



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 03:03 AM UTC

PDB ID : 2UUU / pdb_00002uuu
Title : alkyldihydroxyacetonephosphate synthase in P212121
Authors : Razeto, A.; Mattioli, F.; Carpanelli, E.; Aliverti, A.; Pandini, V.; Coda, A.;
Mattevi, A.
Deposited on : 2007-03-07
Resolution : 1.95 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 : **FAILED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

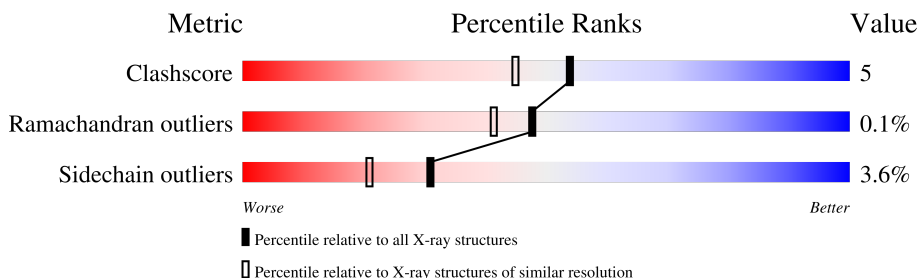
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)

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 $\leq 5\%$

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	584	
1	B	584	
1	C	584	
1	D	584	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19178 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	550	Total	C	N	O	S	0	3	0
			4408	2839	751	798	20			
1	B	540	Total	C	N	O	S	0	1	0
			4329	2788	739	783	19			
1	C	541	Total	C	N	O	S	0	0	0
			4323	2784	735	786	18			
1	D	537	Total	C	N	O	S	0	0	0
			4288	2763	730	776	19			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP O96759
A	-4	ALA	-	expression tag	UNP O96759
A	-3	MET	-	expression tag	UNP O96759
A	-2	GLY	-	expression tag	UNP O96759
A	-1	SER	-	expression tag	UNP O96759
B	-5	GLY	-	expression tag	UNP O96759
B	-4	ALA	-	expression tag	UNP O96759
B	-3	MET	-	expression tag	UNP O96759
B	-2	GLY	-	expression tag	UNP O96759
B	-1	SER	-	expression tag	UNP O96759
C	-5	GLY	-	expression tag	UNP O96759
C	-4	ALA	-	expression tag	UNP O96759
C	-3	MET	-	expression tag	UNP O96759
C	-2	GLY	-	expression tag	UNP O96759
C	-1	SER	-	expression tag	UNP O96759
D	-5	GLY	-	expression tag	UNP O96759
D	-4	ALA	-	expression tag	UNP O96759
D	-3	MET	-	expression tag	UNP O96759
D	-2	GLY	-	expression tag	UNP O96759
D	-1	SER	-	expression tag	UNP O96759

- # FAD
-
- The image displays the chemical structure of Flavin Adenine Dinucleotide (FAD), a crucial coenzyme. The molecule is composed of three main parts: a riboflavin (isoalloxazine) ring system, a ribitol linker, and an adenosine moiety.
- Riboflavin (Isoalloxazine) Ring System:** This is the top part of the structure, featuring a fused bicyclic system with nitrogen atoms (N1, N3, N7, N9) and carbonyl groups (C2=O, C4=O, C6=O). It is attached to a ribitol chain via a glycosidic bond at the N1 position.
 - Ribitol Linker:** A five-carbon chain (C1-C5) that connects the riboflavin to the adenosine moiety. It has hydroxyl groups at C2, C3, and C4, and is linked to the riboflavin at C1 and the adenosine at C5.
 - Adenosine Moiety:** This part consists of an adenine base (a fused bicyclic system with N1, N3, N7, N9 and C2, C4, C6, C8) attached to a ribose sugar (C1'-C5'). The ribose has hydroxyl groups at C2', C3', and C4', and is linked to the ribitol linker at C5'.
- The structure is shown in a 3D representation with stereochemistry indicated by wedge and dash bonds. The overall color scheme uses blue for nitrogen atoms, red for oxygen atoms, and grey for carbon atoms.

PL3

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	C	1	Total	C	O	0	0
			17	16	1		
3	D	1	Total	C	O	0	0
			17	16	1		

- Molecule 4 is water.

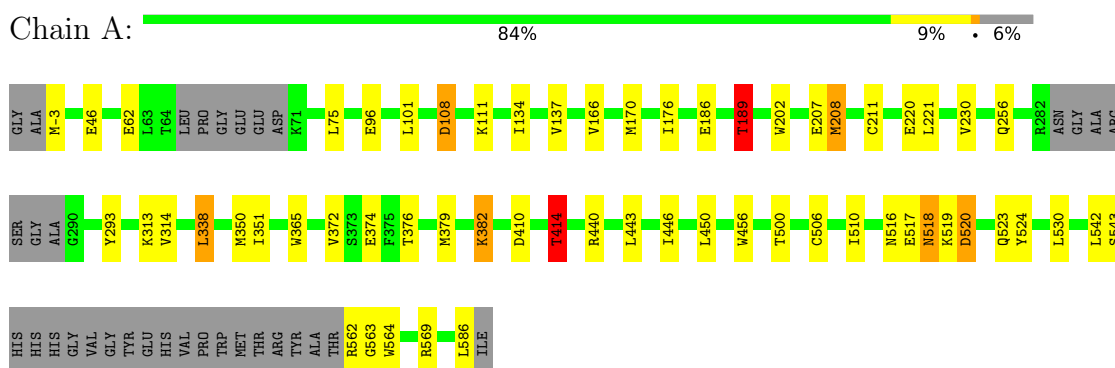
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	484	Total	O	0	0
			484	484		
4	B	385	Total	O	0	0
			385	385		
4	C	333	Total	O	0	0
			333	333		
4	D	348	Total	O	0	0
			348	348		

3 Residue-property plots [i](#)

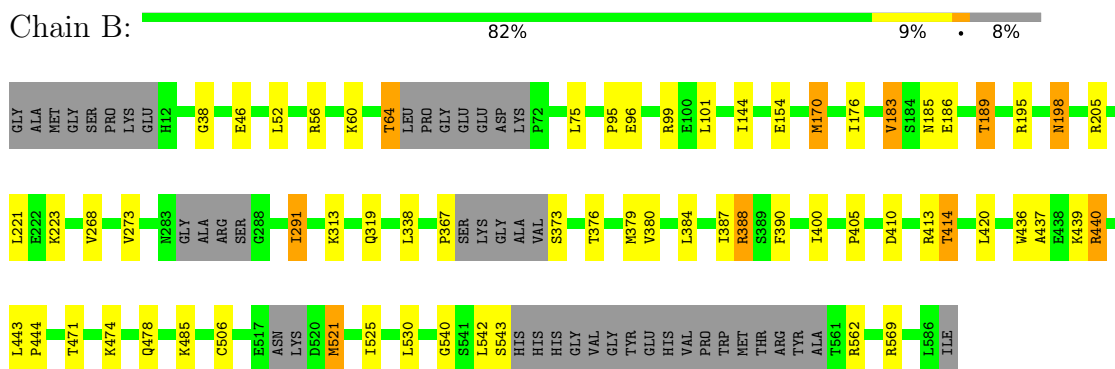
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS failed to run properly.

