



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 03:33 am BST

PDB ID : 1UDY
Title : Medium-Chain Acyl-CoA Dehydrogenase with 3-Thiaoctanoyl-CoA
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Deposited on : 2003-05-07
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

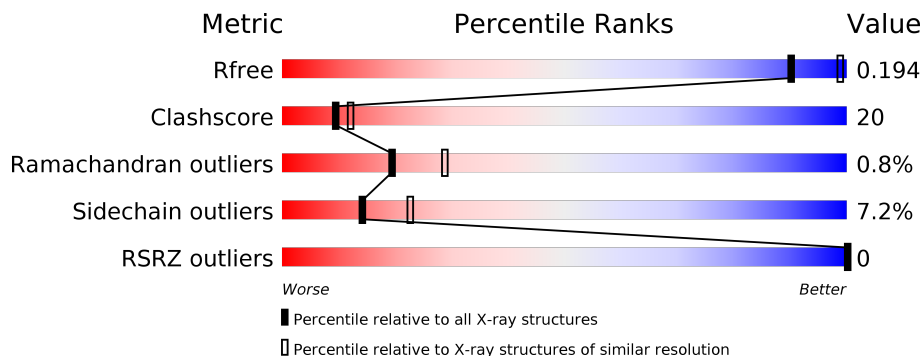
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	396	 63% 30% . .
1	B	396	 59% 34% . .
1	C	396	 62% 31% . .
1	D	396	 63% 30% 5% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12594 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 Acyl-CoA dehydrogenase, medium-chain specific.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	385	2981	1891	514	562	14	0	0	0
1	B	383	2960	1876	511	559	14	0	0	0
1	C	385	2981	1891	514	562	14	0	0	0
1	D	385	2981	1891	514	562	14	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

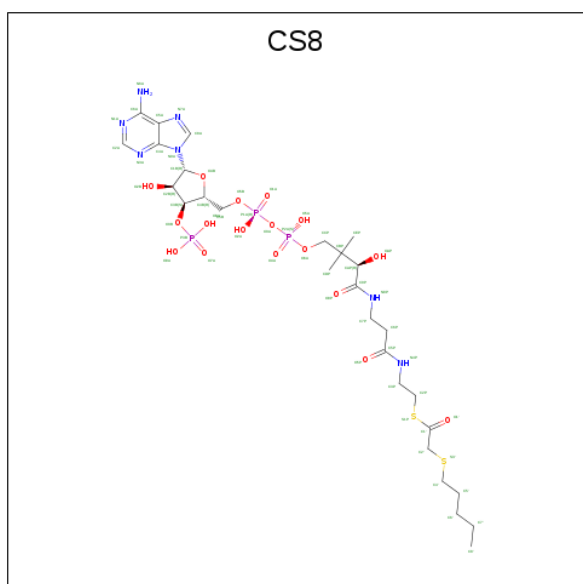
Chain	Residue	Modelled	Actual	Comment	Reference
A	15	GLU	LYS	SEE REMARK 999	UNP P41367
A	258	PRO	SER	SEE REMARK 999	UNP P41367
A	280	GLU	GLY	SEE REMARK 999	UNP P41367
A	306	GLU	ASP	SEE REMARK 999	UNP P41367
B	15	GLU	LYS	SEE REMARK 999	UNP P41367
B	258	PRO	SER	SEE REMARK 999	UNP P41367
B	280	GLU	GLY	SEE REMARK 999	UNP P41367
B	306	GLU	ASP	SEE REMARK 999	UNP P41367
C	15	GLU	LYS	SEE REMARK 999	UNP P41367
C	258	PRO	SER	SEE REMARK 999	UNP P41367
C	280	GLU	GLY	SEE REMARK 999	UNP P41367
C	306	GLU	ASP	SEE REMARK 999	UNP P41367
D	15	GLU	LYS	SEE REMARK 999	UNP P41367
D	258	PRO	SER	SEE REMARK 999	UNP P41367
D	280	GLU	GLY	SEE REMARK 999	UNP P41367
D	306	GLU	ASP	SEE REMARK 999	UNP P41367

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 3 is 3-THIAOCTANOYL-COENZYME A (three-letter code: CS8) (formula: $C_{28}H_{48}N_7O_{17}P_3S_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
3	A	1	Total	C	N	O	P	S	0	0
			57	28	7	17	3	2		
3	B	1	Total	C	N	O	P	S	0	0
			57	28	7	17	3	2		
3	C	1	Total	C	N	O	P	S	0	0
			57	28	7	17	3	2		
3	D	1	Total	C	N	O	P	S	0	0
			57	28	7	17	3	2		

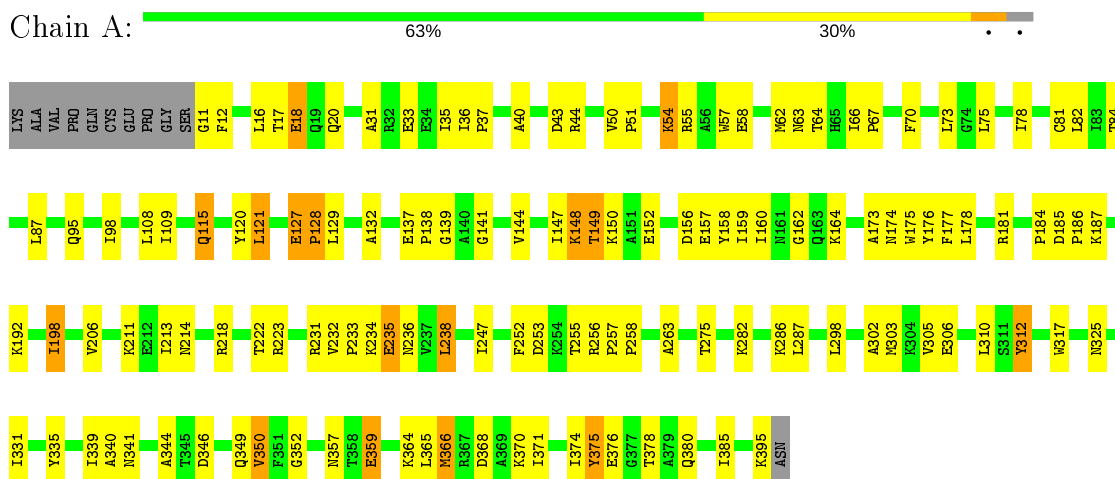
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	60	Total	O	0	0
			60	60		
4	B	63	Total	O	0	0
			63	63		
4	C	52	Total	O	0	0
			52	52		
4	D	76	Total	O	0	0
			76	76		

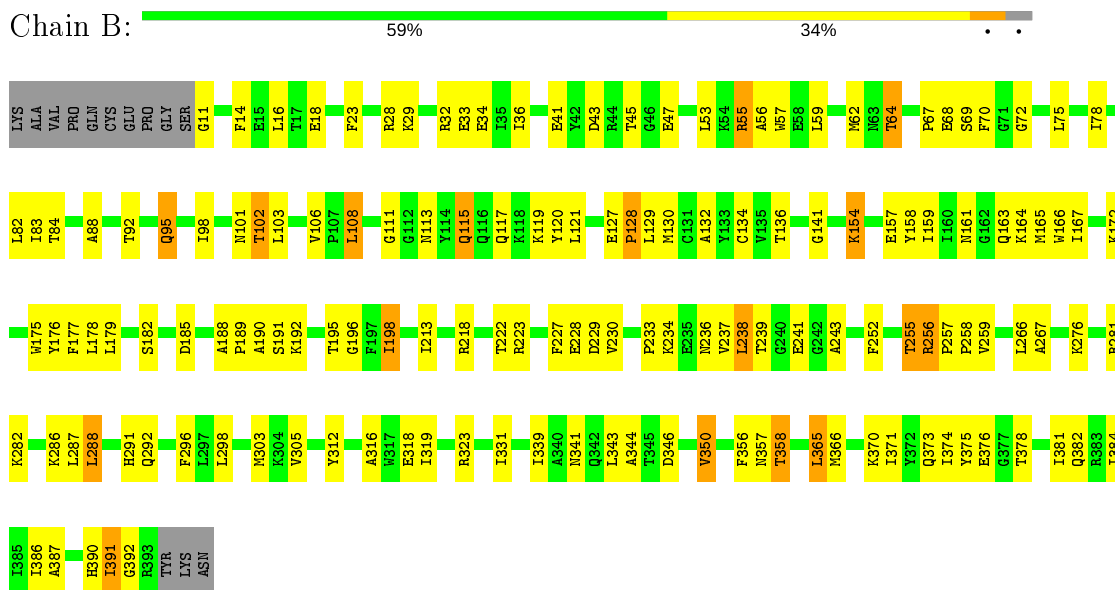
3 Residue-property plots [i](#)

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

- Molecule 1: Acyl-CoA dehydrogenase, medium-chain specific

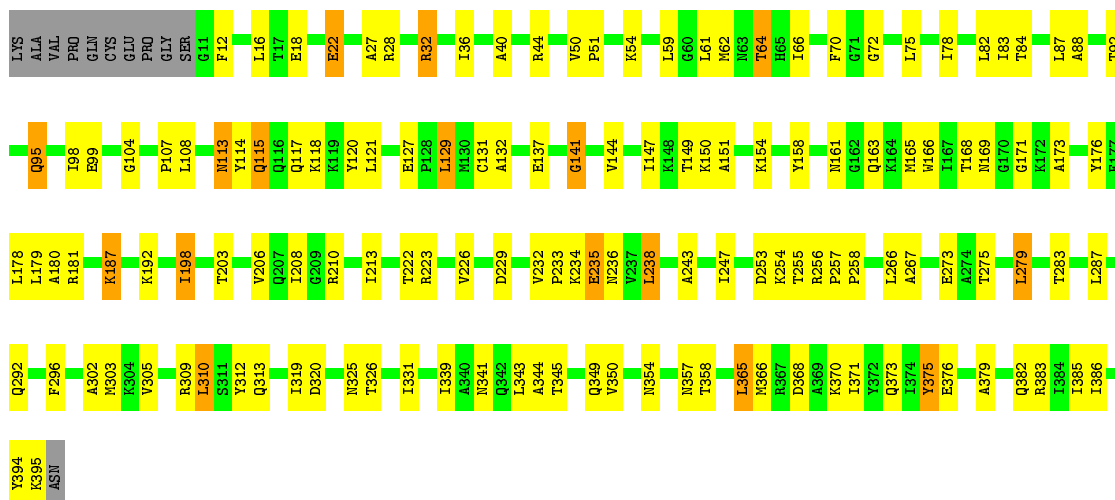


- Molecule 1: Acyl-CoA dehydrogenase, medium-chain specific



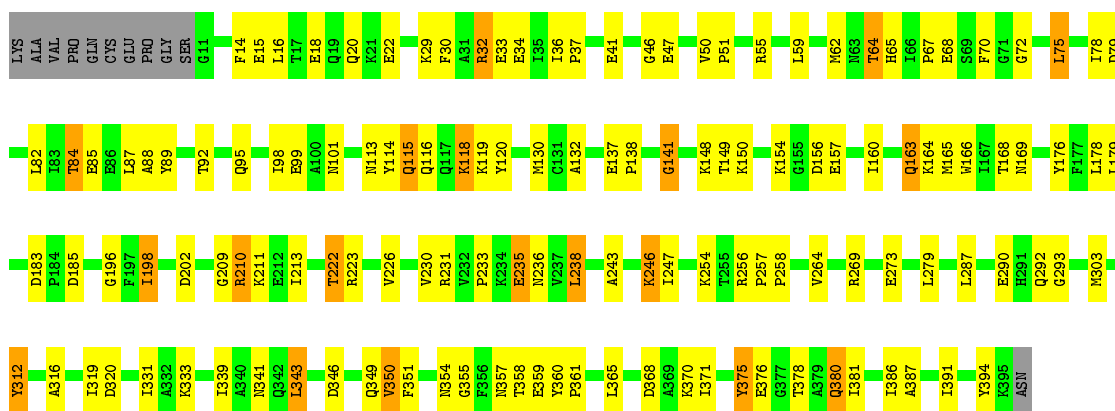
- Molecule 1: Acyl-CoA dehydrogenase, medium-chain specific

Chain C:  62% 31%



• Molecule 1: Acyl-CoA dehydrogenase, medium-chain specific

Chain D:  63% 30% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	99.00Å 110.60Å 147.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 45.89 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.40) 82.2 (45.89-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.29Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.198 , 0.260 0.190 , 0.194	Depositor DCC
R_{free} test set	3019 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	29.6	Xtrriage
Anisotropy	0.499	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 38.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12594	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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: CS8, 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	0.37	0/3038	0.62	0/4101
1	B	0.37	0/3016	0.61	1/4072 (0.0%)
1	C	0.37	0/3038	0.61	0/4101
1	D	0.37	0/3038	0.60	0/4101
All	All	0.37	0/12130	0.61	1/16375 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	177	PHE	N-CA-C	-5.91	95.05	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	2981	0	2974	127	0
1	B	2960	0	2952	139	0
1	C	2981	0	2974	120	0
1	D	2981	0	2974	126	0
2	A	53	0	31	6	0
2	B	53	0	31	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	53	0	31	4	0
2	D	53	0	31	5	0
3	A	57	0	44	3	0
3	B	57	0	44	5	0
3	C	57	0	44	1	0
3	D	57	0	44	0	0
4	A	60	0	0	3	0
4	B	63	0	0	3	0
4	C	52	0	0	0	0
4	D	76	0	0	4	0
All	All	12594	0	12174	481	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 20.

