



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:37 AM UTC

PDB ID : 5AE1 / pdb_00005ae1
Title : Ether Lipid-Generating Enzyme AGPS in complex with inhibitor ZINC69435460
Authors : Piano, V.; Benjamin, D.I.; Valente, S.; Nenci, S.; Marrocco, B.; Mai, A.; Aliverti, A.; Nomura, D.K.; Mattevi, A.
Deposited on : 2015-08-25
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

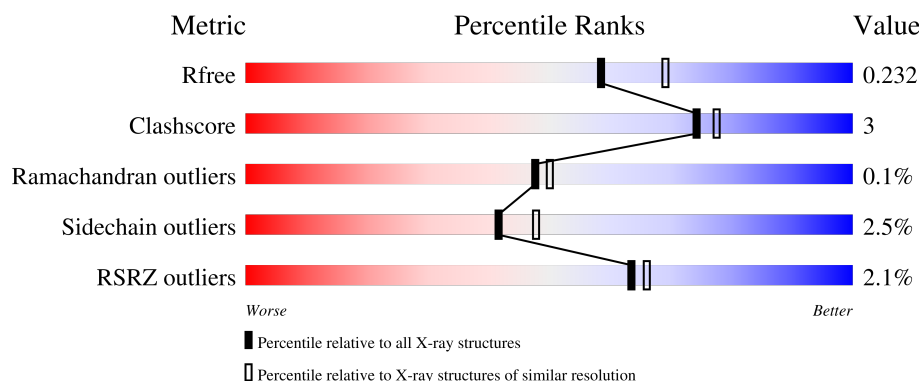
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	658	3% 78% 7% 15%
1	B	658	2% 75% 7% 18%
1	C	658	76% 8% 15%
1	D	658	3% 79% 6% 14%

2 Entry composition [i](#)

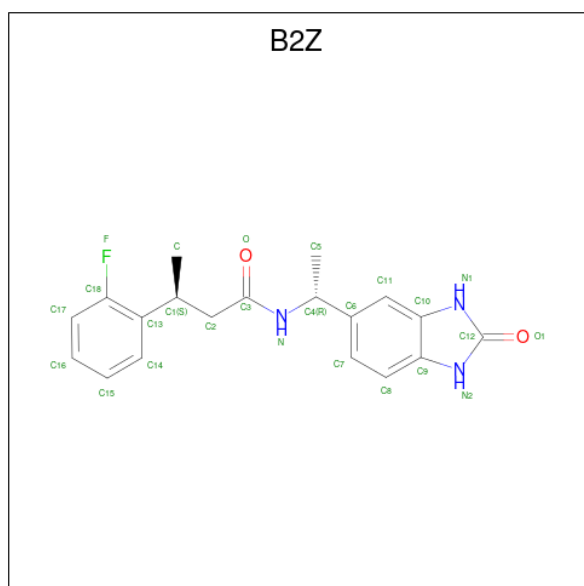
There are 5 unique types of molecules in this entry. The entry contains 18358 atoms, of which 0 are hydrogens and 0 are deuteriums.

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, PEROXISOMAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	560	Total	C	N	O	S	0	1	0
			4410	2810	761	815	24			
1	B	539	Total	C	N	O	S	0	0	0
			4254	2703	740	787	24			
1	C	559	Total	C	N	O	S	0	2	0
			4407	2800	761	822	24			
1	D	564	Total	C	N	O	S	0	0	0
			4395	2786	765	820	24			

- Molecule 2 is (3-(2-FLUOROPHENYL)-N-(1-(2-OXO-2,3-DIHYDRO-1H-BENZO[D]IMIDAZOL-5-YL)ETHYL)BUTANAMIDE) (CCD ID: B2Z) (formula: C₁₉H₂₀FN₃O₂).



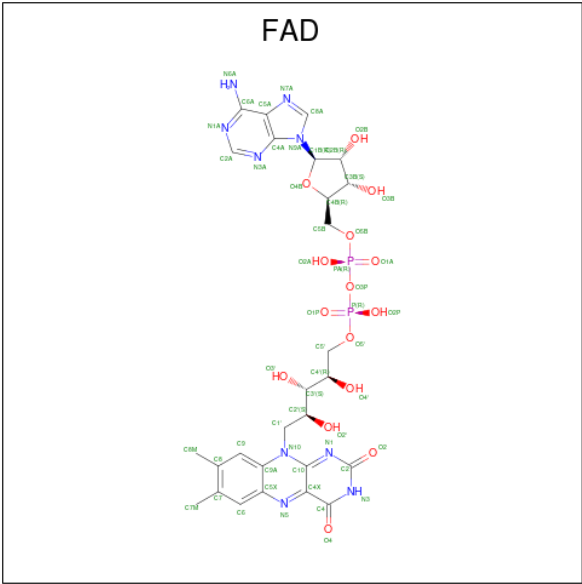
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			25	19	1	3	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	F	N	O	0	0
			25	19	1	3	2		
2	C	1	Total	C	F	N	O	0	0
			25	19	1	3	2		
2	D	1	Total	C	F	N	O	0	0
			25	19	1	3	2		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

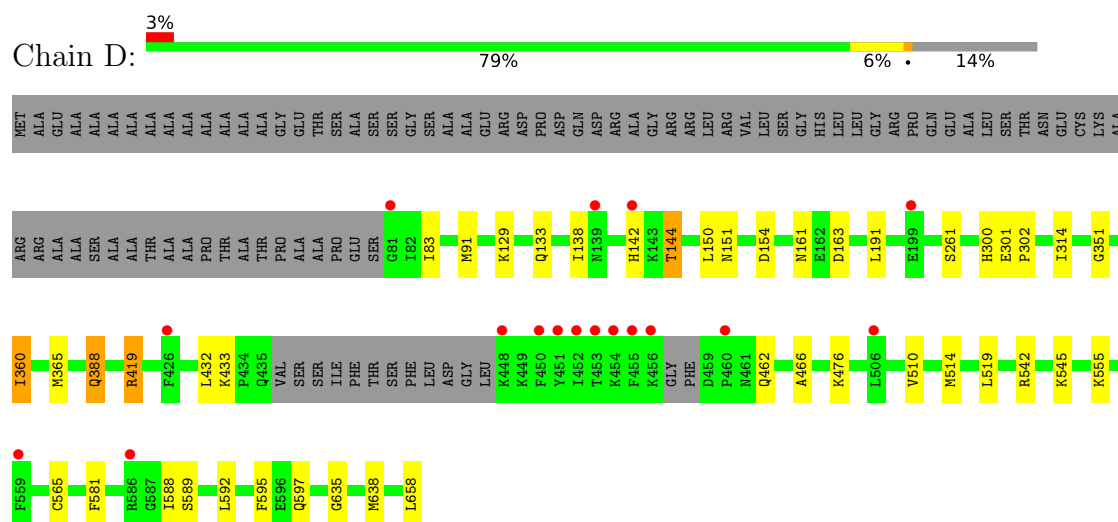
- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	150	Total	O	0	0
			150	150		
5	B	123	Total	O	0	0
			123	123		
5	C	171	Total	O	0	0
			171	171		
5	D	116	Total	O	0	0
			116	116		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	60.79Å 99.02Å 107.02Å 90.64° 89.96° 95.49°	Depositor
Resolution (Å)	107.01 – 2.10 107.01 – 2.10	Depositor EDS
% Data completeness (in resolution range)	93.6 (107.01-2.10) 93.6 (107.01-2.10)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0124	Depositor
R, R_{free}	0.186 , 0.229 0.193 , 0.232	Depositor DCC
R_{free} test set	1484 reflections (1.09%)	wwPDB-VP
Wilson B-factor (Å ²)	26.9	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 35.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.013 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18358	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% 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: B2Z, FAD, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.07	1/4514 (0.0%)	1.07	6/6103 (0.1%)
1	B	1.07	2/4350 (0.0%)	1.02	3/5882 (0.1%)
1	C	1.10	1/4515 (0.0%)	1.05	5/6110 (0.1%)
1	D	1.10	3/4493 (0.1%)	1.06	0/6084
All	All	1.08	7/17872 (0.0%)	1.05	14/24179 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	301	GLU	C-O	-6.07	1.17	1.24
1	A	333	VAL	C-O	-5.66	1.18	1.24
1	B	231	CYS	CA-C	5.48	1.59	1.52
1	B	194	ILE	CA-C	5.43	1.59	1.52
1	D	150	LEU	N-CA	-5.42	1.39	1.46
1	D	388	GLN	CA-C	-5.30	1.46	1.52
1	C	118	TYR	C-O	-5.01	1.19	1.24

