Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2023 – 05:55 AM EDT

PDB ID	:	3MPJ
Title	:	Structure of the glutaryl-coenzyme A dehydrogenase
Authors	:	Wischgoll, S.; Warkentin, E.; Boll, M.; Ermler, U.
Deposited on	:	2010-04-27
Resolution	:	2.10 Å(reported)

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

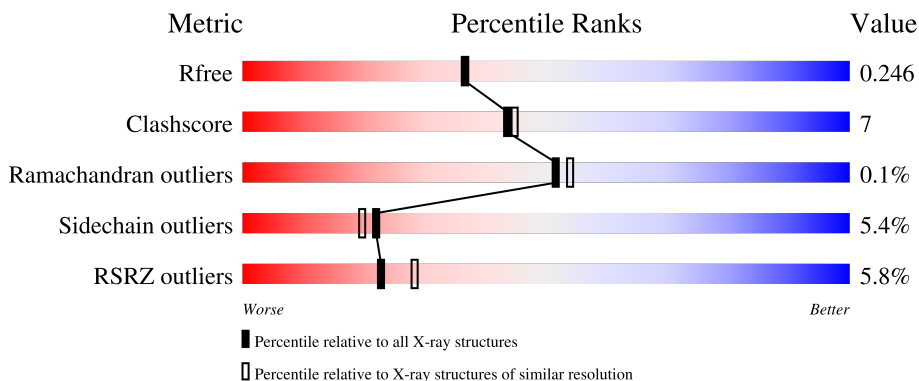|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.10 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.
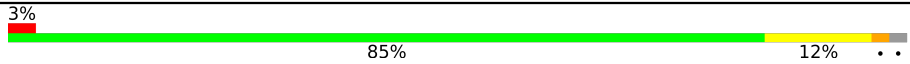
Metric	Percentile Ranks	Value
Rfree		0.246
Clashscore		7
Ramachandran outliers		0.1%
Sidechain outliers		5.4%
RSRZ outliers		5.8%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 <=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	397	81% 15% • •
1	B	397	% 82% 15% • •
1	D	397	10% 83% 14% • •
1	E	397	19% 77% 21% • •
1	F	397	% 86% 10% • •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	397	3% 85% 12%
2	Y	8	50% 12% 62% 25%

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 19170 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 Glutaryl-CoA dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	2	0
			2992	1891	510	571	20			
1	B	393	Total	C	N	O	S	0	2	0
			3026	1913	520	573	20			
1	D	390	Total	C	N	O	S	0	2	0
			3004	1899	515	570	20			
1	E	391	Total	C	N	O	S	0	1	0
			2999	1896	515	568	20			
1	F	390	Total	C	N	O	S	0	2	0
			3001	1898	514	569	20			
1	G	389	Total	C	N	O	S	0	0	0
			2975	1882	508	565	20			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	390	LYS	-	expression tag	UNP C3UVB0
A	391	GLY	-	expression tag	UNP C3UVB0
A	392	HIS	-	expression tag	UNP C3UVB0
A	393	HIS	-	expression tag	UNP C3UVB0
A	394	HIS	-	expression tag	UNP C3UVB0
A	395	HIS	-	expression tag	UNP C3UVB0
A	396	HIS	-	expression tag	UNP C3UVB0
A	397	HIS	-	expression tag	UNP C3UVB0
B	390	LYS	-	expression tag	UNP C3UVB0
B	391	GLY	-	expression tag	UNP C3UVB0
B	392	HIS	-	expression tag	UNP C3UVB0
B	393	HIS	-	expression tag	UNP C3UVB0
B	394	HIS	-	expression tag	UNP C3UVB0
B	395	HIS	-	expression tag	UNP C3UVB0
B	396	HIS	-	expression tag	UNP C3UVB0
B	397	HIS	-	expression tag	UNP C3UVB0
D	390	LYS	-	expression tag	UNP C3UVB0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	391	GLY	-	expression tag	UNP C3UVB0
D	392	HIS	-	expression tag	UNP C3UVB0
D	393	HIS	-	expression tag	UNP C3UVB0
D	394	HIS	-	expression tag	UNP C3UVB0
D	395	HIS	-	expression tag	UNP C3UVB0
D	396	HIS	-	expression tag	UNP C3UVB0
D	397	HIS	-	expression tag	UNP C3UVB0
E	390	LYS	-	expression tag	UNP C3UVB0
E	391	GLY	-	expression tag	UNP C3UVB0
E	392	HIS	-	expression tag	UNP C3UVB0
E	393	HIS	-	expression tag	UNP C3UVB0
E	394	HIS	-	expression tag	UNP C3UVB0
E	395	HIS	-	expression tag	UNP C3UVB0
E	396	HIS	-	expression tag	UNP C3UVB0
E	397	HIS	-	expression tag	UNP C3UVB0
F	390	LYS	-	expression tag	UNP C3UVB0
F	391	GLY	-	expression tag	UNP C3UVB0
F	392	HIS	-	expression tag	UNP C3UVB0
F	393	HIS	-	expression tag	UNP C3UVB0
F	394	HIS	-	expression tag	UNP C3UVB0
F	395	HIS	-	expression tag	UNP C3UVB0
F	396	HIS	-	expression tag	UNP C3UVB0
F	397	HIS	-	expression tag	UNP C3UVB0
G	390	LYS	-	expression tag	UNP C3UVB0
G	391	GLY	-	expression tag	UNP C3UVB0
G	392	HIS	-	expression tag	UNP C3UVB0
G	393	HIS	-	expression tag	UNP C3UVB0
G	394	HIS	-	expression tag	UNP C3UVB0
G	395	HIS	-	expression tag	UNP C3UVB0
G	396	HIS	-	expression tag	UNP C3UVB0
G	397	HIS	-	expression tag	UNP C3UVB0

- Molecule 2 is a protein called Octapeptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	Y	8	72	44	20	8	0	0	0

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

FAD

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	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		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	B	1	Total	Cl	0	0
			1	1		
4	D	1	Total	Cl	0	0
			1	1		
4	E	1	Total	Cl	0	0
			1	1		
4	F	1	Total	Cl	0	0
			1	1		
4	G	1	Total	Cl	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	175	Total 175	O 175	0	0
5	B	179	Total 179	O 179	0	0
5	D	84	Total 84	O 84	0	0
5	E	78	Total 78	O 78	0	0
5	F	143	Total 143	O 143	0	0
5	G	115	Total 115	O 115	0	0
5	Y	3	Total 3	O 3	0	0

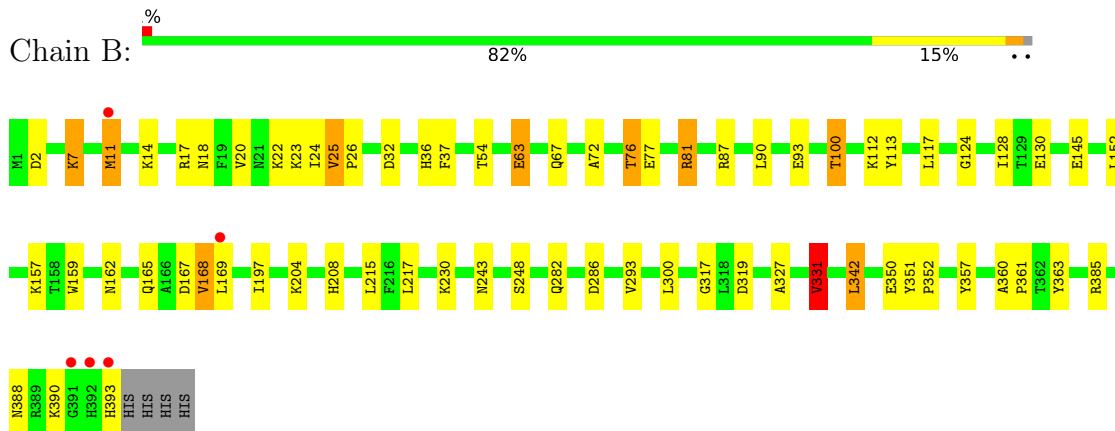# 3 Residue-property plots ⓘ

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.
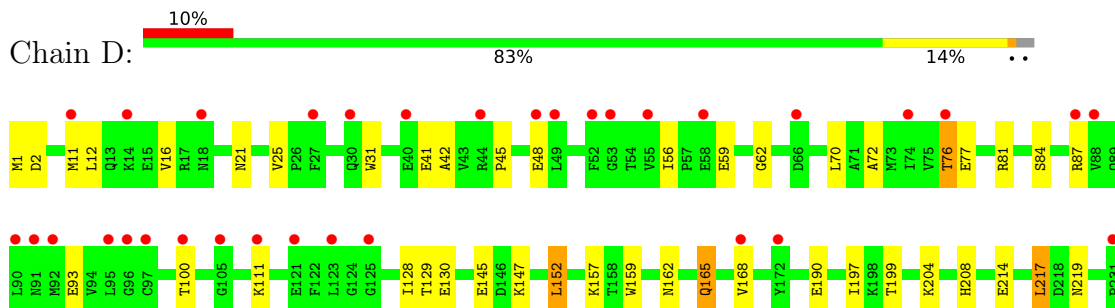
- Molecule 1: Glutaryl-CoA dehydrogenase
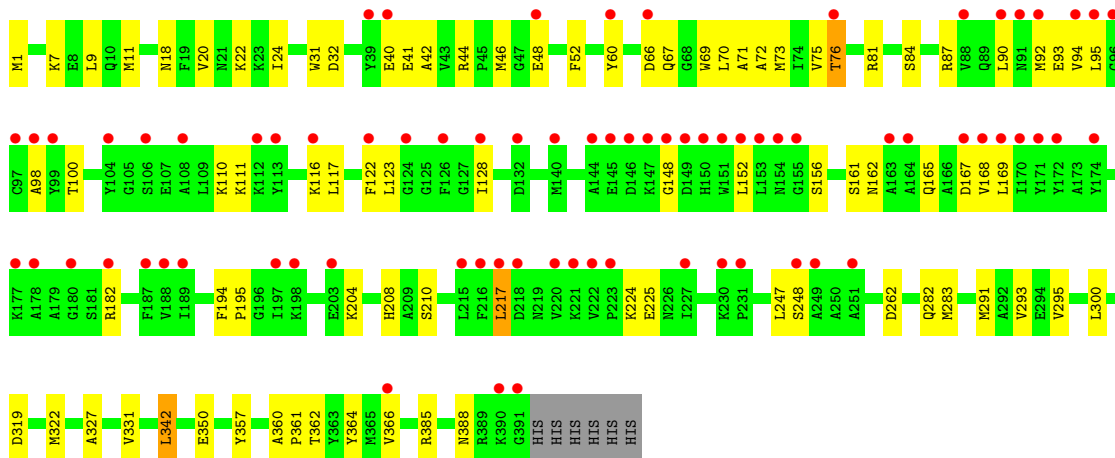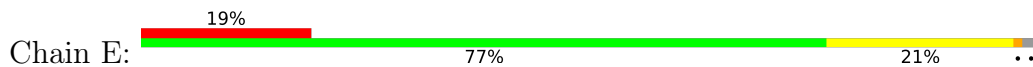

- Molecule 1: Glutaryl-CoA dehydrogenase

- Molecule 1: Glutaryl-CoA dehydrogenase

S241 T245 A251 G255 K266 E270 D280 F281 Q282 M283 L300 D319 A327 V331 L342 Y351 P352 V353 Y357 P361 Y364 N388 R389 K390 GLY HIS HIS HIS HIS HIS HIS

• Molecule 1: Glutaryl-CoA dehydrogenase

Chain E:

19%

77% 21%

M1 K7 E8 L9 Q10 M11 N18 F19 V20 N21 K22 K23 I24 W31 D32 Y39 E40 E41 A42 V43 R44 P45 M46 G47 E48 F52 Y60 D66 Q67 G68 W69 L70 A71 A72 M73 I74 V75 T76 R81 S84 R87 V88 Q89 L90 N91 M92 E93 V94 L95 G96

C97 A98 Y99 T100 Y104 G105 S106 E107 A108 L109 K110 K111 K112 Y113 K116 L117 F122 L123 G124 G125 F126 G127 I128 D132 M140 A144 E145 D146 K147 G148 D149 H150 W151 L152 L153 N154 G155 S156 S161 N162 A163 A164 Q165 A166 D167 V168 L169 I170 Y171 Y172 A173 Y174

