



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:15 AM UTC

PDB ID : 2UUV / pdb_00002uuv
Title : alkylidihydroxyacetonephosphate synthase in P1
Authors : Razeto, A.; Mattioli, F.; Carpanelli, E.; Aliverti, A.; Pandini, V.; Coda, A.;
Mattevi, A.
Deposited on : 2007-03-07
Resolution : 1.99 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

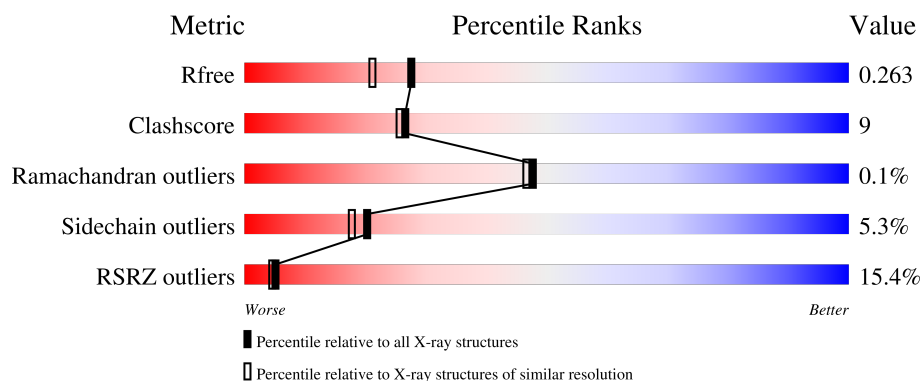
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	584	9% 75% 12% • 10%
1	B	584	10% 74% 13% • 10%
1	C	584	22% 62% 17% • • 16%
1	D	584	14% 74% 15% • 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PL3	D	1586	-	-	X	-

2 Entry composition [i](#)

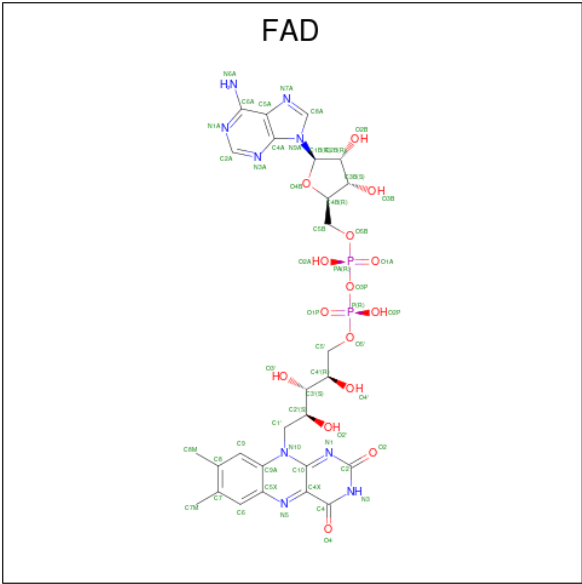
There are 4 unique types of molecules in this entry. The entry contains 17951 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	523	Total	C	N	O	S	0	1	0
			4200	2709	717	756	18			
1	B	523	Total	C	N	O	S	0	1	0
			4186	2695	718	755	18			
1	C	491	Total	C	N	O	S	0	2	0
			3947	2548	677	704	18			
1	D	528	Total	C	N	O	S	0	1	0
			4221	2722	719	762	18			

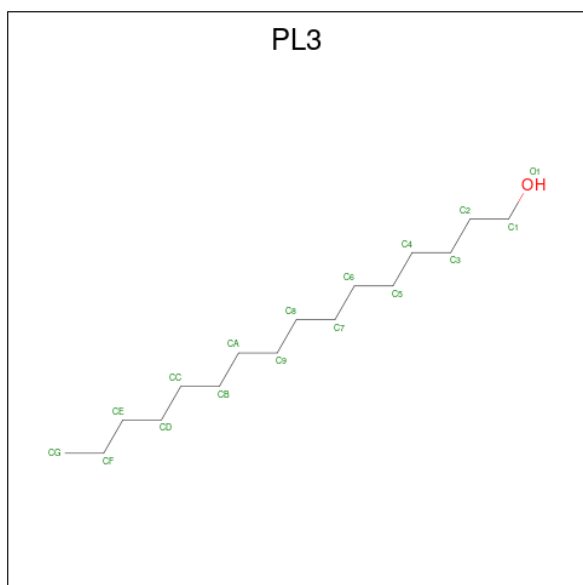
- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

- Molecule 3 is HEXADECAN-1-OL (CCD ID: PL3) (formula: C₁₆H₃₄O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			17	16	1		
3	B	1	Total	C	O	0	0
			17	16	1		
3	D	1	Total	C	O	0	0
			17	16	1		

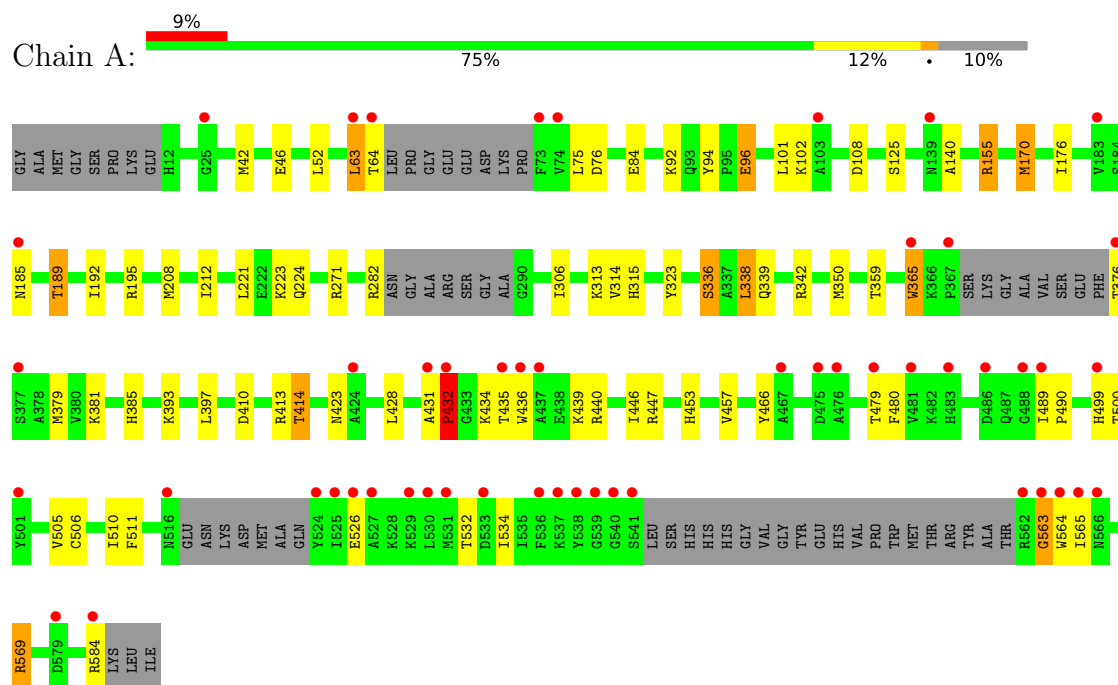
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	318	Total	O	0	0
			318	318		
4	B	265	Total	O	0	0
			265	265		
4	C	239	Total	O	0	0
			239	239		
4	D	312	Total	O	0	0
			312	312		

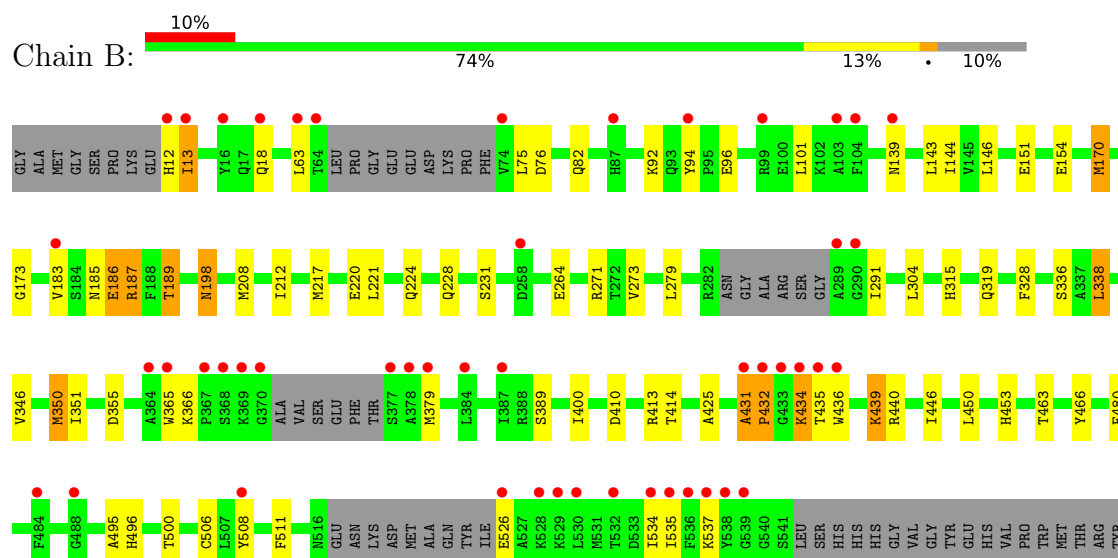
3 Residue-property plots

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: ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE