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	325	ILE	CB-CA-C	-8.24	103.39	111.30
1	A	160	VAL	N-CA-C	7.51	119.13	108.17
1	B	195	PHE	N-CA-C	7.07	119.60	111.11
1	A	590	ASP	CA-C-N	6.12	126.29	119.32
1	A	590	ASP	C-N-CA	6.12	126.29	119.32
1	C	515	ARG	NE-CZ-NH2	-6.07	113.74	119.20
1	B	160	VAL	N-CA-C	5.85	116.71	108.17
1	C	139	ASN	N-CA-C	5.61	119.93	112.30
1	B	261	SER	N-CA-C	5.38	117.89	111.71
1	A	395	PHE	CA-C-N	5.34	125.15	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	395	PHE	C-N-CA	5.34	125.15	119.28
1	C	471	GLU	N-CA-C	5.23	116.79	108.79
1	C	499	ASP	N-CA-C	5.21	116.96	111.28
1	A	159	ILE	CB-CA-C	-5.09	106.40	111.80

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	4410	0	4328	26	0
1	B	4254	0	4191	26	0
1	C	4407	0	4318	38	0
1	D	4395	0	4270	21	0
2	A	25	0	20	4	0
2	B	25	0	20	1	0
2	C	25	0	20	1	0
2	D	25	0	20	0	0
3	A	53	0	31	3	0
3	B	53	0	31	0	0
3	C	53	0	31	0	0
3	D	53	0	31	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
5	A	150	0	0	2	0
5	B	123	0	0	2	0
5	C	171	0	0	9	0
5	D	116	0	0	1	0
All	All	18358	0	17311	110	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 3.