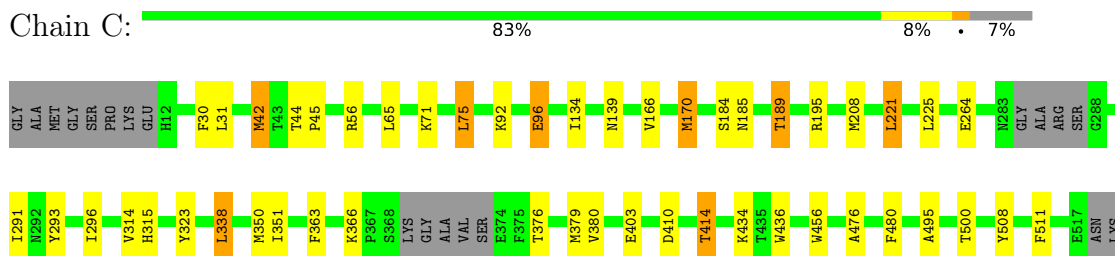
• Molecule 1: ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE

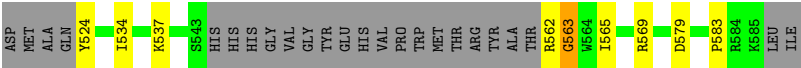


• Molecule 1: ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE

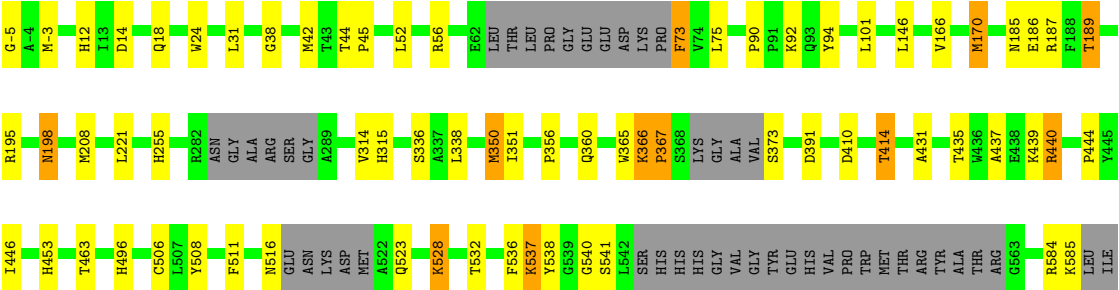
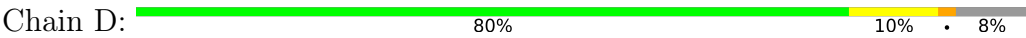


• Molecule 1: ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE





● Molecule 1: ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	103.50Å 108.91Å 216.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.93 – 1.95	Depositor
% Data completeness (in resolution range)	99.8 (29.93-1.95)	Depositor
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.193 , 0.244	Depositor
Wilson B-factor (Å ²)	26.6	Xtriage
Anisotropy	0.573	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.013 for k,h,-l	Xtriage
Total number of atoms	19178	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.20% 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

5.1 Standard geometry

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	0.97	1/4527 (0.0%)	0.90	4/6127 (0.1%)
1	B	0.87	0/4439	0.91	1/6008 (0.0%)
1	C	0.81	0/4431	0.89	1/6000 (0.0%)
1	D	0.83	1/4395 (0.0%)	0.91	9/5948 (0.2%)
All	All	0.87	2/17792 (0.0%)	0.90	15/24083 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	90	PRO	CA-C	6.76	1.55	1.51
1	A	137	VAL	CA-CB	5.07	1.59	1.53

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	THR	N-CA-C	5.92	118.76	108.76
1	D	146	LEU	CA-C-N	5.90	125.81	119.85
1	D	146	LEU	C-N-CA	5.90	125.81	119.85
1	A	293	TYR	N-CA-C	5.67	119.30	112.38
1	D	52	LEU	CA-C-N	5.46	125.11	119.05
1	D	52	LEU	C-N-CA	5.46	125.11	119.05
1	D	94	TYR	CA-C-N	5.33	124.51	118.97
1	D	94	TYR	C-N-CA	5.33	124.51	118.97
1	D	453	HIS	N-CA-C	5.29	116.80	110.44
1	B	540	GLY	N-CA-C	-5.20	105.95	111.93
1	D	431	ALA	CA-C-N	5.18	126.32	119.84
1	D	431	ALA	C-N-CA	5.18	126.32	119.84
1	C	563	GLY	N-CA-C	-5.10	107.62	115.73
1	A	414	THR	N-CA-CB	5.09	117.60	110.12
1	A	519	LYS	N-CA-C	5.08	118.41	111.39

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	4408	0	4422	46	0
1	B	4329	0	4327	43	0
1	C	4323	0	4311	40	0
1	D	4288	0	4283	42	0
2	A	53	0	31	0	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	4	0
3	B	17	0	33	2	0
3	C	17	0	33	0	0
3	D	17	0	33	0	0
4	A	484	0	0	11	0
4	B	385	0	0	9	0
4	C	333	0	0	5	0
4	D	348	0	0	11	0
All	All	19178	0	17599	173	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 5.