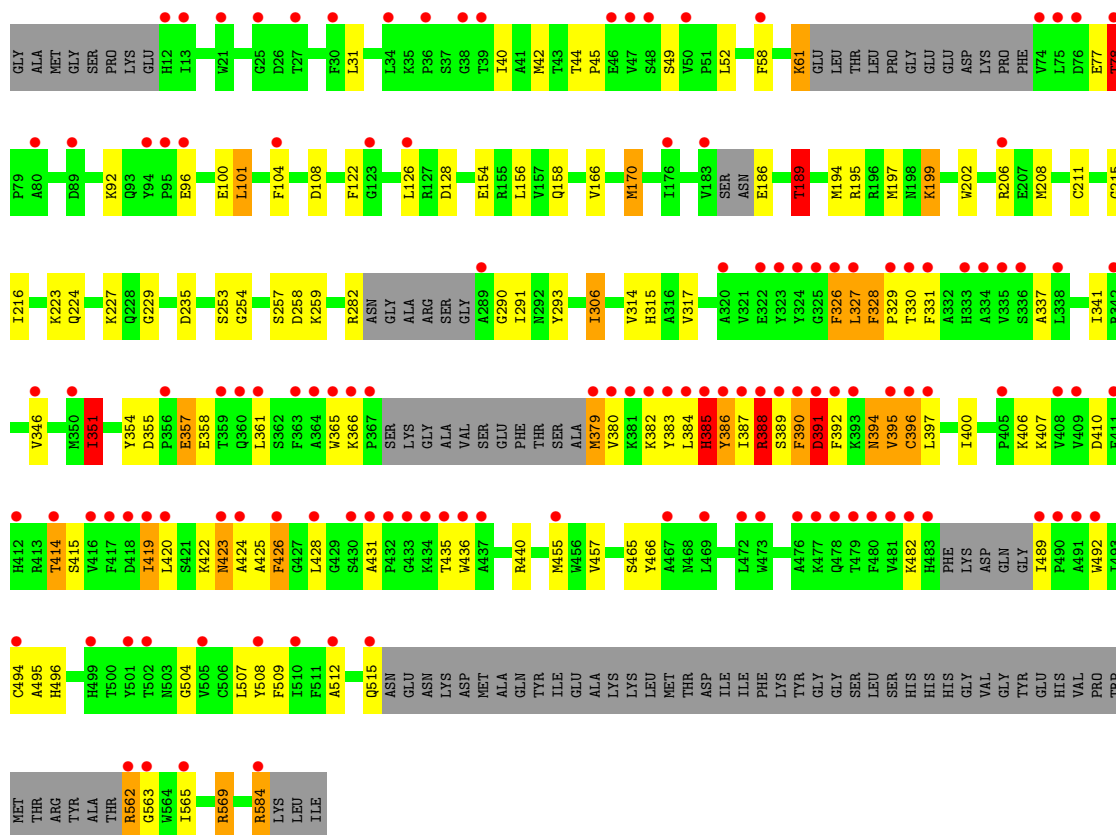


• Molecule 1: ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE

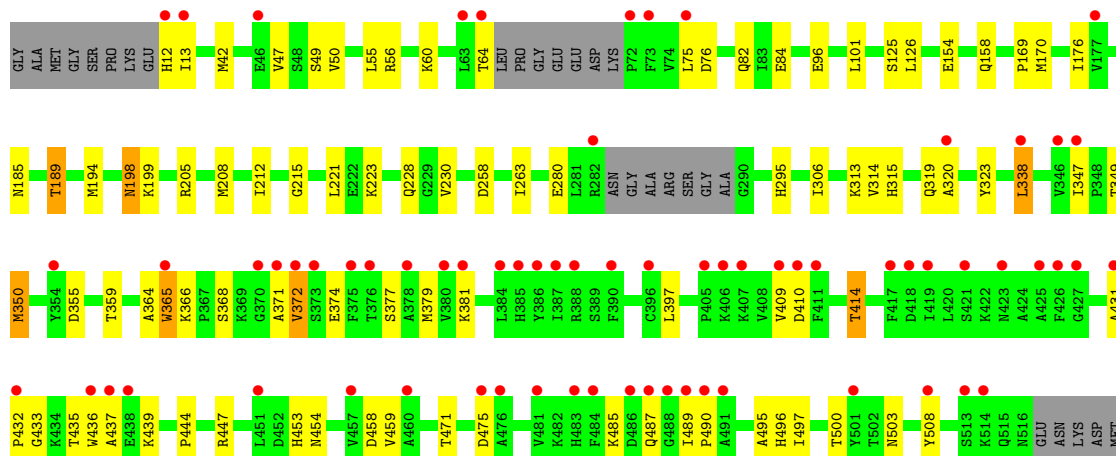
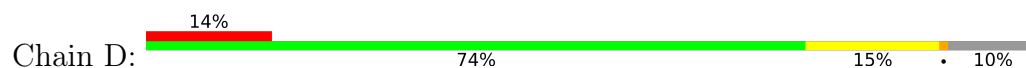


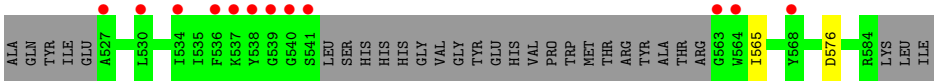


● Molecule 1: ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE



● Molecule 1: ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	77.80Å 98.00Å 107.00Å 114.00° 93.00° 103.00°	Depositor
Resolution (Å)	19.98 – 1.99 19.98 – 1.99	Depositor EDS
% Data completeness (in resolution range)	92.7 (19.98-1.99) 92.6 (19.98-1.99)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.38 (at 1.99Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.226 , 0.264 0.227 , 0.263	Depositor DCC
R_{free} test set	8878 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å ²)	24.9	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 58.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	17951	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% 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: PL3, 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	0.96	1/4308 (0.0%)	1.01	9/5833 (0.2%)
1	B	0.92	2/4292 (0.0%)	0.99	4/5809 (0.1%)
1	C	1.62	52/4051 (1.3%)	1.27	31/5485 (0.6%)
1	D	0.92	1/4331 (0.0%)	0.99	4/5865 (0.1%)
All	All	1.14	56/16982 (0.3%)	1.07	48/22992 (0.2%)

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
1	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	384	LEU	C-N	25.86	1.67	1.33
1	C	61	LYS	C-O	19.89	1.63	1.23
1	C	327	LEU	C-O	19.24	1.48	1.23
1	C	426	PHE	C-N	16.82	1.58	1.33
1	C	388	ARG	C-O	16.81	1.45	1.24
1	C	396	CYS	C-N	16.48	1.56	1.33
1	C	382	LYS	C-N	15.57	1.54	1.33
1	C	389	SER	C-N	15.29	1.53	1.33
1	C	387	ILE	CA-CB	14.20	1.72	1.54
1	C	388	ARG	CD-NE	13.82	1.65	1.46
1	C	385	HIS	CD2-NE2	13.71	1.52	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	78	THR	CB-OG1	13.41	1.65	1.43
1	C	61	LYS	CD-CE	13.06	1.91	1.52
1	C	390	PHE	C-O	-13.03	1.08	1.24
1	C	426	PHE	C-O	12.88	1.38	1.24
1	C	390	PHE	CG-CD1	12.45	1.65	1.38
1	C	391	ASP	CG-OD2	11.83	1.47	1.25
1	C	391	ASP	N-CA	-11.48	1.31	1.46
1	C	395	VAL	CB-CG1	10.83	1.88	1.52
1	C	422	LYS	C-N	9.87	1.47	1.33
1	C	395	VAL	CB-CG2	9.44	1.83	1.52
1	C	390	PHE	CA-CB	8.74	1.66	1.53
1	C	385	HIS	ND1-CE1	8.50	1.41	1.32
1	C	423	ASN	CG-OD1	8.45	1.39	1.23
1	C	385	HIS	CE1-NE2	8.42	1.41	1.32
1	C	327	LEU	CA-C	8.33	1.62	1.52
1	C	61	LYS	CG-CD	8.07	1.76	1.52
1	C	384	LEU	C-O	8.01	1.34	1.24
1	C	388	ARG	CZ-NH1	7.97	1.44	1.32
1	C	389	SER	CA-CB	7.87	1.65	1.53
1	C	390	PHE	CE1-CZ	7.59	1.61	1.38
1	C	327	LEU	C-N	7.33	1.44	1.33
1	C	391	ASP	CB-CG	7.17	1.70	1.52
1	C	394	ASN	CG-OD1	7.15	1.37	1.23
1	C	385	HIS	CG-ND1	7.02	1.46	1.38
1	C	387	ILE	CB-CG1	6.83	1.67	1.53
1	C	385	HIS	C-O	-6.58	1.16	1.24
1	B	434	LYS	C-O	6.02	1.32	1.24
1	A	63	LEU	CA-CB	6.01	1.57	1.53
1	C	326	PHE	C-N	5.98	1.41	1.33
1	C	389	SER	CA-C	5.94	1.60	1.52
1	C	387	ILE	C-O	5.91	1.31	1.24
1	C	391	ASP	CA-C	5.83	1.60	1.52
1	C	383	TYR	CG-CD2	5.77	1.51	1.39
1	C	392	PHE	N-CA	5.66	1.53	1.46
1	C	351	ILE	CA-CB	5.55	1.61	1.54
1	C	389	SER	N-CA	5.49	1.53	1.46
1	B	431	ALA	C-O	5.47	1.31	1.24
1	C	216	ILE	CA-CB	5.38	1.60	1.54
1	C	435	THR	CB-OG1	-5.20	1.35	1.43
1	C	415	SER	CB-OG	5.09	1.52	1.42
1	C	78	THR	CB-CG2	5.09	1.69	1.52
1	C	306	ILE	CA-CB	5.06	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	425	ALA	C-O	5.05	1.30	1.23
1	C	386	TYR	N-CA	5.04	1.52	1.46
1	D	263	ILE	CA-CB	5.02	1.60	1.54

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	389	SER	CA-C-N	-13.37	104.56	123.00
1	C	389	SER	C-N-CA	-13.37	104.56	123.00
1	C	385	HIS	CA-C-O	-13.25	106.89	120.80
1	C	389	SER	O-C-N	13.09	139.90	122.36
1	C	396	CYS	CA-C-O	10.79	132.15	120.71
1	C	61	LYS	CG-CD-CE	-9.85	88.65	111.30
1	C	61	LYS	CA-C-O	-8.11	107.01	120.80
1	C	423	ASN	OD1-CG-ND2	7.60	130.20	122.60
1	A	432	PRO	N-CA-C	-7.37	97.28	112.47
1	C	387	ILE	CA-CB-CG1	7.33	122.87	110.40
1	C	390	PHE	CA-C-O	-7.19	112.55	120.38
1	C	385	HIS	N-CA-C	-7.03	102.18	111.24
1	C	426	PHE	O-C-N	6.85	131.21	123.27
1	C	391	ASP	CA-CB-CG	-6.58	106.02	112.60
1	A	140	ALA	CA-C-N	-6.52	113.57	120.03
1	A	140	ALA	C-N-CA	-6.52	113.57	120.03
1	C	384	LEU	O-C-N	6.51	129.83	122.22
1	C	355	ASP	CA-C-N	-6.33	112.02	119.05
1	C	355	ASP	C-N-CA	-6.33	112.02	119.05
1	C	290	GLY	N-CA-C	-6.06	105.04	112.68
1	B	432	PRO	N-CA-C	-5.92	100.27	112.47
1	C	328	PHE	O-C-N	5.88	127.02	121.38
1	C	504	GLY	N-CA-C	5.76	118.35	110.69
1	C	385	HIS	CB-CG-ND1	-5.76	114.06	122.70
1	A	435	THR	N-CA-C	5.62	117.41	111.28
1	C	385	HIS	O-C-N	5.59	128.60	122.11
1	D	364	ALA	CA-C-N	-5.59	112.09	122.60
1	D	364	ALA	C-N-CA	-5.59	112.09	122.60
1	A	94	TYR	CA-C-N	5.41	125.06	119.05
1	A	94	TYR	C-N-CA	5.41	125.06	119.05
1	C	326	PHE	CA-CB-CG	-5.39	108.41	113.80
1	C	189	THR	N-CA-C	5.38	118.18	109.40
1	C	293	TYR	N-CA-C	5.37	117.88	111.71
1	D	576	ASP	CA-C-N	5.30	124.94	119.05
1	D	576	ASP	C-N-CA	5.30	124.94	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	388	ARG	NE-CZ-NH1	-5.25	116.25	121.50
1	A	52	LEU	CA-C-N	5.17	124.97	119.28
1	A	52	LEU	C-N-CA	5.17	124.97	119.28
1	B	566	ASN	N-CA-C	5.14	117.62	111.71
1	A	563	GLY	N-CA-C	-5.09	106.91	115.62
1	C	253	SER	CA-C-N	5.08	125.52	121.61
1	C	253	SER	C-N-CA	5.08	125.52	121.61
1	C	396	CYS	CA-C-N	-5.08	113.38	122.07
1	C	396	CYS	C-N-CA	-5.08	113.38	122.07
1	B	94	TYR	CA-C-N	5.03	124.47	119.24
1	B	94	TYR	C-N-CA	5.03	124.47	119.24
1	C	254	GLY	N-CA-C	-5.03	103.19	111.38
1	C	257	SER	N-CA-C	5.01	116.82	111.36

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	431	ALA	Peptide
1	B	431	ALA	Peptide
1	C	391	ASP	Sidechain

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	4200	0	4201	70	0
1	B	4186	0	4191	67	0
1	C	3947	0	3956	106	0
1	D	4221	0	4223	70	0
2	A	53	0	31	1	0
2	B	53	0	31	0	0
2	C	53	0	31	0	0
2	D	53	0	31	0	0
3	A	17	0	33	3	0
3	B	17	0	33	8	0
3	D	17	0	33	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	318	0	0	17	0
4	B	265	0	0	26	0
4	C	239	0	0	28	0
4	D	312	0	0	11	0
All	All	17951	0	16794	311	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 9.