All (110) 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:411:GLN:HG2	5:C:2127:HOH:O	1.65	0.95
1:D:300:HIS:ND1	1:D:302:PRO:HD3	1.99	0.78
1:C:386:GLU:CD	5:C:2120:HOH:O	2.31	0.74
1:C:150:LEU:HD22	1:C:180:ASP:HA	1.74	0.70
1:A:133:GLN:HG2	1:A:138:ILE:O	1.94	0.67
1:B:83:ILE:HG23	1:B:91:MET:HE1	1.77	0.67
1:C:83:ILE:HG23	1:C:91:MET:HE1	1.76	0.65
1:D:83:ILE:HG23	1:D:91:MET:HE1	1.79	0.65
1:D:658:LEU:C	5:D:2109:HOH:O	2.38	0.65
1:C:246:MET:SD	5:C:2071:HOH:O	2.55	0.64
1:C:635:GLY:HA2	1:C:638:MET:HE3	1.79	0.63
1:B:425:GLN:HG3	1:B:564:THR:OG1	1.99	0.63
1:C:515:ARG:HD3	5:C:2141:HOH:O	1.99	0.63
1:A:83:ILE:HG23	1:A:91:MET:HE1	1.81	0.62
1:C:428:PHE:CZ	1:C:432:LEU:HD21	2.34	0.62
1:C:635:GLY:HA2	1:C:638:MET:CE	2.29	0.62
1:C:582:ALA:HB2	2:C:888:B2Z:H17	1.82	0.61
1:B:421:MET:HB2	1:B:425:GLN:HB2	1.83	0.60
1:C:317:ARG:NH2	5:C:2092:HOH:O	2.37	0.57
1:D:432:LEU:HD11	1:D:514:MET:HE1	1.86	0.57
1:C:411:GLN:CG	5:C:2127:HOH:O	2.36	0.57
1:C:332:LEU:HB3	1:C:379:ILE:CD1	2.35	0.56
1:A:415:PRO:HB3	1:A:470:PHE:CE2	2.41	0.55
1:D:129:LYS:O	1:D:133:GLN:HG3	2.07	0.55
1:B:582:ALA:HB2	2:B:888:B2Z:H17	1.89	0.54
1:B:635:GLY:HA2	1:B:638:MET:HE3	1.89	0.54
1:C:314:ILE:HG23	1:C:365:MET:HG2	1.89	0.54
1:A:314:ILE:HG23	1:A:365:MET:HG2	1.90	0.54
1:B:397:ASN:HA	1:B:462:GLN:O	2.08	0.54
1:D:161:ASN:OD1	1:D:163:ASP:N	2.41	0.53
1:D:314:ILE:HG23	1:D:365:MET:HG2	1.90	0.53
1:D:635:GLY:HA2	1:D:638:MET:HE2	1.89	0.53
1:D:144:THR:HG21	1:D:519:LEU:O	2.10	0.52
1:B:314:ILE:HG23	1:B:365:MET:HG2	1.92	0.51
1:D:133:GLN:HG2	1:D:138:ILE:O	2.10	0.51
1:A:94:ASN:HA	1:A:197:LEU:HD13	1.92	0.51
1:A:119:PRO:HG2	1:A:506:LEU:HD22	1.93	0.50
2:A:888:B2Z:H51C	3:A:999:FAD:HM81	1.94	0.50
1:D:300:HIS:CE1	1:D:302:PRO:HD3	2.46	0.50
1:A:138:ILE:O	1:A:138:ILE:HD12	2.12	0.50
1:C:150:LEU:CD1	1:C:183:VAL:HG11	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:THR:HG21	1:B:379:ILE:HD12	1.94	0.49
1:C:658:LEU:C	5:C:2163:HOH:O	2.56	0.49
1:B:340:THR:HB	1:B:646:VAL:HG13	1.95	0.49
1:B:463:LEU:C	1:B:463:LEU:HD23	2.38	0.49
1:A:424:GLN:NE2	1:A:562:LEU:HD12	2.28	0.49
1:A:298:THR:HG21	1:A:379:ILE:HD12	1.94	0.48
1:C:425:GLN:HG3	1:C:564:THR:OG1	2.13	0.48
2:A:888:B2Z:H51C	3:A:999:FAD:C8M	2.44	0.47
1:C:429:GLY:O	1:C:503:ARG:NH2	2.47	0.47
1:B:585:TYR:HB2	1:B:591:PRO:HB3	1.95	0.47
2:A:888:B2Z:C5	3:A:999:FAD:HM81	2.44	0.47
1:A:132:ILE:HG22	1:A:138:ILE:HD11	1.95	0.47
1:B:155:THR:N	5:B:2024:HOH:O	2.47	0.47
1:A:317:ARG:NH1	5:A:2070:HOH:O	2.48	0.47
1:B:83:ILE:HD12	5:B:2058:HOH:O	2.15	0.47
1:B:300:HIS:HD2	1:B:313:TRP:CE3	2.33	0.47
1:B:426:PHE:CD1	1:B:465:VAL:HG21	2.49	0.47
1:A:419:ARG:O	1:A:466:ALA:HA	2.15	0.46
1:A:109:GLY:HA3	1:C:268:TRP:CE3	2.50	0.46
1:C:265:ARG:HD3	1:C:279:GLU:OE1	2.16	0.46
1:C:419:ARG:O	1:C:466:ALA:HA	2.15	0.46
1:C:83:ILE:HG23	1:C:91:MET:CE	2.43	0.46
1:A:582:ALA:HB2	2:A:888:B2Z:H17	1.98	0.45
1:A:138:ILE:HD12	1:A:138:ILE:C	2.42	0.45
1:C:515:ARG:CD	5:C:2141:HOH:O	2.61	0.45
5:C:2144:HOH:O	1:D:351:GLY:N	2.49	0.45
1:A:419:ARG:HH22	1:A:508:THR:HG21	1.82	0.44
1:B:323:LYS:HD2	1:B:323:LYS:C	2.42	0.44
1:B:419:ARG:O	1:B:466:ALA:HA	2.17	0.44
1:A:119:PRO:CG	1:A:506:LEU:HD22	2.48	0.44
1:A:442:SER:HB3	1:D:542:ARG:NH1	2.32	0.44
1:C:425:GLN:HE22	1:C:566:ARG:CD	2.31	0.44
1:D:555:LYS:NZ	1:D:597:GLN:OE1	2.46	0.44
1:C:540:LEU:C	1:C:540:LEU:HD23	2.43	0.43
1:C:167:GLU:OE2	1:C:228:TYR:OH	2.28	0.43
1:D:191:LEU:HD23	1:D:595:PHE:CD2	2.53	0.43
1:D:151:ASN:HB3	1:D:154:ASP:OD2	2.18	0.43
1:B:421:MET:HE2	1:B:421:MET:HB3	1.78	0.43
1:B:635:GLY:HA2	1:B:638:MET:CE	2.47	0.43
1:C:150:LEU:HD11	1:C:183:VAL:HG21	2.00	0.43
1:B:83:ILE:CG2	1:B:91:MET:HE1	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:585:TYR:HB2	1:C:591:PRO:HB3	2.01	0.43
1:C:332:LEU:HB3	1:C:379:ILE:HD13	2.01	0.43
1:B:547:ARG:NH1	1:B:605:GLU:OE1	2.48	0.43
1:D:360:ILE:HD13	1:D:360:ILE:HG21	1.75	0.43
1:C:386:GLU:OE1	1:C:474:ARG:NH1	2.52	0.42
1:D:545:LYS:HE3	1:D:565:CYS:SG	2.59	0.42
1:B:98:TYR:CD2	1:B:117:ARG:HD3	2.55	0.42
1:C:189:HIS:O	1:C:515:ARG:NH2	2.52	0.42
1:A:213:THR:C	1:A:263:MET:HG2	2.45	0.42
1:A:630:SER:HA	1:B:348:SER:OG	2.20	0.42
1:C:150:LEU:HG	1:C:151:ASN:N	2.34	0.42
1:A:323:LYS:HD2	1:A:323:LYS:C	2.44	0.41
1:C:323:LYS:HD2	1:C:323:LYS:C	2.45	0.41
1:C:415:PRO:HB3	1:C:470:PHE:CD1	2.55	0.41
1:C:187:HIS:CE1	1:C:197:LEU:HD11	2.55	0.41
1:D:419:ARG:O	1:D:466:ALA:HA	2.21	0.41
1:C:425:GLN:HE22	1:C:566:ARG:HD3	1.85	0.41
1:B:128:PHE:O	1:B:132:ILE:HG13	2.21	0.40
1:A:350:GLN:HA	5:A:2080:HOH:O	2.20	0.40
1:B:259:ASP:OD1	1:B:261:SER:OG	2.35	0.40
1:A:635:GLY:HA2	1:A:638:MET:HE3	2.03	0.40
1:B:83:ILE:HG23	1:B:91:MET:CE	2.50	0.40
1:A:340:THR:HB	1:A:646:VAL:HG13	2.03	0.40
1:A:442:SER:CB	1:D:542:ARG:NH1	2.85	0.40
1:D:83:ILE:HB	1:D:261:SER:HB2	2.04	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	555/658 (84%)	543 (98%)	10 (2%)	2 (0%)	30 28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	533/658 (81%)	522 (98%)	11 (2%)	0	100	100
1	C	557/658 (85%)	547 (98%)	10 (2%)	0	100	100
1	D	558/658 (85%)	549 (98%)	9 (2%)	0	100	100
All	All	2203/2632 (84%)	2161 (98%)	40 (2%)	2 (0%)	48	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	198	ARG
1	A	586	ARG

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	471/545 (86%)	459 (98%)	12 (2%)	42	48
1	B	457/545 (84%)	447 (98%)	10 (2%)	45	53
1	C	474/545 (87%)	462 (98%)	12 (2%)	42	48
1	D	465/545 (85%)	452 (97%)	13 (3%)	38	43
All	All	1867/2180 (86%)	1820 (98%)	47 (2%)	42	48

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	LYS
1	A	120	LEU
1	A	130	ASP
1	A	165	LEU
1	A	360	ILE
1	A	441	THR
1	A	463	LEU
1	A	507	LEU
1	A	508	THR

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Mol	Chain	Res	Type
1	A	589	SER
1	A	599	GLU
1	A	646	VAL
1	B	90	LEU
1	B	134	ASN
1	B	140	LEU
1	B	199	GLU
1	B	360	ILE
1	B	421	MET
1	B	463	LEU
1	B	510	VAL
1	B	599	GLU
1	B	646	VAL
1	C	102	LYS
1	C	138	ILE
1	C	144	THR
1	C	165	LEU
1	C	195	PHE
1	C	360	ILE
1	C	379	ILE
1	C	508	THR
1	C	510	VAL
1	C	515	ARG
1	C	581	PHE
1	C	589	SER
1	D	142	HIS
1	D	144	THR
1	D	360	ILE
1	D	388	GLN
1	D	419	ARG
1	D	433	LYS
1	D	462	GLN
1	D	476	LYS
1	D	510	VAL
1	D	581	PHE
1	D	588	ILE
1	D	589	SER
1	D	592	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	HIS
1	A	272	ASN
1	A	290	GLN
1	A	335	HIS
1	A	424	GLN
1	B	192	HIS
1	B	290	GLN
1	B	400	GLN
1	B	430	HIS
1	B	483	GLN
1	C	139	ASN
1	C	300	HIS
1	C	400	GLN
1	C	423	ASN
1	C	425	GLN
1	C	427	GLN
1	D	133	GLN

5.3.3 RNA [i](#)

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](#)