K177 A178 A179 G180 S181 R182 F187 V188 I189 F194 P195 G196 I197 K198 E203 K204 H208 A209 S210 L215 F216 L217 D218 N219 V220 K221 V222 P223 K224 E225 N226 I227 K230 P231 L247 S248 A249 A250 A251 D262 Q282 M283 M291 A292 V293 E294 V295 L300

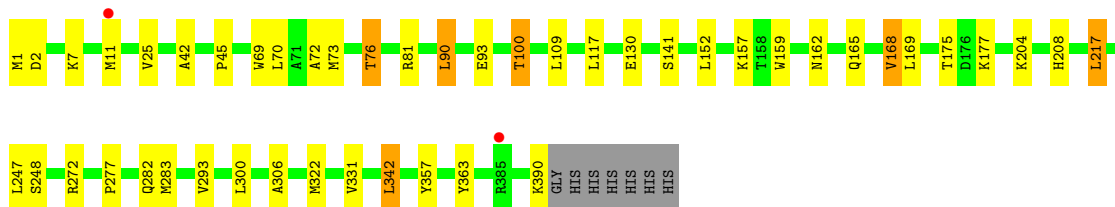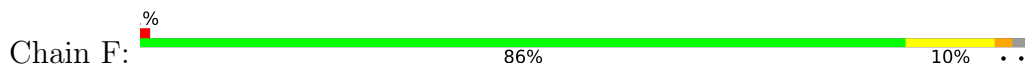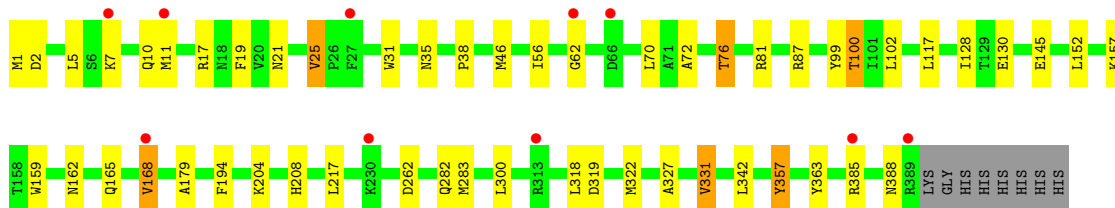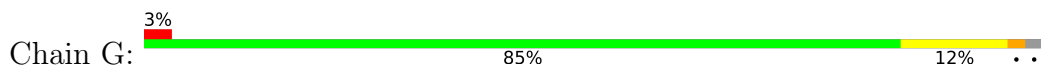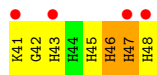D319 M322 A327 V331 L342 E350 Y357 A360 P361 T362 Y363 Y364 M365 V366 R385 N388 R389 K390 G391 HIS HIS HIS HIS HIS HIS

• Molecule 1: Glutaryl-CoA dehydrogenase

Chain F:

%

86% 10%

M1 D2 K7 M11 V25 A42 P45 W69 L70 A71 A72 M73 T76 R81 L90 E93 T100 L109 L117 E130 S141 L152 K157 T158 W159 N162 Q165 V168 L169 T175 D176 K177 K204 H208 L217

L247 S248 R272 P277 Q282 M283 V293 L300 A306 M322 V331 L342 Y357 Y363 R385 K390 GLY HIS HIS HIS HIS HIS HIS

• Molecule 1: Glutaryl-CoA dehydrogenase

Chain G:

3%

85% 12%

M1 D2 L5 S6 K7 Q10 M11 R17 N18 F19 V20 N21 V25 P26 F27 W31 N35 P38 M46 I56 G62 D66 L70 A71 A72 T76 R81 R87 Y99 T100 I101 L102 L117 I128 T129 E130 E145 L152 K157

T158 W159 N162 Q165 V168 A179 F194 K204 H208 L217 K230 D262 Q282 M283 L300 R313 L318 D319 M322 A327 V331 L342 Y357 Y363 R385 N388 R389 LYS GLY HIS HIS HIS HIS HIS HIS

• Molecule 2: Octapeptide

Chain Y:

50%

12% 62% 25%

K41 G42 H43 H44 H45 H46 H47 H48

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	152.40Å 250.60Å 62.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 29.87 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.00-2.10) 99.7 (29.87-2.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.74 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.181 , 0.225 0.217 , 0.246	Depositor DCC
R_{free} test set	7062 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	27.6	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 47.8	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	19170	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.59% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CL, 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	0.94	1/3050 (0.0%)	0.88	8/4117 (0.2%)
1	B	0.90	2/3086 (0.1%)	0.83	4/4163 (0.1%)
1	D	0.68	0/3062	0.71	0/4131
1	E	0.68	0/3057	0.73	2/4124 (0.0%)
1	F	0.83	0/3062	0.79	2/4131 (0.0%)
1	G	0.77	1/3033 (0.0%)	0.77	1/4094 (0.0%)
2	Y	0.77	0/76	0.94	0/98
All	All	0.81	4/18426 (0.0%)	0.79	17/24858 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	Y	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	357	TYR	CD1-CE1	7.49	1.50	1.39
1	A	357	TYR	CD1-CE1	6.58	1.49	1.39
1	B	331	VAL	CB-CG1	-5.24	1.41	1.52
1	G	357	TYR	CD1-CE1	5.04	1.47	1.39

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	192	ARG	NE-CZ-NH1	8.41	124.51	120.30
1	A	358	ARG	NE-CZ-NH1	6.84	123.72	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	342	LEU	CA-CB-CG	6.48	130.21	115.30
1	E	217	LEU	CA-CB-CG	6.07	129.25	115.30
1	A	192	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	A	152	LEU	CA-CB-CG	5.74	128.50	115.30
1	A	358	ARG	NE-CZ-NH2	-5.73	117.43	120.30
1	A	375	MET	CG-SD-CE	-5.71	91.06	100.20
1	A	73	MET	CG-SD-CE	5.71	109.33	100.20
1	B	81	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	271	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	G	217	LEU	CA-CB-CG	5.61	128.21	115.30
1	B	215	LEU	CA-CB-CG	5.34	127.57	115.30
1	B	342	LEU	CA-CB-CG	5.33	127.56	115.30
1	B	286	ASP	CB-CG-OD1	5.33	123.09	118.30
1	F	342	LEU	CA-CB-CG	5.30	127.50	115.30
1	F	217	LEU	CA-CB-CG	5.20	127.26	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	Y	46	HIS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2992	0	2945	45	0
1	B	3026	0	2984	47	0
1	D	3004	0	2967	37	0
1	E	2999	0	2965	52	0
1	F	3001	0	2968	33	1
1	G	2975	0	2937	40	0
2	Y	72	0	55	8	1
3	A	53	0	31	4	0
3	B	53	0	31	4	0
3	D	53	0	31	5	0
3	E	53	0	31	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	53	0	31	5	0
3	G	53	0	31	4	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
5	A	175	0	0	6	0
5	B	179	0	0	6	0
5	D	84	0	0	1	0
5	E	78	0	0	2	0
5	F	143	0	0	4	1
5	G	115	0	0	2	1
5	Y	3	0	0	0	0
All	All	19170	0	18007	245	2

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 7.

