Full wwPDB X-ray Structure Validation Report ⓘ

May 4, 2024 – 09:11 am BST

PDB ID	:	2UUV
Title	:	alkyldihydroxyacetonephosphate synthase in P1
Authors	:	Razeto, A.; Mattiroli, 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:

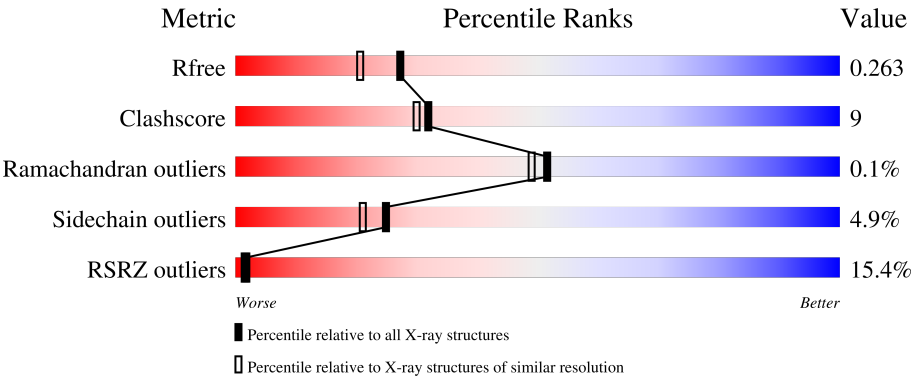
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 <=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% 76% 11% • 10%
1	B	584	13% 75% 13% • 10%
1	C	584	21% 65% 15% • • 16%
1	D	584	11% 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)

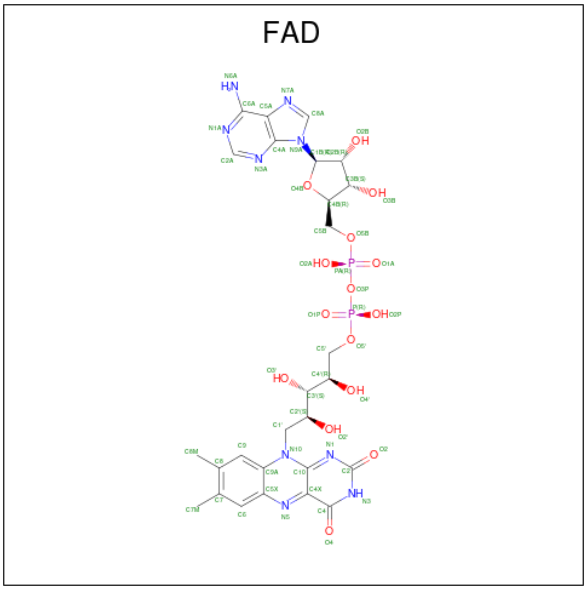
There are 4 unique types of molecules in this entry. The entry contains 17951 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: 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		

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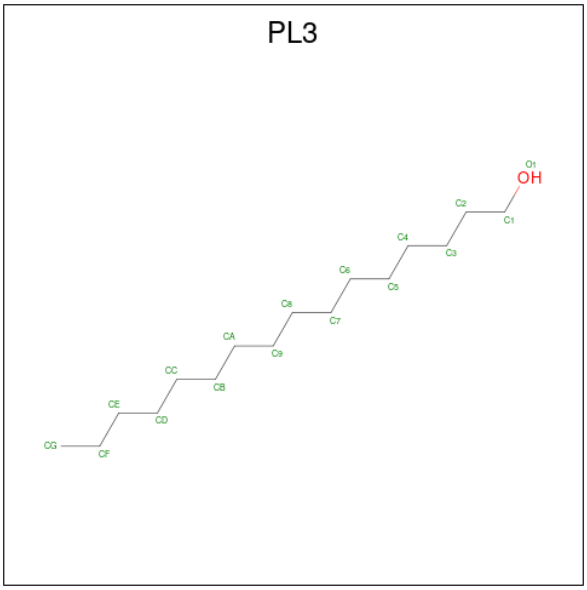
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C N O P 53 27 9 15 2	0	0
2	D	1	Total C N O P 53 27 9 15 2	0	0

- Molecule 3 is HEXADECAN-1-OL (three-letter code: PL3) (formula: $C_{16}H_{34}O$).



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

- Molecule 4 is water.

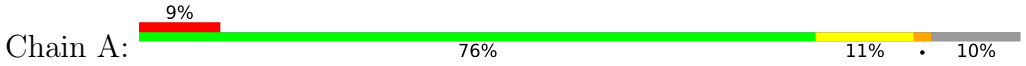
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	318	Total O 318 318	0	0
4	B	265	Total O 265 265	0	0
4	C	239	Total O 239 239	0	0
4	D	312	Total O 312 312	0	0

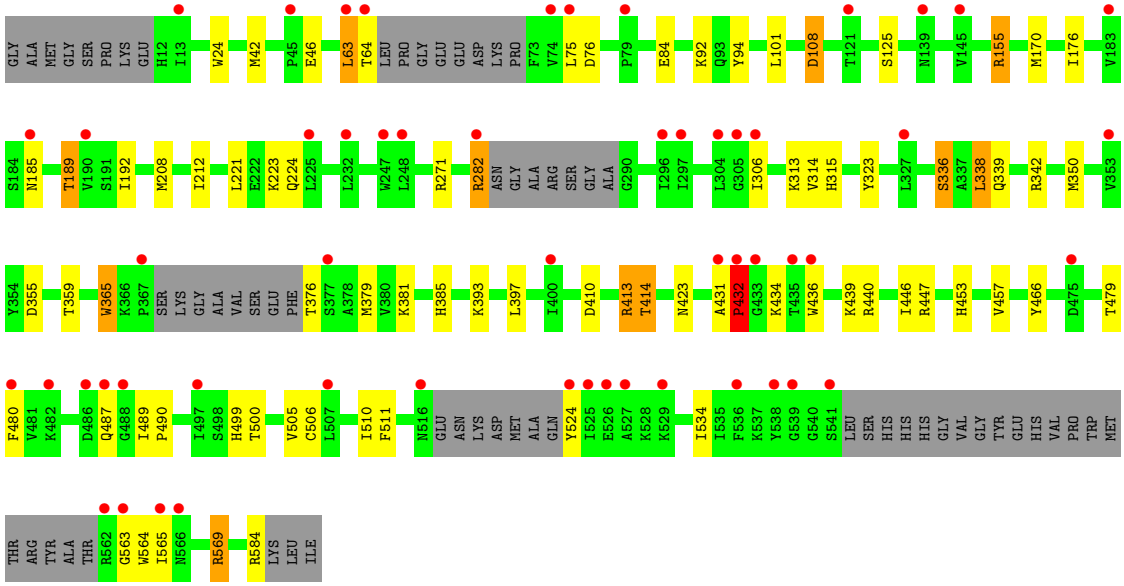
3 Residue-property plots (i)

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 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

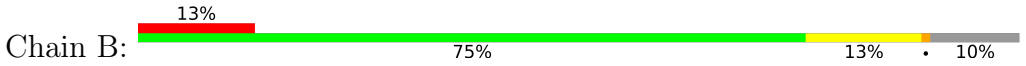
Chain A:

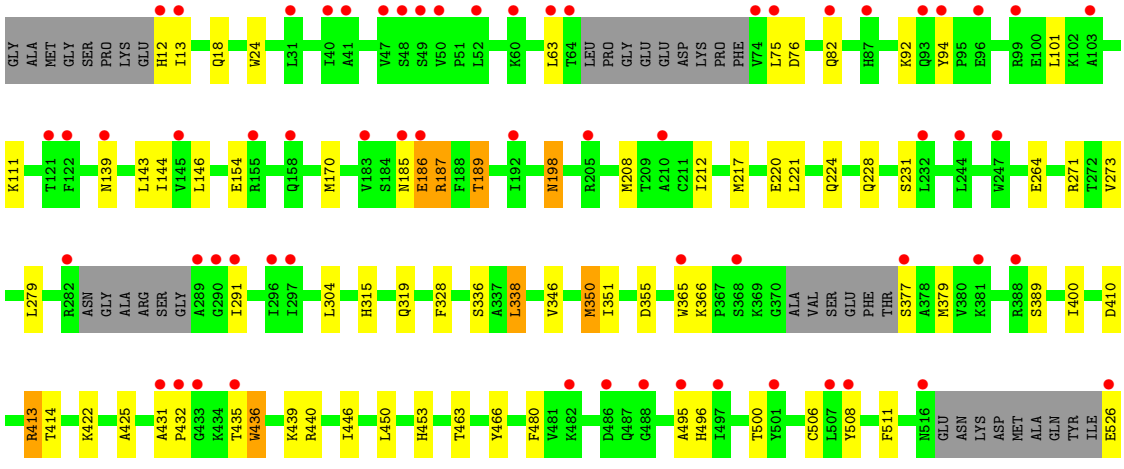


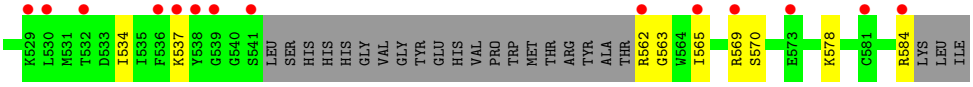


• Molecule 1: ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE

Chain B:

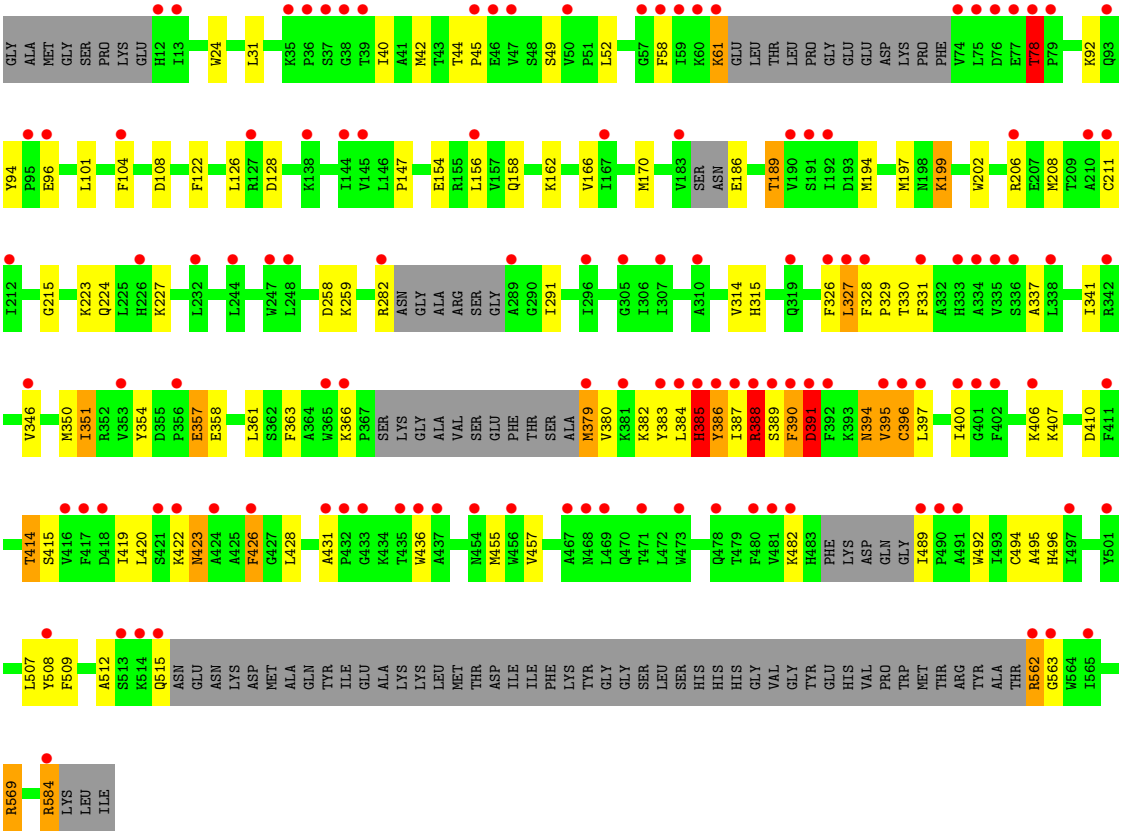






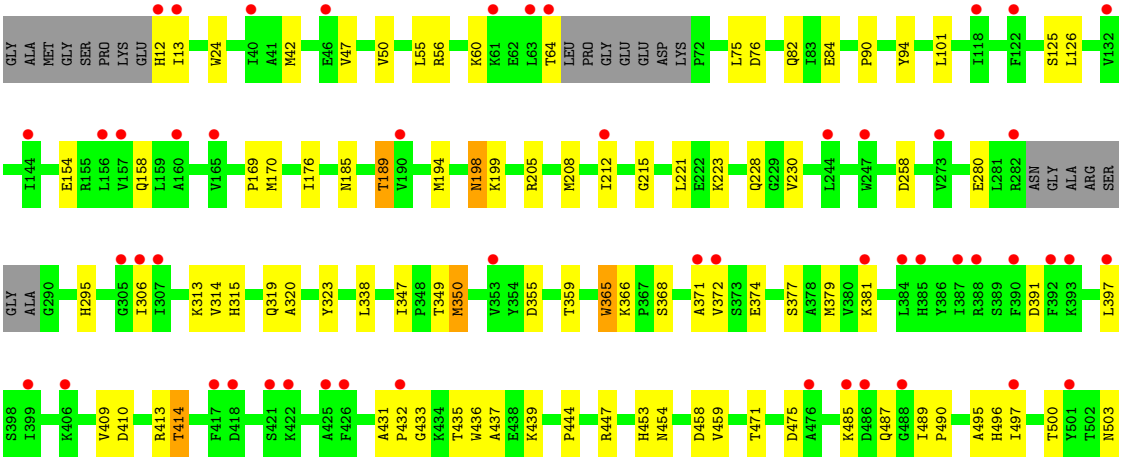
• Molecule 1: ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE

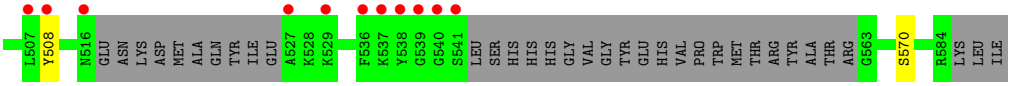
Chain C:



• Molecule 1: ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE

Chain D:




L507
Y508
N516
GLU
ASN
LYS
ASP
MET
ALA
GLN
TYR
ILE
GLU
A527
K528
K529
F536
K537
Y538
G539
G540
S541
LEU
SER
HIS
HIS
HIS
GLY
VAL
GLY
TYR
GLU
HIS
VAL
PRO
TRP
MET
THR
ARG
TYR
ALA
THR
ARG
G563
S570
R584
LYS
LEU
ILE

4 Data and refinement statistics (i)

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) 92.7 (19.98-1.99)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (5.03%)	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)	0.36 , 58.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	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.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (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	0.77	0/4308	0.76	3/5833 (0.1%)
1	B	0.75	1/4292 (0.0%)	0.77	4/5809 (0.1%)
1	C	1.33	37/4051 (0.9%)	0.96	17/5485 (0.3%)
1	D	0.75	0/4331	0.76	2/5865 (0.0%)
All	All	0.93	38/16982 (0.2%)	0.81	26/22992 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	61	LYS	C-O	21.04	1.63	1.23
1	C	390	PHE	CG-CD1	17.50	1.65	1.38
1	C	395	VAL	CB-CG1	16.88	1.88	1.52
1	C	61	LYS	CD-CE	16.15	1.91	1.51
1	C	395	VAL	CB-CG2	14.70	1.83	1.52
1	C	384	LEU	C-N	14.51	1.67	1.34
1	C	426	PHE	C-N	13.89	1.58	1.33
1	C	327	LEU	C-O	13.23	1.48	1.23
1	C	390	PHE	CE1-CZ	12.68	1.61	1.37
1	C	388	ARG	C-O	11.48	1.45	1.23
1	C	388	ARG	CD-NE	11.26	1.65	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	78	THR	CB-OG1	10.98	1.65	1.43
1	C	396	CYS	C-N	9.94	1.56	1.34
1	C	391	ASP	CG-OD2	9.77	1.47	1.25
1	C	383	TYR	CG-CD2	9.48	1.51	1.39
1	C	382	LYS	C-N	8.93	1.54	1.34
1	C	391	ASP	CB-CG	8.68	1.70	1.51
1	C	389	SER	C-N	8.50	1.53	1.34
1	C	388	ARG	CZ-NH1	8.35	1.44	1.33
1	C	389	SER	CA-CB	8.20	1.65	1.52
1	C	426	PHE	C-O	8.09	1.38	1.23
1	C	390	PHE	C-O	-7.95	1.08	1.23
1	C	415	SER	CB-OG	7.75	1.52	1.42
1	C	387	ILE	CA-CB	7.63	1.72	1.54
1	C	391	ASP	N-CA	-7.48	1.31	1.46
1	C	61	LYS	CG-CD	7.12	1.76	1.52
1	C	423	ASN	CG-OD1	7.11	1.39	1.24
1	C	390	PHE	CE2-CZ	6.18	1.49	1.37
1	C	394	ASN	CG-OD1	5.99	1.37	1.24
1	C	422	LYS	C-N	5.96	1.47	1.34
1	C	390	PHE	CA-CB	5.84	1.66	1.53
1	C	383	TYR	CE1-CZ	5.82	1.46	1.38
1	C	384	LEU	C-O	5.66	1.34	1.23
1	C	389	SER	CB-OG	5.53	1.49	1.42
1	B	422	LYS	CD-CE	5.29	1.64	1.51
1	C	385	HIS	CD2-NE2	5.23	1.52	1.42
1	C	78	THR	CB-CG2	5.15	1.69	1.52
1	C	363	PHE	CG-CD2	5.11	1.46	1.38