All (481) 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:161:ASN:ND2	1:B:229:ASP:H	1.59	1.01
1:B:341:ASN:HD21	1:B:370:LYS:HA	1.34	0.92
1:D:378:THR:HG22	1:D:381:ILE:HG12	1.52	0.91
1:A:341:ASN:HD21	1:A:370:LYS:HA	1.36	0.90
1:A:186:PRO:HG2	1:A:187:LYS:HD2	1.54	0.89
1:A:137:GLU:OE2	1:A:149:THR:HG22	1.73	0.88
1:C:32:ARG:HA	1:C:36:ILE:HD12	1.55	0.86
1:B:115:GLN:HE21	1:B:115:GLN:H	1.23	0.86
1:B:292:GLN:HE21	1:D:293:GLY:H	1.23	0.85
1:D:32:ARG:HH11	1:D:32:ARG:HG2	1.40	0.85
1:A:115:GLN:NE2	1:A:115:GLN:H	1.72	0.85
1:C:99:GLU:HB3	3:C:2400:CS8:H7'1	1.58	0.85
1:C:108:LEU:HD23	1:C:238:LEU:HD21	1.59	0.84
1:B:23:PHE:HB3	1:B:83:ILE:HD11	1.59	0.84
1:B:127:GLU:HG3	1:B:129:LEU:HD13	1.61	0.82
1:D:341:ASN:HD21	1:D:370:LYS:HA	1.44	0.81
1:A:282:LYS:HE3	1:A:287:LEU:HD22	1.62	0.81
1:D:163:GLN:NE2	1:D:226:VAL:HG22	1.96	0.80
1:A:78:ILE:O	1:A:82:LEU:HD13	1.82	0.80
1:B:256:ARG:HG2	1:B:256:ARG:HH11	1.45	0.80
1:C:187:LYS:NZ	1:C:187:LYS:HA	1.97	0.80
1:B:55:ARG:O	1:B:59:LEU:HB2	1.83	0.79
1:A:255:THR:O	1:A:258:PRO:HD2	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:ASN:HD21	1:B:229:ASP:H	1.27	0.79
1:C:127:GLU:HG3	1:C:129:LEU:HD22	1.64	0.78
1:A:139:GLY:HA2	1:B:281:ARG:HH12	1.48	0.78
1:A:286:LYS:HE3	4:A:1008:HOH:O	1.84	0.77
1:C:78:ILE:HG13	1:C:320:ASP:OD2	1.84	0.76
1:D:246:LYS:H	1:D:246:LYS:HE3	1.51	0.76
1:C:64:THR:HG23	1:C:75:LEU:HB2	1.68	0.75
1:B:163:GLN:HG2	1:B:164:LYS:N	2.00	0.75
1:A:62:MET:HG3	1:A:98:ILE:HG23	1.69	0.74
1:B:252:PHE:HA	1:B:255:THR:HG23	1.69	0.74
1:B:34:GLU:OE1	1:B:55:ARG:HD3	1.89	0.73
1:B:127:GLU:HG3	1:B:129:LEU:CD1	2.18	0.73
1:B:154:LYS:HD3	1:B:154:LYS:O	1.88	0.73
1:B:292:GLN:HE21	1:D:293:GLY:N	1.85	0.73
1:A:108:LEU:HD12	1:A:238:LEU:HD11	1.69	0.73
1:A:43:ASP:OD1	1:A:218:ARG:HD3	1.89	0.73
1:A:149:THR:HG21	1:A:164:LYS:HE2	1.71	0.72
1:A:159:ILE:CD1	1:A:231:ARG:HG2	2.19	0.72
1:C:32:ARG:HH11	1:C:32:ARG:HG2	1.52	0.72
1:B:331:ILE:HG23	1:C:303:MET:HG3	1.70	0.72
1:D:118:LYS:NZ	1:D:118:LYS:HB2	2.04	0.71
1:A:303:MET:HG3	1:D:331:ILE:HG23	1.72	0.71
1:B:255:THR:O	1:B:258:PRO:HD2	1.90	0.71
1:B:256:ARG:HG2	1:B:256:ARG:NH1	2.05	0.71
1:D:64:THR:HG23	1:D:75:LEU:HB2	1.71	0.71
1:D:378:THR:HG22	1:D:381:ILE:CG1	2.20	0.71
1:D:32:ARG:NH1	1:D:32:ARG:HG2	2.04	0.70
1:B:292:GLN:NE2	1:D:293:GLY:H	1.89	0.70
1:D:29:LYS:O	1:D:33:GLU:HG2	1.92	0.69
1:D:115:GLN:H	1:D:115:GLN:NE2	1.91	0.69
1:D:246:LYS:CE	1:D:246:LYS:H	2.04	0.69
1:D:256:ARG:HG3	1:D:333:LYS:HG3	1.74	0.69
1:D:378:THR:CG2	1:D:381:ILE:HG12	2.22	0.69
1:A:73:LEU:HB3	1:A:75:LEU:HD13	1.74	0.69
1:B:45:THR:OG1	1:B:47:GLU:HG2	1.94	0.68
1:B:257:PRO:HB2	1:B:258:PRO:HD3	1.76	0.68
1:A:331:ILE:HG23	1:D:303:MET:HG3	1.77	0.67
1:B:115:GLN:NE2	1:B:115:GLN:H	1.91	0.67
1:C:341:ASN:HD21	1:C:370:LYS:HA	1.60	0.67
1:A:198:ILE:HG23	1:A:236:ASN:HB3	1.75	0.67
1:B:161:ASN:HD21	1:B:229:ASP:N	1.91	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:LEU:CD2	1:D:82:LEU:HD21	2.23	0.67
1:A:252:PHE:HA	1:A:255:THR:HG22	1.76	0.67
1:A:156:ASP:HA	1:A:234:LYS:HD3	1.77	0.67
1:A:150:LYS:HD2	1:A:181:ARG:O	1.93	0.67
1:C:141:GLY:HA3	2:C:2399:FAD:H5'1	1.76	0.67
1:A:54:LYS:HB2	1:A:54:LYS:NZ	2.09	0.67
1:B:390:HIS:C	1:B:392:GLY:H	1.99	0.66
1:A:62:MET:CG	1:A:98:ILE:HG23	2.25	0.66
1:C:233:PRO:HB2	1:C:235:GLU:OE2	1.95	0.66
1:B:233:PRO:HG2	1:B:236:ASN:OD1	1.94	0.66
1:C:187:LYS:HA	1:C:187:LYS:HZ3	1.61	0.66
1:C:158:TYR:HB2	1:C:232:VAL:CG1	2.26	0.65
1:A:302:ALA:O	1:A:305:VAL:HG12	1.96	0.65
1:C:137:GLU:OE2	1:C:149:THR:HB	1.96	0.65
1:B:55:ARG:NH2	1:B:59:LEU:HD13	2.11	0.65
1:B:57:TRP:CD2	1:B:128:PRO:HG3	2.31	0.65
1:B:84:THR:HG23	1:B:95:GLN:OE1	1.97	0.65
1:B:291:HIS:HD2	4:B:944:HOH:O	1.81	0.64
1:C:257:PRO:HB2	1:C:258:PRO:HD3	1.79	0.64
1:A:17:THR:H	1:A:20:GLN:HE21	1.44	0.64
1:D:163:GLN:HE22	1:D:226:VAL:HG22	1.62	0.64
1:D:222:THR:HB	4:D:860:HOH:O	1.97	0.64
1:B:346:ASP:O	1:B:350:VAL:HG13	1.98	0.63
1:C:158:TYR:HB2	1:C:232:VAL:HG13	1.80	0.63
1:D:55:ARG:O	1:D:59:LEU:HD13	1.98	0.63
1:B:78:ILE:O	1:B:82:LEU:HD13	1.97	0.63
1:C:275:THR:O	1:C:279:LEU:HD22	1.99	0.63
1:A:137:GLU:HB3	1:A:138:PRO:HD2	1.80	0.63
1:C:150:LYS:HG3	1:C:151:ALA:H	1.63	0.62
1:A:395:LYS:NZ	1:A:395:LYS:CB	2.62	0.62
1:B:161:ASN:ND2	1:B:229:ASP:N	2.40	0.62
1:C:115:GLN:H	1:C:115:GLN:CD	2.03	0.62
1:D:41:GLU:HB2	4:D:1025:HOH:O	1.99	0.61
1:C:150:LYS:HD2	1:C:181:ARG:O	2.00	0.61
1:C:357:ASN:HD22	1:C:358:THR:H	1.46	0.61
1:C:187:LYS:HA	1:C:187:LYS:HZ2	1.65	0.61
1:C:345:THR:HA	1:C:366:MET:HE2	1.81	0.61
1:C:370:LYS:HZ3	1:D:349:GLN:HG2	1.64	0.61
1:A:137:GLU:OE2	1:A:147:ILE:HB	2.01	0.61
1:D:387:ALA:O	1:D:391:ILE:HD13	2.01	0.61
1:D:16:LEU:HD22	1:D:82:LEU:HD21	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:LYS:HE2	4:B:901:HOH:O	2.01	0.60
1:A:115:GLN:H	1:A:115:GLN:HE21	1.50	0.60
1:D:233:PRO:HG2	1:D:236:ASN:ND2	2.16	0.60
1:C:370:LYS:NZ	1:D:349:GLN:HG2	2.17	0.60
1:A:206:VAL:O	1:A:206:VAL:HG23	2.01	0.59
1:B:108:LEU:HD22	1:B:238:LEU:HD11	1.83	0.59
1:B:164:LYS:HB3	1:B:167:ILE:HD11	1.83	0.59
1:D:198:ILE:C	1:D:198:ILE:HD13	2.22	0.59
1:B:16:LEU:HD23	1:B:82:LEU:HD21	1.83	0.59
1:A:198:ILE:HG22	1:A:236:ASN:O	2.03	0.59
1:A:375:TYR:O	1:A:376:GLU:HB2	2.02	0.58
1:D:257:PRO:HB2	1:D:258:PRO:HD3	1.84	0.58
1:C:83:ILE:O	1:C:87:LEU:HD13	2.03	0.58
1:A:395:LYS:HZ2	1:A:395:LYS:HB2	1.69	0.58
1:C:50:VAL:O	1:C:54:LYS:HD3	2.04	0.58
1:A:149:THR:HB	1:A:162:GLY:HA3	1.85	0.58
1:C:213:ILE:O	1:D:358:THR:HG22	2.04	0.57
1:B:11:GLY:N	4:B:864:HOH:O	2.37	0.57
1:D:165:MET:HG3	1:D:166:TRP:CD1	2.39	0.57
1:C:171:GLY:HA2	1:C:208:ILE:HD13	1.86	0.57
1:A:78:ILE:HD11	1:A:317:TRP:HA	1.85	0.57
1:A:395:LYS:NZ	1:A:395:LYS:HB2	2.18	0.57
1:D:65:HIS:HE1	1:D:254:LYS:NZ	2.02	0.57
1:A:282:LYS:HE3	1:A:287:LEU:CD2	2.33	0.57
1:B:381:ILE:HG23	3:B:1400:CS8:H133	1.87	0.57
1:A:173:ALA:HB3	1:A:176:TYR:CE1	2.39	0.57
1:D:55:ARG:NH2	1:D:59:LEU:HD11	2.19	0.57
1:D:339:ILE:O	1:D:343:LEU:HD12	2.05	0.57
1:A:368:ASP:O	1:A:371:ILE:HG22	2.05	0.56
1:D:210:ARG:HH11	1:D:210:ARG:HG3	1.69	0.56
1:B:384:ILE:HD11	1:C:292:GLN:HE21	1.69	0.56
1:D:202:ASP:HB3	4:D:1048:HOH:O	2.04	0.56
1:A:375:TYR:HD1	1:A:375:TYR:O	1.88	0.56
1:C:163:GLN:HG2	1:C:226:VAL:HG22	1.86	0.56
1:A:252:PHE:CE1	3:A:400:CS8:H31	2.40	0.56
1:B:117:GLN:O	1:B:121:LEU:HB2	2.06	0.56
1:B:111:GLY:O	1:B:239:THR:HG22	2.05	0.56
1:B:371:ILE:CD1	2:B:1399:FAD:HM83	2.35	0.56
1:D:380:GLN:H	1:D:380:GLN:NE2	2.03	0.56
1:A:252:PHE:O	1:A:256:ARG:HB2	2.04	0.56
1:D:246:LYS:HD3	1:D:246:LYS:N	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:ALA:HB3	1:C:176:TYR:HD1	1.70	0.56
1:C:150:LYS:HG3	1:C:151:ALA:N	2.19	0.56
1:B:163:GLN:HG2	1:B:164:LYS:H	1.71	0.55
1:B:56:ALA:HB3	1:B:62:MET:HE3	1.87	0.55
1:C:368:ASP:O	1:C:371:ILE:HG22	2.05	0.55
1:A:282:LYS:HG3	1:A:287:LEU:HD13	1.88	0.55
1:C:344:ALA:HB1	1:C:366:MET:HA	1.89	0.55
1:C:16:LEU:HD22	1:C:82:LEU:HD21	1.87	0.55
1:D:292:GLN:NE2	4:D:813:HOH:O	2.39	0.55
1:B:16:LEU:HD23	1:B:82:LEU:CD2	2.36	0.55
1:A:132:ALA:HB3	1:A:176:TYR:HD1	1.72	0.55
1:A:152:GLU:O	1:A:158:TYR:HA	2.07	0.55
1:D:378:THR:HG21	2:D:3399:FAD:O2B	2.07	0.55
1:D:114:TYR:HB3	1:D:115:GLN:HE21	1.71	0.55
1:A:43:ASP:HB2	1:A:364:LYS:HE2	1.87	0.54
1:B:103:LEU:HD22	3:B:1400:CS8:H4'1	1.89	0.54
1:C:154:LYS:NZ	1:C:154:LYS:HB3	2.22	0.54
1:C:32:ARG:NH1	1:C:32:ARG:HG2	2.21	0.54
1:A:357:ASN:ND2	1:B:213:ILE:O	2.39	0.54
1:C:357:ASN:HD22	1:C:358:THR:N	2.05	0.54
1:C:255:THR:C	1:C:258:PRO:HD2	2.28	0.54
1:A:16:LEU:HG	1:A:20:GLN:HB2	1.89	0.54
1:A:17:THR:OG1	1:A:20:GLN:HG3	2.07	0.54
2:A:399:FAD:H8A	2:A:399:FAD:O1A	2.08	0.54
1:B:227:PHE:HD2	1:B:230:VAL:HG21	1.72	0.54
1:D:246:LYS:CD	1:D:246:LYS:N	2.71	0.54
1:A:371:ILE:HD12	1:A:374:ILE:HB	1.90	0.54
1:B:175:TRP:CE3	1:B:198:ILE:HD13	2.42	0.54
1:C:287:LEU:H	1:C:287:LEU:HD22	1.73	0.54
1:D:115:GLN:H	1:D:115:GLN:CD	2.11	0.54
1:C:166:TRP:HZ2	1:D:354:ASN:HD22	1.56	0.54
1:A:357:ASN:OD1	1:A:359:GLU:HB2	2.08	0.54
1:C:192:LYS:NZ	1:C:192:LYS:HB2	2.23	0.54
1:C:394:TYR:O	1:C:395:LYS:HB3	2.08	0.54
1:A:159:ILE:HD11	1:A:231:ARG:NH1	2.23	0.53
1:B:292:GLN:HE21	1:D:293:GLY:CA	2.20	0.53
1:C:178:LEU:HD13	1:C:179:LEU:N	2.22	0.53
1:C:357:ASN:ND2	1:C:358:THR:N	2.56	0.53
1:C:394:TYR:O	1:C:395:LYS:CB	2.57	0.53
1:D:16:LEU:HD21	1:D:82:LEU:HD21	1.88	0.53
1:B:43:ASP:CG	1:B:218:ARG:HH21	2.12	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:LEU:H	1:B:16:LEU:HD12	1.72	0.53
1:C:345:THR:HA	1:C:366:MET:CE	2.39	0.53
1:A:233:PRO:HB2	1:A:235:GLU:HG2	1.90	0.53
1:C:255:THR:O	1:C:258:PRO:HD2	2.09	0.53
1:C:371:ILE:HD11	2:C:2399:FAD:HM83	1.91	0.53
1:C:302:ALA:O	1:C:305:VAL:HG12	2.07	0.53
1:B:382:GLN:O	1:B:386:ILE:HG13	2.09	0.53
1:C:161:ASN:ND2	1:C:229:ASP:H	2.07	0.53
1:A:255:THR:C	1:A:258:PRO:HD2	2.29	0.52
1:D:64:THR:HG23	1:D:75:LEU:CB	2.37	0.52
1:C:254:LYS:HD2	1:C:319:ILE:HG12	1.92	0.52
1:A:198:ILE:HG23	1:A:236:ASN:CB	2.39	0.52
1:B:371:ILE:HD11	2:B:1399:FAD:HM83	1.90	0.52
1:C:115:GLN:N	1:C:115:GLN:OE1	2.26	0.52
1:D:55:ARG:CZ	1:D:59:LEU:HD11	2.40	0.52
1:A:177:PHE:HE1	1:A:238:LEU:HD22	1.74	0.52
1:B:292:GLN:HB3	1:D:292:GLN:HB3	1.92	0.52
1:B:370:LYS:HZ2	1:B:373:GLN:NE2	2.08	0.52
1:C:149:THR:HG23	1:C:180:ALA:HA	1.91	0.52
1:A:149:THR:HG21	1:A:164:LYS:CE	2.38	0.52
1:A:40:ALA:O	1:A:44:ARG:HG3	2.10	0.52
1:B:282:LYS:HE2	1:B:287:LEU:HD13	1.91	0.52
1:C:357:ASN:ND2	1:D:213:ILE:O	2.42	0.52
1:D:316:ALA:O	1:D:319:ILE:HG22	2.09	0.52
1:D:118:LYS:HZ2	1:D:118:LYS:HB2	1.74	0.51
1:B:119:LYS:HD3	1:B:120:TYR:CE2	2.45	0.51
1:A:129:LEU:HG	1:A:174:ASN:ND2	2.26	0.51
1:A:255:THR:HG23	1:A:376:GLU:OE2	2.11	0.51
1:C:203:THR:O	1:C:206:VAL:HG13	2.11	0.51
1:B:102:THR:O	1:B:106:VAL:HG23	2.11	0.51
1:B:282:LYS:HG3	1:B:286:LYS:O	2.10	0.51
1:A:317:TRP:CH2	1:D:15:GLU:HG2	2.46	0.51
1:D:371:ILE:HD11	2:D:3399:FAD:HM83	1.91	0.51
1:A:50:VAL:HB	1:A:51:PRO:HD3	1.93	0.51
1:C:117:GLN:O	1:C:121:LEU:HB2	2.10	0.51
1:B:390:HIS:C	1:B:392:GLY:N	2.64	0.51
1:C:62:MET:HG3	1:C:98:ILE:HG23	1.93	0.51
1:D:62:MET:HG3	1:D:98:ILE:HG23	1.92	0.51
1:B:387:ALA:O	1:B:391:ILE:HG13	2.10	0.50
1:C:113:ASN:O	1:C:117:GLN:HG3	2.11	0.50
1:C:357:ASN:ND2	1:C:358:THR:H	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:ASP:HB3	1:A:325:ASN:OD1	2.11	0.50
1:A:213:ILE:HB	1:B:358:THR:HG21	1.94	0.50
1:A:346:ASP:O	1:A:350:VAL:HG13	2.12	0.50
1:D:183:ASP:OD1	1:D:185:ASP:HB3	2.11	0.50
1:B:189:PRO:O	1:B:191:SER:N	2.44	0.50
1:B:158:TYR:CE1	1:B:237:VAL:HG21	2.46	0.50
1:B:88:ALA:HB1	1:B:92:THR:HG22	1.93	0.50
1:C:120:TYR:CE2	1:C:198:ILE:HG12	2.46	0.50
1:D:371:ILE:CD1	2:D:3399:FAD:HM83	2.41	0.50
1:A:158:TYR:HB2	1:A:232:VAL:HG13	1.94	0.50
1:B:165:MET:HG3	1:B:166:TRP:CD1	2.46	0.50
1:B:53:LEU:HD13	1:B:130:MET:CE	2.42	0.50
1:B:198:ILE:HG13	1:B:198:ILE:O	2.11	0.50
1:D:246:LYS:H	1:D:246:LYS:CD	2.25	0.50
1:A:11:GLY:N	4:A:887:HOH:O	2.45	0.50