All (245) 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:G:72:ALA:O	1:G:76:THR:HG22	1.65	0.95
1:F:331:VAL:HG21	1:F:363:TYR:HB2	1.59	0.84
5:B:7089:HOH:O	2:Y:47:HIS:HB3	1.77	0.84
1:E:72:ALA:O	1:E:76:THR:HG22	1.78	0.83
1:B:36:HIS:HD2	2:Y:48:HIS:HA	1.43	0.83
2:Y:46:HIS:HB2	2:Y:48:HIS:HD2	1.44	0.83
2:Y:42:GLY:C	2:Y:43:HIS:CA	2.48	0.81
1:B:77:GLU:OE1	5:B:7219:HOH:O	1.98	0.81
1:D:72:ALA:O	1:D:76:THR:HG22	1.79	0.81
1:D:70:LEU:HD21	1:G:1:MET:HG2	1.63	0.80
1:B:76:THR:HG22	1:B:90:LEU:HD23	1.61	0.80
1:B:11:MET:HE2	1:B:14:LYS:HD2	1.63	0.80
1:F:100:THR:HG21	5:F:7538:HOH:O	1.80	0.79
1:G:327:ALA:O	1:G:331:VAL:HG12	1.84	0.78
2:Y:46:HIS:HB2	2:Y:48:HIS:CD2	2.18	0.77
1:G:72:ALA:O	1:G:76:THR:CG2	2.33	0.77
1:E:72:ALA:O	1:E:76:THR:CG2	2.35	0.75
1:B:327:ALA:O	1:B:331:VAL:HG13	1.86	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:ALA:O	1:A:331:VAL:HG13	1.87	0.73
1:A:77:GLU:OE1	5:A:7266:HOH:O	2.09	0.70
1:D:81[B]:ARG:O	1:D:81[B]:ARG:HG2	1.93	0.68
3:E:400:FAD:H2'	3:E:400:FAD:H9	1.76	0.67
3:D:400:FAD:H2'	3:D:400:FAD:C9	2.25	0.67
3:F:400:FAD:H2'	3:F:400:FAD:H9	1.76	0.67
1:A:81:ARG:HD2	5:A:7957:HOH:O	1.93	0.67
3:F:400:FAD:H2'	3:F:400:FAD:C9	2.24	0.67
1:G:17:ARG:HH12	1:G:81:ARG:HH21	1.40	0.67
3:G:400:FAD:H2'	3:G:400:FAD:C9	2.24	0.66
3:E:400:FAD:H2'	3:E:400:FAD:C9	2.25	0.66
1:A:76:THR:HG22	1:A:90:LEU:HD23	1.77	0.66
1:A:322:MET:CE	1:B:293:VAL:HA	2.24	0.66
1:F:272:ARG:NH1	1:F:277:PRO:HD3	2.13	0.64
1:G:17:ARG:HH12	1:G:81:ARG:NH2	1.95	0.64
1:F:72:ALA:O	1:F:76:THR:HG22	1.97	0.64
1:E:282:GLN:HE21	1:G:283:MET:H	1.46	0.64
1:E:283:MET:H	1:G:282:GLN:HE21	1.46	0.64
1:A:331:VAL:HG21	1:A:363:TYR:HB2	1.80	0.64
1:D:282:GLN:HE21	1:F:283:MET:H	1.45	0.64
1:E:162:ASN:HA	1:E:165:GLN:HE21	1.62	0.63
1:G:5:LEU:O	1:G:10:GLN:NE2	2.31	0.63
1:B:204:LYS:O	1:B:208:HIS:HE1	1.80	0.63
1:F:81:ARG:HD2	5:F:7589:HOH:O	1.98	0.63
3:G:400:FAD:H2'	3:G:400:FAD:H9	1.80	0.63
1:D:283:MET:H	1:F:282:GLN:HE21	1.47	0.62
1:E:81:ARG:HD2	5:E:7641:HOH:O	1.99	0.62
1:E:331:VAL:HG23	1:E:360:ALA:HB1	1.80	0.62
1:E:327:ALA:O	1:E:331:VAL:HG13	2.00	0.61
1:B:36:HIS:CD2	2:Y:48:HIS:HA	2.32	0.61
1:E:20:VAL:HG22	1:E:24:ILE:HD12	1.83	0.61
1:E:293:VAL:HA	1:F:322:MET:HE3	1.83	0.61
1:E:18:ASN:HD21	1:E:22:LYS:NZ	2.00	0.60
3:B:400:FAD:H2'	3:B:400:FAD:C9	2.31	0.60
1:G:204:LYS:O	1:G:208:HIS:HE1	1.84	0.59
1:G:35:ASN:HD22	1:G:208:HIS:HB3	1.66	0.59
1:D:21:ASN:ND2	1:D:81[B]:ARG:HH22	2.00	0.59
1:D:130:GLU:HG2	1:D:157:LYS:HD3	1.85	0.59
1:G:35:ASN:ND2	1:G:208:HIS:HB3	2.17	0.59
1:A:159:TRP:O	3:A:400:FAD:C4X	2.50	0.59
1:G:21:ASN:HA	1:G:25:VAL:HG13	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:162:ASN:HA	1:G:165:GLN:HE21	1.68	0.58
1:E:293:VAL:HA	1:F:322:MET:CE	2.33	0.58
1:F:100:THR:HG22	5:F:7633:HOH:O	2.02	0.58
1:A:21:ASN:HA	1:A:25:VAL:HG13	1.86	0.58
1:E:1:MET:HG2	1:F:70:LEU:HD21	1.85	0.58
1:D:152:LEU:HD21	1:D:219:ASN:HA	1.86	0.57
1:E:282:GLN:HB2	1:G:282:GLN:HB2	1.86	0.57
1:A:17:ARG:HH12	1:A:81:ARG:NH2	2.02	0.57
1:F:72:ALA:O	1:F:76:THR:CG2	2.52	0.57
1:D:1:MET:HG2	1:G:70:LEU:HD21	1.85	0.57
1:E:117:LEU:HD21	1:E:168:VAL:CG1	2.34	0.57
1:D:199:THR:HA	1:D:214:GLU:O	2.05	0.56
1:A:322:MET:HE2	1:B:293:VAL:HG22	1.87	0.56
1:B:319:ASP:H	1:B:388:ASN:HD21	1.54	0.56
1:G:81:ARG:NH1	1:G:262:ASP:OD2	2.38	0.56
1:B:72:ALA:O	1:B:76:THR:CG2	2.53	0.56
1:D:12:LEU:O	1:D:16:VAL:HG23	2.06	0.56
1:A:319:ASP:H	1:A:388:ASN:HD21	1.53	0.56
1:E:44:ARG:NH1	1:E:48:GLU:HG3	2.21	0.56
1:D:319:ASP:H	1:D:388:ASN:HD21	1.53	0.56
1:F:357:TYR:CE2	1:G:357:TYR:CE2	2.94	0.56
1:A:100:THR:HG21	5:A:7065:HOH:O	2.05	0.56
1:E:42:ALA:O	1:E:46:MET:HG3	2.05	0.56
1:D:31:TRP:CZ2	1:D:41:GLU:HG3	2.41	0.55
1:A:72:ALA:O	1:A:76:THR:CG2	2.55	0.55
3:E:400:FAD:H2A	1:F:282:GLN:HE22	1.72	0.55
1:D:147:LYS:HE3	1:D:152:LEU:HD12	1.89	0.55
1:B:124:GLY:HA2	1:B:168:VAL:O	2.06	0.55
1:E:319:ASP:H	1:E:388:ASN:HD21	1.55	0.54
1:B:130:GLU:HG2	1:B:157:LYS:HD3	1.90	0.54
1:A:145[B]:GLU:OE2	1:A:147:LYS:NZ	2.27	0.54
1:A:240:GLY:HA3	5:A:7283:HOH:O	2.07	0.54
1:D:84:SER:O	1:D:87:ARG:HG3	2.07	0.54
1:A:318:LEU:H	1:A:388:ASN:ND2	2.06	0.54
1:E:81:ARG:NH1	1:E:262:ASP:OD2	2.41	0.54
1:G:130:GLU:HG2	1:G:157:LYS:HD3	1.90	0.54
1:D:327:ALA:O	1:D:331:VAL:HG13	2.07	0.53
1:A:72:ALA:O	1:A:76:THR:HG22	2.09	0.53
1:G:17:ARG:NH1	1:G:81:ARG:NH2	2.57	0.53
3:A:400:FAD:C9	3:A:400:FAD:H2'	2.39	0.53
1:B:72:ALA:O	1:B:76:THR:HG22	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:84:SER:O	1:E:87:ARG:HG3	2.09	0.52
1:A:16:VAL:O	1:A:20:VAL:HG23	2.10	0.52
1:E:87:ARG:HD2	1:E:87:ARG:C	2.30	0.52
1:G:318:LEU:O	1:G:322:MET:HG3	2.10	0.52
1:B:162:ASN:HA	1:B:165:GLN:HE21	1.75	0.52
1:B:100:THR:HG21	5:B:7078:HOH:O	2.09	0.52
1:A:100:THR:HG22	5:A:7075:HOH:O	2.09	0.51
1:E:70:LEU:HD21	1:F:1:MET:HG2	1.91	0.51
3:D:400:FAD:H2'	3:D:400:FAD:H9	1.92	0.51
1:D:282:GLN:HB2	1:F:282:GLN:HB2	1.93	0.51
1:B:76:THR:CG2	1:B:90:LEU:HD23	2.37	0.51
1:A:277:PRO:HD2	1:A:280:ASP:OD2	2.11	0.51
1:F:162:ASN:HA	1:F:165:GLN:HE21	1.76	0.50
1:G:100:THR:HG21	5:G:7411:HOH:O	2.10	0.50
3:A:400:FAD:H2A	1:B:282:GLN:HE22	1.76	0.50
1:D:56:ILE:HB	1:D:62:GLY:HA3	1.94	0.50
1:E:116:LYS:HD2	1:E:122:PHE:CZ	2.47	0.50
1:G:117:LEU:HD21	1:G:168:VAL:HG13	1.92	0.50
1:B:167:ASP:OD2	2:Y:45:HIS:HE1	1.95	0.50
1:D:162:ASN:HA	1:D:165:GLN:HE21	1.75	0.50
1:E:283:MET:H	1:G:282:GLN:NE2	2.09	0.50
1:D:21:ASN:HD21	1:D:81[B]:ARG:HH22	1.60	0.49
1:B:243:ASN:HD21	1:B:317:GLY:HA2	1.77	0.49
1:F:73:MET:HG3	1:F:306:ALA:HB2	1.94	0.49
1:B:20:VAL:HG22	1:B:24:ILE:HD12	1.93	0.49
1:A:243:ASN:HB3	5:A:7130:HOH:O	2.13	0.49
1:D:282:GLN:NE2	1:F:283:MET:H	2.10	0.49
1:B:385:ARG:HG3	1:B:385:ARG:HH11	1.78	0.49
1:E:60:TYR:CZ	1:E:110:LYS:HD2	2.48	0.49
1:G:87:ARG:HD2	1:G:87:ARG:C	2.33	0.49
1:E:204:LYS:O	1:E:208:HIS:HE1	1.96	0.48
1:B:112:LYS:HE2	1:B:113:TYR:OH	2.13	0.48
1:E:116:LYS:HB2	1:E:122:PHE:CD2	2.49	0.48
1:G:331:VAL:HG11	1:G:363:TYR:CB	2.44	0.48
1:E:32:ASP:OD1	1:E:208:HIS:HD2	1.97	0.48
1:E:94:VAL:HA	1:E:98:ALA:HB3	1.94	0.48
1:G:56:ILE:HB	1:G:62:GLY:HA3	1.96	0.48
1:F:272:ARG:HH12	1:F:277:PRO:HD3	1.79	0.48
1:A:372:ILE:HA	1:A:375:MET:HE3	1.95	0.48
1:B:331:VAL:HG21	1:B:363:TYR:HB2	1.95	0.48
1:E:71:ALA:O	1:E:75:VAL:HG23	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:73:MET:SD	1:E:247:LEU:HG	2.53	0.48
1:A:32:ASP:OD1	1:A:208:HIS:HD2	1.98	0.47
1:A:322:MET:HE3	1:B:293:VAL:HA	1.94	0.47
1:D:389:ARG:O	1:D:390:LYS:C	2.51	0.47
1:E:92:MET:SD	1:E:161:SER:HB2	2.55	0.47
1:D:357:TYR:CE2	1:E:357:TYR:CE2	3.03	0.47
1:E:282:GLN:HE22	3:F:400:FAD:H2A	1.79	0.47
1:A:127:GLY:O	1:A:157:LYS:HE3	2.15	0.47
1:E:282:GLN:NE2	1:G:283:MET:H	2.13	0.47
1:E:128:ILE:HB	3:E:400:FAD:O2	2.16	0.46
1:B:100:THR:HG22	5:B:7158:HOH:O	2.15	0.46
1:D:152:LEU:CD2	1:D:219:ASN:HA	2.46	0.46
1:A:11:MET:HE2	1:A:14:LYS:HD2	1.96	0.46
1:B:243:ASN:ND2	1:B:317:GLY:HA2	2.30	0.46
1:D:283:MET:H	1:F:282:GLN:NE2	2.12	0.46
3:B:400:FAD:H2'	3:B:400:FAD:H9	1.97	0.46
1:A:204:LYS:O	1:A:208:HIS:HE1	1.98	0.46
1:D:204:LYS:O	1:D:208:HIS:HE1	1.98	0.46
1:E:282:GLN:HB3	1:G:283:MET:HG3	1.98	0.46
1:A:130:GLU:HG2	1:A:157:LYS:HD3	1.98	0.46
1:D:190:GLU:HB3	5:D:7587:HOH:O	2.15	0.46
1:D:197:ILE:HG12	1:D:217:LEU:HD22	1.97	0.46
1:E:18:ASN:HD21	1:E:22:LYS:HZ3	1.62	0.46
1:B:17:ARG:HH12	1:B:81:ARG:NH2	2.14	0.46
1:D:77:GLU:HG2	1:D:255:GLY:HA2	1.97	0.46
1:D:159:TRP:O	3:D:400:FAD:C4X	2.64	0.46
1:E:81:ARG:NH2	5:E:7557:HOH:O	2.46	0.46
3:F:400:FAD:H9	3:F:400:FAD:C2'	2.44	0.46
1:F:76:THR:HG21	1:F:248:SER:OG	2.16	0.45
1:A:8:GLU:HG2	1:A:65:MET:CE	2.46	0.45
1:B:360:ALA:N	1:B:361:PRO:CD	2.80	0.45
1:F:109:LEU:HD12	5:F:7583:HOH:O	2.17	0.45
1:G:194:PHE:N	1:G:194:PHE:CD1	2.83	0.45
1:B:159:TRP:O	3:B:400:FAD:C4X	2.64	0.45
1:D:361:PRO:HA	1:D:364:TYR:CZ	2.52	0.45
1:B:18:ASN:HD21	1:B:22:LYS:NZ	2.14	0.45
1:D:266:LYS:HE2	1:D:270:GLU:OE1	2.16	0.45
1:F:130:GLU:HG2	1:F:157:LYS:HD3	1.98	0.45
1:E:52:PHE:O	1:E:94:VAL:HG21	2.16	0.45
1:F:73:MET:SD	1:F:247:LEU:HG	2.56	0.45
1:F:76:THR:HG22	1:F:90:LEU:HD23	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:ILE:HG12	1:B:217:LEU:HD22	2.00	0.44
1:D:128:ILE:HB	3:D:400:FAD:O2	2.17	0.44
1:A:360:ALA:N	1:A:361:PRO:CD	2.80	0.44
1:A:322:MET:HE2	1:B:293:VAL:HA	1.98	0.44
1:A:159:TRP:O	3:A:400:FAD:C10	2.66	0.44
1:D:129:THR:OG1	3:D:400:FAD:H1'1	2.17	0.44
1:A:17:ARG:HH12	1:A:81:ARG:CZ	2.30	0.44
1:E:69:TRP:O	1:E:73:MET:HG2	2.17	0.44
1:F:204:LYS:O	1:F:208:HIS:HE1	2.01	0.44
1:B:76:THR:HG21	1:B:248:SER:OG	2.18	0.43
1:E:291:MET:O	1:E:295:VAL:HG23	2.18	0.43
1:B:11:MET:HE2	1:B:14:LYS:CD	2.43	0.43
1:B:351:TYR:HB3	1:B:352:PRO:HD2	2.01	0.43
1:F:141:SER:O	1:F:177:LYS:NZ	2.40	0.43
1:E:123:LEU:HD13	1:E:165:GLN:HB3	2.00	0.43
1:F:42:ALA:C	1:F:45:PRO:HD2	2.39	0.43
1:A:145[A]:GLU:HG2	1:A:152:LEU:O	2.18	0.43
1:B:7:LYS:HD2	1:B:7:LYS:HA	1.74	0.43
1:E:194:PHE:HA	1:E:195:PRO:HD3	1.88	0.43
1:E:31:TRP:CZ2	1:E:41:GLU:HG3	2.53	0.43
1:E:95:LEU:HD12	1:E:248:SER:HB2	2.00	0.43
1:G:159:TRP:O	3:G:400:FAD:C4X	2.67	0.43
1:A:76:THR:HG21	1:A:248:SER:OG	2.19	0.43
1:B:72:ALA:O	1:B:76:THR:HG23	2.17	0.43
1:E:361:PRO:HA	1:E:364:TYR:CZ	2.53	0.43
1:F:117:LEU:HD21	1:F:168:VAL:HG13	2.00	0.43
1:A:84:SER:O	1:A:87:ARG:HG3	2.19	0.42
1:G:204:LYS:O	1:G:208:HIS:CE1	2.70	0.42
1:A:72:ALA:O	1:A:76:THR:HG23	2.19	0.42
1:B:54:THR:HA	1:B:63:GLU:HB2	2.01	0.42
1:G:99:TYR:O	1:G:102:LEU:HB3	2.19	0.42
1:G:81:ARG:HD2	5:G:7596:HOH:O	2.18	0.42
1:B:67:GLN:NE2	5:B:7247:HOH:O	2.20	0.42
1:E:9:LEU:HD11	1:E:67:GLN:HE21	1.85	0.42
1:E:116:LYS:HB2	1:E:122:PHE:CE2	2.55	0.42
1:A:75:VAL:O	1:A:79:ILE:HG13	2.20	0.42
1:A:325:TYR:CE1	1:A:374:LYS:HE3	2.55	0.42
1:G:331:VAL:HG11	1:G:363:TYR:HB2	2.02	0.42
1:A:191:PRO:HA	1:A:197:ILE:HD13	2.02	0.42
1:E:122:PHE:HA	1:E:167:ASP:OD2	2.20	0.42
1:B:32:ASP:OD1	1:B:208:HIS:HD2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:ILE:HB	3:B:400:FAD:O2	2.21	0.41
1:G:319:ASP:H	1:G:388:ASN:HD21	1.67	0.41
1:B:25:VAL:N	1:B:26:PRO:CD	2.83	0.41
1:D:31:TRP:HZ2	1:D:41:GLU:HG3	1.82	0.41
1:E:322:MET:HE2	1:F:293:VAL:HA	2.03	0.41
1:A:124:GLY:HA2	1:A:168:VAL:O	2.21	0.41
1:E:362:THR:O	1:E:366:VAL:HG22	2.21	0.41
1:G:128:ILE:HB	3:G:400:FAD:O2	2.20	0.41
1:A:7:LYS:HD2	1:A:7:LYS:HA	1.57	0.41
1:F:69:TRP:O	1:F:73:MET:HG2	2.20	0.41
1:G:19:PHE:CE2	1:G:46:MET:CG	3.03	0.41
1:G:31:TRP:CE3	1:G:38:PRO:HG3	2.56	0.41
1:A:299:ARG:HH11	1:A:299:ARG:HD2	1.70	0.41
1:D:42:ALA:C	1:D:45:PRO:HD2	2.41	0.41
1:F:159:TRP:O	3:F:400:FAD:C4X	2.69	0.41
1:B:117:LEU:HD21	1:B:168:VAL:HG13	2.03	0.40
1:B:37:PHE:HB3	2:Y:47:HIS:H	1.87	0.40
1:B:23:LYS:HE2	1:B:23:LYS:HB3	1.95	0.40
1:A:162:ASN:HA	1:A:165:GLN:HE21	1.87	0.40
1:B:81:ARG:NH2	5:B:8022:HOH:O	2.30	0.40
1:D:70:LEU:CD2	1:G:1:MET:HG2	2.43	0.40
1:A:361:PRO:HA	1:A:364:TYR:CZ	2.57	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:390:LYS:O	2:Y:41:LYS:CG[4_455]	1.78	0.42
5:F:7936:HOH:O	5:G:8014:HOH:O[1_556]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	389/397 (98%)	376 (97%)	13 (3%)	0	100	100
1	B	393/397 (99%)	380 (97%)	13 (3%)	0	100	100
1	D	390/397 (98%)	379 (97%)	11 (3%)	0	100	100
1	E	390/397 (98%)	368 (94%)	21 (5%)	1 (0%)	41	41
1	F	390/397 (98%)	378 (97%)	12 (3%)	0	100	100
1	G	387/397 (98%)	375 (97%)	11 (3%)	1 (0%)	41	41
2	Y	4/8 (50%)	2 (50%)	2 (50%)	0	100	100
All	All	2343/2390 (98%)	2258 (96%)	83 (4%)	2 (0%)	51	54