All (173) 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:220:GLU:HG2	4:A:2203:HOH:O	1.49	1.13
1:C:92:LYS:HE3	1:C:185:ASN:O	1.48	1.11
1:A:256:GLN:HE21	1:A:350:MET:HE3	1.11	1.09
1:A:208:MET:CE	1:A:314:VAL:HG23	1.88	1.03
1:A:256:GLN:NE2	1:A:350:MET:HE3	1.78	0.98
1:B:373:SER:HA	1:B:376:THR:HG22	1.49	0.94
1:B:410:ASP:O	1:B:414:THR:HG23	1.69	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:ASN:HB2	4:C:2128:HOH:O	1.72	0.86
1:D:92:LYS:HE2	1:D:185:ASN:O	1.80	0.81
1:B:373:SER:HA	1:B:376:THR:CG2	2.13	0.79
1:B:379:MET:SD	1:B:436:TRP:CZ2	2.77	0.78
1:A:410:ASP:O	1:A:414:THR:HG23	1.84	0.78
1:D:437:ALA:O	1:D:440:ARG:HD3	1.82	0.77
1:A:208:MET:HE3	1:A:314:VAL:HG23	1.67	0.76
1:C:338:LEU:HG	1:C:500:THR:HG21	1.68	0.75
1:B:379:MET:SD	1:B:436:TRP:CH2	2.78	0.75
1:B:388:ARG:HD3	4:B:2280:HOH:O	1.86	0.74
1:D:410:ASP:O	1:D:414:THR:HG22	1.87	0.74
1:D:-5:GLY:N	4:D:2004:HOH:O	2.20	0.73
1:C:31:LEU:HD23	1:C:42:MET:HE3	1.71	0.73
1:B:542:LEU:O	1:B:543:SER:HB2	1.89	0.71
1:B:223:LYS:HE2	4:B:2169:HOH:O	1.91	0.70
1:D:208:MET:HE3	1:D:314:VAL:HG23	1.72	0.70
1:A:208:MET:HE3	1:A:208:MET:HA	1.74	0.70
1:A:542:LEU:HD23	4:A:2406:HOH:O	1.90	0.70
1:B:569:ARG:NH2	4:B:2368:HOH:O	2.23	0.70
1:D:208:MET:HE2	1:D:315:HIS:HA	1.74	0.69
1:B:319:GLN:HG2	1:B:405:PRO:HA	1.74	0.69
1:C:92:LYS:CE	1:C:185:ASN:O	2.36	0.68
1:A:176:ILE:HG21	3:A:1588:PL3:H1C1	1.77	0.67
1:A:189:THR:HG21	4:A:2195:HOH:O	1.95	0.67
1:B:373:SER:CA	1:B:376:THR:HG22	2.25	0.66
1:C:208:MET:HE2	1:C:315:HIS:HA	1.78	0.65
1:D:496:HIS:CE1	1:D:508:TYR:CD1	2.85	0.64
1:C:562:ARG:HD2	1:C:565:ILE:HG13	1.79	0.64
1:D:166:VAL:HB	1:D:189:THR:HB	1.79	0.64
1:B:474:LYS:HE2	1:B:478:GLN:HE22	1.63	0.63
1:D:185:ASN:HB3	4:D:2119:HOH:O	1.98	0.62
1:A:208:MET:HE2	1:A:314:VAL:HG23	1.78	0.62
1:D:516:ASN:H	1:D:523:GLN:HE22	1.46	0.62
1:C:410:ASP:O	1:C:414:THR:HG23	2.00	0.62
1:B:189:THR:HG21	4:B:2142:HOH:O	1.99	0.61
1:C:323:TYR:HE2	1:C:350:MET:HE3	1.65	0.61
1:C:166:VAL:HB	1:C:189:THR:HB	1.81	0.61
1:C:31:LEU:CD2	1:C:42:MET:HE3	2.31	0.61
1:D:221:LEU:HD22	4:D:2185:HOH:O	2.02	0.60
1:A:256:GLN:HE21	1:A:350:MET:CE	2.02	0.59
1:D:221:LEU:C	1:D:221:LEU:HD23	2.28	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:463:THR:O	1:D:540:GLY:HA2	2.03	0.59
1:B:291:ILE:HD13	1:B:291:ILE:N	2.19	0.58
1:A:256:GLN:NE2	1:A:350:MET:CE	2.60	0.58
1:A:382[B]:LYS:NZ	4:A:2350:HOH:O	2.35	0.58
1:C:569:ARG:HD2	4:C:2320:HOH:O	2.03	0.58
1:D:73:PHE:HA	4:D:2050:HOH:O	2.04	0.57
1:A:443:LEU:O	1:A:446:ILE:HG22	2.05	0.57
1:D:-3:MET:HE2	4:D:2005:HOH:O	2.04	0.57
1:A:510:ILE:HG21	3:A:1588:PL3:HAC1	1.87	0.57
1:C:379:MET:SD	1:C:436:TRP:CZ2	2.98	0.57
1:A:108:ASP:O	1:A:111:LYS:HE2	2.05	0.56
1:D:44:THR:HB	1:D:45:PRO:HD2	1.87	0.56
1:B:38:GLY:O	1:B:56:ARG:HD2	2.06	0.55
1:B:198:ASN:H	1:B:198:ASN:HD22	1.54	0.55
1:D:208:MET:HE2	1:D:315:HIS:CA	2.36	0.55
1:D:189:THR:HG21	4:D:2154:HOH:O	2.06	0.54
1:B:170:MET:HE2	1:B:195:ARG:NH2	2.24	0.53
1:B:380:VAL:O	1:B:384:LEU:HG	2.08	0.53
1:C:170:MET:HE2	1:C:195:ARG:NH2	2.24	0.53
1:A:-3:MET:HE2	4:A:2162:HOH:O	2.09	0.52
1:A:365:TRP:HD1	1:A:365:TRP:O	1.92	0.52
1:B:60:LYS:O	1:B:64:THR:HB	2.09	0.52
1:C:208:MET:HE3	1:C:314:VAL:HG23	1.91	0.52
1:C:579:ASP:O	1:C:583:PRO:HG3	2.10	0.52
3:A:1588:PL3:O1	4:A:2484:HOH:O	2.19	0.51
1:C:221:LEU:HD22	1:C:225:LEU:CD1	2.41	0.51
1:D:373:SER:HA	4:D:2276:HOH:O	2.11	0.51
1:C:366:LYS:HD3	1:C:380:VAL:HG21	1.93	0.51
1:D:186:GLU:HG2	4:D:2153:HOH:O	2.10	0.51
1:A:518:ASN:OD1	1:A:518:ASN:N	2.43	0.51
1:B:471:THR:HG23	4:B:2332:HOH:O	2.12	0.50
1:C:208:MET:HE2	1:C:315:HIS:CA	2.39	0.50
1:D:198:ASN:HD22	1:D:198:ASN:H	1.60	0.50
1:A:376:THR:HA	1:A:379:MET:HE2	1.93	0.50
1:B:474:LYS:HE2	1:B:478:GLN:NE2	2.25	0.50
1:B:183:VAL:HG13	4:B:2141:HOH:O	2.11	0.50
1:D:511:PHE:HZ	1:D:528:LYS:HE2	1.76	0.50
1:C:476:ALA:CB	1:C:534:ILE:HD12	2.42	0.49
1:A:414:THR:HG21	4:A:2168:HOH:O	2.13	0.49
1:B:95:PRO:HB2	1:B:99[B]:ARG:HH12	1.78	0.49
1:B:176:ILE:HG21	3:B:1588:PL3:H2C1	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439:LYS:HD2	4:B:2274:HOH:O	2.11	0.49
1:B:387:ILE:HA	1:B:390:PHE:O	2.12	0.49
1:C:323:TYR:CE2	1:C:350:MET:HE3	2.46	0.49