All (311) 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:C:61:LYS:CG	1:C:61:LYS:CD	1.76	1.62
1:C:395:VAL:CB	1:C:395:VAL:CG2	1.83	1.56
1:C:61:LYS:CD	1:C:61:LYS:CE	1.91	1.49
1:C:395:VAL:CB	1:C:395:VAL:CG1	1.88	1.48
1:C:78:THR:OG1	1:C:78:THR:CB	1.65	1.40
1:A:506:CYS:SG	4:A:2280:HOH:O	1.91	1.26
1:C:390:PHE:C	1:C:391:ASP:N	2.03	1.15
1:B:224[B]:GLN:OE1	4:B:2129:HOH:O	1.59	1.15
1:A:365:TRP:HE1	1:A:446:ILE:CD1	1.64	1.09
1:A:365:TRP:HE1	1:A:446:ILE:HD11	1.16	1.09
1:A:365:TRP:NE1	1:A:446:ILE:HD11	1.70	1.05
1:B:224[B]:GLN:NE2	4:B:2127:HOH:O	1.87	1.05
1:D:126:LEU:H	3:D:1586:PL3:H3C2	1.17	1.03
1:C:584:ARG:HG3	1:C:584:ARG:HH11	1.24	1.01
1:C:330:THR:HB	4:C:2166:HOH:O	1.62	0.99
1:A:342:ARG:HD3	4:A:2223:HOH:O	1.62	0.99
1:D:125:SER:HB2	3:D:1586:PL3:H1C2	1.44	0.98
1:C:330:THR:HG21	4:C:2165:HOH:O	1.64	0.96
1:C:431:ALA:H	1:C:436:TRP:HE1	1.16	0.92
3:B:1586:PL3:H2C2	4:B:2244:HOH:O	1.73	0.87
1:A:410:ASP:O	1:A:414:THR:HG23	1.75	0.87
1:A:42:MET:HE2	1:A:365:TRP:HH2	1.40	0.86
1:B:338:LEU:HG	1:B:500:THR:HG21	1.58	0.85
1:A:338:LEU:HG	1:A:500:THR:HG21	1.57	0.84
1:C:385:HIS:O	1:C:388:ARG:HB2	1.78	0.83
1:D:366:LYS:HD2	1:D:372:VAL:O	1.78	0.83
1:C:61:LYS:CG	1:C:61:LYS:CE	2.57	0.82
1:B:139:ASN:HB3	4:B:2044:HOH:O	1.81	0.81
1:D:126:LEU:N	3:D:1586:PL3:H3C2	1.95	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:126:LEU:H	3:D:1586:PL3:C3	1.92	0.80
1:B:264:GLU:HG3	4:B:2063:HOH:O	1.81	0.80
1:D:410:ASP:O	1:D:414:THR:HG23	1.81	0.80
1:C:61:LYS:CD	1:C:61:LYS:CB	2.62	0.78
1:B:563:GLY:HA2	4:B:2250:HOH:O	1.83	0.78
1:A:563:GLY:HA2	4:A:2302:HOH:O	1.84	0.77
1:A:569:ARG:HH11	1:A:569:ARG:HB3	1.46	0.77
1:C:224:GLN:HG3	4:C:2083:HOH:O	1.85	0.77
1:D:338:LEU:HG	1:D:500:THR:HG21	1.67	0.77
1:A:125:SER:HA	3:A:1586:PL3:H1C1	1.67	0.76
1:D:323:TYR:CE1	1:D:433:GLY:HA2	2.21	0.76
1:C:92:LYS:HE3	4:C:2073:HOH:O	1.85	0.75
1:D:199:LYS:HG2	4:D:2081:HOH:O	1.86	0.75
1:A:208:MET:HE3	1:A:314:VAL:HG23	1.67	0.75
1:D:189:THR:HG21	4:D:2150:HOH:O	1.85	0.75
1:A:569:ARG:HH11	1:A:569:ARG:CB	2.00	0.74
1:C:258:ASP:HB2	4:C:2117:HOH:O	1.88	0.74
1:C:410:ASP:O	1:C:414:THR:HG23	1.88	0.73
1:A:410:ASP:O	1:A:414:THR:CG2	2.37	0.72
1:D:349:THR:O	4:D:2251:HOH:O	2.05	0.72
1:D:508:TYR:HB2	4:D:2284:HOH:O	1.90	0.71
1:C:224:GLN:OE1	1:C:227:LYS:HE2	1.90	0.71
1:C:395:VAL:CG1	1:C:395:VAL:CA	2.70	0.70
1:A:84:GLU:HB2	4:A:2042:HOH:O	1.91	0.69
1:A:379:MET:HA	1:A:379:MET:HE2	1.74	0.69
1:A:189:THR:HG21	4:A:2117:HOH:O	1.93	0.69
1:B:365:TRP:O	1:B:365:TRP:CD1	2.46	0.69
1:A:176:ILE:HG21	3:A:1586:PL3:H3C1	1.75	0.69
1:B:350:MET:HE3	4:B:2146:HOH:O	1.92	0.68
1:B:379:MET:SD	1:B:436:TRP:CZ2	2.86	0.68
1:C:351:ILE:HD12	1:C:400:ILE:HG12	1.75	0.68
1:A:393:LYS:HD2	4:A:2245:HOH:O	1.94	0.68
1:B:139:ASN:HB2	4:B:2099:HOH:O	1.95	0.67
1:D:377:SER:O	1:D:381:LYS:HG2	1.95	0.66
1:B:228:GLN:HG3	4:B:2131:HOH:O	1.94	0.66
1:B:439:LYS:HG2	4:B:2217:HOH:O	1.97	0.65
1:B:212:ILE:HD13	1:B:221:LEU:HD11	1.78	0.65
1:C:395:VAL:CG2	1:C:395:VAL:CA	2.72	0.65
1:B:365:TRP:CZ3	1:B:446:ILE:HD11	2.33	0.64
1:B:562:ARG:HD2	4:B:2251:HOH:O	1.97	0.64
1:B:537:LYS:HG3	1:B:537:LYS:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:426:PHE:N	4:C:2201:HOH:O	2.31	0.64
1:B:189:THR:HG21	4:B:2098:HOH:O	1.97	0.64
1:D:487:GLN:HE21	1:D:489:ILE:HD12	1.62	0.64
1:A:208:MET:HE2	1:A:315:HIS:HA	1.78	0.64
1:C:208:MET:HE2	1:C:315:HIS:HA	1.80	0.64
1:A:569:ARG:HB3	1:A:569:ARG:NH1	2.12	0.63
1:D:379:MET:HE1	1:D:431:ALA:HA	1.80	0.63
1:A:365:TRP:HE1	1:A:446:ILE:HD13	1.61	0.63
1:C:584:ARG:HH11	1:C:584:ARG:CG	2.08	0.63
1:A:42:MET:HE2	1:A:365:TRP:CH2	2.27	0.63
1:D:368:SER:HB2	1:D:377:SER:HA	1.80	0.63
1:A:92:LYS:HE3	1:A:185:ASN:O	1.99	0.62
1:B:220:GLU:HG3	1:B:224[B]:GLN:HE21	1.62	0.62
1:B:414:THR:HG22	4:B:2206:HOH:O	1.98	0.62
1:D:205:ARG:HH12	1:D:228:GLN:HB3	1.64	0.62
1:C:496:HIS:CE1	1:C:508:TYR:CD1	2.88	0.62
1:A:499:HIS:CE1	4:A:2163:HOH:O	2.53	0.62
1:C:328:PHE:CD1	4:C:2200:HOH:O	2.51	0.62
1:C:104:PHE:HB3	4:C:2032:HOH:O	1.99	0.61
1:C:78:THR:CB	1:C:78:THR:HG1	2.08	0.61
1:A:192:ILE:HD12	1:A:306:ILE:HD11	1.81	0.61
1:D:60:LYS:O	1:D:64:THR:HG23	2.00	0.61
1:B:365:TRP:CZ3	1:B:446:ILE:CD1	2.84	0.61
1:D:50:VAL:HG11	1:D:372:VAL:HB	1.83	0.61
1:B:63:LEU:CD1	3:B:1586:PL3:HGC1	2.31	0.60
1:A:510:ILE:HG21	3:A:1586:PL3:HAC1	1.84	0.60
1:C:584:ARG:HG3	1:C:584:ARG:NH1	2.04	0.60
1:B:92:LYS:HE3	1:B:185:ASN:O	2.00	0.60
1:C:61:LYS:CD	1:C:61:LYS:NZ	2.65	0.60
1:B:463:THR:HG22	4:B:2237:HOH:O	2.01	0.60
1:C:330:THR:HG22	1:C:331:PHE:H	1.66	0.59
1:C:208:MET:HE3	1:C:314:VAL:HG23	1.84	0.59
1:B:63:LEU:HD11	3:B:1586:PL3:CG	2.32	0.58
1:B:365:TRP:O	1:B:365:TRP:HD1	1.86	0.58
1:B:410:ASP:O	1:B:414:THR:HG23	2.03	0.58
1:B:63:LEU:HD11	3:B:1586:PL3:HGC1	1.85	0.58
1:B:63:LEU:CD1	3:B:1586:PL3:CG	2.81	0.58
1:D:447:ARG:NH1	3:D:1586:PL3:H5C2	2.19	0.58
1:A:212:ILE:HD13	1:A:221:LEU:HD11	1.86	0.57
1:A:192:ILE:HD12	1:A:306:ILE:CD1	2.34	0.57
1:A:365:TRP:NE1	1:A:446:ILE:CD1	2.42	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:431:ALA:N	1:C:436:TRP:HE1	1.95	0.56
1:C:327:LEU:HD21	1:C:428:LEU:HD11	1.87	0.56
1:D:82:GLN:HB3	1:D:84:GLU:OE2	2.05	0.56
1:C:431:ALA:H	1:C:436:TRP:NE1	1.97	0.56
1:B:351:ILE:HD12	1:B:400:ILE:HG12	1.88	0.56
1:C:96:GLU:OE1	1:C:96:GLU:N	2.33	0.56
1:B:466:TYR:OH	4:B:2231:HOH:O	2.18	0.56
1:C:126:LEU:HB2	4:C:2209:HOH:O	2.06	0.56
1:B:198:ASN:H	1:B:198:ASN:HD22	1.54	0.55
1:C:391:ASP:O	1:C:395:VAL:HG23	2.05	0.55
1:D:439:LYS:HD2	4:D:2261:HOH:O	2.07	0.55
1:C:395:VAL:CG2	1:C:395:VAL:CG1	2.85	0.55
1:A:208:MET:O	1:A:313:LYS:HE2	2.07	0.54
1:A:170:MET:HE2	1:A:195:ARG:NH2	2.23	0.54
1:D:458:ASP:OD2	3:D:1586:PL3:H2C1	2.07	0.54
1:B:562:ARG:HG2	4:B:2254:HOH:O	2.06	0.54
1:D:12:HIS:CE1	4:D:2001:HOH:O	2.61	0.54
1:B:220:GLU:HG3	1:B:224[B]:GLN:NE2	2.23	0.53
1:B:82:GLN:HG2	4:B:2041:HOH:O	2.09	0.53
1:B:562:ARG:HB2	4:B:2249:HOH:O	2.08	0.53
1:D:56:ARG:HB2	4:D:2051:HOH:O	2.09	0.53
1:C:419:ILE:O	1:C:423:ASN:ND2	2.42	0.53
1:D:379:MET:CE	1:D:431:ALA:HA	2.39	0.53
1:C:58:PHE:HZ	4:C:2177:HOH:O	1.90	0.52
1:D:198:ASN:H	1:D:198:ASN:HD22	1.55	0.52
1:D:350:MET:HB3	1:D:436:TRP:CH2	2.44	0.52
1:A:155:ARG:O	1:A:155:ARG:HD3	2.10	0.52
1:C:330:THR:HG23	1:C:394:ASN:HB3	1.92	0.52
1:B:450:LEU:HD11	3:B:1586:PL3:HCC1	1.91	0.52
1:C:259:LYS:N	4:C:2117:HOH:O	2.43	0.52
1:C:166:VAL:HB	1:C:189:THR:HB	1.91	0.51
1:D:208:MET:HE2	1:D:315:HIS:HA	1.92	0.51
1:D:319:GLN:OE1	1:D:319:GLN:HA	2.08	0.51
1:D:176:ILE:HG21	3:D:1586:PL3:H5C1	1.92	0.51
1:A:479:THR:HG21	1:A:534:ILE:HD11	1.92	0.51
1:C:329:PRO:HD3	4:C:2200:HOH:O	2.10	0.51
1:B:496:HIS:CE1	1:B:508:TYR:CD1	2.99	0.51
1:C:194:MET:HE3	1:C:197[B]:MET:HE3	1.92	0.51
1:A:76:ASP:O	1:A:453:HIS:HA	2.11	0.50
1:B:271:ARG:HD2	4:B:2178:HOH:O	2.10	0.50
1:A:155:ARG:HD3	1:A:155:ARG:C	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:GLN:HG3	4:C:2099:HOH:O	2.11	0.50
1:A:379:MET:HE2	1:A:379:MET:CA	2.41	0.50
1:C:223:LYS:HE3	1:C:224:GLN:NE2	2.26	0.50
1:C:326:PHE:HB3	4:C:2201:HOH:O	2.10	0.50
1:C:327:LEU:HB3	1:C:395:VAL:CG1	2.42	0.50
1:A:385:HIS:HE1	4:C:2159:HOH:O	1.94	0.50
1:B:143:LEU:C	1:B:144:ILE:HD12	2.37	0.50
1:B:410:ASP:OD1	1:B:413:ARG:NH2	2.45	0.50
1:C:563:GLY:HA2	4:C:2224:HOH:O	2.12	0.49
1:B:146:LEU:HD23	4:B:2107:HOH:O	2.11	0.49