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	389	SER	O-C-N	10.75	139.90	122.70
1	B	187	ARG	NE-CZ-NH2	-8.97	115.82	120.30
1	C	386	TYR	CB-CG-CD2	-8.38	115.97	121.00
1	C	389	SER	CA-C-N	-8.21	99.13	117.20
1	C	388	ARG	NE-CZ-NH1	-8.09	116.25	120.30
1	B	413	ARG	NE-CZ-NH2	-8.05	116.28	120.30
1	B	187	ARG	NE-CZ-NH1	7.99	124.29	120.30
1	C	61	LYS	CG-CD-CE	-7.75	88.65	111.90
1	C	389	SER	C-N-CA	-6.86	104.56	121.70
1	C	395	VAL	CG1-CB-CG2	-6.74	100.12	110.90
1	D	413	ARG	NE-CZ-NH2	-6.39	117.11	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	396	CYS	CA-C-N	-6.33	103.27	117.20
1	C	385	HIS	CA-C-O	-6.29	106.89	120.10
1	C	387	ILE	CA-CB-CG1	6.25	122.87	111.00
1	C	61	LYS	CA-C-O	-6.23	107.01	120.10
1	C	61	LYS	CD-CE-NZ	-5.93	98.06	111.70
1	D	391	ASP	CB-CG-OD2	5.81	123.53	118.30
1	C	396	CYS	CA-C-O	5.74	132.15	120.10
1	B	413	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	A	432	PRO	N-CA-C	-5.70	97.28	112.10
1	A	413	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	C	391	ASP	CB-CG-OD1	-5.63	113.23	118.30
1	A	63	LEU	CA-CB-CG	5.56	128.10	115.30
1	C	395	VAL	CA-CB-CG1	-5.31	102.93	110.90
1	C	390	PHE	CB-CG-CD2	-5.16	117.19	120.80
1	C	386	TYR	CB-CG-CD1	5.15	124.09	121.00

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4200	0	4201	67	0
1	B	4186	0	4191	66	0
1	C	3947	0	3956	99	0
1	D	4221	0	4223	71	0
2	A	53	0	31	1	0
2	B	53	0	31	1	0
2	C	53	0	31	1	0
2	D	53	0	31	1	0
3	A	17	0	33	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	17	0	33	8	0
3	D	17	0	33	11	0
4	A	318	0	0	18	0
4	B	265	0	0	27	0
4	C	239	0	0	27	0
4	D	312	0	0	11	0
All	All	17951	0	16794	300	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 (300) 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:B:224[B]:GLN:OE1	4:B:2129:HOH:O	1.59	1.15
1:C:390:PHE:C	1:C:391:ASP:N	2.03	1.10
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:126:LEU:N	3:D:1586:PL3:H3C2	1.95	0.81
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:208:MET:HE3	1:A:314:VAL:HG23	1.65	0.76
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: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: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: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:A:208:MET:HE2	1:A:315:HIS:HA	1.78	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:C:208:MET:HE2	1:C:315:HIS:HA	1.80	0.64
1:D:487:GLN:HE21	1:D:489:ILE:HD12	1.62	0.64
1:A:569:ARG:HB3	1:A:569:ARG:NH1	2.12	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: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:C:78:THR:CB	1:C:78:THR:HG1	2.08	0.62
1:B:220:GLU:HG3	1:B:224[B]:GLN:HE21	1.62	0.62
1:D:379:MET:HE1	1:D:431:ALA:HA	1.81	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: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: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:D:24:TRP:CZ3	2:D:1585:FAD:HM83	2.39	0.57
1:C:208:MET:HE3	1:C:314:VAL:HG23	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
1:C:431:ALA:N	1:C:436:TRP:HE1	1.95	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:350:MET:HE3	4:B:2146:HOH:O	2.07	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:D:319:GLN:OE1	1:D:319:GLN:HA	2.08	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:176:ILE:HG21	3:D:1586:PL3:H5C1	1.92	0.51
1:D:208:MET:HE2	1:D:315:HIS:HA	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: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:C:224:GLN:HG3	4:C:2099:HOH:O	2.11	0.50
1:C:223:LYS:HE3	1:C:224:GLN:NE2	2.26	0.50
1:A:42:MET:CE	1:A:365:TRP:HH2	2.25	0.50
1:C:326:PHE:HB3	4:C:2201:HOH:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:327:LEU:HB3	1:C:395:VAL:CG1	2.42	0.50
1:D:379:MET:HE1	1:D:432:PRO:HD2	1.94	0.50
1:A:385:HIS:HE1	4:C:2159:HOH:O	1.94	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: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: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: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:A:24:TRP:CZ3	2:A:1585:FAD:HM83	2.48	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:B:111:LYS:NZ	4:B:2056:HOH:O	2.44	0.47
1:C:194:MET:HE3	1:C:197[B]:MET:HE3	1.96	0.47
1:D:359:THR:HG23	1:D:397:LEU:HB2	1.96	0.47
1:A:379:MET:HE1	4:A:2262:HOH:O	2.13	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:208:MET:HE3	1:D:314:VAL:HG23	1.98	0.46
1:D:374:GLU:OE2	1:D:439:LYS:HA	2.15	0.46
1:A:155:ARG:HD3	1:A:155:ARG:C	2.36	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:271:ARG:HD2	4:A:2198:HOH:O	2.17	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:143:LEU:C	1:B:144:ILE:HD12	2.37	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:D:12:HIS:HE1	4:D:2001:HOH:O	1.99	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:D:76:ASP:HB2	1:D:454:ASN:HB2	2.00	0.44
1:B:63:LEU:CD1	3:B:1586:PL3:HGC2	2.47	0.44
1:D:84:GLU:H	1:D:84:GLU:CD	2.21	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: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:C:24:TRP:CZ3	2:C:1585:FAD:HM83	2.52	0.43
1:D:496:HIS:CE1	1:D:508:TYR:CD1	3.06	0.43
1:C:31:LEU:CD2	1:C:42:MET:HE2	2.48	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:A:223:LYS:HZ2	1:A:224[B]:GLN:NE2	2.16	0.43
1:C:44:THR:HB	1:C:45:PRO:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:31:LEU:HG	1:C:42:MET:HE2	2.01	0.42
1:C:147:PRO:HG2	1:C:197[B]:MET:HE1	1.99	0.42
1:C:194:MET:CE	1:C:197[B]:MET:HE3	2.49	0.42
1:C:199:LYS:HD2	4:C:2081:HOH:O	2.20	0.42
1:D:208:MET:HE1	1:D:230:VAL:HG12	2.01	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:B:24:TRP:CZ3	2:B:1585:FAD:HM83	2.54	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
4:A:2242:HOH:O	1:C:282:ARG:HD2	2.20	0.42
1:B:13:ILE:HG22	1:B:18:GLN:HG3	2.02	0.42
1:A:42:MET:HE2	1:A:365:TRP:HH2	1.85	0.42
1:B:186:GLU:OE1	1:B:187:ARG:HD2	2.19	0.42
1:B:208:MET:HE2	1:B:315:HIS:HA	2.01	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:379:MET:CE	1:A:379:MET:HA	2.50	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:C:282:ARG:C	4:C:2143:HOH:O	2.59	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:162:LYS:NZ	4:C:2031:HOH:O	2.54	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	512/584 (88%)	503 (98%)	8 (2%)	1 (0%)	47	44
1	B	512/584 (88%)	502 (98%)	9 (2%)	1 (0%)	47	44
1	C	477/584 (82%)	462 (97%)	15 (3%)	0	100	100
1	D	519/584 (89%)	511 (98%)	7 (1%)	1 (0%)	47	44
All	All	2020/2336 (86%)	1978 (98%)	39 (2%)	3 (0%)	51	49

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 (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	460/507 (91%)	437 (95%)	23 (5%)	24	20
1	B	458/507 (90%)	431 (94%)	27 (6%)	19	15
1	C	433/507 (85%)	412 (95%)	21 (5%)	25	22
1	D	463/507 (91%)	446 (96%)	17 (4%)	34	32
All	All	1814/2028 (89%)	1726 (95%)	88 (5%)	25	21

All (88) 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	94	TYR
1	A	101	LEU
1	A	108	ASP
1	A	155	ARG
1	A	170	MET

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Mol	Chain	Res	Type
1	A	189	THR
1	A	282	ARG
1	A	336	SER
1	A	338	LEU
1	A	350	MET
1	A	355	ASP
1	A	365	TRP
1	A	381	LYS
1	A	414	THR
1	A	440	ARG
1	A	487	GLN
1	A	524	TYR
1	A	565	ILE
1	A	569	ARG
1	A	584	ARG
1	B	75	LEU
1	B	94	TYR
1	B	101	LEU
1	B	170	MET
1	B	186	GLU
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	377	SER
1	B	389	SER
1	B	435	THR
1	B	436	TRP
1	B	440	ARG
1	B	526	GLU
1	B	534	ILE
1	B	565	ILE
1	B	569	ARG
1	B	570	SER
1	B	584	ARG

