



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2023 – 06:20 PM EDT

PDB ID : 2F1O
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

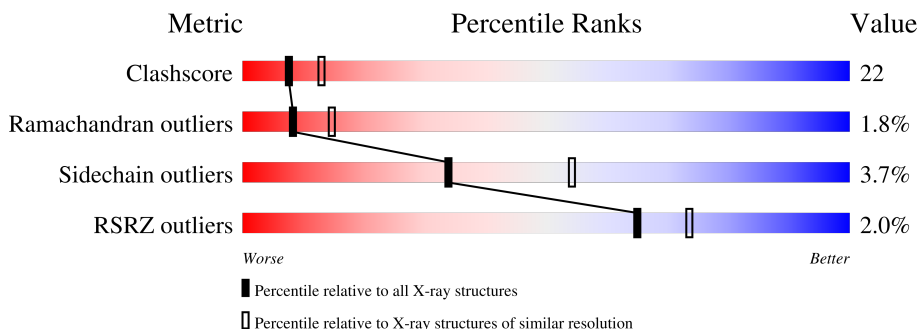
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

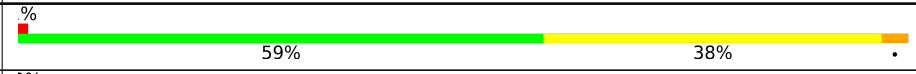

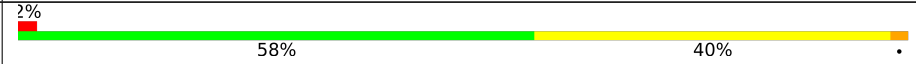
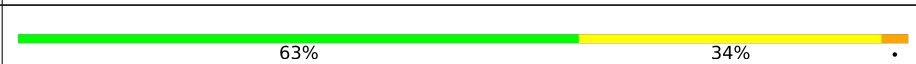

The reported resolution of this entry is 2.75 Å.

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	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	 2% 59% 38%
1	B	273	 2% 53% 45%
1	C	273	 2% 59% 38%
1	D	273	 2% 58% 40%
1	E	273	 63% 34%
1	F	273	 2% 55% 45%

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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

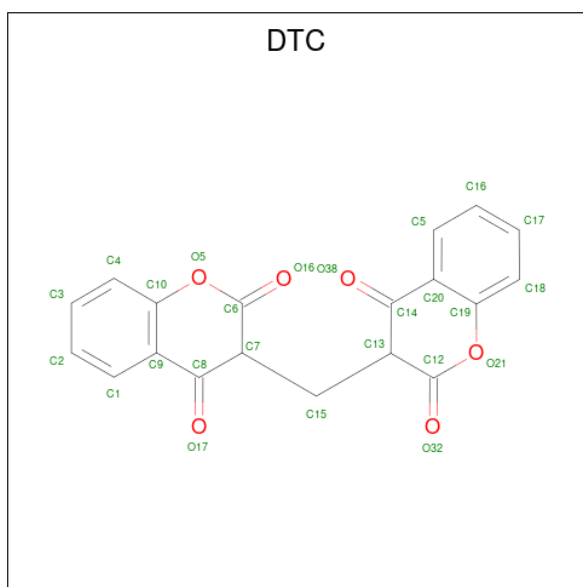
There are 4 unique types of molecules in this entry. The entry contains 18146 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	273	2175	1414	365	389	7	0	0	0
1	B	273	2175	1414	365	389	7	0	0	0
1	C	273	2175	1414	365	389	7	0	0	0
1	D	273	2175	1414	365	389	7	0	0	0
1	E	273	2175	1414	365	389	7	0	0	0
1	F	273	2175	1414	365	389	7	0	0	0
1	G	273	2175	1414	365	389	7	0	0	0
1	H	273	2175	1414	365	389	7	0	0	0

- Molecule 2 is BISHYDROXY[2H-1-BENZOPYRAN-2-ONE,1,2-BENZOPYRONE] (three-letter code: 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 (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 4 is water.

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

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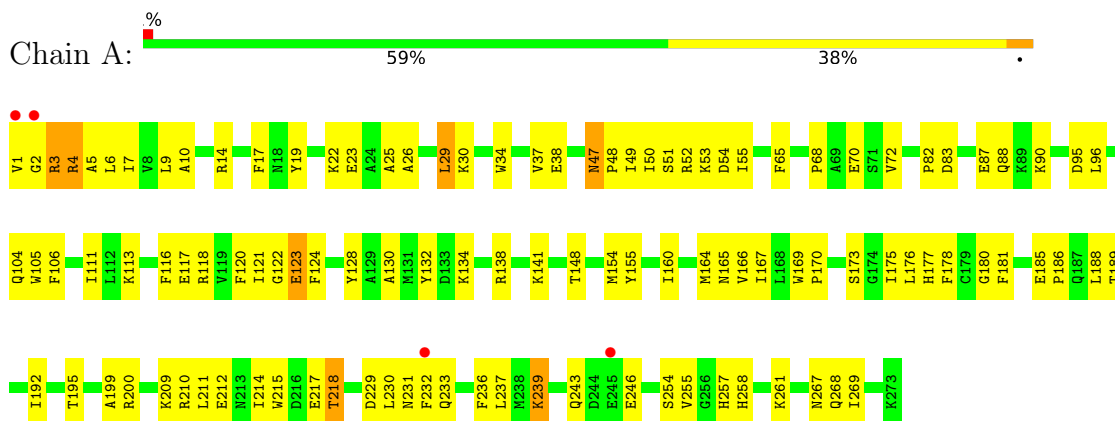
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	18	Total 18	O 18	0	0
4	F	10	Total 10	O 10	0	0
4	G	8	Total 8	O 8	0	0
4	H	8	Total 8	O 8	0	0

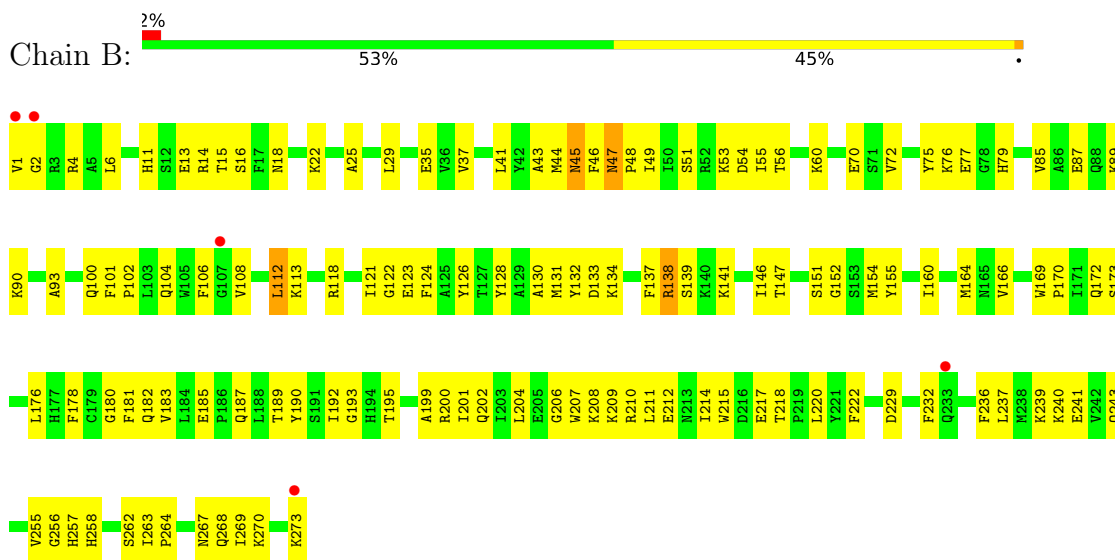
3 Residue-property plots

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.

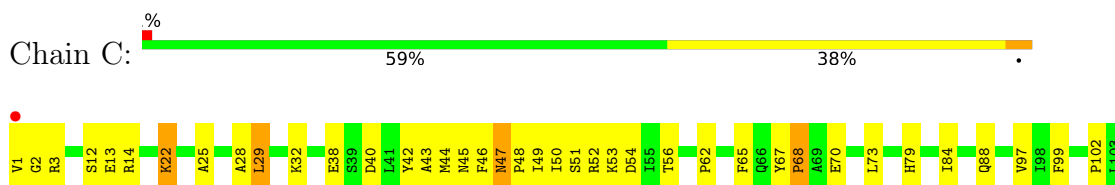
- Molecule 1: NAD(P)H dehydrogenase [quinone] 1

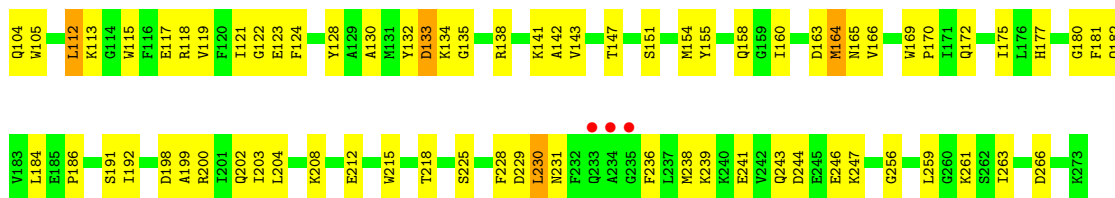


- Molecule 1: NAD(P)H dehydrogenase [quinone] 1

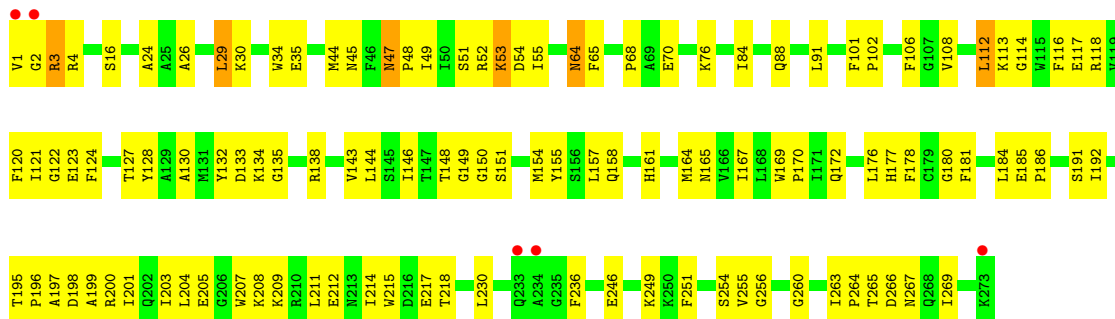


- Molecule 1: NAD(P)H dehydrogenase [quinone] 1

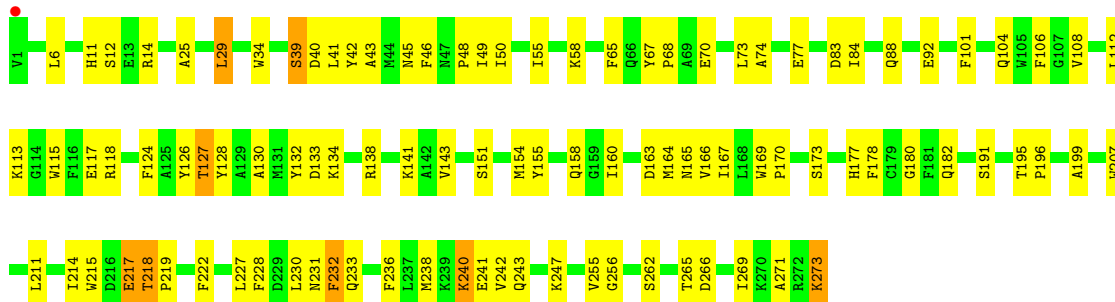




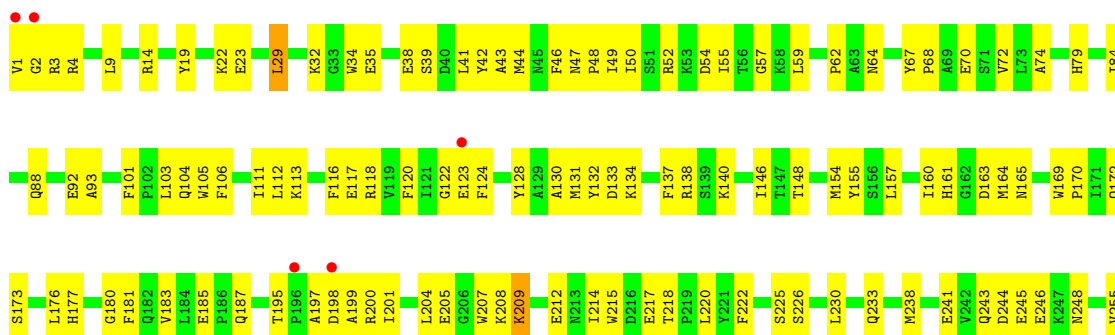
● Molecule 1: NAD(P)H dehydrogenase [quinone] 1



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

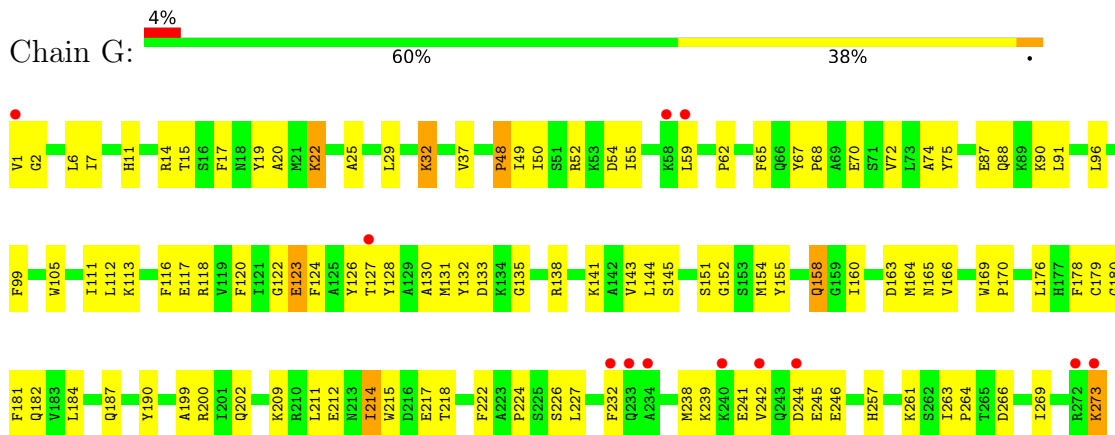


● Molecule 1: NAD(P)H dehydrogenase [quinone] 1

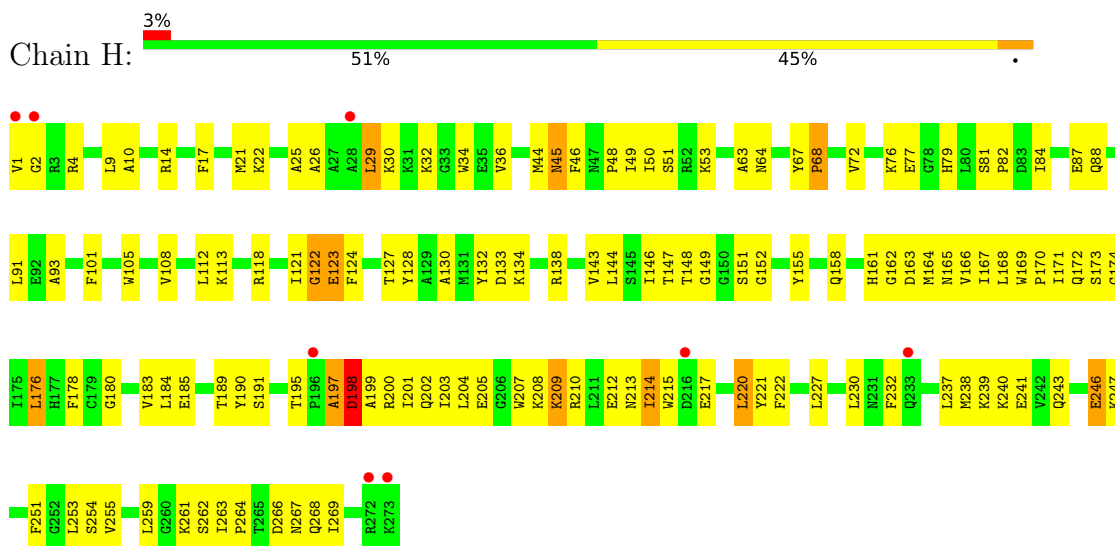




• Molecule 1: NAD(P)H dehydrogenase [quinone] 1



• 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 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (38.66-2.75) 95.1 (38.66-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 2.69Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.219 , 0.282 0.220 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	37.6	Xtrriage
Anisotropy	0.311	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 38.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	18146	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

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	0.41	0/2233	0.65	0/3015
1	B	0.42	0/2233	0.67	0/3015
1	C	0.41	0/2233	0.64	1/3015 (0.0%)
1	D	0.40	0/2233	0.66	0/3015
1	E	0.45	0/2233	0.65	1/3015 (0.0%)
1	F	0.41	0/2233	0.62	0/3015
1	G	0.40	0/2233	0.64	0/3015
1	H	0.41	0/2233	0.64	0/3015
All	All	0.41	0/17864	0.65	2/24120 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	182	GLN	N-CA-C	-5.24	96.86	111.00
1	C	182	GLN	N-CA-C	-5.19	96.98	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2175	0	2179	94	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2175	0	2179	125	0
1	C	2175	0	2179	100	0
1	D	2175	0	2179	116	0
1	E	2175	0	2179	76	0
1	F	2175	0	2179	110	0
1	G	2175	0	2179	97	0
1	H	2175	0	2179	129	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	2	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
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	788	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 22.