2:A:399:FAD:O2'	3:A:400:CS8:H21	2.12	0.50
1:B:108:LEU:HB3	1:B:121:LEU:HD11	1.94	0.50
1:C:108:LEU:CD2	1:C:238:LEU:HD21	2.37	0.50
1:B:384:ILE:HD11	1:C:292:GLN:NE2	2.27	0.50
1:D:88:ALA:HB1	1:D:92:THR:HG22	1.94	0.50
1:C:88:ALA:HB1	1:C:92:THR:HG22	1.93	0.49
1:D:114:TYR:HB3	1:D:115:GLN:NE2	2.26	0.49
1:B:281:ARG:HB3	1:B:288:LEU:HD22	1.94	0.49
1:B:370:LYS:NZ	1:B:373:GLN:NE2	2.60	0.49
1:D:132:ALA:HB3	1:D:176:TYR:HD1	1.77	0.49
1:B:195:THR:HG23	1:B:241:GLU:HA	1.93	0.49
1:C:235:GLU:H	1:C:235:GLU:CD	2.16	0.49
1:D:141:GLY:HA3	2:D:3399:FAD:H5'1	1.94	0.49
1:B:163:GLN:HG2	1:B:164:LYS:O	2.12	0.49
1:A:206:VAL:O	1:A:206:VAL:CG2	2.60	0.49
1:B:196:GLY:C	1:B:238:LEU:HD23	2.33	0.49
1:B:53:LEU:HD13	1:B:130:MET:HE1	1.95	0.49
1:B:141:GLY:HA3	2:B:1399:FAD:H5'1	1.94	0.49
1:D:46:GLY:O	1:D:211:LYS:NZ	2.45	0.49
1:B:292:GLN:HG3	1:B:296:PHE:CE1	2.47	0.49
1:D:78:ILE:HG23	1:D:79:ASP:N	2.27	0.49
1:B:136:THR:OG1	3:B:1400:CS8:H32	2.12	0.49
1:B:132:ALA:HB3	1:B:176:TYR:HD1	1.76	0.49
1:A:349:GLN:HE21	1:B:370:LYS:NZ	2.11	0.49
1:C:192:LYS:O	1:C:192:LYS:HG2	2.13	0.49
1:D:32:ARG:HH11	1:D:32:ARG:CG	2.18	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:ASP:O	1:A:234:LYS:HG3	2.13	0.48
1:C:382:GLN:O	1:C:386:ILE:HG13	2.12	0.48
1:D:375:TYR:O	1:D:376:GLU:HB2	2.13	0.48
1:A:192:LYS:HG2	1:A:192:LYS:O	2.12	0.48
1:B:255:THR:C	1:B:258:PRO:HD2	2.32	0.48
1:B:64:THR:O	1:B:75:LEU:HB2	2.13	0.48
1:C:165:MET:HG3	1:C:166:TRP:CD1	2.49	0.48
1:D:118:LYS:HZ3	1:D:118:LYS:HB2	1.77	0.48
1:A:238:LEU:HD23	1:A:247:ILE:HD13	1.94	0.48
1:D:196:GLY:O	1:D:238:LEU:HD13	2.14	0.48
1:B:182:SER:HB3	1:B:195:THR:OG1	2.13	0.48
1:A:127:GLU:HB3	1:A:129:LEU:HD22	1.96	0.48
1:D:346:ASP:O	1:D:350:VAL:HG13	2.14	0.48
1:A:109:ILE:HG23	4:A:875:HOH:O	2.13	0.48
1:B:175:TRP:HB2	1:B:198:ILE:CD1	2.44	0.48
1:D:154:LYS:O	1:D:157:GLU:HG2	2.13	0.48
1:C:350:VAL:O	2:D:3399:FAD:H51A	2.14	0.47
1:C:131:CYS:HA	1:C:173:ALA:HB1	1.97	0.47
1:A:214:ASN:ND2	1:B:357:ASN:HD22	2.11	0.47
1:B:178:LEU:C	1:B:178:LEU:HD13	2.35	0.47
1:C:114:TYR:HB3	1:C:115:GLN:OE1	2.14	0.47
1:D:119:LYS:HD3	1:D:120:TYR:CE2	2.50	0.47
1:A:371:ILE:HB	1:B:356:PHE:CZ	2.50	0.47
1:B:103:LEU:CD2	3:B:1400:CS8:H2'2	2.44	0.47
1:B:154:LYS:HE3	1:B:157:GLU:OE2	2.14	0.47
1:B:108:LEU:HD12	1:B:117:GLN:HA	1.96	0.47
1:C:178:LEU:C	1:C:178:LEU:HD13	2.35	0.47
1:D:50:VAL:HB	1:D:51:PRO:HD3	1.95	0.47
1:D:85:GLU:HG3	1:D:264:VAL:HG22	1.95	0.47
1:D:67:PRO:HB2	1:D:70:PHE:CD2	2.50	0.47
1:B:303:MET:HG3	1:C:331:ILE:HG23	1.97	0.47
1:C:349:GLN:HE21	1:D:380:GLN:HE22	1.62	0.47
1:D:164:LYS:HE3	1:D:178:LEU:CD2	2.45	0.47
1:B:115:GLN:N	1:B:115:GLN:HE21	2.00	0.47
1:B:134:CYS:SG	1:B:167:ILE:HG21	2.54	0.47
1:D:20:GLN:HB3	1:D:82:LEU:CD2	2.44	0.47
1:A:141:GLY:HA3	2:A:399:FAD:H5'1	1.96	0.47
1:A:16:LEU:HD11	1:A:82:LEU:HD21	1.97	0.47
1:C:120:TYR:CD2	1:C:198:ILE:HG12	2.50	0.46
1:C:266:LEU:CD1	1:C:365:LEU:HG	2.46	0.46
1:C:371:ILE:CD1	2:C:2399:FAD:HM83	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:168:THR:O	1:D:169:ASN:HB2	2.14	0.46
1:A:63:ASN:HB3	1:A:66:ILE:HD12	1.97	0.46
1:D:233:PRO:HB2	1:D:235:GLU:HG2	1.97	0.46
1:A:275:THR:HG21	1:D:394:TYR:CE1	2.50	0.46
1:A:395:LYS:HZ3	1:A:395:LYS:HB3	1.79	0.46
1:B:316:ALA:O	1:B:319:ILE:HG22	2.15	0.46
1:C:309:ARG:HA	1:C:312:TYR:CD2	2.51	0.46
1:A:33:GLU:O	1:A:37:PRO:HG2	2.15	0.46
2:B:1399:FAD:C2	3:B:1400:CS8:H21	2.45	0.46
1:C:27:ALA:HB2	1:C:83:ILE:HG23	1.98	0.46
1:D:312:TYR:CD1	1:D:312:TYR:C	2.88	0.46
1:A:12:PHE:CD1	1:D:14:PHE:HA	2.51	0.46
1:C:256:ARG:HH12	1:C:385:ILE:HD13	1.81	0.46
1:C:40:ALA:O	1:C:44:ARG:HG3	2.16	0.46
1:D:333:LYS:HD3	1:D:333:LYS:O	2.16	0.46
1:A:374:ILE:HA	1:A:378:THR:HG22	1.97	0.46
1:B:29:LYS:HE3	1:B:33:GLU:OE1	2.16	0.46
1:D:78:ILE:HG22	1:D:320:ASP:OD2	2.15	0.46
1:A:380:GLN:HB2	2:A:399:FAD:O2B	2.16	0.46
1:A:67:PRO:HB2	1:A:70:PHE:CD2	2.51	0.46
1:D:157:GLU:OE1	1:D:231:ARG:CZ	2.63	0.46
1:A:159:ILE:HD11	1:A:231:ARG:HH11	1.81	0.45
1:A:257:PRO:HB2	1:A:258:PRO:HD3	1.98	0.45
1:B:163:GLN:CG	1:B:164:LYS:N	2.74	0.45
1:C:379:ALA:O	1:C:383:ARG:HG2	2.16	0.45
1:D:154:LYS:HG2	1:D:154:LYS:O	2.17	0.45
1:A:54:LYS:HB2	1:A:54:LYS:HZ3	1.79	0.45
1:B:267:ALA:HB1	1:B:343:LEU:HD22	1.97	0.45
1:D:36:ILE:HB	1:D:37:PRO:HD3	1.98	0.45
1:D:55:ARG:NE	1:D:59:LEU:HD11	2.31	0.45
1:C:210:ARG:O	1:C:223:ARG:HB2	2.16	0.45
1:C:273:GLU:OE1	1:C:273:GLU:HA	2.16	0.45
1:A:148:LYS:HD3	1:A:148:LYS:N	2.32	0.45
1:A:36:ILE:HB	1:A:37:PRO:HD3	1.98	0.45
1:B:237:VAL:O	1:B:238:LEU:O	2.34	0.45
1:C:22:GLU:OE1	1:C:22:GLU:HA	2.17	0.45
1:A:144:VAL:O	1:A:147:ILE:HG23	2.17	0.45
1:A:31:ALA:HA	1:A:35:ILE:HD12	1.99	0.45
1:B:384:ILE:HD13	1:C:296:PHE:HE1	1.82	0.45
1:D:210:ARG:HD3	1:D:210:ARG:H	1.82	0.45
1:B:292:GLN:HE21	1:D:293:GLY:HA3	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:GLN:HE22	1:D:226:VAL:CG2	2.27	0.45
1:A:108:LEU:CD1	1:A:238:LEU:HD11	2.42	0.45
1:C:132:ALA:HB3	1:C:176:TYR:CD1	2.50	0.45
1:B:111:GLY:O	1:B:239:THR:CG2	2.65	0.45
1:B:344:ALA:HB1	1:B:366:MET:HA	1.98	0.45
1:D:148:LYS:O	1:D:149:THR:C	2.55	0.45
1:C:375:TYR:O	1:C:376:GLU:HB2	2.17	0.45
1:C:50:VAL:HB	1:C:51:PRO:HD3	1.99	0.45
1:C:243:ALA:O	1:C:247:ILE:HG13	2.17	0.44
1:D:113:ASN:OD1	1:D:116:GLN:HG3	2.16	0.44
1:A:63:ASN:HB3	1:A:66:ILE:CD1	2.47	0.44
1:D:341:ASN:HD21	1:D:370:LYS:CA	2.23	0.44
1:A:344:ALA:HB1	1:A:366:MET:HA	1.98	0.44
1:A:371:ILE:CD1	2:A:399:FAD:HM83	2.47	0.44
1:C:61:LEU:HD22	1:C:83:ILE:CG2	2.48	0.44
1:D:55:ARG:HD2	1:D:55:ARG:HA	1.78	0.44
1:B:32:ARG:HA	1:B:36:ILE:HD12	2.00	0.44
1:C:104:GLY:O	1:C:107:PRO:HD2	2.17	0.44
1:D:269:ARG:O	1:D:273:GLU:HG2	2.17	0.44
1:D:68:GLU:HA	1:D:72:GLY:O	2.17	0.44
1:A:121:LEU:HA	1:A:121:LEU:HD12	1.83	0.44
1:A:159:ILE:HD12	1:A:231:ARG:HG2	1.97	0.44
1:B:127:GLU:HA	1:B:128:PRO:HD3	1.82	0.44
1:B:266:LEU:CD1	1:B:365:LEU:HG	2.48	0.44
1:C:144:VAL:O	1:C:147:ILE:HG23	2.17	0.44
1:A:349:GLN:HE21	1:B:370:LYS:HZ1	1.65	0.44
1:B:67:PRO:HG2	1:B:70:PHE:CD2	2.53	0.44
1:A:132:ALA:HB3	1:A:176:TYR:CD1	2.53	0.44
1:A:55:ARG:HD2	1:A:58:GLU:OE1	2.18	0.44
1:B:98:ILE:O	1:B:101:ASN:HB2	2.18	0.44
1:D:178:LEU:HD13	1:D:179:LEU:N	2.33	0.44
1:A:57:TRP:CD2	1:A:128:PRO:HG3	2.52	0.44
1:B:161:ASN:HD22	1:B:228:GLU:HA	1.83	0.44
1:B:64:THR:OG1	1:B:75:LEU:HD22	2.17	0.44
2:C:2399:FAD:H8A	2:C:2399:FAD:O1A	2.18	0.44
1:D:156:ASP:O	1:D:157:GLU:HB3	2.18	0.44
1:A:160:ILE:HD13	1:A:178:LEU:HD23	2.01	0.43
1:D:357:ASN:OD1	1:D:359:GLU:HB2	2.18	0.43
1:A:211:LYS:HB2	1:A:223:ARG:NH2	2.32	0.43
1:A:256:ARG:HD2	1:A:376:GLU:O	2.18	0.43
1:B:371:ILE:HD12	1:B:374:ILE:HB	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:GLN:HE21	1:C:95:GLN:HB3	1.66	0.43
1:D:59:LEU:N	1:D:59:LEU:HD12	2.33	0.43
1:B:154:LYS:HD2	1:B:159:ILE:HD11	2.01	0.43
1:B:189:PRO:O	1:B:192:LYS:N	2.51	0.43
1:C:168:THR:O	1:C:169:ASN:HB2	2.18	0.43
1:C:234:LYS:C	1:C:236:ASN:H	2.20	0.43
1:C:395:LYS:O	1:C:395:LYS:HG3	2.18	0.43
1:D:160:ILE:HB	1:D:230:VAL:HB	1.99	0.43
1:C:198:ILE:HG13	1:C:198:ILE:O	2.17	0.43
1:D:351:PHE:HB3	1:D:355:GLY:N	2.32	0.43
1:B:256:ARG:CG	1:B:256:ARG:HH11	2.18	0.43
1:C:253:ASP:OD1	1:C:326:THR:HA	2.19	0.43
1:A:175:TRP:CE3	1:A:198:ILE:HD13	2.54	0.43
1:B:239:THR:OG1	1:B:243:ALA:HB3	2.19	0.43
1:D:178:LEU:C	1:D:178:LEU:HD13	2.39	0.43
1:D:360:TYR:HB3	1:D:361:PRO:HD2	2.00	0.43
1:D:89:TYR:CE1	1:D:269:ARG:HD3	2.53	0.43
1:A:109:ILE:CG1	1:A:121:LEU:HD21	2.49	0.43
1:A:335:TYR:CE2	1:A:339:ILE:HG21	2.54	0.43
1:B:28:ARG:O	1:B:32:ARG:HG2	2.19	0.43
1:C:166:TRP:HZ2	1:D:354:ASN:ND2	2.15	0.43
1:C:339:ILE:O	1:C:343:LEU:HD13	2.19	0.43
1:A:81:CYS:HB3	1:A:312:TYR:CE1	2.54	0.42
1:A:214:ASN:HD22	1:B:357:ASN:HD22	1.66	0.42
1:C:309:ARG:HA	1:C:312:TYR:CE2	2.54	0.42
1:D:185:ASP:OD2	1:D:185:ASP:C	2.57	0.42
1:A:156:ASP:C	1:A:234:LYS:HG3	2.39	0.42
1:B:282:LYS:HE2	1:B:287:LEU:CD1	2.49	0.42
1:B:41:GLU:O	1:B:45:THR:HG23	2.19	0.42
1:C:267:ALA:HB1	1:C:343:LEU:HD22	2.01	0.42
1:C:253:ASP:HB3	1:C:325:ASN:OD1	2.19	0.42
1:A:395:LYS:HZ3	1:A:395:LYS:CB	2.31	0.42
1:A:303:MET:HE2	1:D:386:ILE:HD13	2.00	0.42
1:B:113:ASN:O	1:B:117:GLN:HG3	2.19	0.42
1:C:370:LYS:NZ	1:C:373:GLN:NE2	2.67	0.42
1:D:287:LEU:O	1:D:290:GLU:HB2	2.19	0.42
1:A:18:GLU:CA	1:A:18:GLU:OE2	2.66	0.42
1:A:385:ILE:HD11	3:A:400:CS8:H142	2.02	0.42
1:B:14:PHE:HA	1:C:12:PHE:CD1	2.54	0.42
1:D:150:LYS:HZ1	1:D:183:ASP:C	2.23	0.42
1:D:164:LYS:HE3	1:D:178:LEU:HD22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:ILE:O	1:C:72:GLY:HA3	2.20	0.42
1:C:32:ARG:N	1:C:32:ARG:HD2	2.35	0.42
1:C:354:ASN:HD22	1:D:166:TRP:HZ2	1.66	0.42
1:D:98:ILE:O	1:D:101:ASN:HB2	2.19	0.42
1:B:339:ILE:HD12	1:B:339:ILE:C	2.40	0.42
1:A:352:GLY:O	1:B:374:ILE:HD13	2.20	0.42
1:C:266:LEU:HD11	1:C:365:LEU:HG	2.02	0.42
1:C:257:PRO:CB	1:C:258:PRO:HD3	2.49	0.42
1:D:209:GLY:O	1:D:223:ARG:HD3	2.20	0.42
1:A:160:ILE:HD13	1:A:178:LEU:CD2	2.50	0.41
1:D:243:ALA:O	1:D:247:ILE:HG13	2.20	0.41
1:D:30:PHE:O	1:D:34:GLU:HB2	2.20	0.41
1:D:65:HIS:HE1	1:D:254:LYS:HZ1	1.66	0.41
1:B:378:THR:O	1:B:382:GLN:HG2	2.20	0.41
1:C:256:ARG:N	1:C:257:PRO:CD	2.83	0.41
1:C:61:LEU:HD22	1:C:83:ILE:HG23	2.03	0.41
1:A:371:ILE:HD13	2:A:399:FAD:HM83	2.01	0.41
1:B:257:PRO:CB	1:B:258:PRO:HD3	2.48	0.41
1:B:130:MET:HB2	1:B:172:LYS:O	2.20	0.41
1:B:192:LYS:HA	1:B:192:LYS:HD2	1.91	0.41
1:D:115:GLN:N	1:D:115:GLN:NE2	2.63	0.41
1:A:305:VAL:HG13	1:A:306:GLU:N	2.36	0.41
1:B:305:VAL:HG23	1:B:343:LEU:HD21	2.01	0.41
1:B:62:MET:C	1:B:64:THR:N	2.72	0.41
1:D:202:ASP:OD2	1:D:202:ASP:C	2.59	0.41
1:D:84:THR:OG1	1:D:99:GLU:OE2	2.39	0.41
1:A:184:PRO:O	1:A:185:ASP:C	2.58	0.41
1:B:185:ASP:HB3	1:B:188:ALA:HB2	2.03	0.41
1:B:68:GLU:HA	1:B:72:GLY:O	2.21	0.41
1:C:28:ARG:HG3	1:C:32:ARG:HD3	2.03	0.41
1:B:16:LEU:HD12	1:B:16:LEU:N	2.36	0.41
1:C:87:LEU:N	1:C:87:LEU:HD12	2.35	0.41
1:D:257:PRO:N	1:D:258:PRO:CD	2.84	0.41
1:A:36:ILE:N	1:A:37:PRO:CD	2.84	0.41
1:A:16:LEU:HG	1:A:20:GLN:CB	2.50	0.40
1:B:195:THR:CG2	1:B:241:GLU:HA	2.51	0.40
1:C:59:LEU:HA	1:C:59:LEU:HD12	1.89	0.40
1:D:368:ASP:O	1:D:371:ILE:HG22	2.21	0.40
1:A:17:THR:HG1	1:A:20:GLN:HG3	1.85	0.40
1:A:238:LEU:HA	1:A:238:LEU:HD12	1.86	0.40
1:B:318:GLU:OE2	1:B:323:ARG:HD2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:VAL:HG21	1:B:376:GLU:HG2	2.03	0.40
1:D:137:GLU:HB3	1:D:138:PRO:HD2	2.04	0.40
1:C:70:PHE:HD1	1:C:118:LYS:HD2	1.86	0.40
1:C:310:LEU:HD12	1:C:313:GLN:HE22	1.85	0.40
1:A:120:TYR:CE2	1:A:198:ILE:HG12	2.56	0.40
1:A:263:ALA:HB1	1:A:340:ALA:HB2	2.02	0.40
1:B:391:ILE:HG22	1:B:391:ILE:O	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	383/396 (97%)	366 (96%)	15 (4%)	2 (0%)	29 41
1	B	381/396 (96%)	350 (92%)	24 (6%)	7 (2%)	8 10
1	C	383/396 (97%)	371 (97%)	10 (3%)	2 (0%)	29 41
1	D	383/396 (97%)	367 (96%)	14 (4%)	2 (0%)	29 41
All	All	1530/1584 (97%)	1454 (95%)	63 (4%)	13 (1%)	19 29

