	1	Total 53	C 27	N 9	O 15	P 2	0	0
3	H	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	19	Total O 19 19	0	0
4	B	23	Total O 23 23	0	0
4	C	23	Total O 23 23	0	0
4	D	13	Total O 13 13	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	18	Total 18	O 18	0	0
4	F	10	Total 10	O 10	0	0
4	G	8	Total 8	O 8	0	0
4	H	8	Total 8	O 8	0	0

3 Residue-property plots

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

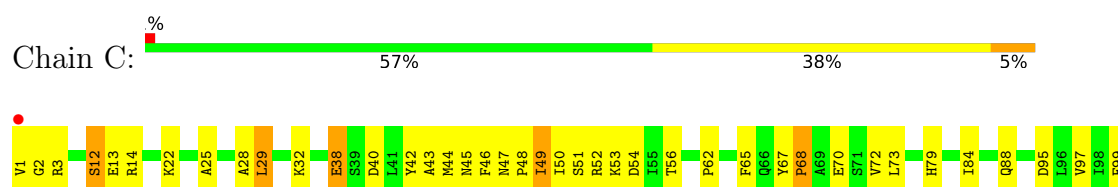
• Molecule 1: NAD(P)H dehydrogenase [quinone] 1

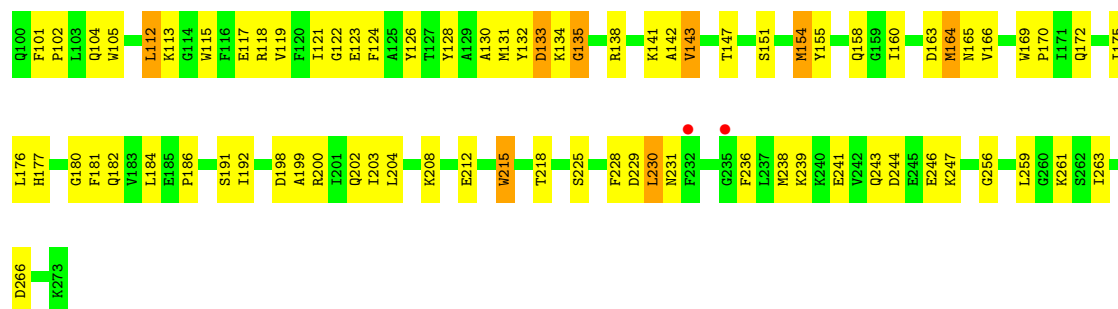


• Molecule 1: NAD(P)H dehydrogenase [quinone] 1

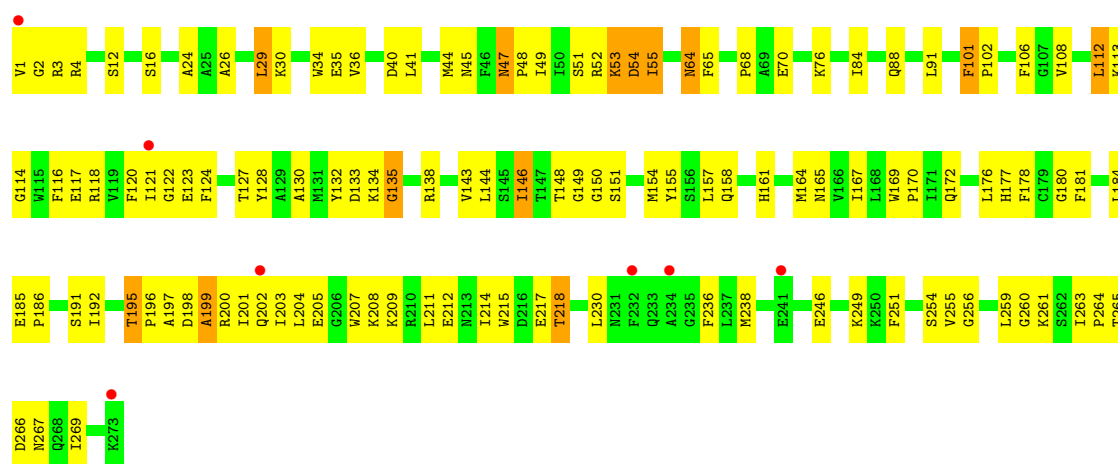


• Molecule 1: NAD(P)H dehydrogenase [quinone] 1

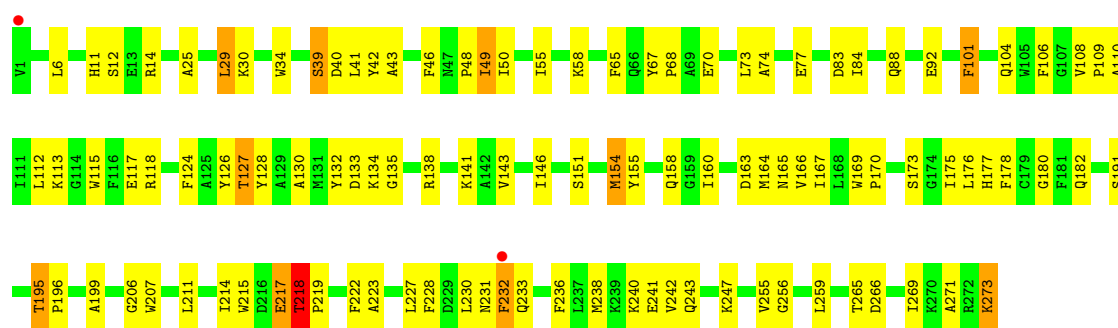




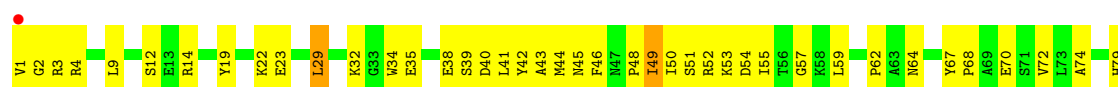
• Molecule 1: NAD(P)H dehydrogenase [quinone] 1

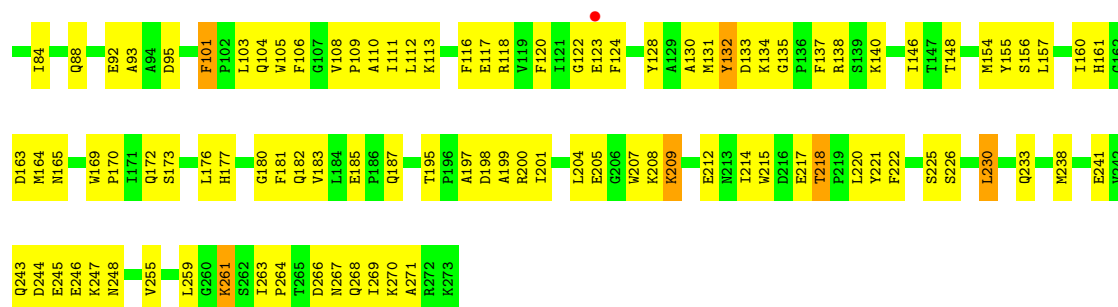


• Molecule 1: NAD(P)H dehydrogenase [quinone] 1

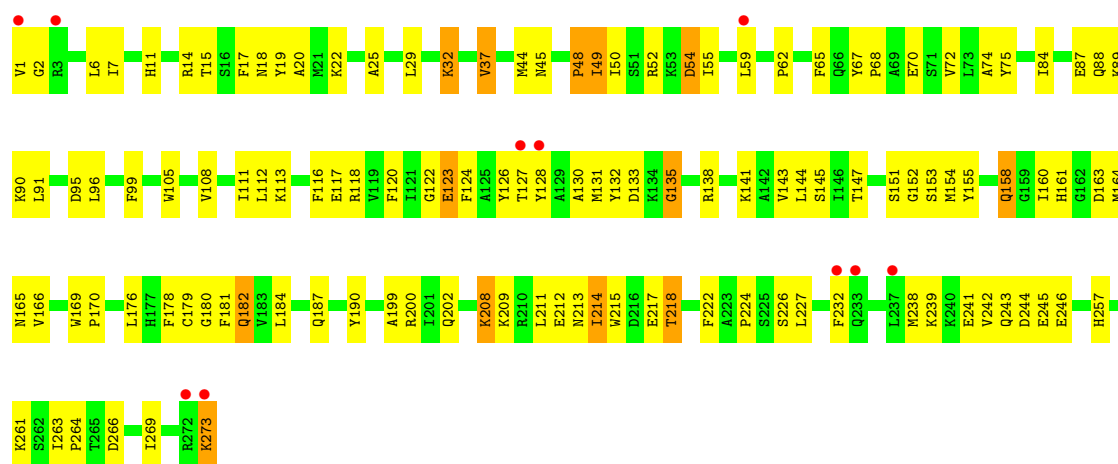


• Molecule 1: NAD(P)H dehydrogenase [quinone] 1

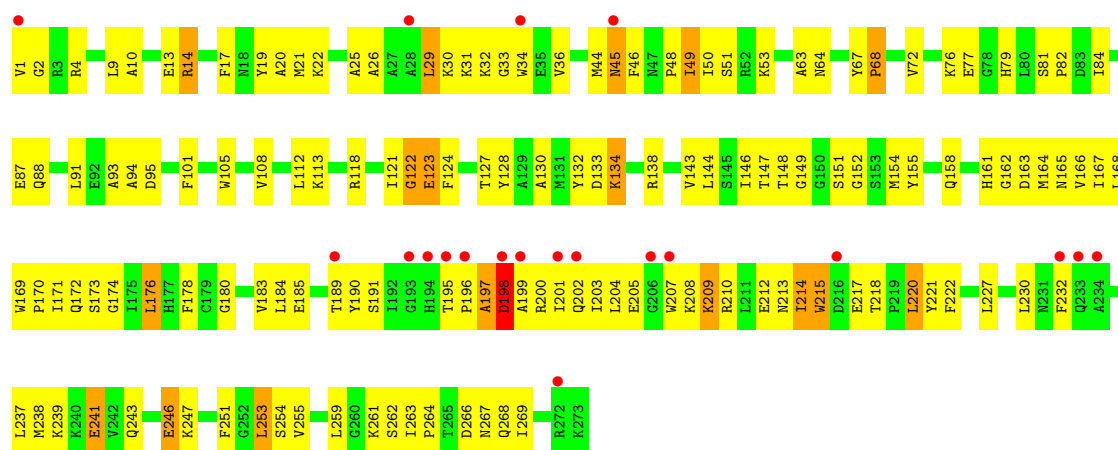




• Molecule 1: NAD(P)H dehydrogenase [quinone] 1



• Molecule 1: NAD(P)H dehydrogenase [quinone] 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	76.24Å 86.19Å 100.56Å 91.14° 107.91° 93.17°	Depositor
Resolution (Å)	38.66 – 2.75 38.66 – 2.75	Depositor EDS
% Data completeness (in resolution range)	(Not available) (38.66-2.75) 96.9 (38.66-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.219 , 0.282 0.218 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	37.6	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 38.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	18146	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DTC, FAD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.48	0/2233	1.04	11/3015 (0.4%)
1	B	0.50	0/2233	1.05	11/3015 (0.4%)
1	C	0.49	0/2233	1.01	13/3015 (0.4%)
1	D	0.48	0/2233	1.06	14/3015 (0.5%)
1	E	0.51	0/2233	1.02	16/3015 (0.5%)
1	F	0.47	0/2233	1.01	15/3015 (0.5%)
1	G	0.47	0/2233	1.05	15/3015 (0.5%)
1	H	0.48	0/2233	0.99	8/3015 (0.3%)
All	All	0.48	0/17864	1.03	103/24120 (0.4%)

There are no bond length outliers.

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	202	GLN	OE1-CD-NE2	-9.78	112.82	122.60
1	B	101	PHE	N-CA-C	9.59	116.76	108.13
1	D	101	PHE	N-CA-C	9.31	116.51	108.13
1	F	101	PHE	N-CA-C	9.13	116.35	108.13
1	G	218	THR	CA-C-N	9.05	129.13	119.89
1	G	218	THR	C-N-CA	9.05	129.13	119.89
1	A	135	GLY	CA-C-N	8.97	128.71	119.56
1	A	135	GLY	C-N-CA	8.97	128.71	119.56
1	A	218	THR	CA-C-N	8.47	128.41	120.03
1	A	218	THR	C-N-CA	8.47	128.41	120.03
1	B	56	THR	N-CA-C	-7.72	99.39	110.59
1	C	182	GLN	N-CA-C	-7.52	96.98	109.24
1	H	49	ILE	N-CA-C	7.51	118.29	106.88
1	A	229	ASP	N-CA-C	-7.42	97.95	109.76
1	E	182	GLN	N-CA-C	-7.17	96.86	108.41
1	E	195	THR	CA-C-N	7.05	127.02	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	195	THR	C-N-CA	7.05	127.02	119.76
1	E	49	ILE	N-CA-C	7.04	117.79	107.37
1	F	12	SER	N-CA-C	7.00	118.99	111.36
1	D	218	THR	CA-C-N	6.95	126.87	119.85
1	D	218	THR	C-N-CA	6.95	126.87	119.85
1	G	54	ASP	N-CA-C	-6.92	104.64	113.23
1	D	135	GLY	CA-C-N	6.79	126.49	119.56
1	D	135	GLY	C-N-CA	6.79	126.49	119.56
1	G	153	SER	N-CA-C	-6.79	103.95	111.82
1	D	202	GLN	CG-CD-NE2	6.66	126.38	116.40
1	C	154	MET	N-CA-C	-6.56	104.75	112.89
1	H	95	ASP	N-CA-C	-6.51	104.39	112.72
1	C	12	SER	N-CA-C	6.42	118.35	111.36
1	B	232	PHE	N-CA-C	6.41	118.27	111.28
1	B	61	ASP	CA-C-N	6.39	126.31	119.28
1	B	61	ASP	C-N-CA	6.39	126.31	119.28
1	F	95	ASP	N-CA-C	-6.38	105.15	113.12
1	G	84	ILE	N-CA-C	-6.33	104.58	110.53
1	C	72	VAL	N-CA-C	-6.25	104.41	110.72
1	G	95	ASP	N-CA-C	-6.25	105.31	113.12
1	G	108	VAL	CA-C-N	6.22	126.17	119.76
1	G	108	VAL	C-N-CA	6.22	126.17	119.76
1	E	175	ILE	N-CA-C	6.17	116.36	110.74
1	F	135	GLY	CA-C-N	6.16	126.35	119.32
1	F	135	GLY	C-N-CA	6.16	126.35	119.32
1	E	135	GLY	CA-C-N	6.13	125.34	118.97
1	E	135	GLY	C-N-CA	6.13	125.34	118.97
1	B	12	SER	N-CA-C	6.13	119.95	112.23
1	H	218	THR	CA-C-N	6.01	126.48	119.99
1	H	218	THR	C-N-CA	6.01	126.48	119.99
1	F	261	LYS	CB-CA-C	-5.98	106.92	114.40
1	F	218	THR	CA-C-N	5.95	126.28	119.92
1	F	218	THR	C-N-CA	5.95	126.28	119.92
1	A	95	ASP	N-CA-C	-5.94	106.16	113.41
1	D	36	VAL	N-CA-C	5.94	117.90	108.87
1	C	101	PHE	N-CA-C	5.93	113.47	108.13
1	B	84	ILE	N-CA-C	-5.91	104.74	110.42
1	H	94	ALA	N-CA-C	5.89	117.90	110.24
1	H	215	TRP	N-CA-C	5.83	118.58	111.82
1	F	182	GLN	N-CA-C	-5.72	99.41	108.73
1	B	95	ASP	N-CA-C	-5.71	106.44	113.41
1	G	135	GLY	CA-C-N	5.69	125.36	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	135	GLY	C-N-CA	5.69	125.36	119.56
1	A	150	GLY	N-CA-C	5.69	120.57	111.64
1	A	182	GLN	N-CA-C	-5.69	99.46	108.73
1	A	49	ILE	N-CA-C	5.64	116.85	108.23
1	E	146	ILE	N-CA-C	5.63	116.85	108.46
1	C	143	VAL	N-CA-C	5.61	115.75	108.35
1	E	223	ALA	CA-C-N	5.57	125.49	119.76
1	E	223	ALA	C-N-CA	5.57	125.49	119.76
1	B	174	GLY	N-CA-C	5.55	119.39	112.73
1	E	154	MET	N-CA-C	-5.50	106.41	113.23
1	B	182	GLN	N-CA-C	-5.49	99.57	108.41
1	F	230	LEU	N-CA-C	5.48	118.06	108.52
1	G	49	ILE	N-CA-C	5.48	115.84	108.17
1	A	174	GLY	N-CA-C	5.45	119.23	112.64
1	H	14	ARG	N-CA-C	-5.45	106.47	113.23
1	C	38	GLU	N-CA-C	5.43	118.56	110.14
1	F	247	LYS	N-CA-C	-5.39	106.78	113.19
1	G	182	GLN	N-CA-C	-5.35	99.05	108.20
1	F	49	ILE	N-CA-C	5.35	116.28	108.58
1	D	146	ILE	N-CA-C	5.34	116.28	108.53
1	C	176	LEU	N-CA-C	5.29	116.91	111.03
1	C	135	GLY	CA-C-N	5.29	124.62	118.85
1	C	135	GLY	C-N-CA	5.29	124.62	118.85
1	F	132	TYR	N-CA-C	5.29	117.02	108.08
1	G	161	HIS	N-CA-C	-5.29	107.00	113.50
1	D	12	SER	N-CA-C	5.27	119.77	113.23
1	E	218	THR	CA-C-N	5.27	126.42	119.84
1	E	218	THR	C-N-CA	5.27	126.42	119.84
1	E	176	LEU	N-CA-C	5.27	116.83	111.14
1	E	206	GLY	N-CA-C	-5.26	106.12	112.49
1	G	208	LYS	N-CA-C	-5.26	105.23	110.97
1	D	195	THR	CA-C-N	5.24	125.15	119.76
1	D	195	THR	C-N-CA	5.24	125.15	119.76
1	C	95	ASP	N-CA-C	-5.23	106.59	113.12
1	D	199	ALA	N-CA-C	-5.20	105.79	111.82
1	D	54	ASP	N-CA-C	-5.19	107.33	113.97
1	E	101	PHE	N-CA-C	5.10	112.72	108.13
1	C	49	ILE	N-CA-C	5.10	115.19	107.80
1	F	221	TYR	N-CA-C	5.08	117.02	108.73
1	C	215	TRP	N-CA-C	5.06	117.69	111.82
1	H	253	LEU	N-CA-C	5.06	116.87	111.36
1	A	263	ILE	CB-CA-C	-5.04	106.25	110.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	45	ASN	N-CA-C	-5.04	105.79	112.24
1	F	45	ASN	N-CA-C	-5.04	105.79	112.24
1	B	119	VAL	N-CA-C	5.00	116.45	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2175	0	2179	100	0
1	B	2175	0	2179	129	0
1	C	2175	0	2179	104	0
1	D	2175	0	2179	122	0
1	E	2175	0	2179	86	0
1	F	2175	0	2179	121	0
1	G	2175	0	2179	105	0
1	H	2175	0	2179	136	0
2	A	25	0	10	1	0
2	B	25	0	10	1	0
2	C	25	0	10	2	0
2	D	25	0	10	1	0
2	E	50	0	20	3	0
2	G	25	0	10	5	0
2	H	25	0	10	3	0
3	A	53	0	31	4	0
3	B	53	0	31	5	0
3	C	53	0	31	6	0
3	D	53	0	31	4	0
3	E	53	0	31	2	0
3	F	53	0	31	2	0
3	G	53	0	31	3	0
3	H	53	0	31	5	0
4	A	19	0	0	1	0
4	B	23	0	0	2	0
4	C	23	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	13	0	0	1	0
4	E	18	0	0	1	0
4	F	10	0	0	2	0
4	G	8	0	0	0	0
4	H	8	0	0	2	0
All	All	18146	0	17760	840	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 23.

