



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2026 – 12:20 PM UTC

PDB ID : 2FON / pdb_00002fon
Title : X-ray crystal structure of LeACX1, an acyl-CoA oxidase from *Lycopersicon esculentum* (tomato)
Authors : Garavito, R.M.; Powers, R.A.
Deposited on : 2006-01-13
Resolution : 2.74 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

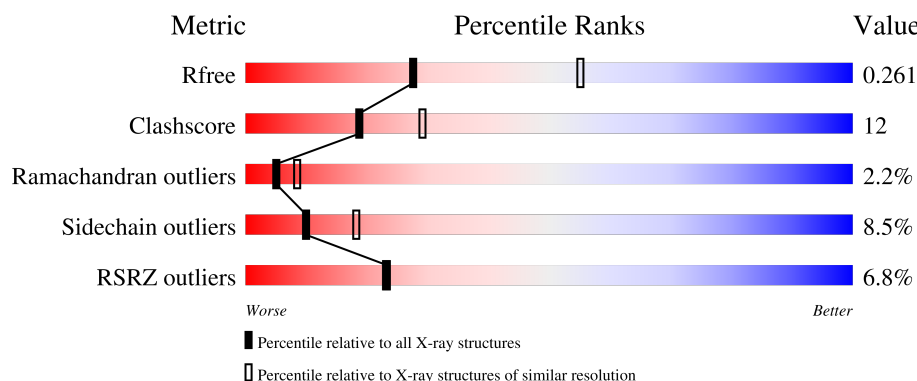
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.74 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}	180053	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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

Mol	Chain	Length	Quality of chain
1	A	683	9% 65% 26% 5% .
1	B	683	4% 69% 22% 5% .
1	C	683	6% 67% 24% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14949 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 peroxisomal acyl-CoA oxidase 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	654	Total	C	N	O	S	0	0	0
			5010	3180	873	932	25			
1	B	656	Total	C	N	O	S	0	0	0
			5040	3198	878	939	25			
1	C	653	Total	C	N	O	S	0	0	0
			4704	2960	828	892	24			

There are 57 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	cloning artifact	UNP Q5D8D3
A	-17	ARG	-	cloning artifact	UNP Q5D8D3
A	-16	GLY	-	cloning artifact	UNP Q5D8D3
A	-15	SER	-	cloning artifact	UNP Q5D8D3
A	-14	HIS	-	cloning artifact	UNP Q5D8D3
A	-13	HIS	-	cloning artifact	UNP Q5D8D3
A	-12	HIS	-	cloning artifact	UNP Q5D8D3
A	-11	HIS	-	cloning artifact	UNP Q5D8D3
A	-10	HIS	-	cloning artifact	UNP Q5D8D3
A	-9	HIS	-	cloning artifact	UNP Q5D8D3
A	-8	GLY	-	cloning artifact	UNP Q5D8D3
A	-7	SER	-	cloning artifact	UNP Q5D8D3
A	-6	ALA	-	cloning artifact	UNP Q5D8D3
A	-5	CYS	-	cloning artifact	UNP Q5D8D3
A	-4	GLU	-	cloning artifact	UNP Q5D8D3
A	-3	LEU	-	cloning artifact	UNP Q5D8D3
A	-2	VAL	-	cloning artifact	UNP Q5D8D3
A	-1	ARG	-	cloning artifact	UNP Q5D8D3
A	0	GLU	-	cloning artifact	UNP Q5D8D3
B	-18	MET	-	cloning artifact	UNP Q5D8D3
B	-17	ARG	-	cloning artifact	UNP Q5D8D3
B	-16	GLY	-	cloning artifact	UNP Q5D8D3
B	-15	SER	-	cloning artifact	UNP Q5D8D3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	cloning artifact	UNP Q5D8D3
B	-13	HIS	-	cloning artifact	UNP Q5D8D3
B	-12	HIS	-	cloning artifact	UNP Q5D8D3
B	-11	HIS	-	cloning artifact	UNP Q5D8D3
B	-10	HIS	-	cloning artifact	UNP Q5D8D3
B	-9	HIS	-	cloning artifact	UNP Q5D8D3
B	-8	GLY	-	cloning artifact	UNP Q5D8D3
B	-7	SER	-	cloning artifact	UNP Q5D8D3
B	-6	ALA	-	cloning artifact	UNP Q5D8D3
B	-5	CYS	-	cloning artifact	UNP Q5D8D3
B	-4	GLU	-	cloning artifact	UNP Q5D8D3
B	-3	LEU	-	cloning artifact	UNP Q5D8D3
B	-2	VAL	-	cloning artifact	UNP Q5D8D3
B	-1	ARG	-	cloning artifact	UNP Q5D8D3
B	0	GLU	-	cloning artifact	UNP Q5D8D3
C	-18	MET	-	cloning artifact	UNP Q5D8D3
C	-17	ARG	-	cloning artifact	UNP Q5D8D3
C	-16	GLY	-	cloning artifact	UNP Q5D8D3
C	-15	SER	-	cloning artifact	UNP Q5D8D3
C	-14	HIS	-	cloning artifact	UNP Q5D8D3
C	-13	HIS	-	cloning artifact	UNP Q5D8D3
C	-12	HIS	-	cloning artifact	UNP Q5D8D3
C	-11	HIS	-	cloning artifact	UNP Q5D8D3
C	-10	HIS	-	cloning artifact	UNP Q5D8D3
C	-9	HIS	-	cloning artifact	UNP Q5D8D3
C	-8	GLY	-	cloning artifact	UNP Q5D8D3
C	-7	SER	-	cloning artifact	UNP Q5D8D3
C	-6	ALA	-	cloning artifact	UNP Q5D8D3
C	-5	CYS	-	cloning artifact	UNP Q5D8D3
C	-4	GLU	-	cloning artifact	UNP Q5D8D3
C	-3	LEU	-	cloning artifact	UNP Q5D8D3
C	-2	VAL	-	cloning artifact	UNP Q5D8D3
C	-1	ARG	-	cloning artifact	UNP Q5D8D3
C	0	GLU	-	cloning artifact	UNP Q5D8D3

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		

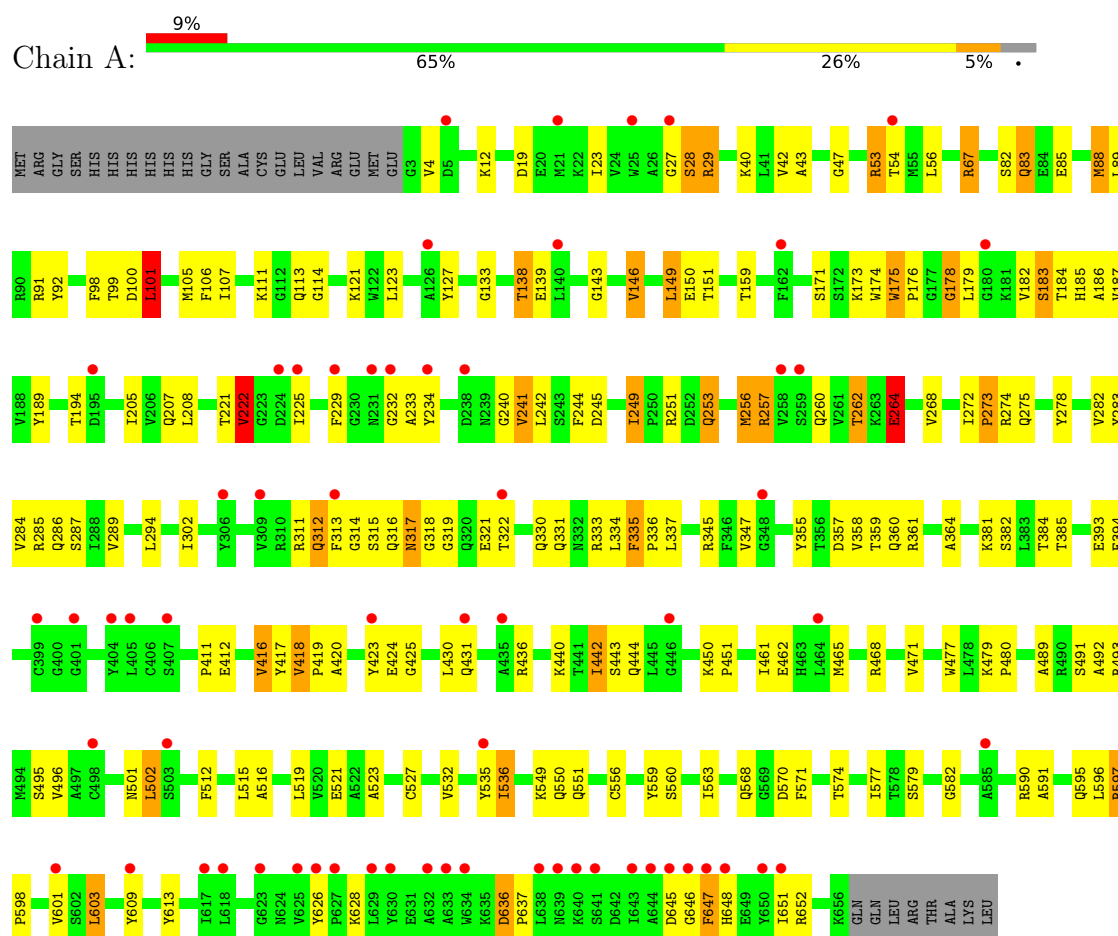
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	14	Total	O	0	0
			14	14		
3	B	22	Total	O	0	0
			22	22		

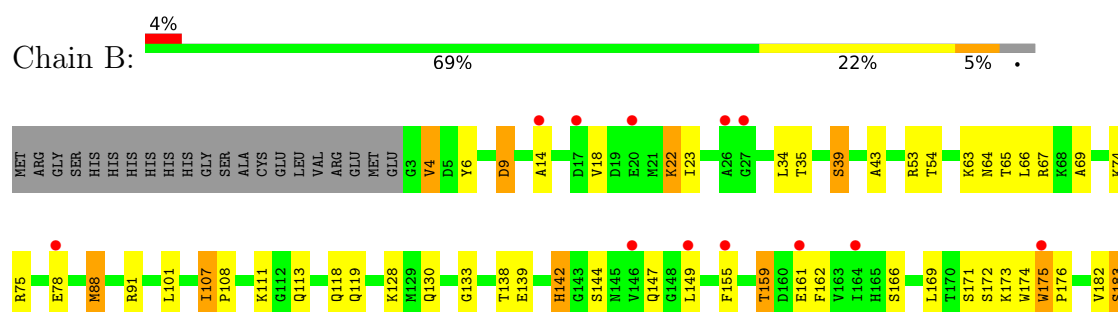
3 Residue-property plots

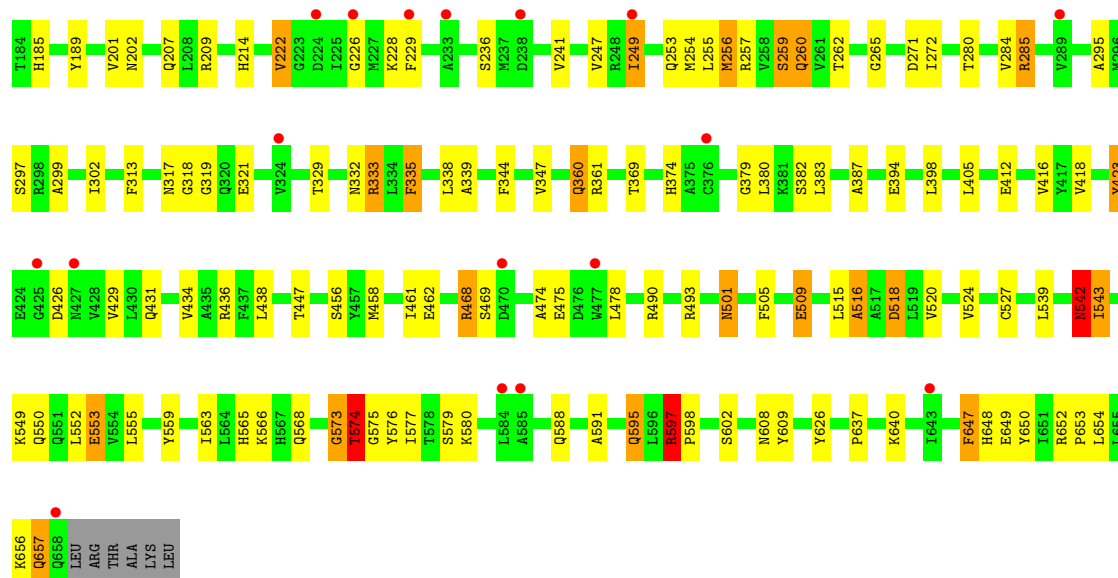
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: peroxisomal acyl-CoA oxidase 1A