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	179	ALA
1	E	148	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	304/309 (98%)	290 (95%)	14 (5%)	27	26
1	B	307/309 (99%)	286 (93%)	21 (7%)	16	13
1	D	305/309 (99%)	287 (94%)	18 (6%)	19	17
1	E	304/309 (98%)	282 (93%)	22 (7%)	14	11
1	F	305/309 (99%)	290 (95%)	15 (5%)	25	23
1	G	302/309 (98%)	289 (96%)	13 (4%)	29	29
2	Y	6/7 (86%)	5 (83%)	1 (17%)	2	1
All	All	1833/1861 (98%)	1729 (94%)	104 (6%)	22	18

All (104) residues with a non-rotameric sidechain are listed below:

Full wwPDB X-ray Structure Validation Report

Mol	Chain	Res	Type
1	A	2	ASP
1	A	11	MET
1	A	66[A]	ASP
1	A	66[B]	ASP
1	A	76	THR
1	A	90	LEU
1	A	93	GLU
1	A	100	THR
1	A	145[A]	GLU
1	A	145[B]	GLU
1	A	152	LEU
1	A	168	VAL
1	A	300	LEU
1	A	342	LEU
1	B	2	ASP
1	B	7	LYS
1	B	11	MET
1	B	25	VAL
1	B	63	GLU
1	B	76	THR
1	B	87	ARG
1	B	93	GLU
1	B	100	THR
1	B	145[A]	GLU
1	B	145[B]	GLU
1	B	152	LEU
1	B	168	VAL
1	B	169	LEU
1	B	230	LYS
1	B	300	LEU
1	B	331	VAL
1	B	342	LEU
1	B	350	GLU
1	B	390	LYS
1	B	393	HIS
1	D	2	ASP
1	D	11	MET
1	D	25	VAL
1	D	48	GLU
1	D	59	GLU
1	D	76	THR
1	D	93	GLU
1	D	100	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	111	LYS
1	D	145[A]	GLU
1	D	145[B]	GLU
1	D	152	LEU
1	D	165	GLN
1	D	168	VAL
1	D	217	LEU
1	D	280	ASP
1	D	300	LEU
1	D	342	LEU
1	E	7	LYS
1	E	11	MET
1	E	40	GLU
1	E	66	ASP
1	E	76	THR
1	E	90	LEU
1	E	93	GLU
1	E	100	THR
1	E	111	LYS
1	E	152	LEU
1	E	156	SER
1	E	169	LEU
1	E	182	ARG
1	E	210	SER
1	E	217	LEU
1	E	224	LYS
1	E	225	GLU
1	E	300	LEU
1	E	342	LEU
1	E	350	GLU
1	E	385[A]	ARG
1	E	385[B]	ARG
1	F	2	ASP
1	F	7	LYS
1	F	11	MET
1	F	25	VAL
1	F	76	THR
1	F	90	LEU
1	F	93	GLU
1	F	100	THR
1	F	152	LEU
1	F	168	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	169	LEU
1	F	175	THR
1	F	217	LEU
1	F	300	LEU
1	F	342	LEU
1	G	2	ASP
1	G	7	LYS
1	G	11	MET
1	G	25	VAL
1	G	76	THR
1	G	100	THR
1	G	145	GLU
1	G	152	LEU
1	G	168	VAL
1	G	300	LEU
1	G	331	VAL
1	G	342	LEU
1	G	385	ARG
2	Y	47	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	21	ASN
1	A	33	ASN
1	A	165	GLN
1	A	208	HIS
1	A	243	ASN
1	A	269	ASN
1	A	282	GLN
1	A	388	ASN
1	B	18	ASN
1	B	21	ASN
1	B	33	ASN
1	B	36	HIS
1	B	165	GLN
1	B	208	HIS
1	B	269	ASN
1	B	282	GLN
1	B	388	ASN
1	D	21	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	165	GLN
1	D	208	HIS
1	D	243	ASN
1	D	269	ASN
1	D	282	GLN
1	D	388	ASN
1	E	18	ASN
1	E	21	ASN
1	E	33	ASN
1	E	67	GLN
1	E	165	GLN
1	E	208	HIS
1	E	243	ASN
1	E	269	ASN
1	E	282	GLN
1	E	388	ASN
1	F	21	ASN
1	F	33	ASN
1	F	165	GLN
1	F	208	HIS
1	F	269	ASN
1	F	282	GLN
1	F	388	ASN
1	G	21	ASN
1	G	33	ASN
1	G	35	ASN
1	G	36	HIS
1	G	89	GLN
1	G	162	ASN
1	G	165	GLN
1	G	208	HIS
1	G	243	ASN
1	G	269	ASN
1	G	282	GLN
1	G	388	ASN
2	Y	45	HIS
2	Y	48	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
3	FAD	E	400	-	53,58,58	1.34	5 (9%)	68,89,89	1.62	14 (20%)
3	FAD	D	400	-	53,58,58	1.68	10 (18%)	68,89,89	1.86	15 (22%)
3	FAD	A	400	-	53,58,58	1.59	9 (16%)	68,89,89	1.86	18 (26%)
3	FAD	G	400	-	53,58,58	1.49	5 (9%)	68,89,89	1.62	11 (16%)
3	FAD	F	400	-	53,58,58	1.32	5 (9%)	68,89,89	1.60	13 (19%)
3	FAD	B	400	-	53,58,58	1.39	7 (13%)	68,89,89	1.67	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
3	FAD	E	400	-	-	2/30/50/50	0/6/6/6
3	FAD	D	400	-	-	9/30/50/50	0/6/6/6
3	FAD	A	400	-	-	6/30/50/50	0/6/6/6
3	FAD	G	400	-	-	5/30/50/50	0/6/6/6
3	FAD	F	400	-	-	7/30/50/50	0/6/6/6
3	FAD	B	400	-	-	7/30/50/50	0/6/6/6

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	400	FAD	C4X-N5	6.43	1.43	1.30
3	A	400	FAD	C2A-N3A	6.09	1.41	1.32
3	D	400	FAD	C4X-N5	5.02	1.40	1.30
3	D	400	FAD	C1'-C2'	5.01	1.59	1.52
3	E	400	FAD	C4X-N5	4.71	1.39	1.30
3	G	400	FAD	C1'-C2'	4.38	1.58	1.52
3	A	400	FAD	C1'-C2'	4.22	1.58	1.52
3	D	400	FAD	O4B-C1B	4.14	1.46	1.41
3	F	400	FAD	C4X-N5	4.13	1.38	1.30
3	B	400	FAD	C2A-N3A	4.00	1.38	1.32
3	F	400	FAD	C2A-N3A	3.92	1.38	1.32
3	E	400	FAD	C1'-C2'	3.74	1.57	1.52
3	E	400	FAD	C2A-N3A	3.66	1.38	1.32
3	B	400	FAD	C1'-C2'	3.62	1.57	1.52
3	G	400	FAD	C2A-N3A	3.57	1.37	1.32
3	A	400	FAD	C2A-N1A	3.43	1.40	1.33
3	D	400	FAD	C10-N1	3.40	1.40	1.33
3	A	400	FAD	C4X-N5	3.27	1.37	1.30
3	F	400	FAD	C2A-N1A	3.26	1.40	1.33
3	B	400	FAD	C4X-N5	3.09	1.36	1.30
3	B	400	FAD	C10-N1	3.02	1.39	1.33
3	D	400	FAD	C2B-C1B	-2.93	1.49	1.53
3	G	400	FAD	C2A-N1A	2.85	1.39	1.33
3	F	400	FAD	C1'-C2'	2.75	1.56	1.52
3	D	400	FAD	C2A-N1A	2.71	1.38	1.33
3	B	400	FAD	C2A-N1A	2.66	1.38	1.33
3	D	400	FAD	PA-O2A	-2.45	1.43	1.55
3	A	400	FAD	P-O2P	-2.41	1.44	1.55
3	E	400	FAD	C2A-N1A	2.39	1.38	1.33
3	D	400	FAD	C2A-N3A	2.37	1.35	1.32
3	G	400	FAD	C10-N1	2.35	1.38	1.33
3	A	400	FAD	C10-N1	2.27	1.37	1.33
3	A	400	FAD	C5'-C4'	2.19	1.54	1.51
3	D	400	FAD	C10-N10	2.17	1.42	1.37
3	B	400	FAD	O4B-C4B	-2.17	1.40	1.45
3	B	400	FAD	C1'-N10	2.12	1.53	1.48
3	F	400	FAD	C5'-C4'	2.08	1.54	1.51
3	D	400	FAD	O4B-C4B	-2.06	1.40	1.45
3	A	400	FAD	C6A-C5A	-2.04	1.35	1.43
3	E	400	FAD	C1'-N10	2.03	1.53	1.48
3	A	400	FAD	C9-C9A	-2.00	1.36	1.39