All (788) 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	1.07	1.15
1:D:47:ASN:HD22	1:D:48:PRO:N	1.51	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:48:PRO:HG3	1:D:49:ILE:HD11	1.41	1.03
1:G:128:TYR:OH	2:G:7280:DTC:O16	1.76	1.01
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:F:255:VAL:HG23	1:F:267:ASN:HD22	1.28	0.94
1:F:238:MET:HE3	1:F:243:GLN:HG2	1.49	0.92
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: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:F:14:ARG:NH2	1:F:43:ALA:HB2	1.93	0.83
1:D:47:ASN:HD22	1:D:47:ASN:C	1.78	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
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:A:47:ASN:C	1:A:47:ASN:HD22	1.84	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:151:SER:H	1:D:154:MET:CE	1.91	0.77
1:E:238:MET:HE3	1:E:243:GLN:HG2	1.65	0.77
1:D:151:SER:N	1:D:154:MET:HE3	1.93	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: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:D:150:GLY:HA2	1:D:154:MET:HE1	1.71	0.72
1:E:49:ILE:HD11	1:F:48:PRO:HG3	1.70	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ASP:OD2	1:A:118:ARG:NH2	2.24	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:F:198:ASP:O	1:F:201:ILE:HB	1.92	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:G:138:ARG:HA	1:G:180:GLY:O	1.95	0.67
1:B:49:ILE:O	1:B:118:ARG:HD3	1.94	0.67
1:A:47:ASN:ND2	1:A:47:ASN:C	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:151:SER:H	1:E:154:MET:HE3	1.64	0.63
1:G:49:ILE:HD11	1:H:48:PRO:HG3	1.81	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:47:ASN:ND2	1:D:47:ASN:C	2.49	0.59
1:B:47:ASN:HD22	1:B:47:ASN:C	2.06	0.58
1:B:54:ASP:CG	1:B:118:ARG:HH11	2.06	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:241:GLU:H	1:F:241:GLU:CD	2.09	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
1:D:169:TRP:HB3	1:D:170:PRO:HD3	1.88	0.56
1:H:238:MET:HE1	1:H:259:LEU:HD21	1.87	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: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:G:151:SER:H	1:G:154:MET:HE3	1.71	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:195:THR:CG2	1:F:199:ALA:HB3	2.37	0.55
1:F:214:ILE:HG23	1:F:215:TRP:N	2.21	0.55
1:B:269:ILE:HG22	1:B:270:LYS:HG2	1.88	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
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: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:C:241:GLU:CD	1:C:241:GLU:H	2.10	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:44:MET:HE1	1:H:87:GLU:OE2	2.08	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
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:E:151:SER:N	1:E:154:MET:HE3	2.23	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: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:72:VAL:HG22	1:B:122:GLY:HA3	1.91	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:232:PHE:CD1	1:B:232:PHE:N	2.78	0.51
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:195:THR:HG22	1:E:199:ALA:HB3	1.91	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: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:A:214:ILE:HD12	1:A:217:GLU:OE2	2.11	0.51
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:C:238:MET:HE3	1:C:243:GLN:HG2	1.93	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: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:G:244:ASP:C	1:G:246:GLU:H	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:214:ILE:HG23	1:G:215:TRP:N	2.27	0.50
1:H:130:ALA:HB1	1:H:134:LYS:O	2.12	0.50
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: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: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:26:ALA:HB1	1:A:30:LYS:HZ2	1.76	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:108:VAL:HB	1:H:112:LEU:HD23	1.95	0.49
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: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:H:132:TYR:C	1:H:134:LYS:H	2.16	0.48
1:H:241:GLU:H	1:H:241:GLU:CD	2.16	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: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: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:B:47:ASN:ND2	1:B:47:ASN:C	2.66	0.47
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:106:PHE:HD2	1:E:167:ILE:CD1	2.27	0.47
1:E:265:THR:O	1:E:266:ASP:C	2.53	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: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:C:45:ASN:CG	1:D:45:ASN:HD21	2.18	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:13:GLU:C	1:B:15:THR:H	2.19	0.46
1:B:102:PRO:O	1:B:102:PRO:HG2	2.15	0.46
1:B:137:PHE:C	1:B:139:SER:H	2.18	0.46
1:C:53:LYS:HZ1	1:D:53:LYS:HZ2	1.62	0.46
1:D:4:ARG:HG2	1:D:35:GLU:OE2	2.15	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:23:GLU:HA	1:A:23:GLU:OE1	2.15	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
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
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:128:TYR:HH	2:G:7280:DTC:C6	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:132:TYR:CD1	1:G:178:PHE:HA	2.49	0.46
1:H:197:ALA:O	1:H:198:ASP:C	2.54	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: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:C:51:SER:C	1:C:53:LYS:H	2.20	0.46
1:A:88:GLN:HB3	1:A:124:PHE:CZ	2.51	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: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: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:C:45:ASN:CG	1:D:45:ASN:ND2	2.69	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:G:244:ASP:C	1:G:246:GLU:N	2.69	0.45
1:H:163:ASP:CG	1:H:165:ASN:HB2	2.36	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ASN:ND2	1:A:269:ILE:HD12	2.31	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:F:263:ILE:O	1:F:264:PRO:C	2.54	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:C:47:ASN:HD22	1:C:47:ASN:C	2.20	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:F:67:TYR:HB3	1:F:68:PRO:HD3	1.98	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: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: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
1:H:238:MET:HE1	1:H:259:LEU:CD2	2.48	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:D:123:GLU:OE2	1:D:123:GLU:HA	2.18	0.44
1:H:174:GLY:O	1:H:178:PHE:HB2	2.18	0.44
1:A:22:LYS:NZ	1:A:38:GLU:OE1	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:273:LYS:HD3	1:E:273:LYS:C	2.38	0.44
1:F:157:LEU:HD23	1:F:163:ASP:HB2	1.99	0.44
1:H:51:SER:OG	1:H:53:LYS:HB3	2.18	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:F:238:MET:CE	1:F:243:GLN:HG2	2.34	0.43
1:A:105:TRP:HB3	1:C:175:ILE:HG12	2.00	0.43
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:C:122:GLY:C	1:C:124:PHE:H	2.21	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:73:LEU:HD11	1:E:77:GLU:CD	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:192:ILE:O	1:D:192:ILE:HG13	2.18	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:165:ASN:OD1	1:C:266:ASP:HA	2.19	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:O	1:G:273:LYS:HD3	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:B:77:GLU:OE1	1:B:79:HIS:CE1	2.70	0.43
1:E:40:ASP:O	1:E:41:LEU:C	2.57	0.43
1:G:135:GLY:HA3	1:G:179:CYS:O	2.19	0.43
1:A:52:ARG:C	1:A:54:ASP:H	2.22	0.43
1:B:44:MET:O	1:B:45:ASN:HB3	2.19	0.43
3:B:1301:FAD:C8M	1:D:68:PRO:HG3	2.49	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:132:TYR:C	1:F:134:LYS:H	2.22	0.42
1:F:233:GLN:HA	1:F:233:GLN:NE2	2.34	0.42
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: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:E:241:GLU:CD	1:E:241:GLU:H	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:238:MET:CE	1:C:259:LEU:HD21	2.49	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:A:52:ARG:C	1:A:54:ASP:N	2.73	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: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:163:ASP:CG	1:E:165:ASN:HB2	2.40	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:128:TYR:CD1	2:G:7280:DTC:C19	3.03	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: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
1:C:229:ASP:O	1:C:231:ASN:N	2.40	0.42
1:F:160:ILE:HG12	1:F:160:ILE:O	2.20	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: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:G:6:LEU:HD13	1:G:37:VAL:HG12	2.02	0.42
1:D:52:ARG:C	1:D:54:ASP:H	2.24	0.41
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:F:9:LEU:CD2	1:F:22:LYS:HD3	2.51	0.41
1:F:64:ASN:HD22	1:F:64:ASN:HA	1.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:91:LEU:HD23	1:G:91:LEU:HA	1.88	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:F:46:PHE:O	1:F:48:PRO:HD3	2.20	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: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
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: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:B:192:ILE:HG23	1:B:193:GLY:N	2.36	0.41
1:C:47:ASN:ND2	1:C:47:ASN:C	2.74	0.41
1:C:54:ASP:CG	1:C:118:ARG:HH11	2.24	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: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: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:D:265:THR:O	1:D:266:ASP:C	2.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:113:LYS:O	1:F:117:GLU:HG3	2.20	0.41
1:F:244:ASP:C	1:F:246:GLU:H	2.23	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:44:MET:O	1:H:45:ASN:C	2.59	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
1:B:240:LYS:HG2	1:B:241:GLU:OE2	2.21	0.40
1:C:45:ASN:CG	1:C:45:ASN:O	2.59	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:H:238:MET:CE	1:H:259:LEU:HD21	2.49	0.40
1:A:160:ILE:HA	1:C:228:PHE:CE2	2.57	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:C:44:MET:O	1:C:45:ASN:HB3	2.21	0.40
1:F:246:GLU:C	1:F:248:ASN:H	2.23	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:E:113:LYS:O	1:E:117:GLU:HG3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:138:ARG:HA	1:F:180:GLY:O	2.22	0.40
1:H:255:VAL:HG21	1:H:268:GLN:HG2	2.02	0.40
1:B:49:ILE:C	1:B:118:ARG:HD3	2.40	0.40
1:B:137:PHE:C	1:B:139:SER:N	2.75	0.40
1:E:46:PHE:HE2	1:E:115:TRP:HA	1.86	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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	271/273 (99%)	247 (91%)	21 (8%)	3 (1%)	14	25
1	B	271/273 (99%)	246 (91%)	21 (8%)	4 (2%)	10	18
1	C	271/273 (99%)	246 (91%)	18 (7%)	7 (3%)	5	8
1	D	271/273 (99%)	239 (88%)	29 (11%)	3 (1%)	14	25
1	E	271/273 (99%)	242 (89%)	23 (8%)	6 (2%)	6	11
1	F	271/273 (99%)	241 (89%)	29 (11%)	1 (0%)	34	53
1	G	271/273 (99%)	245 (90%)	21 (8%)	5 (2%)	8	15
1	H	271/273 (99%)	235 (87%)	25 (9%)	11 (4%)	3	3
All	All	2168/2184 (99%)	1941 (90%)	187 (9%)	40 (2%)	8	15

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

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Mol	Chain	Res	Type
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
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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	227/227 (100%)	219 (96%)	8 (4%)	36	56
1	B	227/227 (100%)	221 (97%)	6 (3%)	46	66
1	C	227/227 (100%)	222 (98%)	5 (2%)	52	70
1	D	227/227 (100%)	220 (97%)	7 (3%)	40	60
1	E	227/227 (100%)	214 (94%)	13 (6%)	20	36
1	F	227/227 (100%)	220 (97%)	7 (3%)	40	60
1	G	227/227 (100%)	218 (96%)	9 (4%)	31	51
1	H	227/227 (100%)	214 (94%)	13 (6%)	20	36
All	All	1816/1816 (100%)	1748 (96%)	68 (4%)	34	54

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	4	ARG
1	A	14	ARG
1	A	29	LEU
1	A	47	ASN
1	A	82	PRO
1	A	189	THR
1	A	218	THR
1	B	22	LYS
1	B	45	ASN
1	B	47	ASN
1	B	112	LEU
1	B	218	THR
1	B	273	LYS
1	C	22	LYS
1	C	29	LEU
1	C	47	ASN
1	C	112	LEU
1	C	218	THR
1	D	3	ARG
1	D	29	LEU
1	D	47	ASN
1	D	64	ASN
1	D	91	LEU

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Mol	Chain	Res	Type
1	D	112	LEU
1	D	198	ASP
1	E	29	LEU
1	E	39	SER
1	E	45	ASN
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	240	LYS
1	E	262	SER
1	E	273	LYS
1	F	29	LEU
1	F	39	SER
1	F	47	ASN
1	F	207	TRP
1	F	209	LYS
1	F	218	THR
1	F	226	SER
1	G	22	LYS
1	G	29	LEU
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	148	THR
1	H	198	ASP
1	H	207	TRP
1	H	209	LYS
1	H	232	PHE

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Mol	Chain	Res	Type
1	H	240	LYS
1	H	246	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	66	GLN
1	A	104	GLN
1	A	158	GLN
1	A	172	GLN
1	A	267	ASN
1	B	45	ASN
1	B	47	ASN
1	B	79	HIS
1	B	172	GLN
1	B	267	ASN
1	C	45	ASN
1	C	47	ASN
1	C	104	GLN
1	C	172	GLN
1	C	267	ASN
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	66	GLN
1	E	158	GLN
1	E	194	HIS
1	F	45	ASN
1	F	47	ASN
1	F	64	ASN
1	F	79	HIS
1	F	104	GLN
1	F	161	HIS
1	F	233	GLN
1	F	267	ASN
1	G	45	ASN

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Mol	Chain	Res	Type
1	G	172	GLN
1	G	177	HIS
1	G	268	GLN
1	H	47	ASN
1	H	64	ASN
1	H	79	HIS
1	H	88	GLN
1	H	172	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 monosaccharides 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	G	7280	-	28,28,28	5.04	22 (78%)	36,41,41	1.55	9 (25%)
3	FAD	F	5301	-	53,58,58	11.82	17 (32%)	68,89,89	2.44	12 (17%)
2	DTC	D	1280	-	28,28,28	5.05	21 (75%)	36,41,41	1.58	9 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FAD	H	7301	-	53,58,58	11.42	15 (28%)	68,89,89	2.48	10 (14%)
3	FAD	C	2301	-	53,58,58	12.26	16 (30%)	68,89,89	2.42	12 (17%)
3	FAD	E	4301	-	53,58,58	12.88	13 (24%)	68,89,89	2.51	13 (19%)
2	DTC	B	3280	-	28,28,28	4.96	21 (75%)	36,41,41	1.61	11 (30%)
3	FAD	B	1301	-	53,58,58	12.17	16 (30%)	68,89,89	2.46	13 (19%)
3	FAD	G	6301	-	53,58,58	11.57	18 (33%)	68,89,89	2.46	13 (19%)
2	DTC	H	6280	-	28,28,28	5.01	22 (78%)	36,41,41	1.57	8 (22%)
3	FAD	D	3301	-	53,58,58	12.04	16 (30%)	68,89,89	2.43	14 (20%)
2	DTC	A	2280	-	28,28,28	4.98	22 (78%)	36,41,41	1.54	8 (22%)
2	DTC	C	280	-	28,28,28	5.07	22 (78%)	36,41,41	1.52	8 (22%)
2	DTC	E	4280	-	28,28,28	5.03	22 (78%)	36,41,41	1.50	8 (22%)
2	DTC	E	5280	-	28,28,28	4.98	22 (78%)	36,41,41	1.61	9 (25%)
3	FAD	A	301	-	53,58,58	11.67	18 (33%)	68,89,89	2.48	13 (19%)

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	G	7280	-	2/2/6/6	2/4/36/36	0/4/4/4
3	FAD	F	5301	-	-	4/30/50/50	0/6/6/6
2	DTC	D	1280	-	2/2/6/6	2/4/36/36	0/4/4/4
3	FAD	H	7301	-	-	7/30/50/50	0/6/6/6
3	FAD	C	2301	-	-	5/30/50/50	0/6/6/6
3	FAD	E	4301	-	-	6/30/50/50	0/6/6/6
2	DTC	B	3280	-	2/2/6/6	1/4/36/36	0/4/4/4
3	FAD	B	1301	-	-	4/30/50/50	0/6/6/6
3	FAD	G	6301	-	-	6/30/50/50	0/6/6/6
2	DTC	H	6280	-	2/2/6/6	2/4/36/36	0/4/4/4
3	FAD	D	3301	-	-	7/30/50/50	0/6/6/6
2	DTC	A	2280	-	2/2/6/6	2/4/36/36	0/4/4/4
2	DTC	C	280	-	2/2/6/6	2/4/36/36	0/4/4/4
2	DTC	E	4280	-	2/2/6/6	2/4/36/36	0/4/4/4
2	DTC	E	5280	-	2/2/6/6	2/4/36/36	0/4/4/4
3	FAD	A	301	-	-	3/30/50/50	0/6/6/6