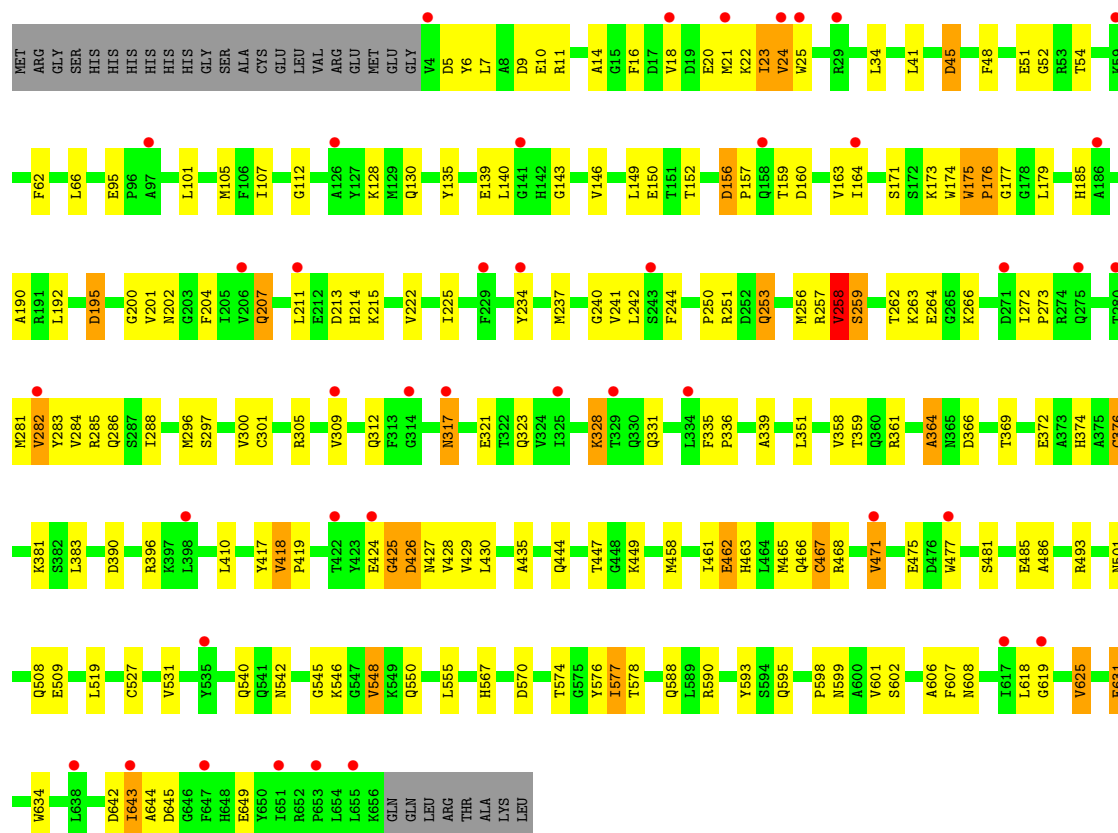


- Molecule 1: peroxisomal acyl-CoA oxidase 1A





• Molecule 1: peroxisomal acyl-CoA oxidase 1A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	120.20Å 240.33Å 89.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.74 30.00 – 2.74	Depositor EDS
% Data completeness (in resolution range)	92.9 (30.00-2.74) 92.7 (30.00-2.74)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.72Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.212 , 0.267 0.205 , 0.261	Depositor DCC
R_{free} test set	3221 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å ²)	70.6	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 61.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14949	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.28% 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: 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	1.19	3/5120 (0.1%)	1.28	29/6948 (0.4%)
1	B	1.17	9/5150 (0.2%)	1.26	34/6988 (0.5%)
1	C	0.81	3/4803 (0.1%)	1.07	16/6552 (0.2%)
All	All	1.08	15/15073 (0.1%)	1.21	79/20488 (0.4%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	107	ILE	CA-CB	-11.51	1.48	1.54
1	A	107	ILE	CA-CB	-7.12	1.50	1.54
1	B	302	ILE	CA-CB	-6.75	1.46	1.54
1	C	107	ILE	CA-CB	6.71	1.57	1.54
1	A	302	ILE	CA-CB	-6.62	1.46	1.54
1	C	163	VAL	CA-CB	5.75	1.62	1.54
1	B	299	ALA	CA-CB	-5.62	1.44	1.53
1	B	524	VAL	CA-CB	5.35	1.60	1.54
1	A	229	PHE	C-O	-5.31	1.17	1.24
1	B	247	VAL	CA-CB	-5.21	1.47	1.54
1	B	295	ALA	CA-C	5.20	1.59	1.52
1	B	387	ALA	N-CA	-5.20	1.40	1.46
1	B	69	ALA	CA-C	5.11	1.59	1.52
1	B	22	LYS	N-CA	-5.10	1.40	1.46
1	C	258	VAL	CA-CB	5.06	1.61	1.54

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	418	VAL	CA-C-N	-9.43	109.94	119.56
1	A	418	VAL	C-N-CA	-9.43	109.94	119.56
1	A	56	LEU	CA-C-N	-9.30	111.28	120.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	LEU	C-N-CA	-9.30	111.28	120.21
1	C	272	ILE	CA-C-N	9.07	131.18	119.84
1	C	272	ILE	C-N-CA	9.07	131.18	119.84
1	A	178	GLY	N-CA-C	-8.21	103.17	115.00
1	B	319	GLY	N-CA-C	7.73	120.83	112.33
1	A	272	ILE	CA-C-N	7.66	129.41	119.84
1	A	272	ILE	C-N-CA	7.66	129.41	119.84
1	A	335	PHE	CA-C-N	-7.50	111.03	119.28
1	A	335	PHE	C-N-CA	-7.50	111.03	119.28
1	C	272	ILE	N-CA-C	7.29	115.80	109.02
1	A	330	GLN	N-CA-C	-7.18	103.38	111.07
1	B	63	LYS	N-CA-C	-7.12	103.45	111.14
1	A	347	VAL	CB-CA-C	-7.02	102.90	111.88
1	A	626	TYR	CA-C-N	-6.80	111.50	119.05
1	A	626	TYR	C-N-CA	-6.80	111.50	119.05
1	A	527	CYS	N-CA-C	6.66	118.54	111.28
1	B	335	PHE	CA-C-N	-6.40	113.03	119.56
1	B	335	PHE	C-N-CA	-6.40	113.03	119.56
1	C	471	VAL	N-CA-C	6.38	116.68	108.12
1	B	171	SER	N-CA-C	-6.28	105.62	113.28
1	C	160	ASP	N-CA-C	6.26	120.03	111.39
1	B	272	ILE	CA-C-N	6.25	127.66	119.84
1	B	272	ILE	C-N-CA	6.25	127.66	119.84
1	B	387	ALA	N-CA-C	-6.19	104.53	111.28
1	B	222	VAL	CB-CA-C	-6.17	100.03	110.71
1	C	201	VAL	N-CA-C	6.13	116.94	108.84
1	A	278	TYR	N-CA-C	-6.07	106.00	113.41
1	A	138	THR	N-CA-C	6.07	118.84	110.35
1	B	416	VAL	CB-CA-C	-6.04	102.80	112.16
1	C	163	VAL	CB-CA-C	6.04	121.19	111.29
1	C	467	CYS	N-CA-C	6.04	120.84	112.45
1	B	626	TYR	CA-C-N	-6.03	112.65	119.28
1	B	626	TYR	C-N-CA	-6.03	112.65	119.28
1	B	226	GLY	N-CA-C	6.00	118.53	111.63
1	B	249	ILE	CA-C-N	-5.94	114.15	120.03
1	B	249	ILE	C-N-CA	-5.94	114.15	120.03
1	B	166	SER	CA-C-N	-5.90	112.94	119.19
1	B	166	SER	C-N-CA	-5.90	112.94	119.19
1	B	183	SER	N-CA-C	5.88	118.53	110.24
1	A	222	VAL	CB-CA-C	-5.86	101.32	110.69
1	B	597	ARG	CA-C-N	-5.71	113.74	119.56
1	B	597	ARG	C-N-CA	-5.71	113.74	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	608	ASN	N-CA-C	5.66	119.48	112.24
1	B	302	ILE	N-CA-C	5.62	115.82	110.42
1	C	14	ALA	N-CA-C	5.61	117.84	109.59
1	A	647	PHE	N-CA-C	5.59	120.54	111.37
1	B	201	VAL	N-CA-C	5.57	116.27	109.30
1	B	423	TYR	N-CA-C	5.53	118.70	110.52
1	A	334	LEU	N-CA-C	5.51	118.12	111.40
1	B	101	LEU	CA-CB-CG	-5.50	97.04	116.30
1	A	43	ALA	CA-C-N	-5.47	115.01	123.17
1	A	43	ALA	C-N-CA	-5.47	115.01	123.17
1	A	603	LEU	N-CA-C	5.47	118.76	111.75
1	B	516	ALA	N-CA-C	5.46	117.93	111.33
1	B	332	ASN	N-CA-C	5.46	117.98	111.71
1	A	496	VAL	N-CA-C	-5.43	104.30	111.09
1	A	636	ASP	CA-C-N	5.43	125.25	119.28
1	A	636	ASP	C-N-CA	5.43	125.25	119.28
1	B	182	VAL	N-CA-C	5.41	116.06	110.82
1	C	200	GLY	N-CA-C	5.35	119.43	112.68
1	A	101	LEU	CA-CB-CG	-5.35	97.58	116.30
1	B	360	GLN	N-CA-C	-5.31	105.16	111.69
1	B	647	PHE	N-CA-C	5.29	117.46	111.11
1	B	142	HIS	N-CA-C	5.20	117.89	108.69
1	A	628	LYS	N-CA-C	5.16	116.60	111.07
1	A	182	VAL	N-CA-C	5.16	116.08	111.90
1	C	625	VAL	N-CA-C	5.13	115.35	110.42
1	B	43	ALA	CA-C-N	-5.13	115.53	123.17
1	B	43	ALA	C-N-CA	-5.13	115.53	123.17
1	C	427	ASN	N-CA-C	5.13	117.27	111.11
1	B	468	ARG	N-CA-C	-5.12	100.36	109.06
1	C	202	ASN	N-CA-C	5.10	117.04	109.69
1	C	256	MET	N-CA-C	5.09	121.25	113.61
1	A	345	ARG	NE-CZ-NH1	-5.05	116.44	121.50
1	C	156	ASP	CA-C-N	5.02	126.12	119.84
1	C	156	ASP	C-N-CA	5.02	126.12	119.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5010	0	4838	130	0
1	B	5040	0	4884	113	0
1	C	4704	0	4258	105	0
2	A	53	0	31	6	0
2	B	53	0	31	5	0
2	C	53	0	31	6	0
3	A	14	0	0	0	0
3	B	22	0	0	2	0
All	All	14949	0	14073	345	0