1:B:379:MET:SD	1:B:436:TRP:HZ2	2.35	0.49
1:D:379:MET:HE1	1:D:432:PRO:HD2	1.94	0.49
1:B:537:LYS:O	1:B:537:LYS:CG	2.60	0.49
1:C:455:MET:N	1:C:515:GLN:HE21	2.09	0.49
1:C:328:PHE:HA	4:C:2200:HOH:O	2.11	0.49
1:A:223:LYS:NZ	1:A:224[B]:GLN:NE2	2.61	0.49
1:D:84:GLU:H	1:D:84:GLU:CD	2.21	0.49
1:C:52:LEU:O	4:C:2015:HOH:O	2.20	0.48
1:C:457:VAL:HG23	1:C:512:ALA:HB2	1.94	0.48
1:A:379:MET:HE1	1:A:428:LEU:O	2.13	0.48
1:C:354:TYR:HD1	1:C:358:GLU:HG2	1.77	0.48
1:C:108:ASP:HA	4:C:2037:HOH:O	2.13	0.48
1:D:55:LEU:HD13	1:D:365:TRP:HB2	1.95	0.48
1:B:562:ARG:CG	4:B:2254:HOH:O	2.60	0.48
1:C:357:GLU:HB2	1:C:494:CYS:HB3	1.95	0.48
1:A:499:HIS:HB2	1:A:506:CYS:HB3	1.96	0.48
1:B:154:GLU:HA	1:B:273:VAL:HG11	1.96	0.48
1:B:506:CYS:HB2	4:B:2237:HOH:O	2.12	0.48
1:D:350:MET:HB3	1:D:436:TRP:CZ2	2.49	0.48
1:D:359:THR:HG23	1:D:397:LEU:HB2	1.96	0.47
1:C:337:ALA:O	1:C:341:ILE:HG13	2.15	0.47
1:A:379:MET:SD	1:A:436:TRP:CZ2	3.07	0.47
1:C:354:TYR:CD1	1:C:358:GLU:HG2	2.50	0.47
1:C:361:LEU:HB2	4:C:2177:HOH:O	2.14	0.47
1:D:320:ALA:HB3	1:D:409:VAL:HG21	1.97	0.47
1:B:12:HIS:N	4:B:2001:HOH:O	2.48	0.47
1:B:228:GLN:CG	4:B:2131:HOH:O	2.60	0.47
1:C:194:MET:HE3	1:C:197[B]:MET:CE	2.45	0.47
1:D:212:ILE:HD13	1:D:221:LEU:HD11	1.96	0.47
1:D:154:GLU:O	1:D:158:GLN:HG3	2.15	0.47
1:D:208:MET:HE3	1:D:314:VAL:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:323:TYR:HE2	1:D:350:MET:SD	2.38	0.47
1:C:330:THR:HG22	1:C:331:PHE:N	2.28	0.47
1:C:386:TYR:HE2	4:C:2063:HOH:O	1.98	0.46
1:B:328:PHE:CE1	1:B:425:ALA:HB2	2.50	0.46
1:C:101:LEU:HD11	1:C:156:LEU:HD13	1.98	0.46
1:C:31:LEU:HG	1:C:42:MET:CE	2.46	0.46
1:C:379:MET:HE2	1:C:436:TRP:CZ3	2.49	0.46
1:A:92:LYS:CE	1:A:185:ASN:O	2.63	0.46
1:B:76:ASP:O	1:B:453:HIS:HA	2.15	0.46
1:C:366:LYS:HD3	1:C:380:VAL:HG11	1.97	0.46
1:D:374:GLU:OE2	1:D:439:LYS:HA	2.15	0.46
1:A:359:THR:HG23	1:A:397:LEU:HB2	1.98	0.46
1:C:569:ARG:HA	4:C:2228:HOH:O	2.16	0.46
1:A:208:MET:HE2	1:A:315:HIS:CA	2.46	0.46
2:A:1585:FAD:HM71	2:A:1585:FAD:HM83	1.79	0.46
1:C:282:ARG:C	4:C:2143:HOH:O	2.59	0.46
1:A:223:LYS:HZ2	1:A:224[B]:GLN:NE2	2.13	0.45
1:A:271:ARG:HD2	4:A:2198:HOH:O	2.17	0.45
1:C:31:LEU:HG	1:C:42:MET:HE2	1.98	0.45
1:C:154:GLU:O	1:C:158:GLN:HG3	2.16	0.45
1:C:354:TYR:O	1:C:396:CYS:HB3	2.16	0.45
1:B:480:PHE:CZ	1:B:511:PHE:HB2	2.52	0.45
1:D:169:PRO:HG3	1:D:306:ILE:HD12	1.99	0.45
1:D:444:PRO:HA	3:D:1586:PL3:HAC1	1.98	0.45
1:C:202:TRP:CE2	1:C:211:CYS:HB2	2.52	0.45
1:C:208:MET:HE1	1:C:315:HIS:C	2.42	0.45
1:D:12:HIS:HE1	4:D:2001:HOH:O	1.99	0.45
1:B:151:GLU:CD	1:B:151:GLU:H	2.25	0.45
1:A:339:GLN:HG3	1:A:466:TYR:CZ	2.51	0.44
1:A:499:HIS:HE1	4:A:2163:HOH:O	1.95	0.44
1:B:231:SER:HB3	1:B:315:HIS:CE1	2.52	0.44
1:C:31:LEU:CD2	1:C:42:MET:HE2	2.47	0.44
1:C:357:GLU:N	1:C:357:GLU:CD	2.75	0.44
1:D:76:ASP:HB2	1:D:454:ASN:HB2	2.00	0.44
1:C:194:MET:CE	1:C:197[B]:MET:HE1	2.47	0.44
1:B:63:LEU:CD1	3:B:1586:PL3:HGC2	2.47	0.44
1:D:459:VAL:CG2	3:D:1586:PL3:H6C1	2.48	0.44
1:A:564:TRP:CH2	1:B:279:LEU:HD13	2.53	0.44
1:C:194:MET:O	1:C:215:GLY:HA3	2.17	0.44
1:C:492:TRP:HZ2	4:C:2177:HOH:O	2.01	0.44
1:A:96:GLU:CD	1:A:96:GLU:H	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:258:ASP:HB2	4:D:2251:HOH:O	2.17	0.44
1:C:326:PHE:HD2	1:C:400:ILE:HD12	1.83	0.43
1:C:327:LEU:HB3	1:C:395:VAL:HG12	2.00	0.43
1:A:439:LYS:HE3	4:A:2268:HOH:O	2.19	0.43
1:D:496:HIS:CE1	1:D:508:TYR:CD1	3.06	0.43
1:C:365:TRP:NE1	4:C:2178:HOH:O	2.51	0.43
1:A:480:PHE:CZ	1:A:511:PHE:HB2	2.53	0.43
1:B:212:ILE:HD13	1:B:221:LEU:CD1	2.48	0.43
1:D:205:ARG:NH1	1:D:228:GLN:HB3	2.30	0.43
1:C:44:THR:HB	1:C:45:PRO:HD2	2.01	0.43
1:C:122:PHE:HB3	1:C:128:ASP:HB3	2.01	0.43
1:A:223:LYS:NZ	1:A:224[B]:GLN:HE21	2.16	0.43
1:A:315:HIS:HB3	4:A:2204:HOH:O	2.19	0.43
1:B:170:MET:HE3	1:B:173:GLY:N	2.34	0.43
1:D:435:THR:O	1:D:439:LYS:HD3	2.19	0.43
1:A:108:ASP:HB2	4:A:2126:HOH:O	2.18	0.43
1:B:186:GLU:CD	1:B:187:ARG:HD2	2.43	0.43
1:C:562:ARG:N	1:D:280:GLU:H	2.16	0.43
1:C:379:MET:HB2	1:C:428:LEU:HB3	2.00	0.43
1:A:432:PRO:O	1:A:432:PRO:CD	2.66	0.42
1:B:63:LEU:HD12	3:B:1586:PL3:HGC2	2.01	0.42
1:B:198:ASN:HD22	1:B:198:ASN:N	2.15	0.42
1:D:323:TYR:CD1	1:D:433:GLY:HA2	2.54	0.42
1:D:447:ARG:HH12	3:D:1586:PL3:H5C2	1.83	0.42
1:C:199:LYS:HD2	4:C:2081:HOH:O	2.20	0.42
1:D:350:MET:HG2	1:D:436:TRP:CE2	2.53	0.42
1:A:489:ILE:HB	4:A:2288:HOH:O	2.19	0.42
1:A:432:PRO:O	1:A:432:PRO:HD2	2.18	0.42
1:A:500:THR:HG22	1:A:505:VAL:HG12	2.01	0.42
1:C:235:ASP:CG	1:C:440:ARG:HH22	2.27	0.42
4:A:2242:HOH:O	1:C:282:ARG:HD2	2.20	0.42
1:D:208:MET:HE1	1:D:230:VAL:HG12	2.02	0.42
1:B:208:MET:HE2	1:B:315:HIS:HA	2.01	0.42
1:B:13:ILE:HG22	1:B:18:GLN:HG3	2.02	0.42
1:B:186:GLU:OE1	1:B:187:ARG:HD2	2.19	0.42
1:C:170:MET:HE2	1:C:195:ARG:NH2	2.35	0.42
1:C:291[A]:ILE:HG23	1:D:295:HIS:O	2.20	0.42
1:C:495:ALA:HA	1:C:508:TYR:O	2.20	0.42
1:A:376:THR:HG21	4:A:2037:HOH:O	2.20	0.41
1:A:379:MET:CE	4:A:2262:HOH:O	2.67	0.41
1:D:205:ARG:NH1	1:D:228:GLN:O	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:ILE:HD12	4:A:2288:HOH:O	2.20	0.41
1:C:78:THR:OG1	1:C:78:THR:CG2	2.60	0.41
1:C:229:GLY:C	1:C:317:VAL:HG23	2.45	0.41
1:C:326:PHE:CD2	1:C:400:ILE:HD12	2.54	0.41
1:C:326:PHE:CE2	1:C:420:LEU:HD13	2.55	0.41
1:C:326:PHE:O	1:C:397:LEU:HD12	2.20	0.41
1:D:76:ASP:O	1:D:453:HIS:HA	2.20	0.41
1:D:489:ILE:HA	1:D:490:PRO:HD3	1.94	0.41
1:A:323:TYR:CE1	1:A:434:LYS:HG2	2.56	0.41
1:A:379:MET:SD	1:A:436:TRP:HZ2	2.43	0.41
1:B:365:TRP:CZ3	1:B:446:ILE:HG12	2.56	0.41
1:C:194:MET:CE	1:C:197[B]:MET:CE	2.98	0.41
1:C:424:ALA:C	4:C:2200:HOH:O	2.62	0.41
1:C:507:LEU:HD21	1:C:509:PHE:CZ	2.55	0.41
1:D:47:VAL:HG21	1:D:371:ALA:CB	2.50	0.41
1:D:223:LYS:HD3	4:D:2171:HOH:O	2.20	0.41
1:A:282:ARG:HD2	4:B:2252:HOH:O	2.20	0.41
1:A:410:ASP:OD1	1:A:413:ARG:NH2	2.51	0.41
1:B:495:ALA:HA	1:B:508:TYR:O	2.20	0.41
1:D:495:ALA:HA	1:D:508:TYR:O	2.20	0.41
1:C:407:LYS:HG3	4:C:2164:HOH:O	2.19	0.41
1:D:125:SER:HA	3:D:1586:PL3:H3C1	2.02	0.41
1:D:471:THR:O	1:D:475:ASP:HB2	2.19	0.41
1:C:40:ILE:HG22	1:C:52:LEU:HD12	2.02	0.41
1:C:208:MET:CE	1:C:315:HIS:CA	2.99	0.41
1:D:487:GLN:NE2	1:D:489:ILE:HD12	2.32	0.41
1:B:187:ARG:NH2	1:B:578:LYS:O	2.54	0.40
1:B:304:LEU:HA	4:B:2176:HOH:O	2.20	0.40
1:D:194:MET:O	1:D:215:GLY:HA3	2.21	0.40
1:C:206:ARG:O	1:D:503:ASN:HB2	2.21	0.40
1:D:338:LEU:HD21	1:D:497:ILE:HG21	2.02	0.40
1:A:336:SER:HB3	1:A:423:ASN:OD1	2.21	0.40
1:A:447:ARG:HG3	1:A:457:VAL:CG1	2.51	0.40
1:D:185:ASN:ND2	4:D:2153:HOH:O	2.51	0.40
1:A:63:LEU:HA	1:A:490:PRO:HB3	2.02	0.40
1:C:465:SER:O	1:C:466:TYR:C	2.65	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	512/584 (88%)	503 (98%)	8 (2%)	1 (0%)	43	42
1	B	512/584 (88%)	502 (98%)	9 (2%)	1 (0%)	43	42
1	C	477/584 (82%)	462 (97%)	15 (3%)	0	100	100
1	D	519/584 (89%)	511 (98%)	7 (1%)	1 (0%)	43	42
All	All	2020/2336 (86%)	1978 (98%)	39 (2%)	3 (0%)	48	46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	437	ALA
1	A	432	PRO
1	B	432	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	460/507 (91%)	439 (95%)	21 (5%)	24	22
1	B	458/507 (90%)	427 (93%)	31 (7%)	14	11
1	C	433/507 (85%)	408 (94%)	25 (6%)	18	15
1	D	463/507 (91%)	444 (96%)	19 (4%)	27	26
All	All	1814/2028 (89%)	1718 (95%)	96 (5%)	20	18