1:C:403:GLU:OE2	1:C:434:LYS:HE3	2.12	0.49
1:C:184:SER:HB3	4:C:2132:HOH:O	2.11	0.49
1:C:456:TRP:CG	1:C:524:TYR:HE2	2.30	0.49
1:B:439:LYS:C	1:B:439:LYS:HD3	2.39	0.48
1:A:207:GLU:O	1:A:313:LYS:NZ	2.43	0.48
1:C:44:THR:HB	1:C:45:PRO:HD2	1.96	0.48
1:A:365:TRP:O	1:A:365:TRP:CD1	2.67	0.48
1:A:456:TRP:CD1	1:A:524:TYR:HE2	2.31	0.48
1:B:443:LEU:N	1:B:444:PRO:HD2	2.28	0.48
1:D:187:ARG:O	1:D:189:THR:HG22	2.14	0.47
1:D:356:PRO:O	1:D:360:GLN:HG3	2.13	0.47
1:A:506:CYS:HB2	4:A:2441:HOH:O	2.13	0.47
1:D:12:HIS:HE1	1:D:14:ASP:OD1	1.96	0.47
1:C:563:GLY:HA2	4:C:2317:HOH:O	2.14	0.47
1:A:166:VAL:HB	1:A:189:THR:HB	1.96	0.47
1:B:221:LEU:C	1:B:221:LEU:HD23	2.39	0.47
1:B:410:ASP:OD1	1:B:413:ARG:NH2	2.41	0.47
1:C:495:ALA:HA	1:C:508:TYR:O	2.15	0.47
1:D:92:LYS:CE	1:D:185:ASN:O	2.56	0.46
1:D:366:LYS:O	1:D:366:LYS:HG2	2.14	0.46
1:A:208:MET:HE1	1:A:230:VAL:CG1	2.45	0.45
1:A:62:GLU:HA	1:A:62:GLU:OE1	2.16	0.45
1:A:108:ASP:OD1	1:A:108:ASP:C	2.58	0.45
1:B:410:ASP:O	1:B:414:THR:CG2	2.54	0.45
1:D:537:LYS:O	1:D:537:LYS:HG2	2.17	0.45
1:C:476:ALA:HA	1:C:534:ILE:HD12	1.99	0.45
1:B:205:ARG:HD2	4:B:2154:HOH:O	2.15	0.45
1:D:255:HIS:HB3	1:D:350:MET:CE	2.46	0.45
1:B:52:LEU:HD23	1:B:367:PRO:HA	1.98	0.45
3:B:1588:PL3:H4C2	3:B:1588:PL3:H1C1	1.57	0.45
1:B:198:ASN:HD22	1:B:198:ASN:N	2.12	0.44
1:C:134:ILE:HG23	4:C:2096:HOH:O	2.17	0.44
1:A:374:GLU:HB3	4:A:2343:HOH:O	2.17	0.44
1:C:350:MET:HG2	1:C:351:ILE:N	2.33	0.44
1:C:363:PHE:HD1	1:C:380:VAL:HG22	1.83	0.44
1:A:517:GLU:O	1:A:517:GLU:HG3	2.18	0.44
1:D:42:MET:HE2	1:D:365:TRP:HH2	1.83	0.44
1:C:30:PHE:C	1:C:42:MET:HE2	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:366:LYS:HA	1:D:367:PRO:HD3	1.74	0.43
1:C:96:GLU:CD	1:C:96:GLU:H	2.25	0.43
1:C:410:ASP:O	1:C:414:THR:CG2	2.66	0.43
1:A:530:LEU:C	1:A:530:LEU:HD23	2.44	0.43
1:D:506:CYS:HB2	4:D:2320:HOH:O	2.18	0.43
1:A:520:ASP:O	1:A:523:GLN:HG2	2.19	0.43
1:D:350:MET:HG3	1:D:351:ILE:N	2.34	0.43
1:A:563:GLY:HA2	4:A:2466:HOH:O	2.18	0.43
1:A:221:LEU:C	1:A:221:LEU:HD23	2.44	0.43
1:A:134:ILE:HG23	4:A:2141:HOH:O	2.17	0.43
1:A:208:MET:HE2	1:A:314:VAL:C	2.44	0.43
1:A:450:LEU:HD11	3:A:1588:PL3:HDC2	2.01	0.43
1:A:562:ARG:C	1:A:564:TRP:H	2.25	0.42
1:B:183:VAL:O	1:B:183:VAL:CG1	2.68	0.42
1:B:268:VAL:CG2	1:B:313:LYS:HG3	2.49	0.42
1:A:338:LEU:HD12	1:A:351:ILE:HD13	2.01	0.42
1:B:154:GLU:HA	1:B:273:VAL:HG11	2.01	0.42
1:C:456:TRP:CD1	1:C:524:TYR:HE2	2.38	0.42
1:D:24:TRP:CG	1:D:444:PRO:HB2	2.54	0.42
1:D:31:LEU:HD12	1:D:446:ILE:HA	2.02	0.42
1:D:536:PHE:C	1:D:538:TYR:H	2.28	0.42
1:A:338:LEU:HG	1:A:500:THR:HG21	2.01	0.42
1:B:291:ILE:N	1:B:291:ILE:CD1	2.83	0.42
1:D:463:THR:OG1	1:D:541:SER:HB3	2.20	0.42
1:A:542:LEU:O	1:A:543:SER:HB3	2.20	0.42
1:D:170:MET:HE2	1:D:195:ARG:NH2	2.35	0.41
1:C:293:TYR:HD2	1:C:296:ILE:HD12	1.84	0.41
1:D:511:PHE:HZ	1:D:528:LYS:CE	2.32	0.41
1:A:516:ASN:ND2	1:A:518:ASN:OD1	2.54	0.41
1:B:437:ALA:O	1:B:440:ARG:HD3	2.20	0.41
1:C:208:MET:HE2	1:C:315:HIS:C	2.46	0.41
1:C:480:PHE:CZ	1:C:511:PHE:HB2	2.55	0.41
1:A:202:TRP:CE2	1:A:211:CYS:HB2	2.56	0.41
1:C:56:ARG:NH1	1:C:75:LEU:HD22	2.36	0.41
1:D:38:GLY:O	1:D:56:ARG:NH1	2.53	0.41
1:A:376:THR:HA	1:A:379:MET:CE	2.51	0.41
1:B:400:ILE:HD12	1:B:420:LEU:HD11	2.03	0.41
1:D:18:GLN:HG2	4:D:2022:HOH:O	2.21	0.41
1:D:391:ASP:HB2	4:D:2278:HOH:O	2.21	0.41
1:C:534:ILE:O	1:C:537:LYS:HB3	2.22	0.40
1:B:144:ILE:N	1:B:144:ILE:HD12	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:521:MET:HE3	1:B:521:MET:HB2	1.95	0.40
1:B:506:CYS:CB	4:B:2325:HOH:O	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	545/584 (93%)	538 (99%)	7 (1%)	0	100	100
1	B	529/584 (91%)	518 (98%)	10 (2%)	1 (0%)	43	36
1	C	531/584 (91%)	525 (99%)	6 (1%)	0	100	100
1	D	525/584 (90%)	513 (98%)	10 (2%)	2 (0%)	30	21
All	All	2130/2336 (91%)	2094 (98%)	33 (2%)	3 (0%)	48	41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	537	LYS
1	B	562	ARG
1	D	367	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	484/507 (96%)	465 (96%)	19 (4%)	28	18
1	B	474/507 (94%)	454 (96%)	20 (4%)	26	16
1	C	472/507 (93%)	459 (97%)	13 (3%)	38	30
1	D	468/507 (92%)	450 (96%)	18 (4%)	29	19
All	All	1898/2028 (94%)	1828 (96%)	70 (4%)	31	20