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

All (345) 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:A:29:ARG:HG3	1:A:29:ARG:HH11	1.15	1.07
1:C:361:ARG:HD2	1:C:369:THR:HG21	1.47	0.97
1:A:29:ARG:HH11	1:A:29:ARG:CG	1.77	0.96
1:B:361:ARG:HD3	1:B:369:THR:HG21	1.45	0.94
1:B:285:ARG:HG3	1:B:285:ARG:HH11	1.35	0.90
1:B:516:ALA:O	1:B:520:VAL:HG23	1.72	0.90
1:A:316:GLN:O	1:A:317:ASN:O	1.90	0.88
1:C:475:GLU:HA	1:C:588:GLN:NE2	1.90	0.87
1:A:91:ARG:HG3	1:A:91:ARG:HH11	1.40	0.85
1:A:29:ARG:HG3	1:A:29:ARG:NH1	1.92	0.84
1:A:412:GLU:O	1:A:416:VAL:HG12	1.78	0.84
1:B:539:LEU:HD13	1:B:553:GLU:HG3	1.61	0.81
1:A:317:ASN:O	1:A:319:GLY:N	2.13	0.79
1:C:372:GLU:O	1:C:376:CYS:HB2	1.83	0.79
1:C:475:GLU:HA	1:C:588:GLN:HE22	1.48	0.78
1:A:442:ILE:O	1:A:444:GLN:N	2.16	0.78
1:B:490:ARG:HD3	3:B:2013:HOH:O	1.84	0.76
1:A:88:MET:HE1	1:A:91:ARG:HE	1.48	0.76
1:C:419:PRO:HB3	2:C:3000:FAD:HM71	1.67	0.76
1:A:113:GLN:O	1:A:257:ARG:HB2	1.86	0.75
1:A:333:ARG:HD2	1:A:394:GLU:OE2	1.85	0.75
1:B:595:GLN:O	1:B:598:PRO:HD2	1.85	0.74
1:A:516:ALA:HA	1:A:519:LEU:HD12	1.67	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:637:PRO:O	1:B:640:LYS:HG3	1.87	0.74
1:B:656:LYS:O	1:B:657:GLN:HG2	1.89	0.72
1:C:485:GLU:HG2	1:C:576:TYR:OH	1.89	0.72
1:C:286:GLN:HG2	1:C:351:LEU:HB3	1.70	0.71
1:A:316:GLN:C	1:A:317:ASN:O	2.32	0.71
1:C:296:MET:O	1:C:300:VAL:HG23	1.91	0.71
1:C:631:GLU:HA	1:C:634:TRP:HD1	1.56	0.71
1:B:333:ARG:HB2	1:B:398:LEU:HD21	1.73	0.70
1:B:34:LEU:HD23	1:B:88:MET:HG2	1.73	0.70
1:B:285:ARG:HG3	1:B:285:ARG:NH1	2.06	0.70
1:C:381:LYS:NZ	1:C:425:GLY:O	2.23	0.70
1:A:143:GLY:HA3	2:A:1000:FAD:O2P	1.92	0.69
1:B:174:TRP:C	1:B:176:PRO:HD3	2.17	0.69
1:B:91:ARG:HG3	1:B:91:ARG:HH11	1.58	0.69
1:C:179:LEU:HB3	1:C:240:GLY:HA3	1.75	0.69
1:A:568:GLN:NE2	1:A:582:GLY:HA3	2.08	0.68
1:B:35:THR:OG1	1:B:88:MET:HE3	1.93	0.68
1:C:105:MET:HB3	1:C:135:TYR:HB2	1.75	0.68
1:A:185:HIS:NE2	1:A:207:GLN:HG3	2.08	0.68
1:A:442:ILE:HD11	1:A:495:SER:HB3	1.73	0.68
1:A:105:MET:HA	1:A:105:MET:HE2	1.75	0.68
1:C:20:GLU:HA	1:C:23:ILE:HD12	1.75	0.68
1:C:458:MET:HG2	1:C:461:ILE:HD11	1.75	0.68
1:A:101:LEU:HD23	1:A:105:MET:HG3	1.75	0.68
1:A:431:GLN:HG3	1:A:523:ALA:HB1	1.76	0.68
1:A:88:MET:HE3	1:A:88:MET:HA	1.74	0.67
1:A:138:THR:OG1	2:A:1000:FAD:H1'1	1.94	0.67
1:A:502:LEU:HD12	1:A:515:LEU:HD12	1.77	0.67
1:C:284:VAL:HG12	1:C:288:ILE:HD11	1.76	0.67
1:A:502:LEU:HD12	1:A:515:LEU:CD1	2.24	0.66
1:B:118:GLN:NE2	1:B:254:MET:O	2.26	0.66
1:A:91:ARG:HG3	1:A:91:ARG:NH1	2.10	0.66
1:B:138:THR:OG1	2:B:2000:FAD:H1'1	1.96	0.66
1:C:339:ALA:HA	1:C:555:LEU:HD22	1.78	0.66
1:A:493:ARG:HD3	1:A:574:THR:HB	1.76	0.66
1:B:542:ASN:CG	1:B:543:ILE:H	2.06	0.64
1:B:176:PRO:HA	2:B:2000:FAD:C4	2.26	0.64
1:A:264:GLU:H	1:A:264:GLU:CD	2.06	0.64
1:C:493:ARG:HD3	1:C:574:THR:HB	1.80	0.64
1:A:436:ARG:HG2	1:A:512:PHE:CZ	2.33	0.63
1:C:112:GLY:O	1:C:257:ARG:HD3	1.97	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:361:ARG:CD	1:C:369:THR:HG21	2.24	0.63
1:A:570:ASP:O	1:A:574:THR:HG23	1.98	0.63
1:B:438:LEU:HD22	1:B:458:MET:HE3	1.81	0.62
1:C:174:TRP:O	1:C:175:TRP:HB2	2.00	0.62
1:A:47:GLY:O	1:A:67:ARG:NH2	2.32	0.62
1:C:242:LEU:HD21	1:C:244:PHE:CE1	2.35	0.62
1:B:361:ARG:CD	1:B:369:THR:HG21	2.24	0.62
1:A:283:TYR:HB2	1:A:355:TYR:CE1	2.36	0.61
2:A:1000:FAD:H2'	2:A:1000:FAD:C9	2.30	0.61
1:A:282:VAL:O	1:A:286:GLN:HB2	2.01	0.60
1:A:595:GLN:O	1:A:598:PRO:HD2	2.01	0.60
1:B:209:ARG:HD3	1:B:214:HIS:O	2.01	0.60
1:C:527:CYS:O	1:C:531:VAL:HG23	2.02	0.60
1:C:618:LEU:HA	1:C:625:VAL:HG13	1.84	0.60
1:B:185:HIS:NE2	1:B:207:GLN:HG3	2.16	0.60
1:A:173:LYS:O	1:A:241:VAL:HA	2.02	0.59
1:A:636:ASP:CG	1:A:637:PRO:HD2	2.28	0.59
1:B:648:HIS:HB3	3:B:2014:HOH:O	2.02	0.59
2:A:1000:FAD:H2'	2:A:1000:FAD:H9	1.84	0.59
1:C:139:GLU:HG3	1:C:149:LEU:HD22	1.83	0.59
1:C:465:MET:HE3	1:C:493:ARG:HG2	1.85	0.59
1:C:374:HIS:C	1:C:374:HIS:CD2	2.81	0.59
1:A:176:PRO:HA	2:A:1000:FAD:C4	2.32	0.59
2:B:2000:FAD:H2'	2:B:2000:FAD:C9	2.33	0.59
1:C:284:VAL:O	1:C:288:ILE:HG13	2.03	0.59
1:A:88:MET:CE	1:A:91:ARG:HE	2.14	0.58
1:B:262:THR:OG1	1:B:265:GLY:O	2.21	0.58
1:A:411:PRO:HB3	1:B:229:PHE:CD2	2.39	0.58
1:C:41:LEU:O	1:C:45:ASP:HB2	2.03	0.58
1:C:297:SER:HB2	1:C:607:PHE:CZ	2.38	0.58
1:C:361:ARG:HA	1:C:364:ALA:HB3	1.86	0.58
1:A:251:ARG:O	1:A:256:MET:HE2	2.04	0.58
1:C:545:GLY:O	1:C:548:VAL:HB	2.05	0.57
1:B:574:THR:OG1	1:B:575:GLY:N	2.37	0.57
1:A:82:SER:OG	1:A:85:GLU:HG3	2.05	0.57
1:A:225:ILE:HD12	1:B:405:LEU:HD21	1.86	0.56
1:A:242:LEU:HD21	1:A:244:PHE:CZ	2.41	0.56
1:B:139:GLU:HG3	1:B:149:LEU:HD22	1.88	0.56
1:B:173:LYS:O	1:B:241:VAL:HA	2.06	0.56
1:C:45:ASP:HB3	1:C:48:PHE:HD1	1.70	0.56
1:C:396:ARG:HA	1:C:410:LEU:HD13	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:ARG:CZ	1:B:398:LEU:HD23	2.35	0.56
1:B:436:ARG:NH2	1:B:509:GLU:OE2	2.38	0.55
1:A:262:THR:OG1	1:A:264:GLU:OE1	2.19	0.55
1:B:139:GLU:HG2	1:B:173:LYS:HD3	1.87	0.55
1:A:568:GLN:HE22	1:A:582:GLY:HA3	1.72	0.55
1:A:150:GLU:HB2	1:A:171:SER:HB3	1.89	0.55
1:C:590:ARG:HG3	1:C:590:ARG:HH11	1.71	0.55
1:B:53:ARG:HH22	1:B:412:GLU:CD	2.11	0.55
2:B:2000:FAD:H2'	2:B:2000:FAD:H9	1.89	0.55
1:B:493:ARG:HD3	1:B:574:THR:HB	1.89	0.54
1:C:173:LYS:HB2	1:C:242:LEU:HB3	1.88	0.54
1:C:418:VAL:N	1:C:419:PRO:HD2	2.22	0.54
1:A:139:GLU:OE2	1:A:151:THR:OG1	2.15	0.54
1:A:442:ILE:C	1:A:444:GLN:H	2.15	0.54
1:A:273:PRO:C	1:A:275:GLN:H	2.15	0.54
1:B:256:MET:HB3	1:B:260:GLN:HB3	1.89	0.54
1:C:185:HIS:NE2	1:C:207:GLN:HG2	2.23	0.54
1:A:431:GLN:HG3	1:A:523:ALA:CB	2.38	0.54
1:B:4:VAL:HG22	1:B:6:TYR:CE1	2.43	0.54
1:B:382:SER:HB3	1:B:431:GLN:HE21	1.73	0.54
1:C:435:ALA:HB1	1:C:519:LEU:HB3	1.90	0.54
1:C:417:TYR:C	1:C:419:PRO:HD2	2.33	0.53
1:B:4:VAL:HG22	1:B:6:TYR:CZ	2.43	0.53
1:A:461:ILE:O	1:A:462:GLU:C	2.50	0.53
1:A:29:ARG:CG	1:A:29:ARG:NH1	2.48	0.53
1:B:329:THR:O	1:B:333:ARG:HG3	2.09	0.53
1:B:493:ARG:HH11	1:B:574:THR:HB	1.74	0.53
1:A:221:THR:O	1:A:242:LEU:HA	2.09	0.52
1:C:297:SER:HB2	1:C:607:PHE:CE2	2.45	0.52
1:C:7:LEU:HD21	1:C:309:VAL:HG22	1.91	0.52
1:C:361:ARG:HB2	1:C:366:ASP:HB3	1.92	0.52
1:B:647:PHE:C	1:B:647:PHE:CD2	2.88	0.52
1:A:174:TRP:O	1:A:175:TRP:HB2	2.08	0.52
1:A:283:TYR:HB2	1:A:355:TYR:HE1	1.74	0.52
1:A:335:PHE:CG	1:A:596:LEU:HD23	2.45	0.52
1:C:152:THR:O	1:C:164:ILE:HA	2.10	0.52
1:A:331:GLN:HG2	1:A:335:PHE:CE1	2.45	0.52
1:A:382:SER:HB3	1:A:431:GLN:OE1	2.10	0.51
1:B:174:TRP:O	1:B:175:TRP:HB2	2.10	0.51
1:B:256:MET:HA	1:B:259:SER:O	2.10	0.51
1:C:471:VAL:HG11	1:C:477:TRP:NE1	2.25	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:486:ALA:HA	1:C:576:TYR:CE2	2.44	0.51
1:B:475:GLU:O	1:B:478:LEU:HB2	2.11	0.51
1:C:234:TYR:O	1:C:237:MET:HB3	2.11	0.51
1:C:419:PRO:CB	2:C:3000:FAD:HM71	2.38	0.51
1:B:474:ALA:C	1:B:588:GLN:HE21	2.19	0.50
1:B:35:THR:OG1	1:B:88:MET:CE	2.58	0.50
1:B:209:ARG:HD2	1:B:214:HIS:CE1	2.46	0.50
1:A:67:ARG:HB2	1:B:650:TYR:CE1	2.46	0.50
1:B:394:GLU:O	1:B:398:LEU:HG	2.12	0.50
1:A:19:ASP:O	1:A:23:ILE:HD13	2.10	0.50
1:B:18:VAL:O	1:B:22:LYS:HG3	2.10	0.50
1:B:518:ASP:OD2	1:B:518:ASP:N	2.44	0.50
1:A:551:GLN:HE21	1:A:603:LEU:HD11	1.77	0.50
1:B:461:ILE:O	1:B:462:GLU:C	2.54	0.50
1:B:542:ASN:O	1:B:543:ILE:HB	2.12	0.50
1:B:559:TYR:O	1:B:563:ILE:HG12	2.11	0.49
1:C:52:GLY:C	1:C:54:THR:H	2.20	0.49
1:C:174:TRP:HD1	1:C:175:TRP:CD1	2.30	0.49
2:C:3000:FAD:O1A	2:C:3000:FAD:H8A	2.12	0.49
1:A:471:VAL:HG21	1:A:477:TRP:CE2	2.46	0.49
1:A:651:ILE:HD13	1:B:66:LEU:HB3	1.94	0.49
1:B:175:TRP:N	1:B:176:PRO:HD3	2.27	0.49
1:B:468:ARG:NH1	1:B:575:GLY:O	2.45	0.49
1:B:128:LYS:HD2	1:B:130:GLN:NE2	2.27	0.49
1:C:128:LYS:HB2	1:C:130:GLN:NE2	2.27	0.49
1:A:521:GLU:CD	1:B:565:HIS:HE2	2.21	0.49
1:C:282:VAL:O	1:C:286:GLN:HB2	2.12	0.49