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	GLU
1	A	64	THR
1	A	75	LEU
1	A	96	GLU
1	A	101	LEU
1	A	102	LYS
1	A	155	ARG
1	A	170	MET
1	A	189	THR
1	A	336	SER
1	A	338	LEU
1	A	350	MET
1	A	365	TRP
1	A	381	LYS
1	A	414	THR
1	A	440	ARG
1	A	526	GLU
1	A	532	THR
1	A	565	ILE
1	A	569	ARG
1	A	584	ARG
1	B	13	ILE
1	B	75	LEU
1	B	96	GLU
1	B	101	LEU
1	B	170	MET
1	B	183	VAL
1	B	186	GLU
1	B	187	ARG
1	B	189	THR
1	B	198	ASN
1	B	217	MET
1	B	291	ILE
1	B	319	GLN
1	B	336	SER
1	B	338	LEU
1	B	346	VAL
1	B	350	MET
1	B	355	ASP
1	B	366	LYS
1	B	389	SER
1	B	434	LYS
1	B	435	THR

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Mol	Chain	Res	Type
1	B	439	LYS
1	B	440	ARG
1	B	526	GLU
1	B	534	ILE
1	B	535	ILE
1	B	565	ILE
1	B	569	ARG
1	B	570	SER
1	B	584	ARG
1	C	49	SER
1	C	77	GLU
1	C	78	THR
1	C	100	GLU
1	C	101	LEU
1	C	170	MET
1	C	186	GLU
1	C	189	THR
1	C	199	LYS
1	C	306	ILE
1	C	346	VAL
1	C	351	ILE
1	C	357	GLU
1	C	379	MET
1	C	385	HIS
1	C	388	ARG
1	C	406	LYS
1	C	414	THR
1	C	419	ILE
1	C	482	LYS
1	C	489	ILE
1	C	562	ARG
1	C	565	ILE
1	C	569	ARG
1	C	584	ARG
1	D	13	ILE
1	D	42	MET
1	D	49	SER
1	D	75	LEU
1	D	96	GLU
1	D	101	LEU
1	D	170	MET
1	D	189	THR

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Mol	Chain	Res	Type
1	D	198	ASN
1	D	313	LYS
1	D	338	LEU
1	D	347	ILE
1	D	350	MET
1	D	355	ASP
1	D	365	TRP
1	D	372	VAL
1	D	414	THR
1	D	485	LYS
1	D	565	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	185	ASN
1	A	256	GLN
1	B	198	ASN
1	B	226	HIS
1	B	256	GLN
1	B	315	HIS
1	B	394	ASN
1	B	453	HIS
1	B	496	HIS
1	B	566	ASN
1	C	82	GLN
1	C	85	ASN
1	C	93	GLN
1	C	255	HIS
1	C	315	HIS
1	C	319	GLN
1	C	340	GLN
1	C	360	GLN
1	C	423	ASN
1	C	470	GLN
1	C	478	GLN
1	C	483	HIS
1	C	499	HIS
1	C	515	GLN
1	D	12	HIS
1	D	82	GLN

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Mol	Chain	Res	Type
1	D	198	ASN
1	D	256	GLN
1	D	315	HIS
1	D	412	HIS
1	D	468	ASN
1	D	487	GLN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

7 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	C	1585	-	58,58,58	1.30	5 (8%)	85,89,89	1.50	12 (14%)
2	FAD	B	1585	-	58,58,58	1.34	7 (12%)	85,89,89	1.70	18 (21%)
3	PL3	D	1586	-	16,16,16	1.00	1 (6%)	15,15,15	0.77	1 (6%)
2	FAD	D	1585	-	58,58,58	1.28	5 (8%)	85,89,89	1.71	13 (15%)
3	PL3	A	1586	-	16,16,16	0.88	1 (6%)	15,15,15	0.85	1 (6%)
3	PL3	B	1586	-	16,16,16	0.94	1 (6%)	15,15,15	0.71	0
2	FAD	A	1585	-	58,58,58	1.35	6 (10%)	85,89,89	1.69	21 (24%)

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	C	1585	-	-	3/34/50/50	0/6/6/6
2	FAD	B	1585	-	-	2/34/50/50	0/6/6/6
3	PL3	D	1586	-	-	4/14/14/14	-
2	FAD	D	1585	-	-	2/34/50/50	0/6/6/6
3	PL3	A	1586	-	-	7/14/14/14	-
3	PL3	B	1586	-	-	11/14/14/14	-
2	FAD	A	1585	-	-	4/34/50/50	0/6/6/6

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1585	FAD	P-O3P	5.18	1.65	1.59
2	D	1585	FAD	P-O3P	4.88	1.64	1.59
2	C	1585	FAD	PA-O3P	4.44	1.64	1.59
2	B	1585	FAD	P-O3P	3.95	1.63	1.59
2	C	1585	FAD	C4X-N5	3.71	1.38	1.30
2	B	1585	FAD	C4X-N5	3.64	1.38	1.30
2	A	1585	FAD	C4X-N5	3.63	1.38	1.30
3	B	1586	PL3	O1-C1	-3.61	1.23	1.42
3	D	1586	PL3	O1-C1	-3.56	1.23	1.42
3	A	1586	PL3	O1-C1	-3.28	1.25	1.42
2	D	1585	FAD	C2A-N3A	3.20	1.39	1.33
2	D	1585	FAD	C4X-N5	2.76	1.36	1.30
2	B	1585	FAD	PA-O3P	2.62	1.62	1.59
2	D	1585	FAD	C1'-C2'	2.61	1.56	1.52
2	C	1585	FAD	C8A-N7A	2.54	1.36	1.31
2	A	1585	FAD	C1'-N10	2.51	1.53	1.47
2	B	1585	FAD	C5A-N7A	-2.48	1.34	1.39
2	A	1585	FAD	C9-C9A	2.47	1.43	1.39
2	B	1585	FAD	C10-N1	2.41	1.38	1.33
2	C	1585	FAD	C10-N1	2.37	1.38	1.33
2	A	1585	FAD	C5A-N7A	-2.29	1.34	1.39
2	B	1585	FAD	C2A-N1A	2.29	1.38	1.33
2	D	1585	FAD	O2-C2	-2.21	1.20	1.24
2	B	1585	FAD	C5'-C4'	2.16	1.54	1.51
2	A	1585	FAD	C1'-C2'	2.12	1.55	1.52
2	C	1585	FAD	C5A-N7A	-2.03	1.35	1.39

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1585	FAD	N3A-C2A-N1A	-6.53	118.70	128.58
2	B	1585	FAD	N3A-C2A-N1A	-6.13	119.31	128.58
2	C	1585	FAD	N3A-C2A-N1A	-6.12	119.32	128.58
2	A	1585	FAD	N9A-C8A-N7A	-4.84	107.08	113.94
2	B	1585	FAD	N9A-C8A-N7A	-4.79	107.14	113.94
2	A	1585	FAD	N3A-C2A-N1A	-4.51	121.76	128.58
2	A	1585	FAD	C4X-C10-N10	4.41	122.80	116.48
2	A	1585	FAD	C5A-N7A-C8A	4.19	110.03	103.45
2	B	1585	FAD	C4X-C10-N10	3.96	122.15	116.48
2	D	1585	FAD	C5A-N7A-C8A	3.96	109.67	103.45
2	D	1585	FAD	O2-C2-N1	-3.90	115.33	121.80
2	B	1585	FAD	C5A-N7A-C8A	3.85	109.50	103.45
2	D	1585	FAD	N9A-C8A-N7A	-3.83	108.51	113.94
2	D	1585	FAD	C4X-C10-N10	3.79	121.90	116.48
2	B	1585	FAD	O2-C2-N1	-3.74	115.58	121.80
2	D	1585	FAD	C4A-C5A-N7A	-3.68	106.37	110.58
2	B	1585	FAD	C10-C4X-N5	-3.66	117.33	124.81
2	D	1585	FAD	C2A-N1A-C6A	3.61	124.66	118.73
2	B	1585	FAD	C4-C4X-N5	3.47	123.00	118.21
2	D	1585	FAD	C4-N3-C2	-3.43	119.55	125.64
2	A	1585	FAD	C10-C4X-N5	-3.40	117.86	124.81
2	D	1585	FAD	C10-C4X-N5	-3.37	117.93	124.81
2	B	1585	FAD	C2A-N1A-C6A	3.36	124.25	118.73
2	A	1585	FAD	C5A-C4A-N3A	-3.36	122.09	126.72
2	C	1585	FAD	C5A-C4A-N3A	-3.18	122.34	126.72
2	B	1585	FAD	C4-N3-C2	-3.09	120.15	125.64
2	A	1585	FAD	C4-N3-C2	-3.08	120.18	125.64
2	A	1585	FAD	C4A-N9A-C8A	3.04	108.93	105.74
2	C	1585	FAD	C4-N3-C2	-3.03	120.27	125.64
2	C	1585	FAD	C2A-N3A-C4A	2.91	118.94	111.83
2	A	1585	FAD	C4-C4X-N5	2.85	122.14	118.21
2	C	1585	FAD	C10-C4X-N5	-2.80	119.09	124.81
2	C	1585	FAD	C4X-C10-N10	2.68	120.31	116.48
2	A	1585	FAD	N3A-C4A-N9A	2.62	131.62	127.17
2	C	1585	FAD	N9A-C8A-N7A	-2.62	110.22	113.94
2	B	1585	FAD	C5A-C4A-N3A	-2.60	123.13	126.72
2	D	1585	FAD	C4-C4X-C10	2.58	121.36	116.93
2	C	1585	FAD	O2P-P-O3P	2.56	114.18	107.27
2	A	1585	FAD	C4A-C5A-N7A	-2.55	107.67	110.58
2	B	1585	FAD	C4A-N9A-C8A	2.52	108.38	105.74
2	D	1585	FAD	C2A-N3A-C4A	2.43	117.77	111.83
2	A	1585	FAD	O4B-C1B-N9A	2.41	112.72	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1585	FAD	O3P-PA-O1A	2.30	117.61	110.70
2	A	1585	FAD	C6A-C5A-C4A	2.29	120.30	117.18
2	B	1585	FAD	O4B-C1B-N9A	2.27	112.44	108.09
2	C	1585	FAD	C2A-N1A-C6A	2.24	122.40	118.73
2	A	1585	FAD	C4X-C4-N3	2.23	118.94	113.25
3	A	1586	PL3	O1-C1-C2	2.23	125.61	111.44
2	B	1585	FAD	C6A-C5A-C4A	2.23	120.22	117.18
2	D	1585	FAD	C5A-C4A-N3A	-2.22	123.65	126.72
2	B	1585	FAD	C4X-C4-N3	2.22	118.91	113.25
2	B	1585	FAD	O2-C2-N3	2.21	122.83	118.58
2	A	1585	FAD	C8M-C8-C9	2.21	123.47	119.57
2	C	1585	FAD	C4X-C4-N3	2.21	118.88	113.25
3	D	1586	PL3	O1-C1-C2	2.20	125.40	111.44
2	B	1585	FAD	C2A-N3A-C4A	2.17	117.13	111.83
2	A	1585	FAD	O3B-C3B-C2B	-2.17	104.86	111.82
2	D	1585	FAD	O3B-C3B-C2B	-2.13	104.97	111.82
2	A	1585	FAD	C2A-N3A-C4A	2.13	117.04	111.83
2	C	1585	FAD	C4-C4X-C10	2.10	120.53	116.93
2	A	1585	FAD	O2P-P-O5'	2.09	117.04	107.57
2	B	1585	FAD	C4A-C5A-N7A	-2.07	108.21	110.58
2	B	1585	FAD	C5B-C4B-C3B	-2.06	107.79	115.21
2	A	1585	FAD	O2-C2-N1	-2.05	118.40	121.80
2	C	1585	FAD	C4X-C10-N1	-2.02	119.64	124.59
2	A	1585	FAD	C4X-C10-N1	-2.02	119.64	124.59