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	190	ALA
1	B	238	LEU
1	C	238	LEU
1	A	238	LEU
1	B	64	THR
1	B	69	SER
1	D	238	LEU
1	B	128	PRO

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Mol	Chain	Res	Type
1	B	234	LYS
1	B	391	ILE
1	A	128	PRO
1	C	141	GLY
1	D	141	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	301/310 (97%)	278 (92%)	23 (8%)	13	20
1	B	299/310 (96%)	279 (93%)	20 (7%)	16	26
1	C	301/310 (97%)	283 (94%)	18 (6%)	19	31
1	D	301/310 (97%)	276 (92%)	25 (8%)	11	17
All	All	1202/1240 (97%)	1116 (93%)	86 (7%)	14	23

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLU
1	A	54	LYS
1	A	64	THR
1	A	84	THR
1	A	87	LEU
1	A	95	GLN
1	A	115	GLN
1	A	121	LEU
1	A	127	GLU
1	A	148	LYS
1	A	149	THR
1	A	157	GLU
1	A	198	ILE
1	A	222	THR
1	A	235	GLU
1	A	298	LEU

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Mol	Chain	Res	Type
1	A	310	LEU
1	A	312	TYR
1	A	350	VAL
1	A	359	GLU
1	A	365	LEU
1	A	366	MET
1	A	375	TYR
1	B	18	GLU
1	B	55	ARG
1	B	95	GLN
1	B	102	THR
1	B	108	LEU
1	B	115	GLN
1	B	154	LYS
1	B	179	LEU
1	B	198	ILE
1	B	222	THR
1	B	223	ARG
1	B	255	THR
1	B	256	ARG
1	B	288	LEU
1	B	298	LEU
1	B	312	TYR
1	B	350	VAL
1	B	358	THR
1	B	365	LEU
1	B	375	TYR
1	C	18	GLU
1	C	22	GLU
1	C	32	ARG
1	C	64	THR
1	C	84	THR
1	C	95	GLN
1	C	113	ASN
1	C	115	GLN
1	C	129	LEU
1	C	187	LYS
1	C	198	ILE
1	C	222	THR
1	C	235	GLU
1	C	279	LEU
1	C	283	THR

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Mol	Chain	Res	Type
1	C	310	LEU
1	C	365	LEU
1	C	375	TYR
1	D	18	GLU
1	D	22	GLU
1	D	32	ARG
1	D	47	GLU
1	D	64	THR
1	D	75	LEU
1	D	84	THR
1	D	87	LEU
1	D	95	GLN
1	D	115	GLN
1	D	118	LYS
1	D	130	MET
1	D	163	GLN
1	D	198	ILE
1	D	210	ARG
1	D	222	THR
1	D	235	GLU
1	D	246	LYS
1	D	279	LEU
1	D	312	TYR
1	D	343	LEU
1	D	350	VAL
1	D	365	LEU
1	D	375	TYR
1	D	380	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	95	GLN
1	A	105	GLN
1	A	115	GLN
1	A	163	GLN
1	A	169	ASN
1	A	174	ASN
1	A	214	ASN
1	A	217	GLN
1	A	236	ASN

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Mol	Chain	Res	Type
1	A	313	GLN
1	A	341	ASN
1	A	349	GLN
1	B	19	GLN
1	B	105	GLN
1	B	115	GLN
1	B	117	GLN
1	B	161	ASN
1	B	169	ASN
1	B	217	GLN
1	B	291	HIS
1	B	292	GLN
1	B	313	GLN
1	B	341	ASN
1	B	373	GLN
1	C	19	GLN
1	C	20	GLN
1	C	65	HIS
1	C	95	GLN
1	C	105	GLN
1	C	161	ASN
1	C	169	ASN
1	C	217	GLN
1	C	313	GLN
1	C	341	ASN
1	C	354	ASN
1	C	357	ASN
1	C	373	GLN
1	C	380	GLN
1	D	19	GLN
1	D	65	HIS
1	D	95	GLN
1	D	105	GLN
1	D	115	GLN
1	D	161	ASN
1	D	163	GLN
1	D	169	ASN
1	D	207	GLN
1	D	217	GLN
1	D	236	ASN
1	D	313	GLN
1	D	341	ASN

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Mol	Chain	Res	Type
1	D	354	ASN
1	D	380	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

8 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	FAD	A	399	-	51,58,58	2.67	21 (41%)	60,89,89	2.40	19 (31%)
3	CS8	C	2400	-	51,59,59	0.91	2 (3%)	61,85,85	2.10	12 (19%)
2	FAD	D	3399	-	51,58,58	2.58	22 (43%)	60,89,89	2.41	17 (28%)
3	CS8	B	1400	-	51,59,59	1.18	4 (7%)	61,85,85	2.20	13 (21%)
3	CS8	D	3400	-	51,59,59	0.89	2 (3%)	61,85,85	2.16	11 (18%)
3	CS8	A	400	-	51,59,59	0.94	2 (3%)	61,85,85	2.10	11 (18%)
2	FAD	C	2399	-	51,58,58	2.39	19 (37%)	60,89,89	2.28	16 (26%)
2	FAD	B	1399	-	51,58,58	2.52	23 (45%)	60,89,89	2.41	17 (28%)

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	FAD	A	399	-	-	6/30/50/50	0/6/6/6
3	CS8	C	2400	-	-	10/53/74/74	0/3/3/3
2	FAD	D	3399	-	-	8/30/50/50	0/6/6/6
3	CS8	B	1400	-	-	13/53/74/74	0/3/3/3
3	CS8	D	3400	-	-	14/53/74/74	0/3/3/3
3	CS8	A	400	-	-	12/53/74/74	0/3/3/3
2	FAD	C	2399	-	-	9/30/50/50	0/6/6/6
2	FAD	B	1399	-	-	8/30/50/50	0/6/6/6

All (95) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	399	FAD	C4X-C10	9.03	1.47	1.38
2	D	3399	FAD	C4X-C10	8.61	1.47	1.38
2	C	2399	FAD	C4X-C10	8.46	1.47	1.38
2	B	1399	FAD	C4X-C10	7.20	1.46	1.38
2	A	399	FAD	O4B-C1B	5.92	1.49	1.41
2	B	1399	FAD	O4B-C1B	5.74	1.49	1.41
2	D	3399	FAD	C2'-C3'	-5.48	1.43	1.53
2	C	2399	FAD	O4B-C1B	5.33	1.48	1.41
2	B	1399	FAD	C2'-C3'	-5.15	1.43	1.53
2	D	3399	FAD	O4B-C1B	5.15	1.48	1.41
2	A	399	FAD	C2'-C3'	-4.96	1.44	1.53
2	A	399	FAD	C9A-N10	4.74	1.44	1.38
2	D	3399	FAD	C9A-N10	4.55	1.44	1.38
2	B	1399	FAD	PA-O2A	-4.44	1.34	1.55
2	D	3399	FAD	PA-O2A	-4.38	1.34	1.55
2	C	2399	FAD	C2'-C3'	-4.36	1.45	1.53
2	D	3399	FAD	C1'-N10	-4.35	1.43	1.48
2	B	1399	FAD	C5'-C4'	-4.33	1.45	1.51
2	C	2399	FAD	PA-O2A	-4.31	1.35	1.55
2	A	399	FAD	PA-O2A	-4.14	1.35	1.55
2	B	1399	FAD	C9A-N10	4.08	1.44	1.38
2	B	1399	FAD	C4-N3	4.03	1.40	1.33
2	B	1399	FAD	C1'-N10	-3.94	1.44	1.48
2	C	2399	FAD	C9A-N10	3.87	1.43	1.38
3	B	1400	CS8	C5P-N4P	3.85	1.42	1.33
2	B	1399	FAD	C10-N1	3.84	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	399	FAD	C4-C4X	3.74	1.47	1.41
2	D	3399	FAD	C5'-C4'	-3.63	1.46	1.51
2	C	2399	FAD	P-O2P	-3.57	1.38	1.55
2	A	399	FAD	P-O2P	-3.53	1.38	1.55
3	A	400	CS8	C5P-N4P	3.47	1.41	1.33
2	A	399	FAD	C4X-N5	3.46	1.38	1.33
2	A	399	FAD	C1'-N10	-3.46	1.44	1.48
2	A	399	FAD	C5X-N5	3.44	1.41	1.35
2	D	3399	FAD	C4-N3	3.39	1.38	1.33
2	A	399	FAD	C4-N3	3.36	1.38	1.33
3	C	2400	CS8	C5P-N4P	3.32	1.40	1.33
3	D	3400	CS8	C5P-N4P	3.25	1.40	1.33
2	D	3399	FAD	P-O2P	-3.20	1.40	1.55
2	A	399	FAD	C5'-C4'	-3.20	1.47	1.51
2	D	3399	FAD	C10-N1	3.18	1.37	1.33
2	B	1399	FAD	P-O2P	-3.13	1.40	1.55
2	C	2399	FAD	C10-N1	3.12	1.37	1.33
2	A	399	FAD	C10-N1	3.12	1.37	1.33
2	D	3399	FAD	C2-N3	3.10	1.44	1.38
2	A	399	FAD	C2-N3	3.09	1.44	1.38
3	B	1400	CS8	C9P-N8P	3.07	1.40	1.33
2	D	3399	FAD	C4X-N5	2.97	1.37	1.33
2	C	2399	FAD	C4-N3	2.91	1.38	1.33
2	C	2399	FAD	C1'-N10	-2.83	1.45	1.48
2	B	1399	FAD	C8-C7	2.82	1.47	1.40
2	D	3399	FAD	C4-C4X	2.82	1.46	1.41
2	C	2399	FAD	C2B-C1B	-2.77	1.49	1.53
2	B	1399	FAD	C4X-N5	2.73	1.37	1.33
2	C	2399	FAD	C2-N3	2.73	1.43	1.38
2	D	3399	FAD	P-O5'	-2.68	1.48	1.59
2	B	1399	FAD	C4-C4X	2.68	1.46	1.41
2	A	399	FAD	C2B-C1B	-2.67	1.49	1.53
2	A	399	FAD	P-O5'	-2.66	1.48	1.59
2	B	1399	FAD	C2-N1	-2.61	1.33	1.38
2	D	3399	FAD	C8-C7	2.60	1.47	1.40
3	A	400	CS8	C9P-N8P	2.53	1.39	1.33
2	C	2399	FAD	C4-C4X	2.52	1.45	1.41
2	A	399	FAD	C8-C7	2.51	1.47	1.40
2	A	399	FAD	C2-N1	-2.51	1.33	1.38
2	B	1399	FAD	P-O5'	-2.49	1.49	1.59
2	C	2399	FAD	C8-C7	2.48	1.47	1.40
2	C	2399	FAD	C4A-N3A	2.38	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2399	FAD	C2-N1	-2.35	1.33	1.38
2	D	3399	FAD	C5B-C4B	2.32	1.58	1.51
3	B	1400	CS8	C2A-N3A	2.32	1.35	1.32
2	C	2399	FAD	C4X-N5	2.31	1.36	1.33
2	C	2399	FAD	C5'-C4'	-2.31	1.48	1.51
3	B	1400	CS8	P3B-O3B	2.27	1.63	1.59
2	B	1399	FAD	C2-N3	2.26	1.42	1.38
2	D	3399	FAD	C2B-C1B	-2.22	1.50	1.53
2	B	1399	FAD	C5X-N5	2.22	1.39	1.35
2	D	3399	FAD	C4A-N3A	2.21	1.38	1.35
2	B	1399	FAD	C2B-C1B	-2.21	1.50	1.53
3	C	2400	CS8	C9P-N8P	2.18	1.38	1.33
3	D	3400	CS8	C9P-N8P	2.18	1.38	1.33
2	B	1399	FAD	C2A-N3A	2.17	1.35	1.32
2	A	399	FAD	C2A-N3A	2.15	1.35	1.32
2	D	3399	FAD	C2A-N3A	2.15	1.35	1.32
2	A	399	FAD	C4'-C3'	-2.14	1.49	1.53
2	D	3399	FAD	C2-N1	-2.14	1.33	1.38
2	B	1399	FAD	C2A-N1A	2.13	1.37	1.33
2	C	2399	FAD	P-O5'	-2.12	1.50	1.59
2	B	1399	FAD	O3B-C3B	-2.11	1.38	1.43
2	D	3399	FAD	C5X-N5	2.11	1.38	1.35
2	C	2399	FAD	C2A-N3A	2.11	1.35	1.32
2	A	399	FAD	C2A-N1A	2.08	1.37	1.33
2	B	1399	FAD	C4A-N3A	2.05	1.38	1.35
2	B	1399	FAD	C5B-C4B	2.03	1.57	1.51
2	D	3399	FAD	C2A-N1A	2.03	1.37	1.33