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	400	FAD	N3A-C2A-N1A	-7.15	117.51	128.68
3	G	400	FAD	N3A-C2A-N1A	-6.20	118.99	128.68
3	F	400	FAD	N3A-C2A-N1A	-5.71	119.76	128.68
3	B	400	FAD	N3A-C2A-N1A	-5.55	120.00	128.68
3	D	400	FAD	N3A-C2A-N1A	-5.53	120.03	128.68
3	D	400	FAD	O2'-C2'-C1'	5.30	122.61	109.80
3	B	400	FAD	O2'-C2'-C1'	5.25	122.51	109.80
3	A	400	FAD	O2'-C2'-C1'	5.22	122.42	109.80
3	E	400	FAD	N3A-C2A-N1A	-4.99	120.88	128.68
3	D	400	FAD	C4-N3-C2	-4.44	117.43	125.64
3	G	400	FAD	C9A-C5X-N5	-4.18	117.89	122.43
3	G	400	FAD	O2'-C2'-C1'	3.93	119.31	109.80
3	G	400	FAD	C5X-C9A-N10	3.77	121.85	117.95
3	D	400	FAD	C10-N1-C2	3.77	124.44	116.90
3	F	400	FAD	O4'-C4'-C3'	-3.51	100.56	109.10
3	D	400	FAD	C4X-C4-N3	3.50	122.09	113.19
3	A	400	FAD	O3'-C3'-C2'	3.45	117.14	108.81
3	B	400	FAD	C1B-N9A-C4A	-3.42	120.63	126.64
3	E	400	FAD	C4-N3-C2	-3.39	119.37	125.64
3	A	400	FAD	C1B-N9A-C4A	-3.37	120.72	126.64
3	E	400	FAD	O2'-C2'-C1'	3.31	117.79	109.80
3	F	400	FAD	C4X-C10-N10	3.28	121.27	116.48
3	D	400	FAD	O4-C4-C4X	-3.26	117.95	126.60
3	D	400	FAD	C4X-C10-N1	-3.20	117.31	124.73
3	B	400	FAD	C9A-C5X-N5	-3.20	118.95	122.43
3	E	400	FAD	C5X-C9A-N10	3.20	121.25	117.95
3	D	400	FAD	O3'-C3'-C2'	3.09	116.28	108.81
3	F	400	FAD	P-O3P-PA	-3.09	122.22	132.83
3	F	400	FAD	O3'-C3'-C4'	-2.93	101.72	108.81
3	F	400	FAD	O2'-C2'-C3'	2.93	116.22	109.10
3	B	400	FAD	O4'-C4'-C3'	-2.91	102.02	109.10
3	A	400	FAD	C9A-C5X-N5	-2.91	119.27	122.43
3	E	400	FAD	C4X-C10-N1	-2.91	117.98	124.73
3	B	400	FAD	C4-C4X-C10	2.90	121.66	116.79
3	E	400	FAD	C1'-C2'-C3'	2.88	117.84	109.79
3	F	400	FAD	O3'-C3'-C2'	2.87	115.75	108.81
3	F	400	FAD	C10-C4X-N5	-2.86	118.79	124.86
3	A	400	FAD	N6A-C6A-N1A	2.85	124.48	118.57
3	E	400	FAD	C4X-C10-N10	2.79	120.56	116.48
3	A	400	FAD	O4'-C4'-C3'	-2.77	102.35	109.10
3	B	400	FAD	C4-N3-C2	-2.75	120.56	125.64
3	E	400	FAD	P-O3P-PA	-2.74	123.42	132.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	400	FAD	C4X-C4-N3	2.73	120.13	113.19
3	A	400	FAD	C10-C4X-N5	-2.71	119.11	124.86
3	D	400	FAD	C10-C4X-N5	-2.63	119.27	124.86
3	F	400	FAD	C4-N3-C2	-2.62	120.80	125.64
3	A	400	FAD	C4X-C10-N10	2.62	120.31	116.48
3	A	400	FAD	C6-C5X-C9A	2.60	122.61	118.94
3	B	400	FAD	C10-C4X-N5	-2.57	119.40	124.86
3	A	400	FAD	C2A-N1A-C6A	2.56	123.13	118.75
3	A	400	FAD	O3B-C3B-C4B	-2.56	103.66	111.05
3	E	400	FAD	C4-C4X-C10	2.55	121.08	116.79
3	D	400	FAD	C9A-C5X-N5	-2.55	119.66	122.43
3	B	400	FAD	C5X-N5-C4X	2.50	122.23	118.07
3	G	400	FAD	C4X-C4-N3	2.49	119.52	113.19
3	D	400	FAD	C4X-C10-N10	2.43	120.04	116.48
3	G	400	FAD	C9-C9A-N10	-2.39	118.61	121.84
3	A	400	FAD	C4X-C10-N1	-2.38	119.20	124.73
3	G	400	FAD	C4-N3-C2	-2.34	121.32	125.64
3	F	400	FAD	C4-C4X-N5	2.33	121.56	118.23
3	E	400	FAD	O4B-C1B-C2B	-2.32	103.54	106.93
3	E	400	FAD	C6-C5X-C9A	2.28	122.16	118.94
3	A	400	FAD	C5X-N5-C4X	2.27	121.85	118.07
3	E	400	FAD	C9A-C5X-N5	-2.25	119.98	122.43
3	A	400	FAD	O4B-C1B-C2B	2.25	110.21	106.93
3	B	400	FAD	C2A-N1A-C6A	2.24	122.59	118.75
3	D	400	FAD	C5B-C4B-C3B	-2.23	106.81	115.18
3	E	400	FAD	C10-C4X-N5	-2.23	120.12	124.86
3	A	400	FAD	C5X-C6-C7	-2.22	116.63	120.71
3	G	400	FAD	C2A-N1A-C6A	2.15	122.43	118.75
3	D	400	FAD	C4'-C3'-C2'	-2.14	108.91	113.36
3	F	400	FAD	O3B-C3B-C4B	-2.14	104.87	111.05
3	A	400	FAD	P-O3P-PA	-2.12	125.53	132.83
3	F	400	FAD	C9A-C5X-N5	-2.12	120.12	122.43
3	B	400	FAD	C5A-C6A-N6A	2.12	123.57	120.35
3	A	400	FAD	O2'-C2'-C3'	2.09	114.17	109.10
3	G	400	FAD	C6-C5X-C9A	2.08	121.88	118.94
3	F	400	FAD	C1B-N9A-C4A	-2.08	122.99	126.64
3	G	400	FAD	O4-C4-C4X	-2.06	121.12	126.60
3	D	400	FAD	O2P-P-O5'	2.05	117.28	107.75
3	G	400	FAD	C8M-C8-C9	-2.03	115.74	119.49
3	B	400	FAD	C4X-C10-N10	2.03	119.44	116.48
3	D	400	FAD	P-O3P-PA	-2.01	125.94	132.83
3	B	400	FAD	O4-C4-C4X	-2.00	121.29	126.60

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	400	FAD	C1'-C2'-C3'-O3'
3	A	400	FAD	C1'-C2'-C3'-C4'
3	A	400	FAD	O4'-C4'-C5'-O5'
3	B	400	FAD	C2'-C1'-N10-C10
3	B	400	FAD	C1'-C2'-C3'-O3'
3	B	400	FAD	C1'-C2'-C3'-C4'
3	D	400	FAD	C1'-C2'-C3'-O3'
3	D	400	FAD	C1'-C2'-C3'-C4'
3	D	400	FAD	O4'-C4'-C5'-O5'
3	E	400	FAD	C2'-C1'-N10-C10
3	F	400	FAD	C2'-C1'-N10-C10
3	F	400	FAD	C1'-C2'-C3'-C4'
3	G	400	FAD	C1'-C2'-C3'-C4'
3	A	400	FAD	O3'-C3'-C4'-O4'
3	F	400	FAD	O3'-C3'-C4'-O4'
3	F	400	FAD	O4'-C4'-C5'-O5'
3	A	400	FAD	O3'-C3'-C4'-C5'
3	D	400	FAD	O3'-C3'-C4'-C5'
3	D	400	FAD	O3'-C3'-C4'-O4'
3	F	400	FAD	O3'-C3'-C4'-C5'
3	F	400	FAD	C2'-C3'-C4'-O4'
3	D	400	FAD	C4'-C5'-O5'-P
3	B	400	FAD	PA-O3P-P-O5'
3	D	400	FAD	PA-O3P-P-O5'
3	G	400	FAD	PA-O3P-P-O5'
3	G	400	FAD	C1'-C2'-C3'-O3'
3	G	400	FAD	C4'-C5'-O5'-P
3	B	400	FAD	C4'-C5'-O5'-P
3	F	400	FAD	PA-O3P-P-O5'
3	D	400	FAD	C5'-O5'-P-O3P
3	B	400	FAD	O3'-C3'-C4'-O4'
3	E	400	FAD	C4'-C5'-O5'-P
3	A	400	FAD	C2'-C1'-N10-C10
3	B	400	FAD	O4'-C4'-C5'-O5'
3	D	400	FAD	C2'-C1'-N10-C10
3	G	400	FAD	C2'-C1'-N10-C10

There are no ring outliers.

6 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	400	FAD	4	0
3	D	400	FAD	5	0
3	A	400	FAD	4	0
3	G	400	FAD	4	0
3	F	400	FAD	5	0
3	B	400	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand FAD E 400