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1585	FAD	N10-C1'-C2'-O2'
2	A	1585	FAD	N10-C1'-C2'-C3'
2	B	1585	FAD	N10-C1'-C2'-O2'
2	B	1585	FAD	N10-C1'-C2'-C3'
2	C	1585	FAD	N10-C1'-C2'-O2'
2	C	1585	FAD	N10-C1'-C2'-C3'
2	D	1585	FAD	N10-C1'-C2'-O2'
2	D	1585	FAD	N10-C1'-C2'-C3'
3	B	1586	PL3	C3-C4-C5-C6
3	D	1586	PL3	C8-C9-CA-CB
3	B	1586	PL3	CC-CD-CE-CF
3	B	1586	PL3	C9-CA-CB-CC
3	B	1586	PL3	CA-CB-CC-CD

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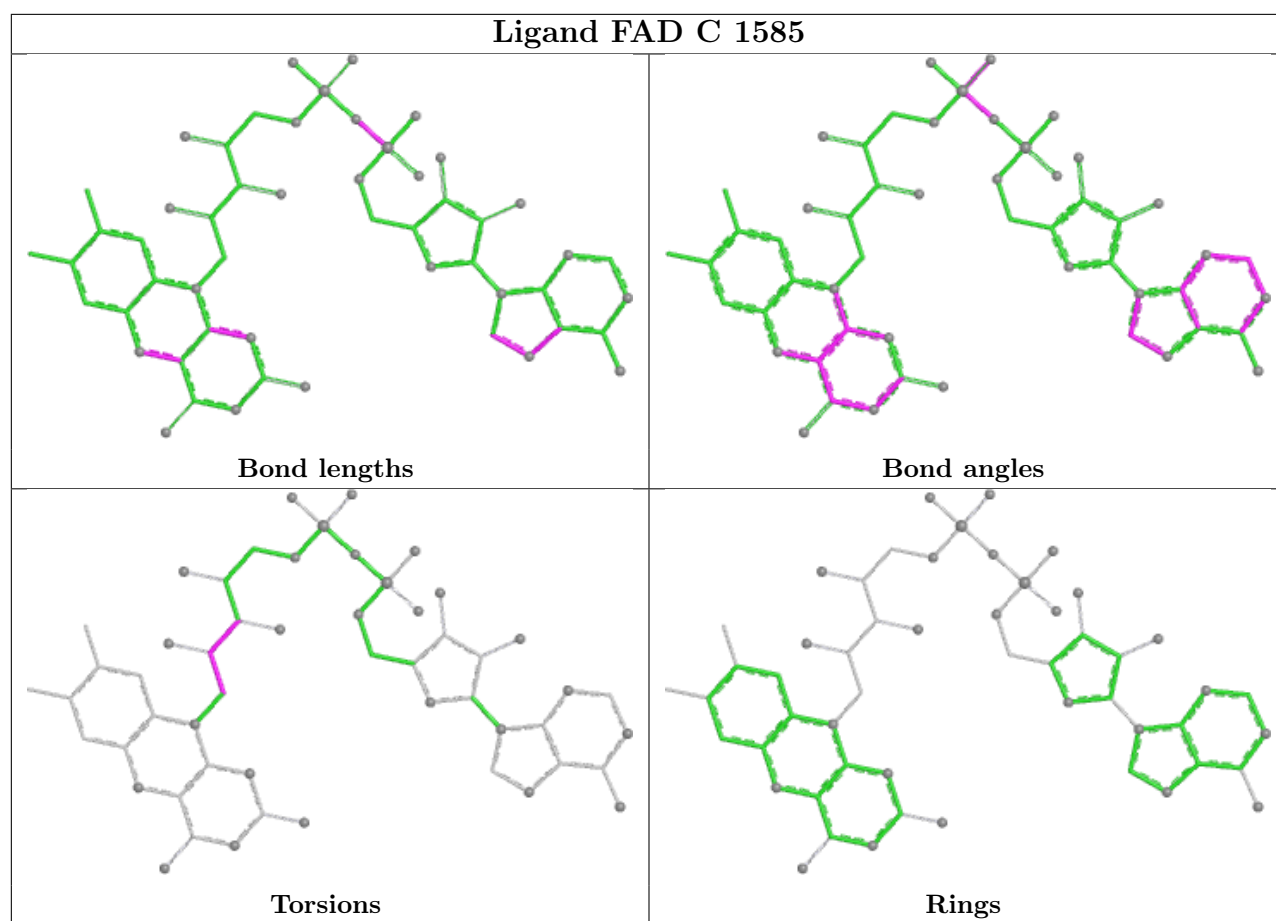
Mol	Chain	Res	Type	Atoms
3	B	1586	PL3	CB-CC-CD-CE
3	D	1586	PL3	O1-C1-C2-C3
3	D	1586	PL3	C4-C5-C6-C7
3	A	1586	PL3	C5-C6-C7-C8
3	B	1586	PL3	C1-C2-C3-C4
3	A	1586	PL3	C1-C2-C3-C4
3	A	1586	PL3	C9-CA-CB-CC
3	B	1586	PL3	C4-C5-C6-C7
3	A	1586	PL3	C3-C4-C5-C6
3	A	1586	PL3	CB-CC-CD-CE
3	B	1586	PL3	CD-CE-CF-CG
3	B	1586	PL3	O1-C1-C2-C3
3	B	1586	PL3	C6-C7-C8-C9
2	A	1585	FAD	PA-O3P-P-O1P
2	A	1585	FAD	PA-O3P-P-O2P
3	A	1586	PL3	C7-C8-C9-CA
3	B	1586	PL3	C8-C9-CA-CB
3	D	1586	PL3	C9-CA-CB-CC
2	C	1585	FAD	O2'-C2'-C3'-O3'
3	A	1586	PL3	CC-CD-CE-CF

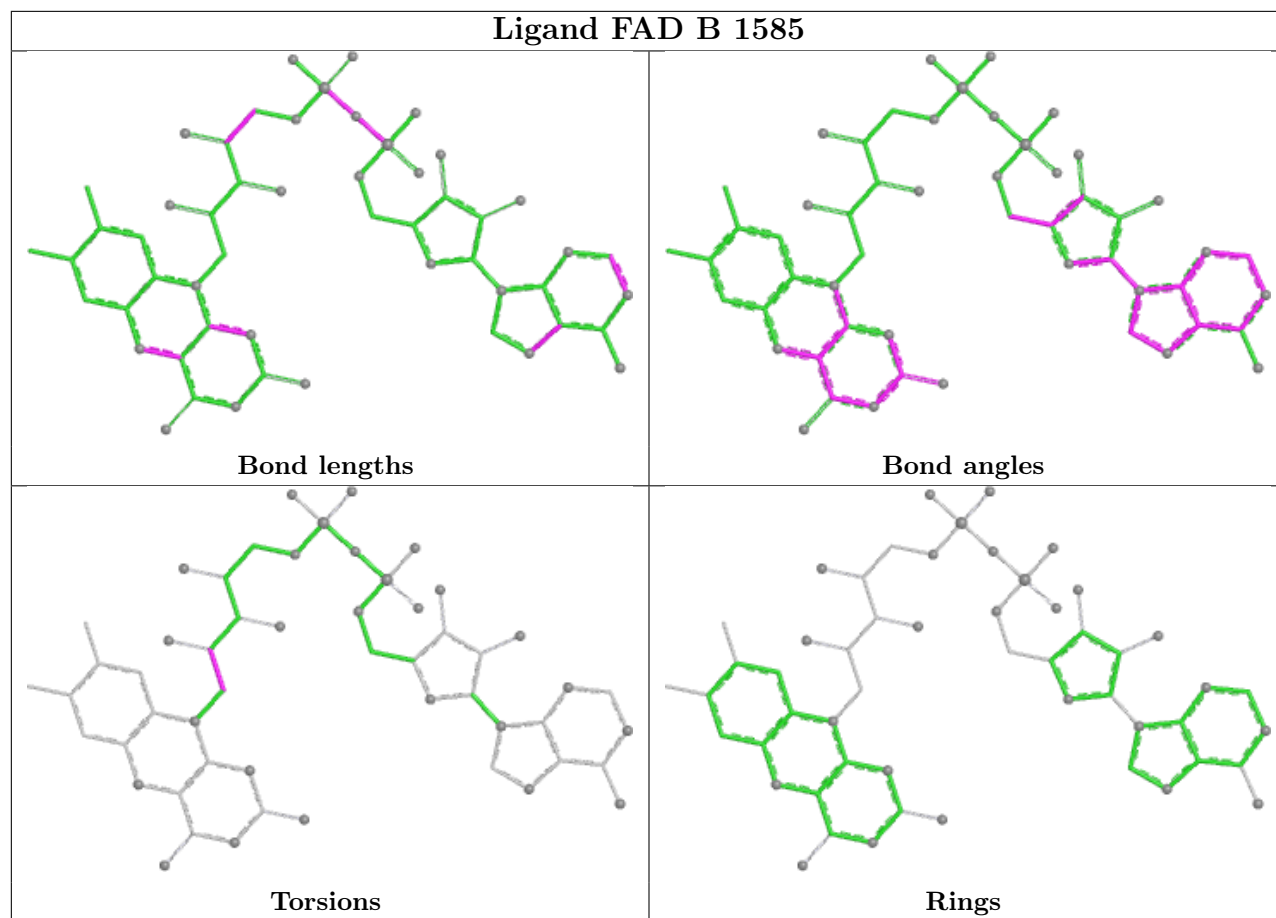
There are no ring outliers.

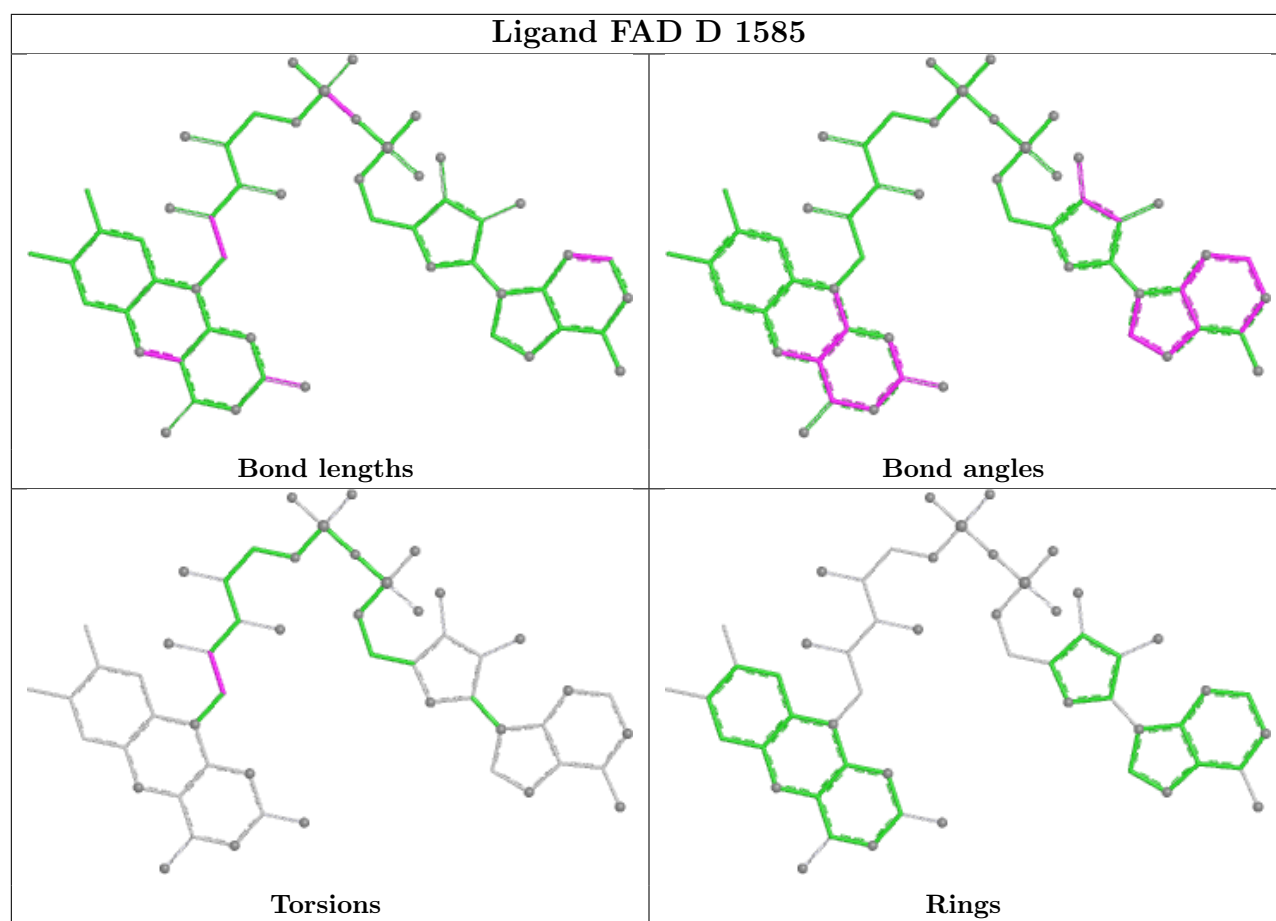
4 monomers are involved in 23 short contacts:

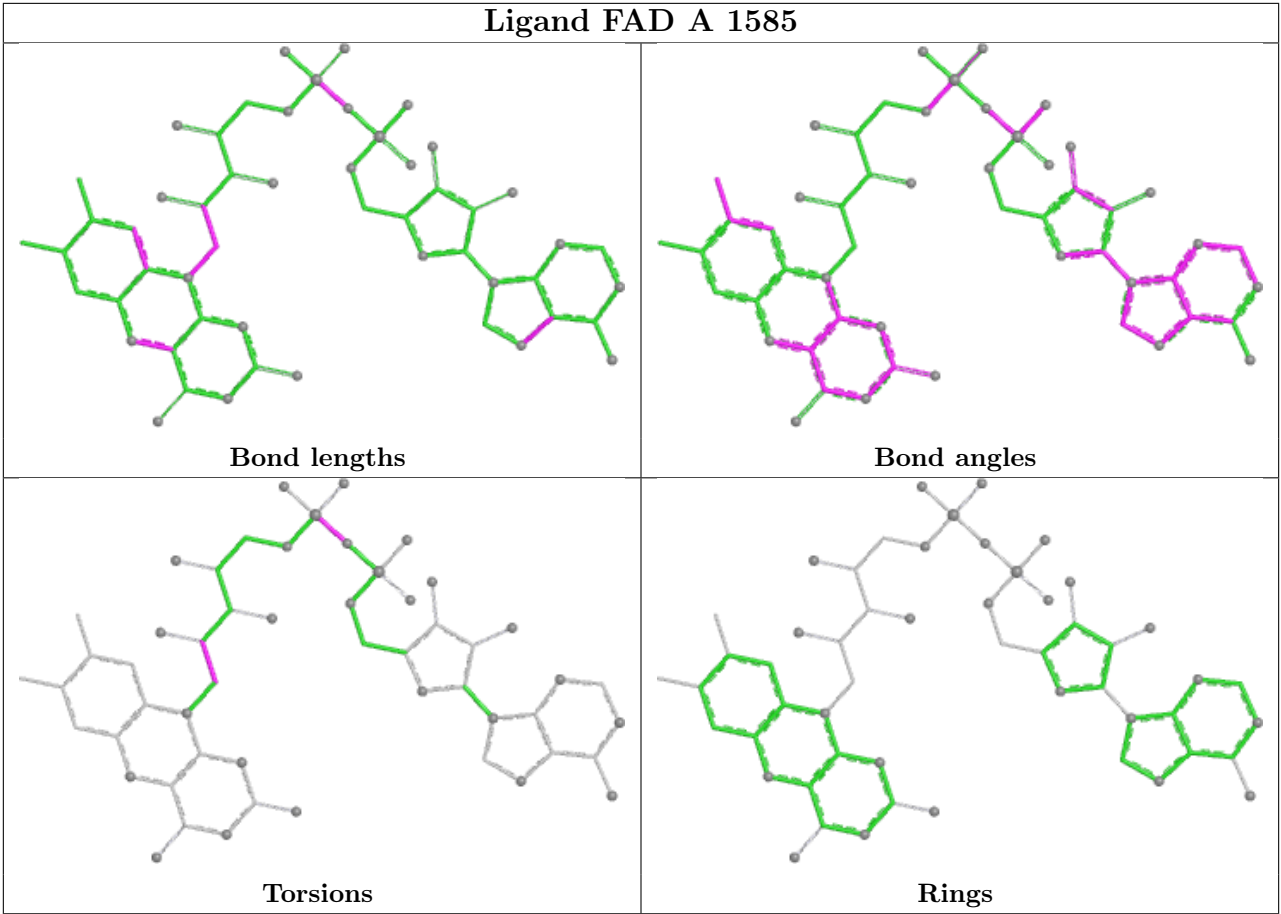
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1586	PL3	11	0
3	A	1586	PL3	3	0
3	B	1586	PL3	8	0
2	A	1585	FAD	1	0

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	390:PHE	C	391:ASP	N	2.03
1	C	384:LEU	C	385:HIS	N	1.67

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	523/584 (89%)	0.72	52 (9%) 13 11	10, 25, 53, 86	1 (0%)
1	B	523/584 (89%)	0.91	56 (10%) 11 10	11, 26, 56, 85	1 (0%)
1	C	491/584 (84%)	1.49	129 (26%) 1 1	14, 33, 58, 79	2 (0%)
1	D	528/584 (90%)	0.98	81 (15%) 5 4	9, 25, 51, 68	1 (0%)
All	All	2065/2336 (88%)	1.02	318 (15%) 5 4	9, 26, 55, 86	5 (0%)

All (318) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	436	TRP	8.1
1	A	63	LEU	6.9
1	A	524	TYR	6.4
1	C	390	PHE	6.0
1	C	386	TYR	5.9
1	A	525	ILE	5.5
1	A	527	ALA	5.5
1	C	501	TYR	5.4
1	C	365	TRP	5.4
1	B	370	GLY	5.3
1	C	388	ARG	5.3
1	C	384	LEU	5.3
1	C	387	ILE	5.2
1	C	39	THR	5.2
1	C	356	PRO	5.1
1	C	389	SER	5.0
1	C	480	PHE	4.9
1	D	63	LEU	4.9
1	B	536	PHE	4.8
1	C	383	TYR	4.8
1	A	432	PRO	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	289	ALA	4.6
1	C	395	VAL	4.6
1	B	431	ALA	4.5
1	D	371	ALA	4.4
1	C	36	PRO	4.4
1	C	481	VAL	4.3
1	C	426	PHE	4.2
1	D	372	VAL	4.2
1	B	432	PRO	4.2
1	A	436	TRP	4.2
1	D	425	ALA	4.1
1	B	538	TYR	4.0
1	C	38	GLY	4.0
1	B	530	LEU	4.0
1	C	392	PHE	4.0
1	A	536	PHE	4.0
1	C	74	VAL	4.0
1	C	385	HIS	3.9
1	C	483	HIS	3.9
1	C	327	LEU	3.9
1	A	538	TYR	3.9
1	D	508	TYR	3.9
1	C	489	ILE	3.9
1	D	384	LEU	3.8
1	C	381	LYS	3.8
1	B	581	CYS	3.8
1	D	476	ALA	3.8
1	C	336	SER	3.8
1	D	501	TYR	3.7
1	D	426	PHE	3.7
1	C	289	ALA	3.7
1	C	431	ALA	3.7
1	C	419	ILE	3.7
1	C	391	ASP	3.6
1	C	379	MET	3.6
1	D	538	TYR	3.6
1	C	428	LEU	3.6
1	D	489	ILE	3.6
1	A	64	THR	3.5
1	A	565	ILE	3.5
1	D	534	ILE	3.5
1	C	411	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	397	LEU	3.5
1	A	435	THR	3.5
1	D	12	HIS	3.5
1	D	365	TRP	3.4
1	D	346	VAL	3.4
1	C	434	LYS	3.4
1	B	562	ARG	3.4
1	B	139	ASN	3.4
1	C	326	PHE	3.4
1	B	99	ARG	3.3
1	D	282	ARG	3.3
1	A	564	TRP	3.3
1	C	508	TYR	3.2
1	A	431	ALA	3.2
1	C	418	ASP	3.2
1	C	330	THR	3.2
1	A	377	SER	3.2
1	A	539	GLY	3.2
1	C	478	GLN	3.2
1	C	562	ARG	3.2
1	A	475	ASP	3.2
1	D	72	PRO	3.2
1	A	74	VAL	3.1
1	B	63	LEU	3.1
1	C	380	VAL	3.1
1	C	479	THR	3.1
1	D	432	PRO	3.1
1	D	527	ALA	3.1
1	C	490	PRO	3.1
1	D	387	ILE	3.0
1	C	47	VAL	3.0
1	C	382	LYS	3.0
1	C	417	PHE	3.0
1	C	408	VAL	3.0
1	B	12	HIS	3.0
1	B	64	THR	3.0
1	D	375	PHE	3.0
1	D	536	PHE	3.0
1	B	367	PRO	3.0
1	C	424	ALA	3.0
1	D	437	ALA	2.9
1	C	176	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	75	LEU	2.9
1	C	76	ASP	2.9
1	A	488	GLY	2.9
1	C	437	ALA	2.9
1	B	365	TRP	2.9
1	C	12	HIS	2.9
1	D	385	HIS	2.9
1	D	388	ARG	2.9
1	B	87	HIS	2.9
1	B	103	ALA	2.9
1	C	476	ALA	2.9
1	B	528	LYS	2.9
1	D	407	LYS	2.9
1	B	436	TRP	2.9
1	D	451	LEU	2.9
1	B	435	THR	2.8
1	C	50	VAL	2.8
1	C	334	ALA	2.8
1	C	435	THR	2.8
1	C	346	VAL	2.8
1	D	457	VAL	2.8
1	C	48	SER	2.8
1	C	396	CYS	2.8
1	C	25	GLY	2.8
1	C	472	LEU	2.8
1	A	365	TRP	2.8
1	D	491	ALA	2.8
1	A	516	ASN	2.8
1	C	482	LYS	2.8
1	B	535	ILE	2.8
1	C	477	LYS	2.7
1	C	27	THR	2.7
1	A	541	SER	2.7
1	C	473	TRP	2.7
1	C	46	GLU	2.7
1	C	467	ALA	2.7
1	A	531	MET	2.7
1	B	368	SER	2.7
1	C	416	VAL	2.7
1	B	539	GLY	2.7
1	C	325	GLY	2.7
1	D	390	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	376	THR	2.7
1	D	64	THR	2.7
1	A	529	LYS	2.7
1	A	183	VAL	2.7
1	C	433	GLY	2.6
1	C	350	MET	2.6
1	A	73	PHE	2.6
1	C	432	PRO	2.6
1	D	537	LYS	2.6
1	C	565	ILE	2.6
1	B	584	ARG	2.6
1	A	526	GLU	2.6
1	B	526	GLU	2.6
1	D	386	TYR	2.6
1	A	566	ASN	2.6
1	B	379	MET	2.6
1	B	573	GLU	2.6
1	C	183	VAL	2.6
1	D	381	LYS	2.6
1	C	95	PRO	2.6
1	D	436	TRP	2.6
1	A	533	ASP	2.6
1	A	537	LYS	2.6
1	B	74	VAL	2.6
1	C	363	PHE	2.5
1	D	13	ILE	2.5
1	C	323	TYR	2.5
1	C	34	LEU	2.5
1	D	530	LEU	2.5
1	D	539	GLY	2.5
1	B	534	ILE	2.5
1	B	565	ILE	2.5
1	C	512	ALA	2.5
1	A	367	PRO	2.5
1	A	540	GLY	2.5
1	C	331	PHE	2.5
1	D	370	GLY	2.5
1	C	21	TRP	2.5
1	D	564	TRP	2.5
1	D	320	ALA	2.5
1	A	479	THR	2.5
1	D	376	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	563	GLY	2.4
1	B	16	TYR	2.4
1	B	580	ILE	2.4
1	B	529	LYS	2.4
1	B	532	THR	2.4
1	B	488	GLY	2.4
1	D	396	CYS	2.4
1	C	324	TYR	2.4
1	C	469	LEU	2.4
1	C	58	PHE	2.4
1	D	431	ALA	2.4
1	C	335	VAL	2.4
1	D	563	GLY	2.4
1	C	510	ILE	2.4
1	A	437	ALA	2.4
1	C	126	LEU	2.3
1	A	476	ALA	2.3
1	D	423	ASN	2.3
1	D	405	PRO	2.3
1	D	541	SER	2.3
1	D	486	ASP	2.3
1	C	420	LEU	2.3
1	D	75	LEU	2.3
1	D	417	PHE	2.3
1	D	484	PHE	2.3
1	C	80	ALA	2.3
1	A	489	ILE	2.3
1	B	13	ILE	2.3
1	C	13	ILE	2.3
1	B	433	GLY	2.3
1	B	183	VAL	2.3
1	A	530	LEU	2.3
1	C	502	THR	2.3
1	B	578	LYS	2.3
1	D	514	LYS	2.3
1	C	405	PRO	2.3
1	C	584	ARG	2.3
1	D	427	GLY	2.3
1	D	46	GLU	2.3
1	D	418	ASP	2.3
1	C	409	VAL	2.3
1	D	481	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	499	HIS	2.3
1	D	338	LEU	2.3
1	B	94	TYR	2.2
1	B	508	TYR	2.2
1	C	94	TYR	2.2
1	C	367	PRO	2.2
1	D	568	TYR	2.2
1	D	421	SER	2.2
1	D	419	ILE	2.2
1	D	483	HIS	2.2
1	D	487	GLN	2.2
1	C	491	ALA	2.2
1	D	347	ILE	2.2
1	A	584	ARG	2.2
1	C	494	CYS	2.2
1	C	89	ASP	2.2
1	C	430	SER	2.2
1	D	373	SER	2.2
1	A	139	ASN	2.2
1	C	412	HIS	2.2
1	C	455	MET	2.2
1	D	406	LYS	2.2
1	C	206	ARG	2.2
1	A	481	VAL	2.2
1	D	380	VAL	2.2
1	B	290	GLY	2.2
1	B	378	ALA	2.2
1	C	320	ALA	2.2
1	D	378	ALA	2.2
1	A	483	HIS	2.1
1	A	499	HIS	2.1
1	C	342	ARG	2.2
1	C	393	LYS	2.2
1	B	484	PHE	2.1
1	C	96	GLU	2.1
1	D	73	PHE	2.1
1	C	78	THR	2.1
1	C	359	THR	2.1
1	A	563	GLY	2.1
1	D	488	GLY	2.1
1	B	384	LEU	2.1
1	C	338	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	333	HIS	2.1
1	A	467	ALA	2.1
1	C	423	ASN	2.1
1	C	30	PHE	2.1
1	C	515	GLN	2.1
1	A	579	ASP	2.1
1	D	409	VAL	2.1
1	C	366	LYS	2.1
1	A	185	ASN	2.1
1	A	424	ALA	2.1
1	B	104	PHE	2.1
1	C	104	PHE	2.1
1	A	486	ASP	2.1
1	B	387	ILE	2.1
1	D	354	TYR	2.1
1	D	410	ASP	2.1
1	D	475	ASP	2.1
1	B	369	LYS	2.1
1	B	434	LYS	2.1
1	D	438	GLU	2.1
1	D	540	GLY	2.1
1	C	492	TRP	2.1
1	B	18	GLN	2.1
1	C	329	PRO	2.1
1	C	360	GLN	2.1
1	C	361	LEU	2.1
1	C	364	ALA	2.1
1	D	460	ALA	2.1
1	B	258	ASP	2.1
1	C	322	GLU	2.0
1	D	513	SER	2.0
1	C	414	THR	2.0
1	D	490	PRO	2.0
1	B	564	TRP	2.0
1	A	103	ALA	2.0
1	A	562	ARG	2.0
1	B	364	ALA	2.0
1	B	537	LYS	2.0
1	B	377	SER	2.0
1	D	411	PHE	2.0
1	A	25	GLY	2.0
1	C	123	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	501	TYR	2.0
1	C	505	VAL	2.0
1	D	177	VAL	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](#)