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Mol	Chain	Res	Type
1	C	49	SER
1	C	78	THR
1	C	94	TYR
1	C	170	MET
1	C	186	GLU
1	C	189	THR
1	C	199	LYS
1	C	346	VAL
1	C	350	MET
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	482	LYS
1	C	489	ILE
1	C	562	ARG
1	C	569	ARG
1	C	584	ARG
1	D	13	ILE
1	D	42	MET
1	D	75	LEU
1	D	90	PRO
1	D	94	TYR
1	D	101	LEU
1	D	170	MET
1	D	189	THR
1	D	198	ASN
1	D	313	LYS
1	D	347	ILE
1	D	350	MET
1	D	355	ASP
1	D	365	TRP
1	D	414	THR
1	D	485	LYS
1	D	570	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	136	GLN
1	A	139	ASN
1	A	185	ASN
1	A	256	GLN
1	A	412	HIS
1	B	198	ASN
1	B	315	HIS
1	B	453	HIS
1	C	82	GLN
1	C	85	ASN
1	C	93	GLN
1	C	255	HIS
1	C	315	HIS
1	C	340	GLN
1	C	423	ASN
1	C	499	HIS
1	C	515	GLN
1	D	82	GLN
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 monosaccharides 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	B	1585	-	53,58,58	1.25	5 (9%)	68,89,89	1.61	10 (14%)
3	PL3	D	1586	-	16,16,16	0.98	1 (6%)	15,15,15	0.74	1 (6%)
3	PL3	B	1586	-	16,16,16	0.93	1 (6%)	15,15,15	0.69	0
2	FAD	C	1585	-	53,58,58	1.21	4 (7%)	68,89,89	1.44	9 (13%)
2	FAD	A	1585	-	53,58,58	1.26	6 (11%)	68,89,89	1.53	14 (20%)
2	FAD	D	1585	-	53,58,58	1.20	4 (7%)	68,89,89	1.69	13 (19%)
3	PL3	A	1586	-	16,16,16	0.86	1 (6%)	15,15,15	0.83	1 (6%)

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	1585	-	-	2/30/50/50	0/6/6/6
3	PL3	D	1586	-	-	4/14/14/14	-
3	PL3	B	1586	-	-	11/14/14/14	-
2	FAD	C	1585	-	-	2/30/50/50	0/6/6/6
2	FAD	A	1585	-	-	4/30/50/50	0/6/6/6
2	FAD	D	1585	-	-	2/30/50/50	0/6/6/6
3	PL3	A	1586	-	-	7/14/14/14	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1585	FAD	C2A-N3A	4.67	1.39	1.32
2	C	1585	FAD	C4X-N5	4.13	1.38	1.30
2	B	1585	FAD	C4X-N5	4.04	1.38	1.30
2	A	1585	FAD	C4X-N5	4.04	1.38	1.30
3	B	1586	PL3	O1-C1	-3.56	1.23	1.42
3	D	1586	PL3	O1-C1	-3.51	1.23	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1585	FAD	C2A-N3A	3.31	1.37	1.32
3	A	1586	PL3	O1-C1	-3.24	1.25	1.42
2	D	1585	FAD	C4X-N5	3.07	1.36	1.30
2	B	1585	FAD	C2A-N3A	2.88	1.36	1.32
2	A	1585	FAD	C2A-N3A	2.60	1.36	1.32
2	D	1585	FAD	C1'-C2'	2.57	1.56	1.52
2	A	1585	FAD	C9-C9A	2.45	1.43	1.39
2	B	1585	FAD	C10-N1	2.38	1.38	1.33
2	C	1585	FAD	C10-N1	2.35	1.38	1.33
2	D	1585	FAD	O2-C2	-2.31	1.20	1.24
2	A	1585	FAD	C1'-N10	2.28	1.53	1.48
2	B	1585	FAD	C2A-N1A	2.20	1.38	1.33
2	C	1585	FAD	C2B-C1B	-2.12	1.50	1.53
2	A	1585	FAD	C1'-C2'	2.09	1.55	1.52
2	B	1585	FAD	C5'-C4'	2.08	1.54	1.51
2	A	1585	FAD	C8A-N7A	-2.02	1.31	1.34

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1585	FAD	N3A-C2A-N1A	-6.38	118.70	128.68
2	B	1585	FAD	N3A-C2A-N1A	-6.00	119.31	128.68
2	C	1585	FAD	N3A-C2A-N1A	-5.99	119.32	128.68
2	A	1585	FAD	N3A-C2A-N1A	-4.43	121.76	128.68
2	A	1585	FAD	C4X-C10-N10	4.32	122.80	116.48
2	D	1585	FAD	O2-C2-N1	-3.92	115.33	121.83
2	B	1585	FAD	C4X-C10-N10	3.88	122.15	116.48
2	B	1585	FAD	O2-C2-N1	-3.77	115.58	121.83
2	D	1585	FAD	C4X-C10-N10	3.71	121.90	116.48
2	B	1585	FAD	C10-C4X-N5	-3.55	117.33	124.86
2	D	1585	FAD	C2A-N1A-C6A	3.45	124.66	118.75
2	B	1585	FAD	C4-C4X-N5	3.35	123.00	118.23
2	A	1585	FAD	C10-C4X-N5	-3.30	117.86	124.86
2	D	1585	FAD	C4-N3-C2	-3.30	119.55	125.64
2	D	1585	FAD	C10-C4X-N5	-3.26	117.93	124.86
2	B	1585	FAD	C2A-N1A-C6A	3.21	124.25	118.75
2	B	1585	FAD	C4-N3-C2	-2.97	120.15	125.64
2	A	1585	FAD	C4-N3-C2	-2.96	120.18	125.64
2	C	1585	FAD	C4-N3-C2	-2.91	120.27	125.64
2	D	1585	FAD	C4A-C5A-N7A	-2.91	106.37	109.40
2	A	1585	FAD	C4-C4X-N5	2.75	122.14	118.23
2	D	1585	FAD	C4-C4X-C10	2.72	121.36	116.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1585	FAD	C10-C4X-N5	-2.72	119.09	124.86
2	D	1585	FAD	C1B-N9A-C4A	-2.65	121.99	126.64
2	C	1585	FAD	C4X-C10-N10	2.62	120.31	116.48
2	A	1585	FAD	P-O3P-PA	-2.58	123.97	132.83
2	C	1585	FAD	C1B-N9A-C4A	-2.56	122.14	126.64
2	A	1585	FAD	O2'-C2'-C1'	2.50	115.83	109.80
2	B	1585	FAD	C1B-N9A-C4A	-2.41	122.40	126.64
2	D	1585	FAD	C5A-C6A-N6A	2.33	123.89	120.35
2	A	1585	FAD	C4X-C4-N3	2.26	118.94	113.19
2	B	1585	FAD	C4X-C4-N3	2.25	118.91	113.19
2	C	1585	FAD	C4X-C4-N3	2.24	118.88	113.19
2	C	1585	FAD	C4-C4X-C10	2.23	120.53	116.79
2	D	1585	FAD	P-O3P-PA	-2.21	125.23	132.83
2	C	1585	FAD	C4X-C10-N1	-2.19	119.64	124.73
2	A	1585	FAD	C4X-C10-N1	-2.19	119.64	124.73
2	A	1585	FAD	C5A-C6A-N6A	2.19	123.68	120.35
2	A	1585	FAD	C8M-C8-C9	2.15	123.47	119.49
2	A	1585	FAD	O3B-C3B-C2B	-2.15	104.86	111.82
2	B	1585	FAD	O2-C2-N3	2.15	122.83	118.65
2	C	1585	FAD	C2A-N1A-C6A	2.13	122.40	118.75
3	A	1586	PL3	O1-C1-C2	2.12	125.61	111.66
2	D	1585	FAD	O3B-C3B-C2B	-2.12	104.97	111.82
3	D	1586	PL3	O1-C1-C2	2.09	125.40	111.66
2	D	1585	FAD	C4X-C10-N1	-2.07	119.93	124.73
2	A	1585	FAD	O2-C2-N1	-2.07	118.40	121.83
2	A	1585	FAD	O2P-P-O5'	2.00	117.04	107.75

There are no chirality outliers.

All (32) 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	C9-CA-CB-CC

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

There are no ring outliers.