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD D 400

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD A 400

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD G 400

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD F 400

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD B 400

Bond lengths

Bond angles

Torsions

Rings
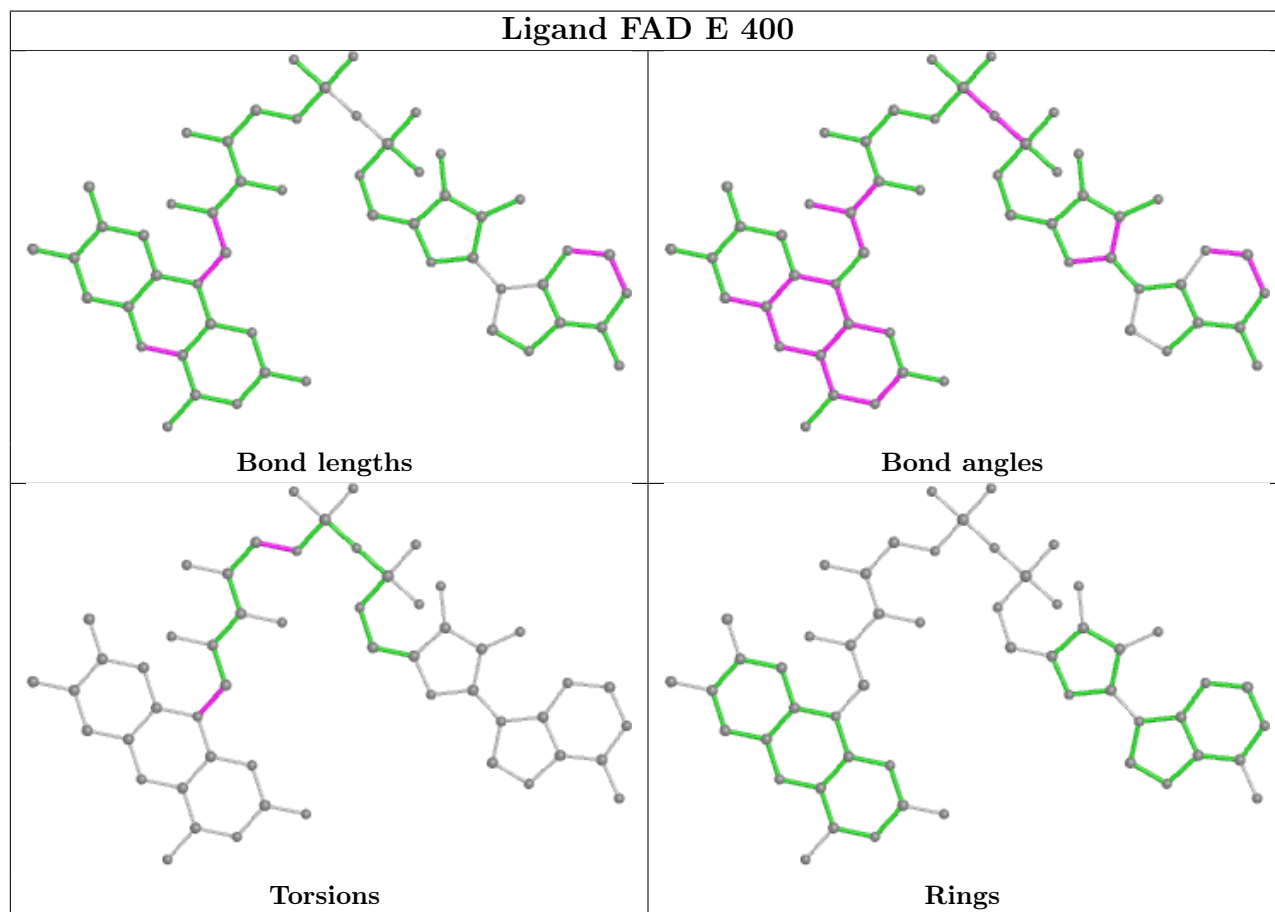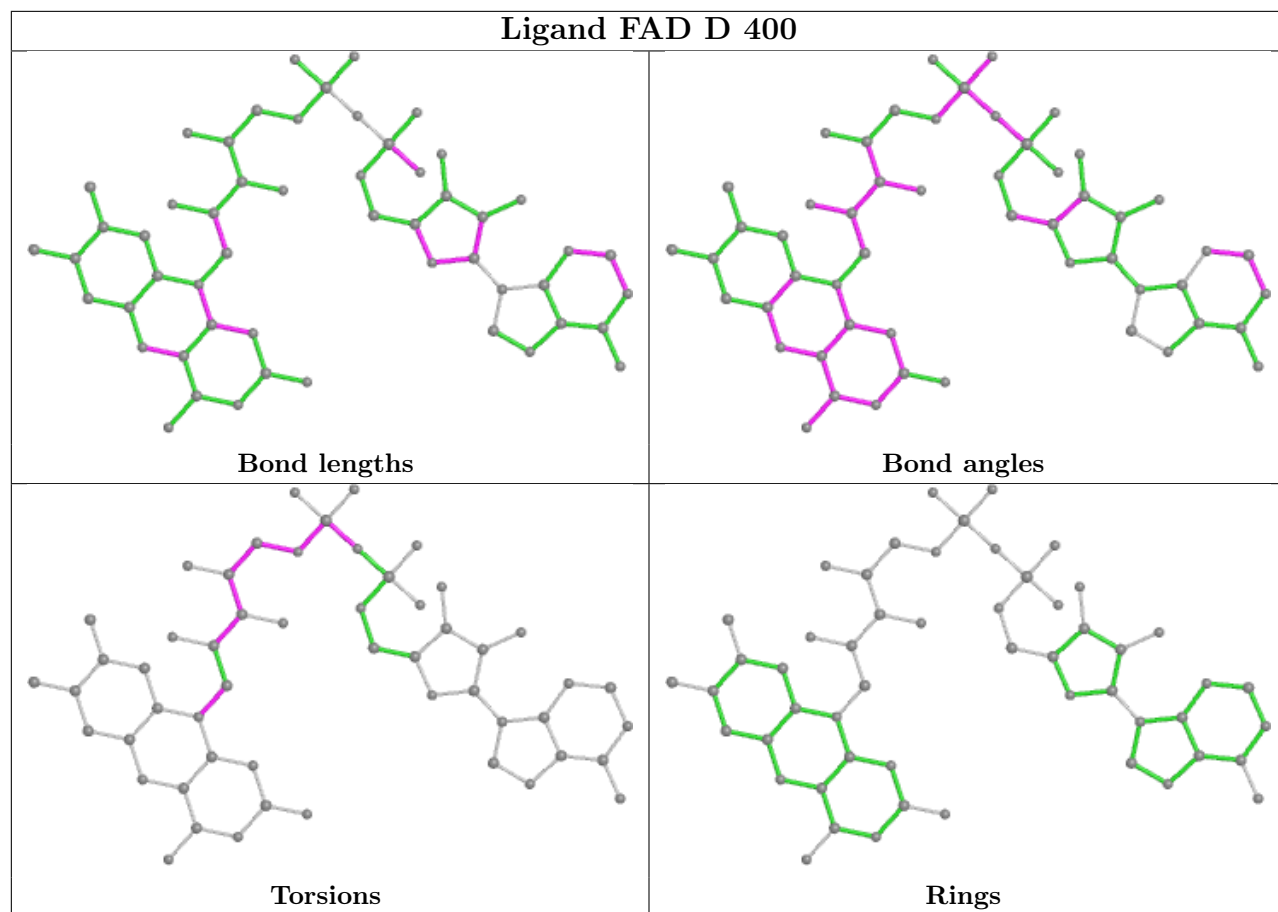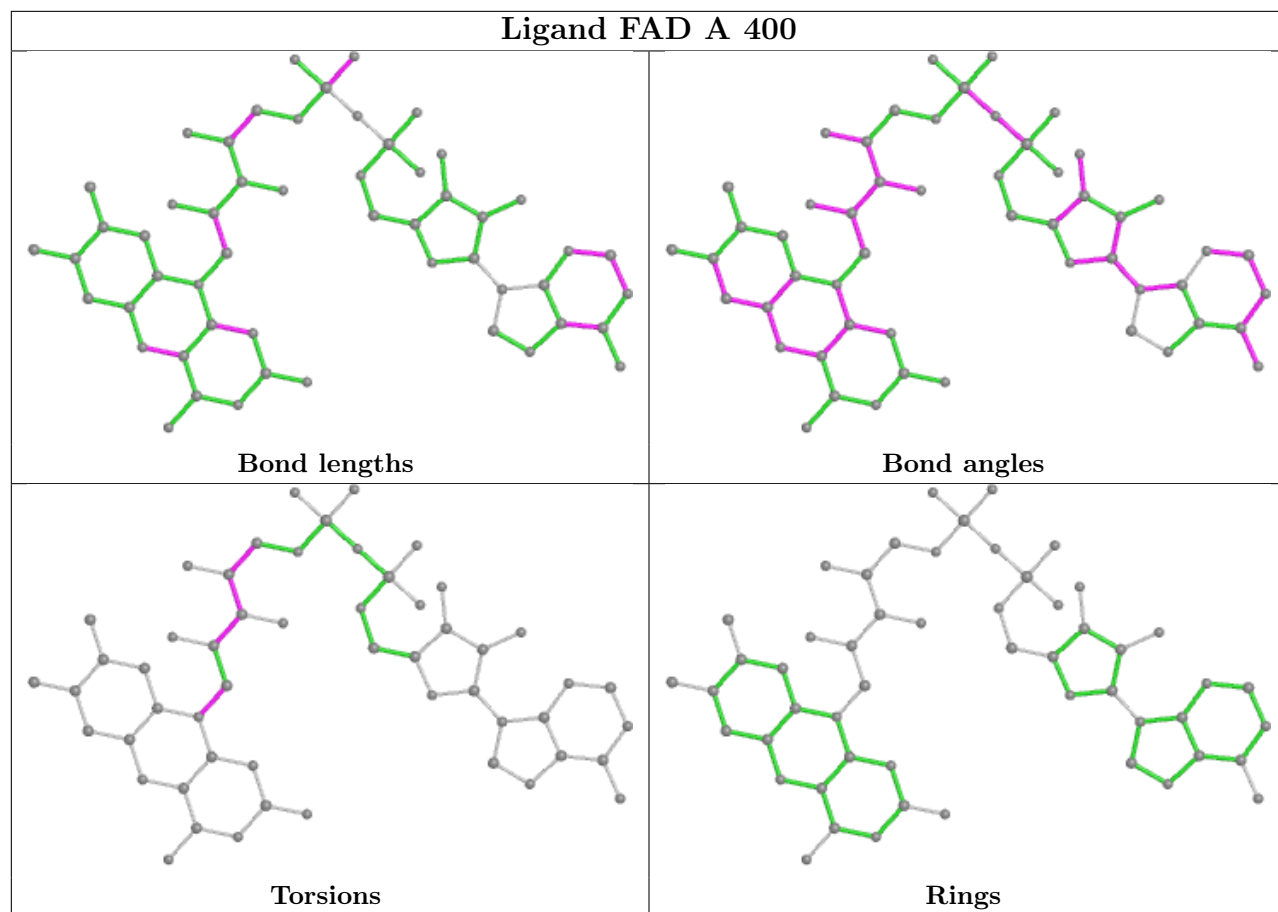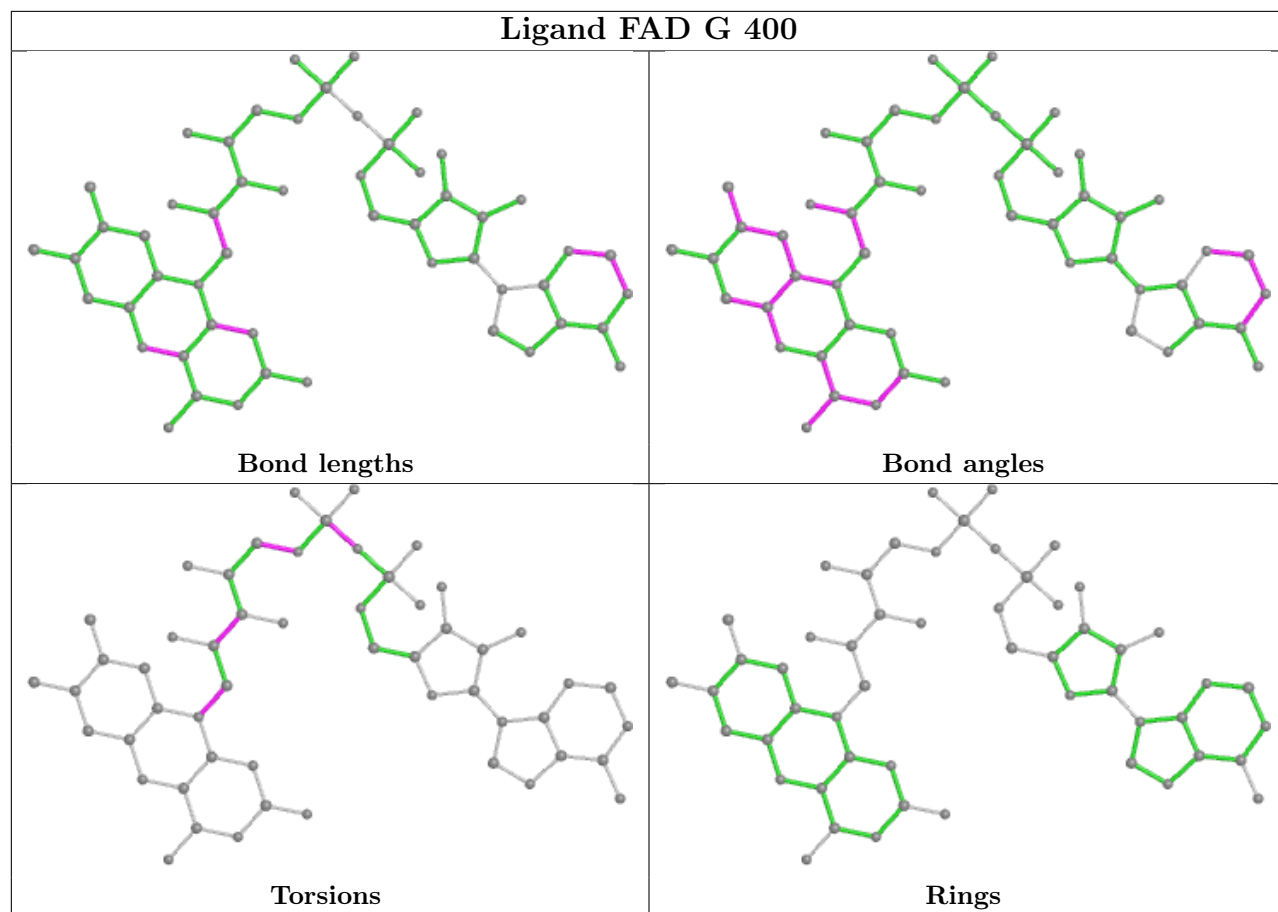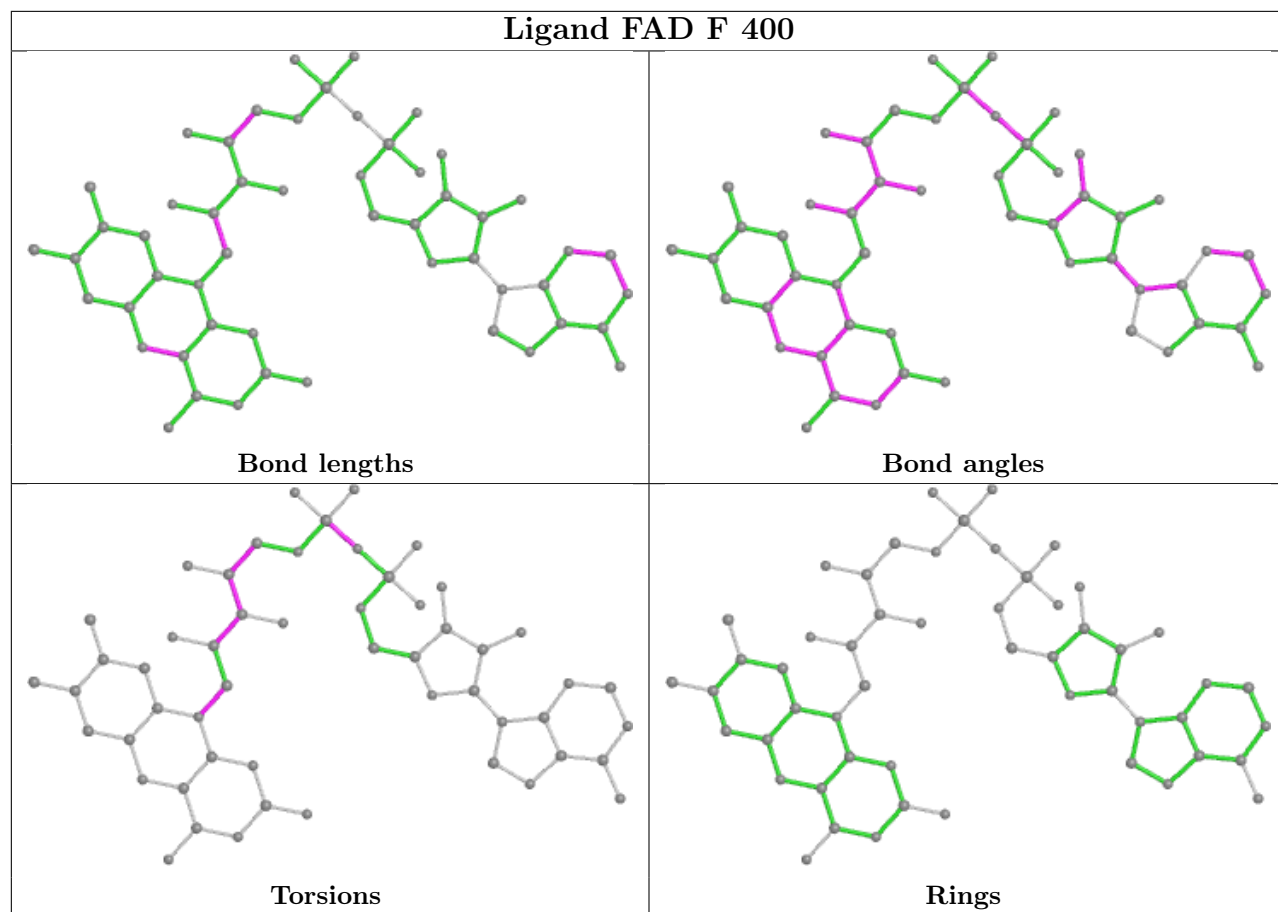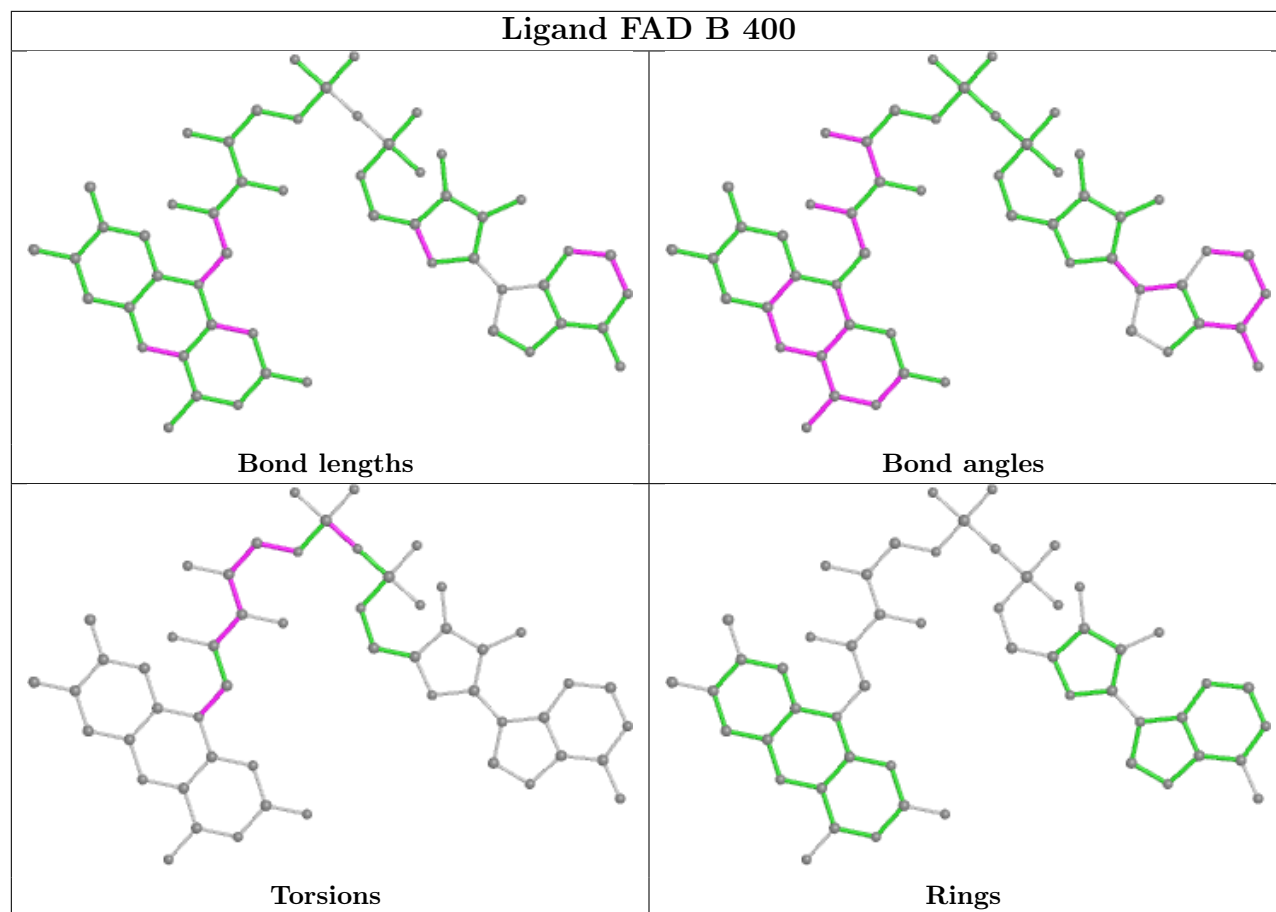
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	389/397 (97%)	-0.32	1 (0%)	94	94	13, 25, 43, 57	0
1	B	393/397 (98%)	-0.15	5 (1%)	77	80	13, 27, 48, 92	0
1	D	390/397 (98%)	0.75	39 (10%)	7	9	23, 47, 75, 88	0
1	E	391/397 (98%)	0.87	76 (19%)	1	1	18, 51, 99, 141	0
1	F	390/397 (98%)	-0.14	2 (0%)	91	92	16, 31, 50, 64	0
1	G	389/397 (97%)	0.24	10 (2%)	56	61	22, 39, 61, 77	0
2	Y	8/8 (100%)	1.92	4 (50%)	0	0	29, 48, 58, 76	0
All	All	2350/2390 (98%)	0.21	137 (5%)	23	28	13, 35, 73, 141	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	393	HIS	5.4
1	E	108	ALA	5.0
1	E	155	GLY	5.0
1	E	169	LEU	4.8
2	Y	41	LYS	4.7
1	D	11	MET	4.6
1	E	144	ALA	4.5
1	E	90	LEU	4.3
1	E	122	PHE	4.3
1	E	170	ILE	4.3
1	D	40	GLU	4.2
1	E	189	ILE	4.2
1	E	96	GLY	4.0
1	E	227	ILE	4.0
1	D	390	LYS	4.0
1	D	95	LEU	3.8
1	E	150	HIS	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	168	VAL	3.7
1	E	88	VAL	3.6
1	E	217	LEU	3.4
1	E	148	GLY	3.4
1	D	245	THR	3.3
1	D	90	LEU	3.3
1	E	153	LEU	3.3
1	E	391	GLY	3.2
1	E	187	PHE	3.2
1	E	222	VAL	3.2
1	E	92	MET	3.2
1	E	40	GLU	3.2
1	E	151	TRP	3.2
1	D	92	MET	3.2
1	D	76	THR	3.1
1	E	97	CYS	3.1
1	E	116	LYS	3.1
1	D	58	GLU	3.1
1	E	95	LEU	3.0
1	B	391	GLY	3.0
1	E	180	GLY	3.0
1	G	66	ASP	3.0
1	D	91	ASN	3.0
1	D	66	ASP	3.0
1	E	188	VAL	3.0
1	E	152	LEU	2.9
1	E	218	ASP	2.9
1	E	126	PHE	2.9
1	G	389	ARG	2.8
1	E	221	LYS	2.8
1	D	97	CYS	2.8
1	G	313	ARG	2.8
1	B	11	MET	2.8
1	E	171	TYR	2.8
1	D	52	PHE	2.8
2	Y	48	HIS	2.8
1	E	104	TYR	2.8
1	D	27	PHE	2.8
1	E	174	TYR	2.8
1	E	249	ALA	2.7
1	E	146	ASP	2.7
1	D	30	GLN	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	98	ALA	2.7
1	E	178	ALA	2.7
1	D	351	TYR	2.7
1	B	392	HIS	2.7
1	D	123	LEU	2.7
1	D	44	ARG	2.7
1	E	220	VAL	2.7
1	E	106	SER	2.7
1	G	230	LYS	2.7
1	E	215	LEU	2.7
1	E	94	VAL	2.6
1	G	385	ARG	2.6
1	D	121	GLU	2.6
2	Y	43	HIS	2.6
1	E	124	GLY	2.6
1	G	27	PHE	2.6
2	Y	47	HIS	2.6
1	E	198	LYS	2.5
1	E	164	ALA	2.5
1	G	11	MET	2.5
1	E	177	LYS	2.5
1	E	132	ASP	2.5
1	D	100	THR	2.5