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	GLU
1	A	75	LEU
1	A	96	GLU
1	A	101	LEU
1	A	108	ASP
1	A	170	MET
1	A	186	GLU
1	A	189	THR
1	A	208	MET
1	A	338	LEU
1	A	372	VAL
1	A	382[A]	LYS
1	A	382[B]	LYS
1	A	414	THR
1	A	440	ARG
1	A	518	ASN
1	A	520	ASP
1	A	569	ARG
1	A	586	LEU
1	B	46	GLU
1	B	64	THR
1	B	75	LEU
1	B	96	GLU
1	B	101	LEU
1	B	170	MET
1	B	183	VAL
1	B	185	ASN
1	B	186	GLU
1	B	189	THR
1	B	198	ASN
1	B	291	ILE
1	B	338	LEU
1	B	388	ARG

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Mol	Chain	Res	Type
1	B	414	THR
1	B	440	ARG
1	B	485	LYS
1	B	521	MET
1	B	525	ILE
1	B	530	LEU
1	C	42	MET
1	C	65	LEU
1	C	71	LYS
1	C	75	LEU
1	C	96	GLU
1	C	170	MET
1	C	189	THR
1	C	221	LEU
1	C	264	GLU
1	C	291	ILE
1	C	338	LEU
1	C	376	THR
1	C	414	THR
1	D	73	PHE
1	D	75	LEU
1	D	101	LEU
1	D	170	MET
1	D	189	THR
1	D	198	ASN
1	D	336	SER
1	D	338	LEU
1	D	350	MET
1	D	366	LYS
1	D	414	THR
1	D	435	THR
1	D	439	LYS
1	D	440	ARG
1	D	528	LYS
1	D	532	THR
1	D	584	ARG
1	D	585	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	HIS

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Mol	Chain	Res	Type
1	A	82	GLN
1	A	93	GLN
1	A	161	HIS
1	A	226	HIS
1	A	256	GLN
1	A	315	HIS
1	A	470	GLN
1	A	499	HIS
1	A	523	GLN
1	B	12	HIS
1	B	33	GLN
1	B	161	HIS
1	B	198	ASN
1	B	256	GLN
1	B	283	ASN
1	B	315	HIS
1	B	340	GLN
1	B	423	ASN
1	B	478	GLN
1	B	499	HIS
1	C	12	HIS
1	C	82	GLN
1	C	87	HIS
1	C	224	GLN
1	C	283	ASN
1	C	454	ASN
1	C	487	GLN
1	C	499	HIS
1	D	12	HIS
1	D	17	GLN
1	D	85	ASN
1	D	198	ASN
1	D	315	HIS
1	D	394	ASN
1	D	487	GLN
1	D	523	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](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FAD	B	1587	-	58,58,58	1.42	8 (13%)	85,89,89	1.82	22 (25%)
2	FAD	A	1587	-	58,58,58	1.43	8 (13%)	85,89,89	1.61	16 (18%)
3	PL3	C	1587	-	16,16,16	0.95	1 (6%)	15,15,15	0.88	0
3	PL3	A	1588	-	16,16,16	0.92	1 (6%)	15,15,15	0.84	0
3	PL3	D	1587	-	16,16,16	0.94	1 (6%)	15,15,15	0.74	0
3	PL3	B	1588	-	16,16,16	0.99	1 (6%)	15,15,15	0.73	0
2	FAD	C	1586	-	58,58,58	1.42	10 (17%)	85,89,89	1.51	13 (15%)
2	FAD	D	1586	-	58,58,58	1.37	7 (12%)	85,89,89	1.63	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	B	1587	-	-	3/34/50/50	0/6/6/6
2	FAD	A	1587	-	-	2/34/50/50	0/6/6/6
3	PL3	C	1587	-	-	5/14/14/14	-
3	PL3	A	1588	-	-	8/14/14/14	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PL3	D	1587	-	-	8/14/14/14	-
3	PL3	B	1588	-	-	8/14/14/14	-
2	FAD	C	1586	-	-	4/34/50/50	0/6/6/6
2	FAD	D	1586	-	-	4/34/50/50	0/6/6/6

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1586	FAD	P-O3P	4.63	1.64	1.59
2	A	1587	FAD	C4X-N5	4.54	1.40	1.30
2	C	1586	FAD	C4X-N5	4.22	1.39	1.30
2	B	1587	FAD	C2A-N3A	4.14	1.41	1.33
2	D	1586	FAD	P-O3P	4.06	1.63	1.59
2	B	1587	FAD	C4X-N5	3.94	1.39	1.30
2	D	1586	FAD	C4X-N5	3.87	1.39	1.30
2	A	1587	FAD	C10-N1	3.84	1.41	1.33
3	B	1588	PL3	O1-C1	-3.84	1.22	1.42
3	C	1587	PL3	O1-C1	-3.69	1.23	1.42
3	D	1587	PL3	O1-C1	-3.68	1.23	1.42
3	A	1588	PL3	O1-C1	-3.64	1.23	1.42
2	A	1587	FAD	C1'-C2'	3.59	1.57	1.52
2	B	1587	FAD	C1'-C2'	3.57	1.57	1.52
2	D	1586	FAD	C2A-N1A	3.49	1.40	1.33
2	A	1587	FAD	C2A-N3A	3.15	1.39	1.33
2	D	1586	FAD	C5'-C4'	2.94	1.55	1.51
2	B	1587	FAD	C8A-N7A	2.93	1.37	1.31
2	B	1587	FAD	C2A-N1A	2.72	1.38	1.33
2	C	1586	FAD	C1'-N10	2.72	1.54	1.47
2	A	1587	FAD	C9-C8	2.71	1.43	1.39
2	C	1586	FAD	C10-N1	2.65	1.38	1.33
2	B	1587	FAD	C6-C5X	2.57	1.43	1.40
2	D	1586	FAD	C1'-N10	2.37	1.53	1.47
2	D	1586	FAD	C5A-N7A	-2.37	1.34	1.39
2	C	1586	FAD	PA-O3P	2.31	1.62	1.59
2	B	1587	FAD	PA-O3P	2.27	1.62	1.59
2	C	1586	FAD	C5'-C4'	2.22	1.54	1.51
2	C	1586	FAD	C8A-N7A	2.21	1.35	1.31
2	D	1586	FAD	PA-O3P	2.19	1.61	1.59
2	C	1586	FAD	C5X-N5	-2.17	1.35	1.39
2	C	1586	FAD	C4A-N3A	2.08	1.38	1.34
2	A	1587	FAD	C8A-N7A	2.08	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1587	FAD	C6-C5X	2.07	1.43	1.40
2	B	1587	FAD	C2'-C3'	2.05	1.57	1.53
2	C	1586	FAD	C2A-N3A	2.01	1.37	1.33
2	A	1587	FAD	C4X-C10	-2.00	1.38	1.44