All (840) 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)
1:B:255:VAL:HG23	1:B:267:ASN:HD22	1.05	1.17
1:D:151:SER:H	1:D:154:MET:HE3	0.97	1.08
1:D:47:ASN:HD22	1:D:48:PRO:N	1.51	1.08
1:A:48:PRO:HG3	1:C:49:ILE:HD11	1.37	1.06
1:G:1:VAL:HG12	1:G:2:GLY:H	1.17	1.06
1:G:128:TYR:OH	2:G:7280:DTC:O16	1.76	1.03
1:B:48:PRO:HG3	1:D:49:ILE:HD11	1.41	1.03
1:H:50:ILE:HG22	1:H:118:ARG:HG2	1.45	0.98
1:F:14:ARG:HH21	1:F:43:ALA:HB2	1.25	0.98
1:D:151:SER:N	1:D:154:MET:HE3	1.79	0.96
1:F:255:VAL:HG23	1:F:267:ASN:HD22	1.28	0.94
1:H:1:VAL:HG22	1:H:2:GLY:H	1.36	0.91
1:B:1:VAL:HG12	1:B:2:GLY:H	1.34	0.91
1:D:47:ASN:ND2	1:D:49:ILE:H	1.67	0.91
1:B:108:VAL:HB	1:B:112:LEU:HD12	1.52	0.90
1:D:47:ASN:HD21	1:D:49:ILE:H	1.19	0.89
1:B:255:VAL:HG23	1:B:267:ASN:ND2	1.87	0.89
1:D:47:ASN:HD22	1:D:47:ASN:C	1.78	0.88
1:D:108:VAL:HB	1:D:112:LEU:HD12	1.53	0.87
1:A:255:VAL:HG23	1:A:267:ASN:HD22	1.41	0.85
1:C:143:VAL:HG22	1:C:184:LEU:HB2	1.57	0.85
1:A:51:SER:OG	1:A:53:LYS:HG2	1.76	0.84
1:A:47:ASN:C	1:A:47:ASN:HD22	1.84	0.84
1:C:238:MET:HE1	1:C:259:LEU:HD21	1.60	0.84
1:F:14:ARG:NH2	1:F:43:ALA:HB2	1.93	0.83
1:E:160:ILE:HD12	1:F:230:LEU:HD21	1.60	0.82
1:C:200:ARG:HH11	3:C:2301:FAD:H1B	1.45	0.81
1:A:50:ILE:HG22	1:A:118:ARG:HG2	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ILE:HD11	1:C:48:PRO:HG3	1.62	0.81
1:D:76:LYS:HE2	1:D:123:GLU:HG3	1.62	0.81
1:D:1:VAL:HG12	1:D:2:GLY:H	1.45	0.81
1:H:255:VAL:HG23	1:H:267:ASN:HD22	1.46	0.80
1:E:48:PRO:HG3	1:F:49:ILE:HD11	1.63	0.80
1:A:47:ASN:ND2	1:A:49:ILE:H	1.79	0.80
1:G:72:VAL:HG22	1:G:122:GLY:O	1.82	0.80
1:B:255:VAL:H	1:B:267:ASN:ND2	1.80	0.80
1:G:1:VAL:HG12	1:G:2:GLY:N	1.97	0.80
1:G:48:PRO:HG3	1:H:49:ILE:HD11	1.64	0.80
1:H:238:MET:HE1	1:H:259:LEU:HD21	1.62	0.79
1:A:3:ARG:HE	1:A:3:ARG:HA	1.45	0.79
1:H:14:ARG:N	1:H:14:ARG:HD2	1.97	0.79
1:F:50:ILE:HG22	1:F:118:ARG:HG2	1.63	0.79
1:H:239:LYS:O	1:H:243:GLN:HG3	1.83	0.79
1:B:138:ARG:HA	1:B:180:GLY:O	1.83	0.78
1:B:49:ILE:HD11	1:D:48:PRO:HG3	1.64	0.78
1:E:231:ASN:OD1	1:E:233:GLN:HG3	1.84	0.78
1:G:227:LEU:HB3	1:G:242:VAL:HG11	1.65	0.78
1:F:163:ASP:OD2	1:F:165:ASN:HB2	1.84	0.78
1:H:32:LYS:HE3	1:H:212:GLU:HB3	1.65	0.77
1:G:128:TYR:OH	2:G:7280:DTC:C6	2.33	0.77
1:D:200:ARG:HH11	3:D:3301:FAD:H1B	1.50	0.76
1:D:143:VAL:HG22	1:D:184:LEU:HB2	1.67	0.75
1:C:151:SER:OG	1:C:154:MET:HG3	1.85	0.75
1:H:143:VAL:HG22	1:H:184:LEU:HB2	1.68	0.75
1:E:138:ARG:HA	1:E:180:GLY:O	1.86	0.75
1:F:1:VAL:HG22	1:F:2:GLY:H	1.50	0.75
1:H:243:GLN:O	1:H:247:LYS:HG3	1.87	0.74
1:C:138:ARG:HA	1:C:180:GLY:O	1.88	0.74
1:G:214:ILE:HD12	1:G:217:GLU:OE2	1.87	0.74
1:A:238:MET:HE1	1:A:259:LEU:HD21	1.71	0.73
1:D:113:LYS:O	1:D:117:GLU:HG3	1.88	0.73
1:D:138:ARG:HA	1:D:180:GLY:O	1.87	0.73
1:E:49:ILE:HD11	1:F:48:PRO:HG3	1.70	0.72
1:H:44:MET:HE1	1:H:87:GLU:OE2	1.90	0.72
1:A:237:LEU:HD22	1:C:158:GLN:HB2	1.71	0.72
1:G:209:LYS:O	1:G:212:GLU:HB2	1.88	0.72
1:E:160:ILE:HD12	1:F:230:LEU:CD2	2.19	0.72
1:B:47:ASN:ND2	1:B:49:ILE:H	1.88	0.72
1:A:47:ASN:HD22	1:A:48:PRO:N	1.88	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:176:LEU:O	1:F:181:PHE:HB2	1.89	0.71
1:E:166:VAL:HG11	1:F:169:TRP:CD1	2.25	0.71
1:H:214:ILE:O	1:H:217:GLU:HB2	1.89	0.71
1:H:155:TYR:HB3	1:H:164:MET:HB2	1.73	0.71
1:A:26:ALA:HB1	1:A:30:LYS:NZ	2.05	0.71
1:B:237:LEU:HD22	1:D:158:GLN:HB2	1.73	0.71
1:H:209:LYS:HE3	1:H:212:GLU:OE1	1.91	0.71
1:F:54:ASP:OD2	1:F:118:ARG:HD2	1.92	0.70
1:E:240:LYS:H	1:E:240:LYS:HD2	1.55	0.70
1:H:128:TYR:CE1	4:H:7482:HOH:O	2.43	0.70
1:E:163:ASP:OD2	1:E:165:ASN:HB2	1.90	0.70
1:D:84:ILE:HD11	1:D:118:ARG:NH1	2.07	0.70
1:F:267:ASN:ND2	1:F:268:GLN:HE21	1.89	0.70
1:D:151:SER:H	1:D:154:MET:CE	1.91	0.69
1:D:165:ASN:OD1	1:D:269:ILE:HG13	1.92	0.69
1:B:132:TYR:OH	1:D:161:HIS:HD2	1.75	0.69
1:F:169:TRP:HB3	1:F:170:PRO:HD3	1.74	0.69
1:A:47:ASN:C	1:A:47:ASN:ND2	2.48	0.69
1:A:83:ASP:OD2	1:A:118:ARG:NH2	2.24	0.69
3:B:1301:FAD:HM82	1:D:68:PRO:HG3	1.74	0.69
1:C:200:ARG:NH1	3:C:2301:FAD:H1B	2.08	0.69
1:D:55:ILE:HD12	1:D:55:ILE:N	2.08	0.69
1:C:40:ASP:HB3	1:C:43:ALA:HB3	1.74	0.69
1:E:50:ILE:HG22	1:E:118:ARG:HG2	1.73	0.69
1:A:238:MET:HE1	1:A:259:LEU:CD2	2.23	0.68
1:F:198:ASP:O	1:F:201:ILE:HB	1.92	0.68
1:D:47:ASN:ND2	1:D:47:ASN:C	2.49	0.68
1:H:202:GLN:O	1:H:205:GLU:HB2	1.93	0.68
1:A:176:LEU:O	1:A:181:PHE:HB2	1.93	0.68
1:D:51:SER:OG	1:D:53:LYS:HG2	1.94	0.68
1:H:77:GLU:OE1	1:H:79:HIS:CE1	2.46	0.68
1:A:155:TYR:HB3	1:A:164:MET:HB2	1.74	0.68
1:B:262:SER:HB2	1:D:260:GLY:O	1.93	0.68
1:B:60:LYS:O	1:B:60:LYS:HG2	1.94	0.68
1:H:1:VAL:HG22	1:H:2:GLY:N	2.07	0.68
1:D:201:ILE:O	1:D:205:GLU:HG2	1.93	0.68
1:H:195:THR:HG22	1:H:199:ALA:HB3	1.74	0.68
1:C:198:ASP:O	1:C:202:GLN:HG2	1.94	0.67
1:A:200:ARG:HH11	3:A:301:FAD:H1B	1.59	0.67
1:F:238:MET:HE3	1:F:243:GLN:HG2	1.76	0.67
1:G:138:ARG:HA	1:G:180:GLY:O	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:ILE:O	1:B:118:ARG:HD3	1.94	0.67
1:C:132:TYR:O	1:C:134:LYS:N	2.28	0.66
1:D:199:ALA:O	1:D:203:ILE:HG13	1.95	0.66
1:H:128:TYR:CD1	4:H:7482:HOH:O	2.47	0.66
1:B:147:THR:HG22	1:B:189:THR:OG1	1.95	0.66
1:B:176:LEU:O	1:B:181:PHE:HB2	1.95	0.66
1:B:201:ILE:HD13	1:G:14:ARG:HD2	1.78	0.66
1:H:17:PHE:HB2	3:H:7301:FAD:H51A	1.77	0.66
1:H:32:LYS:HE3	1:H:212:GLU:CB	2.26	0.66
1:F:214:ILE:HD12	1:F:217:GLU:OE2	1.95	0.65
1:B:183:VAL:HG12	1:B:220:LEU:HD12	1.77	0.65
1:H:1:VAL:HA	1:H:215:TRP:NE1	2.10	0.65
1:C:32:LYS:HE3	1:C:212:GLU:HB3	1.79	0.65
1:F:59:LEU:HB2	1:F:62:PRO:HG3	1.78	0.65
1:H:144:LEU:HD21	1:H:176:LEU:HD11	1.79	0.65
1:H:201:ILE:O	1:H:205:GLU:HG2	1.98	0.64
1:A:214:ILE:HA	1:A:217:GLU:OE2	1.97	0.64
1:E:55:ILE:HG23	1:E:74:ALA:HB2	1.78	0.64
1:A:186:PRO:HB2	1:A:188:LEU:HD21	1.79	0.64
1:A:111:ILE:HB	1:C:49:ILE:HD12	1.80	0.64
1:B:76:LYS:HE3	1:B:123:GLU:HG3	1.79	0.64
1:F:185:GLU:OE2	1:F:270:LYS:HA	1.98	0.63
1:C:1:VAL:HG12	1:C:2:GLY:H	1.62	0.63
1:B:47:ASN:C	1:B:47:ASN:HD22	2.06	0.63
1:G:49:ILE:HD11	1:H:48:PRO:HG3	1.81	0.63
1:B:54:ASP:CG	1:B:118:ARG:HH11	2.06	0.63
1:H:128:TYR:HD2	2:H:6280:DTC:C20	2.12	0.63
1:F:130:ALA:HB1	1:F:134:LYS:O	1.99	0.63
1:A:230:LEU:CD2	1:C:160:ILE:HD12	2.29	0.62
1:B:47:ASN:HD22	1:B:48:PRO:N	1.95	0.62
1:H:254:SER:HB2	1:H:267:ASN:HD21	1.63	0.62
1:B:1:VAL:HG12	1:B:2:GLY:N	2.11	0.62
1:F:225:SER:HB2	1:F:230:LEU:HD11	1.81	0.62
1:G:239:LYS:HB2	1:G:242:VAL:CG2	2.30	0.62
1:G:6:LEU:HD12	1:G:37:VAL:O	1.99	0.62
1:H:164:MET:HA	1:H:167:ILE:HD12	1.81	0.62
1:H:173:SER:HB2	1:H:222:PHE:CE1	2.35	0.62
1:A:54:ASP:OD1	1:A:118:ARG:NH1	2.33	0.62
1:C:84:ILE:O	1:C:88:GLN:HG3	2.00	0.62
1:B:29:LEU:HD13	1:B:211:LEU:HD13	1.82	0.61
1:E:151:SER:H	1:E:154:MET:HE3	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:127:THR:HB	1:G:130:ALA:HB3	1.81	0.61
1:C:50:ILE:HG22	1:C:118:ARG:HG2	1.82	0.61
1:E:130:ALA:HB1	1:E:134:LYS:O	2.00	0.61
1:G:75:TYR:CZ	1:G:124:PHE:HB2	2.34	0.61
1:G:239:LYS:HB2	1:G:242:VAL:HG23	1.82	0.61
1:C:1:VAL:HG12	1:C:2:GLY:N	2.15	0.61
1:H:163:ASP:OD2	1:H:165:ASN:HB2	2.01	0.61
1:C:155:TYR:HB3	1:C:164:MET:HB2	1.83	0.61
1:D:44:MET:O	1:D:45:ASN:HB3	2.01	0.61
1:F:241:GLU:H	1:F:241:GLU:CD	2.09	0.61
1:H:72:VAL:HG22	1:H:122:GLY:HA3	1.82	0.61
1:H:84:ILE:O	1:H:88:GLN:HG3	2.00	0.61
1:H:128:TYR:CD2	2:H:6280:DTC:C20	2.83	0.60
1:B:160:ILE:HD12	1:D:230:LEU:HD21	1.84	0.60
1:B:183:VAL:CG1	1:B:220:LEU:HD12	2.32	0.60
1:C:104:GLN:HA	3:C:2301:FAD:N5	2.15	0.60
1:G:199:ALA:O	1:G:202:GLN:HB3	2.02	0.60
1:D:47:ASN:ND2	1:D:49:ILE:N	2.46	0.60
1:D:127:THR:OG1	1:D:130:ALA:HB3	2.01	0.60
1:B:201:ILE:CD1	1:G:14:ARG:HD2	2.31	0.60
1:E:25:ALA:O	1:E:29:LEU:HD22	2.02	0.60
1:E:151:SER:OG	1:E:154:MET:HG3	2.02	0.60
1:B:108:VAL:CB	1:B:112:LEU:HD12	2.29	0.60
1:D:108:VAL:CB	1:D:112:LEU:HD12	2.29	0.60
1:B:51:SER:O	1:B:54:ASP:HB2	2.02	0.60
1:F:32:LYS:HE3	1:F:212:GLU:HB3	1.82	0.60
1:F:42:TYR:HB2	4:F:7330:HOH:O	2.01	0.60
1:F:173:SER:HB2	1:F:222:PHE:CE1	2.37	0.60
1:H:67:TYR:HB3	1:H:68:PRO:HD3	1.83	0.60
1:A:267:ASN:ND2	1:A:268:GLN:HE21	2.00	0.59
1:E:169:TRP:CZ2	1:E:256:GLY:HA3	2.36	0.59
1:G:128:TYR:HB3	2:G:7280:DTC:C16	2.32	0.59
1:G:238:MET:HB2	1:H:158:GLN:HB3	1.84	0.59
1:H:14:ARG:N	1:H:14:ARG:CD	2.65	0.59
1:A:230:LEU:HD21	1:C:160:ILE:HD12	1.82	0.59
1:G:7:ILE:HG21	1:G:22:LYS:HG2	1.84	0.59
1:H:132:TYR:CD1	1:H:178:PHE:HA	2.37	0.59
1:G:151:SER:O	1:G:154:MET:HB2	2.01	0.59
1:G:152:GLY:HA2	1:G:190:TYR:CD1	2.38	0.59
1:B:255:VAL:N	1:B:267:ASN:ND2	2.50	0.59
1:G:166:VAL:HG11	1:H:169:TRP:CD1	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:ILE:HD12	1:C:230:LEU:HD21	1.85	0.59
1:B:214:ILE:HG23	1:B:215:TRP:N	2.17	0.59
1:E:155:TYR:HB3	1:E:164:MET:HB2	1.85	0.59
1:A:132:TYR:CD1	1:A:178:PHE:HA	2.38	0.59
4:C:7378:HOH:O	1:D:53:LYS:HD3	2.03	0.59
1:E:238:MET:HE3	1:E:243:GLN:HG2	1.84	0.58
1:C:241:GLU:CD	1:C:241:GLU:H	2.10	0.58
1:G:155:TYR:CD1	1:G:164:MET:HE2	2.38	0.58
1:A:231:ASN:OD1	1:A:233:GLN:HB2	2.04	0.58
1:B:77:GLU:OE1	1:B:79:HIS:HE1	1.87	0.58
1:D:200:ARG:NH1	3:D:3301:FAD:H1B	2.18	0.58
1:G:222:PHE:O	1:G:224:PRO:HD3	2.03	0.58
1:C:12:SER:HB3	1:C:42:TYR:CE1	2.39	0.58
1:C:115:TRP:O	1:C:119:VAL:HG23	2.03	0.58
1:G:65:PHE:CE1	1:G:70:GLU:HG3	2.39	0.58
1:H:197:ALA:O	1:H:199:ALA:N	2.36	0.58
1:A:229:ASP:O	1:A:236:PHE:HA	2.04	0.58
4:B:7390:HOH:O	1:G:15:THR:HB	2.02	0.58
1:G:122:GLY:O	1:G:123:GLU:CB	2.51	0.58
1:D:26:ALA:O	1:D:30:LYS:HG3	2.03	0.58
1:D:1:VAL:HA	1:D:215:TRP:CD1	2.39	0.57
1:A:6:LEU:HD12	1:A:37:VAL:O	2.04	0.57
1:D:47:ASN:ND2	1:D:48:PRO:N	2.37	0.57
1:B:169:TRP:HB3	1:B:170:PRO:HD3	1.86	0.57
1:C:12:SER:HB3	1:C:42:TYR:CD1	2.40	0.57
1:C:122:GLY:O	1:C:123:GLU:HB2	2.04	0.57
1:C:132:TYR:HA	1:C:177:HIS:O	2.03	0.57
1:A:132:TYR:O	1:A:180:GLY:HA2	2.04	0.57
1:H:26:ALA:O	1:H:30:LYS:HG3	2.05	0.57
1:F:214:ILE:HA	1:F:217:GLU:OE2	2.05	0.57
1:B:77:GLU:HB2	1:B:79:HIS:CE1	2.39	0.57
1:A:175:ILE:HG12	1:C:105:TRP:HB3	1.86	0.56
1:C:45:ASN:ND2	1:D:45:ASN:HD21	2.03	0.56
1:H:1:VAL:CG2	1:H:2:GLY:H	2.15	0.56
1:A:55:ILE:CD1	1:A:70:GLU:HB3	2.35	0.56
1:F:74:ALA:HA	1:F:79:HIS:CE1	2.40	0.56
1:H:132:TYR:O	1:H:134:LYS:N	2.38	0.56
1:F:22:LYS:HD2	1:F:38:GLU:OE1	2.05	0.56
1:H:199:ALA:O	1:H:202:GLN:HB2	2.05	0.56
1:G:99:PHE:HB2	1:G:144:LEU:HD23	1.88	0.56
1:A:47:ASN:ND2	1:A:49:ILE:N	2.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:169:TRP:HB3	1:D:170:PRO:HD3	1.88	0.56
1:B:232:PHE:HD1	1:B:232:PHE:H	1.54	0.56
1:D:84:ILE:O	1:D:88:GLN:HG3	2.06	0.56
1:C:1:VAL:HA	1:C:215:TRP:NE1	2.21	0.56
1:F:84:ILE:O	1:F:88:GLN:HG3	2.06	0.56
1:F:238:MET:CE	1:F:243:GLN:HG2	2.34	0.56
1:D:169:TRP:CZ2	1:D:256:GLY:HA3	2.41	0.56
1:A:209:LYS:O	1:A:212:GLU:HB2	2.06	0.55
1:C:25:ALA:O	1:C:29:LEU:HB2	2.06	0.55
1:F:267:ASN:HD21	1:F:268:GLN:HE21	1.53	0.55
1:A:258:HIS:CD2	1:C:263:ILE:HD12	2.41	0.55
1:D:172:GLN:HE22	1:D:186:PRO:HB3	1.71	0.55
1:B:128:TYR:HB3	2:B:3280:DTC:C16	2.36	0.55
1:C:47:ASN:ND2	1:C:49:ILE:H	2.04	0.55
1:D:54:ASP:OD1	1:D:118:ARG:NH1	2.39	0.55
1:D:101:PHE:CZ	1:D:146:ILE:HG12	2.41	0.55
1:E:240:LYS:HD2	1:E:240:LYS:N	2.21	0.55
1:C:67:TYR:HB3	1:C:68:PRO:HD3	1.88	0.55
2:E:4280:DTC:C16	1:F:128:TYR:HB3	2.37	0.55
1:G:6:LEU:HA	1:G:37:VAL:O	2.07	0.55
1:B:106:PHE:HE2	1:B:155:TYR:HE1	1.55	0.55
1:F:88:GLN:HB3	1:F:124:PHE:CZ	2.42	0.55
1:F:195:THR:CG2	1:F:199:ALA:HB3	2.37	0.55
1:G:244:ASP:C	1:G:246:GLU:H	2.13	0.55
1:B:269:ILE:HG22	1:B:270:LYS:HG2	1.88	0.55
1:F:214:ILE:HG23	1:F:215:TRP:N	2.21	0.55
1:A:113:LYS:O	1:A:117:GLU:HG3	2.07	0.54
1:B:54:ASP:OD2	1:B:118:ARG:HD2	2.07	0.54
1:C:45:ASN:ND2	1:D:45:ASN:ND2	2.55	0.54
1:D:76:LYS:HE2	1:D:123:GLU:CG	2.36	0.54
1:G:59:LEU:O	1:G:62:PRO:HD3	2.08	0.54
1:A:246:GLU:O	1:A:261:LYS:NZ	2.40	0.54
1:E:11:HIS:O	1:E:14:ARG:NH2	2.39	0.54
1:F:165:ASN:ND2	1:F:266:ASP:HA	2.22	0.54
1:B:101:PHE:CE2	1:B:108:VAL:HG12	2.43	0.54
1:B:255:VAL:CG2	1:B:267:ASN:HD22	1.98	0.54
1:D:65:PHE:CD1	1:D:70:GLU:HG3	2.42	0.54
1:E:106:PHE:HD2	1:E:167:ILE:HD13	1.72	0.54
1:G:128:TYR:O	1:G:131:MET:HG3	2.07	0.54
1:G:163:ASP:OD1	1:G:165:ASN:ND2	2.39	0.54
1:B:169:TRP:O	1:B:173:SER:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:29:LEU:O	1:H:34:TRP:HB2	2.08	0.54
1:D:255:VAL:HG23	1:D:267:ASN:HB3	1.90	0.54
1:E:218:THR:O	1:E:271:ALA:HB2	2.07	0.54
1:E:243:GLN:O	1:E:247:LYS:HG3	2.06	0.54
1:C:169:TRP:CZ2	1:C:256:GLY:HA3	2.43	0.54
1:E:236:PHE:CD2	1:F:154:MET:HE3	2.43	0.54
1:F:197:ALA:HA	1:F:200:ARG:NE	2.23	0.54
1:A:17:PHE:CD2	1:A:192:ILE:HG12	2.43	0.54
1:B:172:GLN:HB3	1:B:183:VAL:HG11	1.90	0.54
1:B:209:LYS:HD2	1:B:212:GLU:OE2	2.08	0.54
1:D:130:ALA:HB1	1:D:134:LYS:O	2.08	0.54
1:D:255:VAL:H	1:D:267:ASN:HD22	1.56	0.54
1:E:101:PHE:CZ	1:E:108:VAL:HG12	2.43	0.54
1:F:14:ARG:HD3	1:F:19:TYR:CE1	2.43	0.54
1:G:25:ALA:HA	1:G:211:LEU:HD13	1.90	0.54
1:H:241:GLU:H	1:H:241:GLU:CD	2.16	0.54
1:B:187:GLN:HG2	1:B:207:TRP:CE3	2.44	0.53
1:B:267:ASN:ND2	1:B:268:GLN:HE21	2.07	0.53
1:C:133:ASP:OD1	1:C:225:SER:HB3	2.07	0.53
1:E:65:PHE:CD1	1:E:70:GLU:HG3	2.43	0.53
1:D:197:ALA:HA	1:D:200:ARG:NH2	2.22	0.53
1:E:128:TYR:HB3	2:E:5280:DTC:C16	2.38	0.53
1:F:197:ALA:HA	1:F:200:ARG:CZ	2.38	0.53
1:A:1:VAL:HG12	1:A:2:GLY:N	2.24	0.53
1:B:169:TRP:CZ2	1:B:256:GLY:HA3	2.43	0.53
1:E:169:TRP:HB3	1:E:170:PRO:HD3	1.89	0.53
1:F:173:SER:HB2	1:F:222:PHE:HE1	1.74	0.53
1:B:122:GLY:O	1:B:123:GLU:HB2	2.09	0.53
1:E:240:LYS:H	1:E:240:LYS:CD	2.20	0.53
1:H:4:ARG:HE	1:H:93:ALA:HB1	1.72	0.53
1:H:132:TYR:C	1:H:134:LYS:H	2.16	0.53
1:A:47:ASN:HD21	1:A:49:ILE:H	1.52	0.53
1:B:151:SER:OG	1:B:154:MET:HG3	2.08	0.53
1:D:128:TYR:HB3	2:D:1280:DTC:C16	2.38	0.53
1:H:227:LEU:O	1:H:239:LYS:HG3	2.08	0.53
1:D:246:GLU:OE2	1:D:249:LYS:HG3	2.09	0.53
1:F:4:ARG:HE	1:F:93:ALA:HB1	1.74	0.53
1:F:105:TRP:O	1:F:106:PHE:HB2	2.09	0.53
1:D:197:ALA:HA	1:D:200:ARG:HH21	1.74	0.53
1:B:118:ARG:O	1:B:121:ILE:HD11	2.09	0.53
1:F:154:MET:O	1:F:161:HIS:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:165:ASN:OD1	1:F:269:ILE:HG13	2.09	0.53
1:D:47:ASN:HD21	1:D:49:ILE:N	1.98	0.53
1:G:1:VAL:CG1	1:G:2:GLY:H	2.02	0.53
1:G:246:GLU:O	1:G:261:LYS:NZ	2.42	0.53
1:F:165:ASN:HD21	1:F:266:ASP:HA	1.72	0.52
1:H:204:LEU:O	1:H:208:LYS:HG3	2.09	0.52
1:C:1:VAL:HA	1:C:215:TRP:CD1	2.44	0.52
1:E:236:PHE:CG	1:F:154:MET:HE3	2.44	0.52
1:E:14:ARG:NH1	1:E:40:ASP:OD2	2.41	0.52
1:F:88:GLN:O	1:F:92:GLU:HG3	2.09	0.52
1:F:255:VAL:H	1:F:267:ASN:ND2	2.08	0.52
1:G:14:ARG:HG2	1:G:19:TYR:CZ	2.44	0.52
1:E:126:TYR:CD2	1:E:178:PHE:HE2	2.27	0.52
1:B:46:PHE:CE2	1:B:47:ASN:O	2.62	0.52
1:B:47:ASN:ND2	1:B:47:ASN:C	2.66	0.52
1:B:72:VAL:HG22	1:B:122:GLY:HA3	1.91	0.52
1:C:53:LYS:HZ1	1:D:53:LYS:HZ2	1.57	0.52
1:F:122:GLY:O	1:F:123:GLU:HB3	2.09	0.52
1:H:173:SER:HB2	1:H:222:PHE:HE1	1.72	0.52
1:C:3:ARG:NH1	4:C:7428:HOH:O	2.41	0.52
1:E:265:THR:O	1:E:266:ASP:C	2.53	0.52
1:H:151:SER:HA	1:H:190:TYR:HB3	1.91	0.52
1:A:106:PHE:HD2	1:A:167:ILE:CD1	2.23	0.52
1:E:104:GLN:HA	3:E:4301:FAD:C5X	2.40	0.52
1:F:214:ILE:CG2	1:F:215:TRP:N	2.73	0.52
1:H:138:ARG:HA	1:H:180:GLY:O	2.10	0.52
1:H:167:ILE:O	1:H:170:PRO:HD2	2.09	0.52
1:A:25:ALA:O	1:A:29:LEU:HB2	2.10	0.52
1:A:148:THR:HB	3:A:301:FAD:O2	2.09	0.52
1:E:29:LEU:HB3	1:E:34:TRP:HB2	1.92	0.52
1:B:6:LEU:HA	1:B:37:VAL:O	2.11	0.52
1:E:65:PHE:CE1	1:E:70:GLU:HG3	2.45	0.52
1:A:25:ALA:HA	1:A:211:LEU:CD1	2.40	0.51
1:E:46:PHE:CE2	1:E:115:TRP:HA	2.45	0.51
1:B:229:ASP:O	1:B:236:PHE:HA	2.10	0.51
1:C:45:ASN:CG	1:D:45:ASN:HD21	2.18	0.51
1:H:46:PHE:O	1:H:48:PRO:HD3	2.10	0.51
1:H:200:ARG:NH1	3:H:7301:FAD:H1B	2.26	0.51
1:A:26:ALA:HB1	1:A:30:LYS:HZ2	1.74	0.51
1:B:232:PHE:CD1	1:B:232:PHE:N	2.78	0.51
1:D:238:MET:HE1	1:D:259:LEU:CD1	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:50:ILE:HG22	1:G:118:ARG:HG2	1.91	0.51
1:B:18:ASN:OD1	1:B:100:GLN:NE2	2.40	0.51
1:D:148:THR:HB	3:D:3301:FAD:O2	2.10	0.51
1:E:151:SER:HG	1:E:154:MET:HG3	1.73	0.51
1:E:195:THR:HG22	1:E:199:ALA:HB3	1.91	0.51
1:B:137:PHE:C	1:B:139:SER:H	2.18	0.51
1:G:158:GLN:HB2	1:H:237:LEU:HD22	1.92	0.51
1:H:50:ILE:HG13	1:H:50:ILE:O	2.09	0.51
1:A:130:ALA:HB1	1:A:134:LYS:O	2.10	0.51
1:A:243:GLN:OE1	1:C:158:GLN:HG2	2.11	0.51
1:B:13:GLU:C	1:B:15:THR:H	2.19	0.51
1:B:6:LEU:HD13	1:B:37:VAL:HG12	1.93	0.51
1:B:76:LYS:CE	1:B:123:GLU:HG3	2.40	0.51
1:C:169:TRP:HB3	1:C:170:PRO:HD3	1.92	0.51
1:E:88:GLN:HG2	1:E:124:PHE:CE2	2.46	0.51
1:H:25:ALA:O	1:H:29:LEU:HB2	2.11	0.51
1:H:128:TYR:CD2	2:H:6280:DTC:C19	2.93	0.51
1:H:197:ALA:O	1:H:198:ASP:C	2.54	0.51
1:A:214:ILE:HD12	1:A:217:GLU:OE2	2.11	0.51
1:C:51:SER:C	1:C:53:LYS:H	2.20	0.50
1:C:65:PHE:CE1	1:C:70:GLU:HG3	2.45	0.50
1:F:4:ARG:HG2	1:F:35:GLU:HB2	1.93	0.50
1:F:183:VAL:HG12	1:F:220:LEU:HD12	1.92	0.50
1:G:111:ILE:HB	1:H:49:ILE:HD12	1.93	0.50
1:H:204:LEU:HD11	3:H:7301:FAD:N1A	2.26	0.50
1:A:47:ASN:HD22	1:A:49:ILE:H	1.58	0.50
1:A:7:ILE:HG21	1:A:22:LYS:HG2	1.92	0.50
1:B:204:LEU:O	1:B:208:LYS:HG3	2.11	0.50
1:D:238:MET:HE1	1:D:259:LEU:HD11	1.91	0.50
1:E:167:ILE:O	1:E:170:PRO:HD2	2.12	0.50
1:C:28:ALA:HB2	1:C:208:LYS:HE2	1.93	0.50
1:E:173:SER:HB2	1:E:222:PHE:CE1	2.46	0.50
1:E:58:LYS:HA	4:E:7367:HOH:O	2.12	0.50
1:H:9:LEU:HD12	1:H:10:ALA:H	1.76	0.50
1:A:186:PRO:HB2	1:A:188:LEU:CD2	2.42	0.50
1:A:254:SER:HB2	1:A:267:ASN:HD21	1.77	0.50
1:B:200:ARG:NH1	3:B:1301:FAD:H1B	2.26	0.50
1:C:45:ASN:CG	1:D:45:ASN:ND2	2.69	0.50
1:G:214:ILE:HG23	1:G:215:TRP:N	2.27	0.50
1:G:244:ASP:C	1:G:246:GLU:N	2.69	0.50
1:H:130:ALA:HB1	1:H:134:LYS:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:TYR:HB3	2:A:2280:DTC:C16	2.42	0.50
1:B:55:ILE:HD13	1:B:70:GLU:HB3	1.93	0.50
1:E:55:ILE:HG23	1:E:74:ALA:CB	2.40	0.50
1:F:55:ILE:HD13	1:F:70:GLU:HB3	1.93	0.50
1:G:238:MET:HE2	1:G:243:GLN:HG2	1.94	0.50
1:H:163:ASP:CG	1:H:165:ASN:HB2	2.36	0.50
1:A:160:ILE:HG12	1:A:160:ILE:O	2.12	0.50
1:C:22:LYS:HD3	1:C:38:GLU:OE1	2.11	0.50
1:C:104:GLN:HA	3:C:2301:FAD:C5X	2.42	0.50
1:H:1:VAL:HA	1:H:215:TRP:HE1	1.77	0.50
1:H:214:ILE:HD12	1:H:217:GLU:OE2	2.12	0.50
1:B:4:ARG:HG2	1:B:35:GLU:OE1	2.12	0.50
1:F:50:ILE:HG13	1:F:50:ILE:O	2.12	0.50
1:H:200:ARG:HD3	3:H:7301:FAD:N3A	2.27	0.50
1:C:53:LYS:HZ1	1:D:53:LYS:NZ	2.09	0.49
1:G:49:ILE:O	1:G:118:ARG:HD3	2.12	0.49
1:B:258:HIS:CD2	1:D:263:ILE:HD12	2.48	0.49
1:A:185:GLU:HG2	1:A:269:ILE:O	2.12	0.49
1:B:152:GLY:HA2	1:B:190:TYR:CD1	2.47	0.49
1:C:47:ASN:HD22	1:C:47:ASN:C	2.20	0.49
1:F:185:GLU:OE2	1:F:271:ALA:N	2.40	0.49
1:C:128:TYR:HB3	2:C:280:DTC:C16	2.42	0.49
1:D:106:PHE:HD2	1:D:167:ILE:HD13	1.76	0.49
1:H:144:LEU:CD2	1:H:176:LEU:HD11	2.42	0.49
1:A:169:TRP:HB3	1:A:170:PRO:HD3	1.95	0.49
1:D:266:ASP:HB3	1:D:269:ILE:HB	1.94	0.49