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1399	FAD	C5'-C4'-C3'	-10.43	92.05	112.20
2	D	3399	FAD	C5'-C4'-C3'	-9.97	92.95	112.20
2	A	399	FAD	C5'-C4'-C3'	-9.53	93.79	112.20
2	C	2399	FAD	C5'-C4'-C3'	-9.23	94.38	112.20
3	B	1400	CS8	O1'-C1'-S1P	-8.73	111.27	122.61
2	A	399	FAD	C4-N3-C2	8.06	121.94	115.14
3	B	1400	CS8	C2'-C1'-S1P	7.98	123.95	113.58
3	A	400	CS8	C2'-C1'-S1P	7.88	123.81	113.58
2	C	2399	FAD	C4-N3-C2	7.85	121.77	115.14
3	D	3400	CS8	C2'-C1'-S1P	7.82	123.74	113.58
3	D	3400	CS8	O1'-C1'-S1P	-7.75	112.55	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	400	CS8	O1'-C1'-S1P	-7.50	112.88	122.61
2	D	3399	FAD	C4-N3-C2	7.49	121.47	115.14
2	B	1399	FAD	C4-N3-C2	7.41	121.40	115.14
3	C	2400	CS8	O1'-C1'-S1P	-7.34	113.08	122.61
3	C	2400	CS8	C2'-C1'-S1P	7.02	122.70	113.58
3	C	2400	CS8	O6A-CCP-CBP	7.01	121.81	110.55
3	D	3400	CS8	O6A-CCP-CBP	6.68	121.28	110.55
3	A	400	CS8	O6A-CCP-CBP	6.31	120.69	110.55
3	D	3400	CS8	C3P-N4P-C5P	-6.29	111.16	122.84
3	B	1400	CS8	O6A-CCP-CBP	5.73	119.75	110.55
3	A	400	CS8	C3P-N4P-C5P	-5.71	112.24	122.84
3	B	1400	CS8	C3P-N4P-C5P	-5.62	112.41	122.84
3	C	2400	CS8	C3P-N4P-C5P	-5.42	112.78	122.84
2	A	399	FAD	C4X-C4-N3	-4.84	116.81	123.43
2	D	3399	FAD	C4X-C4-N3	-4.52	117.26	123.43
2	C	2399	FAD	C4X-C4-N3	-4.48	117.30	123.43
2	B	1399	FAD	C4X-C4-N3	-4.46	117.33	123.43
2	A	399	FAD	O4B-C1B-C2B	-4.46	100.41	106.93
2	D	3399	FAD	C1'-C2'-C3'	-4.26	97.88	109.79
2	A	399	FAD	C1'-C2'-C3'	-4.17	98.14	109.79
2	C	2399	FAD	C1'-C2'-C3'	-3.96	98.73	109.79
2	D	3399	FAD	C1'-N10-C10	3.91	121.91	118.41
2	B	1399	FAD	C1'-C2'-C3'	-3.90	98.87	109.79
2	B	1399	FAD	O4B-C1B-C2B	-3.84	101.31	106.93
2	C	2399	FAD	O4B-C1B-C2B	-3.80	101.37	106.93
2	A	399	FAD	C4-C4X-C10	-3.72	117.49	119.95
3	B	1400	CS8	CAP-C9P-N8P	3.60	123.75	116.58
2	D	3399	FAD	C1'-N10-C9A	-3.53	115.52	118.29
2	D	3399	FAD	O4B-C1B-C2B	-3.49	101.83	106.93
3	C	2400	CS8	P1A-O3A-P2A	-3.31	121.47	132.83
2	B	1399	FAD	C4-C4X-C10	-3.28	117.78	119.95
3	C	2400	CS8	CAP-C9P-N8P	3.23	123.01	116.58
2	B	1399	FAD	C1'-N10-C10	3.21	121.29	118.41
3	A	400	CS8	CAP-C9P-N8P	3.20	122.94	116.58
2	C	2399	FAD	C4-C4X-C10	-3.14	117.87	119.95
2	D	3399	FAD	C4-C4X-C10	-3.04	117.94	119.95
2	B	1399	FAD	O5'-C5'-C4'	3.03	117.45	109.36
2	D	3399	FAD	O5B-PA-O1A	-3.02	97.26	109.07
3	D	3400	CS8	C7P-N8P-C9P	-3.01	117.21	122.59
2	B	1399	FAD	C4'-C3'-C2'	2.97	119.54	113.36
3	D	3400	CS8	CAP-C9P-N8P	2.95	122.45	116.58
2	C	2399	FAD	O5B-PA-O1A	-2.95	97.56	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3399	FAD	C4'-C3'-C2'	2.88	119.35	113.36
2	C	2399	FAD	C1'-N10-C10	2.87	120.98	118.41
2	D	3399	FAD	O5'-C5'-C4'	2.84	116.93	109.36
2	C	2399	FAD	C4'-C3'-C2'	2.83	119.25	113.36
3	A	400	CS8	P1A-O3A-P2A	-2.80	123.23	132.83
2	A	399	FAD	C1'-N10-C10	2.74	120.87	118.41
3	A	400	CS8	C7P-N8P-C9P	-2.74	117.69	122.59
2	A	399	FAD	C4'-C3'-C2'	2.74	119.06	113.36
3	D	3400	CS8	C1B-N9A-C4A	-2.73	121.85	126.64
2	B	1399	FAD	O5B-PA-O1A	-2.71	98.48	109.07
3	D	3400	CS8	P1A-O3A-P2A	-2.70	123.56	132.83
2	A	399	FAD	O5B-PA-O1A	-2.63	98.78	109.07
2	D	3399	FAD	C5A-C6A-N6A	2.62	124.34	120.35
3	B	1400	CS8	P1A-O3A-P2A	-2.62	123.84	132.83
3	C	2400	CS8	O5P-C5P-C6P	-2.57	117.32	122.02
3	A	400	CS8	O5P-C5P-C6P	-2.56	117.33	122.02
3	A	400	CS8	C1B-N9A-C4A	-2.56	122.15	126.64
3	B	1400	CS8	C3B-C2B-C1B	2.54	105.52	99.89
3	C	2400	CS8	O5P-C5P-N4P	2.52	127.77	123.01
3	B	1400	CS8	C7P-N8P-C9P	-2.52	118.10	122.59
3	D	3400	CS8	O5P-C5P-C6P	-2.51	117.42	122.02
3	C	2400	CS8	C7P-N8P-C9P	-2.51	118.11	122.59
3	C	2400	CS8	C6P-C7P-N8P	-2.49	106.87	111.90
2	D	3399	FAD	C5A-C6A-N1A	-2.47	114.76	120.35
2	C	2399	FAD	O5'-C5'-C4'	2.46	115.94	109.36
2	B	1399	FAD	C5A-C6A-N1A	-2.46	114.77	120.35
3	C	2400	CS8	C1B-N9A-C4A	-2.45	122.33	126.64
2	B	1399	FAD	C1'-N10-C9A	-2.45	116.36	118.29
2	A	399	FAD	C5A-C6A-N1A	-2.44	114.81	120.35
2	C	2399	FAD	O3'-C3'-C4'	-2.44	102.91	108.81
3	A	400	CS8	O5P-C5P-N4P	2.41	127.56	123.01
2	D	3399	FAD	C2A-N1A-C6A	2.40	122.86	118.75
3	B	1400	CS8	O5P-C5P-N4P	2.39	127.52	123.01
3	D	3400	CS8	O5P-C5P-N4P	2.38	127.51	123.01
2	B	1399	FAD	O3'-C3'-C4'	-2.37	103.09	108.81
2	D	3399	FAD	O3'-C3'-C4'	-2.36	103.10	108.81
2	B	1399	FAD	C2A-N1A-C6A	2.36	122.79	118.75
2	A	399	FAD	C4-C4X-N5	2.36	121.29	118.60
2	A	399	FAD	O3'-C3'-C4'	-2.35	103.13	108.81
2	A	399	FAD	C2A-N1A-C6A	2.33	122.74	118.75
2	C	2399	FAD	C5A-C6A-N1A	-2.32	115.09	120.35
3	B	1400	CS8	C1B-N9A-C4A	-2.30	122.59	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2399	FAD	C2A-N1A-C6A	2.29	122.67	118.75
2	A	399	FAD	P-O3P-PA	2.28	140.66	132.83
2	A	399	FAD	C1'-N10-C9A	-2.26	116.51	118.29
2	A	399	FAD	C5A-C6A-N6A	2.26	123.79	120.35
2	A	399	FAD	O5'-C5'-C4'	2.26	115.40	109.36
2	B	1399	FAD	C5A-C6A-N6A	2.26	123.78	120.35
2	A	399	FAD	O3B-C3B-C2B	2.23	119.04	111.82
3	B	1400	CS8	O5A-P2A-O4A	-2.22	101.25	112.24
2	B	1399	FAD	C5X-C9A-N10	-2.20	116.12	117.72
2	D	3399	FAD	O4'-C4'-C5'	2.18	114.83	109.92
3	B	1400	CS8	O5P-C5P-C6P	-2.14	118.11	122.02
2	B	1399	FAD	O4'-C4'-C5'	2.13	114.71	109.92
2	D	3399	FAD	C4X-C10-N10	-2.12	118.12	120.30
2	C	2399	FAD	O4'-C4'-C5'	2.11	114.67	109.92
3	D	3400	CS8	O5A-P2A-O4A	-2.08	101.97	112.24
3	B	1400	CS8	C7P-C6P-C5P	2.06	115.78	112.36
2	C	2399	FAD	C4A-C5A-N7A	2.05	111.54	109.40
2	A	399	FAD	O4'-C4'-C5'	2.04	114.50	109.92
3	C	2400	CS8	O5A-P2A-O4A	-2.03	102.18	112.24
2	C	2399	FAD	C5A-C6A-N6A	2.03	123.43	120.35
3	A	400	CS8	O5A-P2A-O4A	-2.01	102.29	112.24

There are no chirality outliers.

All (80) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	399	FAD	O4B-C4B-C5B-O5B
2	A	399	FAD	C3B-C4B-C5B-O5B
3	C	2400	CS8	CAP-CBP-CCP-O6A
3	C	2400	CS8	CEP-CBP-CCP-O6A
3	C	2400	CS8	CCP-O6A-P2A-O4A
3	C	2400	CS8	CCP-O6A-P2A-O5A
3	C	2400	CS8	CCP-O6A-P2A-O3A
2	D	3399	FAD	O4B-C4B-C5B-O5B
2	D	3399	FAD	C3B-C4B-C5B-O5B
3	B	1400	CS8	O1'-C1'-S1P-C2P
3	B	1400	CS8	C2'-C1'-S1P-C2P
3	B	1400	CS8	CCP-O6A-P2A-O4A
3	B	1400	CS8	CCP-O6A-P2A-O3A
3	B	1400	CS8	O4B-C4B-C5B-O5B
3	D	3400	CS8	CAP-CBP-CCP-O6A
3	D	3400	CS8	CCP-O6A-P2A-O4A

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Mol	Chain	Res	Type	Atoms
3	D	3400	CS8	CCP-O6A-P2A-O5A
3	D	3400	CS8	CCP-O6A-P2A-O3A
3	A	400	CS8	C1'-C2'-S3'-C4'
3	A	400	CS8	CAP-CBP-CCP-O6A
3	A	400	CS8	CCP-O6A-P2A-O4A
3	A	400	CS8	CCP-O6A-P2A-O5A
3	A	400	CS8	CCP-O6A-P2A-O3A
2	C	2399	FAD	O4B-C4B-C5B-O5B
2	C	2399	FAD	C3B-C4B-C5B-O5B
2	C	2399	FAD	C5'-O5'-P-O3P
2	B	1399	FAD	O4B-C4B-C5B-O5B
2	B	1399	FAD	C3B-C4B-C5B-O5B
3	B	1400	CS8	C3B-C4B-C5B-O5B
3	B	1400	CS8	C2B-C3B-O3B-P3B
3	C	2400	CS8	CDP-CBP-CCP-O6A
3	D	3400	CS8	CDP-CBP-CCP-O6A
3	D	3400	CS8	CEP-CBP-CCP-O6A
3	A	400	CS8	CEP-CBP-CCP-O6A
3	B	1400	CS8	C4B-C3B-O3B-P3B
3	C	2400	CS8	S1P-C2P-C3P-N4P
3	D	3400	CS8	C1'-C2'-S3'-C4'
3	A	400	CS8	CDP-CBP-CCP-O6A
3	D	3400	CS8	C5'-C6'-C7'-C8'
2	C	2399	FAD	PA-O3P-P-O1P
2	B	1399	FAD	PA-O3P-P-O1P
2	B	1399	FAD	C4B-C5B-O5B-PA
3	B	1400	CS8	C1'-C2'-S3'-C4'
2	D	3399	FAD	C4B-C5B-O5B-PA
3	A	400	CS8	C5'-C6'-C7'-C8'
3	D	3400	CS8	C5P-C6P-C7P-N8P
3	D	3400	CS8	C3B-O3B-P3B-O9A
2	A	399	FAD	P-O3P-PA-O2A
2	D	3399	FAD	P-O3P-PA-O2A
2	C	2399	FAD	P-O3P-PA-O2A
2	B	1399	FAD	P-O3P-PA-O2A
2	C	2399	FAD	C4B-C5B-O5B-PA
3	B	1400	CS8	CCP-O6A-P2A-O5A
2	C	2399	FAD	C5'-O5'-P-O2P
3	C	2400	CS8	C4'-C5'-C6'-C7'
3	A	400	CS8	S1P-C2P-C3P-N4P
3	C	2400	CS8	C5'-C6'-C7'-C8'
2	A	399	FAD	PA-O3P-P-O2P

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Mol	Chain	Res	Type	Atoms
3	C	2400	CS8	P1A-O3A-P2A-O5A
2	D	3399	FAD	PA-O3P-P-O1P
2	D	3399	FAD	PA-O3P-P-O2P
2	A	399	FAD	C4B-C5B-O5B-PA
3	A	400	CS8	C5P-C6P-C7P-N8P
3	D	3400	CS8	P1A-O3A-P2A-O5A
3	A	400	CS8	P1A-O3A-P2A-O4A
2	C	2399	FAD	PA-O3P-P-O2P
3	B	1400	CS8	O9P-C9P-N8P-C7P
3	D	3400	CS8	C4B-C3B-O3B-P3B
2	A	399	FAD	C5'-O5'-P-O3P
2	D	3399	FAD	C5'-O5'-P-O3P
2	B	1399	FAD	C5'-O5'-P-O3P
3	A	400	CS8	C4'-C5'-C6'-C7'
2	D	3399	FAD	P-O3P-PA-O1A
3	D	3400	CS8	P1A-O3A-P2A-O4A
2	C	2399	FAD	P-O3P-PA-O1A
2	B	1399	FAD	P-O3P-PA-O1A
2	B	1399	FAD	PA-O3P-P-O2P
3	B	1400	CS8	CAP-C9P-N8P-C7P
3	D	3400	CS8	S1P-C2P-C3P-N4P
3	B	1400	CS8	C4'-C5'-C6'-C7'