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1587	FAD	N3A-C2A-N1A	-6.73	118.39	128.58
2	D	1586	FAD	N3A-C2A-N1A	-6.69	118.45	128.58
2	C	1586	FAD	N3A-C2A-N1A	-6.05	119.43	128.58
2	A	1587	FAD	N3A-C2A-N1A	-5.81	119.78	128.58
2	D	1586	FAD	N9A-C8A-N7A	-4.33	107.79	113.94
2	B	1587	FAD	C4X-C10-N10	4.30	122.64	116.48
2	C	1586	FAD	N9A-C8A-N7A	-3.57	108.88	113.94
2	B	1587	FAD	C5X-C9A-N10	3.48	121.11	117.97
2	B	1587	FAD	O4'-C4'-C5'	-3.47	102.33	109.99
2	D	1586	FAD	C5A-N7A-C8A	3.44	108.85	103.45
2	A	1587	FAD	C4X-C10-N10	3.42	121.38	116.48
2	C	1586	FAD	C4-N3-C2	-3.34	119.72	125.64
2	D	1586	FAD	O2P-P-O5'	3.22	122.18	107.57
2	D	1586	FAD	C4A-N9A-C8A	3.13	109.03	105.74
2	D	1586	FAD	C4X-C10-N10	3.13	120.96	116.48
2	B	1587	FAD	C10-C4X-N5	-3.06	118.56	124.81
2	C	1586	FAD	C5A-C4A-N3A	-3.01	122.57	126.72
2	A	1587	FAD	N9A-C8A-N7A	-2.99	109.69	113.94
2	A	1587	FAD	C4A-C5A-N7A	-2.99	107.16	110.58
2	B	1587	FAD	C2A-N1A-C6A	2.99	123.64	118.73
2	D	1586	FAD	C10-C4X-N5	-2.99	118.71	124.81
2	C	1586	FAD	C2A-N3A-C4A	2.97	119.07	111.83
2	C	1586	FAD	C10-C4X-N5	-2.91	118.87	124.81
2	B	1587	FAD	C8M-C8-C9	-2.90	114.46	119.57
2	B	1587	FAD	C2A-N3A-C4A	2.88	118.86	111.83
2	A	1587	FAD	C5A-N7A-C8A	2.85	107.93	103.45
2	C	1586	FAD	C4X-C4-N3	2.85	120.50	113.25
2	B	1587	FAD	C5A-C4A-N3A	-2.82	122.83	126.72
2	B	1587	FAD	C4A-C5A-N7A	-2.81	107.37	110.58
2	A	1587	FAD	C5A-C4A-N3A	-2.81	122.85	126.72
2	D	1586	FAD	C2A-N1A-C6A	2.79	123.32	118.73
2	B	1587	FAD	N9A-C8A-N7A	-2.78	109.98	113.94
2	D	1586	FAD	C2A-N3A-C4A	2.77	118.60	111.83
2	C	1586	FAD	C4-C4X-N5	2.77	122.04	118.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1587	FAD	C9-C9A-N10	-2.74	118.17	121.85
2	B	1587	FAD	C5A-N7A-C8A	2.70	107.70	103.45
2	D	1586	FAD	C9A-C5X-N5	-2.70	119.59	122.45
2	B	1587	FAD	C4-N3-C2	-2.67	120.89	125.64
2	A	1587	FAD	C4X-C4-N3	2.67	120.05	113.25
2	B	1587	FAD	O2P-P-O3P	2.67	114.49	107.27
2	D	1586	FAD	C5X-C9A-N10	2.66	120.37	117.97
2	A	1587	FAD	C2A-N1A-C6A	2.62	123.03	118.73
2	B	1587	FAD	O4B-C1B-N9A	-2.62	103.06	108.09
2	D	1586	FAD	C5A-C4A-N3A	-2.61	123.12	126.72
2	A	1587	FAD	C4-N3-C2	-2.61	121.00	125.64
2	A	1587	FAD	C2A-N3A-C4A	2.60	118.19	111.83
2	C	1586	FAD	C4X-C10-N10	2.60	120.20	116.48
2	B	1587	FAD	C9A-N10-C10	-2.58	116.81	120.75
2	A	1587	FAD	O4B-C1B-N9A	-2.58	103.14	108.09
2	B	1587	FAD	O2-C2-N1	-2.51	117.63	121.80
2	B	1587	FAD	C4-C4X-N5	2.45	121.59	118.21
2	B	1587	FAD	C5'-C4'-C3'	2.43	116.81	112.22
2	D	1586	FAD	C4-C4X-N5	2.38	121.50	118.21
2	A	1587	FAD	C8M-C8-C9	-2.36	115.41	119.57
2	A	1587	FAD	C2'-C1'-N10	2.36	121.36	110.20
2	A	1587	FAD	C5X-C9A-N10	2.36	120.10	117.97
2	D	1586	FAD	N3A-C4A-N9A	2.36	131.18	127.17
2	C	1586	FAD	C4A-N9A-C8A	2.34	108.20	105.74
2	C	1586	FAD	C5A-N7A-C8A	2.32	107.10	103.45
2	B	1587	FAD	C9A-C5X-N5	-2.29	120.02	122.45
2	A	1587	FAD	O2-C2-N1	-2.21	118.13	121.80
2	B	1587	FAD	O3'-C3'-C4'	-2.13	104.08	108.93
2	C	1586	FAD	C9A-C5X-N5	-2.13	120.20	122.45
2	C	1586	FAD	N3A-C4A-N9A	2.06	130.66	127.17
2	D	1586	FAD	C4-N3-C2	-2.02	122.06	125.64
2	B	1587	FAD	C4X-C10-N1	-2.01	119.67	124.59

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1587	FAD	N10-C1'-C2'-O2'
2	A	1587	FAD	N10-C1'-C2'-C3'
2	B	1587	FAD	N10-C1'-C2'-O2'
2	B	1587	FAD	N10-C1'-C2'-C3'
2	C	1586	FAD	N10-C1'-C2'-O2'