1:F:238:MET:HE1	1:F:259:LEU:CD2	2.43	0.49
1:B:255:VAL:H	1:B:267:ASN:HD22	1.60	0.49
1:C:246:GLU:O	1:C:261:LYS:NZ	2.46	0.49
1:D:1:VAL:HG12	1:D:2:GLY:N	2.20	0.49
1:H:208:LYS:O	1:H:212:GLU:HG3	2.13	0.49
1:H:238:MET:HE1	1:H:259:LEU:CD2	2.36	0.49
1:F:50:ILE:HB	1:F:67:TYR:CE1	2.48	0.49
1:G:169:TRP:CD1	1:H:166:VAL:HG11	2.47	0.49
1:H:17:PHE:HE1	1:H:200:ARG:HB3	1.78	0.49
1:H:77:GLU:OE1	1:H:79:HIS:HE1	1.96	0.49
1:D:29:LEU:HD12	1:D:34:TRP:CD1	2.48	0.49
1:D:114:GLY:O	1:D:118:ARG:HG3	2.13	0.49
1:D:116:PHE:O	1:D:120:PHE:HB2	2.13	0.49
1:D:255:VAL:H	1:D:267:ASN:ND2	2.11	0.49
1:H:108:VAL:HB	1:H:112:LEU:HD23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:160:ILE:CD1	1:H:230:LEU:HD21	2.42	0.49
1:H:17:PHE:CE1	1:H:200:ARG:HB3	2.48	0.49
1:H:255:VAL:HG23	1:H:267:ASN:ND2	2.23	0.49
1:C:53:LYS:NZ	1:D:53:LYS:NZ	2.61	0.48
1:D:197:ALA:CA	1:D:200:ARG:HH21	2.26	0.48
1:E:273:LYS:HD3	1:E:273:LYS:C	2.38	0.48
1:F:49:ILE:O	1:F:118:ARG:HD3	2.12	0.48
1:G:160:ILE:HD12	1:H:230:LEU:HD21	1.95	0.48
1:A:87:GLU:O	1:A:90:LYS:N	2.44	0.48
1:C:122:GLY:C	1:C:124:PHE:H	2.21	0.48
1:A:3:ARG:HA	1:A:3:ARG:NE	2.22	0.48
1:E:104:GLN:HA	3:E:4301:FAD:N5	2.28	0.48
1:F:263:ILE:O	1:F:264:PRO:C	2.54	0.48
1:B:29:LEU:CD1	1:B:211:LEU:HB3	2.44	0.48
1:B:192:ILE:HD11	1:B:200:ARG:HG2	1.95	0.48
1:F:1:VAL:HG22	1:F:2:GLY:N	2.21	0.48
1:H:9:LEU:HD12	1:H:10:ALA:N	2.27	0.48
1:C:204:LEU:O	1:C:208:LYS:HG3	2.14	0.48
1:H:221:TYR:HE2	1:H:253:LEU:O	1.96	0.48
1:B:258:HIS:CE1	1:D:157:LEU:HD22	2.48	0.48
1:E:73:LEU:HD11	1:E:77:GLU:CD	2.39	0.48
1:A:1:VAL:HG12	1:A:2:GLY:H	1.79	0.48
1:A:200:ARG:NH1	3:A:301:FAD:H1B	2.26	0.48
1:B:75:TYR:CZ	1:B:124:PHE:HB2	2.49	0.48
1:D:65:PHE:CE1	1:D:70:GLU:HG3	2.49	0.48
1:D:200:ARG:HH11	3:D:3301:FAD:C1B	2.24	0.48
1:F:104:GLN:HA	3:F:5301:FAD:N5	2.29	0.48
1:G:232:PHE:HD1	1:G:232:PHE:H	1.60	0.48
1:H:32:LYS:HE3	1:H:212:GLU:CG	2.44	0.48
1:H:251:PHE:HD1	1:H:262:SER:HB3	1.78	0.48
1:E:207:TRP:CH2	1:E:211:LEU:HD21	2.48	0.48
1:D:29:LEU:HB3	1:D:34:TRP:HB2	1.96	0.48
1:G:155:TYR:HB3	1:G:164:MET:HB2	1.96	0.48
1:H:210:ARG:NE	1:H:214:ILE:HD13	2.29	0.48
1:B:4:ARG:NH1	1:B:93:ALA:O	2.45	0.47
1:B:76:LYS:HE2	1:B:123:GLU:OE1	2.14	0.47
1:C:192:ILE:CG2	3:C:2301:FAD:H5'1	2.44	0.47
1:H:72:VAL:HG13	1:H:123:GLU:HG2	1.96	0.47
1:H:198:ASP:O	1:H:202:GLN:HG2	2.14	0.47
1:E:40:ASP:O	1:E:41:LEU:C	2.57	0.47
1:A:52:ARG:C	1:A:54:ASP:H	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:165:ASN:HD21	1:H:266:ASP:HA	1.79	0.47
1:B:130:ALA:HB1	1:B:134:LYS:O	2.15	0.47
1:E:106:PHE:HD2	1:E:167:ILE:CD1	2.27	0.47
2:G:7280:DTC:O38	1:H:154:MET:HE1	2.14	0.47
1:H:198:ASP:HA	1:H:201:ILE:HD12	1.95	0.47
1:A:239:LYS:O	1:A:243:GLN:HG3	2.15	0.47
1:F:132:TYR:C	1:F:134:LYS:H	2.22	0.47
1:D:218:THR:O	1:D:218:THR:HG23	2.15	0.47
1:A:68:PRO:O	1:A:72:VAL:HG23	2.15	0.47
1:B:113:LYS:NZ	1:D:108:VAL:O	2.48	0.47
1:B:257:HIS:HA	4:B:7430:HOH:O	2.15	0.47
1:C:53:LYS:NZ	4:C:7378:HOH:O	2.48	0.47
1:E:227:LEU:HB3	1:E:242:VAL:HG11	1.96	0.47
1:E:241:GLU:CD	1:E:241:GLU:H	2.23	0.47
1:B:154:MET:HE3	1:D:236:PHE:CD1	2.49	0.47
1:E:163:ASP:CG	1:E:165:ASN:HB2	2.40	0.47
1:H:185:GLU:O	1:H:210:ARG:NH2	2.41	0.47
1:D:209:LYS:HA	1:D:212:GLU:OE2	2.15	0.47
1:F:201:ILE:O	1:F:205:GLU:HG2	2.15	0.47
1:D:130:ALA:O	1:D:135:GLY:HA2	2.15	0.46
1:F:101:PHE:O	1:F:146:ILE:HA	2.16	0.46
1:B:102:PRO:O	1:B:102:PRO:HG2	2.15	0.46
1:D:4:ARG:HG2	1:D:35:GLU:OE2	2.15	0.46
1:D:52:ARG:C	1:D:54:ASP:H	2.24	0.46
1:F:104:GLN:HA	3:F:5301:FAD:C5X	2.44	0.46
1:G:32:LYS:HE3	1:G:212:GLU:HG2	1.97	0.46
1:H:246:GLU:O	1:H:261:LYS:NZ	2.48	0.46
1:A:116:PHE:O	1:A:120:PHE:HB2	2.16	0.46
1:C:200:ARG:HD2	3:C:2301:FAD:N3A	2.30	0.46
1:D:209:LYS:O	1:D:212:GLU:HB2	2.16	0.46
1:F:50:ILE:CG2	1:F:118:ARG:HG2	2.41	0.46
1:G:88:GLN:HB3	1:G:124:PHE:CZ	2.51	0.46
1:G:113:LYS:O	1:G:117:GLU:HG3	2.16	0.46
3:G:6301:FAD:HM82	1:H:68:PRO:HG3	1.98	0.46
1:C:62:PRO:HG2	1:G:202:GLN:OE1	2.15	0.46
1:G:169:TRP:HB3	1:G:170:PRO:HD3	1.96	0.46
1:G:257:HIS:CD2	1:H:162:GLY:HA2	2.51	0.46
1:H:172:GLN:HB3	1:H:183:VAL:HG11	1.96	0.46
1:A:9:LEU:HD21	1:A:19:TYR:HD1	1.81	0.46
1:D:55:ILE:N	1:D:55:ILE:CD1	2.78	0.46
1:F:128:TYR:O	1:F:131:MET:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:132:TYR:HA	1:F:177:HIS:O	2.15	0.46
1:G:17:PHE:HB2	3:G:6301:FAD:H51A	1.97	0.46
1:G:132:TYR:CD1	1:G:178:PHE:HA	2.49	0.46
1:B:1:VAL:CG1	1:B:2:GLY:H	2.16	0.46
1:C:46:PHE:CE2	1:C:115:TRP:HA	2.51	0.46
1:C:236:PHE:CZ	2:C:280:DTC:H16	2.51	0.46
1:D:204:LEU:O	1:D:208:LYS:HG3	2.16	0.46
1:F:238:MET:HE1	1:F:259:LEU:HD21	1.98	0.46
1:A:121:ILE:O	1:A:124:PHE:HB3	2.15	0.46
1:B:11:HIS:CE1	1:B:16:SER:HB3	2.51	0.46
1:A:88:GLN:HB3	1:A:124:PHE:CZ	2.51	0.46
1:C:54:ASP:CG	1:C:118:ARG:HH11	2.24	0.46
1:B:106:PHE:CE2	1:B:155:TYR:HE1	2.33	0.46
1:G:266:ASP:HB3	1:G:269:ILE:HB	1.98	0.46
1:H:22:LYS:O	1:H:25:ALA:HB3	2.15	0.46
1:H:168:LEU:O	1:H:172:GLN:HG3	2.16	0.46
1:A:55:ILE:HD13	1:A:70:GLU:HB3	1.96	0.45
1:B:195:THR:CG2	1:B:199:ALA:HB3	2.46	0.45
1:D:149:GLY:O	1:D:191:SER:HA	2.16	0.45
1:D:254:SER:HB2	1:D:267:ASN:HD21	1.81	0.45
1:D:265:THR:O	1:D:266:ASP:C	2.59	0.45
1:E:127:THR:HG22	1:E:130:ALA:N	2.31	0.45
1:E:166:VAL:CG1	1:F:169:TRP:CD1	2.98	0.45
1:F:244:ASP:C	1:F:246:GLU:H	2.23	0.45
1:A:23:GLU:HA	1:A:23:GLU:OE1	2.15	0.45
1:A:104:GLN:HA	3:A:301:FAD:C5X	2.46	0.45
1:B:25:ALA:HA	1:B:211:LEU:CD1	2.47	0.45
1:C:73:LEU:HD23	4:C:7335:HOH:O	2.15	0.45
1:E:166:VAL:O	1:E:170:PRO:HD3	2.16	0.45
1:F:246:GLU:HG3	4:F:7318:HOH:O	2.16	0.45
1:H:209:LYS:O	1:H:212:GLU:HG3	2.17	0.45
1:G:6:LEU:CD1	1:G:37:VAL:HG12	2.47	0.45
1:G:55:ILE:HG12	1:G:74:ALA:HB2	1.99	0.45
1:G:55:ILE:CD1	1:G:70:GLU:HB3	2.45	0.45
1:D:155:TYR:HB3	1:D:164:MET:HB2	1.97	0.45
1:F:23:GLU:HA	1:F:23:GLU:OE1	2.17	0.45
1:C:45:ASN:CG	1:C:45:ASN:O	2.59	0.45
1:E:40:ASP:HB3	1:E:43:ALA:HB3	1.98	0.45
1:B:141:LYS:HD2	1:B:215:TRP:CZ3	2.51	0.45
1:B:214:ILE:HD12	1:B:217:GLU:OE2	2.17	0.45
1:B:239:LYS:O	1:B:243:GLN:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:195:THR:HA	1:E:196:PRO:HD3	1.76	0.45
1:F:116:PHE:O	1:F:120:PHE:HB2	2.16	0.45
1:H:221:TYR:OH	1:H:253:LEU:HD22	2.17	0.45
1:A:165:ASN:ND2	1:A:269:ILE:HD12	2.31	0.45
1:B:49:ILE:C	1:B:118:ARG:HD3	2.40	0.45
1:B:104:GLN:HA	3:B:1301:FAD:N5	2.31	0.45
1:D:214:ILE:HD12	1:D:217:GLU:OE2	2.16	0.45
1:H:1:VAL:HA	1:H:215:TRP:CD1	2.52	0.45
1:H:146:ILE:HG22	1:H:147:THR:N	2.32	0.45
1:B:137:PHE:C	1:B:139:SER:N	2.75	0.45
1:C:47:ASN:ND2	1:C:47:ASN:C	2.74	0.45
1:E:12:SER:HB3	1:E:42:TYR:CE1	2.52	0.45
1:E:236:PHE:HB2	1:F:154:MET:HG2	1.97	0.45
1:F:9:LEU:HD22	1:F:22:LYS:HD3	1.98	0.45
1:F:72:VAL:HG22	1:F:122:GLY:HA3	1.99	0.45
1:A:218:THR:HG23	4:A:7406:HOH:O	2.16	0.45
1:B:132:TYR:OH	1:D:161:HIS:CD2	2.64	0.45
1:C:113:LYS:O	1:C:117:GLU:HG3	2.16	0.45
1:C:244:ASP:O	1:C:247:LYS:HG3	2.17	0.45
1:D:144:LEU:HD12	1:D:172:GLN:NE2	2.32	0.45
1:D:150:GLY:HA2	1:D:154:MET:CE	2.47	0.45
1:F:67:TYR:HB3	1:F:68:PRO:HD3	1.98	0.45
1:F:246:GLU:C	1:F:248:ASN:H	2.23	0.45
1:H:108:VAL:HG13	1:H:171:ILE:HD13	1.99	0.45
1:B:200:ARG:HD2	3:B:1301:FAD:N3A	2.31	0.45
1:F:245:GLU:HA	1:F:245:GLU:OE1	2.16	0.45
1:A:122:GLY:O	1:A:123:GLU:CB	2.65	0.44
1:A:166:VAL:HG13	1:C:166:VAL:HG13	1.99	0.44
1:H:105:TRP:CD1	3:H:7301:FAD:H6	2.52	0.44
1:A:138:ARG:HA	1:A:180:GLY:O	2.16	0.44
1:D:122:GLY:O	1:D:124:PHE:N	2.45	0.44
1:D:132:TYR:HA	1:D:177:HIS:O	2.17	0.44
1:E:207:TRP:O	1:E:211:LEU:HG	2.18	0.44
1:G:11:HIS:NE2	3:G:6301:FAD:O2P	2.38	0.44
1:G:141:LYS:HD3	1:G:184:LEU:HD21	1.98	0.44
1:G:273:LYS:HD3	1:G:273:LYS:C	2.42	0.44
1:H:251:PHE:HD1	1:H:262:SER:CB	2.30	0.44
1:B:155:TYR:HB3	1:B:164:MET:HB2	2.00	0.44
1:E:151:SER:N	1:E:154:MET:HE3	2.29	0.44
1:E:266:ASP:HB3	1:E:269:ILE:HB	1.98	0.44
1:G:87:GLU:O	1:G:90:LYS:HB2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:200:ARG:O	1:H:201:ILE:C	2.60	0.44
1:D:132:TYR:CD1	1:D:178:PHE:HA	2.53	0.44
1:E:141:LYS:NZ	1:E:215:TRP:O	2.50	0.44
1:F:132:TYR:O	1:F:180:GLY:HA2	2.18	0.44
1:H:21:MET:SD	1:H:204:LEU:HD23	2.57	0.44
1:H:44:MET:O	1:H:45:ASN:C	2.59	0.44
1:D:123:GLU:OE2	1:D:123:GLU:HA	2.18	0.44
1:G:44:MET:HE1	1:G:87:GLU:OE2	2.18	0.44
1:H:174:GLY:O	1:H:178:PHE:HB2	2.18	0.44
1:C:56:THR:O	1:C:79:HIS:HB3	2.18	0.44
1:F:106:PHE:N	1:F:106:PHE:CD1	2.86	0.44
1:C:102:PRO:HA	1:C:147:THR:OG1	2.17	0.44
1:F:157:LEU:HD23	1:F:163:ASP:HB2	1.99	0.44
1:G:49:ILE:C	1:G:118:ARG:HD3	2.43	0.44
1:H:51:SER:OG	1:H:53:LYS:HB3	2.18	0.44
1:A:238:MET:HE1	1:A:259:LEU:HD22	2.00	0.44
1:B:15:THR:HG21	1:G:200:ARG:HH12	1.82	0.44
1:B:56:THR:O	1:B:79:HIS:CD2	2.71	0.44
1:C:199:ALA:O	1:C:203:ILE:HG13	2.17	0.44
1:F:155:TYR:HB3	1:F:164:MET:HB2	1.98	0.44
1:G:126:TYR:CD2	1:G:178:PHE:HE2	2.36	0.44
1:H:101:PHE:CZ	1:H:146:ILE:HG12	2.53	0.44
1:H:121:ILE:HG22	1:H:122:GLY:N	2.32	0.44
1:A:195:THR:CG2	1:A:199:ALA:HB3	2.48	0.44
1:A:254:SER:OG	1:A:257:HIS:HB2	2.17	0.44
1:B:141:LYS:HG2	1:B:182:GLN:HB2	2.00	0.44
1:D:121:ILE:HG22	1:D:122:GLY:N	2.33	0.44
1:F:41:LEU:O	1:F:44:MET:HB2	2.18	0.44
1:F:111:ILE:HG23	1:F:112:LEU:N	2.33	0.44
1:G:25:ALA:HA	1:G:211:LEU:CD1	2.48	0.44
1:G:176:LEU:O	1:G:181:PHE:HB2	2.18	0.44
1:G:214:ILE:CD1	1:G:217:GLU:OE2	2.62	0.44
1:H:266:ASP:HB3	1:H:269:ILE:HB	1.99	0.44
1:E:166:VAL:O	1:E:169:TRP:HB3	2.18	0.43
1:F:1:VAL:HA	1:F:215:TRP:NE1	2.33	0.43
1:A:65:PHE:HB3	1:C:13:GLU:OE1	2.19	0.43
1:A:106:PHE:HD2	1:A:167:ILE:HD11	1.83	0.43
1:B:214:ILE:CG2	1:B:215:TRP:N	2.80	0.43
1:F:122:GLY:O	1:F:123:GLU:CB	2.66	0.43
1:A:52:ARG:C	1:A:54:ASP:N	2.73	0.43
1:A:105:TRP:HB3	1:C:175:ILE:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:PHE:CZ	1:B:108:VAL:HG12	2.53	0.43
1:C:118:ARG:O	1:C:121:ILE:HD11	2.18	0.43
1:E:6:LEU:HD11	1:E:39:SER:HB2	1.99	0.43
1:A:50:ILE:HG13	1:A:50:ILE:O	2.18	0.43
1:E:151:SER:OG	1:E:154:MET:HE3	2.18	0.43
1:E:166:VAL:HA	1:E:255:VAL:HG11	2.01	0.43
1:H:155:TYR:HD2	1:H:190:TYR:CE1	2.36	0.43
1:H:200:ARG:O	1:H:203:ILE:N	2.52	0.43
1:A:4:ARG:NH1	1:A:4:ARG:HG3	2.33	0.43
1:D:24:ALA:O	1:D:208:LYS:HE3	2.18	0.43
1:D:47:ASN:HD22	1:D:48:PRO:CD	2.28	0.43
1:F:137:PHE:HB3	1:F:140:LYS:HD2	2.00	0.43
1:G:163:ASP:HB3	1:G:166:VAL:HG23	2.00	0.43
1:B:146:ILE:HG22	1:B:147:THR:N	2.34	0.43
1:B:152:GLY:HA2	1:B:190:TYR:CE1	2.53	0.43
1:C:131:MET:HE3	1:C:131:MET:HB2	1.95	0.43
1:C:165:ASN:OD1	1:C:266:ASP:HA	2.19	0.43
1:E:238:MET:HE1	1:E:259:LEU:HD21	1.99	0.43
1:G:17:PHE:O	1:G:20:ALA:HB3	2.19	0.43
1:G:160:ILE:HG12	1:G:160:ILE:O	2.18	0.43
1:A:5:ALA:HB2	1:A:34:TRP:CE3	2.53	0.43
1:A:95:ASP:HB3	1:A:215:TRP:CH2	2.53	0.43
1:B:85:VAL:CG1	1:B:89:LYS:HE3	2.49	0.43
1:C:14:ARG:HA	1:C:14:ARG:HD3	1.88	0.43
1:G:273:LYS:HD3	1:G:273:LYS:O	2.18	0.43
1:H:169:TRP:HB3	1:H:170:PRO:HD3	1.99	0.43
1:B:263:ILE:H	1:B:263:ILE:HG13	1.66	0.43
1:F:1:VAL:HA	1:F:215:TRP:CD1	2.53	0.43
1:F:51:SER:C	1:F:53:LYS:N	2.77	0.43
1:B:77:GLU:OE1	1:B:79:HIS:CE1	2.70	0.43
1:G:135:GLY:HA3	1:G:179:CYS:O	2.19	0.43
1:B:44:MET:O	1:B:45:ASN:HB3	2.19	0.43
1:C:132:TYR:O	1:C:135:GLY:N	2.51	0.43
1:D:64:ASN:HD22	1:D:64:ASN:HA	1.50	0.43
1:G:55:ILE:HD13	1:G:70:GLU:HB3	2.00	0.43
1:H:152:GLY:O	1:H:155:TYR:N	2.49	0.43
1:H:213:ASN:O	1:H:215:TRP:N	2.52	0.43
1:D:196:PRO:O	1:D:199:ALA:N	2.52	0.42
1:F:40:ASP:O	1:F:41:LEU:C	2.62	0.42
1:F:233:GLN:HA	1:F:233:GLN:NE2	2.34	0.42
1:A:40:ASP:O	1:A:41:LEU:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:THR:HG22	1:B:199:ALA:HB3	2.00	0.42
1:C:142:ALA:HB2	1:C:181:PHE:CE1	2.54	0.42
1:D:192:ILE:O	1:D:192:ILE:HG13	2.18	0.42
1:D:251:PHE:HB3	1:D:264:PRO:HG3	2.02	0.42
1:E:67:TYR:HB3	1:E:68:PRO:HD3	2.00	0.42
1:E:132:TYR:HA	1:E:177:HIS:O	2.19	0.42
1:A:163:ASP:CG	1:A:165:ASN:HB2	2.44	0.42
1:B:263:ILE:HD11	1:D:263:ILE:HD11	2.01	0.42
1:B:263:ILE:HA	1:B:264:PRO:HD3	1.89	0.42
1:E:132:TYR:OH	1:F:161:HIS:HD2	2.02	0.42
1:F:163:ASP:CG	1:F:165:ASN:HB2	2.44	0.42
1:H:165:ASN:ND2	1:H:266:ASP:HA	2.34	0.42
1:A:47:ASN:HD21	1:A:49:ILE:N	2.15	0.42
1:B:54:ASP:CG	1:B:118:ARG:NH1	2.76	0.42
1:B:72:VAL:O	1:B:75:TYR:HB3	2.18	0.42
1:C:97:VAL:HG12	1:C:99:PHE:CE1	2.55	0.42
1:D:185:GLU:HG3	4:D:7305:HOH:O	2.19	0.42
1:E:126:TYR:CG	1:E:178:PHE:HE2	2.37	0.42
1:F:9:LEU:HD22	1:F:22:LYS:HB2	2.01	0.42
1:F:204:LEU:O	1:F:208:LYS:HG3	2.20	0.42
1:B:166:VAL:HG11	1:D:169:TRP:CD1	2.53	0.42
1:B:199:ALA:O	1:B:202:GLN:HB3	2.19	0.42
1:H:31:LYS:C	1:H:33:GLY:H	2.27	0.42
1:C:45:ASN:HD21	1:D:45:ASN:HD21	1.66	0.42
1:D:165:ASN:OD1	1:D:266:ASP:HA	2.19	0.42
1:E:84:ILE:HD11	1:E:118:ARG:NH1	2.34	0.42
1:E:151:SER:CB	1:E:154:MET:HE3	2.49	0.42
1:F:52:ARG:H	1:F:52:ARG:HG2	1.70	0.42
1:F:172:GLN:HB3	1:F:183:VAL:HG11	2.01	0.42
1:F:187:GLN:HA	1:F:187:GLN:OE1	2.19	0.42
1:G:18:ASN:HD21	1:G:147:THR:HG1	1.62	0.42
1:G:128:TYR:CD1	2:G:7280:DTC:C19	3.03	0.42
1:G:208:LYS:O	1:G:209:LYS:C	2.62	0.42
1:G:244:ASP:O	1:G:246:GLU:N	2.53	0.42
1:D:102:PRO:HG2	1:D:102:PRO:O	2.20	0.42
1:F:195:THR:HG23	1:F:199:ALA:HB3	2.01	0.42
1:G:32:LYS:CE	1:G:212:GLU:HG2	2.49	0.42
1:G:67:TYR:HB3	1:G:68:PRO:HD3	2.02	0.42
1:H:213:ASN:O	1:H:214:ILE:C	2.63	0.42
1:B:126:TYR:CD2	1:B:178:PHE:HE2	2.38	0.42
1:C:112:LEU:HD22	1:C:112:LEU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:TYR:C	1:C:134:LYS:H	2.27	0.42
1:C:229:ASP:O	1:C:231:ASN:N	2.40	0.42
1:G:54:ASP:OD2	1:G:118:ARG:HD2	2.20	0.42
1:A:122:GLY:O	1:A:123:GLU:HB3	2.19	0.42
1:G:88:GLN:O	1:G:89:LYS:C	2.62	0.42
1:H:13:GLU:C	1:H:14:ARG:HD2	2.43	0.42
1:A:209:LYS:O	1:A:210:ARG:C	2.63	0.42
1:C:62:PRO:HD2	1:G:202:GLN:NE2	2.34	0.42
1:C:143:VAL:CG2	1:C:184:LEU:HB2	2.38	0.42
1:E:109:PRO:O	1:E:110:ALA:C	2.62	0.42
1:G:6:LEU:HD13	1:G:37:VAL:HG12	2.02	0.42
1:D:176:LEU:O	1:D:181:PHE:HB2	2.20	0.41
1:E:50:ILE:CG2	1:E:118:ARG:HG2	2.44	0.41
1:F:209:LYS:O	1:F:212:GLU:HG3	2.20	0.41
1:A:9:LEU:HD12	1:A:10:ALA:N	2.35	0.41
1:B:40:ASP:O	1:B:41:LEU:C	2.62	0.41
1:B:103:LEU:HD11	1:B:106:PHE:C	2.45	0.41
1:F:9:LEU:CD2	1:F:22:LYS:HD3	2.51	0.41
1:F:160:ILE:O	1:F:160:ILE:HG12	2.20	0.41
1:F:244:ASP:C	1:F:246:GLU:N	2.78	0.41
1:D:40:ASP:O	1:D:41:LEU:C	2.63	0.41
1:F:64:ASN:HD22	1:F:64:ASN:HA	1.61	0.41
1:G:91:LEU:HD23	1:G:91:LEU:HA	1.88	0.41
1:G:151:SER:H	1:G:154:MET:HE3	1.85	0.41
1:A:1:VAL:HA	1:A:215:TRP:NE1	2.35	0.41
1:B:14:ARG:HH21	1:B:43:ALA:CB	2.34	0.41
1:B:87:GLU:O	1:B:90:LYS:HB2	2.20	0.41
1:D:112:LEU:O	1:D:112:LEU:HD22	2.21	0.41
1:G:141:LYS:HG2	1:G:182:GLN:HB2	2.01	0.41
1:B:185:GLU:O	1:B:210:ARG:NH2	2.47	0.41
1:C:54:ASP:OD1	1:C:118:ARG:NH1	2.54	0.41
1:D:195:THR:CG2	1:D:199:ALA:HB3	2.51	0.41
1:D:246:GLU:O	1:D:261:LYS:NZ	2.43	0.41
1:E:155:TYR:CG	1:E:164:MET:HE2	2.54	0.41
1:F:46:PHE:O	1:F:48:PRO:HD3	2.20	0.41
1:H:19:TYR:O	1:H:20:ALA:C	2.62	0.41
1:B:137:PHE:O	1:B:139:SER:N	2.54	0.41
1:B:206:GLY:O	1:B:209:LYS:HB3	2.20	0.41
1:C:238:MET:HE3	1:C:243:GLN:HG2	2.02	0.41
1:D:207:TRP:O	1:D:211:LEU:HG	2.21	0.41
1:F:3:ARG:NH1	1:F:3:ARG:HG2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:22:LYS:HE3	1:G:22:LYS:HB3	1.94	0.41
1:G:116:PHE:O	1:G:120:PHE:HB2	2.20	0.41
1:G:213:ASN:O	1:G:214:ILE:C	2.63	0.41
1:H:155:TYR:CE1	1:H:161:HIS:CD2	3.09	0.41
1:A:96:LEU:HA	1:A:141:LYS:O	2.21	0.41
1:C:47:ASN:O	1:C:118:ARG:NE	2.52	0.41
1:D:3:ARG:HE	1:D:3:ARG:HA	1.85	0.41
1:A:185:GLU:O	1:A:210:ARG:NH2	2.33	0.41
1:E:228:PHE:CD1	1:E:228:PHE:N	2.88	0.41
1:F:29:LEU:O	1:F:34:TRP:HB2	2.21	0.41
1:F:156:SER:O	1:F:157:LEU:C	2.63	0.41
1:G:96:LEU:HD11	1:G:143:VAL:HG23	2.02	0.41
1:H:122:GLY:O	1:H:124:PHE:N	2.53	0.41
1:A:154:MET:HG2	1:C:236:PHE:HB2	2.02	0.41
1:B:6:LEU:HD22	1:B:90:LYS:HB3	2.03	0.41
1:B:185:GLU:OE2	1:B:270:LYS:HA	2.21	0.41
1:C:1:VAL:CG1	1:C:2:GLY:H	2.33	0.41
1:C:126:TYR:CD2	1:C:126:TYR:C	2.99	0.41
1:C:141:LYS:HD3	1:C:184:LEU:HD21	2.01	0.41
1:C:142:ALA:HB2	1:C:181:PHE:CD1	2.56	0.41
1:C:172:GLN:HE22	1:C:186:PRO:HB3	1.85	0.41
1:D:122:GLY:O	1:D:123:GLU:HB2	2.21	0.41
1:E:132:TYR:HD1	1:E:177:HIS:CD2	2.38	0.41
1:E:214:ILE:HD12	1:E:217:GLU:OE2	2.20	0.41
2:E:5280:DTC:HC3	1:F:105:TRP:CZ2	2.56	0.41
1:F:103:LEU:CB	1:F:148:THR:HG22	2.51	0.41
1:F:113:LYS:O	1:F:117:GLU:HG3	2.20	0.41
1:G:122:GLY:O	1:G:123:GLU:HB2	2.20	0.41
1:G:263:ILE:HA	1:G:264:PRO:HD3	1.95	0.41
1:H:17:PHE:CE1	1:H:204:LEU:HD21	2.56	0.41
1:H:149:GLY:O	1:H:191:SER:HA	2.21	0.41
1:H:263:ILE:HA	1:H:264:PRO:HD2	1.89	0.41
1:A:173:SER:HA	1:A:177:HIS:HB3	2.03	0.41
1:B:173:SER:HB2	1:B:222:PHE:HE1	1.85	0.41
1:F:14:ARG:HH21	1:F:43:ALA:CB	2.12	0.41
1:G:65:PHE:CD1	1:G:70:GLU:HG3	2.56	0.41
1:H:72:VAL:HG12	1:H:76:LYS:HE3	2.03	0.41
1:H:195:THR:CG2	1:H:199:ALA:HB3	2.46	0.41
1:B:53:LYS:O	1:B:53:LYS:HG2	2.22	0.40
1:B:72:VAL:HG22	1:B:122:GLY:CA	2.52	0.40
1:B:169:TRP:CE2	1:B:256:GLY:HA3	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:LYS:HG2	1:B:241:GLU:OE2	2.21	0.40
1:C:65:PHE:CD1	1:C:70:GLU:HG3	2.56	0.40
1:D:101:PHE:CE1	1:D:146:ILE:HG12	2.55	0.40
1:F:57:GLY:HA3	1:F:79:HIS:CD2	2.56	0.40
1:G:105:TRP:HB2	1:H:113:LYS:HE3	2.03	0.40
1:G:145:SER:HA	1:G:187:GLN:HB3	2.03	0.40
1:H:147:THR:HA	1:H:189:THR:OG1	2.21	0.40
1:A:87:GLU:O	1:A:88:GLN:C	2.64	0.40
1:A:160:ILE:HA	1:C:228:PHE:CE2	2.57	0.40
1:B:122:GLY:C	1:B:124:PHE:H	2.28	0.40
1:C:130:ALA:HB1	1:C:134:LYS:O	2.20	0.40
1:C:163:ASP:OD2	1:C:165:ASN:HB2	2.22	0.40
1:D:230:LEU:HA	1:D:236:PHE:CD2	2.56	0.40
1:E:83:ASP:OD2	1:E:118:ARG:NH2	2.46	0.40
1:F:103:LEU:HB3	1:F:148:THR:HG22	2.02	0.40
1:G:226:SER:O	1:G:239:LYS:HE3	2.21	0.40
1:B:25:ALA:HA	1:B:211:LEU:HD12	2.03	0.40
1:H:26:ALA:CB	1:H:36:VAL:HG11	2.50	0.40
1:H:174:GLY:O	1:H:178:PHE:CB	2.70	0.40
1:H:183:VAL:HG12	1:H:220:LEU:HD12	2.03	0.40
1:B:200:ARG:NH1	3:B:1301:FAD:N3A	2.56	0.40
1:C:53:LYS:NZ	1:D:53:LYS:HZ2	2.20	0.40
1:E:113:LYS:O	1:E:117:GLU:HG3	2.22	0.40
1:F:138:ARG:HA	1:F:180:GLY:O	2.22	0.40
1:F:246:GLU:C	1:F:248:ASN:N	2.77	0.40
1:H:196:PRO:O	1:H:197:ALA:C	2.64	0.40
1:H:255:VAL:HG21	1:H:268:GLN:HG2	2.02	0.40
1:C:44:MET:O	1:C:45:ASN:HB3	2.21	0.40
1:E:14:ARG:HH12	1:E:40:ASP:CG	2.29	0.40
1:E:29:LEU:O	1:E:30:LYS:C	2.64	0.40
1:E:46:PHE:HE2	1:E:115:TRP:HA	1.86	0.40
1:F:109:PRO:O	1:F:110:ALA:C	2.63	0.40
1:G:130:ALA:O	1:G:135:GLY:HA2	2.22	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	271/273 (99%)	247 (91%)	21 (8%)	3 (1%)	11	22
1	B	271/273 (99%)	246 (91%)	21 (8%)	4 (2%)	8	15
1	C	271/273 (99%)	246 (91%)	18 (7%)	7 (3%)	4	7
1	D	271/273 (99%)	239 (88%)	29 (11%)	3 (1%)	11	22
1	E	271/273 (99%)	242 (89%)	23 (8%)	6 (2%)	5	10
1	F	271/273 (99%)	241 (89%)	29 (11%)	1 (0%)	30	50
1	G	271/273 (99%)	245 (90%)	21 (8%)	5 (2%)	6	13
1	H	271/273 (99%)	235 (87%)	25 (9%)	11 (4%)	2	3
All	All	2168/2184 (99%)	1941 (90%)	187 (9%)	40 (2%)	6	13