All (303) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	4301	FAD	PA-O2A	92.90	5.91	1.55
3	C	2301	FAD	PA-O2A	88.30	5.69	1.55
3	B	1301	FAD	PA-O2A	87.65	5.66	1.55
3	D	3301	FAD	PA-O2A	86.76	5.62	1.55
3	F	5301	FAD	PA-O2A	85.05	5.54	1.55
3	A	301	FAD	PA-O2A	83.87	5.48	1.55
3	G	6301	FAD	PA-O2A	83.20	5.45	1.55
3	H	7301	FAD	PA-O2A	82.13	5.40	1.55
2	C	280	DTC	O17-C8	13.49	1.41	1.22
2	H	6280	DTC	O17-C8	13.44	1.41	1.22
2	G	7280	DTC	O17-C8	13.29	1.40	1.22
2	A	2280	DTC	O17-C8	13.23	1.40	1.22
2	D	1280	DTC	O17-C8	13.21	1.40	1.22
2	B	3280	DTC	O17-C8	12.97	1.40	1.22
2	E	5280	DTC	O17-C8	12.94	1.40	1.22
2	E	4280	DTC	O17-C8	12.92	1.40	1.22
2	E	4280	DTC	O38-C14	12.35	1.39	1.22
2	C	280	DTC	O38-C14	12.30	1.39	1.22
2	H	6280	DTC	O38-C14	12.12	1.39	1.22
2	D	1280	DTC	O38-C14	12.11	1.39	1.22
2	E	5280	DTC	O38-C14	12.06	1.39	1.22
2	G	7280	DTC	O38-C14	11.90	1.39	1.22
2	A	2280	DTC	O38-C14	11.78	1.38	1.22
2	B	3280	DTC	O38-C14	11.60	1.38	1.22
2	E	4280	DTC	O32-C12	8.44	1.42	1.21
2	A	2280	DTC	O32-C12	8.37	1.42	1.21
2	G	7280	DTC	O32-C12	8.35	1.42	1.21
2	C	280	DTC	O32-C12	8.34	1.42	1.21
2	E	5280	DTC	O32-C12	8.27	1.42	1.21
2	B	3280	DTC	O32-C12	8.27	1.42	1.21
2	D	1280	DTC	O32-C12	8.27	1.42	1.21
2	H	6280	DTC	O32-C12	8.21	1.41	1.21
2	G	7280	DTC	O16-C6	7.55	1.40	1.21
2	D	1280	DTC	O16-C6	7.50	1.40	1.21
2	C	280	DTC	C15-C13	-7.41	1.31	1.54
2	E	4280	DTC	O16-C6	7.40	1.39	1.21
2	E	5280	DTC	O16-C6	7.38	1.39	1.21
2	C	280	DTC	O16-C6	7.35	1.39	1.21
2	B	3280	DTC	O16-C6	7.29	1.39	1.21
2	A	2280	DTC	O16-C6	7.26	1.39	1.21
2	D	1280	DTC	C15-C13	-7.22	1.31	1.54
2	H	6280	DTC	O16-C6	7.16	1.39	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	5280	DTC	C15-C13	-7.06	1.32	1.54
2	A	2280	DTC	C15-C13	-7.05	1.32	1.54
2	H	6280	DTC	C15-C13	-6.94	1.32	1.54
2	E	4280	DTC	C15-C13	-6.90	1.32	1.54
2	B	3280	DTC	C15-C13	-6.84	1.32	1.54
2	G	7280	DTC	C15-C13	-6.77	1.32	1.54
2	C	280	DTC	C9-C10	5.69	1.51	1.40
2	G	7280	DTC	C9-C10	5.52	1.51	1.40
2	H	6280	DTC	C9-C10	5.52	1.51	1.40
2	E	4280	DTC	C9-C10	5.50	1.51	1.40
2	B	3280	DTC	C9-C10	5.39	1.50	1.40
2	D	1280	DTC	C9-C10	5.33	1.50	1.40
2	A	2280	DTC	C9-C10	5.27	1.50	1.40
2	E	5280	DTC	C9-C10	5.18	1.50	1.40
3	F	5301	FAD	O4B-C1B	5.06	1.48	1.41
3	G	6301	FAD	O4B-C1B	4.83	1.47	1.41
3	A	301	FAD	O4B-C1B	4.82	1.47	1.41
2	E	4280	DTC	O21-C12	4.70	1.44	1.36
3	D	3301	FAD	O4B-C1B	4.54	1.47	1.41
3	H	7301	FAD	O4B-C1B	4.48	1.47	1.41
3	C	2301	FAD	O4B-C1B	4.47	1.47	1.41
2	G	7280	DTC	O21-C12	4.45	1.43	1.36
2	G	7280	DTC	O5-C6	4.36	1.43	1.36
2	B	3280	DTC	C18-C19	4.36	1.48	1.39
2	A	2280	DTC	O21-C12	4.36	1.43	1.36
2	D	1280	DTC	O5-C6	4.35	1.43	1.36
2	H	6280	DTC	O21-C12	4.33	1.43	1.36
3	C	2301	FAD	C9A-N10	4.33	1.48	1.41
2	B	3280	DTC	O5-C6	4.30	1.43	1.36
2	B	3280	DTC	C5-C20	4.30	1.46	1.39
2	D	1280	DTC	O21-C12	4.29	1.43	1.36
2	A	2280	DTC	O21-C19	4.29	1.45	1.38
2	E	5280	DTC	O21-C12	4.29	1.43	1.36
2	D	1280	DTC	O21-C19	4.27	1.45	1.38
2	B	3280	DTC	O21-C12	4.26	1.43	1.36
3	B	1301	FAD	O4B-C1B	4.26	1.47	1.41
2	E	4280	DTC	C18-C19	4.25	1.48	1.39
2	G	7280	DTC	O21-C19	4.25	1.45	1.38
2	C	280	DTC	O5-C6	4.24	1.43	1.36
2	E	4280	DTC	O5-C6	4.23	1.43	1.36
2	E	5280	DTC	C5-C20	4.21	1.46	1.39
2	G	7280	DTC	C5-C20	4.20	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	6280	DTC	C5-C20	4.19	1.46	1.39
2	E	4280	DTC	O21-C19	4.18	1.45	1.38
2	A	2280	DTC	C18-C19	4.15	1.48	1.39
2	H	6280	DTC	O5-C6	4.13	1.43	1.36
2	D	1280	DTC	C5-C20	4.13	1.46	1.39
3	E	4301	FAD	O4B-C1B	4.11	1.46	1.41
3	E	4301	FAD	O5'-C5'	4.10	1.60	1.44
2	C	280	DTC	O21-C12	4.10	1.43	1.36
3	E	4301	FAD	C9A-N10	4.09	1.48	1.41
2	E	5280	DTC	O5-C6	4.07	1.43	1.36
2	G	7280	DTC	C18-C19	4.07	1.48	1.39
2	E	4280	DTC	C5-C20	4.04	1.46	1.39
2	D	1280	DTC	C18-C19	4.03	1.48	1.39
2	E	5280	DTC	C18-C19	4.03	1.48	1.39
2	C	280	DTC	C18-C19	4.03	1.48	1.39
2	B	3280	DTC	O21-C19	4.02	1.44	1.38
2	C	280	DTC	O21-C19	4.02	1.44	1.38
3	H	7301	FAD	O5'-C5'	3.98	1.60	1.44
3	A	301	FAD	O5'-C5'	3.94	1.59	1.44
3	C	2301	FAD	O5'-C5'	3.89	1.59	1.44
2	A	2280	DTC	O5-C6	3.86	1.42	1.36
2	A	2280	DTC	C5-C20	3.84	1.46	1.39
2	C	280	DTC	C5-C20	3.83	1.46	1.39
2	H	6280	DTC	C18-C19	3.80	1.47	1.39
3	D	3301	FAD	O5'-C5'	3.78	1.59	1.44
3	A	301	FAD	O5B-C5B	-3.78	1.30	1.44
3	B	1301	FAD	O5B-C5B	-3.77	1.30	1.44
2	E	5280	DTC	O21-C19	3.77	1.44	1.38
3	C	2301	FAD	O5B-C5B	-3.70	1.30	1.44
2	H	6280	DTC	O21-C19	3.65	1.44	1.38
3	G	6301	FAD	O5B-C5B	-3.64	1.30	1.44
3	G	6301	FAD	C9A-N10	3.59	1.47	1.41
2	D	1280	DTC	O5-C10	3.54	1.44	1.38
3	G	6301	FAD	O5'-C5'	3.53	1.58	1.44
3	F	5301	FAD	O5B-C5B	-3.53	1.31	1.44
3	A	301	FAD	C9A-N10	3.52	1.47	1.41
3	E	4301	FAD	O5B-C5B	-3.51	1.31	1.44
3	H	7301	FAD	O5B-C5B	-3.49	1.31	1.44
3	C	2301	FAD	P-O2P	-3.47	1.39	1.55
3	F	5301	FAD	O5'-C5'	3.46	1.58	1.44
2	B	3280	DTC	C16-C5	3.44	1.46	1.38
2	H	6280	DTC	O5-C10	3.39	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1301	FAD	P-O2P	-3.37	1.39	1.55
3	F	5301	FAD	P-O2P	-3.33	1.39	1.55
3	D	3301	FAD	O5B-C5B	-3.32	1.32	1.44
2	E	4280	DTC	C16-C5	3.30	1.45	1.38
3	H	7301	FAD	C9A-N10	3.28	1.46	1.41
3	G	6301	FAD	P-O2P	-3.28	1.39	1.55
3	B	1301	FAD	C4X-N5	3.27	1.37	1.30
2	G	7280	DTC	O5-C10	3.26	1.43	1.38
2	A	2280	DTC	C16-C5	3.25	1.45	1.38
2	E	4280	DTC	C20-C19	3.25	1.46	1.40
3	H	7301	FAD	PA-O5B	-3.25	1.46	1.59
2	G	7280	DTC	C16-C5	3.25	1.45	1.38
3	D	3301	FAD	P-O2P	-3.25	1.40	1.55
2	E	5280	DTC	C16-C5	3.22	1.45	1.38
2	E	5280	DTC	C16-C17	3.22	1.46	1.38
2	A	2280	DTC	C16-C17	3.20	1.46	1.38
3	A	301	FAD	P-O2P	-3.19	1.40	1.55
2	E	5280	DTC	C13-C12	-3.16	1.44	1.53
2	E	5280	DTC	O5-C10	3.16	1.43	1.38
2	C	280	DTC	C20-C19	3.15	1.46	1.40
2	D	1280	DTC	C16-C17	3.14	1.46	1.38
2	E	4280	DTC	C16-C17	3.14	1.46	1.38
2	D	1280	DTC	C13-C12	-3.14	1.44	1.53
2	C	280	DTC	C16-C17	3.13	1.46	1.38
2	A	2280	DTC	C20-C19	3.12	1.46	1.40
2	G	7280	DTC	C16-C17	3.12	1.46	1.38
3	B	1301	FAD	C9A-N10	3.10	1.46	1.41
2	C	280	DTC	C16-C5	3.09	1.45	1.38
3	E	4301	FAD	P-O2P	-3.09	1.40	1.55
2	H	6280	DTC	C16-C17	3.08	1.46	1.38
3	F	5301	FAD	C9A-N10	3.07	1.46	1.41
2	B	3280	DTC	C16-C17	3.06	1.46	1.38
2	B	3280	DTC	C20-C19	3.06	1.46	1.40
2	C	280	DTC	O5-C10	3.05	1.43	1.38
2	A	2280	DTC	O5-C10	3.04	1.43	1.38
2	G	7280	DTC	C20-C19	3.03	1.46	1.40
3	B	1301	FAD	PA-O5B	-3.03	1.47	1.59
2	D	1280	DTC	C16-C5	3.03	1.45	1.38
2	B	3280	DTC	O5-C10	3.03	1.43	1.38
2	D	1280	DTC	C1-C9	3.01	1.44	1.39
3	F	5301	FAD	C4X-N5	3.01	1.36	1.30
2	C	280	DTC	C13-C12	-3.00	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1301	FAD	O5'-C5'	3.00	1.56	1.44
3	H	7301	FAD	P-O2P	-3.00	1.41	1.55
2	D	1280	DTC	C17-C18	2.99	1.45	1.38
3	A	301	FAD	PA-O5B	-2.99	1.47	1.59
2	H	6280	DTC	C17-C18	2.97	1.45	1.38
2	H	6280	DTC	C16-C5	2.96	1.45	1.38
2	E	4280	DTC	O5-C10	2.94	1.43	1.38
2	A	2280	DTC	C17-C18	2.92	1.45	1.38
2	B	3280	DTC	C2-C1	2.91	1.45	1.38
2	B	3280	DTC	C13-C12	-2.91	1.45	1.53
2	E	5280	DTC	C20-C19	2.91	1.46	1.40
2	H	6280	DTC	C13-C12	-2.90	1.45	1.53
2	B	3280	DTC	C17-C18	2.89	1.45	1.38
3	H	7301	FAD	C8-C7	2.89	1.48	1.40
3	C	2301	FAD	C4X-N5	2.89	1.36	1.30
3	E	4301	FAD	C4X-N5	2.89	1.36	1.30
2	H	6280	DTC	C1-C9	2.87	1.44	1.39
2	E	4280	DTC	C1-C9	2.86	1.44	1.39
3	G	6301	FAD	PA-O5B	-2.86	1.47	1.59
2	G	7280	DTC	C3-C4	2.85	1.44	1.38
2	E	5280	DTC	C17-C18	2.84	1.44	1.38
2	H	6280	DTC	C20-C19	2.83	1.46	1.40
3	A	301	FAD	C9A-C5X	2.82	1.45	1.41
2	H	6280	DTC	C3-C4	2.81	1.44	1.38
2	E	4280	DTC	C17-C18	2.80	1.44	1.38
2	D	1280	DTC	C3-C4	2.80	1.44	1.38
2	G	7280	DTC	C13-C12	-2.80	1.45	1.53
2	D	1280	DTC	C2-C1	2.80	1.44	1.38
3	H	7301	FAD	O2-C2	-2.79	1.19	1.24
2	G	7280	DTC	C1-C9	2.79	1.44	1.39
2	G	7280	DTC	C17-C18	2.78	1.44	1.38
2	C	280	DTC	C3-C4	2.78	1.44	1.38
2	B	3280	DTC	C1-C9	2.78	1.44	1.39
2	B	3280	DTC	C3-C4	2.76	1.44	1.38
2	E	5280	DTC	C1-C9	2.73	1.44	1.39
2	D	1280	DTC	C20-C19	2.73	1.45	1.40
3	B	1301	FAD	C2B-C1B	-2.73	1.49	1.53
2	E	5280	DTC	C3-C4	2.72	1.44	1.38
3	F	5301	FAD	PA-O5B	-2.72	1.48	1.59
2	A	2280	DTC	C2-C1	2.72	1.44	1.38
2	A	2280	DTC	C1-C9	2.72	1.44	1.39
2	H	6280	DTC	C2-C1	2.71	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2301	FAD	O2-C2	-2.71	1.19	1.24
3	H	7301	FAD	C4X-N5	2.69	1.36	1.30
3	C	2301	FAD	PA-O5B	-2.69	1.48	1.59
3	D	3301	FAD	C4A-N3A	2.67	1.39	1.35
2	E	4280	DTC	C2-C1	2.67	1.44	1.38
2	C	280	DTC	C17-C18	2.67	1.44	1.38
3	B	1301	FAD	C5'-C4'	-2.67	1.48	1.51
2	E	5280	DTC	C2-C1	2.66	1.44	1.38
2	A	2280	DTC	C13-C12	-2.64	1.46	1.53
2	A	2280	DTC	C3-C4	2.64	1.44	1.38
3	D	3301	FAD	PA-O5B	-2.63	1.48	1.59
2	E	4280	DTC	C13-C12	-2.62	1.46	1.53
3	A	301	FAD	C9-C9A	2.62	1.43	1.39
3	F	5301	FAD	C2A-N3A	2.60	1.36	1.32
3	A	301	FAD	C2A-N3A	2.60	1.36	1.32
3	D	3301	FAD	C2A-N3A	2.59	1.36	1.32
3	D	3301	FAD	C4X-N5	2.59	1.35	1.30
2	E	4280	DTC	C3-C4	2.59	1.44	1.38
3	E	4301	FAD	O2-C2	-2.59	1.19	1.24
2	E	5280	DTC	C9-C8	-2.57	1.43	1.48
2	C	280	DTC	C2-C1	2.56	1.44	1.38
2	C	280	DTC	C1-C9	2.56	1.44	1.39
3	A	301	FAD	C1'-C2'	2.56	1.56	1.52
3	G	6301	FAD	C4X-N5	2.55	1.35	1.30
3	F	5301	FAD	P-O5'	-2.53	1.49	1.59
2	G	7280	DTC	C2-C1	2.52	1.44	1.38
3	F	5301	FAD	C9A-C5X	2.51	1.45	1.41
3	H	7301	FAD	C9A-C5X	2.51	1.45	1.41
3	E	4301	FAD	PA-O5B	-2.50	1.49	1.59
3	B	1301	FAD	P-O5'	-2.50	1.49	1.59
2	E	5280	DTC	C3-C2	2.49	1.44	1.38
2	D	1280	DTC	C3-C2	2.47	1.44	1.38
2	H	6280	DTC	C3-C2	2.47	1.44	1.38
2	C	280	DTC	C3-C2	2.46	1.44	1.38
3	F	5301	FAD	C8-C7	2.44	1.47	1.40
3	B	1301	FAD	C2-N3	2.44	1.44	1.39
3	F	5301	FAD	C2-N3	2.42	1.44	1.39
3	D	3301	FAD	C2B-C1B	-2.41	1.50	1.53
2	G	7280	DTC	C3-C2	2.40	1.44	1.38
3	G	6301	FAD	C4A-N3A	2.40	1.39	1.35
3	E	4301	FAD	C2-N3	2.38	1.44	1.39
3	A	301	FAD	C10-N1	2.38	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	FAD	C9-C8	2.37	1.43	1.39
3	G	6301	FAD	O2-C2	-2.37	1.19	1.24
2	B	3280	DTC	C3-C2	2.36	1.44	1.38
3	G	6301	FAD	C1'-C2'	2.35	1.56	1.52
3	B	1301	FAD	C6-C5X	2.35	1.43	1.40
3	A	301	FAD	C4A-N3A	2.35	1.38	1.35
3	D	3301	FAD	C9A-C5X	2.34	1.45	1.41
2	E	4280	DTC	C9-C8	-2.33	1.44	1.48
2	E	4280	DTC	C3-C2	2.32	1.44	1.38
2	C	280	DTC	C9-C8	-2.32	1.44	1.48
3	A	301	FAD	P-O5'	-2.32	1.49	1.59
2	A	2280	DTC	C3-C2	2.32	1.44	1.38
3	A	301	FAD	C8-C7	2.31	1.46	1.40
3	G	6301	FAD	P-O5'	-2.31	1.49	1.59
3	G	6301	FAD	C8-C7	2.30	1.46	1.40
3	B	1301	FAD	C4A-N3A	2.29	1.38	1.35
3	C	2301	FAD	C6-C5X	2.29	1.43	1.40
3	A	301	FAD	C4X-N5	2.29	1.35	1.30
3	G	6301	FAD	C9-C8	2.29	1.42	1.39
3	G	6301	FAD	C2A-N3A	2.27	1.35	1.32
3	D	3301	FAD	C2-N3	2.26	1.44	1.39
3	G	6301	FAD	C6-C5X	2.26	1.43	1.40
3	H	7301	FAD	P-O1P	2.24	1.58	1.50
3	D	3301	FAD	C8-C7	2.23	1.46	1.40
3	H	7301	FAD	C1'-C2'	2.23	1.55	1.52
3	F	5301	FAD	C4A-N3A	2.23	1.38	1.35
3	C	2301	FAD	C2-N3	2.23	1.44	1.39
3	C	2301	FAD	C2B-C1B	-2.23	1.50	1.53
3	D	3301	FAD	C10-N1	2.22	1.37	1.33
2	G	7280	DTC	C9-C8	-2.21	1.44	1.48
3	G	6301	FAD	C9A-C5X	2.20	1.44	1.41
3	C	2301	FAD	C1'-C2'	2.18	1.55	1.52
2	A	2280	DTC	C9-C8	-2.17	1.44	1.48
3	F	5301	FAD	C1'-C2'	2.17	1.55	1.52
3	D	3301	FAD	P-O5'	-2.15	1.50	1.59
3	E	4301	FAD	C10-N1	2.15	1.37	1.33
3	D	3301	FAD	C2A-N1A	2.13	1.37	1.33
3	B	1301	FAD	O2-C2	-2.13	1.20	1.24
3	C	2301	FAD	C10-N1	2.11	1.37	1.33
3	E	4301	FAD	C2B-C1B	-2.10	1.50	1.53
3	E	4301	FAD	C8-C7	2.10	1.46	1.40
3	H	7301	FAD	C10-N1	2.09	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1301	FAD	C9A-C5X	2.09	1.44	1.41
3	H	7301	FAD	C2A-N3A	2.06	1.35	1.32
3	C	2301	FAD	C8-C7	2.05	1.46	1.40
3	F	5301	FAD	C6-C5X	2.05	1.43	1.40
3	C	2301	FAD	C2A-N3A	2.03	1.35	1.32
3	G	6301	FAD	C10-N1	2.02	1.37	1.33
3	A	301	FAD	O2-C2	-2.02	1.20	1.24
3	F	5301	FAD	C2A-N1A	2.01	1.37	1.33
2	H	6280	DTC	C9-C8	-2.00	1.44	1.48