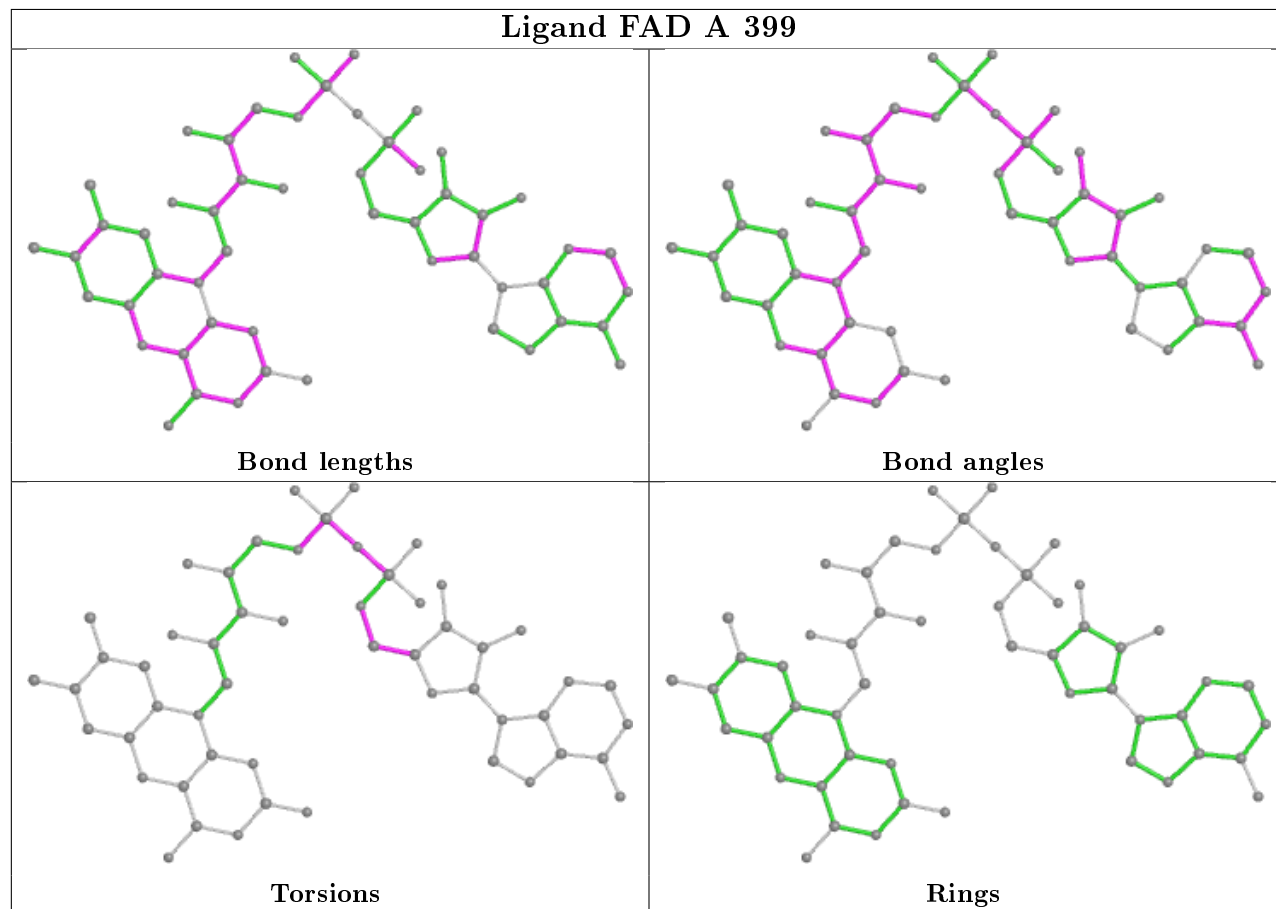
There are no ring outliers.

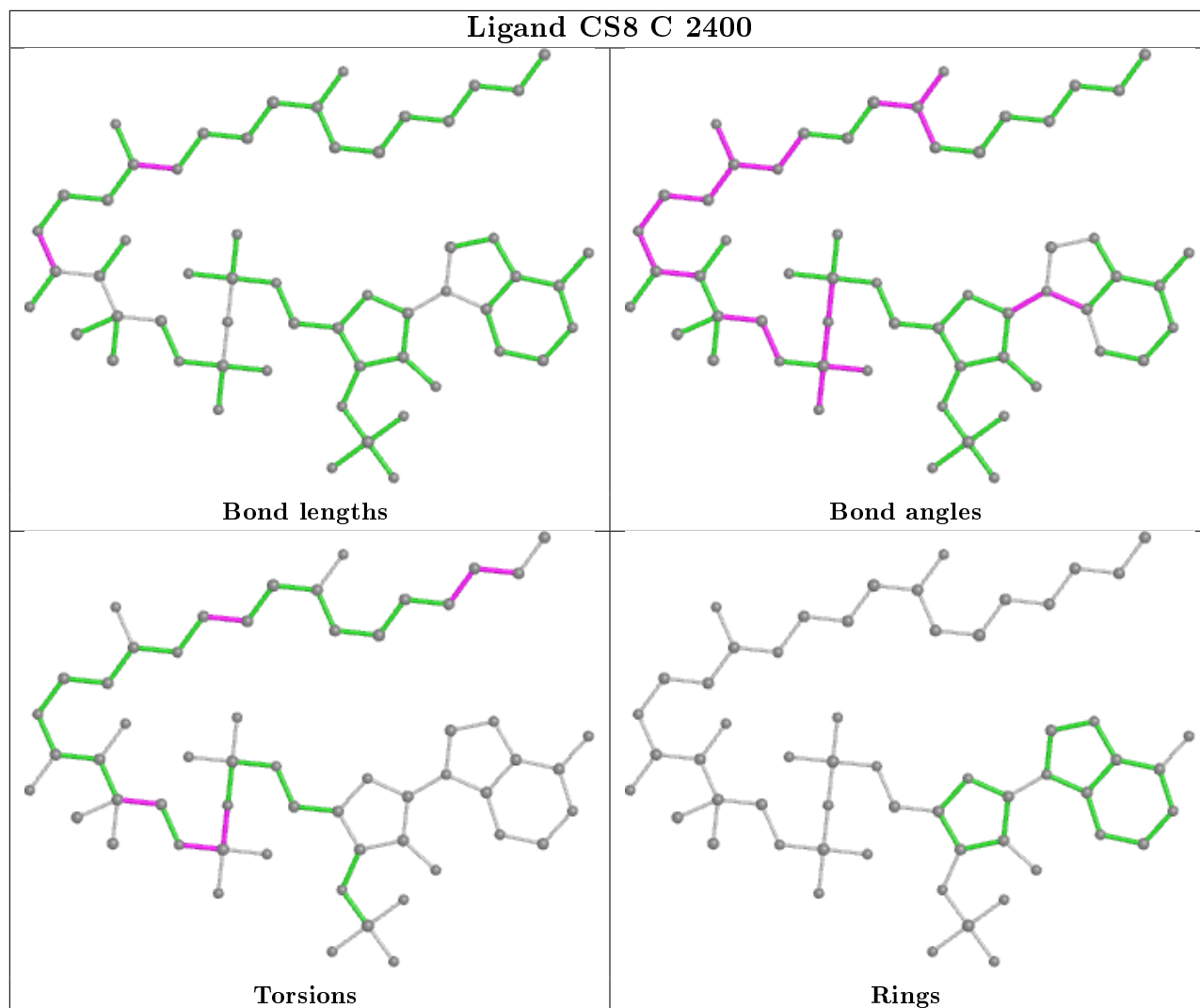
7 monomers are involved in 26 short contacts:

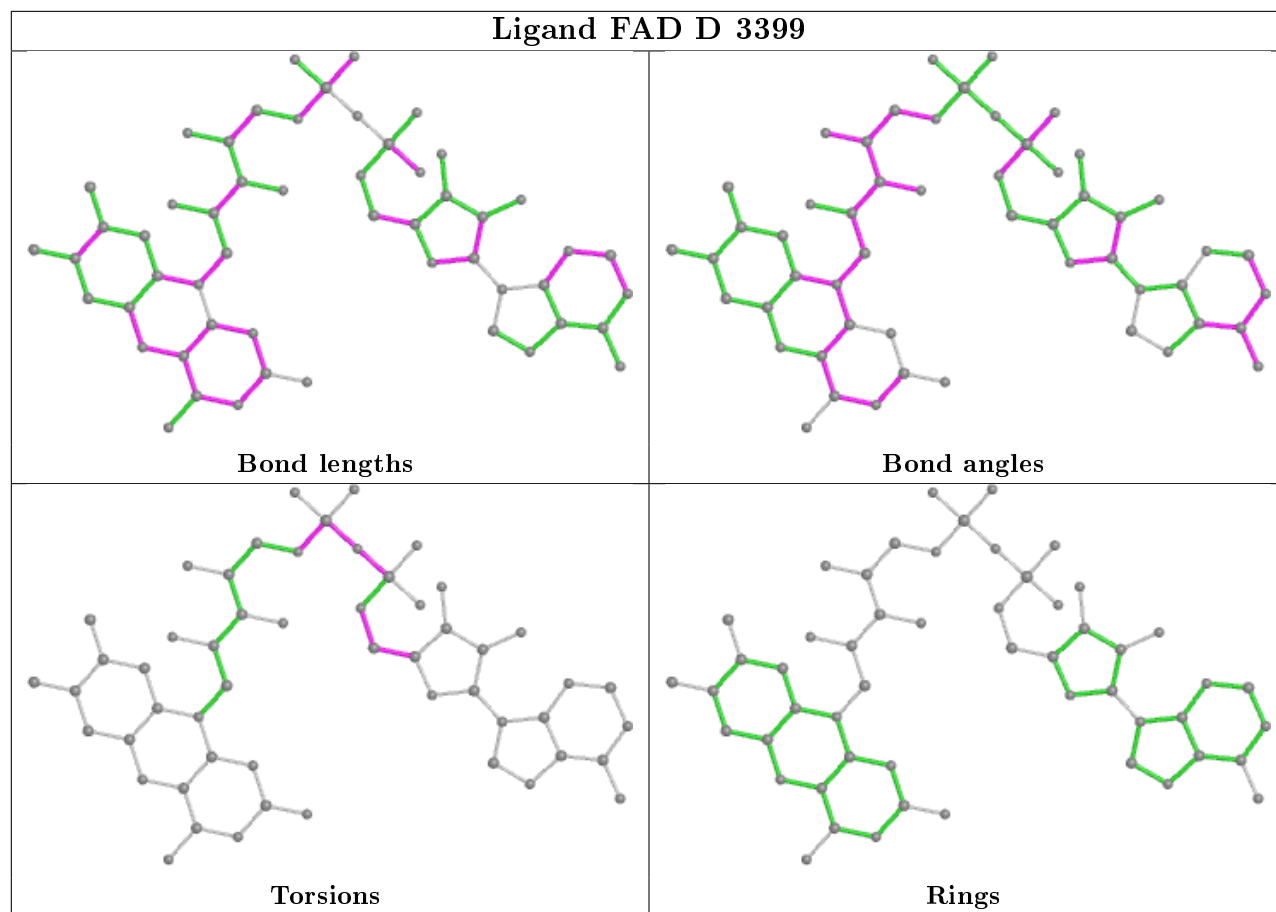
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	399	FAD	6	0
3	C	2400	CS8	1	0
2	D	3399	FAD	5	0
3	B	1400	CS8	5	0
3	A	400	CS8	3	0
2	C	2399	FAD	4	0
2	B	1399	FAD	4	0

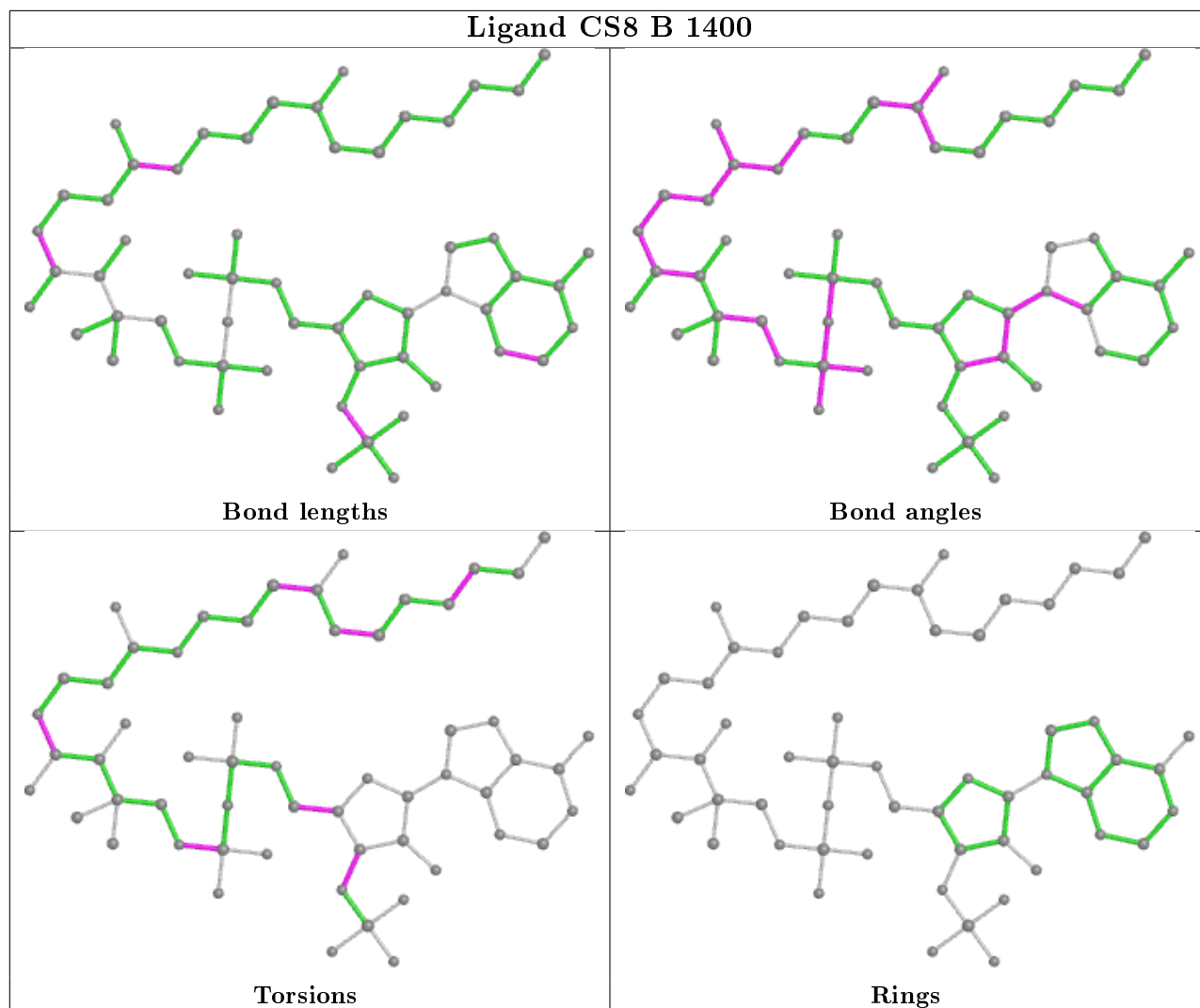
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