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	133	ASP
1	C	230	LEU
1	H	63	ALA
1	H	133	ASP
1	H	197	ALA
1	H	198	ASP
1	H	214	ILE
1	A	239	LYS
1	D	16	SER
1	D	133	ASP
1	F	133	ASP
1	G	123	GLU
1	G	133	ASP
1	B	41	LEU
1	B	133	ASP
1	E	133	ASP
1	E	232	PHE

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Mol	Chain	Res	Type
1	G	32	LYS
1	A	123	GLU
1	A	232	PHE
1	B	131	MET
1	B	138	ARG
1	C	164	MET
1	C	191	SER
1	C	239	LYS
1	H	123	GLU
1	H	220	LEU
1	C	52	ARG
1	D	53	LYS
1	E	191	SER
1	E	217	GLU
1	E	230	LEU
1	G	245	GLU
1	H	45	ASN
1	H	176	LEU
1	E	219	PRO
1	C	68	PRO
1	G	214	ILE
1	H	68	PRO
1	H	122	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	227/227 (100%)	219 (96%)	8 (4%)	32	56
1	B	227/227 (100%)	222 (98%)	5 (2%)	45	67
1	C	227/227 (100%)	224 (99%)	3 (1%)	61	76
1	D	227/227 (100%)	220 (97%)	7 (3%)	35	59
1	E	227/227 (100%)	217 (96%)	10 (4%)	25	47
1	F	227/227 (100%)	219 (96%)	8 (4%)	32	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	227/227 (100%)	218 (96%)	9 (4%)	28	50
1	H	227/227 (100%)	213 (94%)	14 (6%)	16	31
All	All	1816/1816 (100%)	1752 (96%)	64 (4%)	32	56

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	14	ARG
1	A	29	LEU
1	A	47	ASN
1	A	82	PRO
1	A	108	VAL
1	A	189	THR
1	A	218	THR
1	B	37	VAL
1	B	47	ASN
1	B	112	LEU
1	B	218	THR
1	B	273	LYS
1	C	29	LEU
1	C	112	LEU
1	C	218	THR
1	D	29	LEU
1	D	47	ASN
1	D	55	ILE
1	D	64	ASN
1	D	91	LEU
1	D	112	LEU
1	D	198	ASP
1	E	29	LEU
1	E	39	SER
1	E	92	GLU
1	E	112	LEU
1	E	127	THR
1	E	143	VAL
1	E	158	GLN
1	E	218	THR
1	E	232	PHE
1	E	273	LYS
1	F	29	LEU

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Mol	Chain	Res	Type
1	F	39	SER
1	F	108	VAL
1	F	207	TRP
1	F	209	LYS
1	F	218	THR
1	F	226	SER
1	F	261	LYS
1	G	29	LEU
1	G	37	VAL
1	G	48	PRO
1	G	52	ARG
1	G	112	LEU
1	G	158	GLN
1	G	218	THR
1	G	241	GLU
1	G	273	LYS
1	H	29	LEU
1	H	64	ASN
1	H	81	SER
1	H	82	PRO
1	H	91	LEU
1	H	127	THR
1	H	134	LYS
1	H	148	THR
1	H	198	ASP
1	H	207	TRP
1	H	209	LYS
1	H	232	PHE
1	H	241	GLU
1	H	246	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	47	ASN
1	A	66	GLN
1	A	88	GLN
1	A	158	GLN
1	A	172	GLN
1	A	267	ASN
1	B	18	ASN

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Mol	Chain	Res	Type
1	B	45	ASN
1	B	47	ASN
1	B	79	HIS
1	B	100	GLN
1	B	172	GLN
1	B	267	ASN
1	C	18	ASN
1	C	45	ASN
1	C	47	ASN
1	C	100	GLN
1	C	104	GLN
1	C	172	GLN
1	C	182	GLN
1	C	267	ASN
1	C	268	GLN
1	D	45	ASN
1	D	47	ASN
1	D	64	ASN
1	D	79	HIS
1	D	161	HIS
1	D	172	GLN
1	D	267	ASN
1	E	45	ASN
1	E	47	ASN
1	E	66	GLN
1	E	104	GLN
1	E	158	GLN
1	E	187	GLN
1	F	45	ASN
1	F	47	ASN
1	F	64	ASN
1	F	79	HIS
1	F	88	GLN
1	F	104	GLN
1	F	161	HIS
1	F	233	GLN
1	F	267	ASN
1	F	268	GLN
1	G	45	ASN
1	G	66	GLN
1	G	104	GLN
1	G	172	GLN

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Mol	Chain	Res	Type
1	G	177	HIS
1	G	202	GLN
1	H	47	ASN
1	H	64	ASN
1	H	79	HIS
1	H	172	GLN
1	H	182	GLN
1	H	233	GLN
1	H	267	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	DTC	H	6280	-	28,28,28	5.33	22 (78%)	36,41,41	2.68	10 (27%)
2	DTC	B	3280	-	28,28,28	5.28	21 (75%)	36,41,41	2.71	12 (33%)
3	FAD	D	3301	-	58,58,58	11.71	17 (29%)	85,89,89	2.70	13 (15%)
3	FAD	H	7301	-	58,58,58	11.19	19 (32%)	85,89,89	2.87	12 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FAD	A	301	-	58,58,58	11.39	20 (34%)	85,89,89	2.85	14 (16%)
2	DTC	E	4280	-	28,28,28	5.35	22 (78%)	36,41,41	2.62	9 (25%)
3	FAD	F	5301	-	58,58,58	11.54	19 (32%)	85,89,89	2.73	14 (16%)
2	DTC	E	5280	-	28,28,28	5.30	22 (78%)	36,41,41	2.71	10 (27%)
3	FAD	G	6301	-	58,58,58	11.31	20 (34%)	85,89,89	2.85	16 (18%)
3	FAD	B	1301	-	58,58,58	11.88	17 (29%)	85,89,89	2.73	12 (14%)
2	DTC	G	7280	-	28,28,28	5.35	22 (78%)	36,41,41	2.70	10 (27%)
2	DTC	A	2280	-	28,28,28	5.29	22 (78%)	36,41,41	2.66	9 (25%)
2	DTC	D	1280	-	28,28,28	5.38	22 (78%)	36,41,41	2.68	10 (27%)
3	FAD	C	2301	-	58,58,58	11.97	17 (29%)	85,89,89	2.66	14 (16%)
3	FAD	E	4301	-	58,58,58	12.55	16 (27%)	85,89,89	2.62	13 (15%)
2	DTC	C	280	-	28,28,28	5.39	22 (78%)	36,41,41	2.59	9 (25%)

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
2	DTC	H	6280	-	2/2/6/6	2/4/36/36	0/4/4/4
2	DTC	B	3280	-	2/2/6/6	2/4/36/36	0/4/4/4
3	FAD	D	3301	-	-	9/34/50/50	0/6/6/6
3	FAD	H	7301	-	-	10/34/50/50	0/6/6/6
3	FAD	A	301	-	-	6/34/50/50	0/6/6/6
2	DTC	E	4280	-	2/2/6/6	2/4/36/36	0/4/4/4
3	FAD	F	5301	-	-	7/34/50/50	0/6/6/6
2	DTC	E	5280	-	2/2/6/6	2/4/36/36	0/4/4/4
3	FAD	G	6301	-	-	9/34/50/50	0/6/6/6
3	FAD	B	1301	-	-	6/34/50/50	0/6/6/6
2	DTC	G	7280	-	2/2/6/6	2/4/36/36	0/4/4/4
2	DTC	A	2280	-	2/2/6/6	2/4/36/36	0/4/4/4
2	DTC	D	1280	-	2/2/6/6	2/4/36/36	0/4/4/4
3	FAD	C	2301	-	-	6/34/50/50	0/6/6/6
3	FAD	E	4301	-	-	7/34/50/50	0/6/6/6
2	DTC	C	280	-	2/2/6/6	2/4/36/36	0/4/4/4

All (320) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	4301	FAD	PA-O2A	94.12	5.91	1.55
3	C	2301	FAD	PA-O2A	89.45	5.69	1.55
3	B	1301	FAD	PA-O2A	88.79	5.66	1.55
3	D	3301	FAD	PA-O2A	87.89	5.62	1.55
3	F	5301	FAD	PA-O2A	86.16	5.54	1.55
3	A	301	FAD	PA-O2A	84.96	5.48	1.55
3	G	6301	FAD	PA-O2A	84.28	5.45	1.55
3	H	7301	FAD	PA-O2A	83.20	5.40	1.55
2	C	280	DTC	O17-C8	14.34	1.41	1.22
2	H	6280	DTC	O17-C8	14.30	1.41	1.22
2	G	7280	DTC	O17-C8	14.13	1.40	1.22
2	A	2280	DTC	O17-C8	14.07	1.40	1.22
2	D	1280	DTC	O17-C8	14.05	1.40	1.22
2	B	3280	DTC	O17-C8	13.80	1.40	1.22
2	E	5280	DTC	O17-C8	13.77	1.40	1.22
2	E	4280	DTC	O17-C8	13.74	1.40	1.22
2	E	4280	DTC	O38-C14	13.14	1.39	1.22
2	C	280	DTC	O38-C14	13.08	1.39	1.22
2	H	6280	DTC	O38-C14	12.89	1.39	1.22
2	D	1280	DTC	O38-C14	12.89	1.39	1.22
3	H	7301	FAD	P-O3P	-12.88	1.45	1.59
2	E	5280	DTC	O38-C14	12.83	1.39	1.22
2	G	7280	DTC	O38-C14	12.66	1.39	1.22
2	A	2280	DTC	O38-C14	12.53	1.38	1.22
2	B	3280	DTC	O38-C14	12.34	1.38	1.22
3	B	1301	FAD	P-O3P	-12.15	1.46	1.59
3	G	6301	FAD	P-O3P	-11.73	1.46	1.59
3	C	2301	FAD	P-O3P	-11.64	1.46	1.59
3	F	5301	FAD	P-O3P	-11.63	1.46	1.59
3	A	301	FAD	P-O3P	-11.62	1.46	1.59
3	E	4301	FAD	P-O3P	-11.00	1.47	1.59
3	D	3301	FAD	P-O3P	-9.50	1.49	1.59
2	E	4280	DTC	O32-C12	8.40	1.42	1.21
2	C	280	DTC	C15-C13	-8.40	1.31	1.54
2	A	2280	DTC	O32-C12	8.32	1.42	1.21
2	G	7280	DTC	O32-C12	8.31	1.42	1.21
2	C	280	DTC	O32-C12	8.29	1.42	1.21
2	E	5280	DTC	O32-C12	8.23	1.42	1.21
2	B	3280	DTC	O32-C12	8.23	1.42	1.21
2	D	1280	DTC	O32-C12	8.22	1.42	1.21
2	D	1280	DTC	C15-C13	-8.18	1.31	1.54
2	H	6280	DTC	O32-C12	8.16	1.41	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	5280	DTC	C15-C13	-8.01	1.32	1.54
2	A	2280	DTC	C15-C13	-8.00	1.32	1.54
2	H	6280	DTC	C15-C13	-7.87	1.32	1.54
2	E	4280	DTC	C15-C13	-7.82	1.32	1.54
2	B	3280	DTC	C15-C13	-7.75	1.32	1.54
2	G	7280	DTC	C15-C13	-7.68	1.32	1.54
2	G	7280	DTC	O16-C6	7.50	1.40	1.21
2	D	1280	DTC	O16-C6	7.45	1.40	1.21
2	E	4280	DTC	O16-C6	7.36	1.39	1.21
2	E	5280	DTC	O16-C6	7.34	1.39	1.21
2	C	280	DTC	O16-C6	7.30	1.39	1.21
2	B	3280	DTC	O16-C6	7.25	1.39	1.21
2	A	2280	DTC	O16-C6	7.22	1.39	1.21
2	H	6280	DTC	O16-C6	7.11	1.39	1.21
2	C	280	DTC	C9-C10	5.84	1.51	1.40
2	G	7280	DTC	C9-C10	5.67	1.51	1.40
2	H	6280	DTC	C9-C10	5.67	1.51	1.40
2	E	4280	DTC	C9-C10	5.65	1.51	1.40
2	B	3280	DTC	C9-C10	5.54	1.50	1.40
2	D	1280	DTC	C9-C10	5.47	1.50	1.40
2	A	2280	DTC	C9-C10	5.42	1.50	1.40
2	E	5280	DTC	C9-C10	5.32	1.50	1.40
2	E	4280	DTC	O21-C12	5.04	1.44	1.36
2	G	7280	DTC	O21-C12	4.78	1.43	1.36
2	G	7280	DTC	O5-C6	4.68	1.43	1.36
2	A	2280	DTC	O21-C12	4.67	1.43	1.36
2	D	1280	DTC	O5-C6	4.66	1.43	1.36
2	H	6280	DTC	O21-C12	4.64	1.43	1.36
2	B	3280	DTC	O5-C6	4.62	1.43	1.36
2	D	1280	DTC	O21-C12	4.60	1.43	1.36
2	E	5280	DTC	O21-C12	4.60	1.43	1.36
2	B	3280	DTC	O21-C12	4.57	1.43	1.36
2	C	280	DTC	O5-C6	4.55	1.43	1.36
2	E	4280	DTC	O5-C6	4.54	1.43	1.36
2	A	2280	DTC	O21-C19	4.49	1.45	1.38
2	B	3280	DTC	C5-C20	4.48	1.46	1.39
2	D	1280	DTC	O21-C19	4.47	1.45	1.38
2	G	7280	DTC	O21-C19	4.45	1.45	1.38
2	H	6280	DTC	O5-C6	4.44	1.43	1.36
2	B	3280	DTC	C18-C19	4.42	1.48	1.39
2	C	280	DTC	O21-C12	4.40	1.43	1.36
2	E	5280	DTC	C5-C20	4.39	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2301	FAD	C9A-N10	4.39	1.48	1.41
2	G	7280	DTC	C5-C20	4.38	1.46	1.39
2	H	6280	DTC	C5-C20	4.37	1.46	1.39
2	E	4280	DTC	O21-C19	4.37	1.45	1.38
2	E	5280	DTC	O5-C6	4.37	1.43	1.36
2	E	4280	DTC	C18-C19	4.31	1.48	1.39
2	D	1280	DTC	C5-C20	4.30	1.46	1.39
2	B	3280	DTC	C16-C5	4.25	1.46	1.38
3	E	4301	FAD	O5'-C5'	4.21	1.60	1.44
2	A	2280	DTC	C18-C19	4.21	1.48	1.39
2	E	4280	DTC	C5-C20	4.21	1.46	1.39
2	B	3280	DTC	O21-C19	4.21	1.44	1.38
2	C	280	DTC	O21-C19	4.20	1.44	1.38
3	E	4301	FAD	C9A-N10	4.14	1.48	1.41
2	A	2280	DTC	O5-C6	4.14	1.42	1.36
2	G	7280	DTC	C18-C19	4.12	1.48	1.39
2	D	1280	DTC	C18-C19	4.09	1.48	1.39
3	H	7301	FAD	O5'-C5'	4.09	1.60	1.44
2	E	5280	DTC	C18-C19	4.09	1.48	1.39
2	C	280	DTC	C18-C19	4.09	1.48	1.39
2	E	4280	DTC	C16-C5	4.07	1.45	1.38
3	A	301	FAD	O5'-C5'	4.05	1.59	1.44
2	A	2280	DTC	C16-C5	4.02	1.45	1.38
2	G	7280	DTC	C16-C5	4.01	1.45	1.38
2	A	2280	DTC	C5-C20	4.00	1.46	1.39
3	C	2301	FAD	O5'-C5'	3.99	1.59	1.44
2	C	280	DTC	C5-C20	3.99	1.46	1.39
2	E	5280	DTC	C16-C5	3.98	1.45	1.38
2	E	5280	DTC	O21-C19	3.95	1.44	1.38
3	D	3301	FAD	O5'-C5'	3.89	1.59	1.44
2	H	6280	DTC	C18-C19	3.85	1.47	1.39
2	H	6280	DTC	O21-C19	3.82	1.44	1.38
2	C	280	DTC	C16-C5	3.82	1.45	1.38
3	A	301	FAD	O5B-C5B	-3.80	1.30	1.44
3	B	1301	FAD	O5B-C5B	-3.79	1.30	1.44
2	E	5280	DTC	C16-C17	3.78	1.46	1.38
2	A	2280	DTC	C16-C17	3.75	1.46	1.38
2	D	1280	DTC	C16-C5	3.74	1.45	1.38
3	C	2301	FAD	O5B-C5B	-3.71	1.30	1.44
2	D	1280	DTC	O5-C10	3.71	1.44	1.38
2	D	1280	DTC	C17-C18	3.69	1.45	1.38
2	D	1280	DTC	C16-C17	3.68	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	4280	DTC	C16-C17	3.68	1.46	1.38
2	C	280	DTC	C16-C17	3.67	1.46	1.38
2	H	6280	DTC	C17-C18	3.67	1.45	1.38
2	G	7280	DTC	C16-C17	3.66	1.46	1.38
2	H	6280	DTC	C16-C5	3.66	1.45	1.38
3	G	6301	FAD	O5B-C5B	-3.65	1.30	1.44
3	G	6301	FAD	C9A-N10	3.63	1.47	1.41
3	G	6301	FAD	O5'-C5'	3.63	1.58	1.44
2	H	6280	DTC	C16-C17	3.61	1.46	1.38
2	A	2280	DTC	C17-C18	3.60	1.45	1.38
2	B	3280	DTC	C2-C1	3.60	1.45	1.38
2	B	3280	DTC	C16-C17	3.58	1.46	1.38
2	B	3280	DTC	C17-C18	3.57	1.45	1.38
3	A	301	FAD	C9A-N10	3.56	1.47	1.41
3	F	5301	FAD	O5'-C5'	3.56	1.58	1.44
2	H	6280	DTC	O5-C10	3.55	1.43	1.38
3	F	5301	FAD	O5B-C5B	-3.54	1.31	1.44
2	G	7280	DTC	C3-C4	3.52	1.44	1.38
3	E	4301	FAD	O5B-C5B	-3.52	1.31	1.44
3	C	2301	FAD	P-O2P	-3.52	1.39	1.55
3	H	7301	FAD	O5B-C5B	-3.50	1.31	1.44
2	E	5280	DTC	C17-C18	3.50	1.44	1.38
2	H	6280	DTC	C3-C4	3.47	1.44	1.38
2	E	4280	DTC	C17-C18	3.46	1.44	1.38
2	D	1280	DTC	C3-C4	3.46	1.44	1.38
2	D	1280	DTC	C2-C1	3.45	1.44	1.38
2	G	7280	DTC	C17-C18	3.44	1.44	1.38
2	C	280	DTC	C3-C4	3.44	1.44	1.38
3	B	1301	FAD	P-O2P	-3.42	1.39	1.55
2	G	7280	DTC	O5-C10	3.42	1.43	1.38
2	B	3280	DTC	C3-C4	3.41	1.44	1.38
3	H	7301	FAD	PA-O5B	-3.39	1.46	1.59
3	F	5301	FAD	P-O2P	-3.37	1.39	1.55
2	E	5280	DTC	C3-C4	3.36	1.44	1.38
2	A	2280	DTC	C2-C1	3.36	1.44	1.38
2	H	6280	DTC	C2-C1	3.35	1.44	1.38
2	E	4280	DTC	C20-C19	3.35	1.46	1.40
3	D	3301	FAD	O5B-C5B	-3.33	1.32	1.44
3	G	6301	FAD	P-O2P	-3.32	1.39	1.55
3	H	7301	FAD	C9A-N10	3.32	1.46	1.41
2	E	5280	DTC	O5-C10	3.31	1.43	1.38
2	E	4280	DTC	C2-C1	3.30	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	280	DTC	C17-C18	3.30	1.44	1.38
3	D	3301	FAD	P-O2P	-3.30	1.40	1.55
2	E	5280	DTC	C2-C1	3.29	1.44	1.38
2	E	5280	DTC	C13-C12	-3.28	1.44	1.52
2	D	1280	DTC	C13-C12	-3.26	1.44	1.52
2	A	2280	DTC	C3-C4	3.26	1.44	1.38
2	C	280	DTC	C20-C19	3.24	1.46	1.40
3	A	301	FAD	P-O2P	-3.24	1.40	1.55
2	A	2280	DTC	C20-C19	3.21	1.46	1.40
2	C	280	DTC	O5-C10	3.21	1.43	1.38
2	E	4280	DTC	C3-C4	3.20	1.44	1.38
2	A	2280	DTC	O5-C10	3.19	1.43	1.38
2	B	3280	DTC	O5-C10	3.18	1.43	1.38
2	C	280	DTC	C2-C1	3.17	1.44	1.38
3	B	1301	FAD	PA-O5B	-3.16	1.47	1.59
2	B	3280	DTC	C20-C19	3.14	1.46	1.40
3	B	1301	FAD	C9A-N10	3.14	1.46	1.41
3	E	4301	FAD	P-O2P	-3.14	1.40	1.55
2	D	1280	DTC	C1-C9	3.13	1.44	1.39
2	G	7280	DTC	C20-C19	3.12	1.46	1.40
2	C	280	DTC	C13-C12	-3.12	1.45	1.52
2	G	7280	DTC	C2-C1	3.11	1.44	1.38
3	A	301	FAD	PA-O5B	-3.11	1.47	1.59
3	F	5301	FAD	C9A-N10	3.11	1.46	1.41
3	B	1301	FAD	O5'-C5'	3.09	1.56	1.44
2	E	4280	DTC	O5-C10	3.09	1.43	1.38
3	H	7301	FAD	P-O2P	-3.04	1.41	1.55
2	B	3280	DTC	C13-C12	-3.02	1.45	1.52
2	H	6280	DTC	C13-C12	-3.01	1.45	1.52
3	H	7301	FAD	PA-O3P	-3.00	1.56	1.59
2	E	5280	DTC	C20-C19	2.99	1.46	1.40
2	H	6280	DTC	C1-C9	2.98	1.44	1.39
3	G	6301	FAD	PA-O5B	-2.98	1.47	1.59
3	H	7301	FAD	C8-C7	2.98	1.48	1.40
2	E	4280	DTC	C1-C9	2.97	1.44	1.39
3	B	1301	FAD	C4X-N5	2.93	1.37	1.30
3	A	301	FAD	C9A-C5X	2.93	1.45	1.41
2	H	6280	DTC	C20-C19	2.91	1.46	1.40
2	G	7280	DTC	C13-C12	-2.90	1.45	1.52
2	E	5280	DTC	C3-C2	2.90	1.44	1.38
2	G	7280	DTC	C1-C9	2.89	1.44	1.39
2	B	3280	DTC	C1-C9	2.88	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1280	DTC	C3-C2	2.87	1.44	1.38
2	H	6280	DTC	C3-C2	2.87	1.44	1.38
2	C	280	DTC	C3-C2	2.86	1.44	1.38
2	E	5280	DTC	C1-C9	2.84	1.44	1.39
3	F	5301	FAD	PA-O5B	-2.84	1.48	1.59
2	A	2280	DTC	C1-C9	2.82	1.44	1.39
2	D	1280	DTC	C20-C19	2.80	1.45	1.40
3	C	2301	FAD	PA-O5B	-2.80	1.48	1.59
2	G	7280	DTC	C3-C2	2.79	1.44	1.38
3	B	1301	FAD	C5'-C4'	-2.79	1.48	1.51
3	D	3301	FAD	PA-O5B	-2.75	1.48	1.59
2	B	3280	DTC	C3-C2	2.74	1.44	1.38
2	A	2280	DTC	C13-C12	-2.74	1.46	1.52
2	E	4280	DTC	C13-C12	-2.72	1.46	1.52
3	H	7301	FAD	C5A-C6A	2.72	1.48	1.41
2	E	5280	DTC	C9-C8	-2.70	1.43	1.48
3	F	5301	FAD	C4X-N5	2.70	1.36	1.30
2	E	4280	DTC	C3-C2	2.69	1.44	1.38
2	A	2280	DTC	C3-C2	2.69	1.44	1.38
3	H	7301	FAD	O2-C2	-2.67	1.19	1.24
3	F	5301	FAD	O4B-C1B	2.66	1.48	1.42
2	C	280	DTC	C1-C9	2.66	1.44	1.39
3	F	5301	FAD	P-O5'	-2.64	1.49	1.59
3	D	3301	FAD	C4A-N3A	2.63	1.39	1.34
3	A	301	FAD	C5A-C6A	2.63	1.48	1.41
3	A	301	FAD	C9-C9A	2.63	1.43	1.39
3	E	4301	FAD	PA-O5B	-2.61	1.49	1.59
3	B	1301	FAD	P-O5'	-2.61	1.49	1.59
3	B	1301	FAD	C2-N3	2.60	1.44	1.39
3	F	5301	FAD	C9A-C5X	2.60	1.45	1.41
3	H	7301	FAD	C9A-C5X	2.60	1.45	1.41
3	G	6301	FAD	PA-O3P	-2.60	1.56	1.59
3	C	2301	FAD	O2-C2	-2.59	1.19	1.24
3	C	2301	FAD	C4X-N5	2.59	1.36	1.30
3	E	4301	FAD	C4X-N5	2.59	1.36	1.30
3	A	301	FAD	C1'-C2'	2.59	1.56	1.52
3	F	5301	FAD	C2-N3	2.59	1.44	1.39
3	E	4301	FAD	C2-N3	2.54	1.44	1.39
3	A	301	FAD	C9-C8	2.53	1.43	1.39
3	G	6301	FAD	O4B-C1B	2.52	1.47	1.42
3	A	301	FAD	O4B-C1B	2.51	1.47	1.42
3	F	5301	FAD	C8-C7	2.51	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2301	FAD	PA-O3P	-2.48	1.56	1.59
3	E	4301	FAD	O2-C2	-2.48	1.19	1.24
2	E	4280	DTC	C9-C8	-2.45	1.44	1.48
2	C	280	DTC	C9-C8	-2.44	1.44	1.48
3	G	6301	FAD	C4A-N3A	2.43	1.39	1.34
3	G	6301	FAD	C9-C8	2.43	1.42	1.39
3	D	3301	FAD	C9A-C5X	2.43	1.45	1.41
3	B	1301	FAD	C6-C5X	2.42	1.43	1.40
3	A	301	FAD	P-O5'	-2.42	1.49	1.59
3	H	7301	FAD	C4X-N5	2.42	1.36	1.30
3	G	6301	FAD	P-O5'	-2.41	1.49	1.59
3	D	3301	FAD	C2-N3	2.41	1.44	1.39
3	A	301	FAD	C10-N1	2.40	1.38	1.33
3	A	301	FAD	C4A-N3A	2.39	1.38	1.34
3	G	6301	FAD	C1'-C2'	2.39	1.56	1.52
3	C	2301	FAD	C2-N3	2.38	1.44	1.39
3	A	301	FAD	C8-C7	2.38	1.46	1.40
3	C	2301	FAD	C6-C5X	2.37	1.43	1.40
3	G	6301	FAD	C8-C7	2.36	1.46	1.40
3	B	1301	FAD	C4A-N3A	2.35	1.38	1.34
3	D	3301	FAD	O4B-C1B	2.34	1.47	1.42
3	D	3301	FAD	C4X-N5	2.33	1.35	1.30
3	G	6301	FAD	C6-C5X	2.33	1.43	1.40
2	G	7280	DTC	C9-C8	-2.33	1.44	1.48
3	H	7301	FAD	P-O1P	2.31	1.58	1.50
3	F	5301	FAD	C4A-N3A	2.31	1.38	1.34
3	H	7301	FAD	O4B-C1B	2.31	1.47	1.42
3	C	2301	FAD	O4B-C1B	2.30	1.47	1.42
3	D	3301	FAD	C8-C7	2.30	1.46	1.40
3	G	6301	FAD	C4X-N5	2.29	1.35	1.30
2	A	2280	DTC	C9-C8	-2.28	1.44	1.48
3	G	6301	FAD	O2-C2	-2.27	1.19	1.24
3	G	6301	FAD	C9A-C5X	2.27	1.44	1.41
3	H	7301	FAD	C1'-C2'	2.27	1.55	1.52
3	D	3301	FAD	P-O5'	-2.25	1.50	1.59
3	D	3301	FAD	C10-N1	2.24	1.37	1.33
3	C	2301	FAD	C1'-C2'	2.21	1.55	1.52
3	D	3301	FAD	C2A-N1A	2.21	1.37	1.33
3	F	5301	FAD	C5A-C6A	2.20	1.47	1.41
3	F	5301	FAD	C1'-C2'	2.20	1.55	1.52
3	E	4301	FAD	C10-N1	2.17	1.37	1.33
3	B	1301	FAD	O4B-C1B	2.17	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	4301	FAD	C8-C7	2.16	1.46	1.40
3	B	1301	FAD	C9A-C5X	2.16	1.44	1.41
3	F	5301	FAD	C5A-C4A	2.15	1.42	1.39
3	B	1301	FAD	C5A-C6A	2.14	1.47	1.41
3	C	2301	FAD	C10-N1	2.13	1.37	1.33
3	D	3301	FAD	C5A-C6A	2.13	1.46	1.41
3	F	5301	FAD	C6-C5X	2.11	1.43	1.40
3	H	7301	FAD	C10-N1	2.11	1.37	1.33
3	E	4301	FAD	PA-O3P	-2.11	1.57	1.59
3	C	2301	FAD	C8-C7	2.11	1.46	1.40
2	H	6280	DTC	C9-C8	-2.10	1.44	1.48
3	F	5301	FAD	C2A-N1A	2.09	1.37	1.33
3	E	4301	FAD	C5A-C6A	2.08	1.46	1.41
3	E	4301	FAD	O4B-C1B	2.08	1.46	1.42
3	D	3301	FAD	P-O1P	2.06	1.58	1.50
3	A	301	FAD	C2A-N1A	2.06	1.37	1.33
3	A	301	FAD	C4X-N5	2.06	1.35	1.30
3	G	6301	FAD	C2-N3	2.05	1.43	1.39
3	B	1301	FAD	O2-C2	-2.05	1.20	1.24
3	G	6301	FAD	C10-N1	2.04	1.37	1.33
3	C	2301	FAD	C5A-C6A	2.03	1.46	1.41
2	D	1280	DTC	C9-C8	-2.02	1.44	1.48
3	E	4301	FAD	C1'-C2'	2.02	1.55	1.52
3	H	7301	FAD	C4A-N3A	2.02	1.38	1.34
3	A	301	FAD	C2-N3	2.01	1.43	1.39
3	H	7301	FAD	C6-C5X	2.00	1.43	1.40