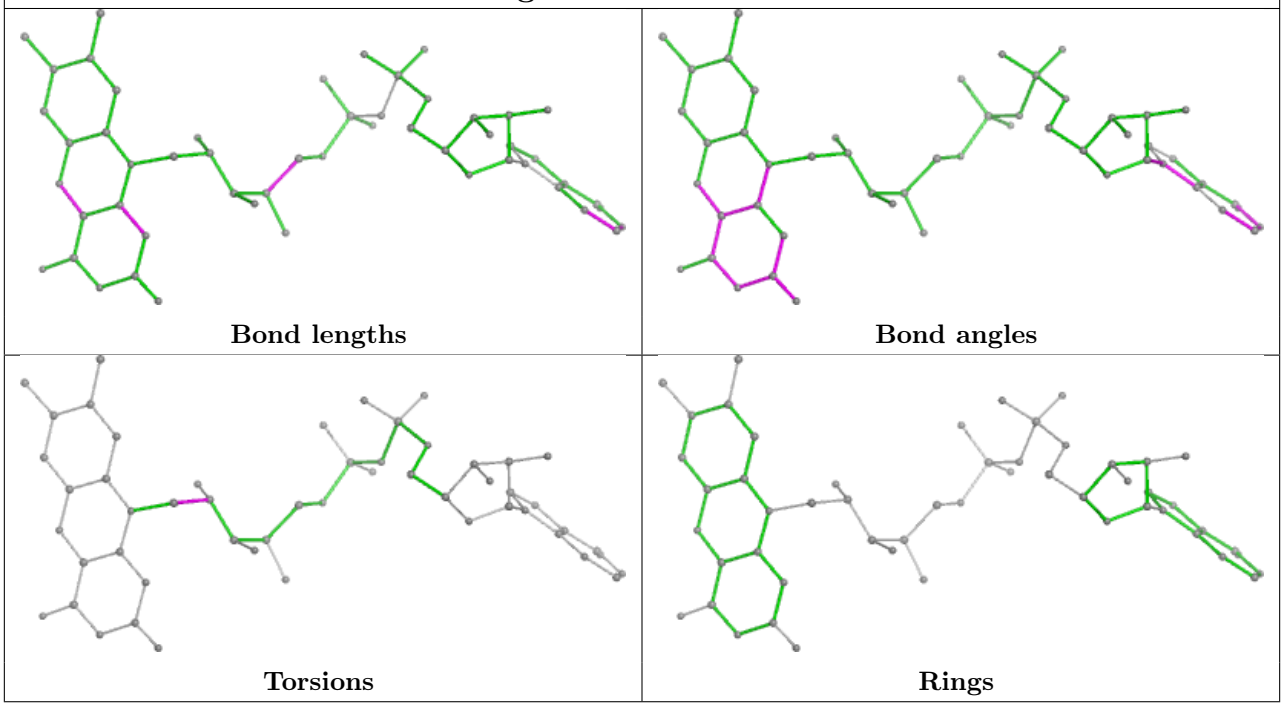
7 monomers are involved in 26 short contacts:

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

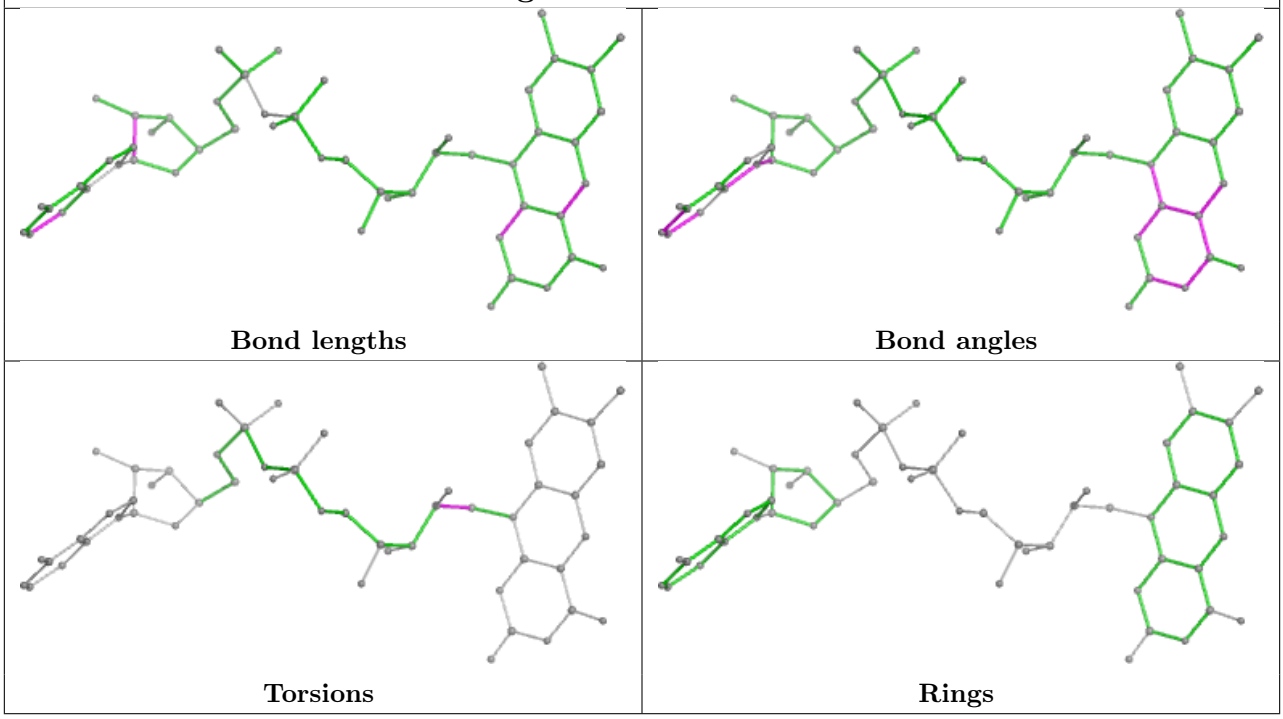
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