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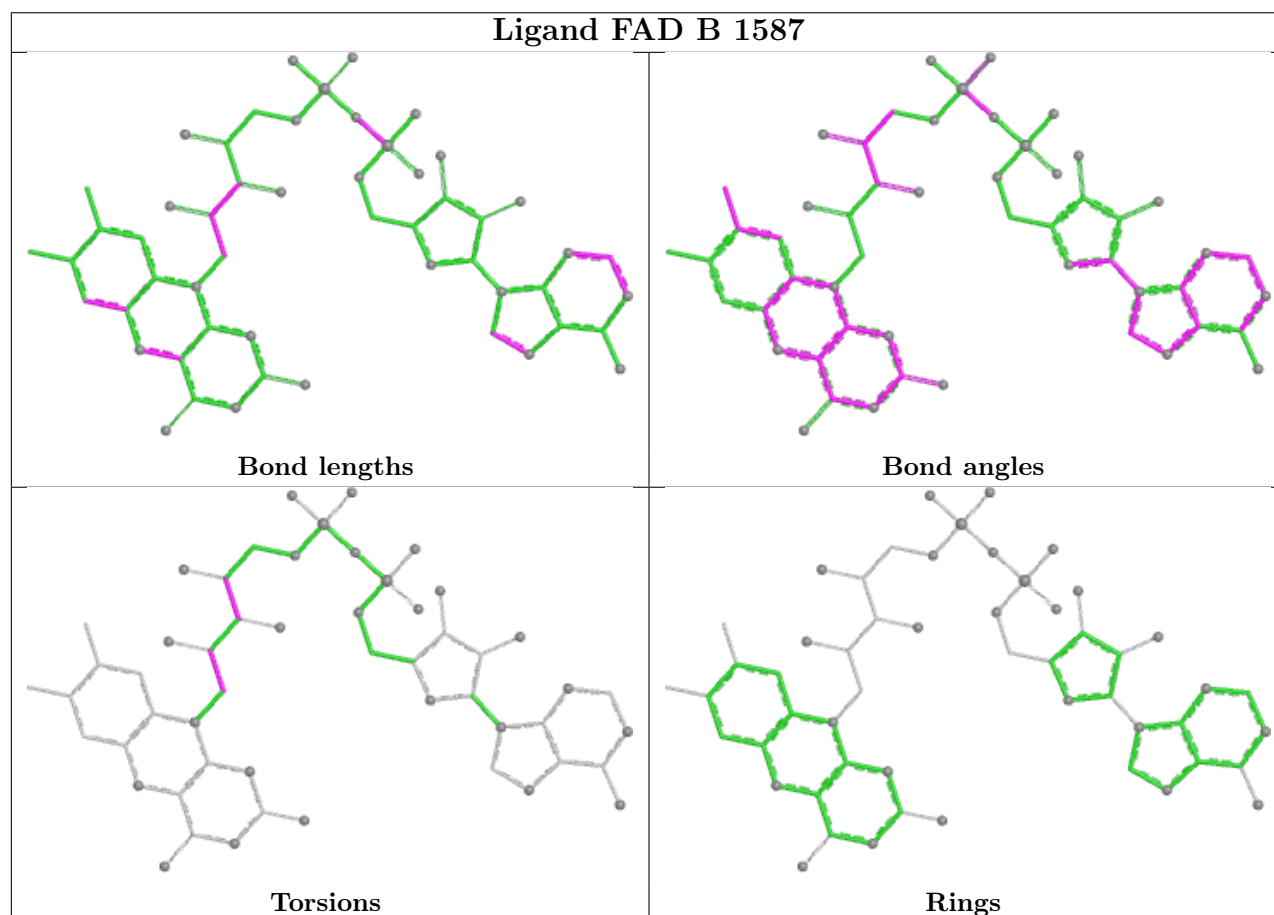
Mol	Chain	Res	Type	Atoms
2	C	1586	FAD	N10-C1'-C2'-C3'
2	D	1586	FAD	N10-C1'-C2'-O2'
2	D	1586	FAD	N10-C1'-C2'-C3'
3	B	1588	PL3	C1-C2-C3-C4
3	A	1588	PL3	CB-CC-CD-CE
3	B	1588	PL3	CC-CD-CE-CF
3	A	1588	PL3	C1-C2-C3-C4
3	B	1588	PL3	C4-C5-C6-C7
3	B	1588	PL3	C3-C4-C5-C6
3	D	1587	PL3	C9-CA-CB-CC
3	A	1588	PL3	CC-CD-CE-CF
3	C	1587	PL3	C4-C5-C6-C7
3	D	1587	PL3	CB-CC-CD-CE
3	A	1588	PL3	C8-C9-CA-CB
3	D	1587	PL3	C2-C3-C4-C5
3	D	1587	PL3	O1-C1-C2-C3
3	D	1587	PL3	C4-C5-C6-C7
3	A	1588	PL3	C4-C5-C6-C7
3	C	1587	PL3	C9-CA-CB-CC
3	D	1587	PL3	C7-C8-C9-CA
3	B	1588	PL3	C5-C6-C7-C8
3	D	1587	PL3	C5-C6-C7-C8
3	A	1588	PL3	C5-C6-C7-C8
3	B	1588	PL3	C6-C7-C8-C9
3	D	1587	PL3	CC-CD-CE-CF
3	C	1587	PL3	C2-C3-C4-C5
3	B	1588	PL3	CA-CB-CC-CD
3	A	1588	PL3	C9-CA-CB-CC
3	B	1588	PL3	O1-C1-C2-C3
2	C	1586	FAD	PA-O3P-P-O2P
3	C	1587	PL3	C3-C4-C5-C6
3	A	1588	PL3	O1-C1-C2-C3
2	D	1586	FAD	PA-O3P-P-O1P
2	D	1586	FAD	PA-O3P-P-O2P
2	B	1587	FAD	C2'-C3'-C4'-C5'
3	C	1587	PL3	CB-CC-CD-CE
2	C	1586	FAD	PA-O3P-P-O1P

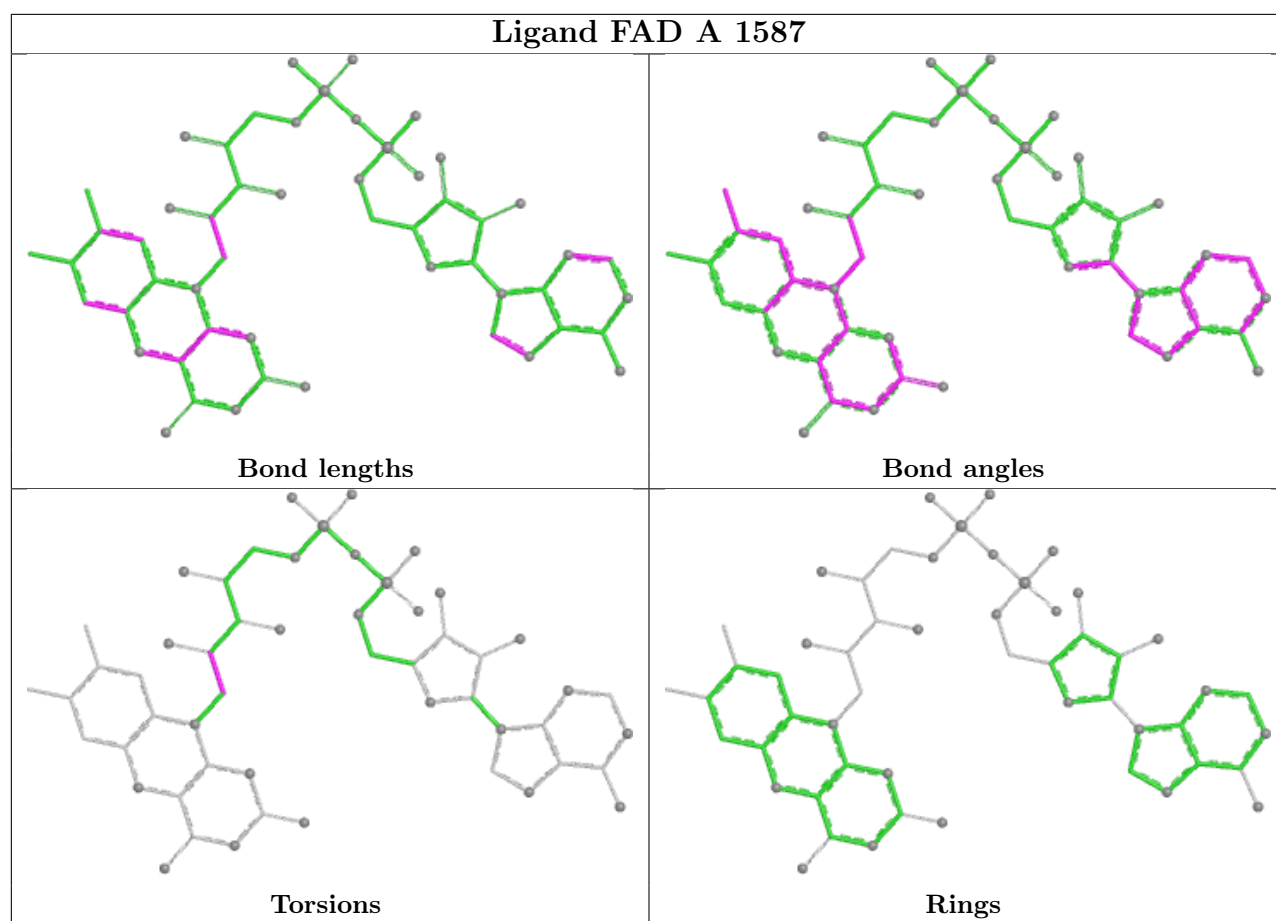
There are no ring outliers.