1:B:159:THR:HG21	1:B:161:GLU:OE1	2.12	0.49
1:A:111:LYS:HZ1	1:A:127:TYR:HH	1.57	0.49
1:A:314:GLY:O	1:A:315:SER:C	2.55	0.49
1:B:474:ALA:HB1	1:B:588:GLN:HB2	1.94	0.49
1:B:542:ASN:CG	1:B:543:ILE:N	2.68	0.49
1:B:505:PHE:HE1	1:B:515:LEU:HD11	1.77	0.49
1:A:442:ILE:C	1:A:444:GLN:N	2.71	0.49
1:C:16:PHE:HZ	1:C:602:SER:O	1.95	0.48
1:B:107:ILE:HB	1:B:108:PRO:HD3	1.95	0.48
1:A:88:MET:CE	1:A:91:ARG:NE	2.77	0.48
1:B:159:THR:CG2	1:B:161:GLU:OE1	2.60	0.48
1:A:535:TYR:CE2	1:A:556:CYS:HB2	2.48	0.48
1:B:379:GLY:HA3	1:B:527:CYS:SG	2.53	0.48
1:A:187:VAL:HG12	1:A:189:TYR:CE1	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:648:HIS:HD2	1:A:652:ARG:HD2	1.79	0.48
1:C:331:GLN:OE1	1:C:593:TYR:HB3	2.12	0.48
1:C:361:ARG:HD3	1:C:366:ASP:OD2	2.14	0.48
1:C:465:MET:HE3	1:C:493:ARG:CG	2.44	0.48
1:A:355:TYR:C	1:A:355:TYR:CD2	2.91	0.48
1:B:64:ASN:OD1	1:B:67:ARG:NH1	2.47	0.48
1:C:23:ILE:O	1:C:24:VAL:C	2.57	0.48
1:C:25:TRP:CD1	1:C:607:PHE:HA	2.49	0.48
1:C:22:LYS:HA	1:C:606:ALA:O	2.12	0.48
1:A:382:SER:CB	1:A:431:GLN:OE1	2.62	0.47
1:B:493:ARG:HH11	1:B:574:THR:CB	2.27	0.47
1:B:133:GLY:HA2	1:B:185:HIS:O	2.13	0.47
1:B:175:TRP:N	1:B:176:PRO:CD	2.77	0.47
1:C:150:GLU:HB2	1:C:171:SER:HB3	1.96	0.47
1:A:106:PHE:CD1	1:A:133:GLY:HA3	2.48	0.47
1:A:420:ALA:HA	1:A:423:TYR:CE2	2.49	0.47
1:A:249:ILE:HG13	1:A:253:GLN:NE2	2.30	0.47
1:B:14:ALA:HB2	1:B:602:SER:OG	2.14	0.47
1:C:234:TYR:CE2	1:C:237:MET:HE3	2.50	0.47
1:C:251:ARG:C	1:C:253:GLN:H	2.23	0.47
1:B:169:LEU:O	1:B:172:SER:HB2	2.15	0.47
1:B:297:SER:OG	1:B:609:TYR:OH	2.17	0.47
1:B:447:THR:O	1:B:447:THR:HG22	2.15	0.47
1:B:426:ASP:HB3	1:B:429:VAL:HB	1.97	0.47
1:A:42:VAL:HG11	1:A:92:TYR:C	2.40	0.46
1:A:111:LYS:NZ	1:A:127:TYR:OH	2.35	0.46
1:A:335:PHE:CD1	1:A:596:LEU:HD23	2.49	0.46
2:A:1000:FAD:H2A	1:B:329:THR:OG1	2.16	0.46
1:C:105:MET:HA	1:C:105:MET:HE2	1.97	0.46
1:A:178:GLY:O	1:A:183:SER:HB2	2.15	0.46
1:A:597:ARG:HD2	1:A:597:ARG:C	2.40	0.46
1:A:179:LEU:HD23	1:A:240:GLY:HA3	1.98	0.46
1:A:568:GLN:NE2	1:A:582:GLY:CA	2.78	0.46
1:B:111:LYS:O	1:B:119:GLN:NE2	2.48	0.46
1:C:372:GLU:O	1:C:372:GLU:HG2	2.15	0.46
1:A:273:PRO:C	1:A:275:GLN:N	2.73	0.46
1:A:284:VAL:O	1:A:287:SER:HB3	2.16	0.46
1:B:469:SER:HB2	1:B:576:TYR:CE2	2.51	0.45
1:B:573:GLY:O	1:B:575:GLY:N	2.49	0.45
1:C:10:GLU:OE2	1:C:323:GLN:NE2	2.49	0.45
1:A:114:GLY:O	1:A:257:ARG:HG3	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:SER:O	1:A:492:ALA:C	2.58	0.45
1:C:328:LYS:HA	1:C:328:LYS:HD2	1.59	0.45
1:A:232:GLY:O	1:A:233:ALA:C	2.59	0.45
1:B:9:ASP:OD1	1:B:9:ASP:N	2.44	0.45
1:C:567:HIS:HB3	1:C:570:ASP:OD2	2.16	0.45
1:B:374:HIS:C	1:B:374:HIS:CD2	2.94	0.45
1:B:652:ARG:O	1:B:653:PRO:C	2.59	0.45
1:C:358:VAL:O	1:C:361:ARG:HG2	2.17	0.45
1:A:294:LEU:HD21	1:A:613:TYR:OH	2.16	0.45
1:B:579:SER:O	1:B:580:LYS:C	2.58	0.45
1:A:245:ASP:C	1:A:245:ASP:OD1	2.60	0.45
1:B:313:PHE:O	1:B:321:GLU:HB3	2.17	0.45
1:B:436:ARG:HH22	1:B:509:GLU:CD	2.24	0.45
1:B:339:ALA:HA	1:B:555:LEU:HD22	1.99	0.45
1:C:21:MET:HG3	1:C:606:ALA:HB1	1.98	0.45
1:C:101:LEU:HD22	2:C:3000:FAD:O4	2.17	0.45
1:C:467:CYS:HG	1:C:576:TYR:HE1	1.65	0.45
1:A:418:VAL:O	1:A:419:PRO:C	2.56	0.44
1:B:280:THR:O	1:B:284:VAL:HG23	2.17	0.44
1:C:20:GLU:HB2	1:C:548:VAL:HG21	2.00	0.44
1:C:577:ILE:HG23	1:C:578:THR:O	2.16	0.44
1:C:643:ILE:HG12	1:C:644:ALA:N	2.31	0.44
1:A:289:VAL:HG13	1:A:384:THR:HG21	1.99	0.44
1:A:502:LEU:HD12	1:A:515:LEU:HD13	1.98	0.44
1:C:105:MET:HB3	1:C:135:TYR:CB	2.44	0.44
1:C:176:PRO:HA	2:C:3000:FAD:C4	2.47	0.44
1:C:301:CYS:O	1:C:305:ARG:HG3	2.18	0.44
1:B:75:ARG:HD2	1:B:75:ARG:HA	1.77	0.44
1:B:597:ARG:HB3	1:B:598:PRO:HD3	1.99	0.44
1:C:285:ARG:HA	1:C:288:ILE:HD12	1.99	0.44
1:C:631:GLU:O	1:C:631:GLU:HG2	2.17	0.44
1:A:205:ILE:HB	1:A:253:GLN:HG2	1.99	0.44
1:B:447:THR:O	1:B:447:THR:CG2	2.65	0.44
1:A:311:ARG:HA	1:A:322:THR:O	2.17	0.44
1:B:34:LEU:CD2	1:B:88:MET:HG2	2.45	0.44
1:A:479:LYS:HA	1:A:480:PRO:HD2	1.85	0.44
1:B:344:PHE:HA	1:B:347:VAL:HG12	2.00	0.44
1:C:462:GLU:HG3	1:C:463:HIS:H	1.81	0.44
1:A:312:GLN:O	1:A:313:PHE:HB2	2.18	0.44
1:B:74:LYS:O	1:B:78:GLU:HG3	2.18	0.44
1:A:27:GLY:O	1:A:28:SER:HB3	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:425:GLY:HA3	1:C:430:LEU:HD21	1.99	0.43
1:A:559:TYR:O	1:A:563:ILE:HG12	2.18	0.43
1:B:4:VAL:CG2	1:B:6:TYR:CZ	3.01	0.43
1:C:258:VAL:CG2	1:C:259:SER:N	2.81	0.43
1:C:447:THR:OG1	1:C:449:LYS:HB3	2.18	0.43
1:A:113:GLN:C	1:A:257:ARG:HB2	2.42	0.43
1:A:381:LYS:NZ	1:A:425:GLY:O	2.41	0.43
1:A:417:TYR:C	1:A:419:PRO:HD2	2.43	0.43
1:A:186:ALA:HB2	1:A:208:LEU:HD11	1.99	0.43
1:A:381:LYS:O	1:A:385:THR:HG23	2.18	0.43
1:A:98:PHE:O	1:A:99:THR:C	2.60	0.43
1:C:101:LEU:HD12	1:C:101:LEU:H	1.82	0.43
1:C:281:MET:O	1:C:283:TYR:N	2.52	0.43
1:B:335:PHE:N	1:B:335:PHE:CD2	2.85	0.43
1:B:656:LYS:C	1:B:657:GLN:HG2	2.44	0.43
1:A:294:LEU:HD12	1:A:609:TYR:OH	2.19	0.43
1:C:5:ASP:OD1	1:C:11:ARG:NH1	2.52	0.43
1:B:113:GLN:O	1:B:255:LEU:HB3	2.19	0.42
1:B:189:TYR:HA	1:B:202:ASN:O	2.19	0.42
1:C:509:GLU:OE1	1:C:509:GLU:HA	2.19	0.42
1:B:35:THR:O	1:B:39:SER:HB2	2.18	0.42
1:A:590:ARG:O	1:A:591:ALA:C	2.60	0.42
1:B:591:ALA:O	1:B:595:GLN:HG2	2.19	0.42
1:A:249:ILE:HG13	1:A:253:GLN:HE21	1.84	0.42
1:C:213:ASP:C	1:C:215:LYS:H	2.27	0.42
1:B:501:ASN:HD22	1:B:501:ASN:HA	1.50	0.42
1:C:101:LEU:HD13	1:C:177:GLY:HA3	2.02	0.42
1:C:426:ASP:OD2	2:C:3000:FAD:H2B	2.19	0.42
1:A:242:LEU:HD21	1:A:244:PHE:HZ	1.84	0.42
1:C:156:ASP:HA	1:C:157:PRO:HD3	1.82	0.42
1:C:190:ALA:HB3	1:C:204:PHE:CE1	2.54	0.42
1:C:262:THR:HG22	1:C:263:LYS:H	1.84	0.42
1:A:283:TYR:O	1:A:286:GLN:HB3	2.20	0.42
1:A:646:GLY:HA3	1:B:66:LEU:HD12	2.01	0.42
1:C:95:GLU:HA	1:C:95:GLU:OE1	2.19	0.42
1:A:335:PHE:O	1:A:336:PRO:C	2.61	0.42
1:A:337:LEU:HD23	1:A:337:LEU:HA	1.60	0.42
1:B:155:PHE:HB2	1:B:162:PHE:CE2	2.55	0.42
1:C:195:ASP:OD1	1:C:195:ASP:N	2.52	0.42
1:A:83:GLN:HA	1:A:83:GLN:HE21	1.85	0.41
1:A:222:VAL:HA	1:A:241:VAL:O	2.18	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:GLY:CA	1:B:434:VAL:HG21	2.50	0.41
1:B:383:LEU:HD12	1:B:383:LEU:HA	1.80	0.41
1:A:381:LYS:HD2	1:A:430:LEU:CD1	2.50	0.41
1:C:176:PRO:HB2	1:C:179:LEU:HB2	2.02	0.41
1:A:184:THR:O	1:A:208:LEU:N	2.43	0.41
1:A:532:VAL:O	1:A:536:ILE:HD12	2.20	0.41
1:A:285:ARG:O	1:A:286:GLN:C	2.64	0.41
1:B:65:THR:OG1	1:B:236:SER:HB2	2.21	0.41
1:C:435:ALA:CB	1:C:519:LEU:HB3	2.48	0.41
1:C:595:GLN:O	1:C:598:PRO:HD2	2.21	0.41
1:A:357:ASP:O	1:A:361:ARG:HG3	2.20	0.41
1:A:450:LYS:HA	1:A:451:PRO:HD3	1.93	0.41
1:A:647:PHE:CE1	1:B:214:HIS:CE1	3.09	0.41
1:A:489:ALA:O	1:A:493:ARG:HD2	2.21	0.41
1:C:312:GLN:HA	1:C:321:GLU:OE2	2.20	0.41
1:A:83:GLN:HE21	1:A:83:GLN:CA	2.34	0.41
1:B:552:LEU:HD23	1:B:552:LEU:HA	1.94	0.41
1:B:576:TYR:HD2	1:B:577:ILE:HG23	1.86	0.41
1:A:98:PHE:C	1:A:100:ASP:N	2.78	0.40
1:A:571:PHE:HB2	1:A:577:ILE:HD11	2.02	0.40
1:B:380:LEU:HD23	1:B:380:LEU:HA	1.85	0.40
1:A:146:VAL:O	1:A:149:LEU:HG	2.21	0.40
1:C:175:TRP:O	1:C:176:PRO:C	2.65	0.40
1:C:383:LEU:HD22	1:C:527:CYS:HB2	2.02	0.40
1:A:179:LEU:HD11	1:A:242:LEU:HD22	2.02	0.40
1:A:603:LEU:HA	1:A:603:LEU:HD23	1.84	0.40
1:B:144:SER:HB2	2:B:2000:FAD:O1A	2.22	0.40
1:C:335:PHE:N	1:C:336:PRO:CD	2.84	0.40
1:B:539:LEU:O	1:B:549:LYS:HE3	2.21	0.40
1:C:426:ASP:OD1	1:C:426:ASP:C	2.64	0.40
1:C:643:ILE:HG12	1:C:645:ASP:H	1.87	0.40
1:A:321:GLU:OE1	1:B:142:HIS:NE2	2.38	0.40
1:A:393:GLU:HA	1:A:393:GLU:OE1	2.21	0.40
1:C:62:PHE:O	1:C:66:LEU:HG	2.21	0.40
1:C:305:ARG:NH1	1:C:619:GLY:O	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	652/683 (96%)	591 (91%)	47 (7%)	14 (2%)	5	9
1	B	654/683 (96%)	617 (94%)	27 (4%)	10 (2%)	8	14
1	C	651/683 (95%)	560 (86%)	71 (11%)	20 (3%)	3	5
All	All	1957/2049 (96%)	1768 (90%)	145 (7%)	44 (2%)	5	8