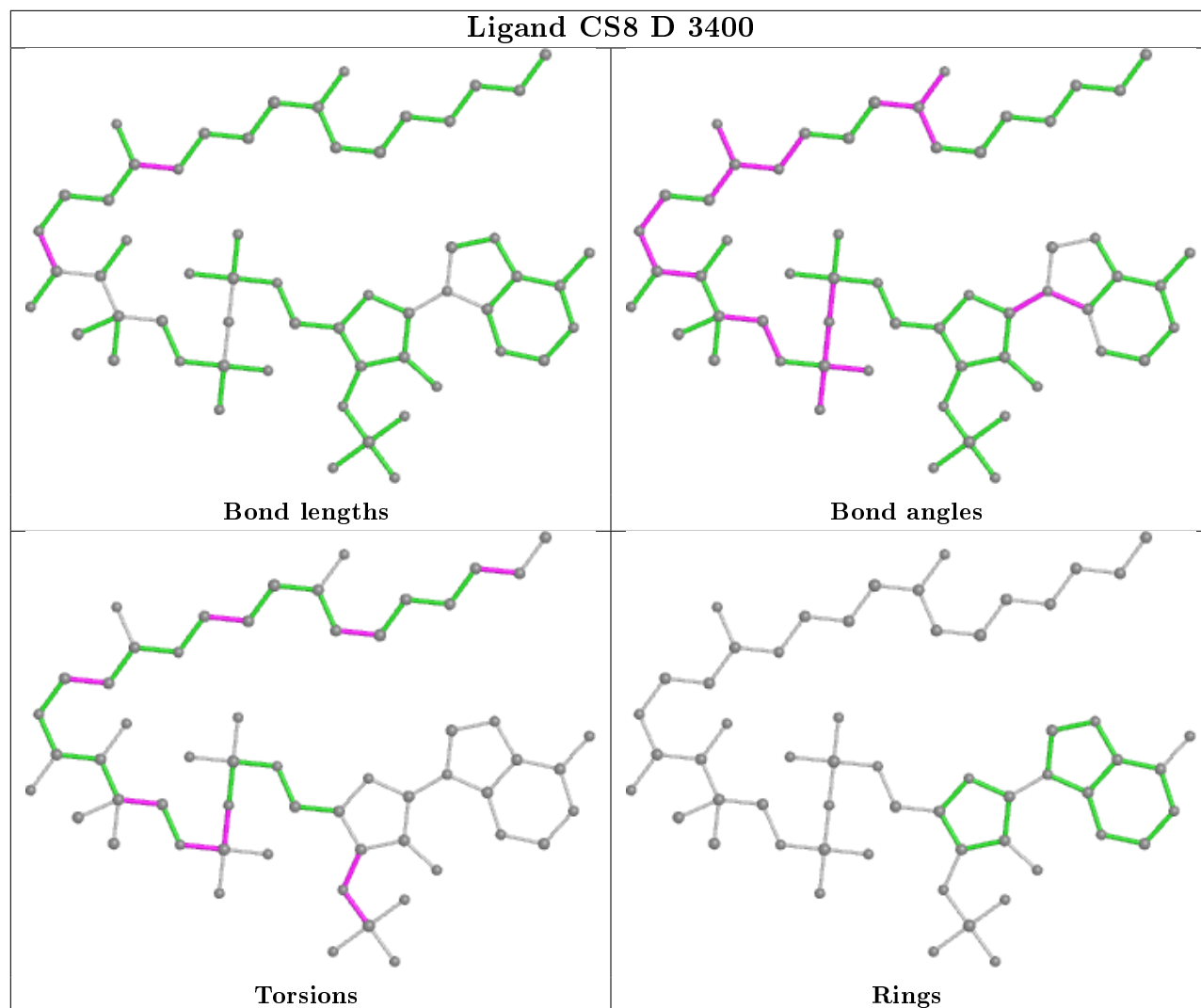
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers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

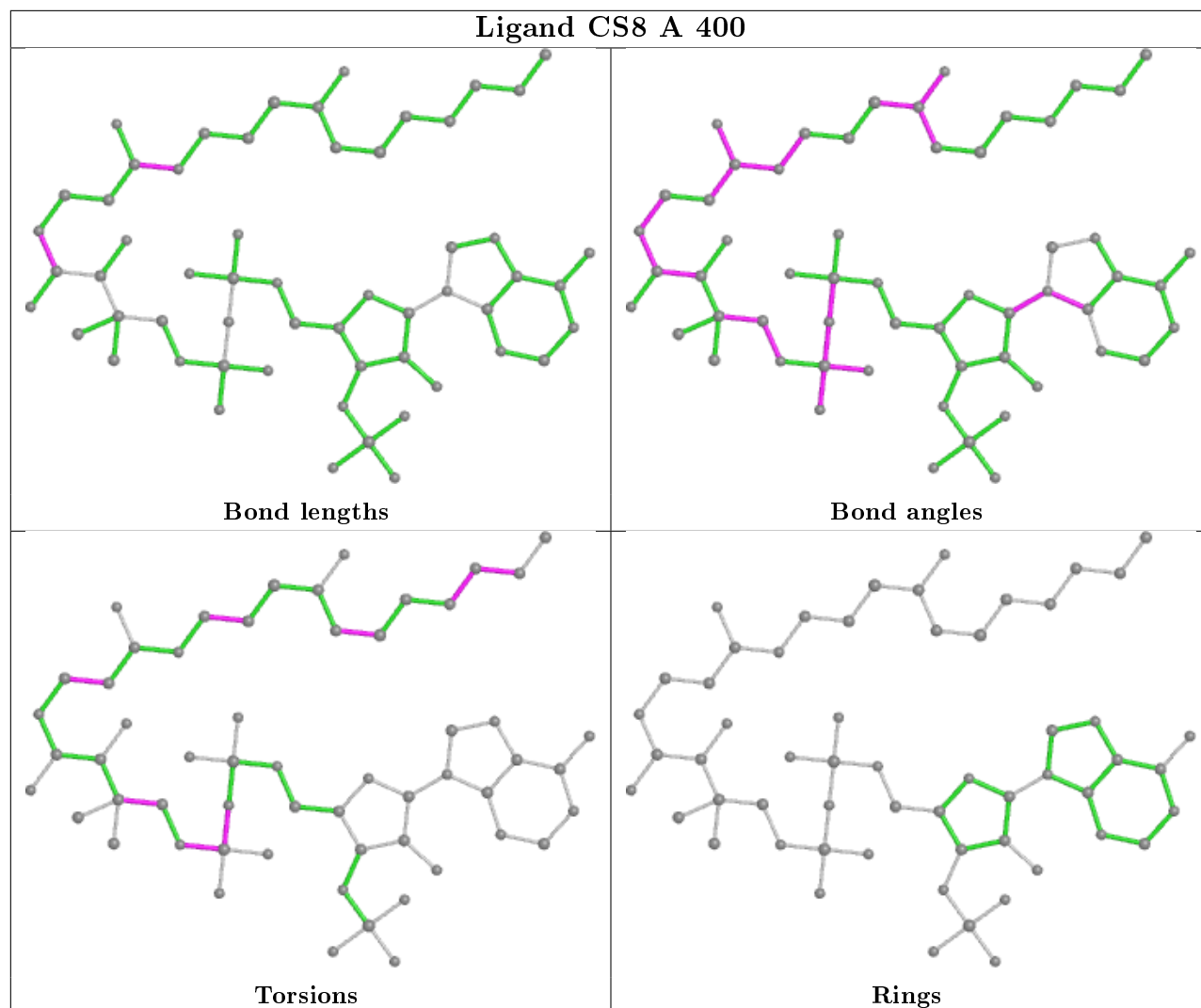


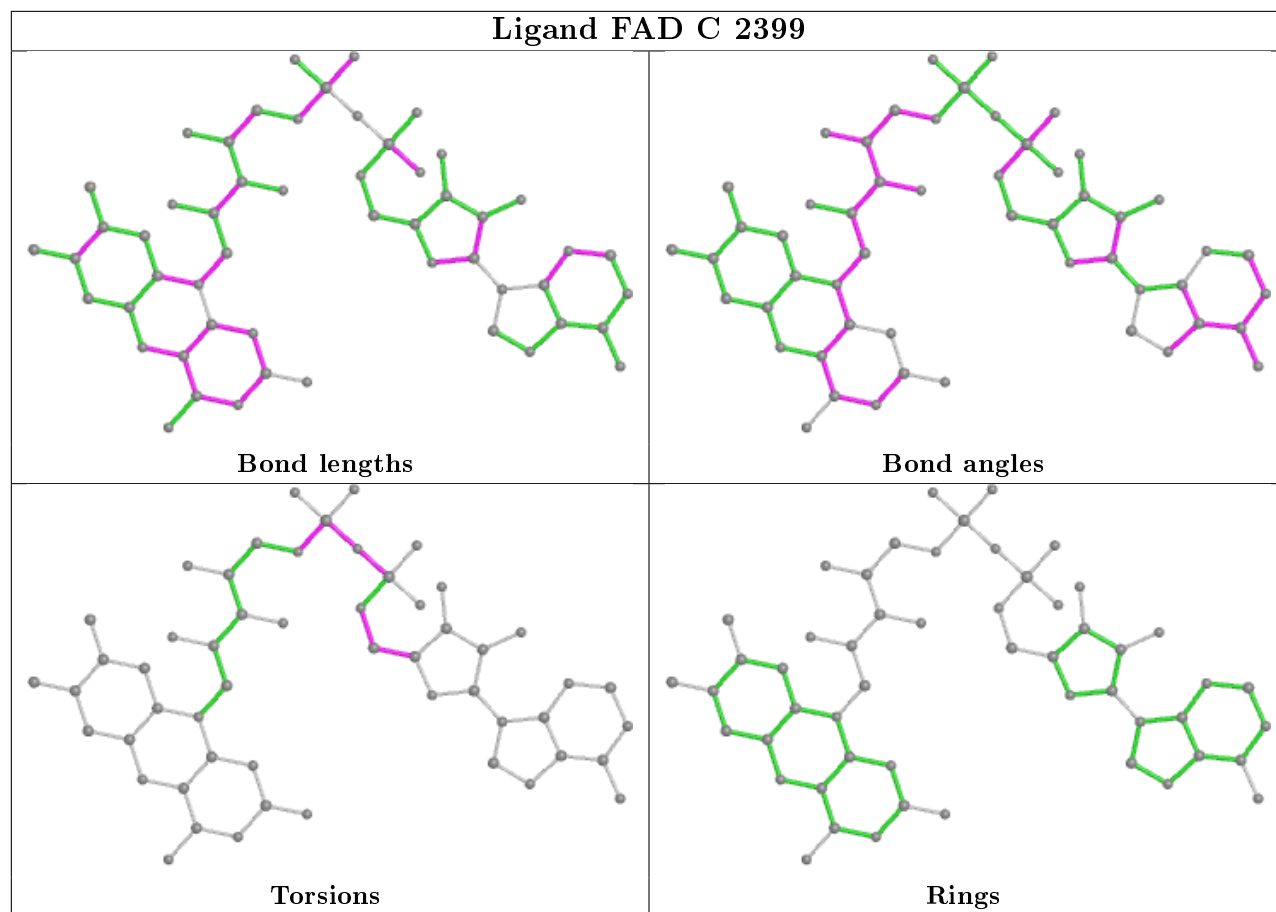


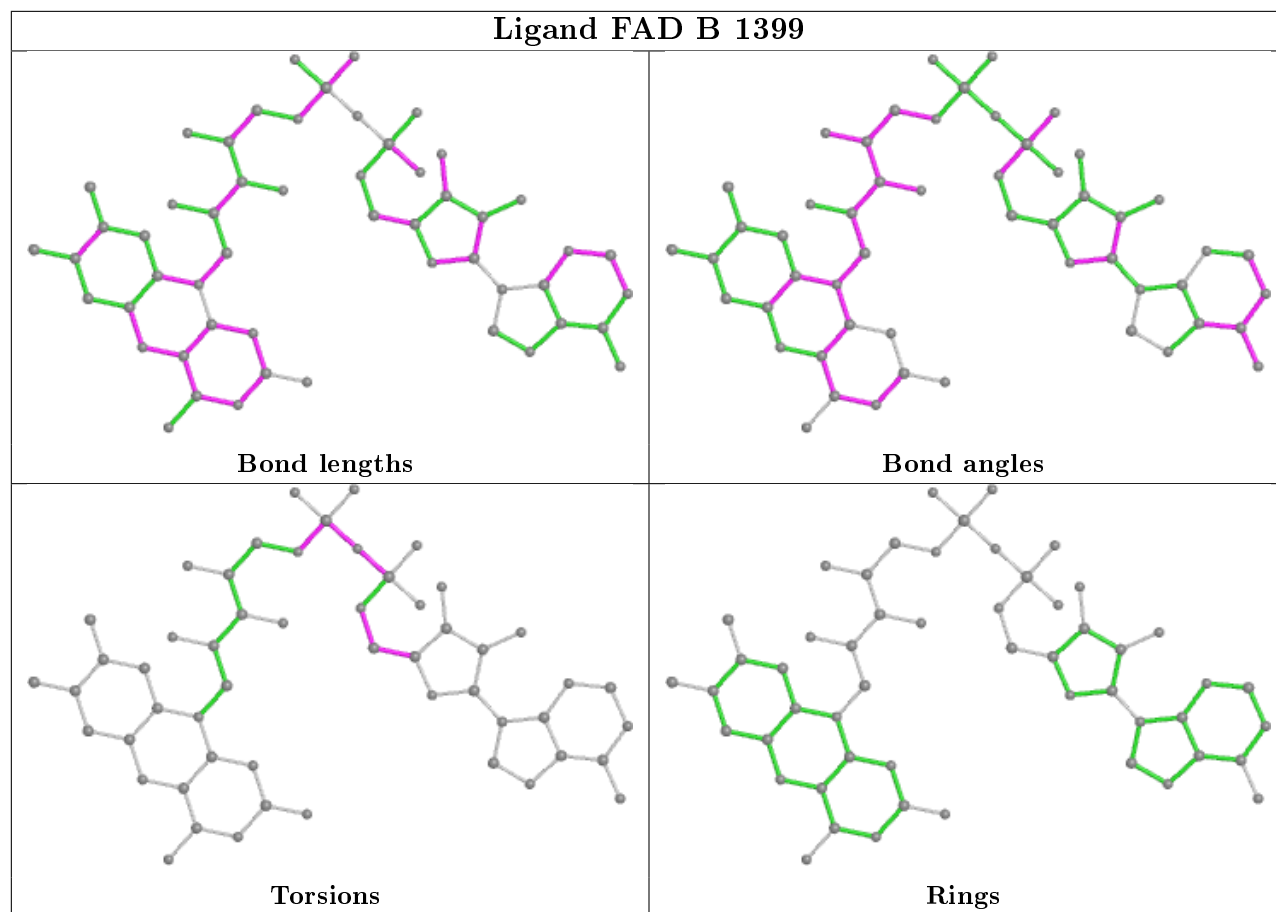












5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	385/396 (97%)	-0.74	0 100 100	14, 26, 38, 50	0
1	B	383/396 (96%)	-0.62	0 100 100	17, 30, 44, 58	0
1	C	385/396 (97%)	-0.76	0 100 100	14, 25, 38, 46	0
1	D	385/396 (97%)	-0.71	0 100 100	14, 25, 40, 49	0
All	All	1538/1584 (97%)	-0.71	0 100 100	14, 27, 41, 58	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