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

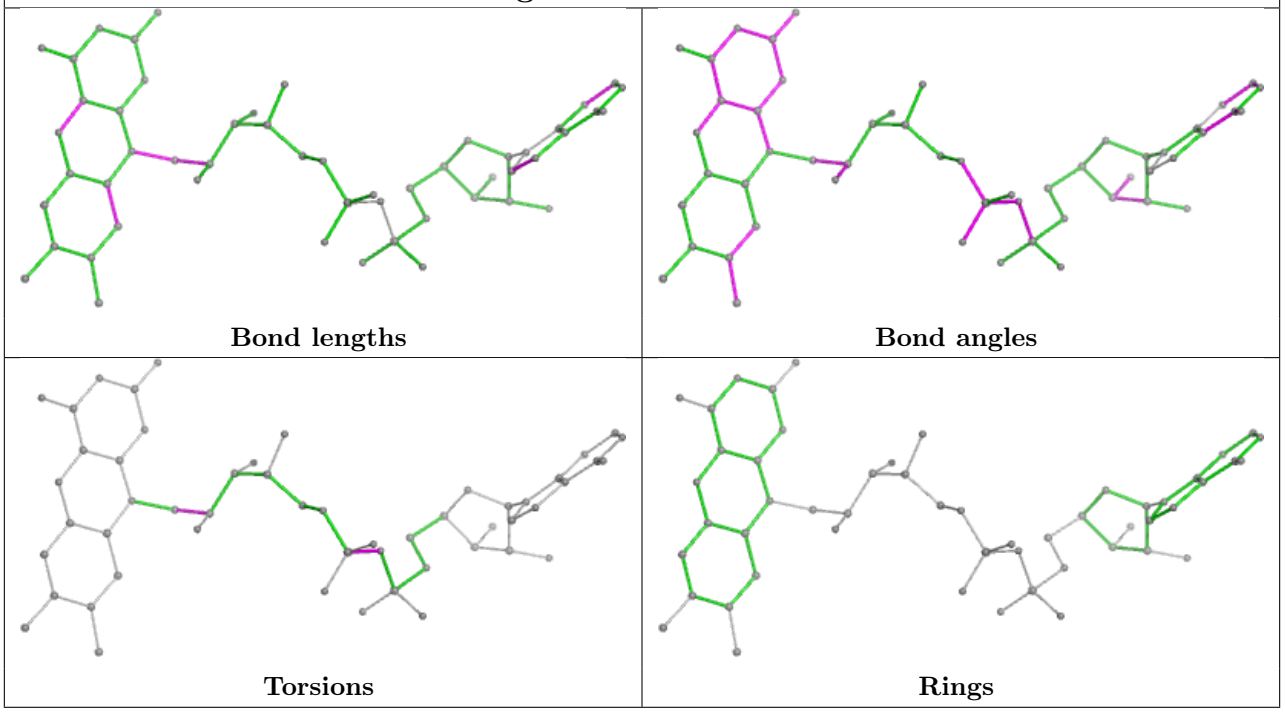
Ligand FAD B 1585



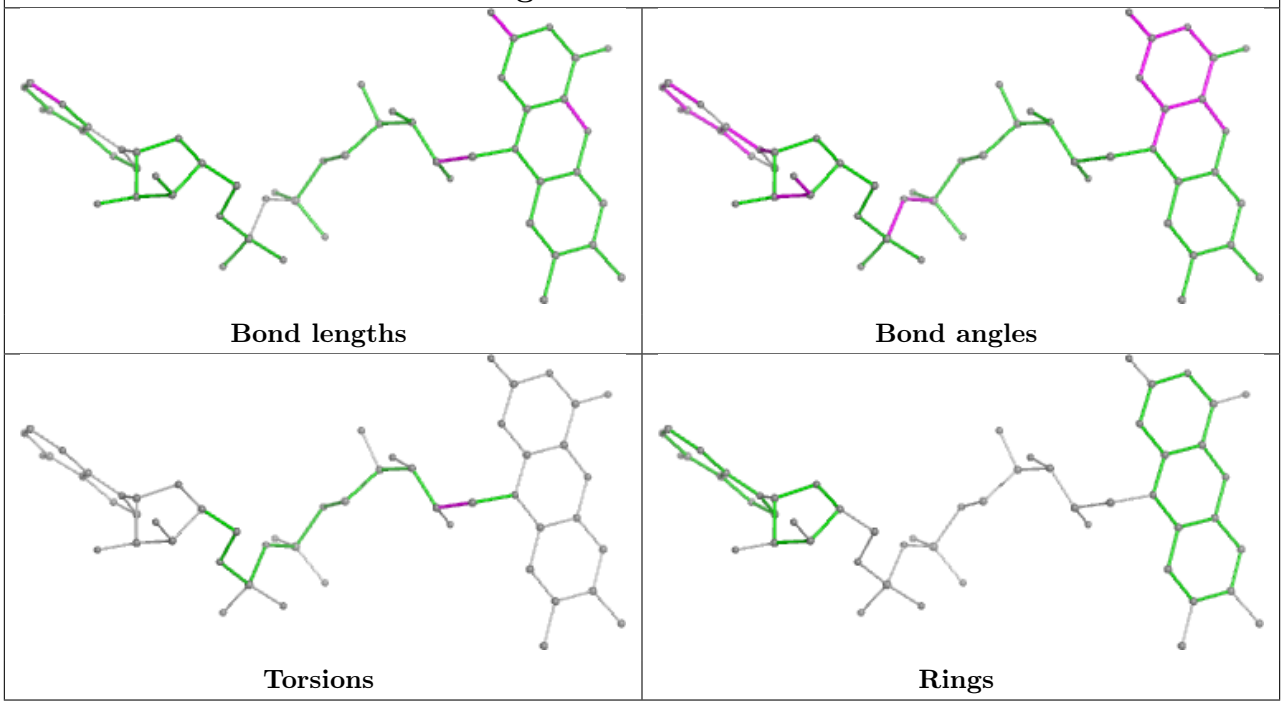
Ligand FAD C 1585



Ligand FAD A 1585



Ligand FAD D 1585



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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, 95^{th} 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%)	0.79	55 (10%)	6 5	11, 25, 53, 86	0
1	B	523/584 (89%)	0.90	76 (14%)	2 2	11, 26, 56, 85	0
1	C	491/584 (84%)	1.36	124 (25%)	0 0	17, 33, 58, 79	0
1	D	528/584 (90%)	0.78	62 (11%)	4 4	9, 25, 51, 68	0
All	All	2065/2336 (88%)	0.95	317 (15%)	2 1	9, 26, 55, 86	0

All (317) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	74	VAL	8.8
1	C	35	LYS	6.9
1	D	282	ARG	6.9
1	A	63	LEU	6.5
1	C	183	VAL	6.4
1	C	501	TYR	6.4
1	C	432	PRO	6.3
1	B	536	PHE	6.1
1	C	489	ILE	6.1
1	C	436	TRP	5.7
1	B	432	PRO	5.6
1	D	536	PHE	5.5
1	C	38	GLY	5.4
1	A	525	ILE	5.3
1	C	36	PRO	5.3
1	B	562	ARG	5.3
1	C	379	MET	5.2
1	C	76	ASP	5.2
1	B	282	ARG	5.1
1	C	562	ARG	5.1
1	D	388	ARG	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	432	PRO	5.1
1	C	282	ARG	5.0
1	A	524	TYR	4.9
1	B	12	HIS	4.9
1	C	46	GLU	4.8
1	B	289	ALA	4.7
1	A	431	ALA	4.7
1	A	541	SER	4.7
1	D	501	TYR	4.6
1	A	565	ILE	4.5
1	B	103	ALA	4.5
1	D	384	LEU	4.4
1	D	12	HIS	4.4
1	B	185	ASN	4.3
1	C	39	THR	4.3
1	C	366	LYS	4.3
1	A	297	ILE	4.3
1	B	99	ARG	4.3
1	C	60	LYS	4.2
1	C	397	LEU	4.2
1	A	64	THR	4.2
1	C	387	ILE	4.2
1	C	478	GLN	4.2
1	C	327	LEU	4.1
1	C	514	LYS	4.1
1	C	388	ARG	4.1
1	C	390	PHE	4.1
1	C	12	HIS	4.1
1	C	400	ILE	4.1
1	C	482	LYS	4.1
1	D	421	SER	4.0
1	B	532	THR	4.0
1	D	488	GLY	4.0
1	B	377	SER	4.0
1	D	13	ILE	4.0
1	C	58	PHE	3.9
1	C	365	TRP	3.9
1	C	456	TRP	3.9
1	B	516	ASN	3.9
1	B	565	ILE	3.9
1	C	336	SER	3.9
1	C	13	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	63	LEU	3.8
1	A	536	PHE	3.8
1	D	165	VAL	3.8
1	C	289	ALA	3.8
1	C	426	PHE	3.8
1	C	75	LEU	3.8
1	C	389	SER	3.7
1	C	384	LEU	3.7
1	B	13	ILE	3.7
1	C	356	PRO	3.7
1	C	326	PHE	3.7
1	D	190	VAL	3.7
1	B	488	GLY	3.6
1	B	486	ASP	3.6
1	C	392	PHE	3.6
1	D	486	ASP	3.6
1	A	185	ASN	3.6
1	B	497	ILE	3.6
1	B	435	THR	3.6
1	D	353	VAL	3.5
1	C	490	PRO	3.5
1	C	418	ASP	3.5
1	C	383	TYR	3.5
1	C	61	LYS	3.5
1	C	480	PHE	3.5
1	D	432	PRO	3.4
1	C	93	GLN	3.4
1	A	538	TYR	3.4
1	C	386	TYR	3.4
1	A	527	ALA	3.4
1	C	508	TYR	3.4
1	A	282	ARG	3.3
1	C	334	ALA	3.3
1	C	565	ILE	3.3
1	B	87	HIS	3.3
1	D	539	GLY	3.3
1	B	381	LYS	3.3
1	B	186	GLU	3.3
1	C	331	PHE	3.3
1	C	145	VAL	3.3
1	A	13	ILE	3.3
1	B	482	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	118	ILE	3.3
1	C	78	THR	3.3
1	A	232	LEU	3.2
1	C	396	CYS	3.2
1	C	385	HIS	3.2
1	C	206	ARG	3.2
1	C	584	ARG	3.2
1	B	433	GLY	3.2
1	C	353	VAL	3.2
1	B	232	LEU	3.1
1	B	145	VAL	3.1
1	C	497	ILE	3.1
1	D	422	LYS	3.1
1	A	562	ARG	3.1
1	D	527	ALA	3.1
1	B	183	VAL	3.1
1	C	395	VAL	3.0
1	B	526	GLU	3.0
1	C	190	VAL	3.0
1	A	145	VAL	3.0
1	C	47	VAL	3.0
1	A	529	LYS	3.0
1	B	537	LYS	3.0
1	C	431	ALA	3.0
1	D	381	LYS	3.0
1	D	393	LYS	2.9
1	A	488	GLY	2.9
1	D	537	LYS	2.9
1	B	40	ILE	2.9
1	C	307	ILE	2.9
1	D	244	LEU	2.9
1	B	205	ARG	2.9
1	B	539	GLY	2.9
1	A	435	THR	2.9
1	C	435	THR	2.9
1	D	497	ILE	2.9
1	D	508	TYR	2.9
1	C	45	PRO	2.9
1	C	406	LYS	2.9
1	C	416	VAL	2.8
1	C	296	ILE	2.8
1	C	156	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	304	LEU	2.8
1	A	486	ASP	2.8
1	B	569	ARG	2.8
1	A	247	TRP	2.8
1	D	387	ILE	2.8
1	D	385	HIS	2.8
1	D	392	PHE	2.8
1	A	516	ASN	2.8
1	D	61	LYS	2.7
1	B	368	SER	2.7
1	C	167	ILE	2.7
1	C	417	PHE	2.7
1	D	426	PHE	2.7
1	A	74	VAL	2.7
1	A	183	VAL	2.7
1	B	41	ALA	2.7
1	C	212	ILE	2.7
1	C	95	PRO	2.7
1	C	424	ALA	2.7
1	C	515	GLN	2.7
1	C	468	ASN	2.7
1	D	156	LEU	2.7
1	B	431	ALA	2.7
1	C	191	SER	2.7
1	A	190	VAL	2.7
1	C	319	GLN	2.7
1	D	507	LEU	2.7
1	B	158	GLN	2.6
1	C	138	LYS	2.6
1	D	160	ALA	2.6
1	C	433	GLY	2.6
1	D	372	VAL	2.6
1	B	507	LEU	2.6
1	C	381	LYS	2.6
1	B	64	THR	2.6
1	C	192	ILE	2.6
1	D	40	ILE	2.6
1	A	305	GLY	2.6
1	B	139	ASN	2.6
1	B	247	TRP	2.6
1	B	365	TRP	2.6
1	B	244	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	539	GLY	2.6
1	D	144	ILE	2.6
1	B	541	SER	2.6
1	A	75	LEU	2.6
1	B	60	LYS	2.6
1	C	310	ALA	2.6
1	C	563	GLY	2.6
1	B	93	GLN	2.6
1	B	529	LYS	2.6
1	C	247	TRP	2.6
1	D	64	THR	2.6
1	C	328	PHE	2.5
1	B	155	ARG	2.5
1	D	418	ASP	2.5
1	C	57	GLY	2.5
1	D	307	ILE	2.5
1	B	74	VAL	2.5
1	D	122	PHE	2.5
1	B	82	GLN	2.5
1	C	248	LEU	2.5
1	D	46	GLU	2.5
1	C	305	GLY	2.5
1	B	573	GLU	2.5
1	A	436	TRP	2.5
1	C	144	ILE	2.5
1	D	212	ILE	2.5
1	D	132	VAL	2.5
1	A	248	LEU	2.5
1	C	467	ALA	2.5
1	D	397	LEU	2.5
1	B	49	SER	2.5
1	D	541	SER	2.5
1	C	437	ALA	2.4
1	B	584	ARG	2.4
1	A	377	SER	2.4
1	B	538	TYR	2.4
1	C	104	PHE	2.4
1	A	139	ASN	2.4
1	B	388	ARG	2.4
1	D	476	ALA	2.4
1	C	513	SER	2.4
1	B	297	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	127	ARG	2.4
1	C	244	LEU	2.4
1	B	501	TYR	2.4
1	D	529	LYS	2.4
1	D	157	VAL	2.4
1	B	75	LEU	2.4
1	C	411	PHE	2.4
1	A	475	ASP	2.4
1	C	79	PRO	2.4
1	A	497	ILE	2.4
1	B	47	VAL	2.4
1	C	37	SER	2.3
1	C	402	PHE	2.3
1	B	210	ALA	2.3
1	B	495	ALA	2.3
1	C	469	LEU	2.3
1	B	96	GLU	2.3
1	C	422	LYS	2.3
1	A	353	VAL	2.3
1	B	192	ILE	2.3
1	D	273	VAL	2.3
1	C	96	GLU	2.3
1	C	421	SER	2.3
1	D	485	LYS	2.3
1	C	210	ALA	2.3
1	C	338	LEU	2.3
1	D	516	ASN	2.3
1	D	306	ILE	2.3
1	B	290	GLY	2.2
1	A	367	PRO	2.2
1	D	425	ALA	2.2
1	B	31	LEU	2.2
1	C	335	VAL	2.2
1	C	481	VAL	2.2
1	A	296	ILE	2.2
1	B	508	TYR	2.2
1	A	566	ASN	2.2
1	A	225	LEU	2.2
1	B	581	CYS	2.2
1	C	491	ALA	2.2
1	D	371	ALA	2.2
1	C	50	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	399	ILE	2.2
1	A	563	GLY	2.2
1	D	390	PHE	2.2
1	C	211	CYS	2.2
1	B	48	SER	2.1
1	B	52	LEU	2.1
1	B	63	LEU	2.1
1	C	401	GLY	2.1
1	D	305	GLY	2.1
1	A	482	LYS	2.1
1	B	122	PHE	2.1
1	C	77	GLU	2.1
1	A	507	LEU	2.1
1	D	406	LYS	2.1
1	B	296	ILE	2.1
1	B	530	LEU	2.1
1	C	473	TRP	2.1
1	A	480	PHE	2.1
1	A	526	GLU	2.1
1	D	417	PHE	2.1
1	C	346	VAL	2.1
1	A	306	ILE	2.1
1	C	59	ILE	2.1
1	A	45	PRO	2.1
1	A	121	THR	2.1
1	C	471	THR	2.1
1	B	50	VAL	2.1
1	C	333	HIS	2.1
1	A	433	GLY	2.1
1	B	121	THR	2.0
1	D	538	TYR	2.0
1	C	226	HIS	2.0
1	A	79	PRO	2.0
1	A	400	ILE	2.0
1	B	291	ILE	2.0
1	C	232	LEU	2.0
1	B	94	TYR	2.0
1	C	342	ARG	2.0
1	D	540	GLY	2.0
1	D	247	TRP	2.0
1	A	487	GLN	2.0
1	C	391	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	327	LEU	2.0
1	C	454	ASN	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 monosaccharides in this entry.