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	THR
1	A	175	TRP
1	A	317	ASN
1	A	318	GLY
1	B	175	TRP
1	B	271	ASP
1	B	574	THR
1	C	23	ILE
1	C	175	TRP
1	C	266	LYS
1	C	273	PRO
1	C	282	VAL
1	C	546	LYS
1	A	12	LYS
1	A	53	ARG
1	A	273	PRO
1	A	442	ILE
1	A	443	SER
1	B	318	GLY
1	B	573	GLY
1	C	24	VAL
1	C	51	GLU
1	C	159	THR
1	C	214	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	468	ARG
1	B	317	ASN
1	B	542	ASN
1	C	317	ASN
1	C	364	ALA
1	C	424	GLU
1	A	28	SER
1	A	264	GLU
1	A	274	ARG
1	A	364	ALA
1	A	424	GLU
1	C	608	ASN
1	B	543	ILE
1	B	597	ARG
1	B	657	GLN
1	C	176	PRO
1	C	6	TYR
1	C	143	GLY
1	C	425	GLY
1	C	250	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	509/571 (89%)	464 (91%)	45 (9%)	9	17
1	B	516/571 (90%)	480 (93%)	36 (7%)	14	26
1	C	434/571 (76%)	391 (90%)	43 (10%)	7	14
All	All	1459/1713 (85%)	1335 (92%)	124 (8%)	10	18

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	VAL
1	A	29	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	40	LYS
1	A	53	ARG
1	A	67	ARG
1	A	83	GLN
1	A	88	MET
1	A	89	LEU
1	A	101	LEU
1	A	121	LYS
1	A	123	LEU
1	A	146	VAL
1	A	149	LEU
1	A	159	THR
1	A	183	SER
1	A	194	THR
1	A	222	VAL
1	A	234	TYR
1	A	241	VAL
1	A	249	ILE
1	A	253	GLN
1	A	256	MET
1	A	257	ARG
1	A	260	GLN
1	A	262	THR
1	A	264	GLU
1	A	268	VAL
1	A	312	GLN
1	A	358	VAL
1	A	359	THR
1	A	360	GLN
1	A	416	VAL
1	A	440	LYS
1	A	465	MET
1	A	468	ARG
1	A	501	ASN
1	A	502	LEU
1	A	536	ILE
1	A	549	LYS
1	A	550	GLN
1	A	560	SER
1	A	579	SER
1	A	597	ARG
1	A	601	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	645	ASP
1	B	4	VAL
1	B	9	ASP
1	B	23	ILE
1	B	39	SER
1	B	54	THR
1	B	88	MET
1	B	147	GLN
1	B	159	THR
1	B	183	SER
1	B	222	VAL
1	B	228	LYS
1	B	249	ILE
1	B	253	GLN
1	B	256	MET
1	B	257	ARG
1	B	259	SER
1	B	260	GLN
1	B	285	ARG
1	B	333	ARG
1	B	338	LEU
1	B	360	GLN
1	B	418	VAL
1	B	423	TYR
1	B	456	SER
1	B	501	ASN
1	B	509	GLU
1	B	518	ASP
1	B	542	ASN
1	B	550	GLN
1	B	553	GLU
1	B	566	LYS
1	B	568	GLN
1	B	574	THR
1	B	595	GLN
1	B	649	GLU
1	B	654	LEU
1	C	9	ASP
1	C	18	VAL
1	C	34	LEU
1	C	45	ASP
1	C	140	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	146	VAL
1	C	192	LEU
1	C	195	ASP
1	C	207	GLN
1	C	211	LEU
1	C	222	VAL
1	C	225	ILE
1	C	241	VAL
1	C	253	GLN
1	C	258	VAL
1	C	259	SER
1	C	264	GLU
1	C	317	ASN
1	C	328	LYS
1	C	359	THR
1	C	376	CYS
1	C	390	ASP
1	C	418	VAL
1	C	426	ASP
1	C	428	VAL
1	C	429	VAL
1	C	444	GLN
1	C	462	GLU
1	C	466	GLN
1	C	481	SER
1	C	501	ASN
1	C	508	GLN
1	C	540	GLN
1	C	542	ASN
1	C	548	VAL
1	C	550	GLN
1	C	577	ILE
1	C	599	ASN
1	C	601	VAL
1	C	631	GLU
1	C	642	ASP
1	C	643	ILE
1	C	649	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	113	GLN
1	A	202	ASN
1	A	239	ASN
1	A	253	GLN
1	A	332	ASN
1	A	444	GLN
1	A	473	GLN
1	A	501	ASN
1	A	567	HIS
1	A	568	GLN
1	A	588	GLN
1	A	648	HIS
1	B	113	GLN
1	B	130	GLN
1	B	137	GLN
1	B	202	ASN
1	B	231	ASN
1	B	253	GLN
1	B	260	GLN
1	B	360	GLN
1	B	374	HIS
1	B	444	GLN
1	B	501	ASN
1	B	507	ASN
1	B	542	ASN
1	B	567	HIS
1	B	588	GLN
1	C	145	ASN
1	C	202	ASN
1	C	312	GLN
1	C	332	ASN
1	C	360	GLN
1	C	374	HIS
1	C	463	HIS
1	C	501	ASN
1	C	541	GLN
1	C	551	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	1000	-	58,58,58	1.41	11 (18%)	85,89,89	2.04	27 (31%)
2	FAD	B	2000	-	58,58,58	1.35	8 (13%)	85,89,89	1.89	22 (25%)
2	FAD	C	3000	-	58,58,58	1.20	5 (8%)	85,89,89	1.58	15 (17%)