12 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	B2Z	C	888	-	27,27,27	1.08	3 (11%)	36,38,38	2.34	6 (16%)
4	SO4	B	1659	-	4,4,4	0.75	0	6,6,6	0.73	0
2	B2Z	D	888	-	27,27,27	1.55	3 (11%)	36,38,38	2.29	10 (27%)
4	SO4	A	1659	-	4,4,4	0.41	0	6,6,6	0.58	0
2	B2Z	A	888	-	27,27,27	1.53	5 (18%)	36,38,38	1.99	6 (16%)
4	SO4	D	1659	-	4,4,4	0.56	0	6,6,6	0.85	0
3	FAD	A	999	-	58,58,58	1.84	10 (17%)	85,89,89	1.64	20 (23%)
4	SO4	C	1659	-	4,4,4	0.45	0	6,6,6	0.89	0
3	FAD	B	999	-	58,58,58	1.72	11 (18%)	85,89,89	1.57	18 (21%)
3	FAD	C	999	-	58,58,58	1.80	16 (27%)	85,89,89	1.75	25 (29%)
2	B2Z	B	888	-	27,27,27	1.55	6 (22%)	36,38,38	2.06	9 (25%)
3	FAD	D	999	-	58,58,58	1.50	10 (17%)	85,89,89	1.60	22 (25%)

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	B2Z	C	888	-	-	0/16/16/16	0/3/3/3
2	B2Z	D	888	-	-	0/16/16/16	0/3/3/3
2	B2Z	A	888	-	-	0/16/16/16	0/3/3/3
3	FAD	A	999	-	-	2/34/50/50	0/6/6/6
3	FAD	B	999	-	-	3/34/50/50	0/6/6/6
3	FAD	C	999	-	-	3/34/50/50	0/6/6/6
2	B2Z	B	888	-	-	0/16/16/16	0/3/3/3
3	FAD	D	999	-	-	2/34/50/50	0/6/6/6

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	FAD	C9A-C5X	8.34	1.54	1.41
3	C	999	FAD	C9A-C5X	5.35	1.49	1.41
3	B	999	FAD	C9A-C5X	4.59	1.48	1.41
3	B	999	FAD	C5A-C4A	4.49	1.47	1.39
3	C	999	FAD	C5A-C4A	4.39	1.46	1.39
3	C	999	FAD	P-O3P	4.29	1.64	1.59
3	A	999	FAD	P-O3P	4.25	1.64	1.59
3	B	999	FAD	C4A-N9A	-4.20	1.29	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	FAD	C8-C7	4.20	1.51	1.40
3	A	999	FAD	C5A-C4A	4.15	1.46	1.39
3	D	999	FAD	C5A-C4A	3.93	1.46	1.39
2	A	888	B2Z	C10-N1	-3.85	1.31	1.38
2	D	888	B2Z	C10-N1	-3.75	1.32	1.38
3	C	999	FAD	PA-O3P	3.74	1.63	1.59
3	C	999	FAD	C4-N3	-3.71	1.31	1.38
3	B	999	FAD	C4-N3	-3.70	1.31	1.38
3	D	999	FAD	P-O3P	3.58	1.63	1.59
2	B	888	B2Z	C10-N1	-3.52	1.32	1.38
3	D	999	FAD	C4-N3	-3.48	1.32	1.38
3	D	999	FAD	C4A-N9A	-3.43	1.30	1.37
3	D	999	FAD	C9A-C5X	3.42	1.46	1.41
2	B	888	B2Z	C12-N1	-3.42	1.31	1.37
2	D	888	B2Z	C12-N1	-3.36	1.32	1.37
3	A	999	FAD	C4A-N9A	-3.33	1.30	1.37
2	D	888	B2Z	O1-C12	3.30	1.30	1.23
2	A	888	B2Z	C12-N1	-3.22	1.32	1.37
2	B	888	B2Z	C13-C1	-3.21	1.47	1.52
3	B	999	FAD	C2-N3	-3.16	1.32	1.39
3	A	999	FAD	C4-N3	-3.15	1.33	1.38
3	B	999	FAD	C5X-N5	-3.09	1.33	1.39
3	C	999	FAD	C8A-N7A	2.97	1.37	1.31
2	A	888	B2Z	O1-C12	2.94	1.29	1.23
3	C	999	FAD	C5A-N7A	-2.83	1.33	1.39
2	A	888	B2Z	C7-C6	2.79	1.43	1.39
3	C	999	FAD	PA-O2A	-2.60	1.43	1.55
3	D	999	FAD	C9-C8	-2.59	1.36	1.39
3	B	999	FAD	C8-C7	2.58	1.47	1.40
3	B	999	FAD	C2-N1	-2.56	1.30	1.36
2	B	888	B2Z	C12-N2	-2.53	1.33	1.37
3	C	999	FAD	C6-C5X	2.53	1.43	1.40
2	C	888	B2Z	C7-C6	2.47	1.43	1.39
2	B	888	B2Z	C7-C6	2.43	1.43	1.39
3	D	999	FAD	C5A-N7A	-2.42	1.34	1.39
3	C	999	FAD	C5A-C6A	2.42	1.47	1.41
3	B	999	FAD	C1'-C2'	2.40	1.56	1.52
3	C	999	FAD	O2'-C2'	2.38	1.48	1.43
2	B	888	B2Z	O1-C12	2.36	1.28	1.23
3	D	999	FAD	C5X-N5	-2.36	1.35	1.39
3	D	999	FAD	PA-O3P	2.31	1.62	1.59
3	A	999	FAD	C4X-N5	2.29	1.35	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	999	FAD	O2-C2	2.27	1.28	1.24
2	C	888	B2Z	O1-C12	2.26	1.28	1.23
2	A	888	B2Z	C13-C1	-2.26	1.49	1.52
3	C	999	FAD	C8-C7	2.25	1.46	1.40
3	C	999	FAD	C10-N1	2.25	1.37	1.33
3	C	999	FAD	C2'-C3'	-2.25	1.49	1.53
3	B	999	FAD	C5A-N7A	-2.22	1.35	1.39
3	C	999	FAD	C2-N3	-2.21	1.34	1.39
2	C	888	B2Z	C10-N1	-2.15	1.34	1.38
3	A	999	FAD	C5A-N7A	-2.12	1.35	1.39
3	C	999	FAD	C4A-N9A	-2.11	1.33	1.37
3	A	999	FAD	C8A-N7A	2.10	1.35	1.31
3	A	999	FAD	C4X-C10	2.04	1.50	1.44
3	B	999	FAD	PA-O2A	-2.03	1.45	1.55