6.4 Ligands (i)

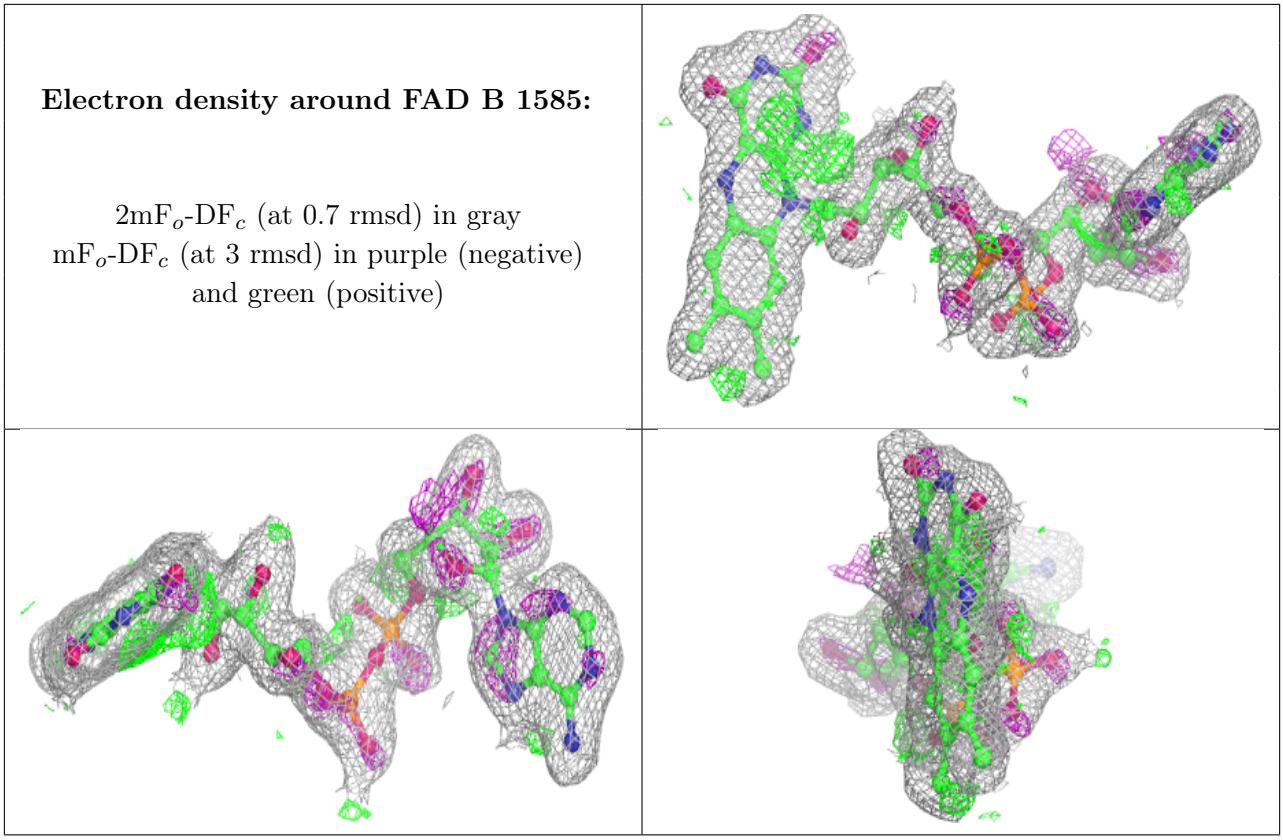
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PL3	A	1586	17/17	0.70	0.24	35,39,44,45	0
3	PL3	D	1586	17/17	0.71	0.20	24,32,34,35	0
3	PL3	B	1586	17/17	0.83	0.19	31,33,45,47	0
2	FAD	B	1585	53/53	0.96	0.08	5,11,13,16	0
2	FAD	A	1585	53/53	0.97	0.07	2,9,12,12	0
2	FAD	C	1585	53/53	0.97	0.08	7,15,19,19	0
2	FAD	D	1585	53/53	0.97	0.08	3,9,12,12	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.