All (170) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	4301	FAD	O2A-PA-O5B	-14.92	38.45	107.75
3	C	2301	FAD	O2A-PA-O5B	-14.28	41.43	107.75
3	B	1301	FAD	O2A-PA-O5B	-14.03	42.59	107.75
3	D	3301	FAD	O2A-PA-O5B	-13.90	43.20	107.75
3	F	5301	FAD	O2A-PA-O5B	-13.82	43.58	107.75
3	A	301	FAD	O2A-PA-O5B	-13.58	44.70	107.75
3	G	6301	FAD	O2A-PA-O5B	-13.45	45.27	107.75
3	H	7301	FAD	O2A-PA-O5B	-12.91	47.80	107.75
3	H	7301	FAD	O2A-PA-O1A	-8.37	70.85	112.24
3	H	7301	FAD	O5B-PA-O1A	-7.53	79.66	109.07
3	A	301	FAD	O2A-PA-O1A	-7.41	75.58	112.24
3	A	301	FAD	O5B-PA-O1A	-7.36	80.30	109.07
3	G	6301	FAD	O5B-PA-O1A	-7.28	80.63	109.07
3	B	1301	FAD	O5B-PA-O1A	-7.00	81.71	109.07
3	F	5301	FAD	O5B-PA-O1A	-6.77	82.61	109.07
3	G	6301	FAD	O2A-PA-O1A	-6.71	79.07	112.24
3	D	3301	FAD	O5B-PA-O1A	-6.70	82.90	109.07
3	E	4301	FAD	O5B-PA-O1A	-6.58	83.36	109.07
3	F	5301	FAD	O2A-PA-O1A	-6.55	79.86	112.24
3	B	1301	FAD	O2A-PA-O1A	-6.46	80.30	112.24
3	C	2301	FAD	O5B-PA-O1A	-6.46	83.83	109.07
3	D	3301	FAD	O2A-PA-O1A	-5.88	83.18	112.24
3	C	2301	FAD	O2A-PA-O1A	-5.30	86.02	112.24
3	E	4301	FAD	O2A-PA-O1A	-5.26	86.21	112.24
3	H	7301	FAD	PA-O5B-C5B	4.68	149.15	121.68
3	D	3301	FAD	PA-O5B-C5B	4.43	147.65	121.68
3	A	301	FAD	PA-O5B-C5B	4.38	147.36	121.68
3	E	4301	FAD	PA-O5B-C5B	4.37	147.31	121.68
3	B	1301	FAD	PA-O5B-C5B	4.37	147.31	121.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	6301	FAD	PA-O5B-C5B	4.36	147.26	121.68
3	F	5301	FAD	O4B-C1B-C2B	-4.32	100.62	106.93
3	F	5301	FAD	PA-O5B-C5B	4.26	146.68	121.68
3	C	2301	FAD	PA-O5B-C5B	4.24	146.55	121.68
2	B	3280	DTC	C15-C7-C6	3.81	123.72	112.36
3	G	6301	FAD	O4B-C1B-C2B	-3.76	101.42	106.93
2	G	7280	DTC	C15-C7-C6	3.74	123.49	112.36
2	E	5280	DTC	C9-C8-C7	3.73	121.82	116.65
2	B	3280	DTC	C9-C8-C7	3.70	121.76	116.65
3	D	3301	FAD	O4B-C1B-C2B	-3.65	101.59	106.93
2	G	7280	DTC	C9-C8-C7	3.64	121.69	116.65
3	C	2301	FAD	O4B-C1B-C2B	-3.63	101.62	106.93
2	C	280	DTC	C15-C7-C6	3.62	123.16	112.36
2	E	5280	DTC	C15-C7-C6	3.61	123.11	112.36
3	H	7301	FAD	O4B-C1B-C2B	-3.60	101.67	106.93
2	D	1280	DTC	C9-C8-C7	3.60	121.63	116.65
2	H	6280	DTC	C15-C7-C6	3.60	123.08	112.36
2	A	2280	DTC	C15-C7-C6	3.59	123.06	112.36
2	E	4280	DTC	C15-C7-C6	3.58	123.02	112.36
2	D	1280	DTC	C15-C7-C6	3.58	123.01	112.36
2	H	6280	DTC	C9-C8-C7	3.53	121.54	116.65
3	E	4301	FAD	O4B-C1B-C2B	-3.52	101.78	106.93
2	A	2280	DTC	C9-C8-C7	3.52	121.52	116.65
2	E	4280	DTC	C9-C8-C7	3.50	121.49	116.65
2	C	280	DTC	C9-C8-C7	3.41	121.36	116.65
3	A	301	FAD	O4B-C1B-C2B	-3.17	102.29	106.93
2	E	5280	DTC	C19-C20-C14	-2.97	118.58	120.48
2	D	1280	DTC	C19-C20-C14	-2.92	118.61	120.48
3	H	7301	FAD	C5A-C6A-N6A	2.91	124.77	120.35
2	C	280	DTC	C19-C20-C14	-2.87	118.65	120.48
2	B	3280	DTC	C19-C20-C14	-2.85	118.66	120.48
2	H	6280	DTC	C19-C20-C14	-2.81	118.69	120.48
3	E	4301	FAD	C5A-C6A-N6A	2.73	124.50	120.35
2	D	1280	DTC	C20-C14-C13	2.70	120.38	116.65
2	G	7280	DTC	C20-C14-C13	2.68	120.36	116.65
2	G	7280	DTC	C19-C20-C14	-2.67	118.77	120.48
2	A	2280	DTC	C20-C14-C13	2.67	120.34	116.65
3	B	1301	FAD	O4B-C1B-C2B	-2.67	103.03	106.93
2	B	3280	DTC	C20-C14-C13	2.64	120.31	116.65
2	E	5280	DTC	C20-C14-C13	2.63	120.29	116.65
3	B	1301	FAD	C5A-C6A-N6A	2.62	124.33	120.35
2	H	6280	DTC	C20-C14-C13	2.62	120.27	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	4301	FAD	C5A-C6A-N1A	-2.61	114.43	120.35
2	H	6280	DTC	O5-C10-C4	2.52	119.60	116.26
3	C	2301	FAD	C2A-N1A-C6A	2.51	123.05	118.75
2	E	4280	DTC	C19-C20-C14	-2.50	118.88	120.48
3	E	4301	FAD	C4-N3-C2	-2.49	121.03	125.64
3	B	1301	FAD	C2A-N1A-C6A	2.48	123.00	118.75
2	E	4280	DTC	C20-C14-C13	2.48	120.08	116.65
2	E	5280	DTC	O5-C10-C4	2.48	119.55	116.26
3	H	7301	FAD	C5A-C6A-N1A	-2.48	114.73	120.35
2	A	2280	DTC	C19-C20-C14	-2.48	118.89	120.48
2	C	280	DTC	C20-C14-C13	2.46	120.06	116.65
2	D	1280	DTC	O5-C10-C4	2.46	119.52	116.26
3	E	4301	FAD	C2A-N1A-C6A	2.45	122.95	118.75
3	H	7301	FAD	C2A-N1A-C6A	2.44	122.93	118.75
3	C	2301	FAD	C5A-C6A-N6A	2.42	124.02	120.35
3	C	2301	FAD	C4-N3-C2	-2.41	121.19	125.64
2	E	5280	DTC	C10-C9-C8	-2.41	118.94	120.48
2	A	2280	DTC	C10-C9-C8	-2.40	118.95	120.48
3	C	2301	FAD	C5A-C6A-N1A	-2.39	114.93	120.35
2	B	3280	DTC	O21-C12-C13	2.39	120.20	116.72
2	D	1280	DTC	C10-C9-C8	-2.37	118.96	120.48
3	A	301	FAD	C4-N3-C2	-2.37	121.27	125.64
3	F	5301	FAD	C4-N3-C2	-2.37	121.27	125.64
3	A	301	FAD	C5A-C6A-N6A	2.36	123.94	120.35
3	G	6301	FAD	C4-N3-C2	-2.35	121.29	125.64
2	H	6280	DTC	O21-C12-C13	2.35	120.14	116.72
2	E	4280	DTC	O21-C12-C13	2.35	120.14	116.72
2	G	7280	DTC	O21-C12-C13	2.34	120.14	116.72
2	B	3280	DTC	C5-C20-C14	2.33	123.29	119.80
3	B	1301	FAD	C5A-C6A-N1A	-2.33	115.07	120.35
2	B	3280	DTC	O5-C10-C4	2.33	119.34	116.26
3	G	6301	FAD	C5X-C9A-N10	-2.32	115.56	117.95
2	A	2280	DTC	O5-C10-C4	2.31	119.33	116.26
3	D	3301	FAD	C4-N3-C2	-2.31	121.38	125.64
2	C	280	DTC	O5-C10-C4	2.30	119.31	116.26
3	B	1301	FAD	C4-N3-C2	-2.30	121.39	125.64
3	D	3301	FAD	C5A-C6A-N1A	-2.30	115.14	120.35
2	E	5280	DTC	O21-C12-C13	2.30	120.07	116.72
3	F	5301	FAD	C5A-C6A-N1A	-2.30	115.14	120.35
2	G	7280	DTC	O5-C10-C4	2.28	119.29	116.26
3	D	3301	FAD	C2A-N1A-C6A	2.27	122.64	118.75
3	G	6301	FAD	C5A-C6A-N1A	-2.27	115.21	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	4280	DTC	O5-C10-C4	2.26	119.25	116.26
3	A	301	FAD	C5X-C9A-N10	-2.26	115.62	117.95
2	E	5280	DTC	C5-C20-C14	2.25	123.17	119.80
3	G	6301	FAD	C2A-N1A-C6A	2.25	122.61	118.75
2	C	280	DTC	O21-C12-C13	2.25	119.99	116.72
2	A	2280	DTC	O21-C12-C13	2.24	119.98	116.72
3	A	301	FAD	C5A-C6A-N1A	-2.23	115.30	120.35
3	E	4301	FAD	P-O3P-PA	2.20	140.39	132.83
2	G	7280	DTC	C10-C9-C8	-2.19	119.08	120.48
2	H	6280	DTC	C10-C9-C8	-2.19	119.08	120.48
3	D	3301	FAD	C5X-C9A-N10	-2.19	115.69	117.95
3	C	2301	FAD	C4'-C3'-C2'	-2.19	108.81	113.36
2	E	5280	DTC	C19-O21-C12	2.19	123.42	121.39
3	A	301	FAD	C4X-C10-N1	-2.17	119.70	124.73
3	D	3301	FAD	C4X-C10-N10	2.16	119.64	116.48
3	H	7301	FAD	C4-N3-C2	-2.16	121.66	125.64
3	G	6301	FAD	C9-C9A-N10	2.15	124.74	121.84
3	A	301	FAD	C2A-N1A-C6A	2.15	122.43	118.75
2	D	1280	DTC	O21-C12-C13	2.15	119.84	116.72
2	B	3280	DTC	C10-C9-C8	-2.14	119.11	120.48
3	B	1301	FAD	C5'-C4'-C3'	-2.13	108.09	112.20
2	D	1280	DTC	C1-C9-C8	2.13	122.98	119.80
3	F	5301	FAD	C2A-N1A-C6A	2.13	122.39	118.75
2	B	3280	DTC	C1-C9-C8	2.13	122.98	119.80
3	D	3301	FAD	C5A-C6A-N6A	2.12	123.58	120.35
3	F	5301	FAD	C4X-C10-N10	2.11	119.57	116.48
2	C	280	DTC	C5-C20-C14	2.11	122.95	119.80
2	H	6280	DTC	C5-C20-C14	2.10	122.94	119.80
2	B	3280	DTC	C19-O21-C12	2.10	123.34	121.39
3	C	2301	FAD	O5'-P-O1P	-2.10	100.88	109.07
2	A	2280	DTC	C1-C9-C8	2.09	122.93	119.80
3	D	3301	FAD	O3B-C3B-C2B	2.08	118.54	111.82
3	B	1301	FAD	C10-N1-C2	2.08	121.05	116.90
3	B	1301	FAD	C4X-C10-N10	2.07	119.51	116.48
3	G	6301	FAD	O3B-C3B-C2B	2.07	118.51	111.82
2	E	4280	DTC	C5-C20-C14	2.07	122.89	119.80
3	F	5301	FAD	C5A-C6A-N6A	2.05	123.47	120.35
3	E	4301	FAD	C10-N1-C2	2.05	121.00	116.90
3	B	1301	FAD	P-O3P-PA	2.05	139.85	132.83
3	D	3301	FAD	O5'-P-O1P	-2.05	101.07	109.07
2	D	1280	DTC	C5-C20-C14	2.04	122.85	119.80
3	F	5301	FAD	O3B-C3B-C2B	2.04	118.41	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	7280	DTC	C5-C20-C14	2.03	122.84	119.80
3	G	6301	FAD	O3B-C3B-C4B	2.03	116.91	111.05
3	E	4301	FAD	O3B-C3B-C2B	2.02	118.37	111.82
3	D	3301	FAD	C10-N1-C2	2.02	120.95	116.90
3	A	301	FAD	O3B-C3B-C2B	2.02	118.37	111.82
2	E	4280	DTC	C10-C9-C8	-2.02	119.19	120.48
2	B	3280	DTC	O21-C19-C18	2.02	118.93	116.26
3	H	7301	FAD	C4X-C10-N10	2.02	119.43	116.48
3	E	4301	FAD	C3B-C2B-C1B	2.01	104.01	100.98
2	C	280	DTC	C10-C9-C8	-2.01	119.20	120.48
3	A	301	FAD	C4X-C10-N10	2.01	119.41	116.48
3	G	6301	FAD	C4X-C10-N10	2.01	119.41	116.48
2	G	7280	DTC	O21-C19-C18	2.00	118.92	116.26
3	C	2301	FAD	O3B-C3B-C2B	2.00	118.31	111.82
3	F	5301	FAD	C5'-C4'-C3'	-2.00	108.33	112.20

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 (57) 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

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Mol	Chain	Res	Type	Atoms
2	C	280	DTC	C12-C13-C15-C7
2	D	1280	DTC	C13-C15-C7-C8
2	D	1280	DTC	C12-C13-C15-C7
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	G	7280	DTC	C12-C13-C15-C7
2	H	6280	DTC	C13-C15-C7-C8
2	H	6280	DTC	C12-C13-C15-C7
3	A	301	FAD	C5B-O5B-PA-O3P
3	B	1301	FAD	C5B-O5B-PA-O3P
3	C	2301	FAD	C5B-O5B-PA-O1A
3	C	2301	FAD	C5B-O5B-PA-O3P
3	C	2301	FAD	C5'-O5'-P-O1P
3	D	3301	FAD	C5B-O5B-PA-O1A
3	D	3301	FAD	C5B-O5B-PA-O3P
3	E	4301	FAD	C5B-O5B-PA-O1A
3	E	4301	FAD	C5B-O5B-PA-O3P
3	F	5301	FAD	C5B-O5B-PA-O3P
3	G	6301	FAD	C5B-O5B-PA-O3P
3	H	7301	FAD	C5B-O5B-PA-O3P
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
2	A	2280	DTC	C12-C13-C15-C7
2	E	4280	DTC	C12-C13-C15-C7
3	H	7301	FAD	C3B-C4B-C5B-O5B
3	C	2301	FAD	C5'-O5'-P-O3P
3	D	3301	FAD	O4B-C4B-C5B-O5B
3	F	5301	FAD	P-O3P-PA-O1A
3	G	6301	FAD	P-O3P-PA-O1A
3	A	301	FAD	C5B-O5B-PA-O1A
3	B	1301	FAD	C5B-O5B-PA-O1A
3	F	5301	FAD	C5B-O5B-PA-O1A
3	G	6301	FAD	C5B-O5B-PA-O1A
3	H	7301	FAD	C5B-O5B-PA-O1A
3	G	6301	FAD	O4B-C4B-C5B-O5B
3	A	301	FAD	P-O3P-PA-O1A
3	C	2301	FAD	P-O3P-PA-O1A

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Mol	Chain	Res	Type	Atoms
3	E	4301	FAD	P-O3P-PA-O1A
3	E	4301	FAD	C3B-C4B-C5B-O5B
3	H	7301	FAD	C4'-C5'-O5'-P
3	D	3301	FAD	C3B-C4B-C5B-O5B
3	F	5301	FAD	O4B-C4B-C5B-O5B
3	G	6301	FAD	C4'-C5'-O5'-P
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	D	3301	FAD	C4'-C5'-O5'-P
3	B	1301	FAD	C5'-O5'-P-O1P
3	D	3301	FAD	C5'-O5'-P-O1P

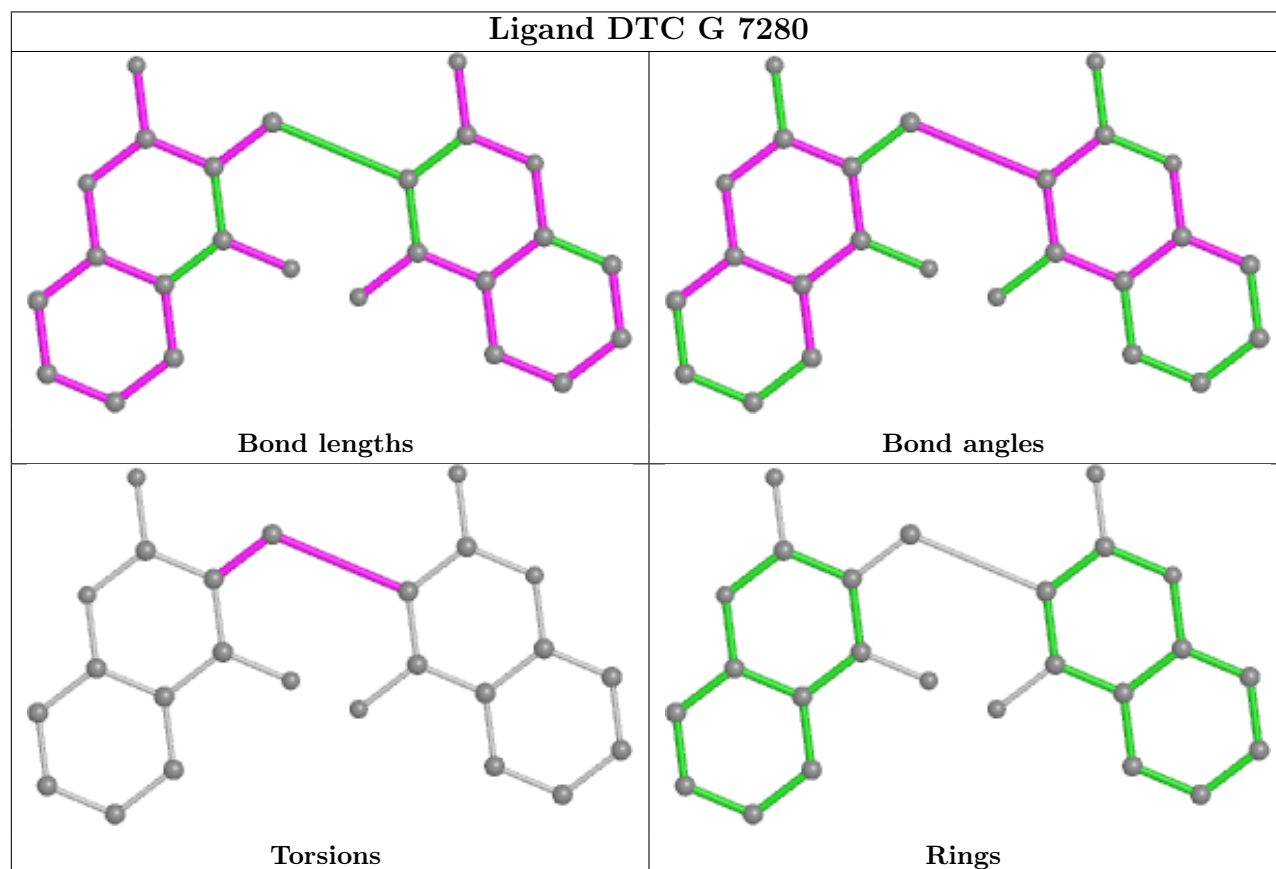
There are no ring outliers.

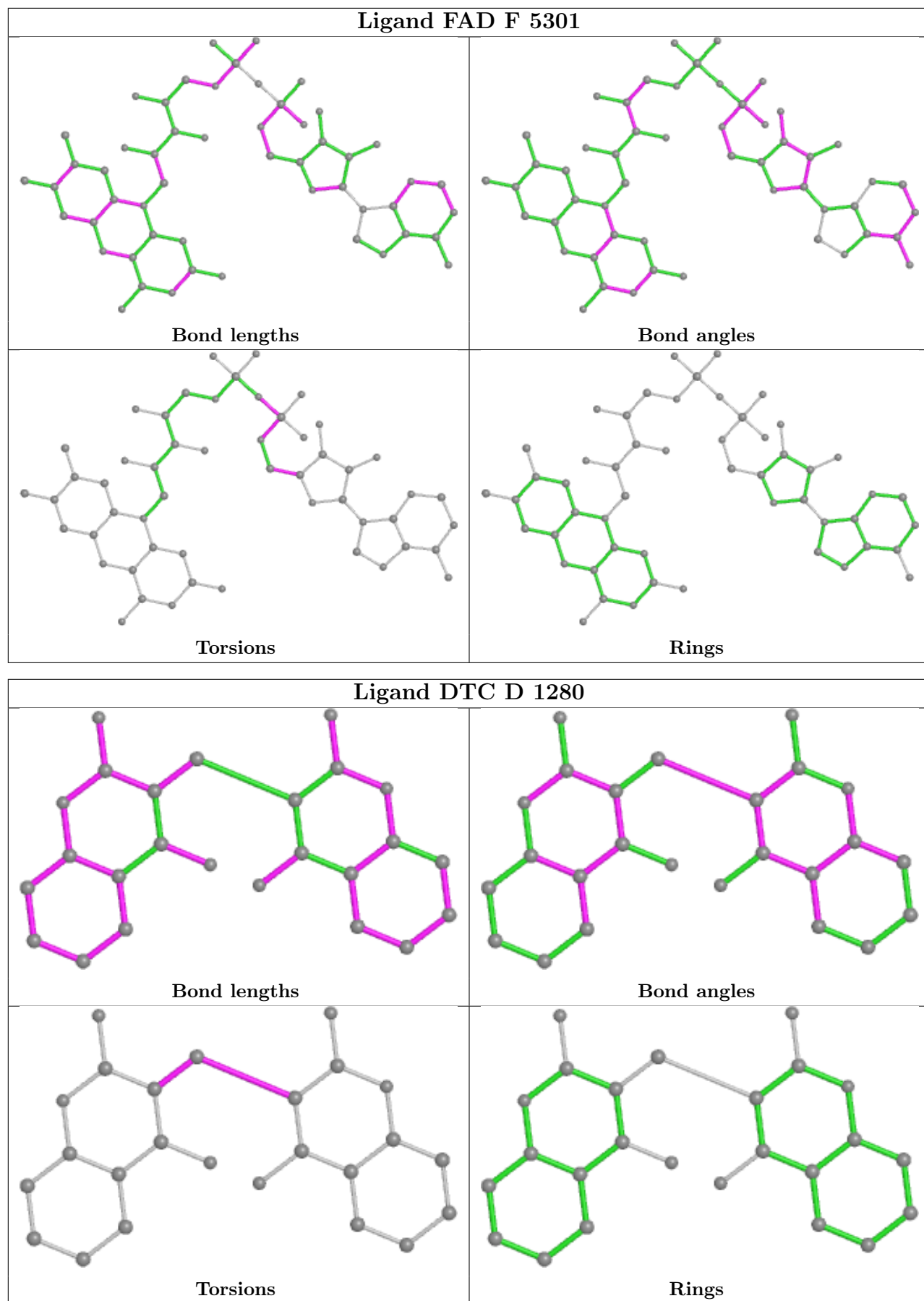
16 monomers are involved in 46 short contacts:

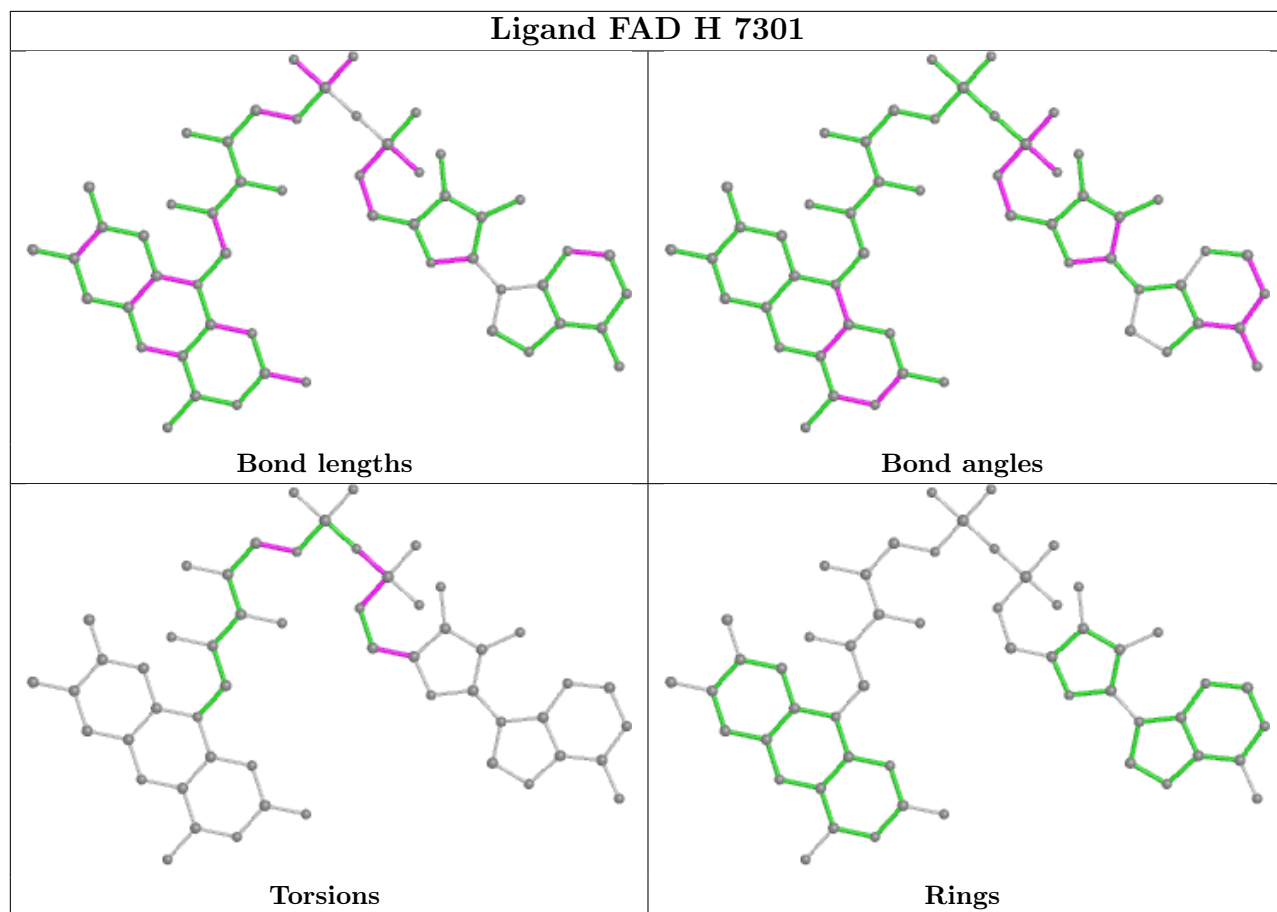
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	7280	DTC	5	0
3	F	5301	FAD	2	0
2	D	1280	DTC	1	0
3	H	7301	FAD	5	0
3	C	2301	FAD	6	0
3	E	4301	FAD	2	0
2	B	3280	DTC	1	0
3	B	1301	FAD	5	0
3	G	6301	FAD	2	0
2	H	6280	DTC	3	0
3	D	3301	FAD	4	0
2	A	2280	DTC	1	0
2	C	280	DTC	2	0
2	E	4280	DTC	1	0
2	E	5280	DTC	2	0
3	A	301	FAD	4	0

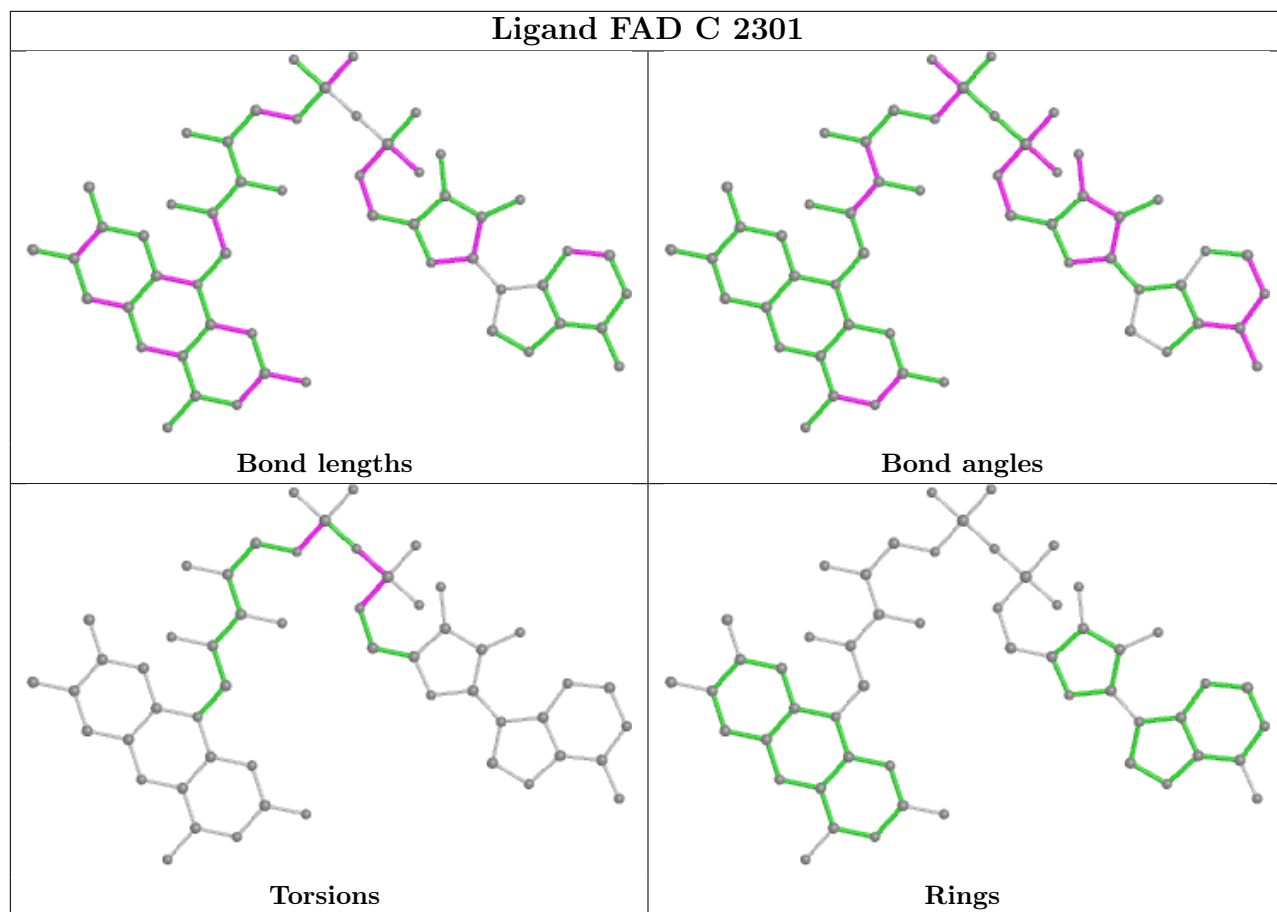
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

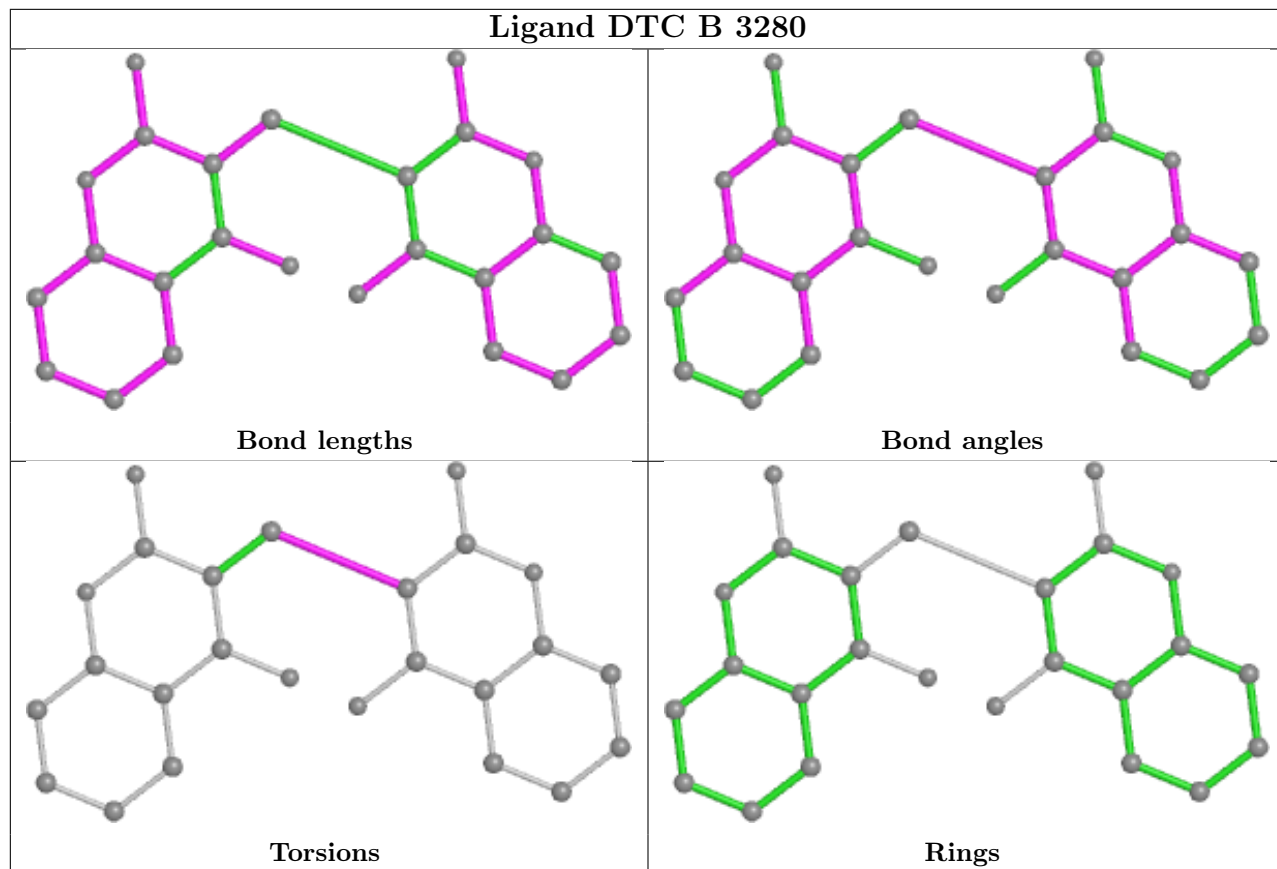
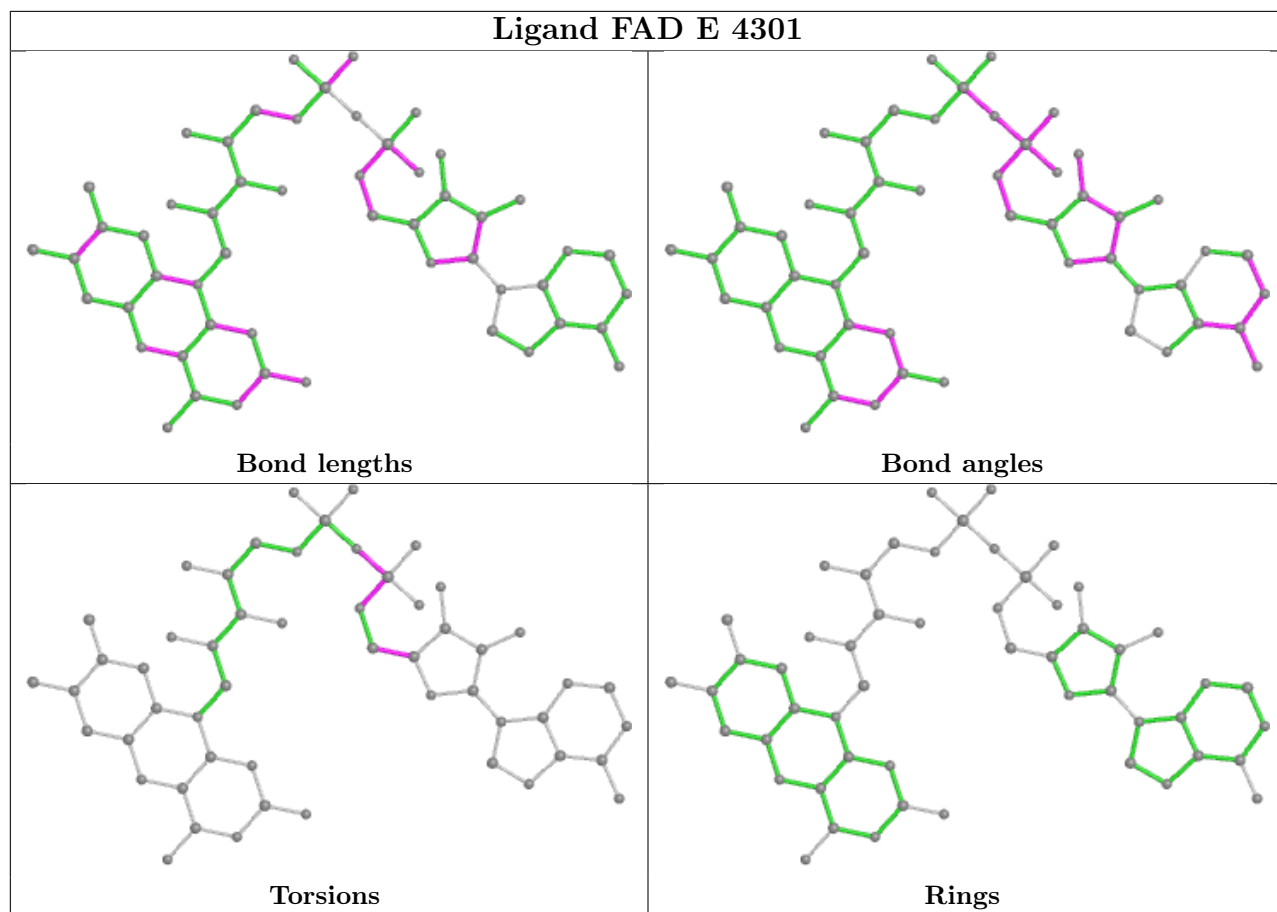
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