All (187) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	7301	FAD	O2A-PA-O3P	16.34	151.44	107.27
3	G	6301	FAD	O2A-PA-O3P	16.14	150.90	107.27
3	A	301	FAD	O2A-PA-O3P	15.79	149.96	107.27
3	E	4301	FAD	O2A-PA-O5B	-15.25	38.45	107.57
3	F	5301	FAD	O2A-PA-O3P	14.72	147.05	107.27
3	C	2301	FAD	O2A-PA-O5B	-14.59	41.43	107.57
3	B	1301	FAD	O2A-PA-O5B	-14.33	42.59	107.57
3	D	3301	FAD	O2A-PA-O3P	14.23	145.73	107.27
3	D	3301	FAD	O2A-PA-O5B	-14.20	43.20	107.57
3	B	1301	FAD	O2A-PA-O3P	14.17	145.58	107.27
3	F	5301	FAD	O2A-PA-O5B	-14.12	43.58	107.57
3	A	301	FAD	O2A-PA-O5B	-13.87	44.70	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	6301	FAD	O2A-PA-O5B	-13.74	45.27	107.57
3	C	2301	FAD	O2A-PA-O3P	13.72	144.37	107.27
3	H	7301	FAD	O2A-PA-O5B	-13.19	47.80	107.57
3	E	4301	FAD	O2A-PA-O3P	12.39	140.75	107.27
2	G	7280	DTC	C15-C13-C14	12.36	128.53	111.08
2	B	3280	DTC	C15-C13-C14	12.16	128.24	111.08
2	E	5280	DTC	C15-C13-C14	12.10	128.15	111.08
2	A	2280	DTC	C15-C13-C14	12.06	128.09	111.08
2	D	1280	DTC	C15-C13-C14	12.01	128.02	111.08
2	H	6280	DTC	C15-C13-C14	11.98	127.98	111.08
2	E	4280	DTC	C15-C13-C14	11.84	127.79	111.08
2	C	280	DTC	C15-C13-C14	11.67	127.55	111.08
3	H	7301	FAD	O2A-PA-O1A	-8.94	70.85	112.44
3	A	301	FAD	O2A-PA-O1A	-7.92	75.58	112.44
3	H	7301	FAD	O5B-PA-O1A	-7.39	79.66	108.94
3	A	301	FAD	O5B-PA-O1A	-7.23	80.30	108.94
3	G	6301	FAD	O2A-PA-O1A	-7.17	79.07	112.44
3	G	6301	FAD	O5B-PA-O1A	-7.14	80.63	108.94
3	F	5301	FAD	O2A-PA-O1A	-7.01	79.86	112.44
3	B	1301	FAD	O2A-PA-O1A	-6.91	80.30	112.44
3	B	1301	FAD	O5B-PA-O1A	-6.87	81.71	108.94
3	F	5301	FAD	O5B-PA-O1A	-6.64	82.61	108.94
3	D	3301	FAD	O5B-PA-O1A	-6.57	82.90	108.94
3	E	4301	FAD	O5B-PA-O1A	-6.45	83.36	108.94
3	C	2301	FAD	O5B-PA-O1A	-6.33	83.83	108.94
3	D	3301	FAD	O2A-PA-O1A	-6.29	83.18	112.44
2	E	4280	DTC	C15-C7-C8	5.75	119.19	111.08
2	H	6280	DTC	C15-C7-C8	5.72	119.15	111.08
3	C	2301	FAD	O2A-PA-O1A	-5.68	86.02	112.44
3	E	4301	FAD	O2A-PA-O1A	-5.64	86.21	112.44
2	A	2280	DTC	C15-C7-C8	5.62	119.01	111.08
2	D	1280	DTC	C15-C7-C8	5.49	118.83	111.08
2	E	5280	DTC	C15-C7-C8	5.49	118.83	111.08
2	B	3280	DTC	C15-C7-C8	5.45	118.77	111.08
2	C	280	DTC	C15-C7-C8	5.44	118.75	111.08
2	G	7280	DTC	C15-C7-C8	5.35	118.63	111.08
3	H	7301	FAD	PA-O5B-C5B	4.85	149.15	121.35
3	D	3301	FAD	PA-O5B-C5B	4.59	147.65	121.35
3	A	301	FAD	PA-O5B-C5B	4.54	147.36	121.35
3	E	4301	FAD	PA-O5B-C5B	4.53	147.31	121.35
3	B	1301	FAD	PA-O5B-C5B	4.53	147.31	121.35
3	G	6301	FAD	PA-O5B-C5B	4.52	147.26	121.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	5301	FAD	PA-O5B-C5B	4.42	146.68	121.35
3	C	2301	FAD	PA-O5B-C5B	4.40	146.55	121.35
2	B	3280	DTC	C15-C7-C6	3.94	123.72	112.31
2	G	7280	DTC	C15-C7-C6	3.86	123.49	112.31
2	C	280	DTC	C15-C7-C6	3.75	123.16	112.31
2	E	5280	DTC	C15-C7-C6	3.73	123.11	112.31
2	H	6280	DTC	C15-C7-C6	3.72	123.08	112.31
2	A	2280	DTC	C15-C7-C6	3.71	123.06	112.31
2	E	4280	DTC	C15-C7-C6	3.70	123.02	112.31
2	D	1280	DTC	C15-C7-C6	3.70	123.01	112.31
2	E	5280	DTC	C9-C8-C7	3.64	121.82	116.69
2	B	3280	DTC	C9-C8-C7	3.60	121.76	116.69
3	A	301	FAD	O4B-C1B-N9A	-3.56	101.25	108.09
2	G	7280	DTC	C9-C8-C7	3.55	121.69	116.69
2	D	1280	DTC	C9-C8-C7	3.50	121.63	116.69
2	H	6280	DTC	C9-C8-C7	3.44	121.54	116.69
2	A	2280	DTC	C9-C8-C7	3.42	121.52	116.69
2	E	4280	DTC	C9-C8-C7	3.40	121.49	116.69
2	C	280	DTC	C9-C8-C7	3.32	121.36	116.69
3	H	7301	FAD	O4B-C1B-N9A	-3.21	101.92	108.09
3	B	1301	FAD	O4B-C1B-N9A	-3.03	102.27	108.09
2	E	5280	DTC	C19-C20-C14	-2.98	118.58	120.48
2	D	1280	DTC	C19-C20-C14	-2.93	118.61	120.48
2	C	280	DTC	C19-C20-C14	-2.87	118.65	120.48
3	D	3301	FAD	O4B-C1B-N9A	-2.87	102.58	108.09
3	C	2301	FAD	C4'-C3'-C2'	-2.86	108.81	113.57
2	B	3280	DTC	C19-C20-C14	-2.85	118.66	120.48
2	H	6280	DTC	C19-C20-C14	-2.82	118.69	120.48
3	G	6301	FAD	O4B-C1B-N9A	-2.80	102.70	108.09
3	F	5301	FAD	O4B-C1B-C2B	-2.80	100.62	106.62
2	G	7280	DTC	C19-C20-C14	-2.68	118.77	120.48
3	C	2301	FAD	O4B-C1B-N9A	-2.67	102.96	108.09
3	G	6301	FAD	C5X-C9A-N10	-2.67	115.56	117.97
3	C	2301	FAD	C2A-N1A-C6A	2.63	123.05	118.73
2	D	1280	DTC	C20-C14-C13	2.62	120.38	116.69
2	G	7280	DTC	C20-C14-C13	2.60	120.36	116.69
3	B	1301	FAD	C2A-N1A-C6A	2.60	123.00	118.73
3	E	4301	FAD	C4-N3-C2	-2.60	121.03	125.64
2	A	2280	DTC	C20-C14-C13	2.59	120.34	116.69
3	A	301	FAD	C5X-C9A-N10	-2.59	115.62	117.97
3	D	3301	FAD	C4'-C3'-C2'	-2.59	109.27	113.57
3	E	4301	FAD	C2A-N1A-C6A	2.57	122.95	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3280	DTC	C20-C14-C13	2.57	120.31	116.69
3	H	7301	FAD	C2A-N1A-C6A	2.56	122.93	118.73
2	E	5280	DTC	C20-C14-C13	2.56	120.29	116.69
3	E	4301	FAD	C4'-C3'-C2'	-2.54	109.34	113.57
2	H	6280	DTC	C20-C14-C13	2.54	120.27	116.69
3	D	3301	FAD	C5X-C9A-N10	-2.52	115.69	117.97
2	H	6280	DTC	O5-C10-C4	2.51	119.60	116.25
3	F	5301	FAD	O4B-C1B-N9A	-2.51	103.27	108.09
3	C	2301	FAD	C4-N3-C2	-2.51	121.19	125.64
2	E	4280	DTC	C19-C20-C14	-2.51	118.88	120.48
2	A	2280	DTC	C19-C20-C14	-2.49	118.89	120.48
2	E	5280	DTC	O5-C10-C4	2.48	119.55	116.25
3	A	301	FAD	C4-N3-C2	-2.46	121.27	125.64
3	F	5301	FAD	C4-N3-C2	-2.46	121.27	125.64
2	D	1280	DTC	O5-C10-C4	2.45	119.52	116.25
3	E	4301	FAD	O4B-C1B-N9A	-2.45	103.38	108.09
3	G	6301	FAD	C4-N3-C2	-2.45	121.29	125.64
2	B	3280	DTC	C5-C20-C14	2.43	123.29	119.89
3	G	6301	FAD	O4B-C1B-C2B	-2.43	101.42	106.62
2	E	5280	DTC	C10-C9-C8	-2.41	118.94	120.48
3	B	1301	FAD	C4'-C3'-C2'	-2.41	109.56	113.57
2	E	4280	DTC	C20-C14-C13	2.41	120.08	116.69
3	D	3301	FAD	C4-N3-C2	-2.40	121.38	125.64
2	A	2280	DTC	C10-C9-C8	-2.40	118.95	120.48
3	B	1301	FAD	C4-N3-C2	-2.39	121.39	125.64
2	C	280	DTC	C20-C14-C13	2.39	120.06	116.69
3	D	3301	FAD	C2A-N1A-C6A	2.38	122.64	118.73
2	D	1280	DTC	C10-C9-C8	-2.38	118.96	120.48
3	G	6301	FAD	C2A-N1A-C6A	2.36	122.61	118.73
2	E	5280	DTC	C5-C20-C14	2.35	123.17	119.89
3	D	3301	FAD	O4B-C1B-C2B	-2.35	101.59	106.62
3	C	2301	FAD	O4B-C1B-C2B	-2.33	101.62	106.62
2	B	3280	DTC	O5-C10-C4	2.33	119.34	116.25
3	H	7301	FAD	O4B-C1B-C2B	-2.31	101.67	106.62
2	A	2280	DTC	O5-C10-C4	2.31	119.33	116.25
2	C	280	DTC	O5-C10-C4	2.30	119.31	116.25
3	F	5301	FAD	C4'-C3'-C2'	-2.30	109.74	113.57
3	G	6301	FAD	C4'-C3'-C2'	-2.29	109.75	113.57
2	G	7280	DTC	O5-C10-C4	2.28	119.29	116.25
3	B	1301	FAD	C5X-C9A-N10	-2.28	115.91	117.97
3	E	4301	FAD	O4B-C1B-C2B	-2.26	101.78	106.62
2	E	4280	DTC	O5-C10-C4	2.26	119.25	116.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	FAD	C2A-N1A-C6A	2.25	122.43	118.73
3	H	7301	FAD	C4-N3-C2	-2.24	121.66	125.64
3	F	5301	FAD	C2A-N1A-C6A	2.23	122.39	118.73
3	F	5301	FAD	C5X-C9A-N10	-2.22	115.97	117.97
2	D	1280	DTC	C1-C9-C8	2.21	122.98	119.89
2	B	3280	DTC	C1-C9-C8	2.21	122.98	119.89
3	E	4301	FAD	C5X-C9A-N10	-2.21	115.97	117.97
3	D	3301	FAD	C4X-C10-N10	2.20	119.64	116.48
2	G	7280	DTC	C10-C9-C8	-2.20	119.08	120.48
2	H	6280	DTC	C10-C9-C8	-2.20	119.08	120.48
2	C	280	DTC	C5-C20-C14	2.19	122.95	119.89
3	B	1301	FAD	C5'-C4'-C3'	-2.19	108.09	112.22
3	G	6301	FAD	C5A-C4A-N9A	-2.18	103.43	105.81
2	H	6280	DTC	C5-C20-C14	2.18	122.94	119.89
2	A	2280	DTC	C1-C9-C8	2.17	122.93	119.89
3	H	7301	FAD	C5X-C9A-N10	-2.16	116.01	117.97
3	F	5301	FAD	C4X-C10-N10	2.16	119.57	116.48
2	E	5280	DTC	C19-O21-C12	2.15	123.42	121.44
2	E	4280	DTC	C5-C20-C14	2.15	122.89	119.89
3	G	6301	FAD	C9-C9A-N10	2.15	124.74	121.85
2	B	3280	DTC	C10-C9-C8	-2.14	119.11	120.48
3	A	301	FAD	C4'-C3'-C2'	-2.13	110.02	113.57
3	C	2301	FAD	C2B-C1B-N9A	2.12	118.57	113.30
2	D	1280	DTC	C5-C20-C14	2.12	122.85	119.89
3	E	4301	FAD	C4B-O4B-C1B	-2.12	104.79	109.47
3	B	1301	FAD	C4X-C10-N10	2.12	119.51	116.48
2	G	7280	DTC	C5-C20-C14	2.11	122.84	119.89
3	D	3301	FAD	O3B-C3B-C2B	2.10	118.54	111.82
3	G	6301	FAD	O3B-C3B-C2B	2.09	118.51	111.82
2	H	6280	DTC	C1-C9-C8	2.07	122.79	119.89
3	H	7301	FAD	C4'-C3'-C2'	-2.07	110.12	113.57
2	B	3280	DTC	C19-O21-C12	2.06	123.34	121.44
3	F	5301	FAD	C5'-C4'-C3'	-2.06	108.33	112.22
3	H	7301	FAD	C4X-C10-N10	2.06	119.43	116.48
3	F	5301	FAD	O3B-C3B-C2B	2.06	118.41	111.82
3	A	301	FAD	C4X-C10-N10	2.05	119.41	116.48
3	G	6301	FAD	C4X-C10-N10	2.05	119.41	116.48
3	E	4301	FAD	O3B-C3B-C2B	2.04	118.37	111.82
3	A	301	FAD	O3B-C3B-C2B	2.04	118.37	111.82
3	C	2301	FAD	O5'-P-O1P	-2.03	100.88	108.94
3	G	6301	FAD	O3B-C3B-C4B	2.03	116.91	111.08
3	C	2301	FAD	O3B-C3B-C2B	2.02	118.31	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	4280	DTC	C10-C9-C8	-2.02	119.19	120.48
3	A	301	FAD	O4B-C1B-C2B	-2.02	102.29	106.62
3	C	2301	FAD	C4B-O4B-C1B	-2.02	105.01	109.47
2	B	3280	DTC	O21-C19-C18	2.02	118.93	116.25
3	A	301	FAD	C2B-C1B-N9A	2.01	118.31	113.30
2	C	280	DTC	C10-C9-C8	-2.01	119.20	120.48
2	G	7280	DTC	O21-C19-C18	2.00	118.92	116.25

All (16) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	2280	DTC	C13
2	A	2280	DTC	C7
2	B	3280	DTC	C13
2	B	3280	DTC	C7
2	C	280	DTC	C13
2	C	280	DTC	C7
2	D	1280	DTC	C13
2	D	1280	DTC	C7
2	E	4280	DTC	C13
2	E	4280	DTC	C7
2	E	5280	DTC	C13
2	E	5280	DTC	C7
2	G	7280	DTC	C13
2	G	7280	DTC	C7
2	H	6280	DTC	C13
2	H	6280	DTC	C7

All (76) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2280	DTC	C13-C15-C7-C8
2	B	3280	DTC	C13-C15-C7-C8
2	C	280	DTC	C13-C15-C7-C8
2	D	1280	DTC	C13-C15-C7-C8
2	E	4280	DTC	C13-C15-C7-C8
2	E	5280	DTC	C13-C15-C7-C8
2	E	5280	DTC	C12-C13-C15-C7
2	G	7280	DTC	C13-C15-C7-C8
2	H	6280	DTC	C13-C15-C7-C8
3	C	2301	FAD	C5B-O5B-PA-O1A
3	C	2301	FAD	C5'-O5'-P-O1P

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Mol	Chain	Res	Type	Atoms
3	D	3301	FAD	C5B-O5B-PA-O1A
3	E	4301	FAD	C5B-O5B-PA-O1A
3	H	7301	FAD	C5B-O5B-PA-O3P
3	H	7301	FAD	C2B-C1B-N9A-C8A
3	H	7301	FAD	C2B-C1B-N9A-C4A
3	H	7301	FAD	O4B-C4B-C5B-O5B
3	B	1301	FAD	P-O3P-PA-O1A
3	D	3301	FAD	P-O3P-PA-O1A
3	H	7301	FAD	P-O3P-PA-O1A
3	E	4301	FAD	O4B-C4B-C5B-O5B
3	H	7301	FAD	C3B-C4B-C5B-O5B
3	A	301	FAD	C2B-C1B-N9A-C8A
3	C	2301	FAD	C2B-C1B-N9A-C8A
3	D	3301	FAD	C2B-C1B-N9A-C8A
3	E	4301	FAD	C2B-C1B-N9A-C8A
3	F	5301	FAD	C2B-C1B-N9A-C8A
3	G	6301	FAD	C2B-C1B-N9A-C8A
3	F	5301	FAD	P-O3P-PA-O1A
3	G	6301	FAD	P-O3P-PA-O1A
2	A	2280	DTC	C12-C13-C15-C7
2	C	280	DTC	C12-C13-C15-C7
2	E	4280	DTC	C12-C13-C15-C7
2	G	7280	DTC	C12-C13-C15-C7
2	H	6280	DTC	C12-C13-C15-C7
3	D	3301	FAD	O4B-C4B-C5B-O5B
3	A	301	FAD	C5B-O5B-PA-O1A
3	A	301	FAD	C5B-O5B-PA-O3P
3	B	1301	FAD	C5B-O5B-PA-O1A
3	B	1301	FAD	C5B-O5B-PA-O3P
3	B	1301	FAD	C5'-O5'-P-O1P
3	C	2301	FAD	C5B-O5B-PA-O3P
3	D	3301	FAD	C5B-O5B-PA-O3P
3	D	3301	FAD	C5'-O5'-P-O1P
3	E	4301	FAD	C5B-O5B-PA-O3P
3	F	5301	FAD	C5B-O5B-PA-O1A
3	F	5301	FAD	C5B-O5B-PA-O3P
3	G	6301	FAD	C5B-O5B-PA-O1A
3	G	6301	FAD	C5B-O5B-PA-O3P
3	H	7301	FAD	C5B-O5B-PA-O1A
3	A	301	FAD	P-O3P-PA-O1A
3	C	2301	FAD	P-O3P-PA-O1A
3	E	4301	FAD	P-O3P-PA-O1A

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Mol	Chain	Res	Type	Atoms
3	A	301	FAD	C2B-C1B-N9A-C4A
3	E	4301	FAD	C3B-C4B-C5B-O5B
3	G	6301	FAD	O4B-C4B-C5B-O5B
3	D	3301	FAD	C3B-C4B-C5B-O5B
3	F	5301	FAD	C2B-C1B-N9A-C4A
3	B	1301	FAD	C2B-C1B-N9A-C8A
3	H	7301	FAD	C4'-C5'-O5'-P
3	D	3301	FAD	C2B-C1B-N9A-C4A
3	G	6301	FAD	C2B-C1B-N9A-C4A
3	E	4301	FAD	P-O3P-PA-O2A
3	G	6301	FAD	P-O3P-PA-O2A
3	H	7301	FAD	P-O3P-PA-O2A
3	A	301	FAD	O4B-C1B-N9A-C8A
3	H	7301	FAD	O4B-C1B-N9A-C8A
3	G	6301	FAD	C4'-C5'-O5'-P
3	F	5301	FAD	O4B-C4B-C5B-O5B
3	G	6301	FAD	O4B-C1B-N9A-C8A
3	D	3301	FAD	C4'-C5'-O5'-P
2	B	3280	DTC	C12-C13-C15-C7
2	D	1280	DTC	C12-C13-C15-C7
3	B	1301	FAD	P-O3P-PA-O2A
3	C	2301	FAD	P-O3P-PA-O2A
3	F	5301	FAD	P-O3P-PA-O2A

There are no ring outliers.