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	1000	-	-	6/34/50/50	0/6/6/6
2	FAD	B	2000	-	-	4/34/50/50	0/6/6/6
2	FAD	C	3000	-	-	12/34/50/50	0/6/6/6

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2000	FAD	C4X-N5	4.26	1.39	1.30
2	A	1000	FAD	C4X-N5	4.21	1.39	1.30
2	C	3000	FAD	C4X-N5	4.02	1.39	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3000	FAD	C2A-N3A	3.87	1.40	1.33
2	C	3000	FAD	C2A-N1A	3.44	1.40	1.33
2	B	2000	FAD	PA-O3P	3.33	1.63	1.59
2	C	3000	FAD	C10-N1	2.57	1.38	1.33
2	B	2000	FAD	C10-N1	2.48	1.38	1.33
2	A	1000	FAD	O2'-C2'	-2.45	1.38	1.43
2	A	1000	FAD	C10-N1	2.44	1.38	1.33
2	A	1000	FAD	P-O3P	2.43	1.62	1.59
2	B	2000	FAD	C2A-N3A	2.36	1.38	1.33
2	A	1000	FAD	C2A-N1A	2.35	1.38	1.33
2	A	1000	FAD	C8A-N7A	2.28	1.36	1.31
2	A	1000	FAD	PA-O3P	2.26	1.61	1.59
2	C	3000	FAD	PA-O3P	2.22	1.61	1.59
2	A	1000	FAD	C2A-N3A	2.16	1.37	1.33
2	B	2000	FAD	O2'-C2'	-2.13	1.38	1.43
2	A	1000	FAD	C4X-C10	-2.12	1.38	1.44
2	A	1000	FAD	C6-C5X	-2.09	1.36	1.40
2	B	2000	FAD	C5A-N7A	-2.05	1.35	1.39
2	A	1000	FAD	C2'-C3'	-2.03	1.49	1.53
2	B	2000	FAD	O3B-C3B	-2.02	1.37	1.43
2	B	2000	FAD	O4B-C4B	-2.02	1.40	1.45

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	FAD	N3A-C2A-N1A	-6.47	118.79	128.58
2	B	2000	FAD	N3A-C2A-N1A	-5.72	119.92	128.58
2	A	1000	FAD	N9A-C8A-N7A	-5.24	106.50	113.94
2	C	3000	FAD	N3A-C2A-N1A	-5.01	120.99	128.58
2	B	2000	FAD	C5'-C4'-C3'	-4.77	103.22	112.22
2	C	3000	FAD	C5A-C4A-N3A	-4.56	120.44	126.72
2	B	2000	FAD	N9A-C8A-N7A	-4.52	107.53	113.94
2	A	1000	FAD	C5A-C4A-N3A	-4.51	120.50	126.72
2	A	1000	FAD	C5'-C4'-C3'	-4.27	104.16	112.22
2	A	1000	FAD	C5A-N7A-C8A	4.19	110.03	103.45
2	A	1000	FAD	O2'-C2'-C3'	-4.18	99.46	109.25
2	B	2000	FAD	C5A-C4A-N3A	-3.94	121.28	126.72
2	A	1000	FAD	C2A-N3A-C4A	3.85	121.24	111.83
2	B	2000	FAD	O5'-C5'-C4'	-3.80	99.22	109.36
2	B	2000	FAD	C4-N3-C2	-3.72	119.03	125.64
2	A	1000	FAD	N3A-C4A-N9A	3.67	133.42	127.17
2	A	1000	FAD	C1'-C2'-C3'	3.64	119.52	109.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	FAD	C4A-N9A-C8A	3.59	109.51	105.74
2	B	2000	FAD	C5A-N7A-C8A	3.49	108.94	103.45
2	C	3000	FAD	N9A-C8A-N7A	-3.46	109.02	113.94
2	C	3000	FAD	N3A-C4A-N9A	3.40	132.95	127.17
2	C	3000	FAD	C5A-N7A-C8A	3.39	108.77	103.45
2	B	2000	FAD	C2A-N3A-C4A	3.38	120.08	111.83
2	A	1000	FAD	C6-C5X-C9A	3.27	123.54	119.05
2	B	2000	FAD	C1'-C2'-C3'	3.25	118.46	109.66
2	B	2000	FAD	C4A-N9A-C8A	3.21	109.11	105.74
2	C	3000	FAD	C2A-N3A-C4A	3.19	119.62	111.83
2	B	2000	FAD	C7M-C7-C6	-3.18	113.97	119.57
2	C	3000	FAD	C4-N3-C2	-3.12	120.10	125.64
2	A	1000	FAD	C9A-C5X-N5	-3.06	119.21	122.45
2	B	2000	FAD	C4X-C10-N10	2.93	120.67	116.48
2	A	1000	FAD	C4X-C4-N3	2.89	120.61	113.25
2	B	2000	FAD	C4X-C4-N3	2.88	120.59	113.25
2	C	3000	FAD	O4-C4-C4X	-2.87	118.96	126.53
2	B	2000	FAD	N3A-C4A-N9A	2.81	131.94	127.17
2	A	1000	FAD	C5X-N5-C4X	2.77	122.57	118.09
2	C	3000	FAD	C4X-C4-N3	2.66	120.03	113.25
2	B	2000	FAD	C10-C4X-N5	-2.62	119.46	124.81
2	A	1000	FAD	C10-C4X-N5	-2.61	119.47	124.81
2	A	1000	FAD	C4-N3-C2	-2.61	121.01	125.64
2	B	2000	FAD	O4-C4-C4X	-2.60	119.66	126.53
2	B	2000	FAD	C4A-C5A-N7A	-2.57	107.64	110.58
2	B	2000	FAD	O2'-C2'-C3'	-2.53	103.34	109.25
2	B	2000	FAD	C4-C4X-N5	2.51	121.67	118.21
2	C	3000	FAD	C4A-C5A-N7A	-2.45	107.78	110.58
2	A	1000	FAD	C2B-C1B-N9A	-2.42	107.28	113.30
2	C	3000	FAD	C4X-C10-N10	2.42	119.94	116.48
2	A	1000	FAD	C10-N1-C2	2.40	122.05	116.85
2	C	3000	FAD	O4B-C1B-N9A	2.37	112.63	108.09
2	A	1000	FAD	C4A-C5A-N7A	-2.36	107.88	110.58
2	A	1000	FAD	O5B-C5B-C4B	-2.34	101.04	108.99
2	A	1000	FAD	C4X-C10-N1	-2.28	118.99	124.59
2	C	3000	FAD	C9A-C5X-N5	-2.21	120.11	122.45
2	A	1000	FAD	O3P-PA-O1A	2.19	117.28	110.70
2	B	2000	FAD	O2P-P-O3P	-2.17	101.40	107.27
2	C	3000	FAD	C5X-C9A-N10	2.17	119.93	117.97
2	B	2000	FAD	O2-C2-N1	-2.15	118.23	121.80
2	A	1000	FAD	O3P-P-O1P	2.12	117.09	110.70
2	A	1000	FAD	C4X-C10-N10	2.10	119.49	116.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	FAD	O3B-C3B-C2B	-2.07	105.19	111.82
2	B	2000	FAD	O3B-C3B-C4B	-2.05	105.19	111.08
2	A	1000	FAD	O4-C4-C4X	-2.05	121.13	126.53
2	A	1000	FAD	O3B-C3B-C4B	-2.04	105.22	111.08
2	C	3000	FAD	C10-C4X-N5	-2.02	120.68	124.81

There are no chirality outliers.

All (22) torsion outliers are listed below:

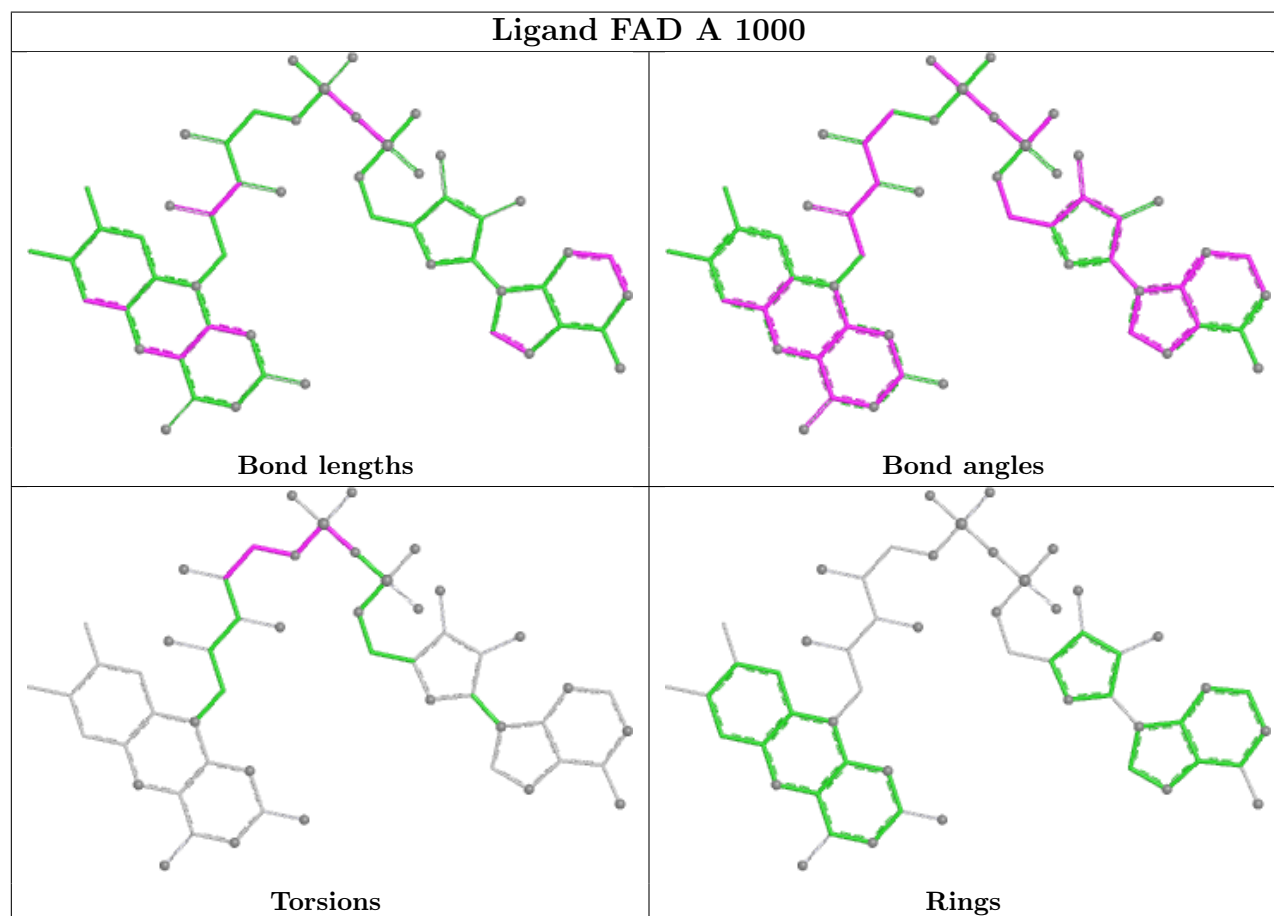
Mol	Chain	Res	Type	Atoms
2	A	1000	FAD	O4'-C4'-C5'-O5'
2	A	1000	FAD	C5'-O5'-P-O3P
2	B	2000	FAD	C5'-O5'-P-O1P
2	B	2000	FAD	C5'-O5'-P-O2P
2	B	2000	FAD	C5'-O5'-P-O3P
2	C	3000	FAD	C5B-O5B-PA-O1A
2	C	3000	FAD	C5B-O5B-PA-O2A
2	C	3000	FAD	C5B-O5B-PA-O3P
2	C	3000	FAD	C1'-C2'-C3'-C4'
2	C	3000	FAD	O4'-C4'-C5'-O5'
2	C	3000	FAD	C5'-O5'-P-O1P
2	C	3000	FAD	C5'-O5'-P-O2P
2	C	3000	FAD	C5'-O5'-P-O3P
2	C	3000	FAD	C3'-C4'-C5'-O5'
2	A	1000	FAD	C4'-C5'-O5'-P
2	C	3000	FAD	C1'-C2'-C3'-O3'
2	A	1000	FAD	C5'-O5'-P-O1P
2	B	2000	FAD	C5B-O5B-PA-O3P
2	A	1000	FAD	C3'-C4'-C5'-O5'
2	A	1000	FAD	PA-O3P-P-O2P
2	C	3000	FAD	P-O3P-PA-O2A
2	C	3000	FAD	P-O3P-PA-O1A

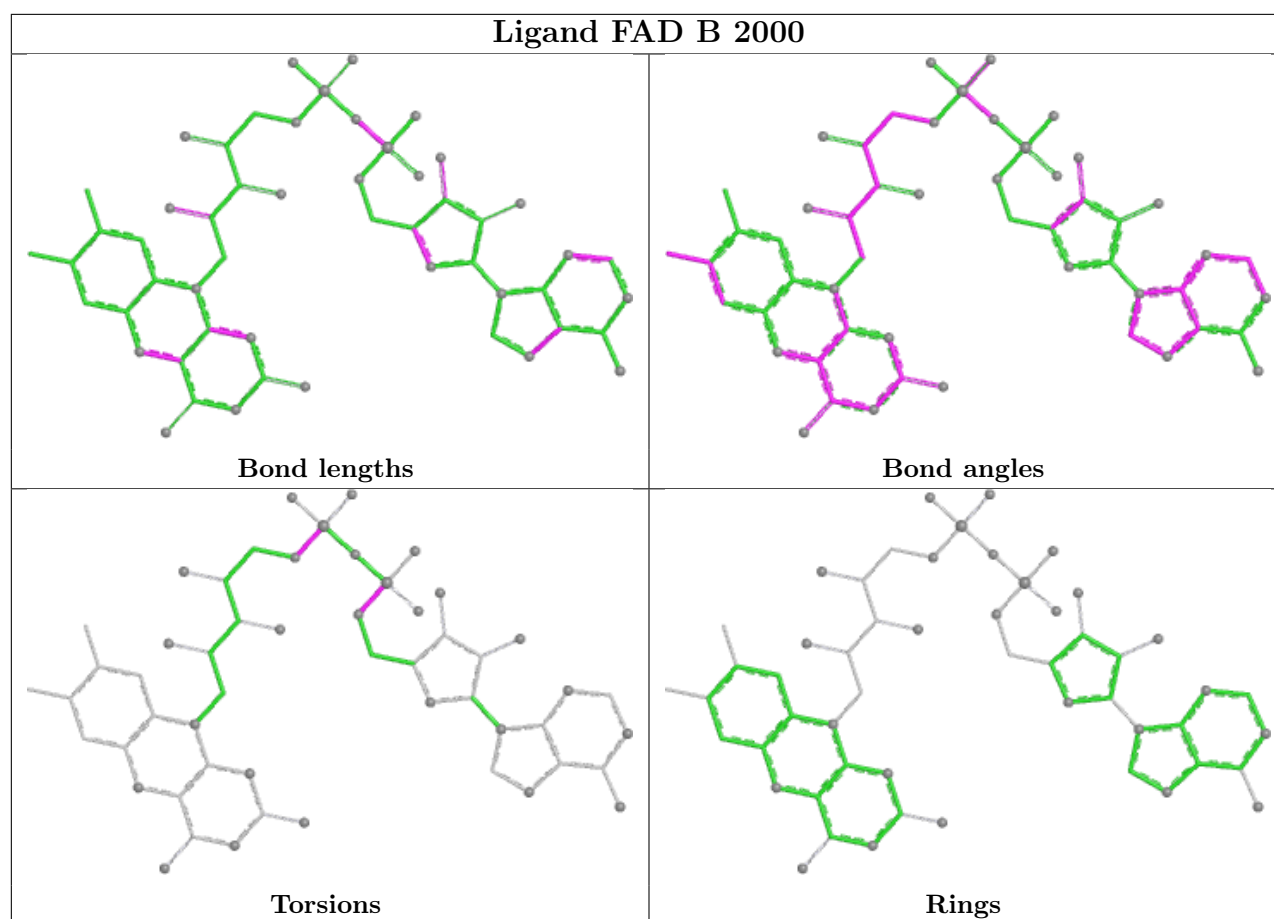
There are no ring outliers.