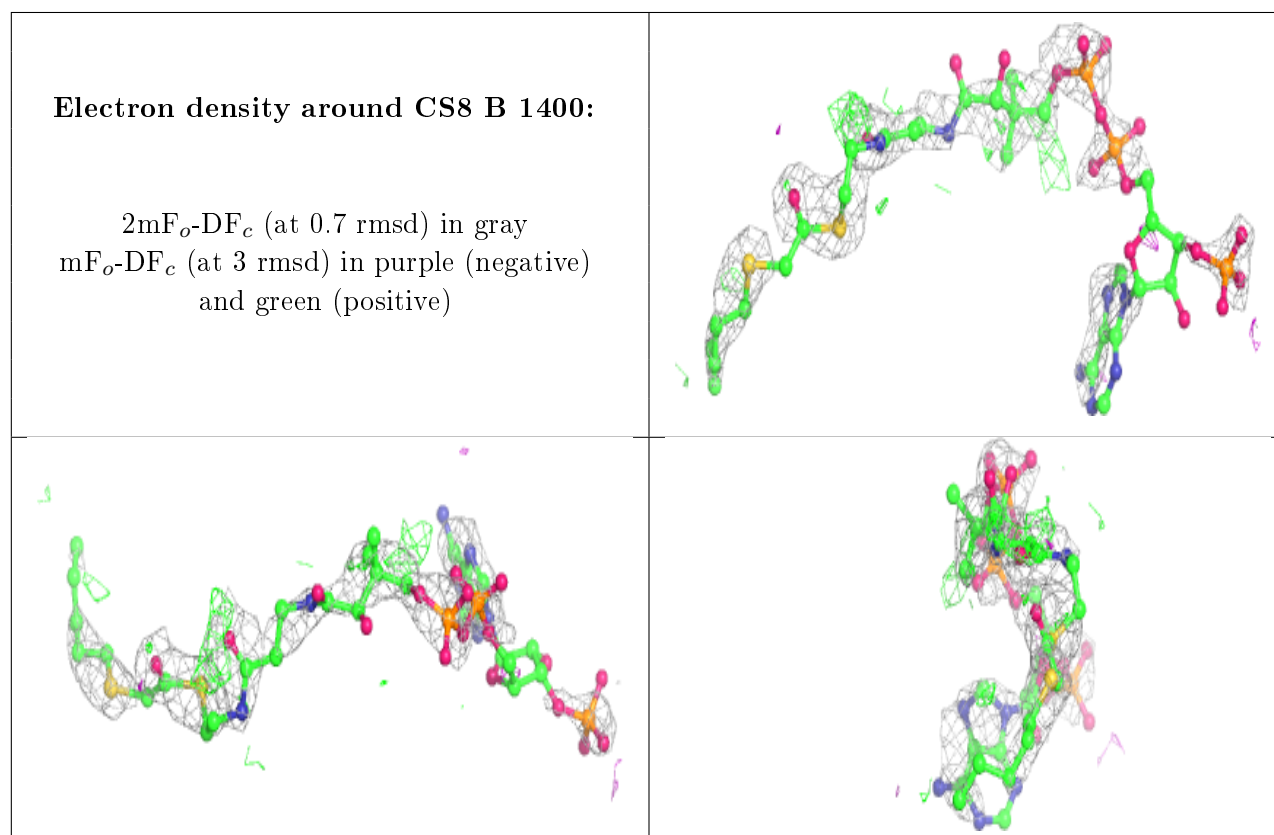
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CS8	B	1400	57/57	0.73	0.36	25,43,49,49	57
2	FAD	B	1399	53/53	0.93	0.14	20,27,33,35	0
2	FAD	A	399	53/53	0.94	0.14	16,23,27,32	0
3	CS8	D	3400	57/57	0.94	0.12	20,29,41,43	57

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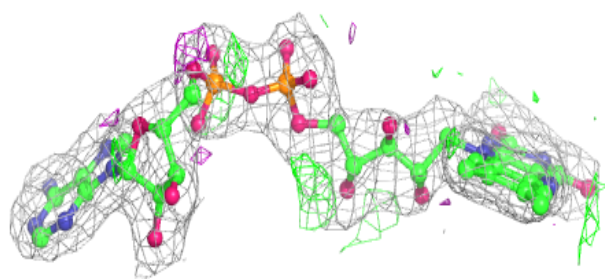
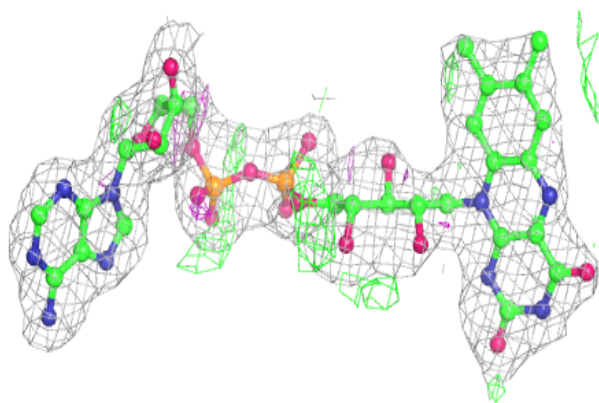
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CS8	A	400	57/57	0.94	0.13	15,30,38,40	57
2	FAD	C	2399	53/53	0.94	0.14	20,24,32,38	0
2	FAD	D	3399	53/53	0.94	0.13	21,25,30,32	0
3	CS8	C	2400	57/57	0.95	0.10	15,29,35,35	0

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

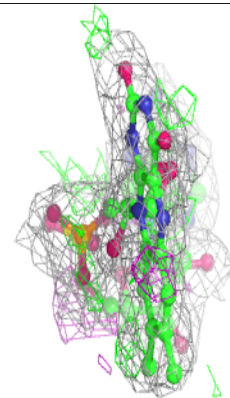
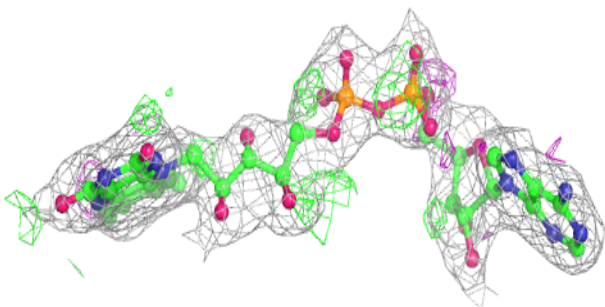
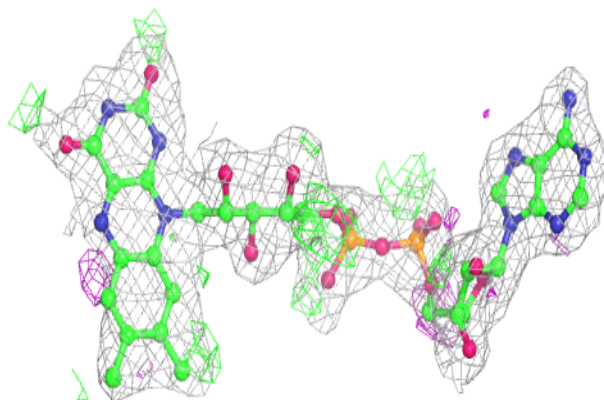


Electron density around FAD B 1399:

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

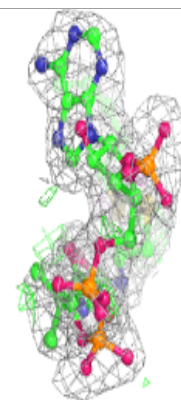
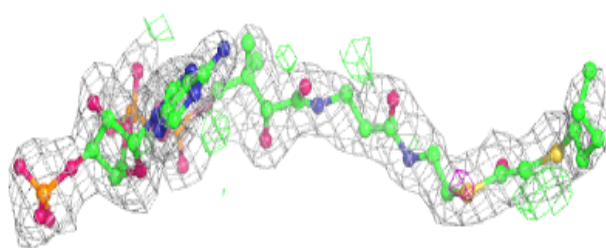
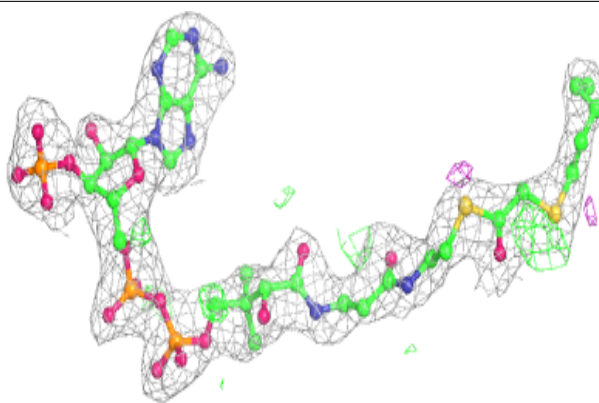
**Electron density around FAD A 399:**

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

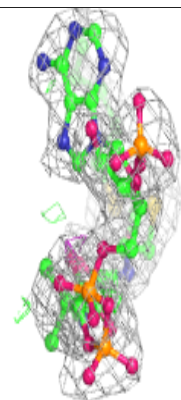
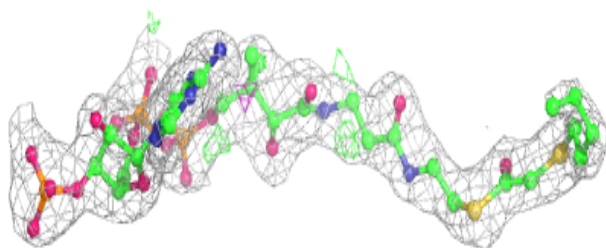
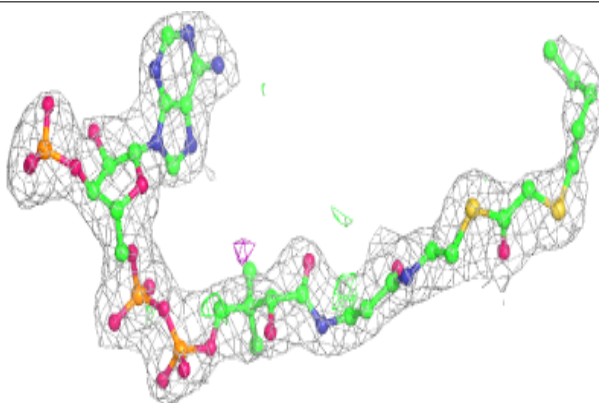


Electron density around CS8 D 3400:

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

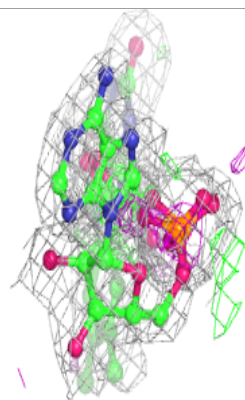
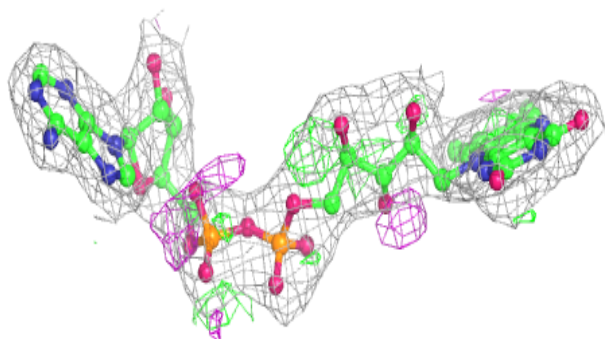
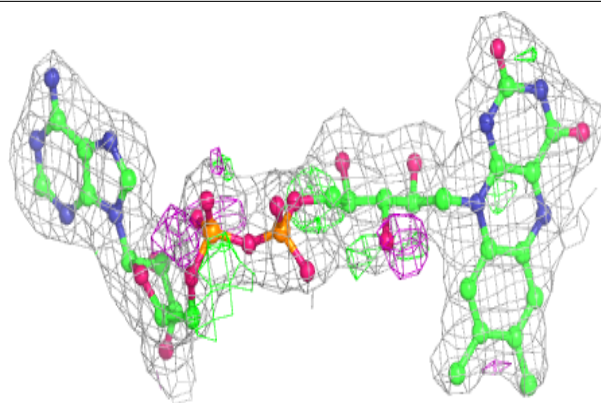
**Electron density around CS8 A 400:**

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

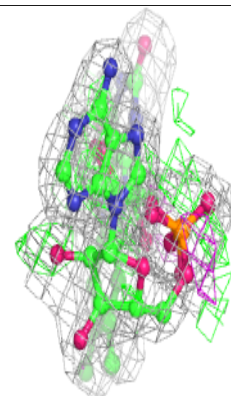
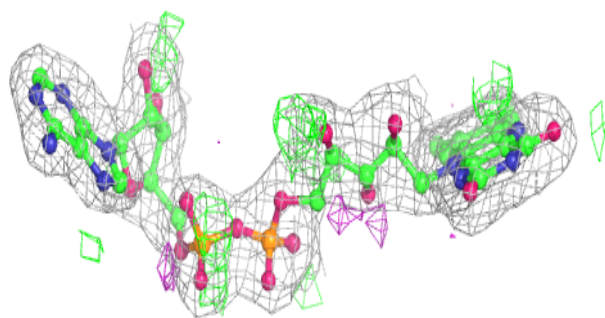
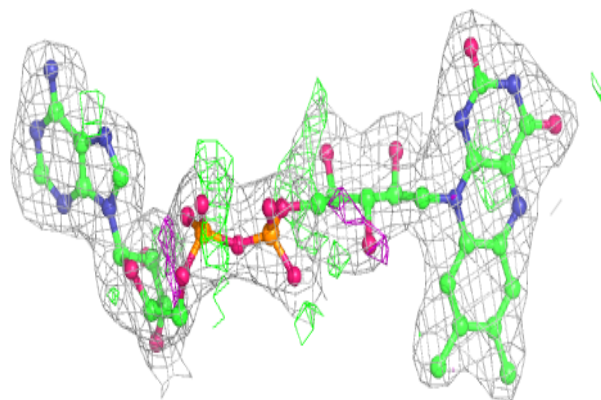


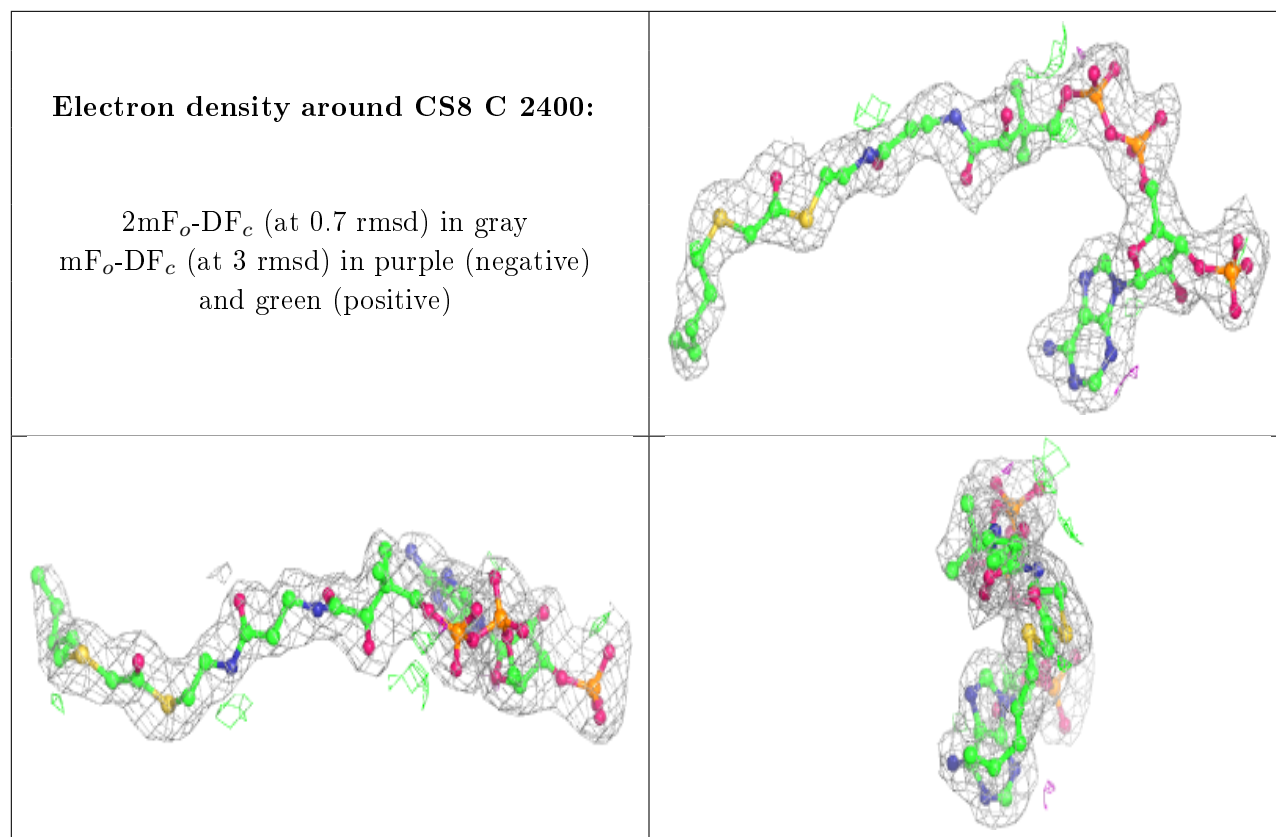
Electron density around FAD C 2399:

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

**Electron density around FAD D 3399:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.