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	888	B2Z	N2-C12-N1	7.53	115.18	106.62
2	D	888	B2Z	O1-C12-N1	-6.80	118.93	126.68
2	C	888	B2Z	C9-N2-C12	-6.76	102.64	110.03
2	C	888	B2Z	O1-C12-N1	-6.41	119.37	126.68
2	D	888	B2Z	C9-N2-C12	-5.56	103.96	110.03
2	A	888	B2Z	N2-C12-N1	5.52	112.89	106.62
2	A	888	B2Z	C9-N2-C12	-5.42	104.11	110.03
2	D	888	B2Z	N2-C12-N1	5.27	112.61	106.62
2	B	888	B2Z	N2-C12-N1	5.14	112.46	106.62
2	A	888	B2Z	O1-C12-N1	-4.92	121.08	126.68
2	B	888	B2Z	O1-C12-N1	-4.76	121.26	126.68
2	B	888	B2Z	C9-N2-C12	-4.62	104.98	110.03
3	A	999	FAD	O4B-C1B-N9A	-4.54	99.37	108.09
3	C	999	FAD	C4A-N9A-C8A	4.15	110.09	105.74
3	B	999	FAD	C5A-C4A-N3A	-4.10	121.08	126.72
3	C	999	FAD	C4-C4X-N5	4.07	123.83	118.21
3	C	999	FAD	N9A-C8A-N7A	-4.01	108.24	113.94
2	B	888	B2Z	C17-C18-C13	-3.88	119.41	123.68
2	D	888	B2Z	C17-C18-C13	-3.83	119.47	123.68
2	C	888	B2Z	C10-N1-C12	-3.83	105.85	110.03
3	A	999	FAD	C5X-C9A-N10	3.70	121.31	117.97
3	B	999	FAD	C4A-N9A-C8A	3.63	109.55	105.74
3	C	999	FAD	C9A-C5X-N5	-3.57	118.67	122.45
3	B	999	FAD	O2A-PA-O1A	3.56	128.98	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	999	FAD	C4-C4X-N5	3.53	123.09	118.21
3	B	999	FAD	N3A-C4A-N9A	3.48	133.08	127.17
2	A	888	B2Z	C17-C18-C13	-3.44	119.90	123.68
2	D	888	B2Z	C4-N-C3	-3.40	118.21	122.90
3	D	999	FAD	C4A-N9A-C8A	3.38	109.29	105.74
3	A	999	FAD	C8M-C8-C9	-3.38	113.62	119.57
3	A	999	FAD	C9A-C5X-N5	-3.36	118.89	122.45
2	D	888	B2Z	C1-C2-C3	-3.30	108.44	113.03
2	B	888	B2Z	C14-C13-C18	3.30	120.38	116.22
2	A	888	B2Z	C14-C13-C18	3.29	120.37	116.22
3	C	999	FAD	C5A-N7A-C8A	3.24	108.54	103.45
3	D	999	FAD	C5A-C4A-N3A	-3.22	122.28	126.72
2	B	888	B2Z	C2-C1-C13	-3.22	103.26	110.84
3	D	999	FAD	C4-C4X-N5	3.21	122.64	118.21
3	A	999	FAD	N3A-C2A-N1A	-3.20	123.73	128.58
3	D	999	FAD	N3A-C2A-N1A	-3.15	123.82	128.58
3	C	999	FAD	O2P-P-O1P	3.14	127.05	112.44
3	A	999	FAD	C4X-C10-N10	3.12	120.95	116.48
3	A	999	FAD	C5'-C4'-C3'	3.08	118.02	112.22
3	A	999	FAD	C4A-N9A-C8A	2.99	108.88	105.74
3	C	999	FAD	C4A-N9A-C1B	-2.98	119.67	126.63
3	D	999	FAD	C2A-N1A-C6A	2.92	123.53	118.73
3	C	999	FAD	C5A-C4A-N3A	-2.90	122.73	126.72
2	C	888	B2Z	C4-N-C3	-2.89	118.91	122.90
3	D	999	FAD	C4A-C5A-N7A	-2.88	107.29	110.58
3	D	999	FAD	C5X-C9A-N10	2.87	120.56	117.97
3	A	999	FAD	C5A-C4A-N3A	-2.84	122.80	126.72
3	B	999	FAD	N3A-C2A-N1A	-2.83	124.31	128.58
3	D	999	FAD	C6A-C5A-N7A	2.78	137.44	132.09
3	B	999	FAD	C2A-N3A-C4A	2.77	118.59	111.83
3	C	999	FAD	O2A-PA-O1A	2.75	125.26	112.44
3	A	999	FAD	O2A-PA-O1A	2.74	125.17	112.44
3	C	999	FAD	O4B-C1B-N9A	-2.72	102.86	108.09
2	B	888	B2Z	C4-N-C3	-2.72	119.15	122.90
3	A	999	FAD	N3A-C4A-N9A	2.70	131.75	127.17
3	C	999	FAD	N3A-C4A-N9A	2.69	131.75	127.17
3	B	999	FAD	C4X-C10-N1	-2.68	118.02	124.59
3	C	999	FAD	C4A-C5A-N7A	-2.67	107.52	110.58
3	D	999	FAD	C4X-C10-N10	2.64	120.26	116.48
3	A	999	FAD	C9A-N10-C10	-2.62	116.75	120.75
2	D	888	B2Z	C2-C1-C13	-2.62	104.66	110.84
3	B	999	FAD	O2P-P-O1P	2.62	124.64	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	999	FAD	C5X-C9A-N10	2.61	120.33	117.97
3	C	999	FAD	O2-C2-N1	-2.58	117.52	121.80
2	B	888	B2Z	C5-C4-C6	2.58	118.28	112.22
3	D	999	FAD	C4A-N9A-C1B	-2.56	120.64	126.63
3	D	999	FAD	N9A-C8A-N7A	-2.55	110.31	113.94
3	D	999	FAD	N3A-C4A-N9A	2.52	131.45	127.17
3	D	999	FAD	O4B-C1B-N9A	-2.52	103.25	108.09
3	A	999	FAD	O2P-P-O1P	2.51	124.14	112.44
3	C	999	FAD	C6A-C5A-N7A	2.51	136.93	132.09
3	D	999	FAD	C10-N1-C2	2.51	122.28	116.85
2	A	888	B2Z	C2-C1-C13	-2.50	104.95	110.84
3	A	999	FAD	C2A-N3A-C4A	2.49	117.92	111.83
3	C	999	FAD	C5X-N5-C4X	2.43	122.02	118.09
3	D	999	FAD	O3'-C3'-C4'	2.42	114.44	108.93
3	C	999	FAD	C4X-C10-N1	-2.42	118.65	124.59
3	A	999	FAD	C8M-C8-C7	2.42	125.69	120.76
3	B	999	FAD	N9A-C8A-N7A	-2.41	110.51	113.94
3	C	999	FAD	C4X-C4-N3	2.41	119.38	113.25
3	A	999	FAD	C4-C4X-N5	2.39	121.50	118.21
3	D	999	FAD	C9A-N10-C10	-2.38	117.13	120.75
3	B	999	FAD	C5X-C9A-N10	2.37	120.11	117.97
3	C	999	FAD	C2A-N1A-C6A	2.37	122.62	118.73
3	B	999	FAD	C10-N1-C2	2.36	121.96	116.85
3	A	999	FAD	C6A-C5A-N7A	2.35	136.62	132.09
3	C	999	FAD	C2A-N3A-C4A	2.30	117.45	111.83
3	B	999	FAD	C9A-C5X-N5	-2.28	120.03	122.45
2	C	888	B2Z	C10-C9-N2	2.28	109.32	106.42
3	D	999	FAD	O2A-PA-O1A	2.26	122.97	112.44
2	D	888	B2Z	C16-C17-C18	2.26	122.00	118.49
3	C	999	FAD	N3A-C2A-N1A	-2.26	125.16	128.58
3	B	999	FAD	C8M-C8-C9	-2.25	115.61	119.57
3	B	999	FAD	C2B-C1B-N9A	2.25	118.89	113.30
3	A	999	FAD	C2A-N1A-C6A	2.20	122.35	118.73
2	B	888	B2Z	C5-C4-N	-2.20	104.98	109.00
3	C	999	FAD	C4X-C10-N10	2.20	119.63	116.48
3	B	999	FAD	O4B-C1B-N9A	-2.19	103.88	108.09
3	D	999	FAD	C2A-N3A-C4A	2.19	117.18	111.83
3	B	999	FAD	C6A-C5A-N7A	2.18	136.30	132.09
2	D	888	B2Z	F-C18-C13	2.18	122.22	118.28
3	C	999	FAD	N6A-C6A-N1A	2.17	123.22	118.38
3	D	999	FAD	C5A-N7A-C8A	2.15	106.83	103.45
3	D	999	FAD	O2A-PA-O3P	2.14	113.05	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	999	FAD	C5'-C4'-C3'	2.11	116.20	112.22
3	A	999	FAD	C6A-C5A-C4A	-2.10	114.31	117.18
3	B	999	FAD	C4X-C4-N3	2.09	118.58	113.25
2	D	888	B2Z	C14-C13-C18	2.06	118.81	116.22
3	A	999	FAD	C4X-C10-N1	-2.05	119.57	124.59
3	D	999	FAD	C4X-C4-N3	2.03	118.42	113.25
3	D	999	FAD	O4'-C4'-C5'	-2.01	105.55	109.99
3	C	999	FAD	O3P-P-O1P	-2.01	104.65	110.70