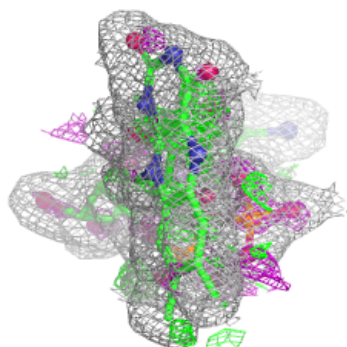
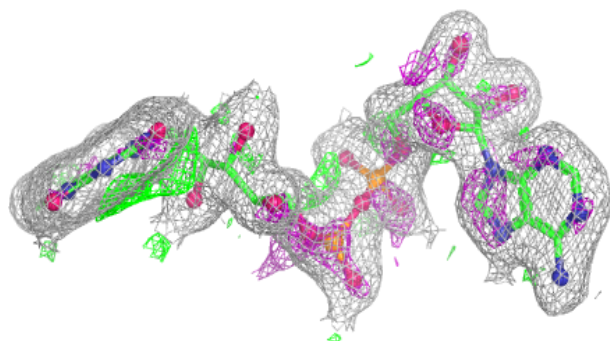
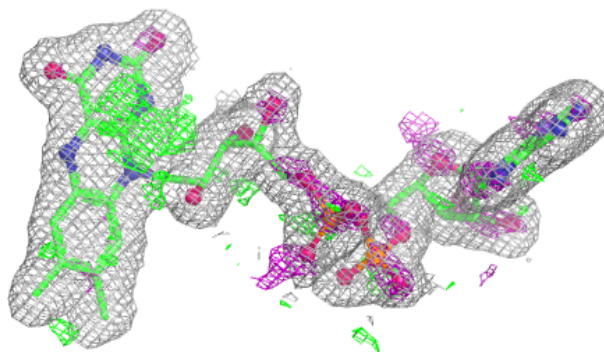
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	PL3	A	1586	17/17	0.73	0.17	35,39,44,45	0
3	PL3	D	1586	17/17	0.79	0.13	24,32,34,35	0
3	PL3	B	1586	17/17	0.85	0.12	31,33,45,47	0
2	FAD	B	1585	53/53	0.95	0.07	5,11,13,16	0
2	FAD	C	1585	53/53	0.96	0.06	7,15,19,19	0
2	FAD	D	1585	53/53	0.97	0.06	3,9,12,12	0
2	FAD	A	1585	53/53	0.97	0.06	2,9,12,12	0

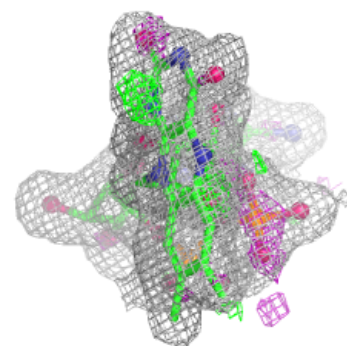
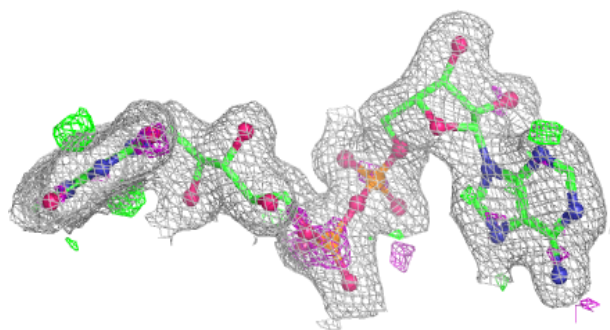
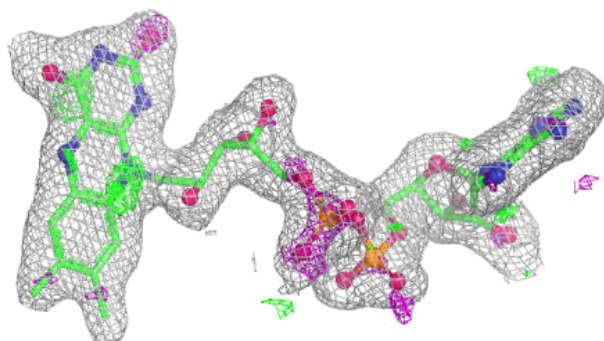
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD B 1585:

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

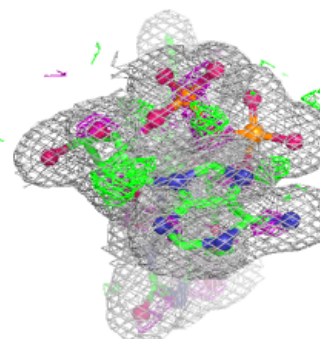
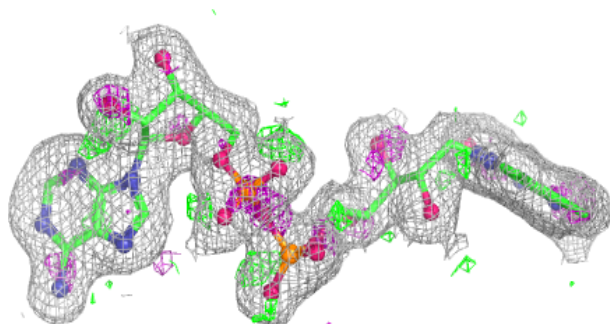
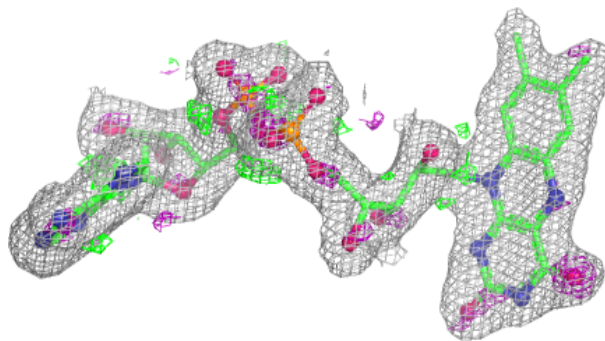
**Electron density around FAD C 1585:**

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

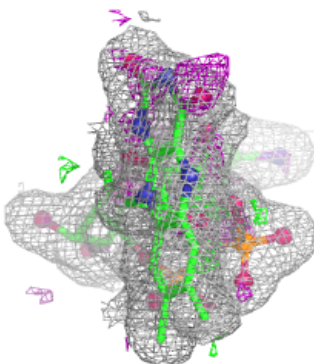
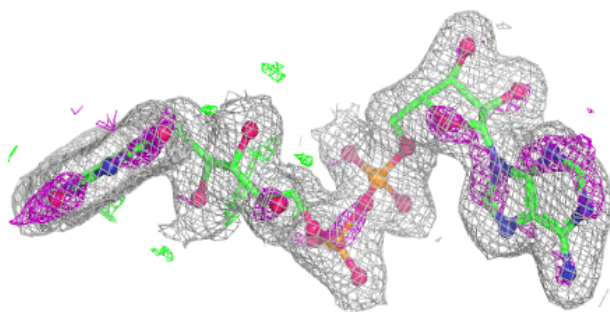
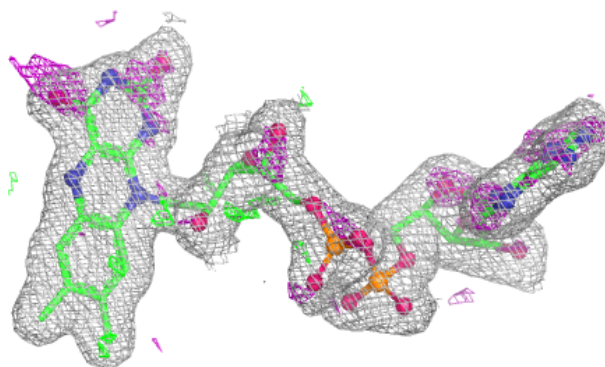


Electron density around FAD D 1585:

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

**Electron density around FAD A 1585:**

$2mF_o-DF_c$ (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.