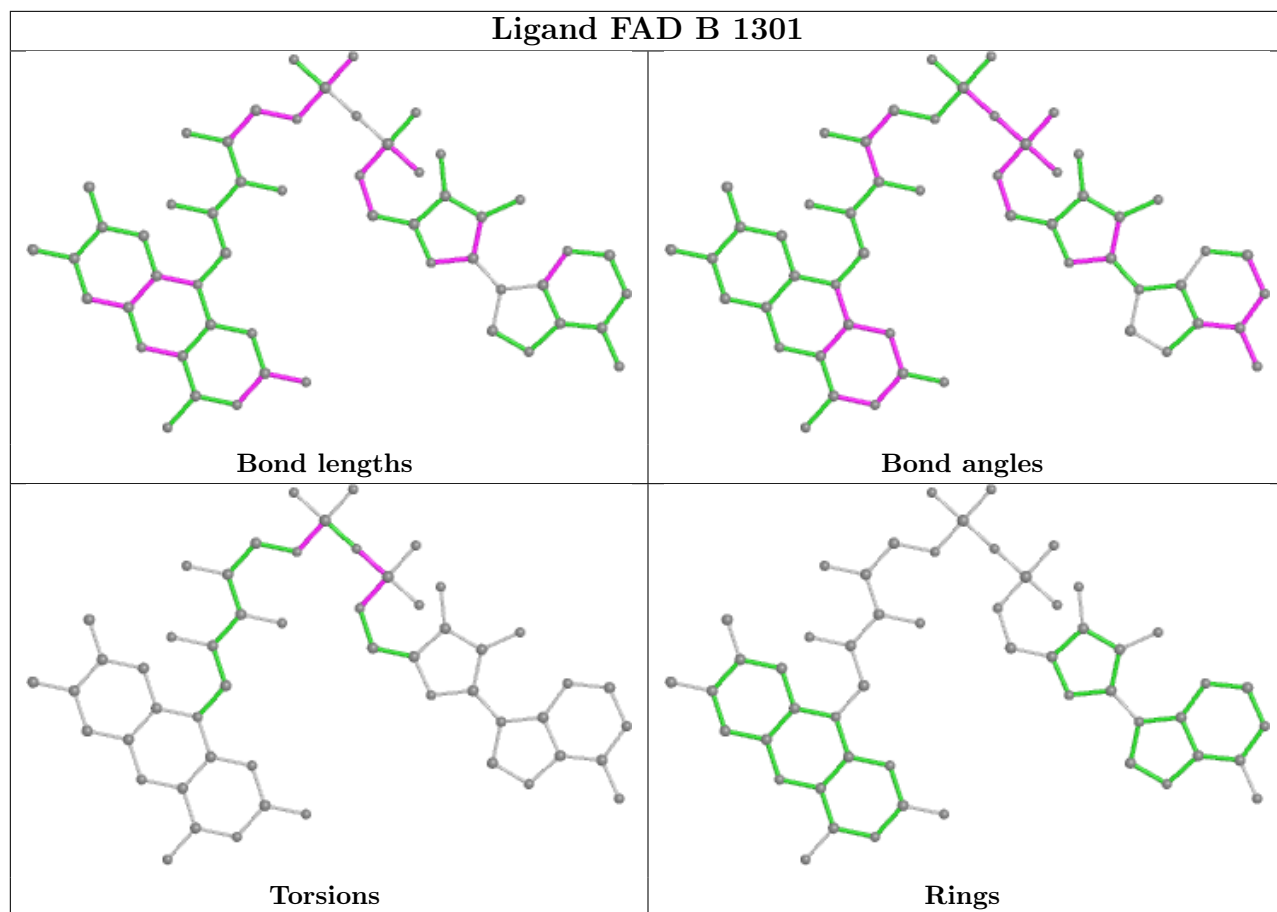


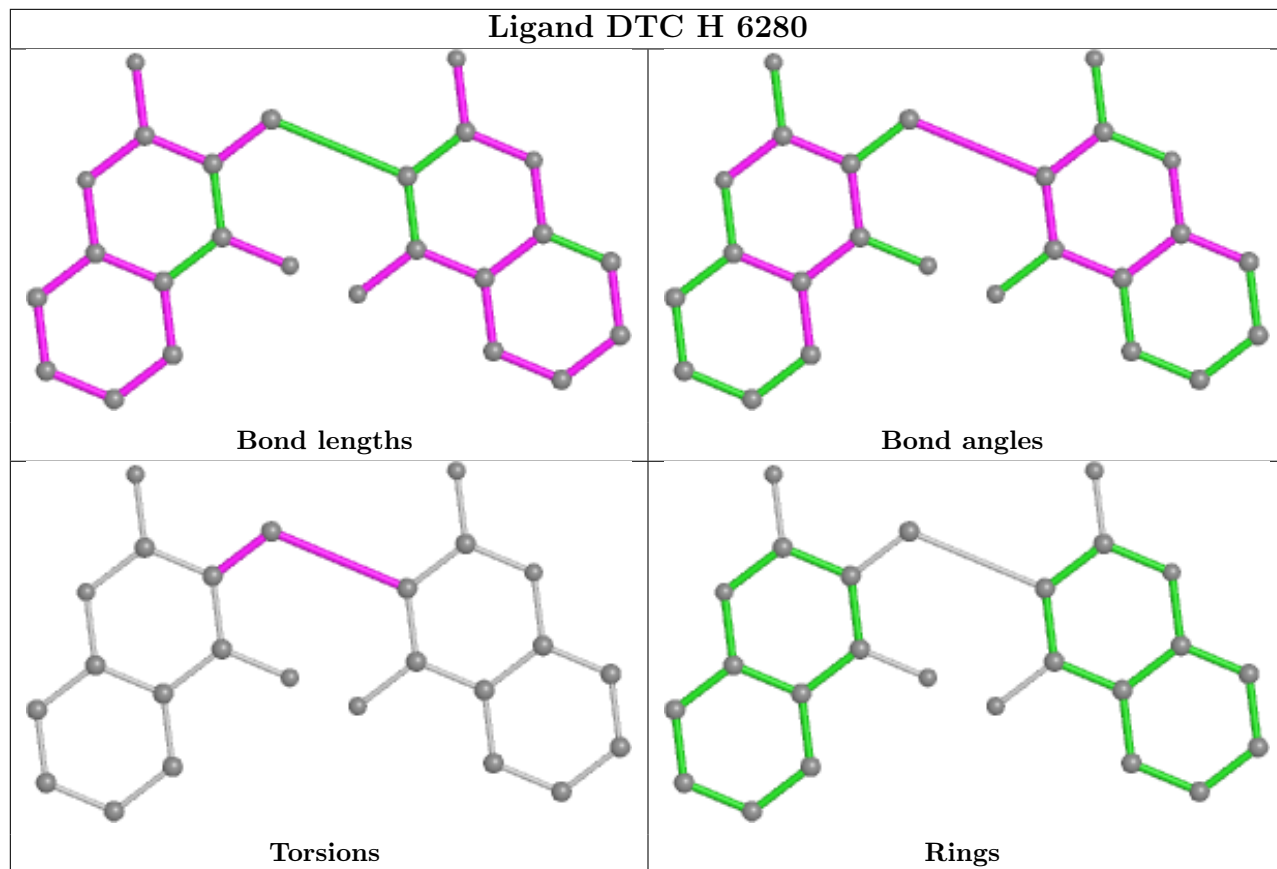
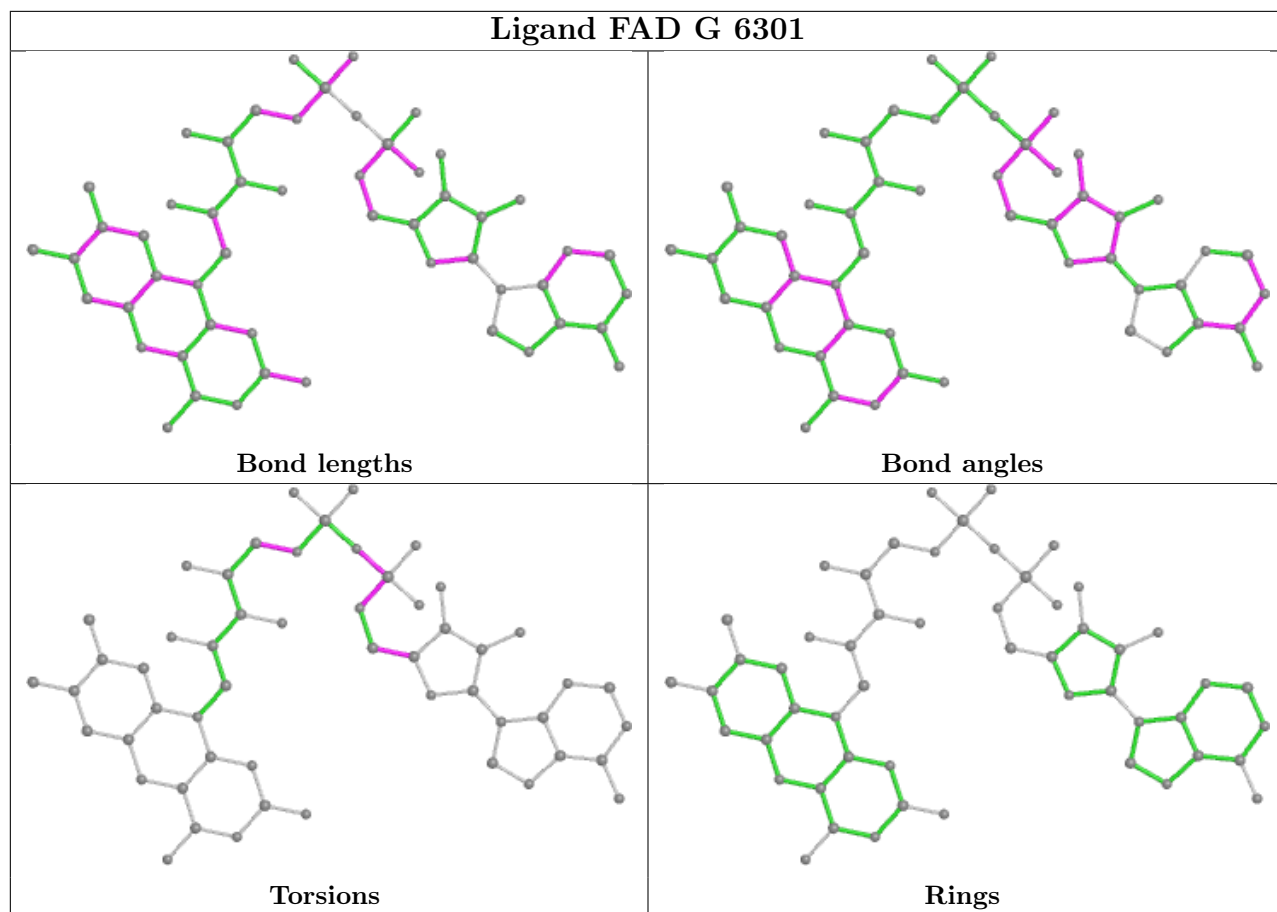


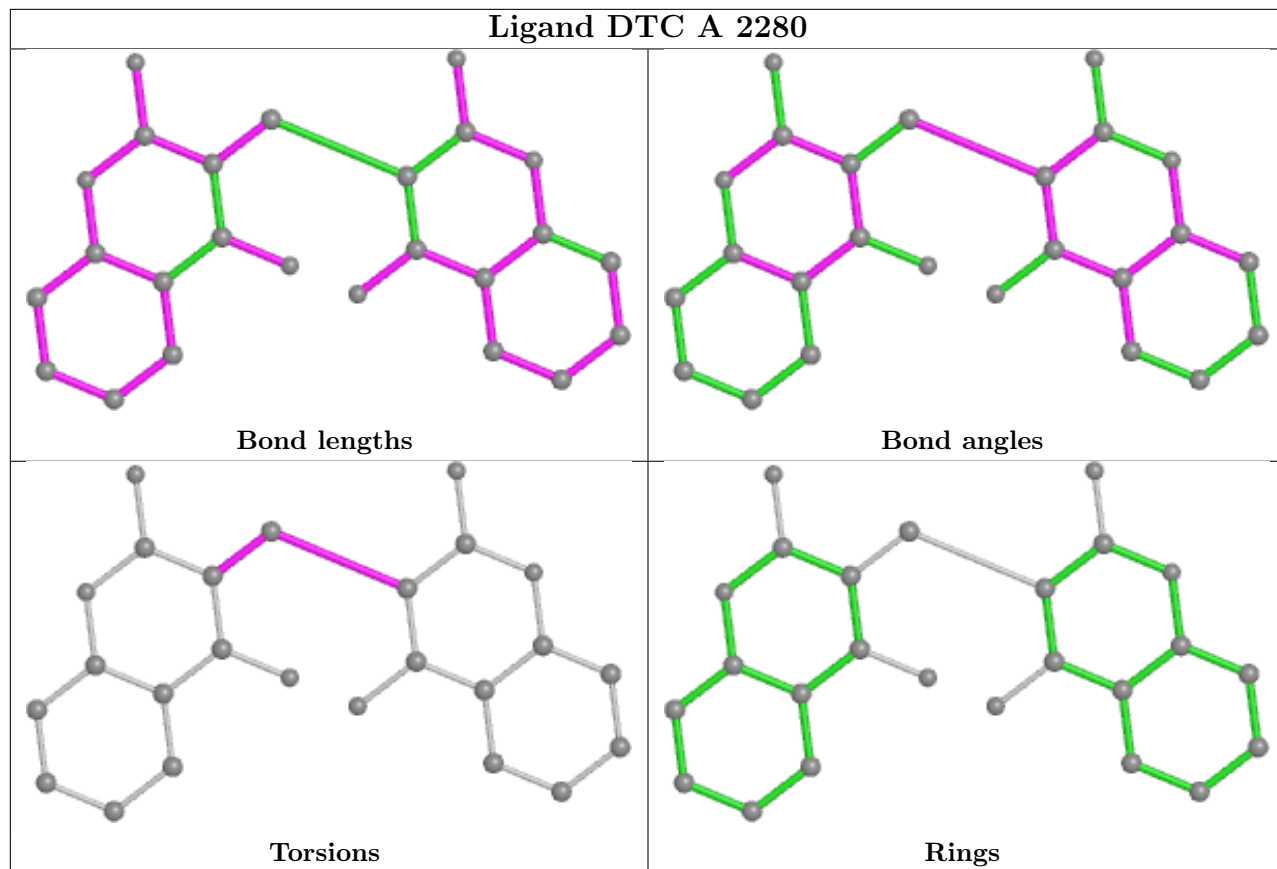
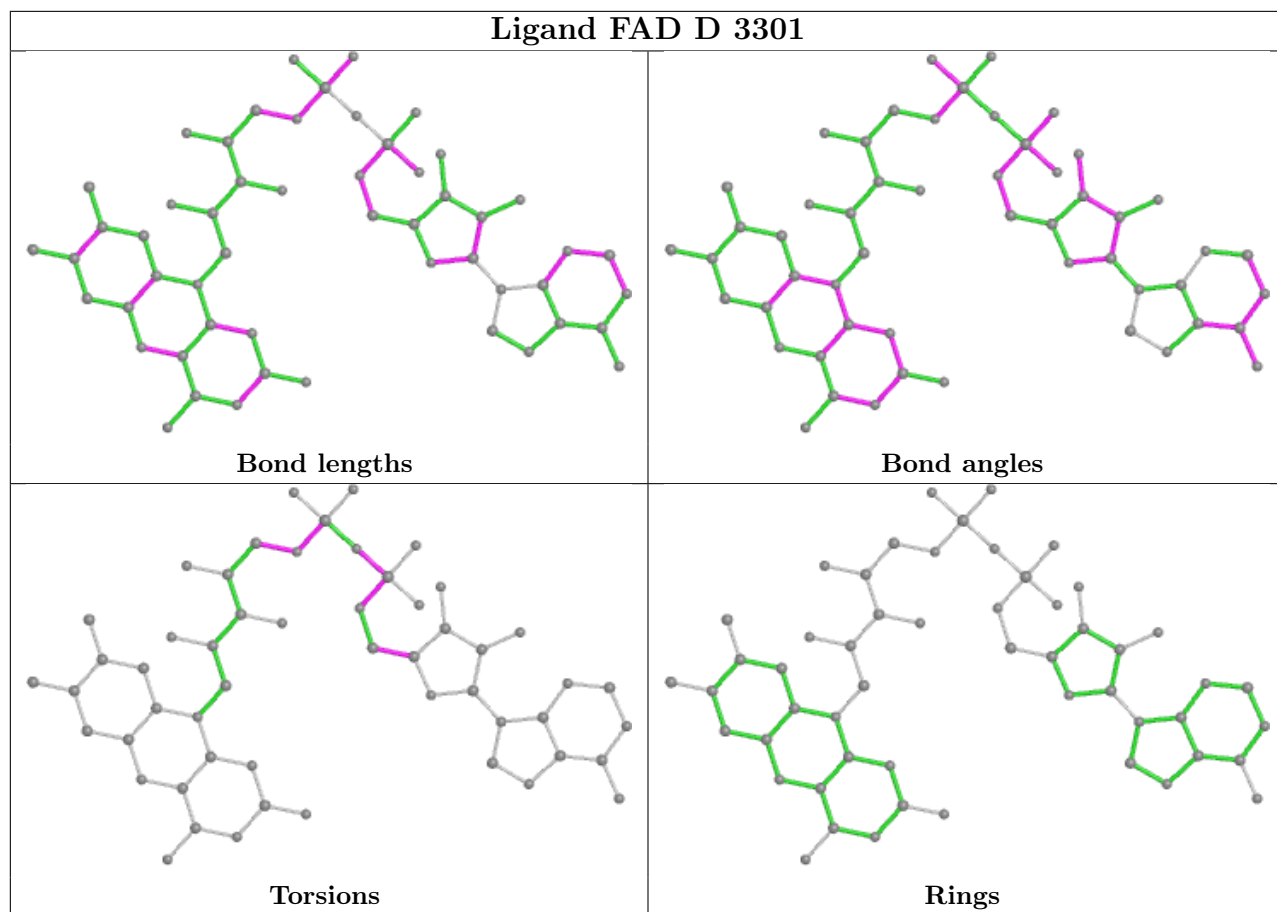


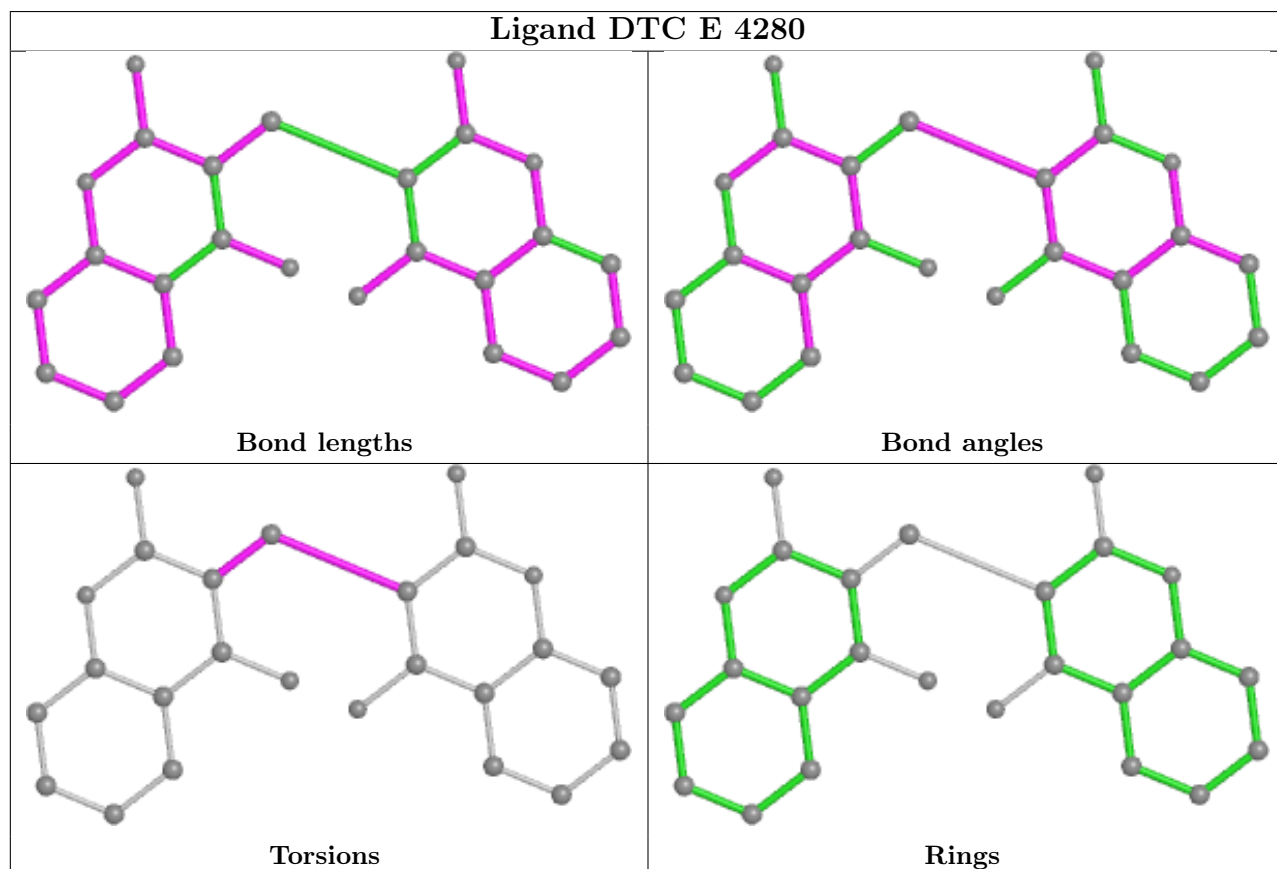
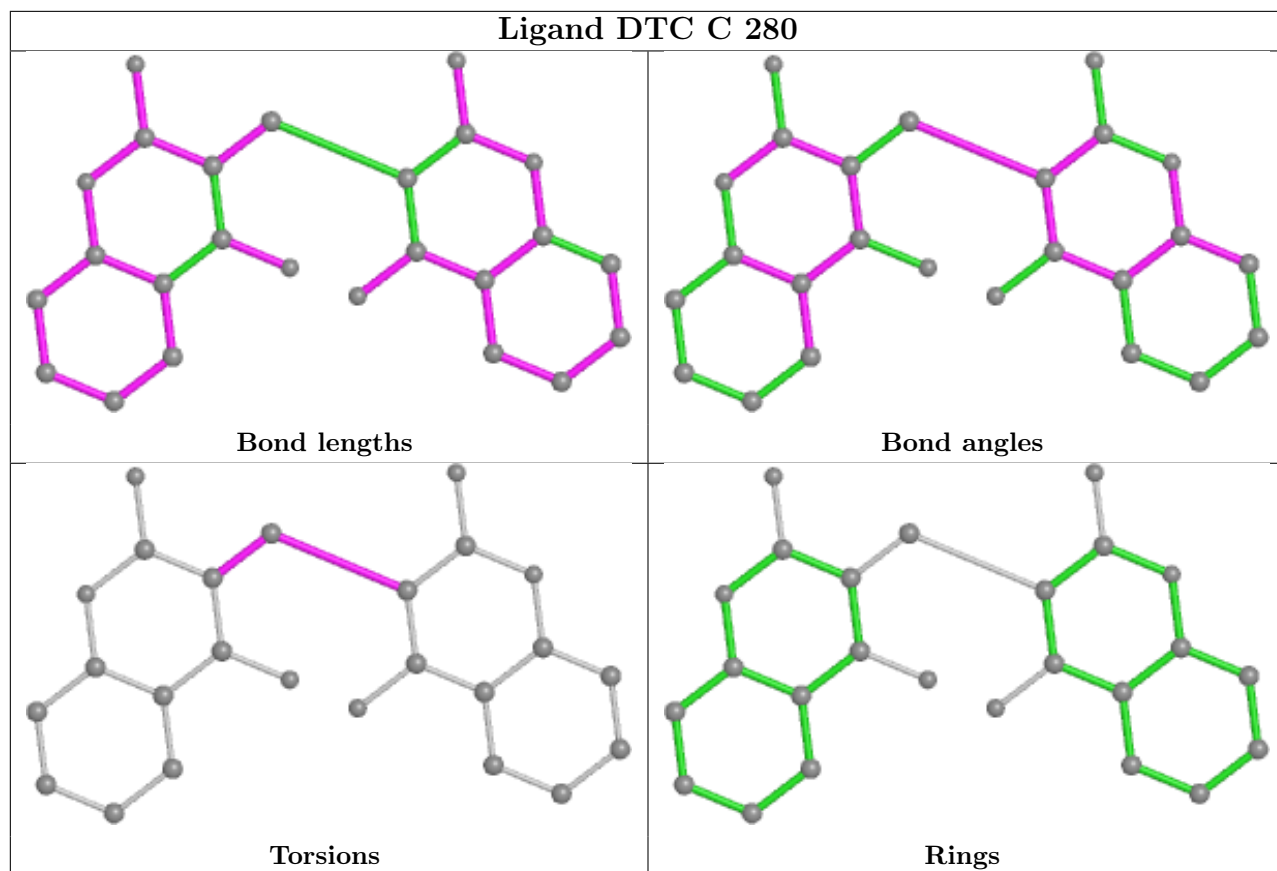