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	999	FAD	N10-C1'-C2'-O2'
3	A	999	FAD	N10-C1'-C2'-C3'
3	B	999	FAD	N10-C1'-C2'-O2'
3	B	999	FAD	N10-C1'-C2'-C3'
3	C	999	FAD	N10-C1'-C2'-O2'
3	C	999	FAD	N10-C1'-C2'-C3'
3	D	999	FAD	N10-C1'-C2'-O2'
3	D	999	FAD	N10-C1'-C2'-C3'
3	B	999	FAD	PA-O3P-P-O2P
3	C	999	FAD	PA-O3P-P-O2P

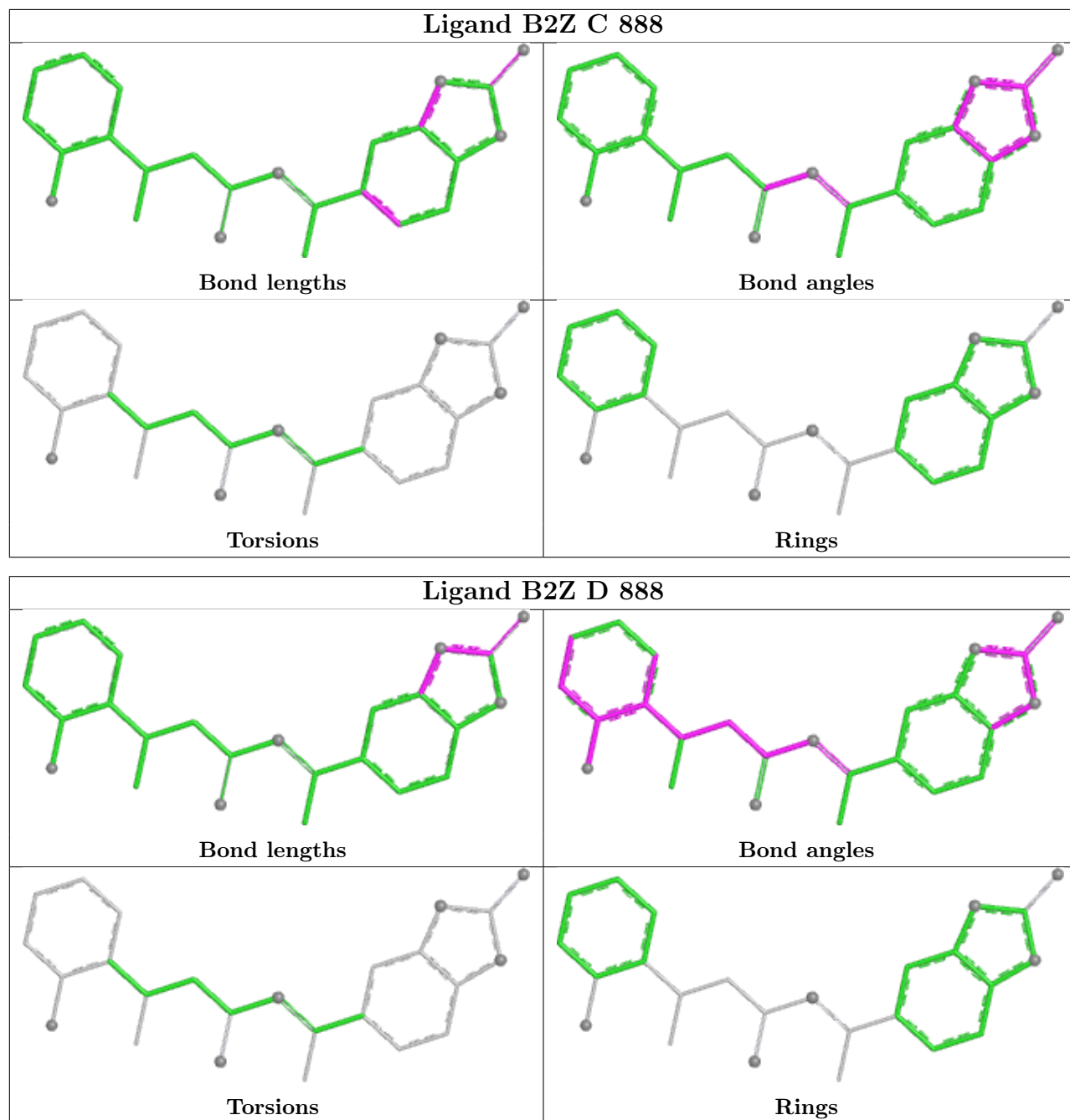
There are no ring outliers.

4 monomers are involved in 6 short contacts:

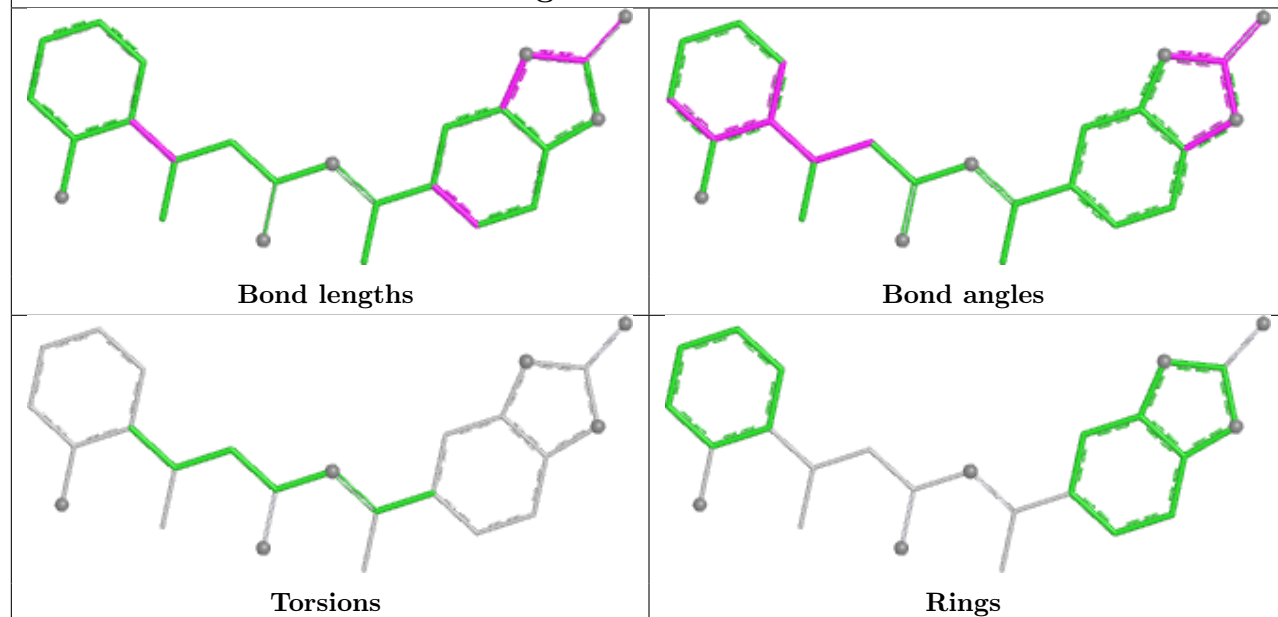
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	888	B2Z	1	0
2	A	888	B2Z	4	0
3	A	999	FAD	3	0
2	B	888	B2Z	1	0