1	E	113	TYR	2.5
1	D	105	GLY	2.5
1	E	66	ASP	2.5
1	E	128	ILE	2.5
1	E	163	ALA	2.5
1	E	366	VAL	2.4
1	E	91	ASN	2.4
1	E	154	ASN	2.4
1	E	145	GLU	2.4
1	D	88	VAL	2.4
1	E	149	ASP	2.4
1	E	223	PRO	2.4
1	E	182	ARG	2.4
1	E	39	TYR	2.4
1	E	197	ILE	2.3
1	E	147	LYS	2.3
1	D	48	GLU	2.3
1	E	203	GLU	2.3
1	E	112	LYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	99	TYR	2.3
1	D	18	ASN	2.3
1	D	87	ARG	2.3
1	F	385[A]	ARG	2.3
1	E	390	LYS	2.3
1	G	7	LYS	2.3
1	D	168	VAL	2.3
1	E	248	SER	2.3
1	D	231	PRO	2.2
1	G	168	VAL	2.2
1	E	230	LYS	2.2
1	E	76	THR	2.2
1	E	216	PHE	2.2
1	D	49	LEU	2.2
1	D	53	GLY	2.2
1	D	14	LYS	2.2
1	D	125	GLY	2.2
1	A	182	ARG	2.2
1	D	251	ALA	2.1
1	D	353	VAL	2.1
1	E	172	TYR	2.1
1	G	62	GLY	2.1
1	D	111	LYS	2.1
1	D	241	SER	2.1
1	E	251	ALA	2.1
1	E	140	MET	2.1
1	F	11	MET	2.1
1	D	96	GLY	2.1
1	E	48	GLU	2.1
1	E	167	ASP	2.1
1	E	231	PRO	2.1
1	E	60	TYR	2.1
1	D	172	TYR	2.0
1	D	55	VAL	2.0
1	B	169	LEU	2.0
1	D	74	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FAD	E	400	53/53	0.89	0.14	32,43,55,62	0
4	CL	E	401	1/1	0.89	0.16	54,54,54,54	0
4	CL	D	401	1/1	0.90	0.06	45,45,45,45	0
3	FAD	G	400	53/53	0.94	0.11	24,29,35,36	0
3	FAD	D	400	53/53	0.95	0.13	21,27,37,39	0
3	FAD	B	400	53/53	0.96	0.10	15,20,25,26	0
3	FAD	A	400	53/53	0.96	0.09	16,20,24,27	0
3	FAD	F	400	53/53	0.97	0.09	19,23,28,32	0
4	CL	A	401	1/1	0.98	0.05	32,32,32,32	0
4	CL	B	401	1/1	0.98	0.07	32,32,32,32	0
4	CL	F	401	1/1	0.98	0.06	36,36,36,36	0
4	CL	G	401	1/1	0.98	0.05	38,38,38,38	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 E 400:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
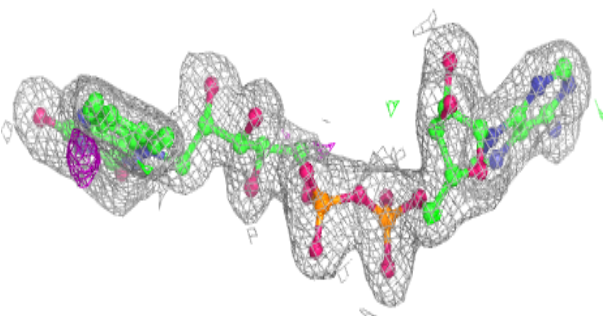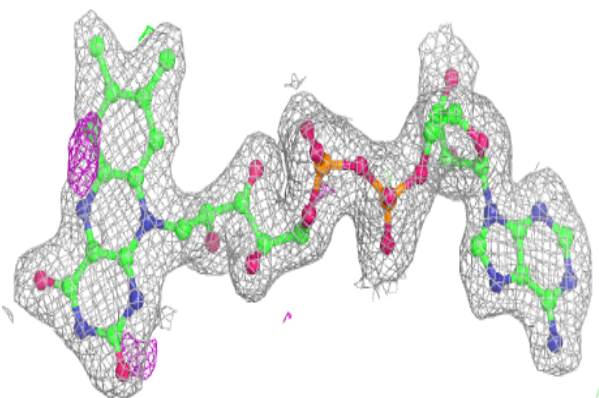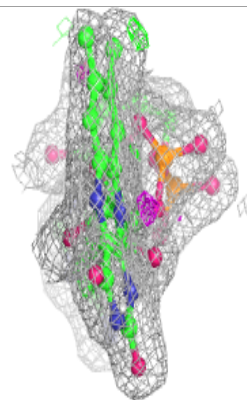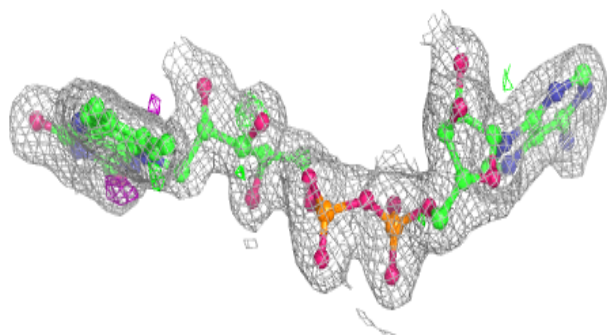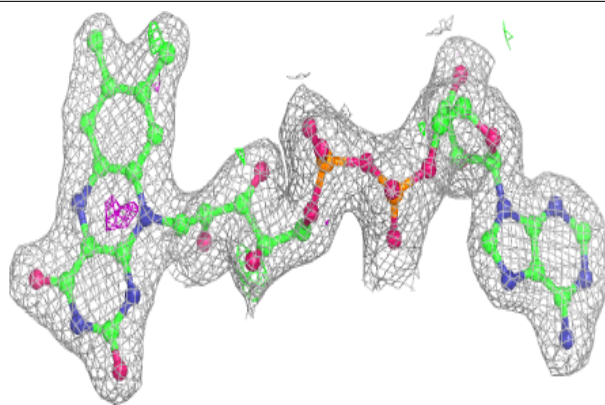mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
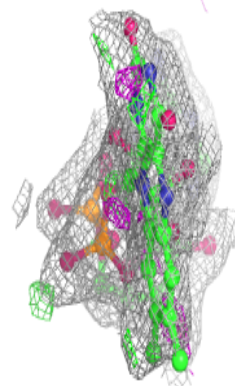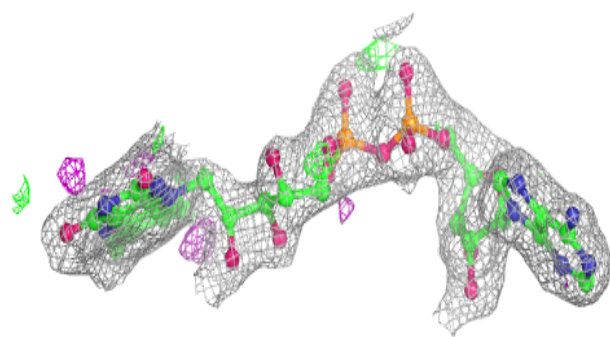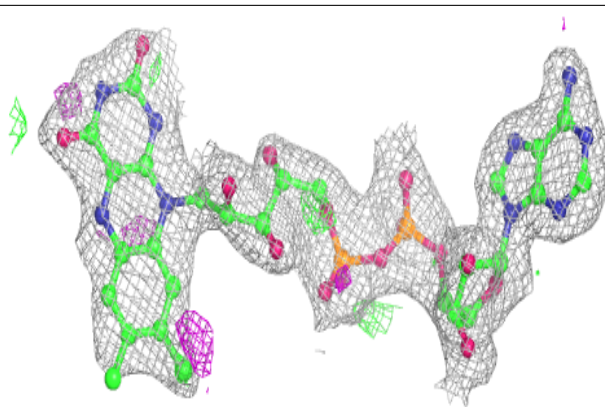
Electron density around FAD G 400:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
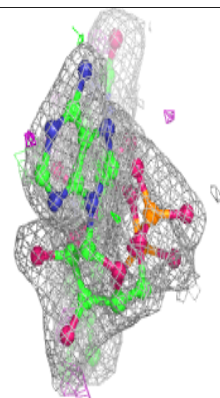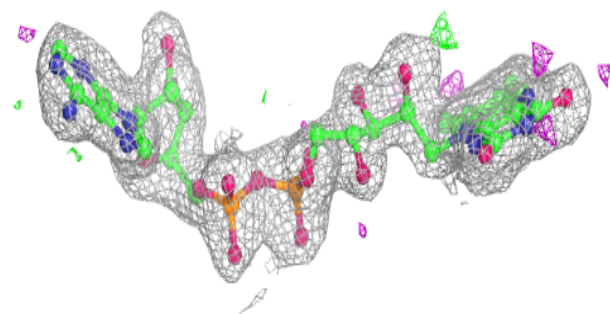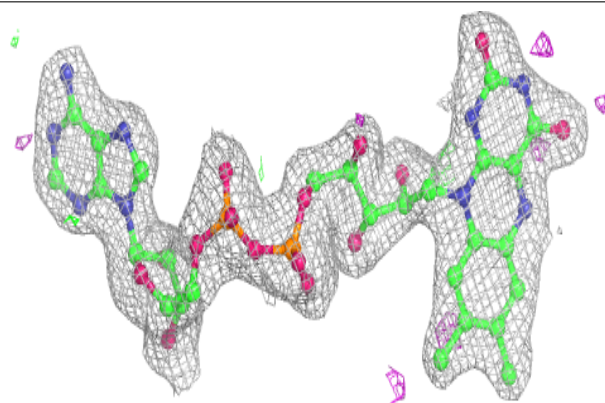
Electron density around FAD D 400:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
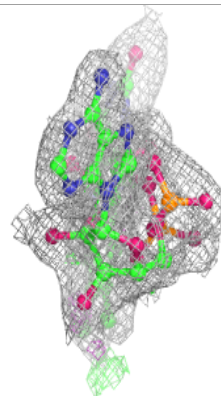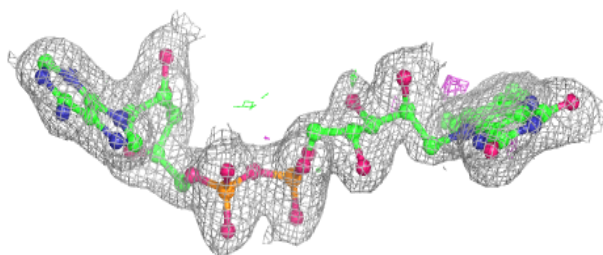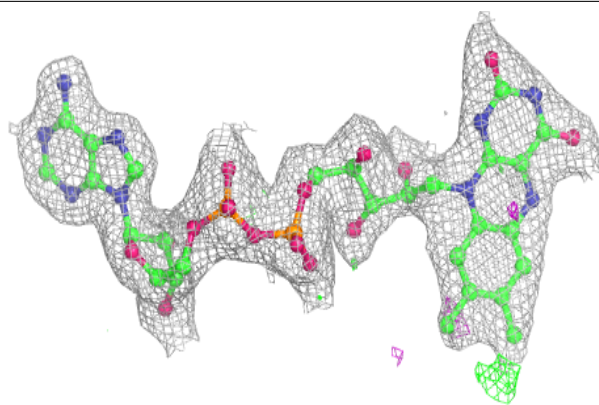
Electron density around FAD B 400:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
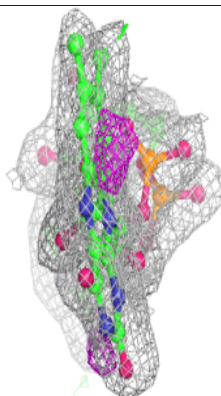
Electron density around FAD A 400:

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

Electron density around FAD F 400:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
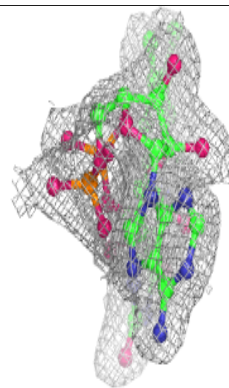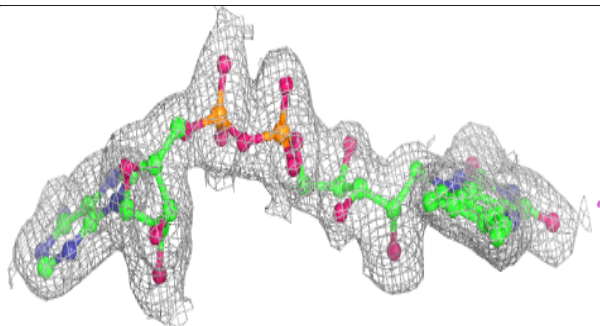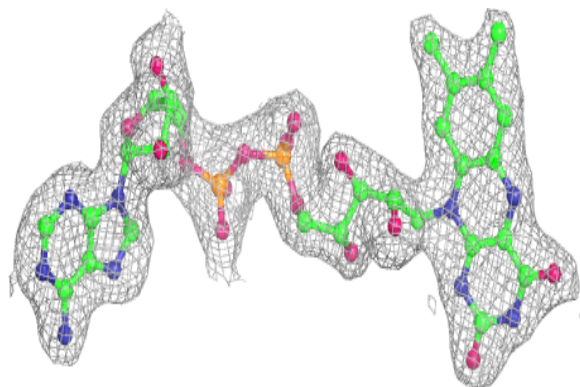
6.5 Other polymers (i)

There are no such residues in this entry.