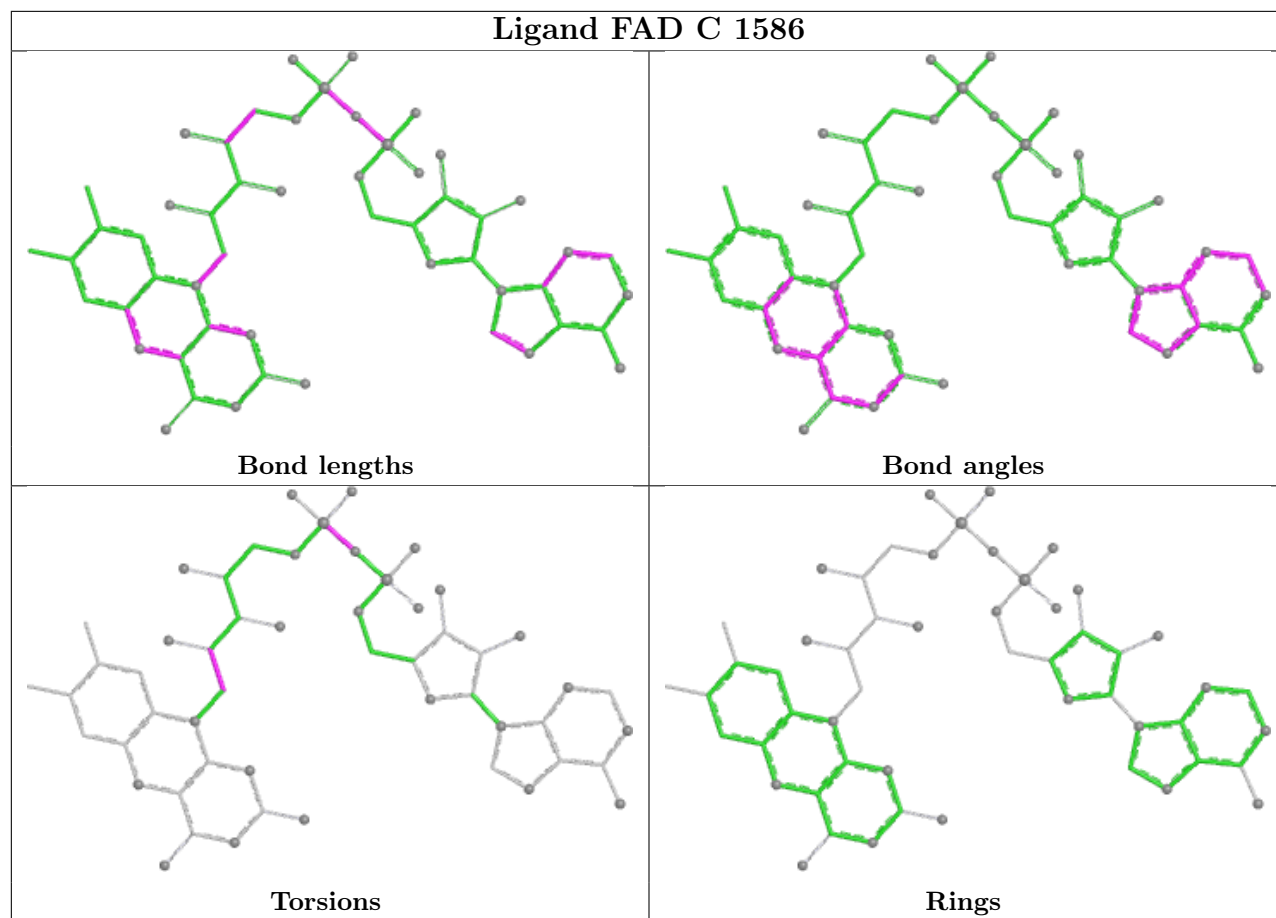
2 monomers are involved in 6 short contacts:

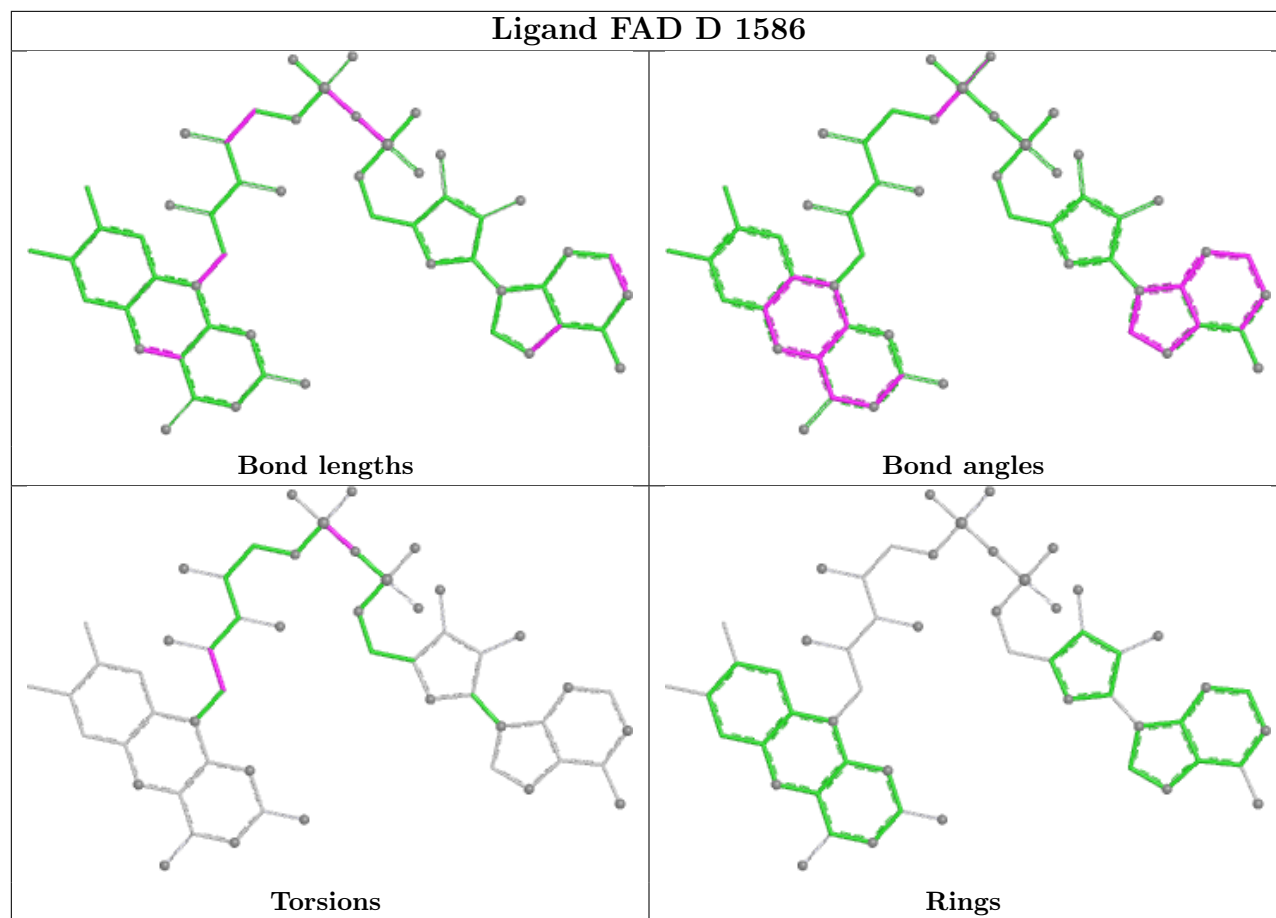
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1588	PL3	4	0
3	B	1588	PL3	2	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.