16 monomers are involved in 47 short contacts:

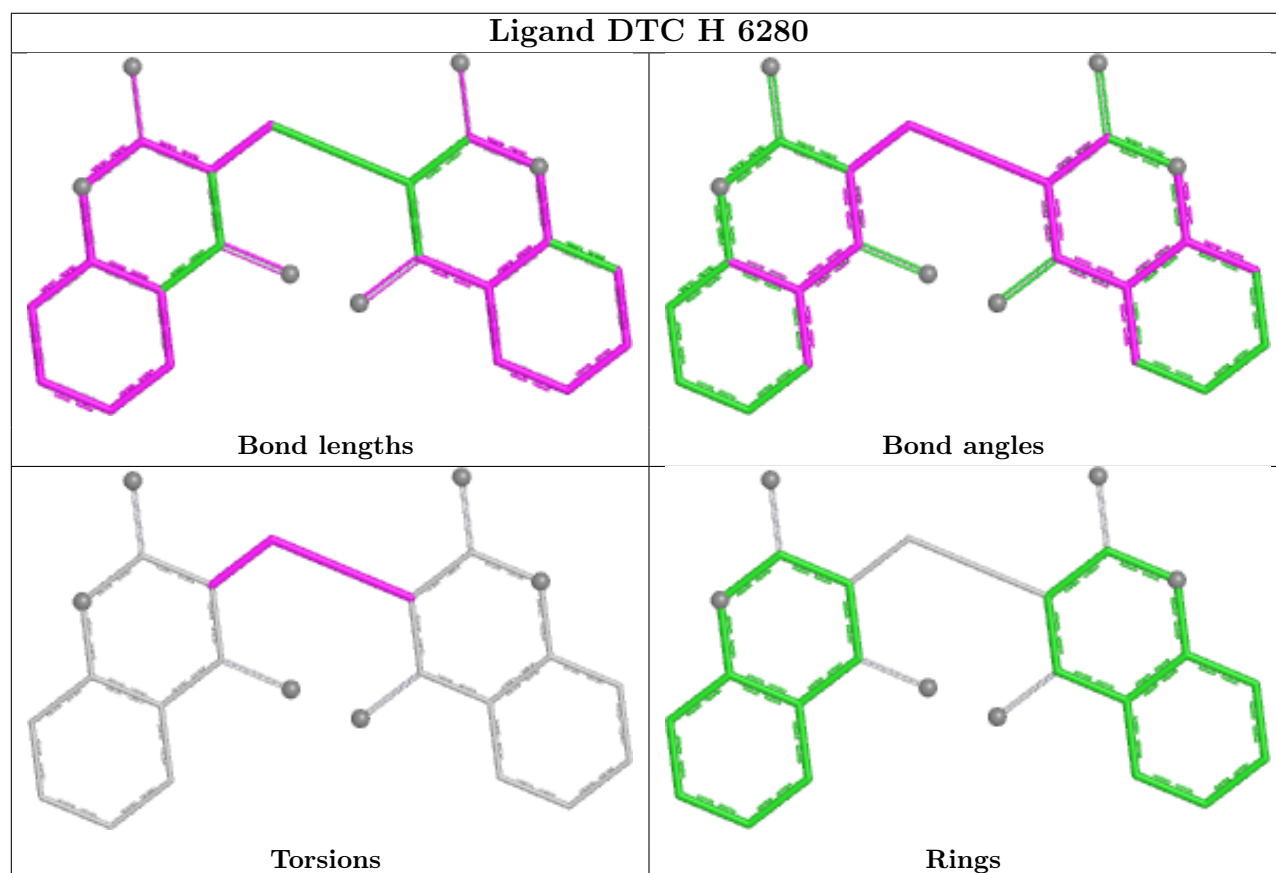
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	6280	DTC	3	0
2	B	3280	DTC	1	0
3	D	3301	FAD	4	0
3	H	7301	FAD	5	0
3	A	301	FAD	4	0
2	E	4280	DTC	1	0
3	F	5301	FAD	2	0
2	E	5280	DTC	2	0
3	G	6301	FAD	3	0
3	B	1301	FAD	5	0
2	G	7280	DTC	5	0
2	A	2280	DTC	1	0
2	D	1280	DTC	1	0
3	C	2301	FAD	6	0

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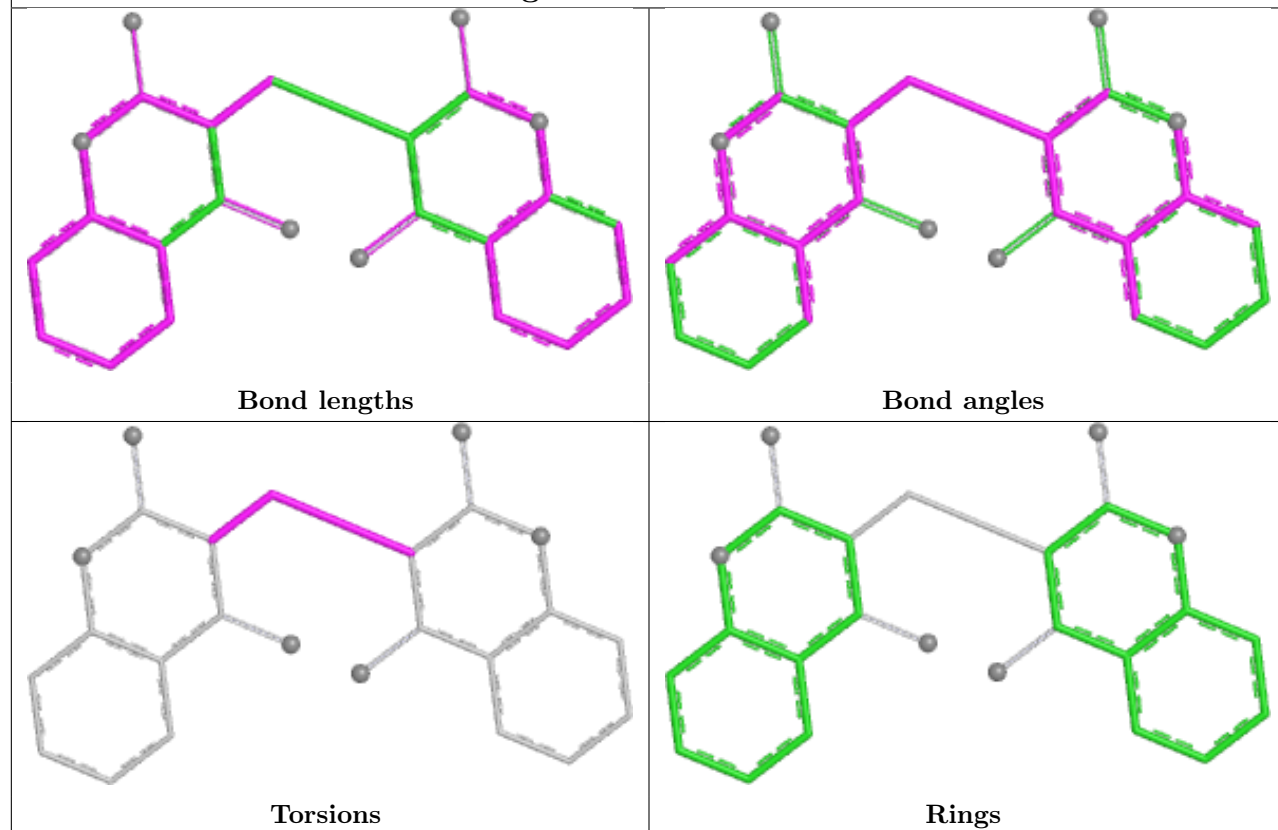
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	4301	FAD	2	0
2	C	280	DTC	2	0

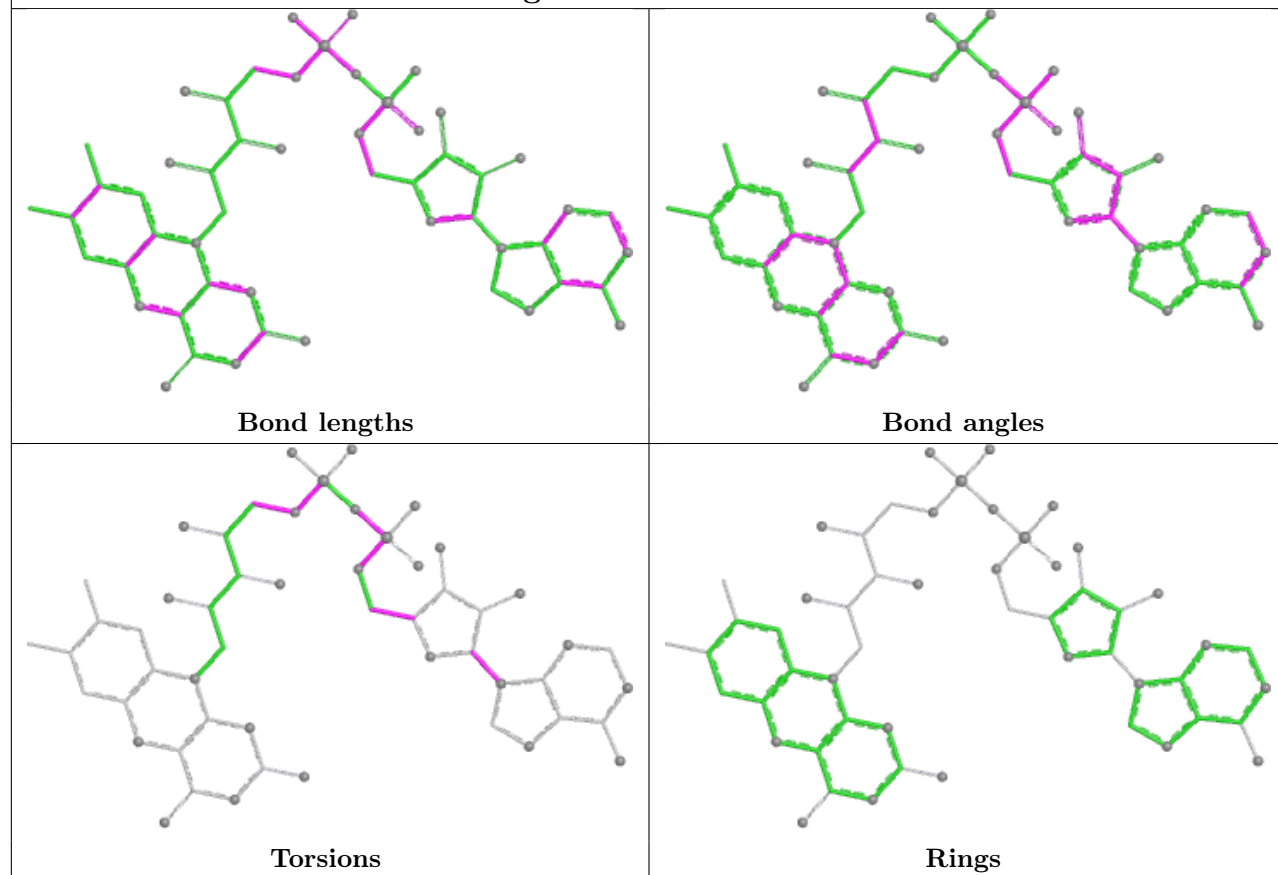
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

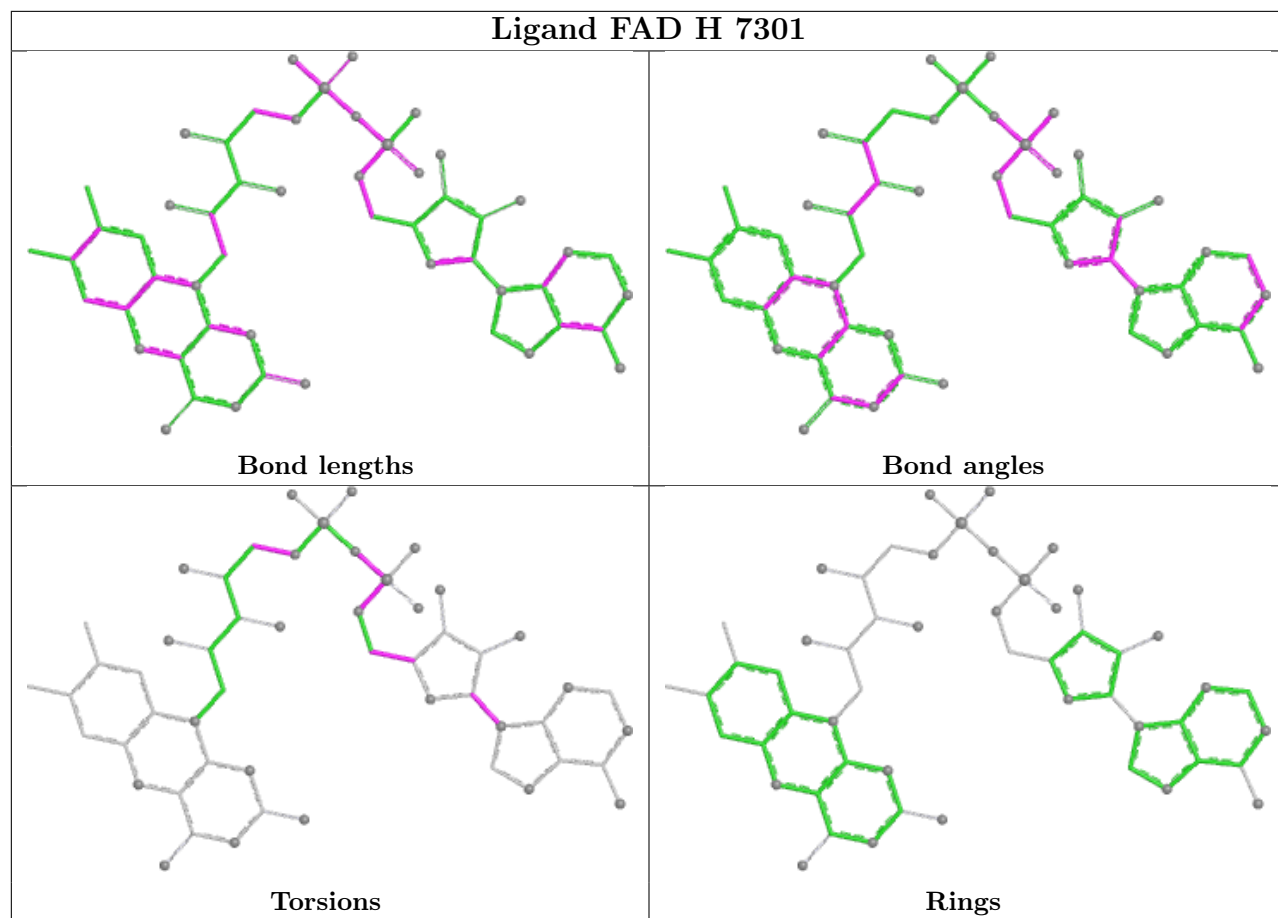


Ligand DTC B 3280

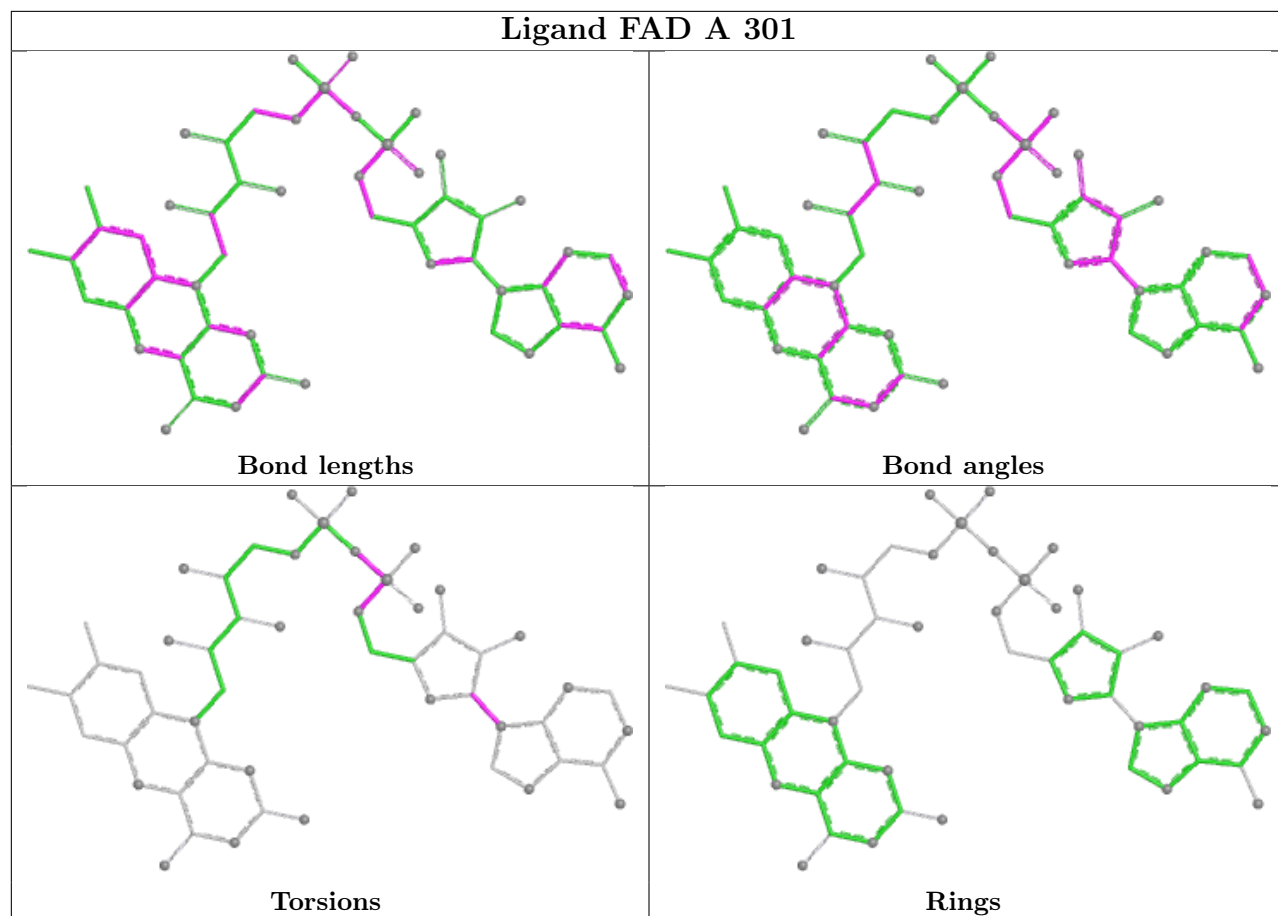


Ligand FAD D 3301

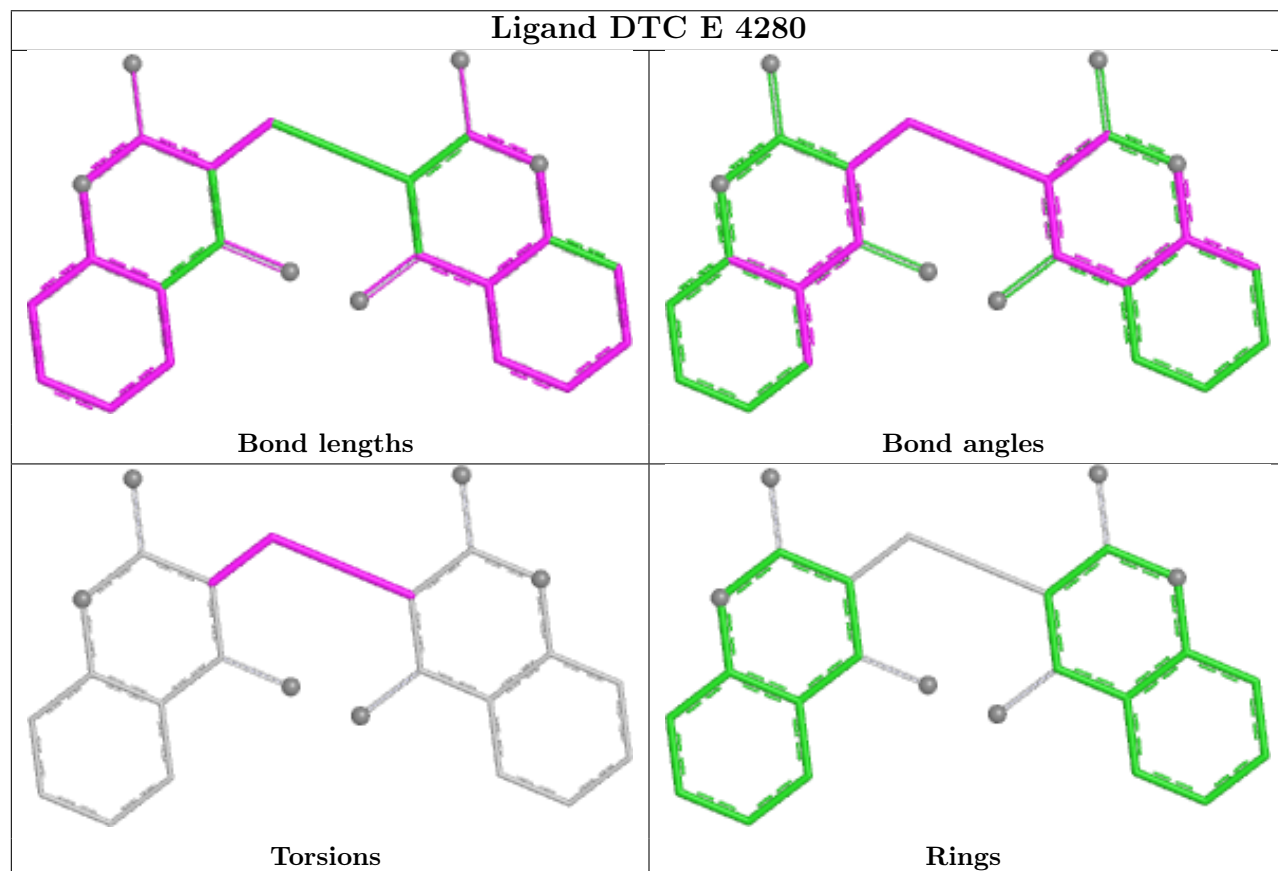


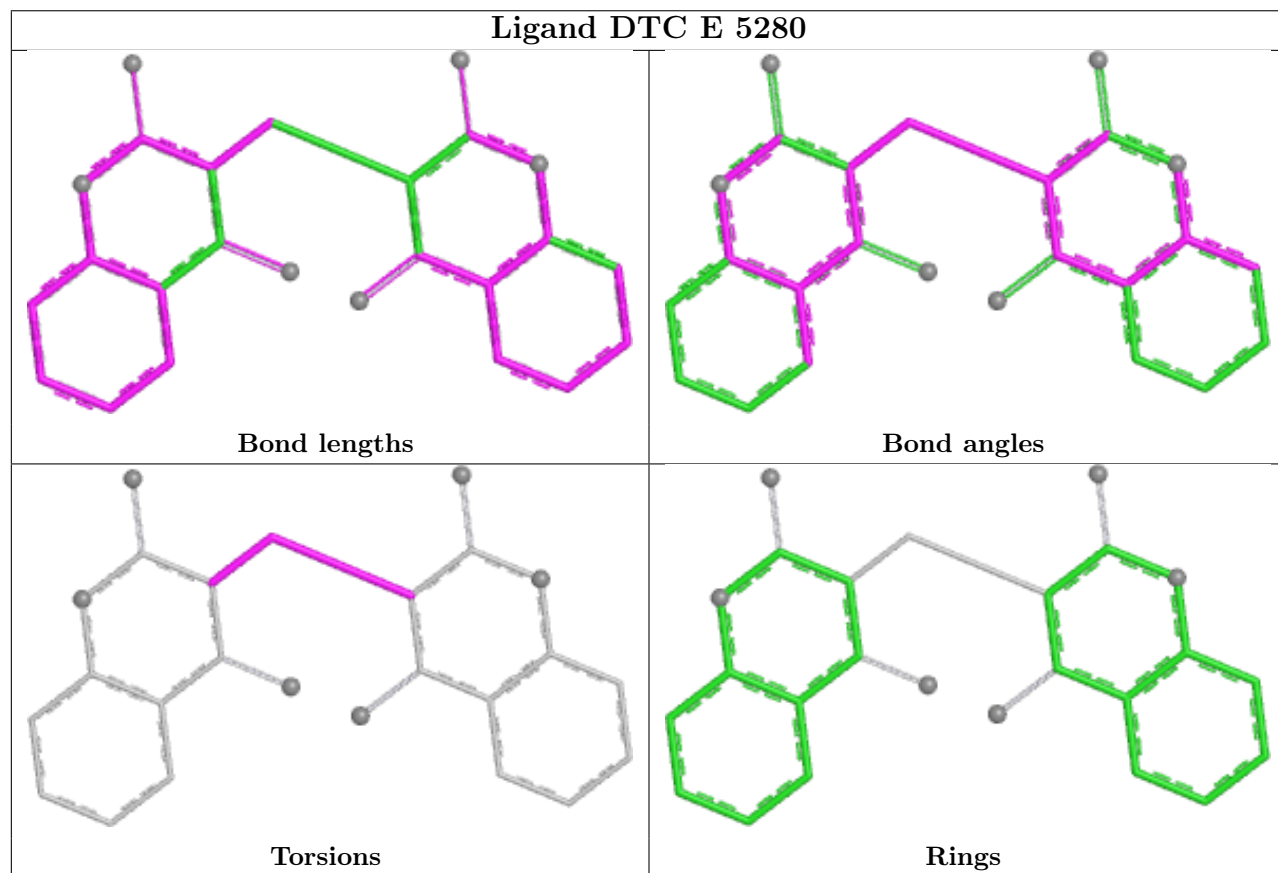
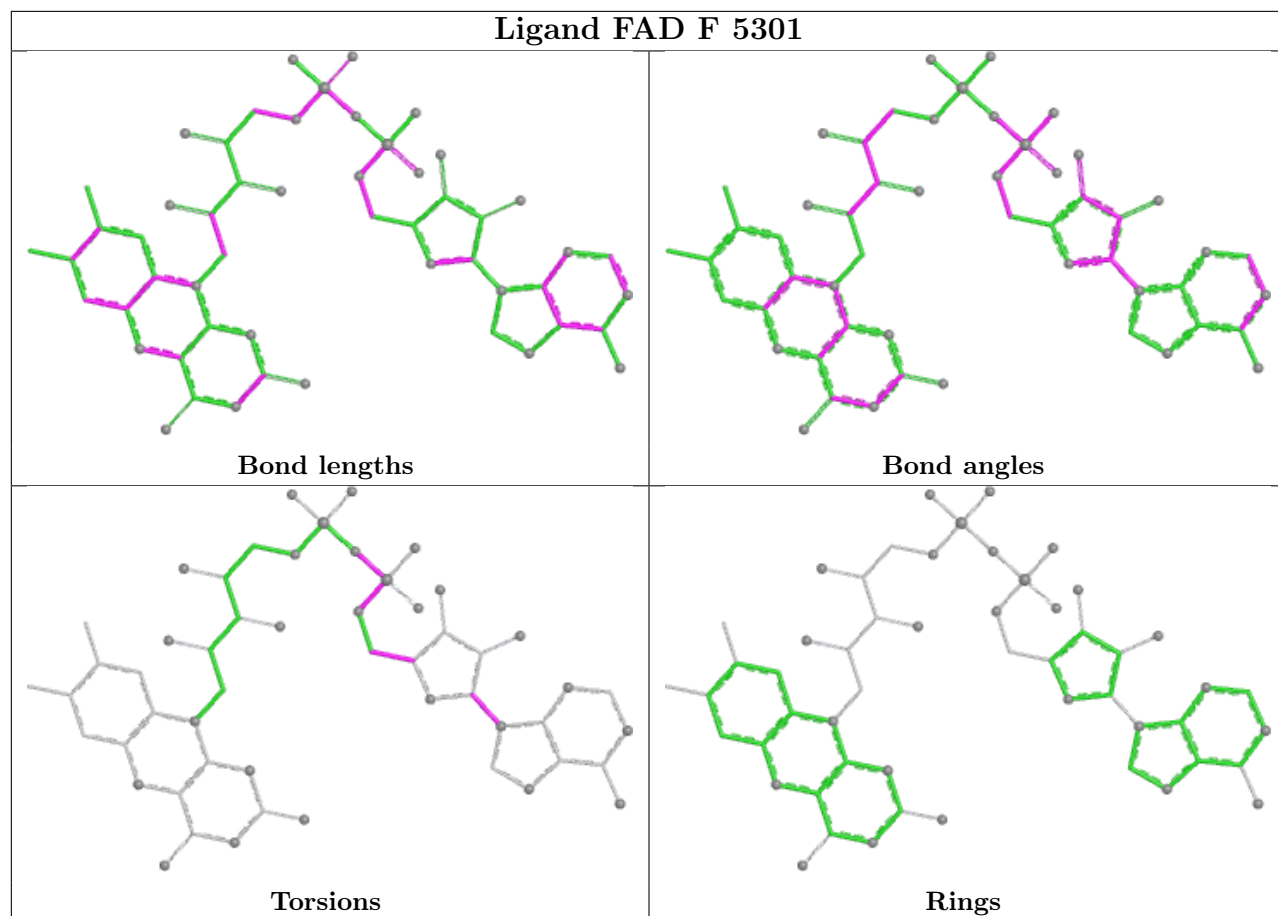