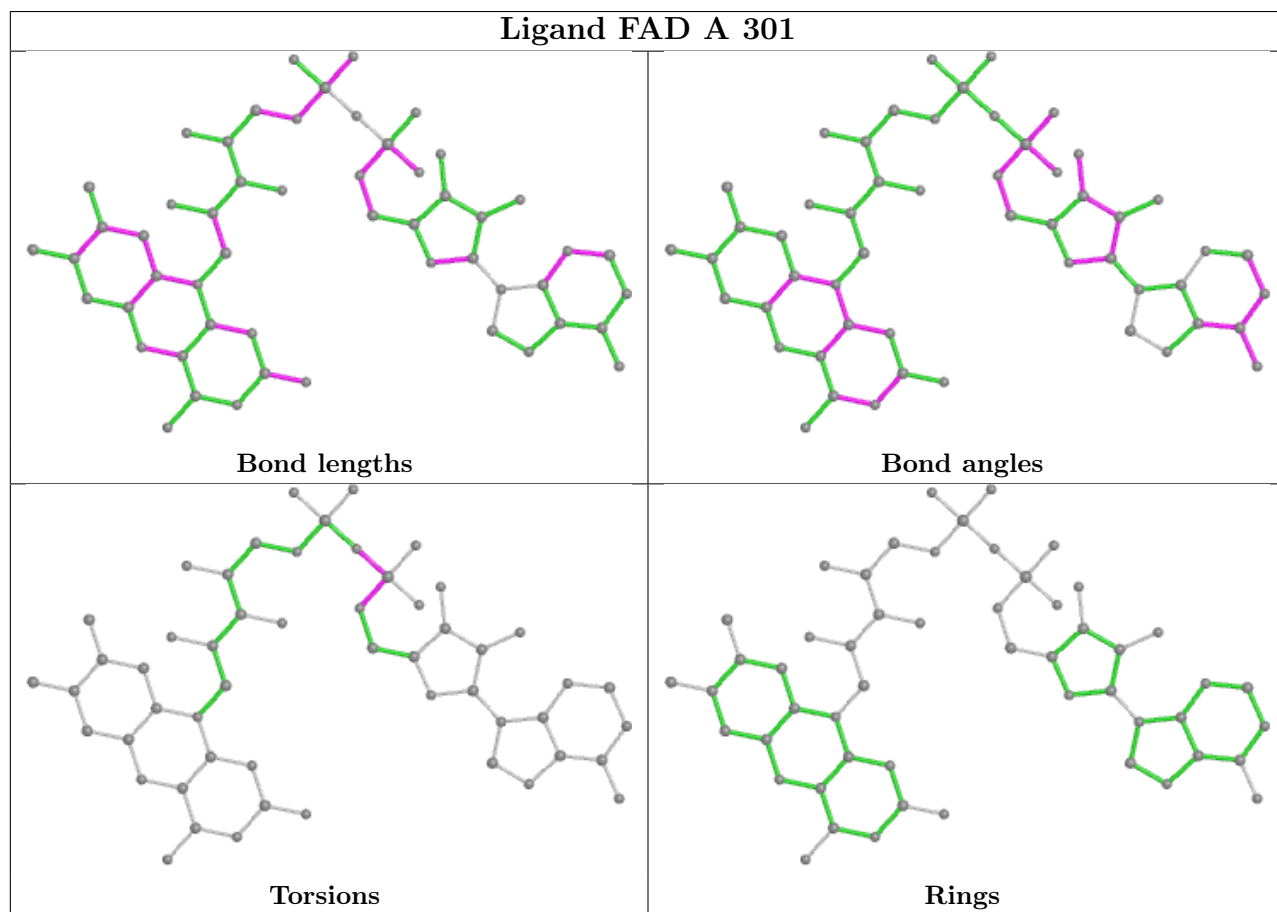
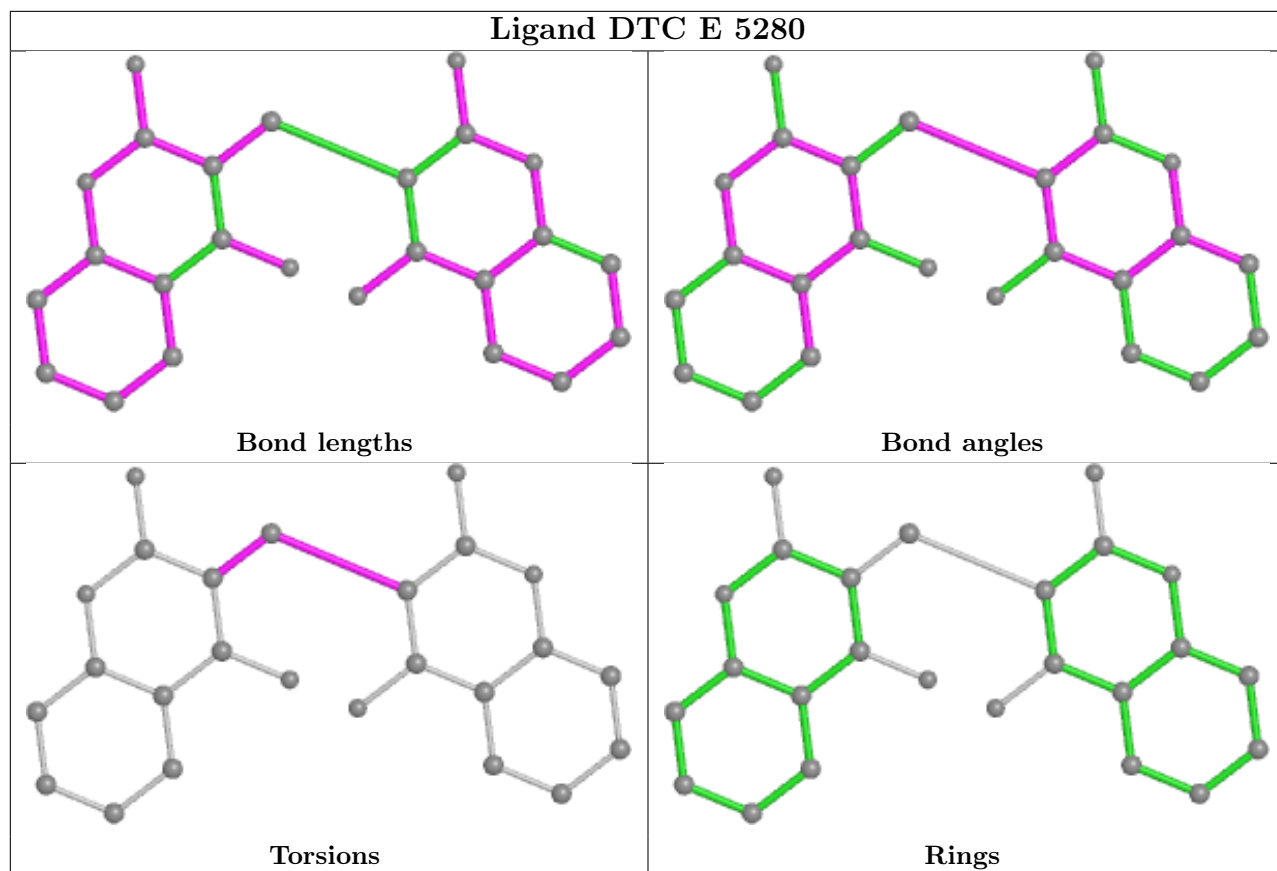












5.7 Other polymers [i](#)

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%)	-0.12	4 (1%) 73 81	13, 31, 50, 78	0
1	B	273/273 (100%)	-0.20	5 (1%) 68 76	14, 29, 47, 74	0
1	C	273/273 (100%)	-0.18	4 (1%) 73 81	12, 28, 53, 71	0
1	D	273/273 (100%)	-0.11	5 (1%) 68 76	13, 33, 52, 80	0
1	E	273/273 (100%)	-0.22	1 (0%) 92 95	11, 27, 52, 69	0
1	F	273/273 (100%)	-0.12	5 (1%) 68 76	15, 32, 53, 68	0
1	G	273/273 (100%)	-0.02	12 (4%) 34 41	15, 35, 65, 81	0
1	H	273/273 (100%)	0.15	8 (2%) 51 61	18, 41, 70, 82	0
All	All	2184/2184 (100%)	-0.10	44 (2%) 65 73	11, 32, 58, 82	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	VAL	9.6
1	E	1	VAL	8.3
1	A	1	VAL	7.0
1	B	1	VAL	6.1
1	D	273	LYS	4.6
1	H	1	VAL	4.5
1	G	1	VAL	4.5
1	G	273	LYS	3.9
1	H	2	GLY	3.8
1	F	1	VAL	3.4
1	C	1	VAL	3.4
1	G	233	GLN	3.3
1	G	59	LEU	3.2
1	G	58	LYS	3.1
1	G	232	PHE	2.9
1	H	233	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	H	273	LYS	2.9
1	H	216	ASP	2.9
1	G	234	ALA	2.7
1	A	2	GLY	2.7
1	H	196	PRO	2.6
1	G	240	LYS	2.6
1	C	235	GLY	2.5
1	C	233	GLN	2.5
1	G	272	ARG	2.5
1	D	233	GLN	2.5
1	H	272	ARG	2.4
1	H	28	ALA	2.4
1	G	242	VAL	2.3
1	F	198	ASP	2.3
1	B	273	LYS	2.2
1	C	234	ALA	2.2
1	G	127	THR	2.2
1	F	123	GLU	2.2
1	G	244	ASP	2.2
1	B	233	GLN	2.2
1	B	107	GLY	2.1
1	B	2	GLY	2.1
1	D	234	ALA	2.1
1	F	2	GLY	2.0
1	A	232	PHE	2.0
1	F	196	PRO	2.0
1	A	245	GLU	2.0
1	D	2	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

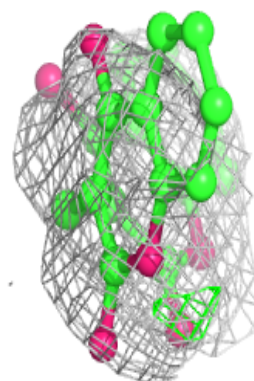
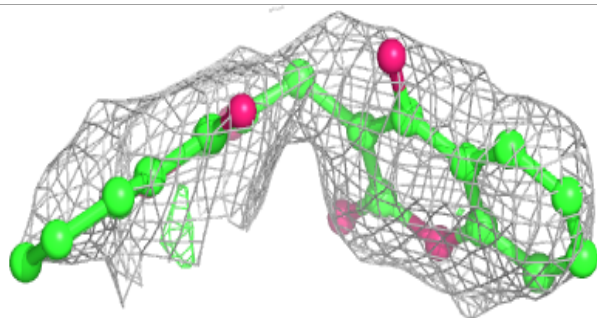
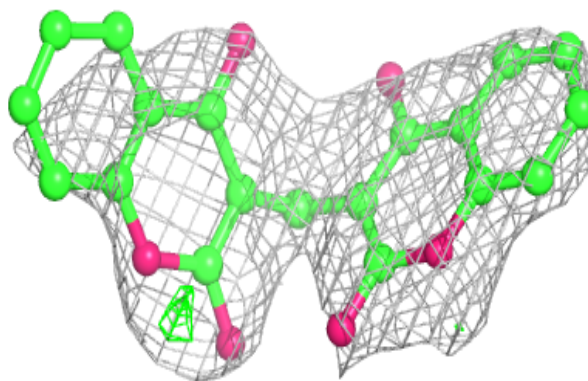
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	DTC	G	7280	25/25	0.77	0.28	34,74,75,75	0
2	DTC	E	5280	25/25	0.79	0.27	34,74,75,75	0
2	DTC	B	3280	25/25	0.81	0.27	34,74,75,75	0
2	DTC	D	1280	25/25	0.81	0.31	34,74,75,75	0
2	DTC	C	280	25/25	0.83	0.28	34,74,75,75	0
2	DTC	H	6280	25/25	0.83	0.27	34,74,75,75	0
2	DTC	A	2280	25/25	0.84	0.28	34,74,75,75	0
2	DTC	E	4280	25/25	0.85	0.29	34,74,75,75	0
3	FAD	H	7301	53/53	0.87	0.18	25,45,53,55	0
3	FAD	A	301	53/53	0.90	0.17	25,34,42,42	0
3	FAD	F	5301	53/53	0.91	0.16	21,30,38,41	0
3	FAD	D	3301	53/53	0.92	0.16	19,28,38,39	0
3	FAD	B	1301	53/53	0.92	0.16	17,22,34,34	0
3	FAD	G	6301	53/53	0.92	0.16	20,28,34,37	0
3	FAD	C	2301	53/53	0.92	0.15	19,27,34,34	0
3	FAD	E	4301	53/53	0.93	0.14	14,23,34,34	0

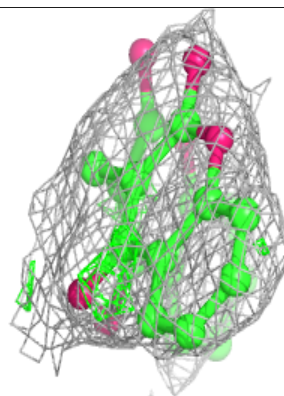
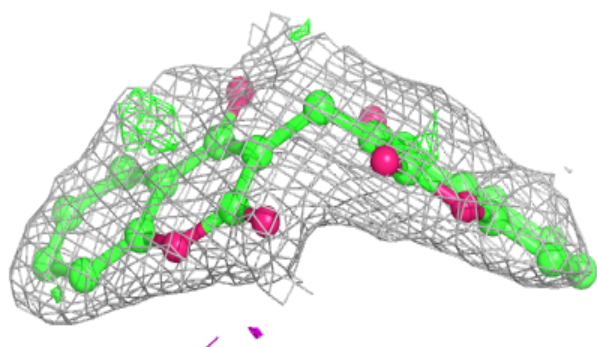
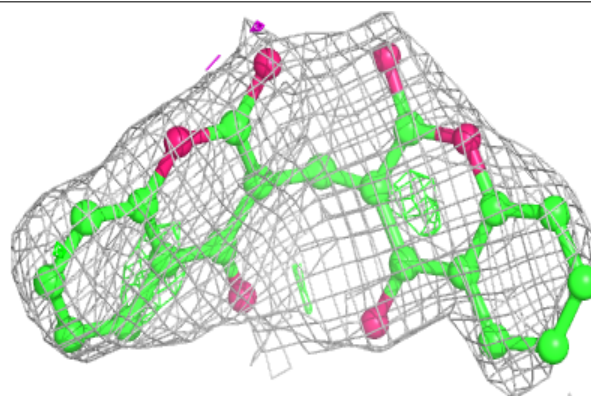
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

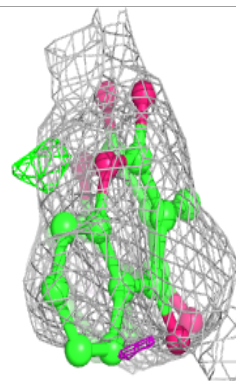
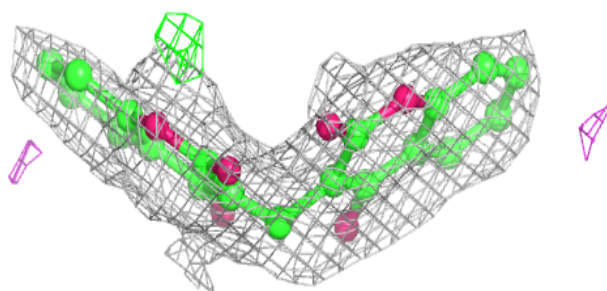
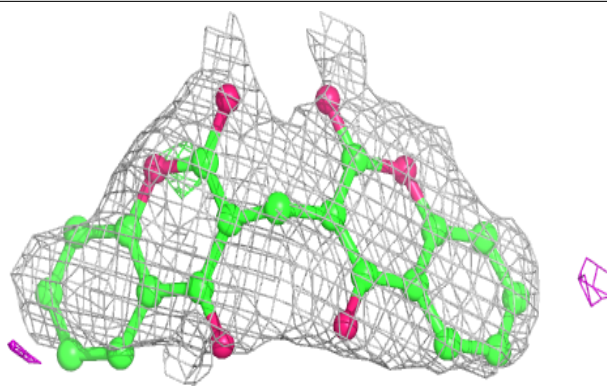
**Electron density around DTC E 5280:**

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

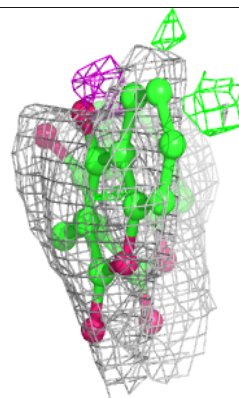
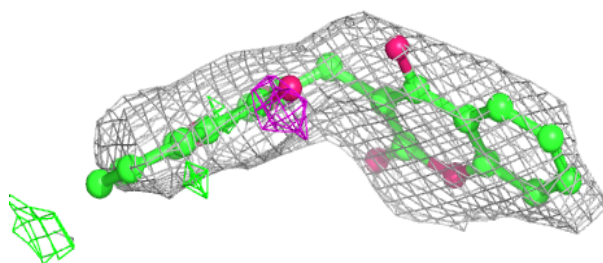
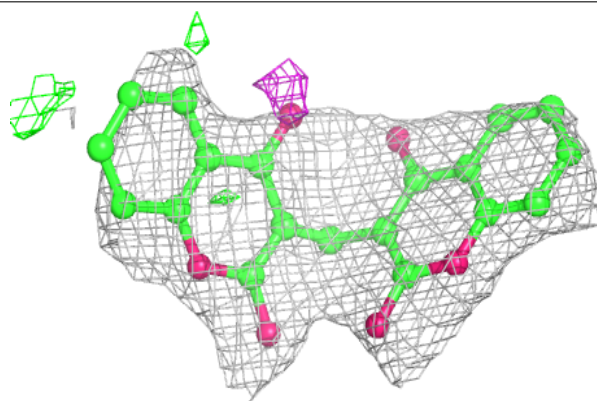


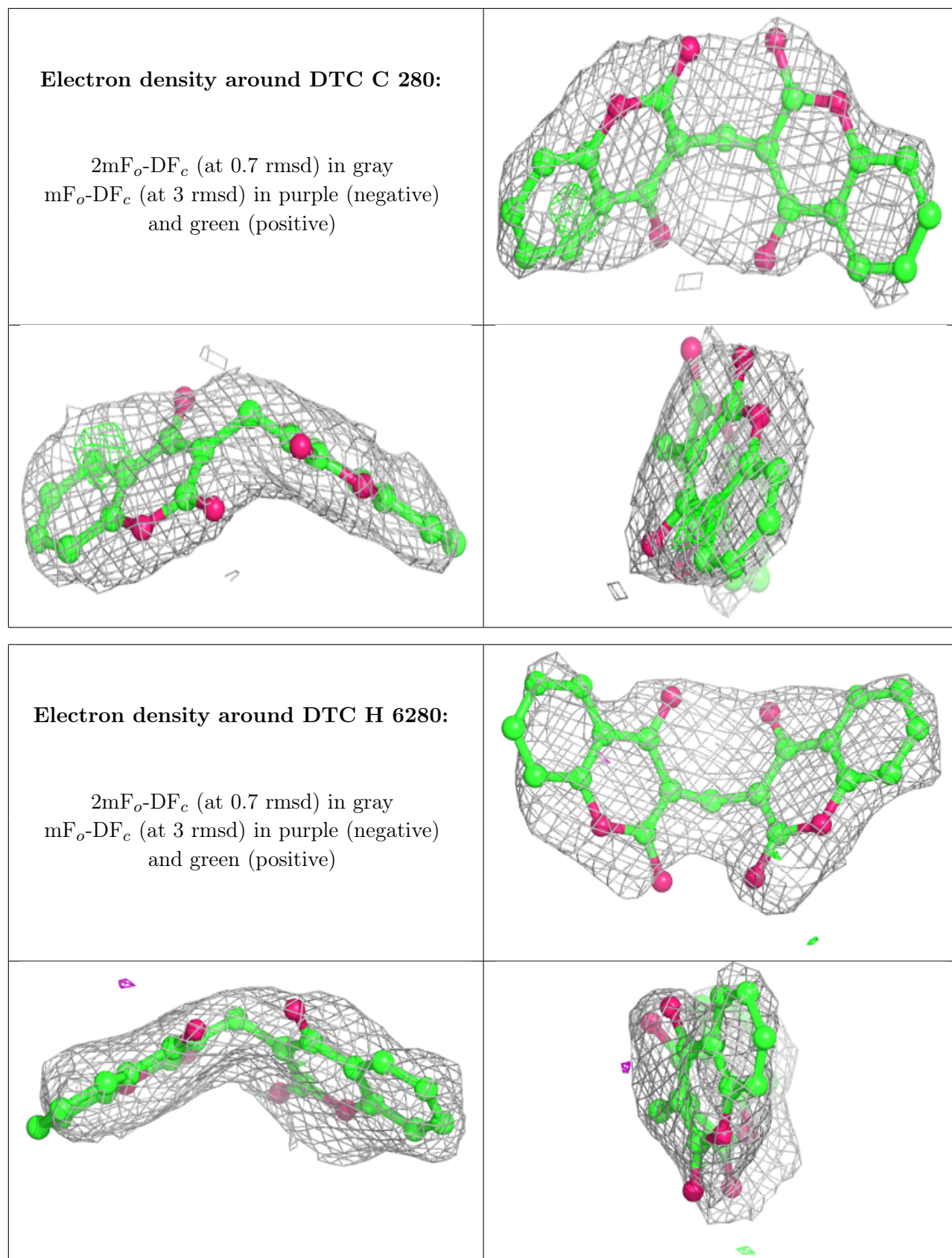
Electron density around DTC B 3280:

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

**Electron density around DTC D 1280:**

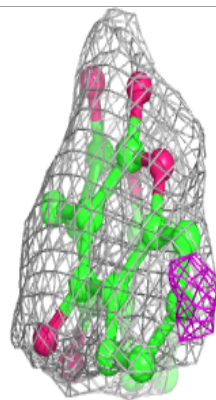
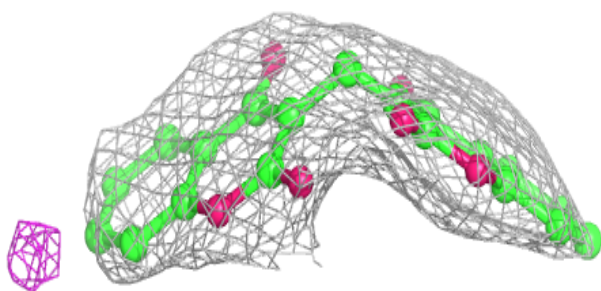
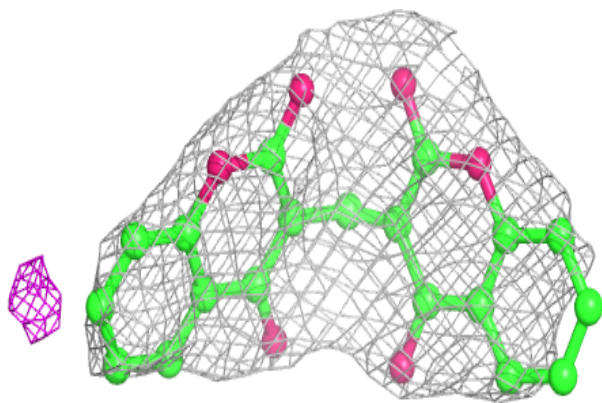
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



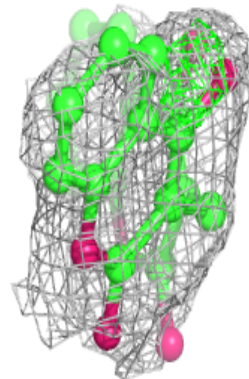
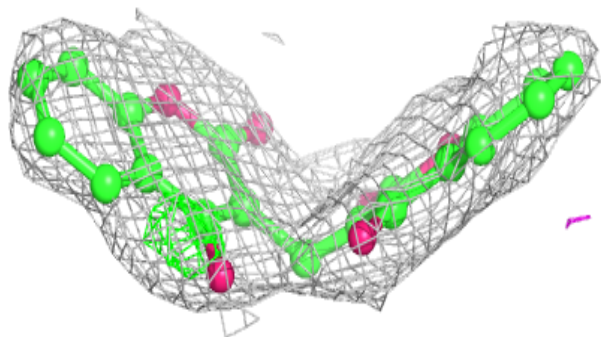
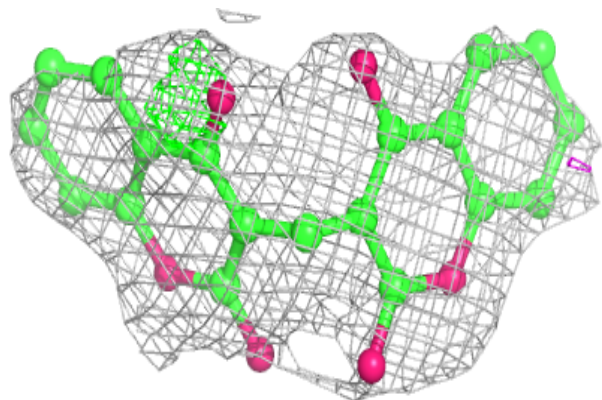


Electron density around DTC A 2280:

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

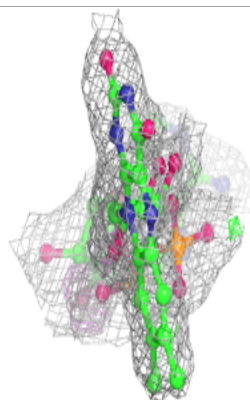
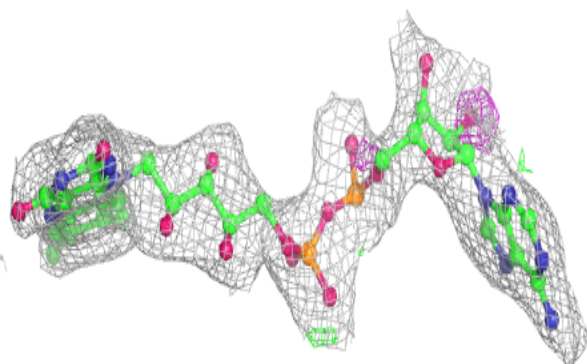
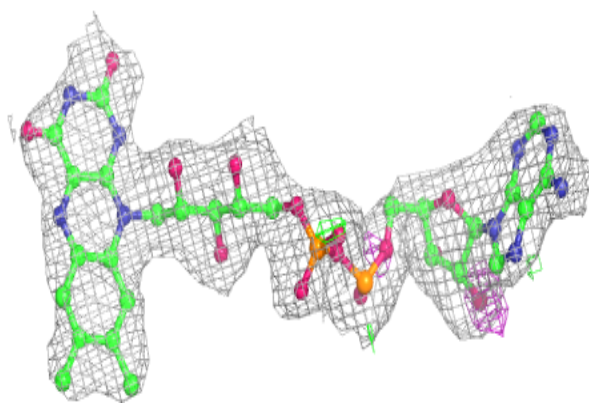
**Electron density around DTC E 4280:**

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

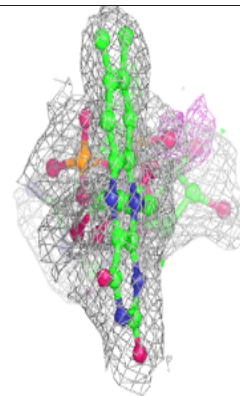
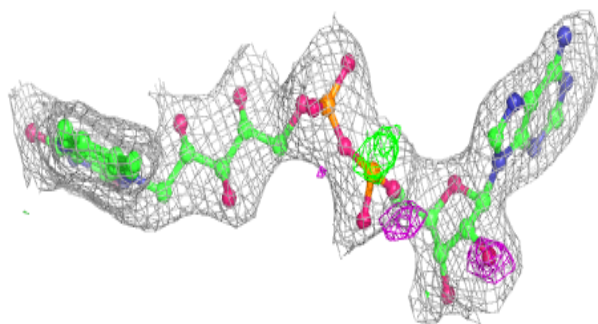
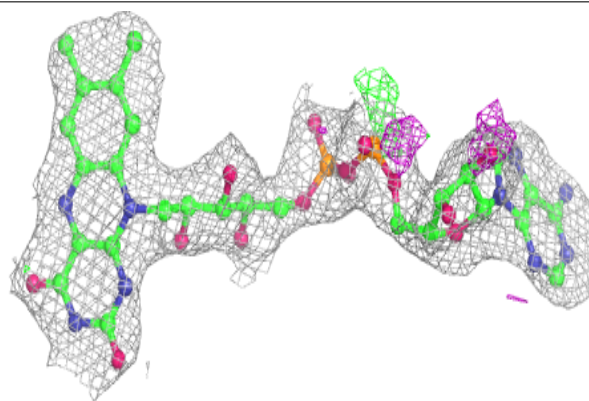


Electron density around FAD H 7301:

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

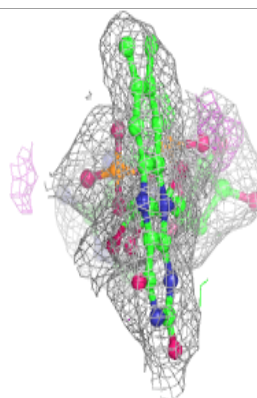
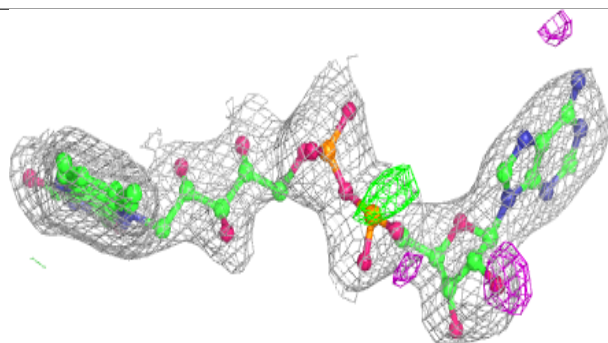
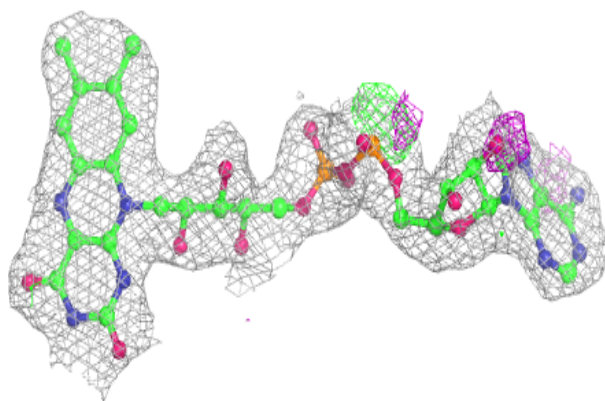
**Electron density around FAD A 301:**

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

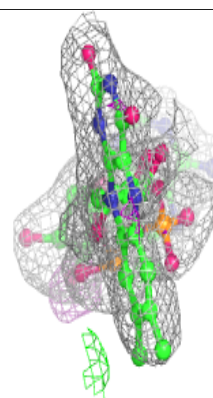
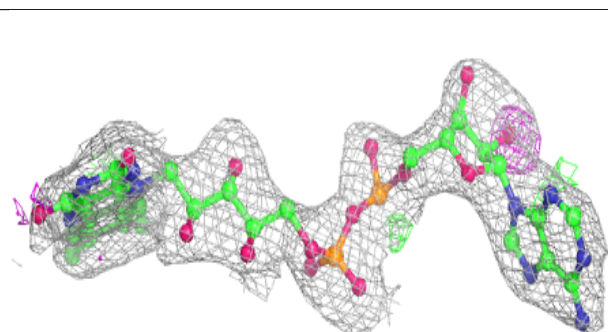
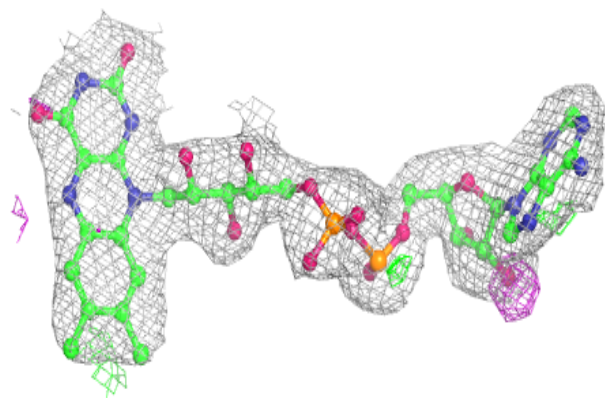


Electron density around FAD F 5301:

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

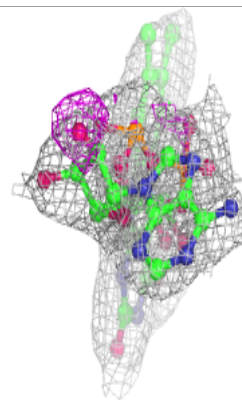
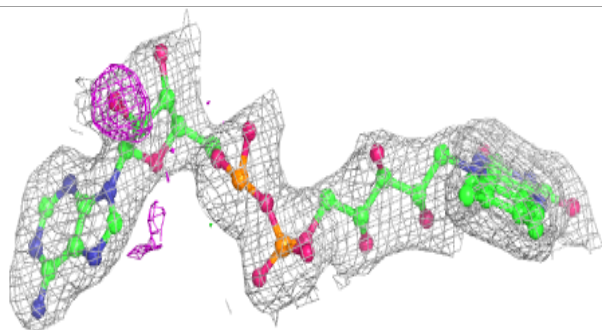
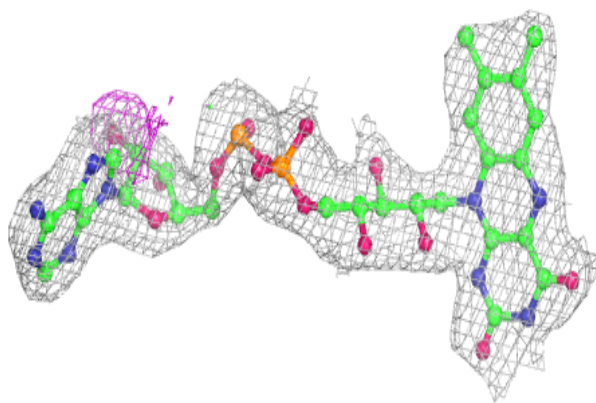
**Electron density around FAD D 3301:**

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

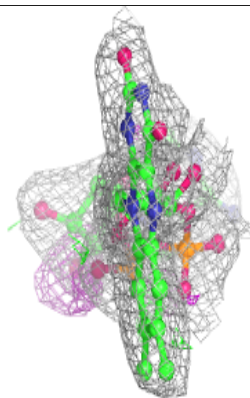
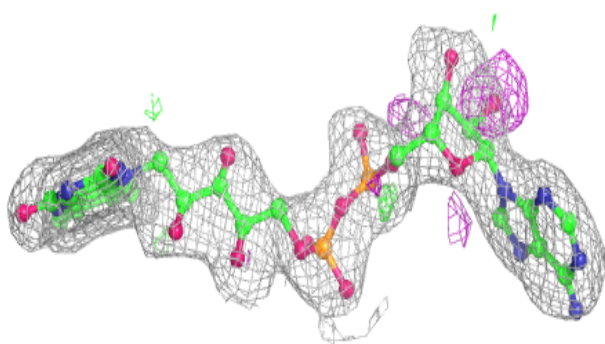
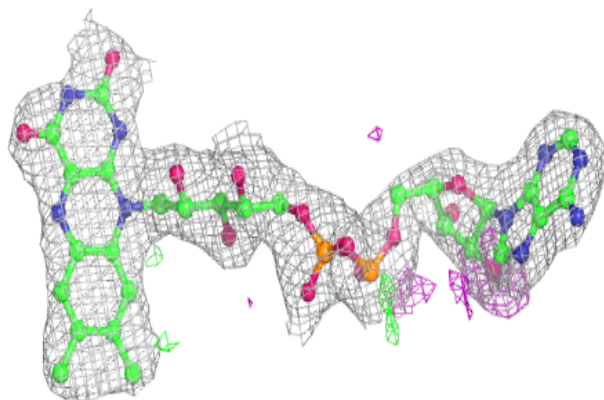


Electron density around FAD B 1301:

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

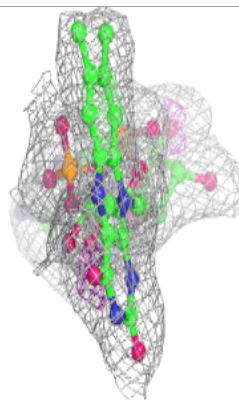
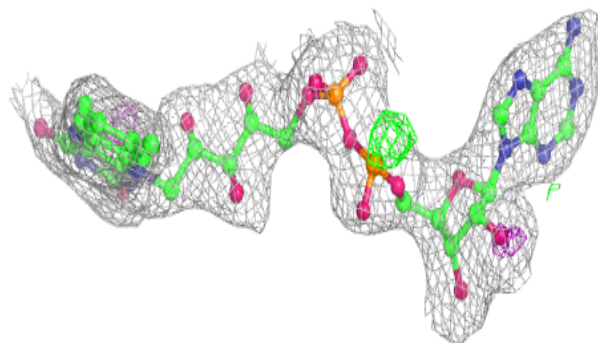
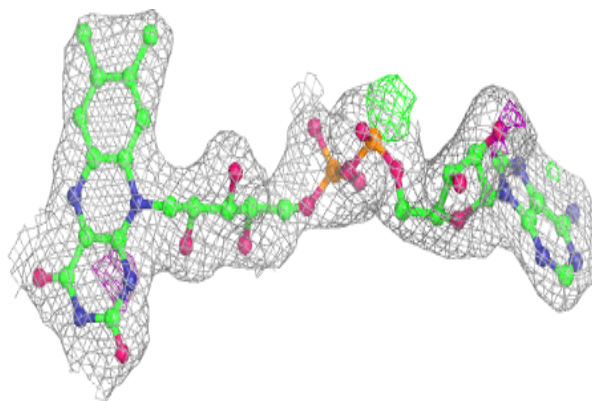
**Electron density around FAD G 6301:**

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

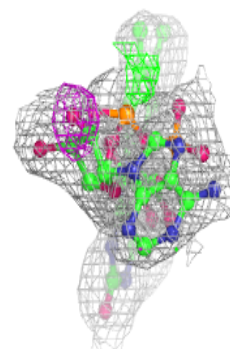
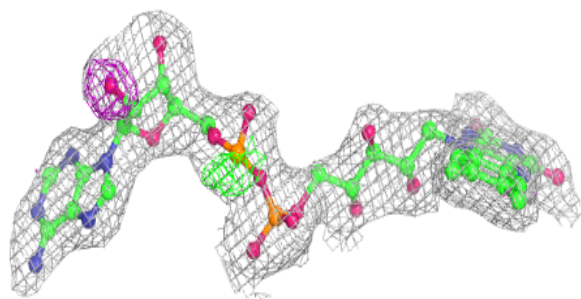
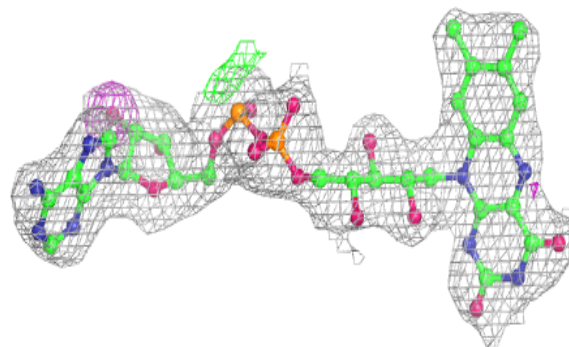


Electron density around FAD C 2301:

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

**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)



6.5 Other polymers

There are no such residues in this entry.