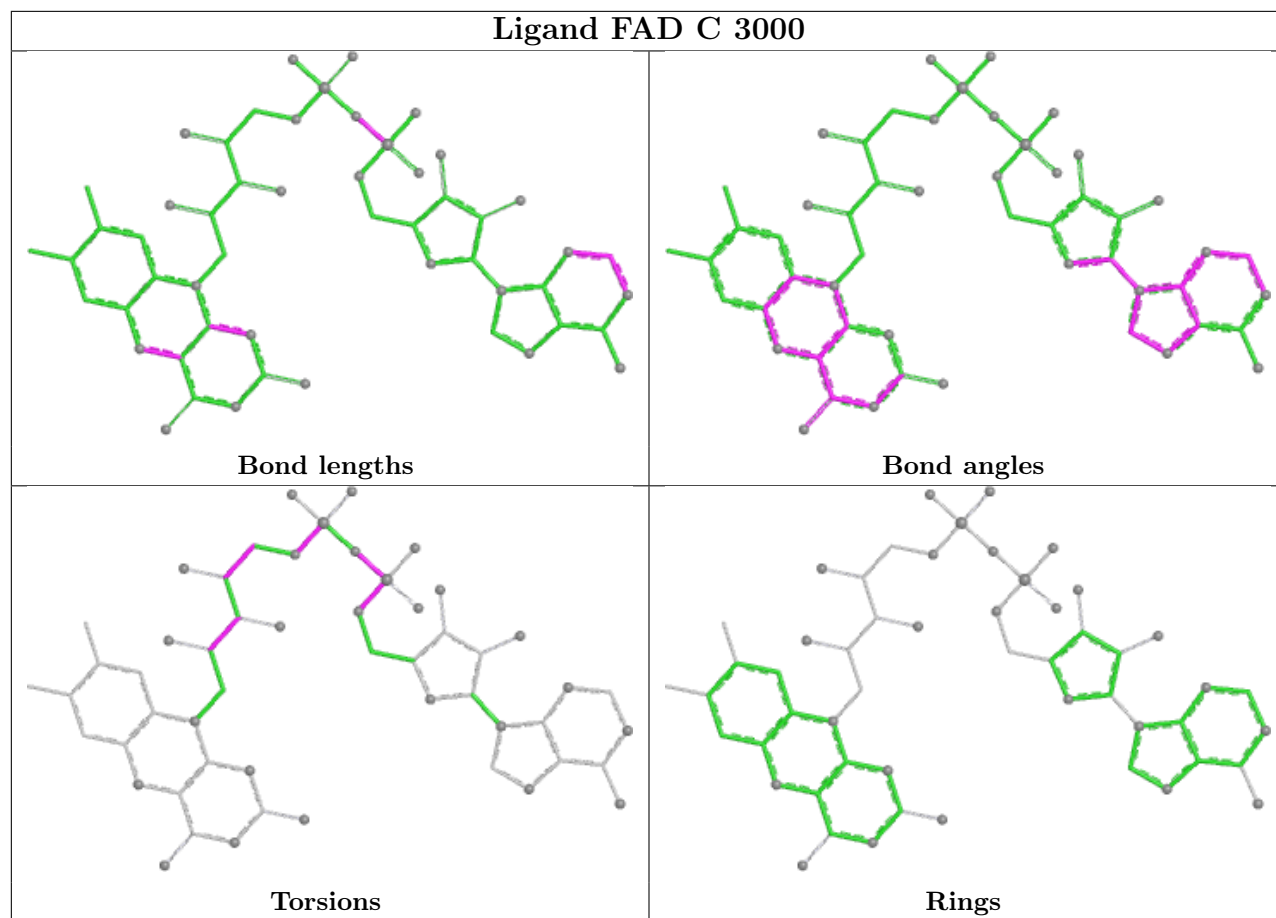
3 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1000	FAD	6	0
2	B	2000	FAD	5	0
2	C	3000	FAD	6	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	654/683 (95%)	0.75	63 (9%)	13	14	49, 67, 78, 91	0
1	B	656/683 (96%)	0.62	29 (4%)	39	38	53, 67, 78, 85	0
1	C	653/683 (95%)	0.59	42 (6%)	25	25	55, 70, 89, 112	0
All	All	1963/2049 (95%)	0.65	134 (6%)	23	23	49, 68, 81, 112	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	585	ALA	6.4
1	C	647	PHE	4.5
1	C	617	ILE	4.4
1	A	651	ILE	4.3
1	A	630	TYR	4.2
1	A	650	TYR	3.9
1	A	27	GLY	3.7
1	C	229	PHE	3.7
1	C	59	LYS	3.6
1	A	21	MET	3.5
1	A	617	ILE	3.5
1	A	238	ASP	3.5
1	C	186	ALA	3.4
1	A	625	VAL	3.4
1	A	633	ALA	3.4
1	A	648	HIS	3.4
1	A	309	VAL	3.4
1	B	224	ASP	3.2
1	A	126	ALA	3.2
1	A	626	TYR	3.2
1	C	334	LEU	3.1
1	B	161	GLU	3.1
1	C	29	ARG	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	585	ALA	3.0
1	A	423	TYR	3.0
1	A	498	CYS	3.0
1	A	646	GLY	3.0
1	A	306	TYR	3.0
1	C	24	VAL	3.0
1	A	629	LEU	2.9
1	A	431	GLN	2.9
1	A	643	ILE	2.9
1	A	601	VAL	2.9
1	A	644	ALA	2.9
1	B	643	ILE	2.9
1	A	634	TRP	2.9
1	A	623	GLY	2.9
1	A	639	ASN	2.8
1	A	348	GLY	2.8
1	A	647	PHE	2.8
1	B	238	ASP	2.8
1	C	4	VAL	2.8
1	A	225	ILE	2.8
1	A	401	GLY	2.8
1	A	464	LEU	2.8
1	C	643	ILE	2.7
1	C	97	ALA	2.7
1	A	503	SER	2.7
1	A	259	SER	2.7
1	C	282	VAL	2.7
1	B	14	ALA	2.6
1	C	271	ASP	2.6
1	C	325	ILE	2.6
1	C	234	TYR	2.6
1	B	324	VAL	2.6
1	B	658	GLN	2.6
1	C	25	TRP	2.6
1	B	584	LEU	2.6
1	A	640	LYS	2.6
1	B	425	GLY	2.6
1	B	155	PHE	2.6
1	C	126	ALA	2.5
1	A	446	GLY	2.5
1	A	632	ALA	2.5
1	B	27	GLY	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	627	PRO	2.5
1	A	618	LEU	2.5
1	C	655	LEU	2.5
1	A	234	TYR	2.5
1	B	226	GLY	2.5
1	C	422	THR	2.4
1	C	329	THR	2.4
1	C	243	SER	2.4
1	C	477	TRP	2.4
1	A	407	SER	2.4
1	A	195	ASP	2.4
1	C	653	PRO	2.4
1	C	619	GLY	2.4
1	B	229	PHE	2.4
1	A	54	THR	2.3
1	A	258	VAL	2.3
1	B	146	VAL	2.3
1	A	313	PHE	2.3
1	B	233	ALA	2.3
1	C	638	LEU	2.3
1	B	249	ILE	2.3
1	C	317	ASN	2.3
1	B	20	GLU	2.3
1	C	398	LEU	2.3
1	B	78	GLU	2.3
1	C	164	ILE	2.2
1	B	17	ASP	2.2
1	A	638	LEU	2.2
1	C	211	LEU	2.2
1	C	424	GLU	2.2
1	A	535	TYR	2.2
1	A	224	ASP	2.2
1	A	641	SER	2.2
1	C	141	GLY	2.2
1	A	162	PHE	2.2
1	A	609	TYR	2.2
1	C	535	TYR	2.2
1	C	275	GLN	2.2
1	B	149	LEU	2.2
1	C	314	GLY	2.2
1	B	376	CYS	2.1
1	B	427	ASN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	404	TYR	2.1
1	A	180	GLY	2.1
1	A	645	ASP	2.1
1	C	309	VAL	2.1
1	A	231	ASN	2.1
1	C	651	ILE	2.1
1	B	477	TRP	2.1
1	B	164	ILE	2.1
1	C	18	VAL	2.1
1	C	206	VAL	2.1
1	A	5	ASP	2.1
1	B	470	ASP	2.1
1	A	322	THR	2.1
1	A	232	GLY	2.1
1	A	25	TRP	2.0
1	C	280	THR	2.0
1	C	21	MET	2.0
1	A	140	LEU	2.0
1	A	405	LEU	2.0
1	C	158	GLN	2.0
1	A	399	CYS	2.0
1	B	289	VAL	2.0
1	C	471	VAL	2.0
1	A	229	PHE	2.0
1	A	435	ALA	2.0
1	B	26	ALA	2.0
1	B	175	TRP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

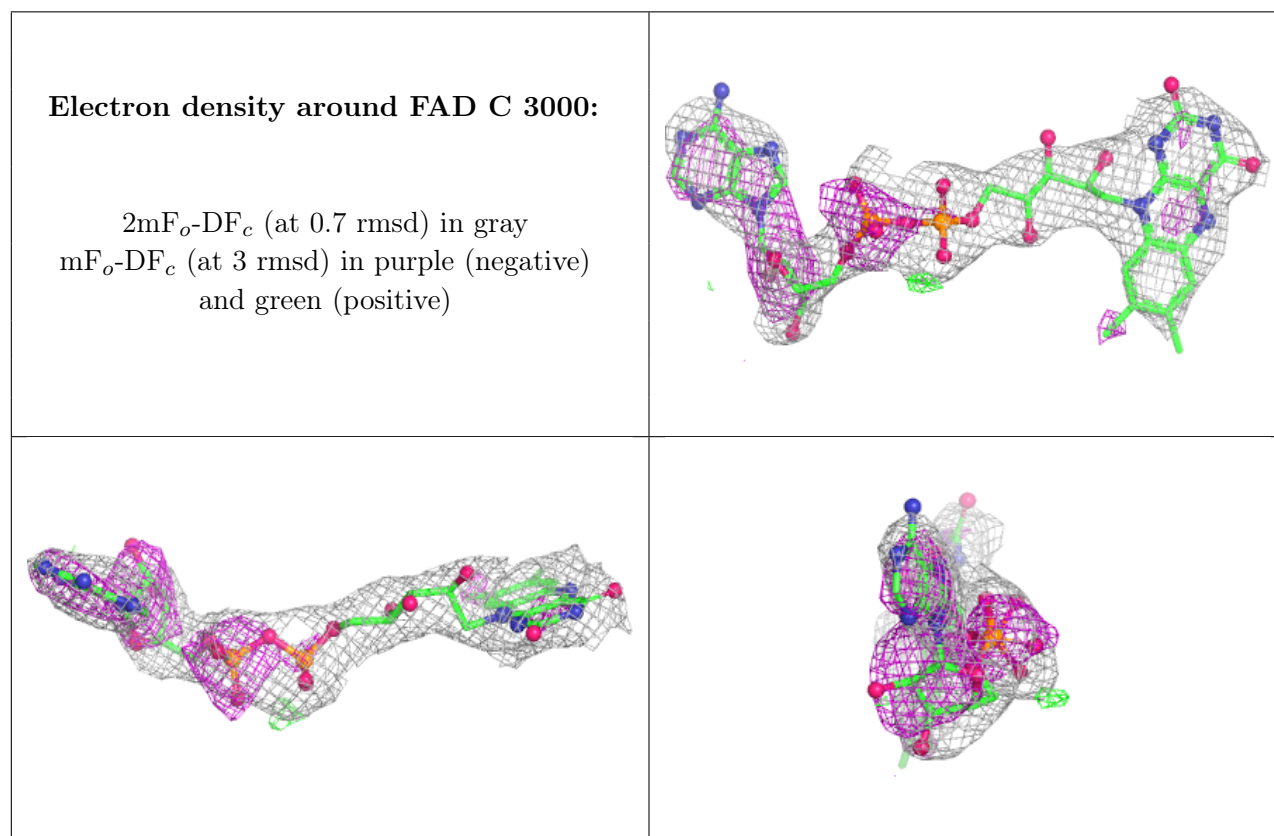
6.4 Ligands [i](#)

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.

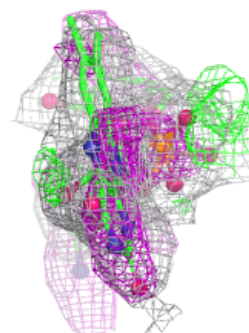
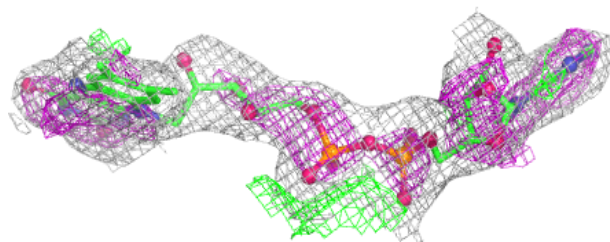
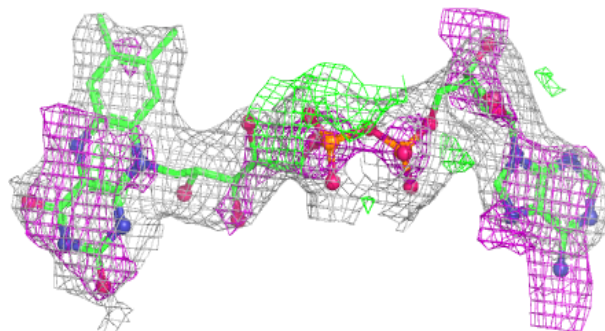
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FAD	C	3000	53/53	0.75	0.15	87,99,107,107	0
2	FAD	A	1000	53/53	0.86	0.13	43,55,59,63	0
2	FAD	B	2000	53/53	0.87	0.12	45,49,55,57	0

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.

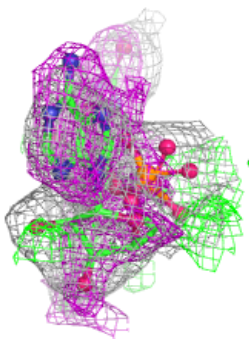
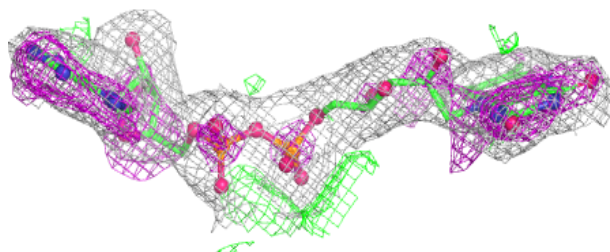
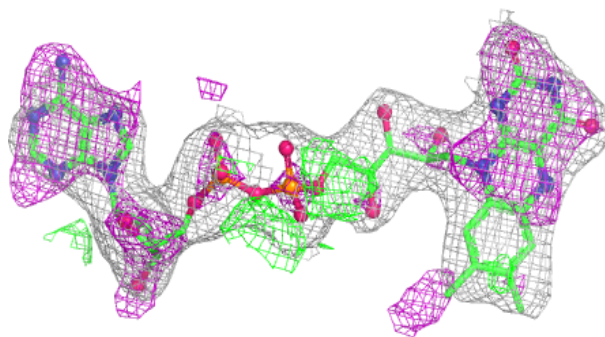


Electron density around FAD A 1000:

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

**Electron density around FAD B 2000:**

$2mF_o-DF_c$ (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.