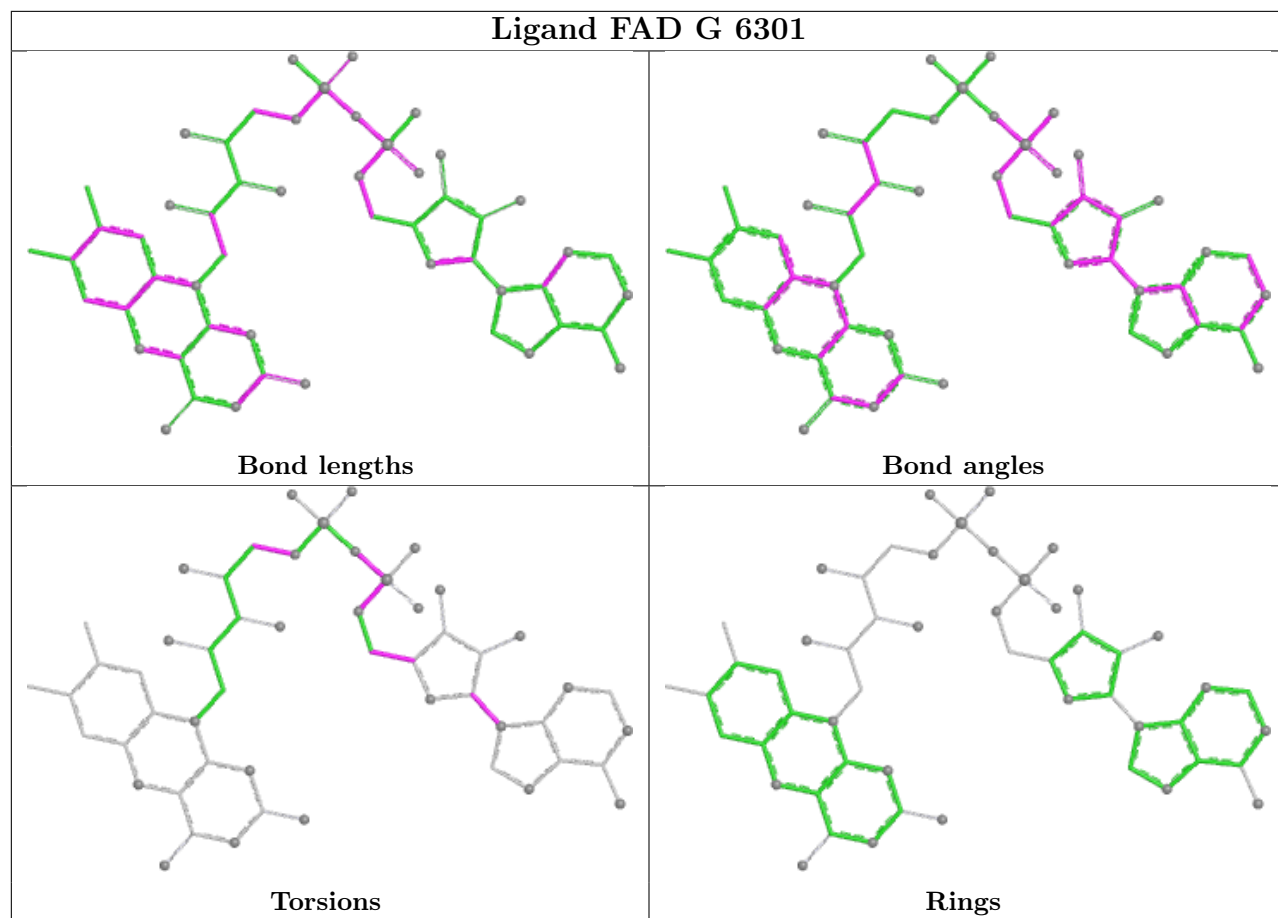
Ligand FAD A 301

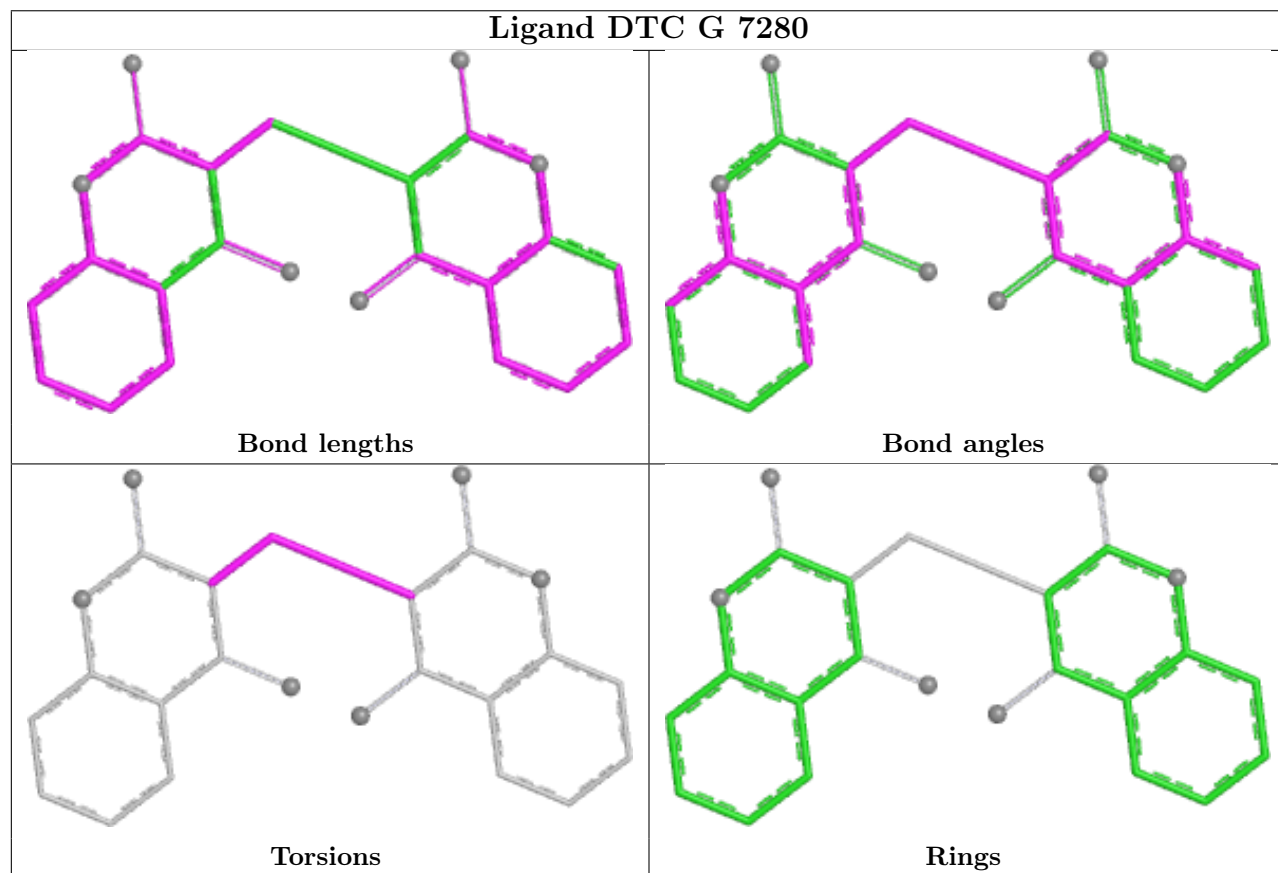
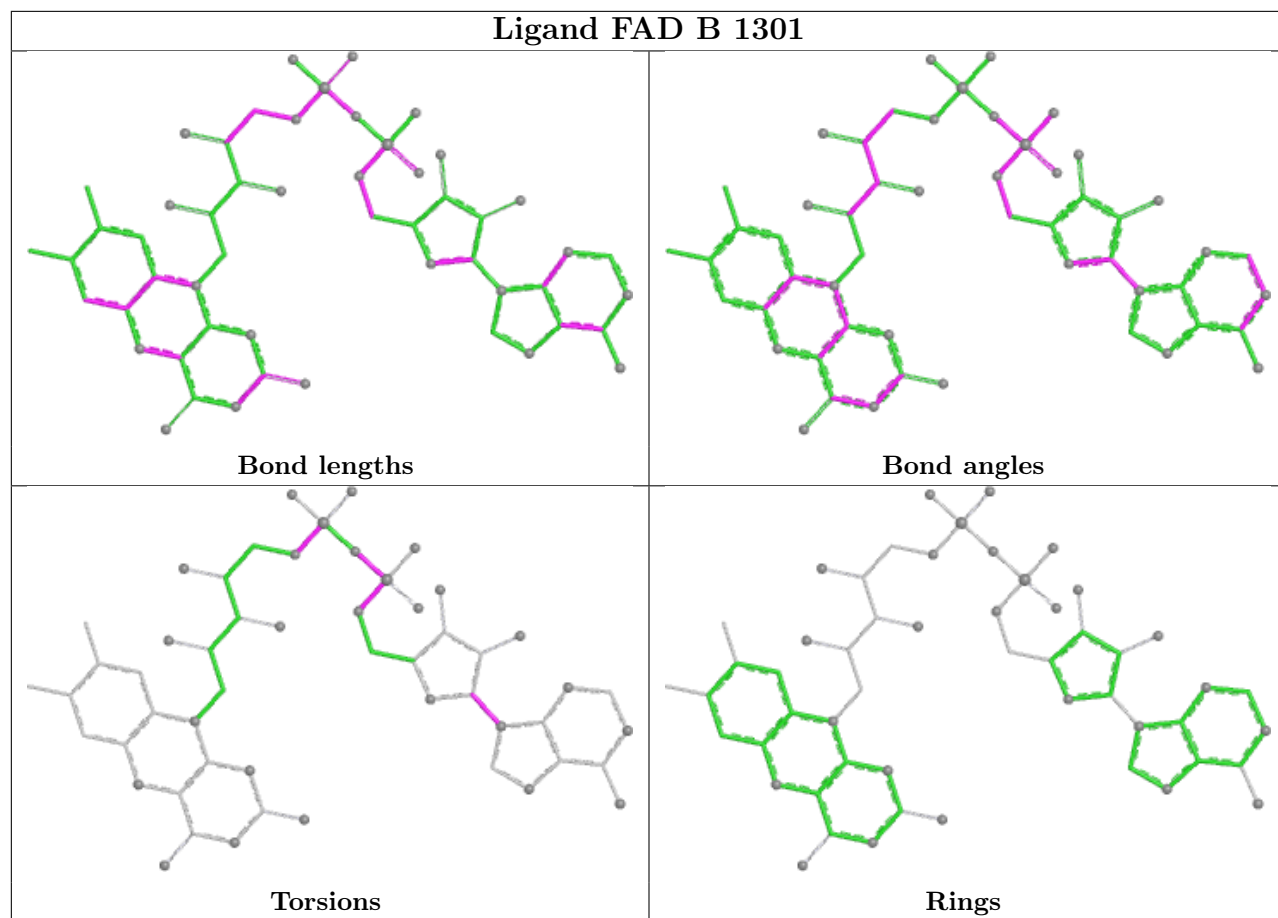


Ligand DTC E 4280

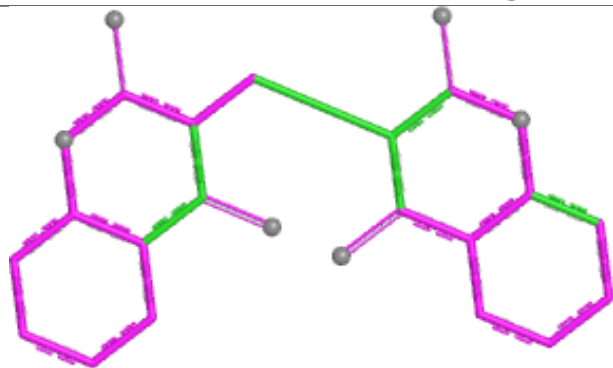




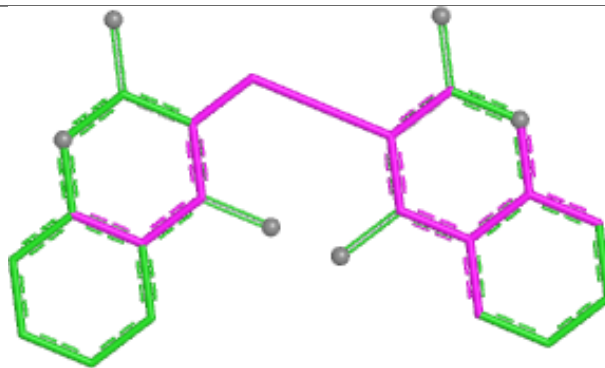




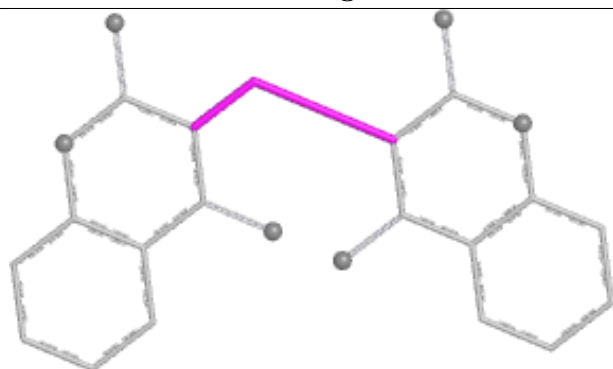
Ligand DTC A 2280



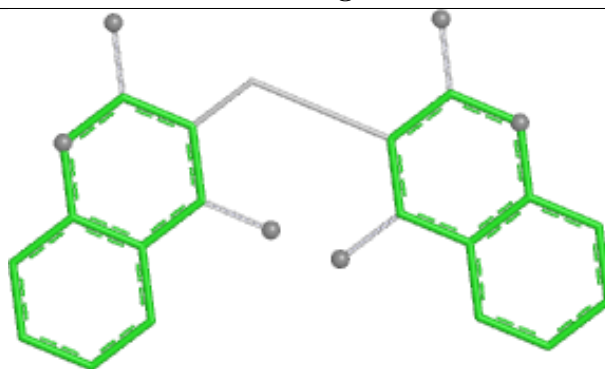
Bond lengths



Bond angles

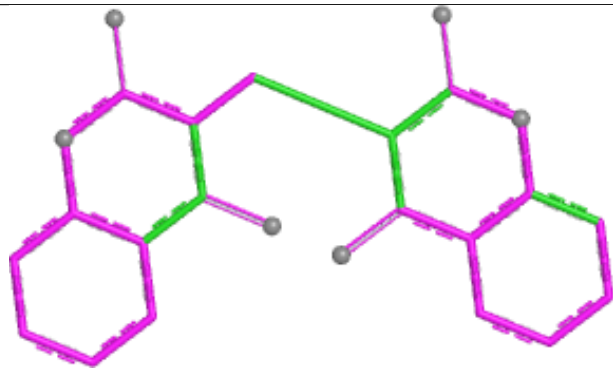


Torsions

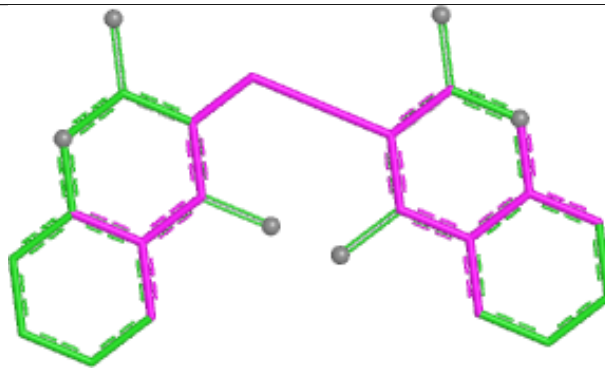


Rings

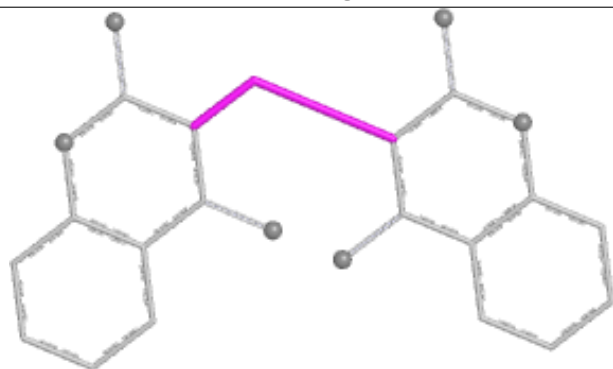
Ligand DTC D 1280



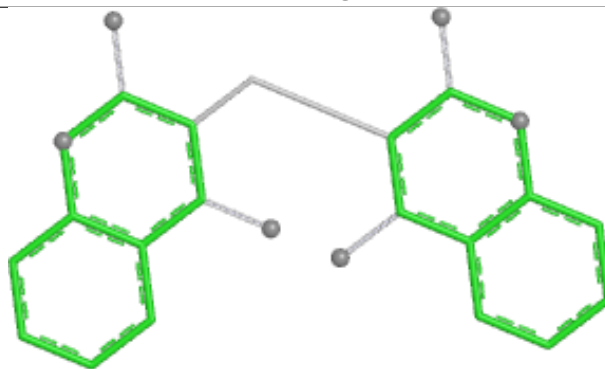
Bond lengths



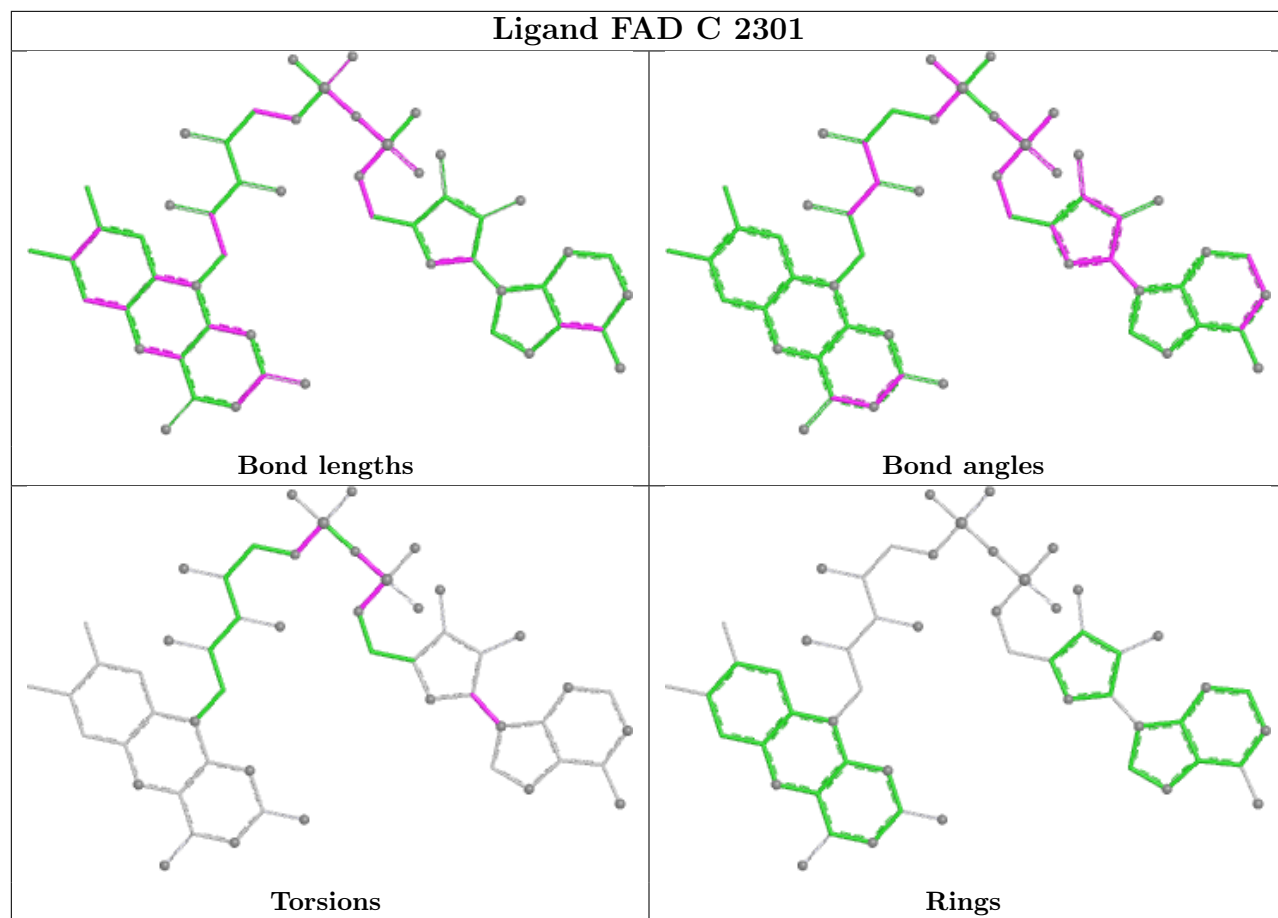
Bond angles

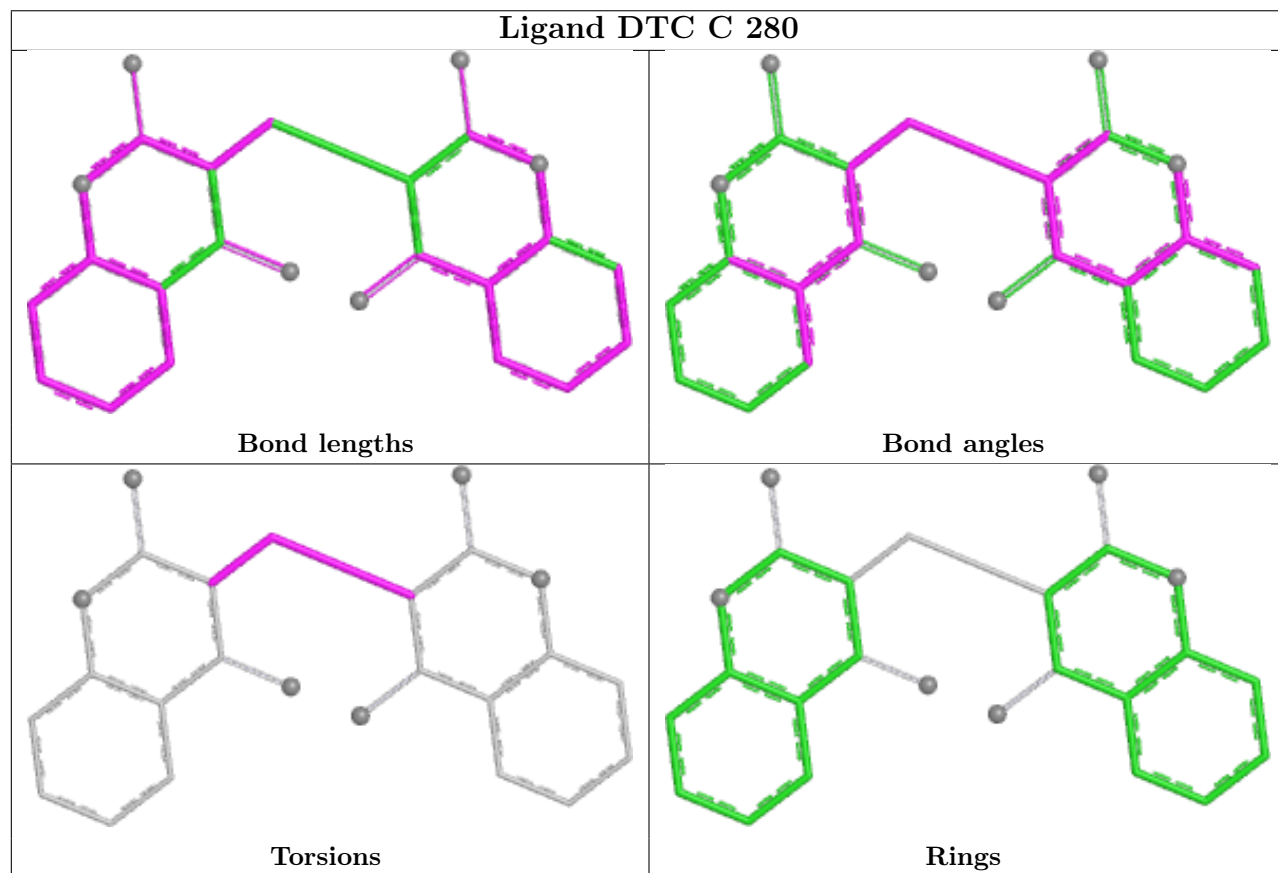
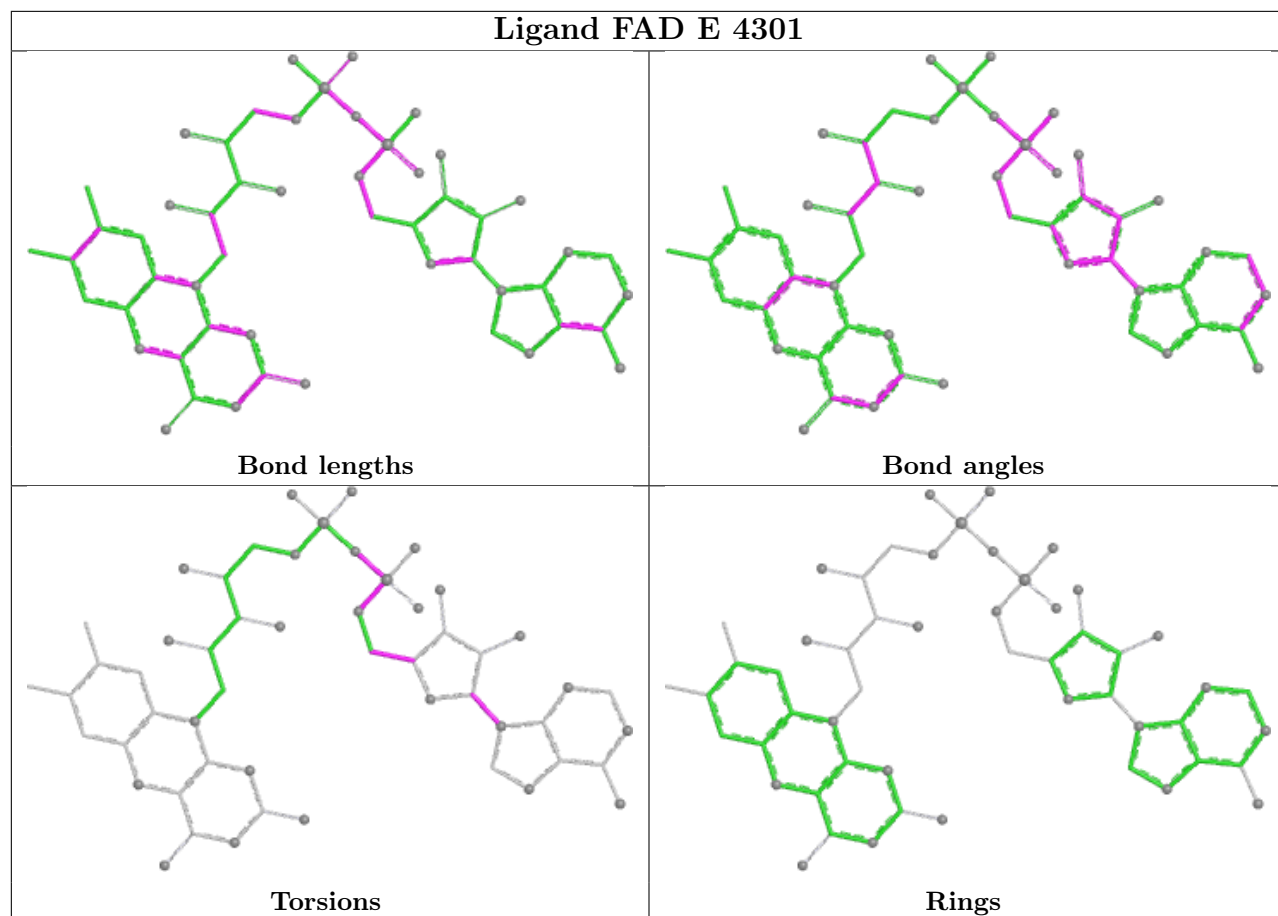