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

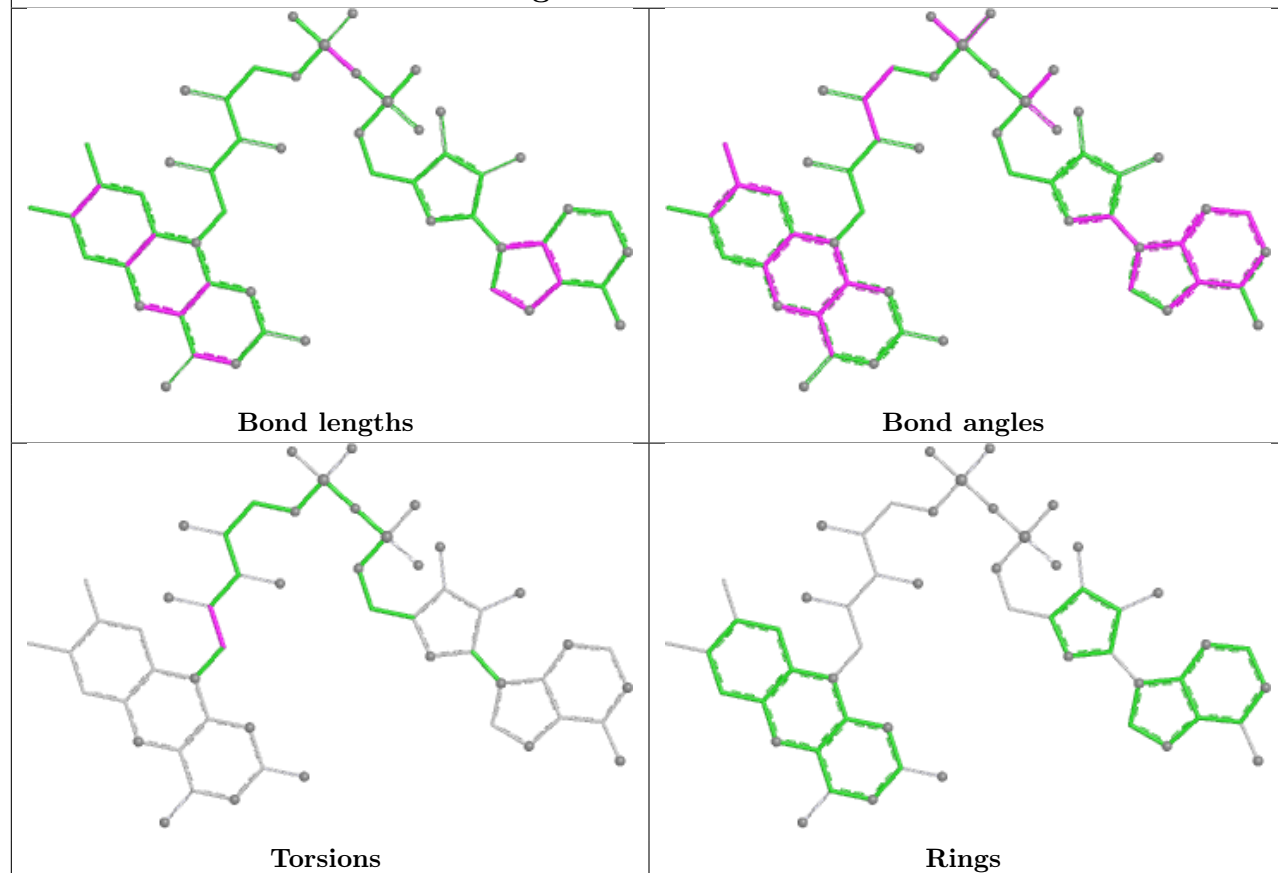
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