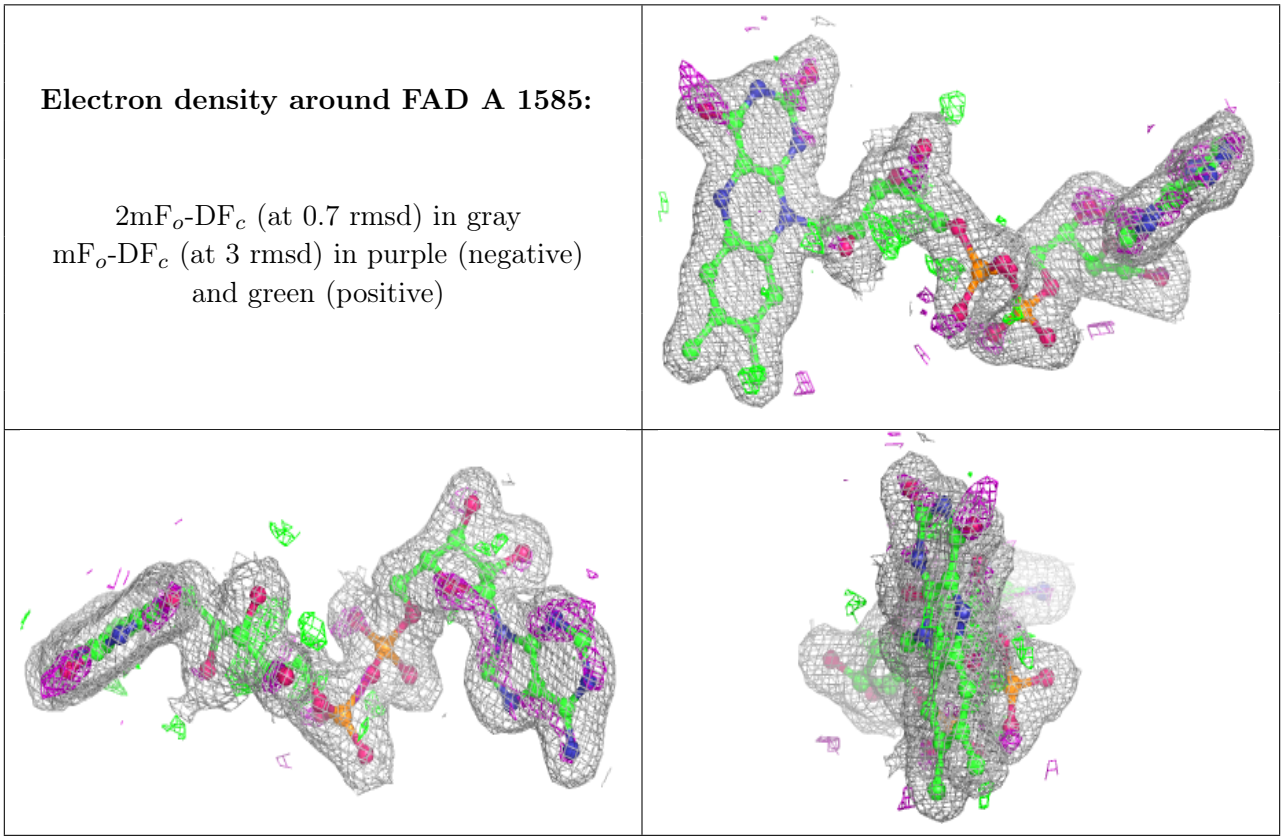
Electron density around FAD B 1585:

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



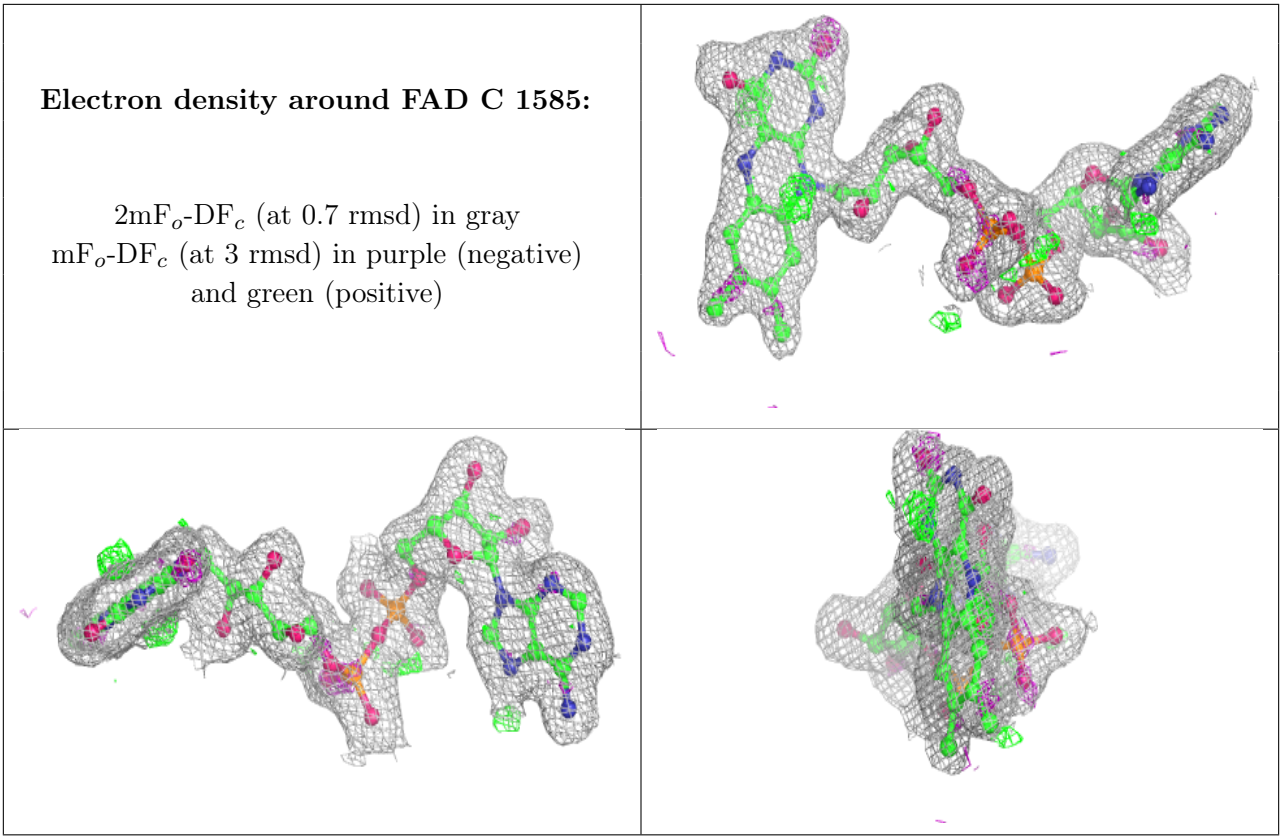
Electron density around FAD A 1585:

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



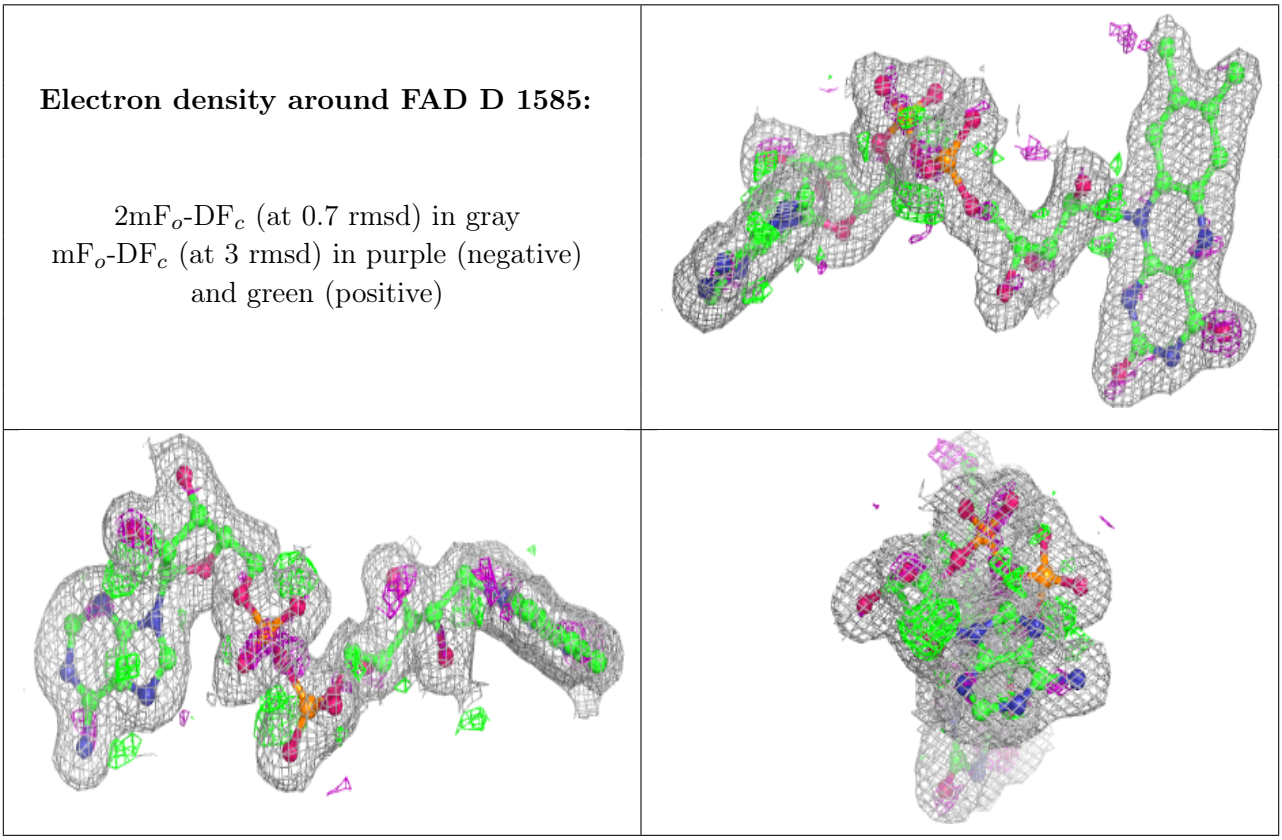
Electron density around FAD C 1585:

$2mF_o$-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)



6.5 Other polymers (i)

There are no such residues in this entry.