Torsions



Rings





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	273/273 (100%)	0.09	4 (1%) 72 71	13, 31, 50, 78	0
1	B	273/273 (100%)	0.08	3 (1%) 78 77	14, 29, 47, 74	0
1	C	273/273 (100%)	0.00	3 (1%) 78 77	12, 28, 53, 71	0
1	D	273/273 (100%)	0.21	7 (2%) 57 55	13, 33, 52, 80	0
1	E	273/273 (100%)	-0.03	2 (0%) 84 84	11, 27, 52, 69	0
1	F	273/273 (100%)	0.12	2 (0%) 84 84	15, 32, 53, 68	0
1	G	273/273 (100%)	0.32	10 (3%) 45 42	15, 35, 65, 81	0
1	H	273/273 (100%)	0.63	20 (7%) 21 21	18, 41, 70, 82	0
All	All	2184/2184 (100%)	0.18	51 (2%) 61 59	11, 32, 58, 82	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	VAL	5.5
1	A	1	VAL	5.3
1	H	196	PRO	4.9
1	A	232	PHE	4.6
1	E	1	VAL	4.6
1	G	1	VAL	4.3
1	D	1	VAL	4.2
1	H	1	VAL	3.7
1	A	2	GLY	3.4
1	H	216	ASP	3.3
1	G	232	PHE	3.2
1	H	198	ASP	3.1
1	D	202	GLN	2.9
1	E	232	PHE	2.9
1	F	1	VAL	2.9
1	H	201	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	H	189	THR	2.8
1	H	199	ALA	2.8
1	F	123	GLU	2.8
1	D	273	LYS	2.6
1	H	233	GLN	2.6
1	G	59	LEU	2.5
1	G	272	ARG	2.5
1	G	233	GLN	2.5
1	H	234	ALA	2.5
1	C	232	PHE	2.4
1	H	232	PHE	2.4
1	H	206	GLY	2.4
1	H	34	TRP	2.3
1	B	14	ARG	2.3
1	H	45	ASN	2.3
1	G	273	LYS	2.3
1	C	1	VAL	2.3
1	H	207	TRP	2.3
1	H	28	ALA	2.2
1	G	127	THR	2.2
1	H	195	THR	2.2
1	C	235	GLY	2.2
1	H	194	HIS	2.2
1	D	234	ALA	2.2
1	A	245	GLU	2.2
1	D	232	PHE	2.2
1	D	241	GLU	2.1
1	H	202	GLN	2.1
1	H	193	GLY	2.1
1	G	128	TYR	2.1
1	G	3	ARG	2.0
1	B	56	THR	2.0
1	D	121	ILE	2.0
1	G	237	LEU	2.0
1	H	272	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

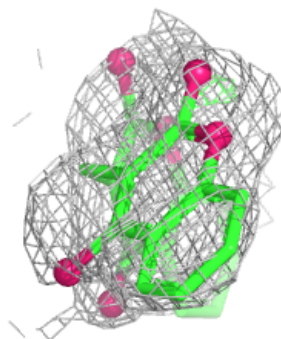
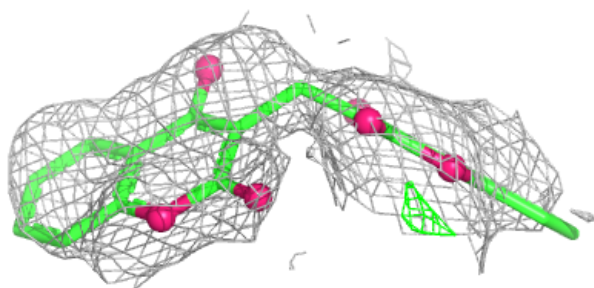
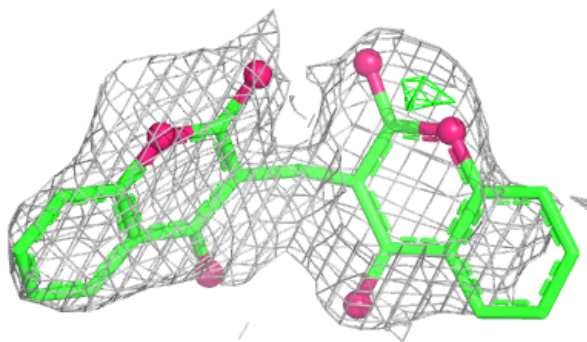
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	DTC	G	7280	25/25	0.79	0.17	34,74,75,75	0
2	DTC	E	5280	25/25	0.84	0.22	34,74,75,75	0
2	DTC	B	3280	25/25	0.86	0.18	34,74,75,75	0
2	DTC	D	1280	25/25	0.86	0.21	34,74,75,75	0
2	DTC	C	280	25/25	0.87	0.19	34,74,75,75	0
3	FAD	H	7301	53/53	0.87	0.12	25,45,53,55	0
2	DTC	E	4280	25/25	0.89	0.22	34,74,75,75	0
2	DTC	H	6280	25/25	0.89	0.18	34,74,75,75	0
2	DTC	A	2280	25/25	0.89	0.20	34,74,75,75	0
3	FAD	D	3301	53/53	0.91	0.10	19,28,38,39	0
3	FAD	A	301	53/53	0.91	0.11	25,34,42,42	0
3	FAD	F	5301	53/53	0.92	0.10	21,30,38,41	0
3	FAD	G	6301	53/53	0.92	0.10	20,28,34,37	0
3	FAD	B	1301	53/53	0.92	0.10	17,22,34,34	0
3	FAD	E	4301	53/53	0.93	0.10	14,23,34,34	0
3	FAD	C	2301	53/53	0.93	0.09	19,27,34,34	0

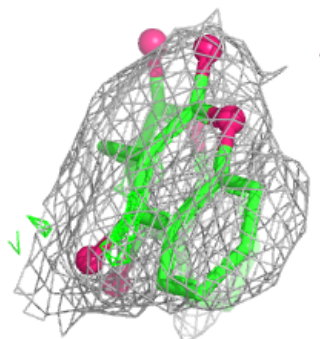
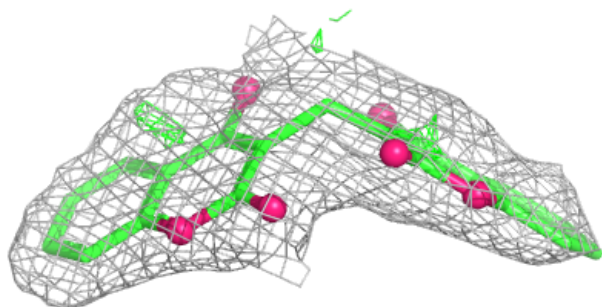
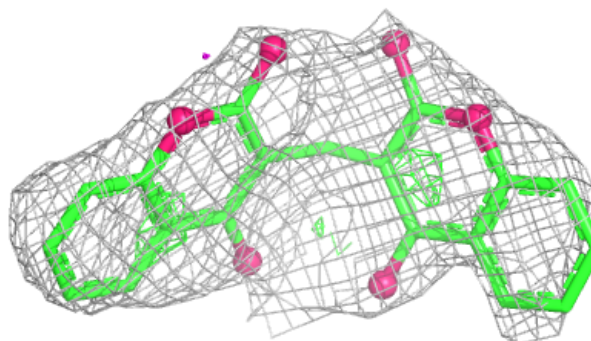
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DTC G 7280:

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

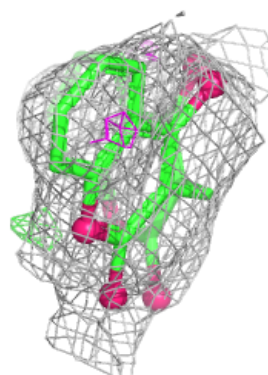
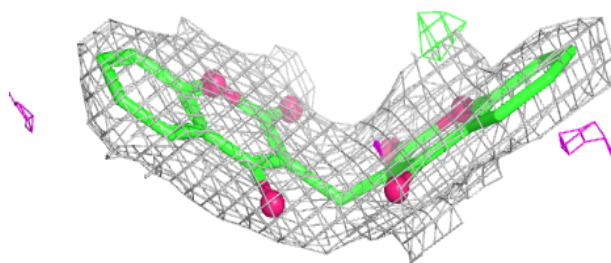
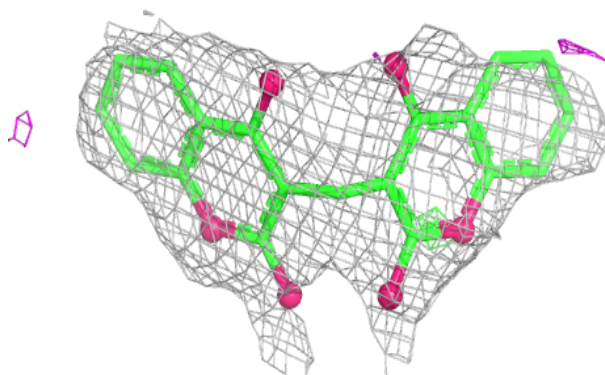
**Electron density around DTC E 5280:**

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

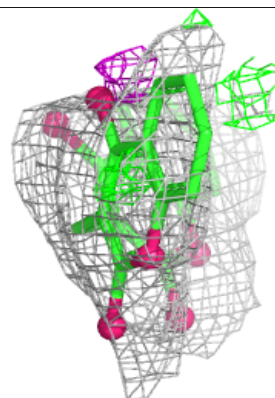
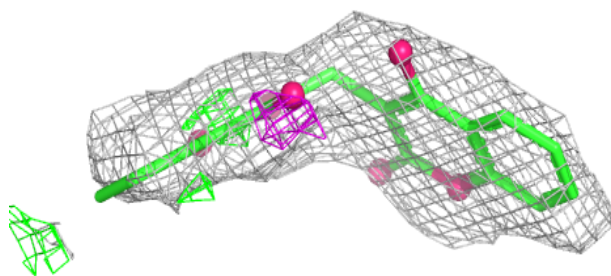
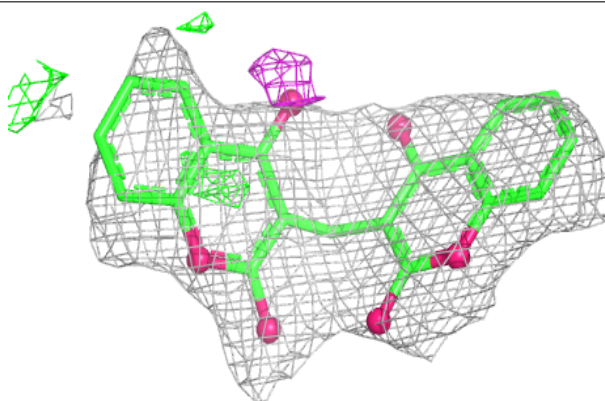


Electron density around DTC B 3280:

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

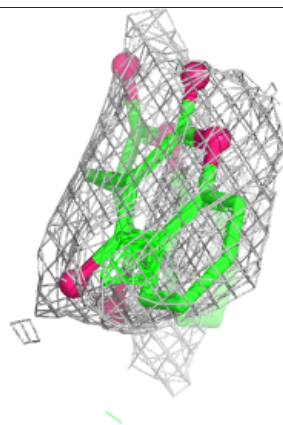
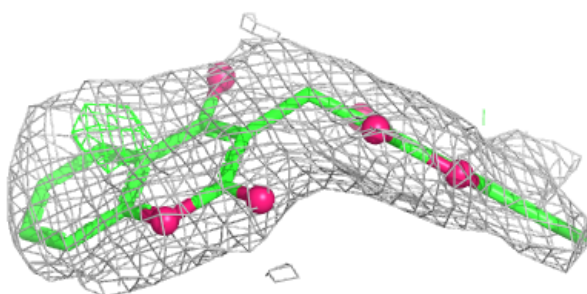
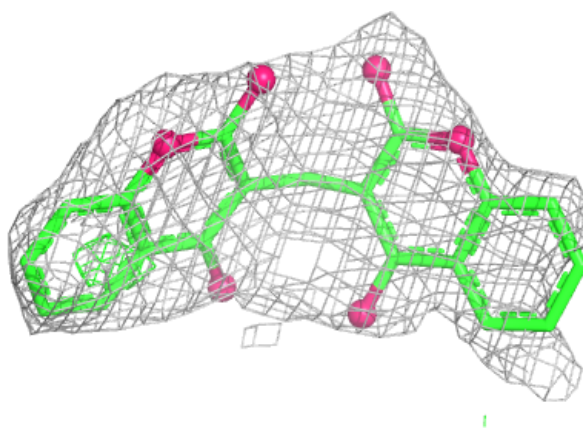
**Electron density around DTC D 1280:**

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

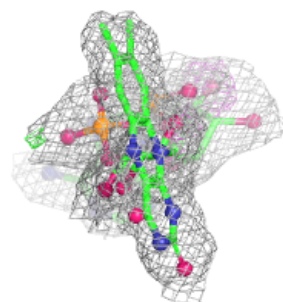
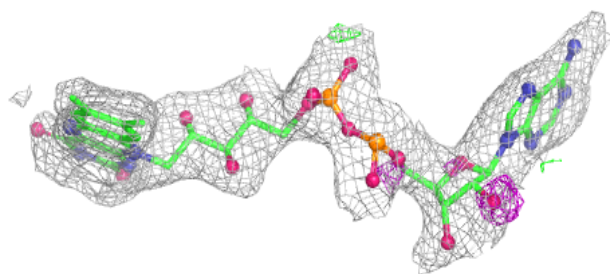
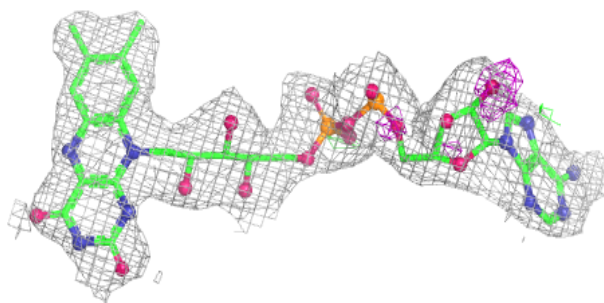


Electron density around DTC C 280:

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and green (positive)

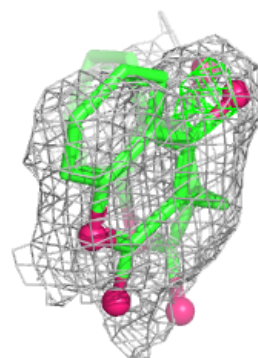
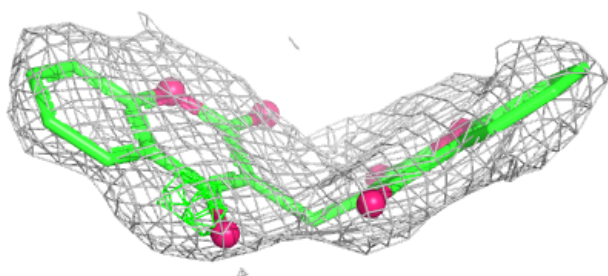
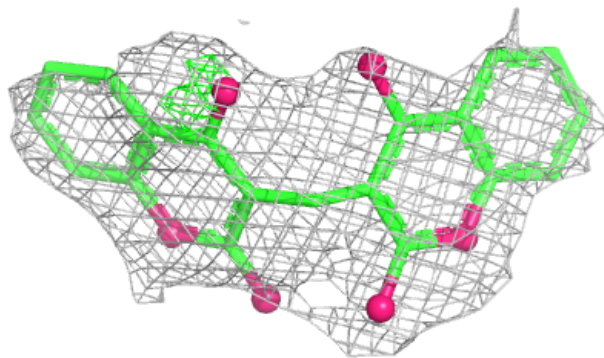
**Electron density around FAD H 7301:**

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

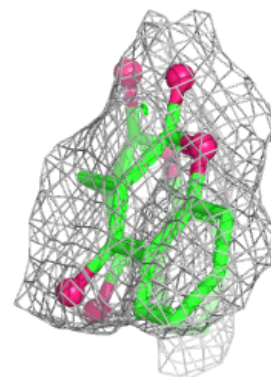
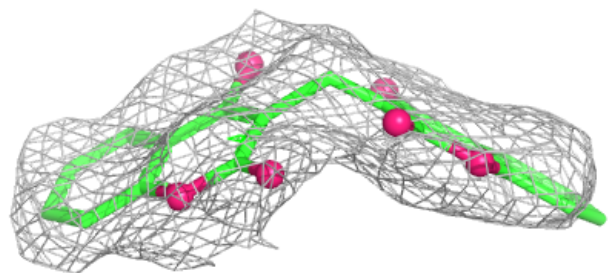
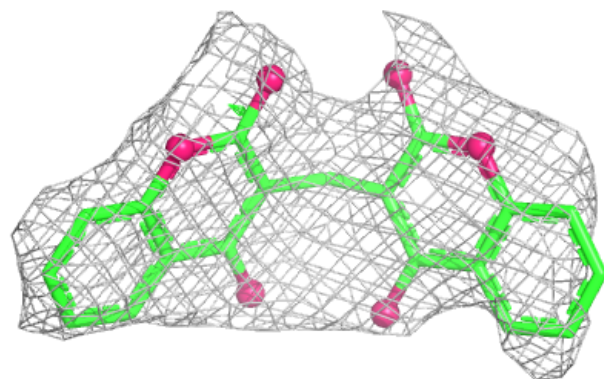


Electron density around DTC E 4280:

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

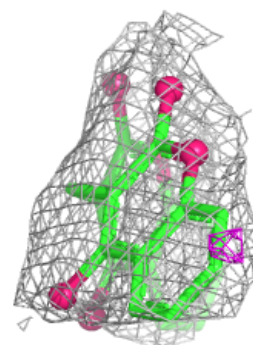
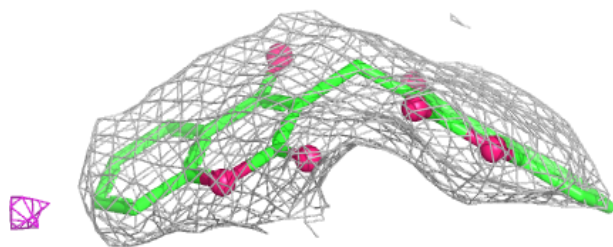
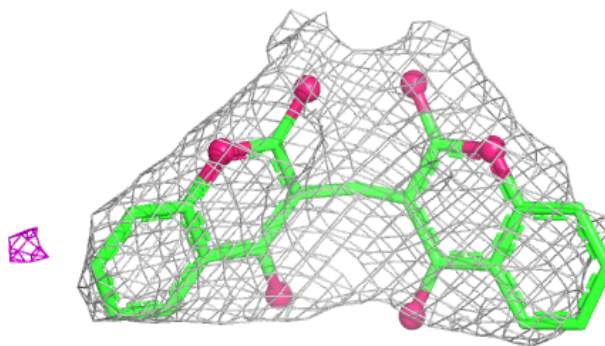
**Electron density around DTC H 6280:**

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

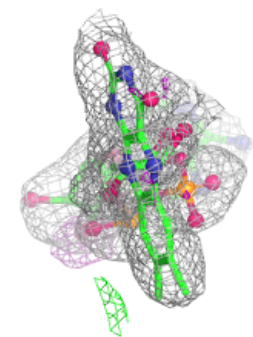
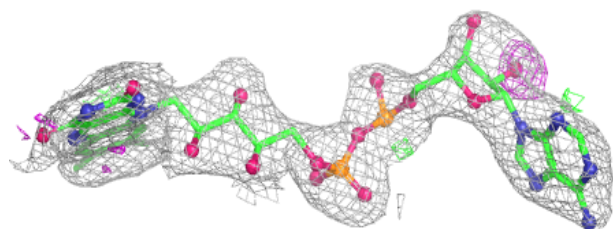
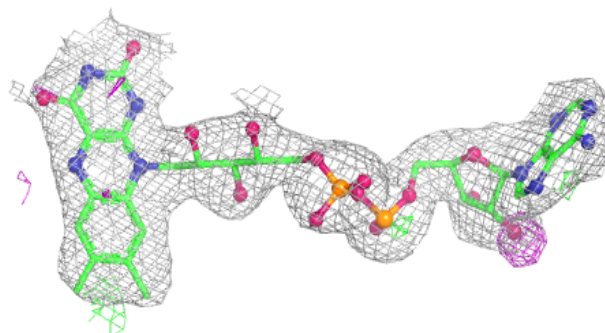


Electron density around DTC A 2280:

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

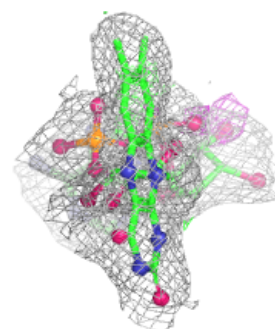
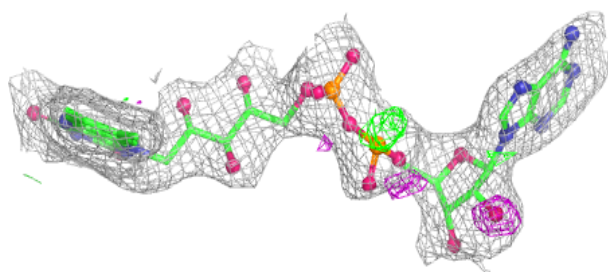
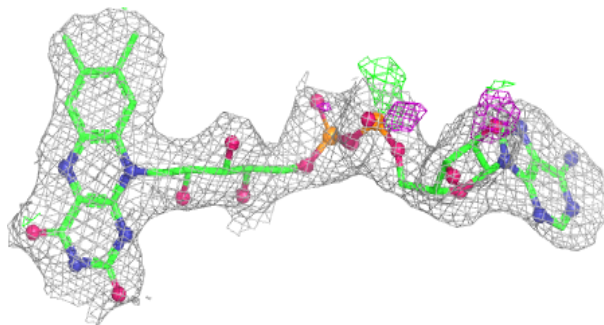
**Electron density around FAD D 3301:**

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

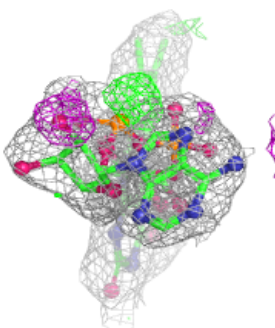
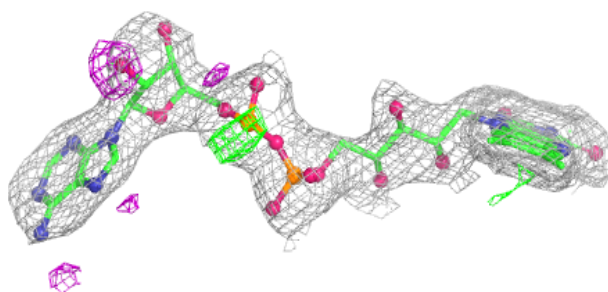
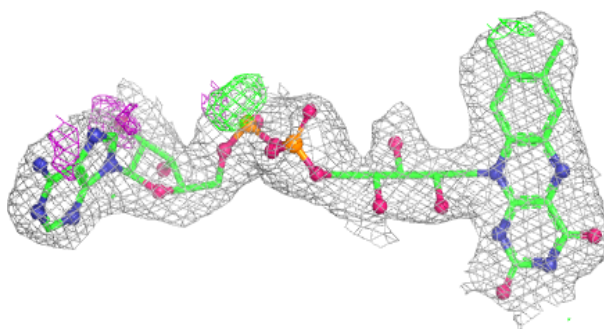


Electron density around FAD A 301:

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

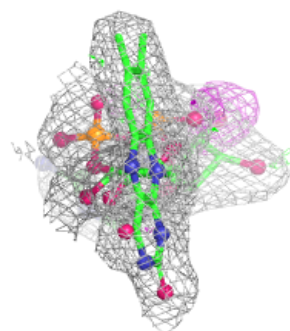
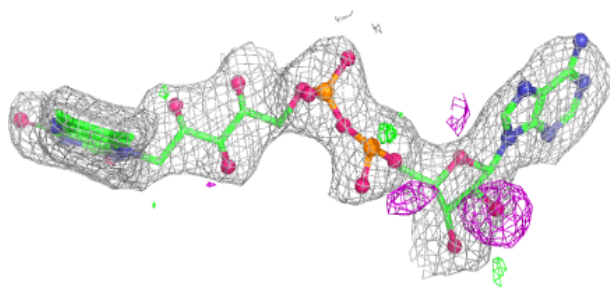
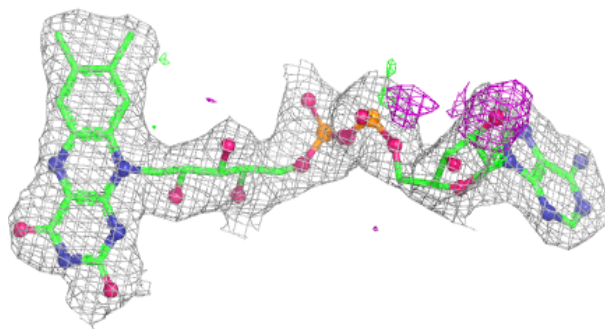
**Electron density around FAD F 5301:**

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

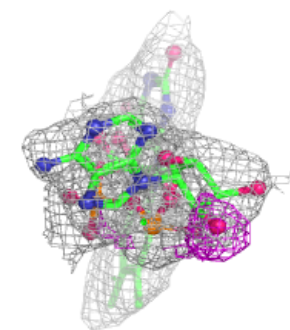
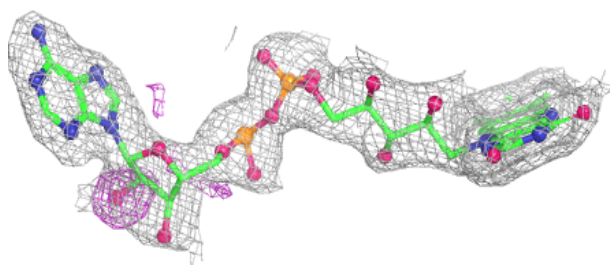
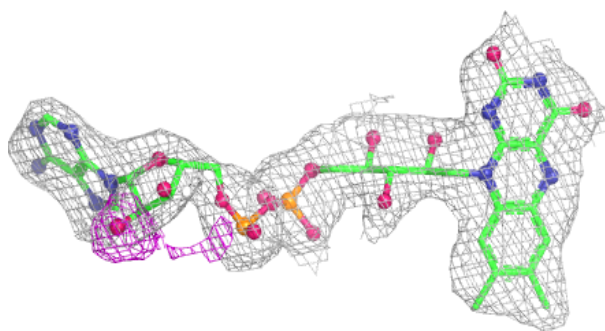


Electron density around FAD G 6301:

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

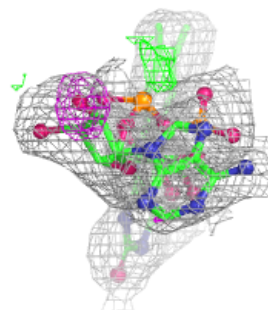
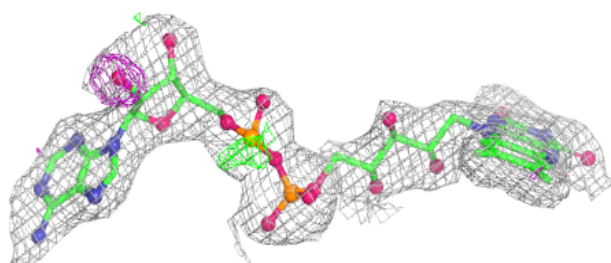
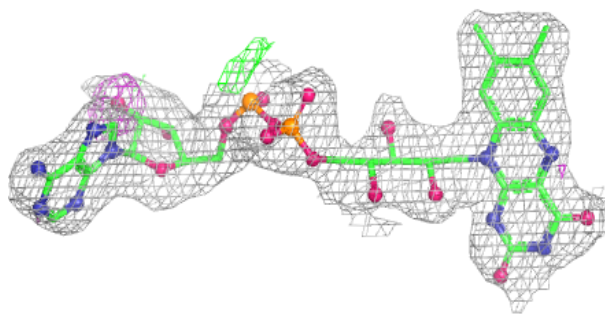
**Electron density around FAD B 1301:**

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

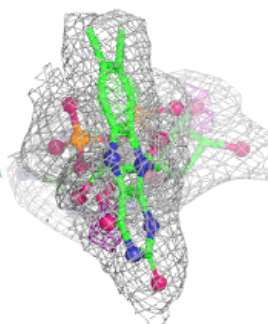
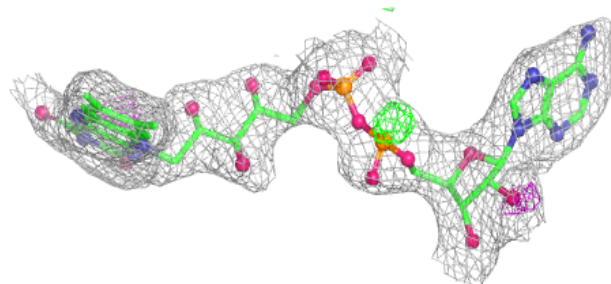
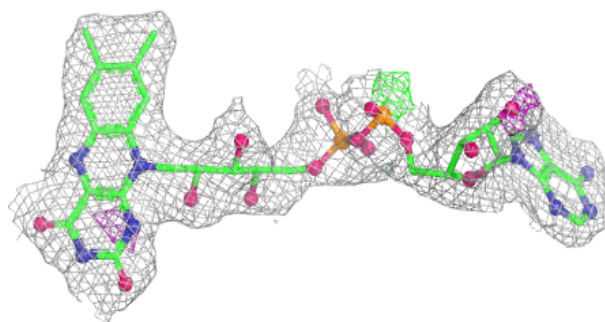


Electron density around FAD E 4301:

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

**Electron density around FAD C 2301:**

$2mF_o-DF_c$ (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.