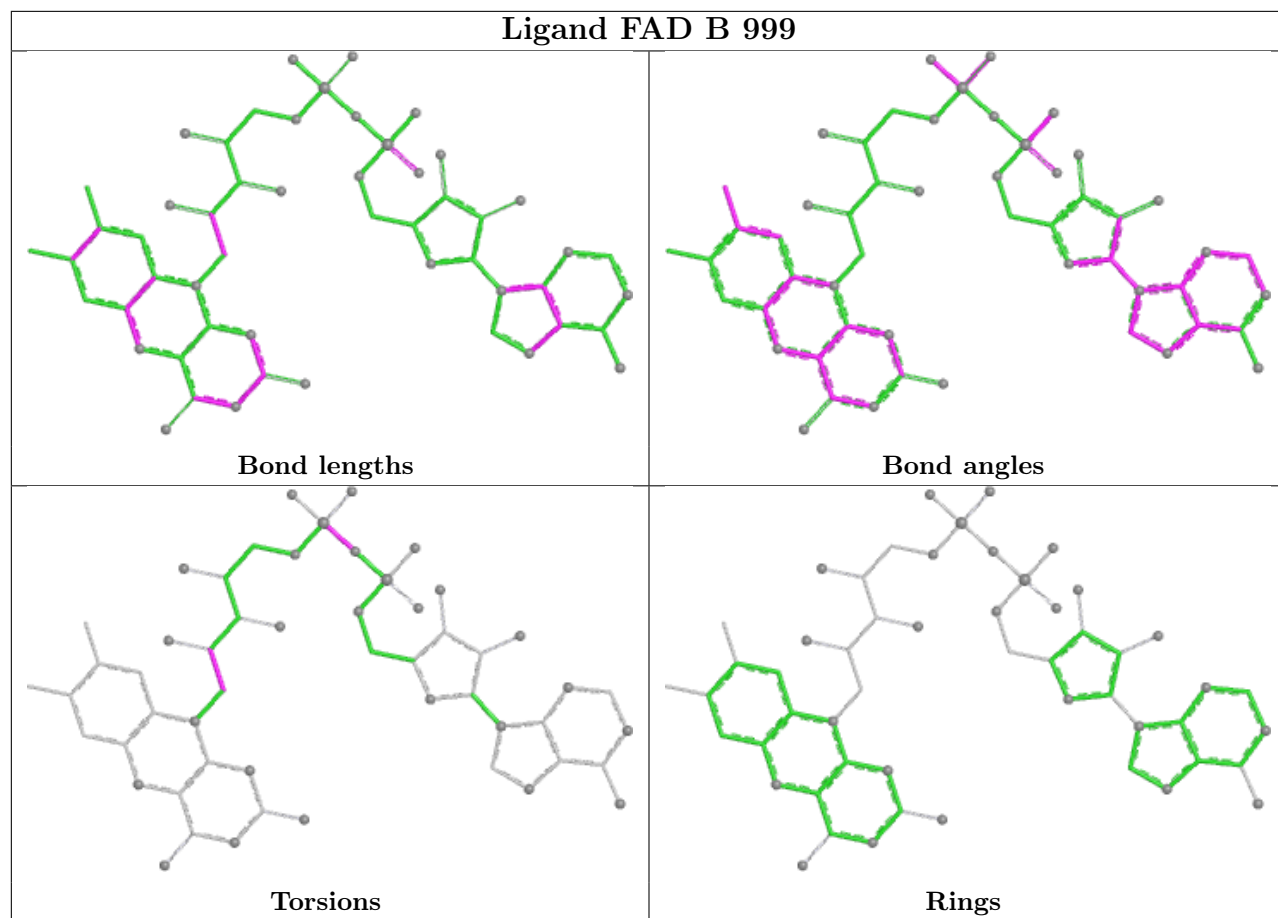


Ligand B2Z A 888

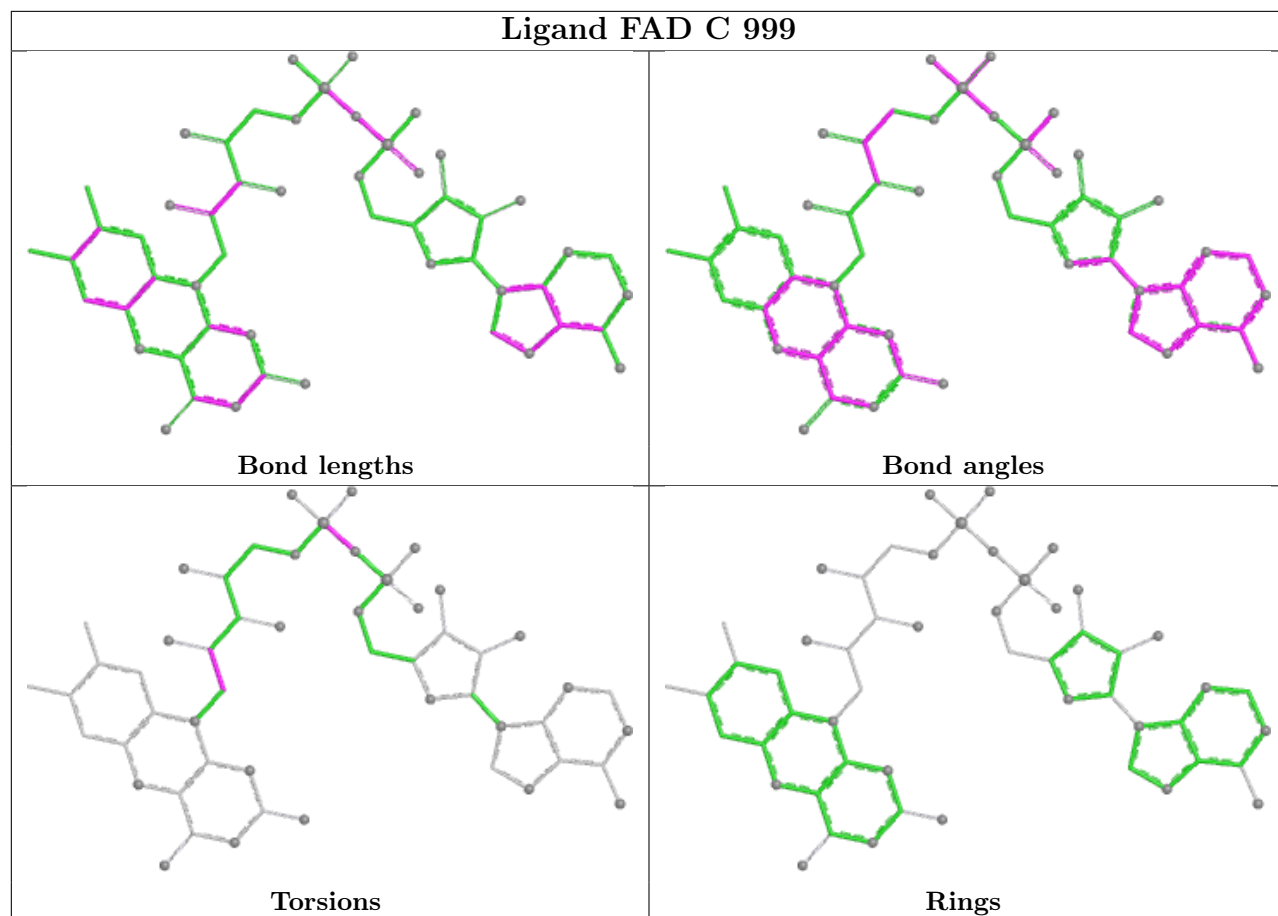


Ligand FAD A 999

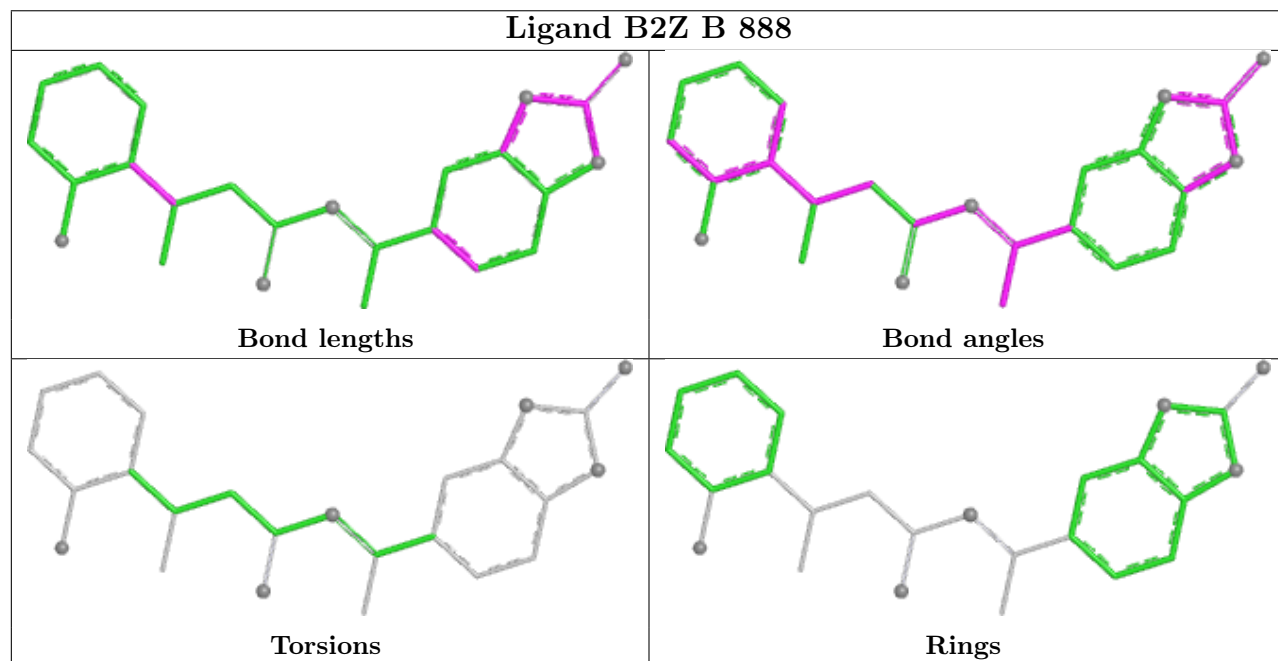


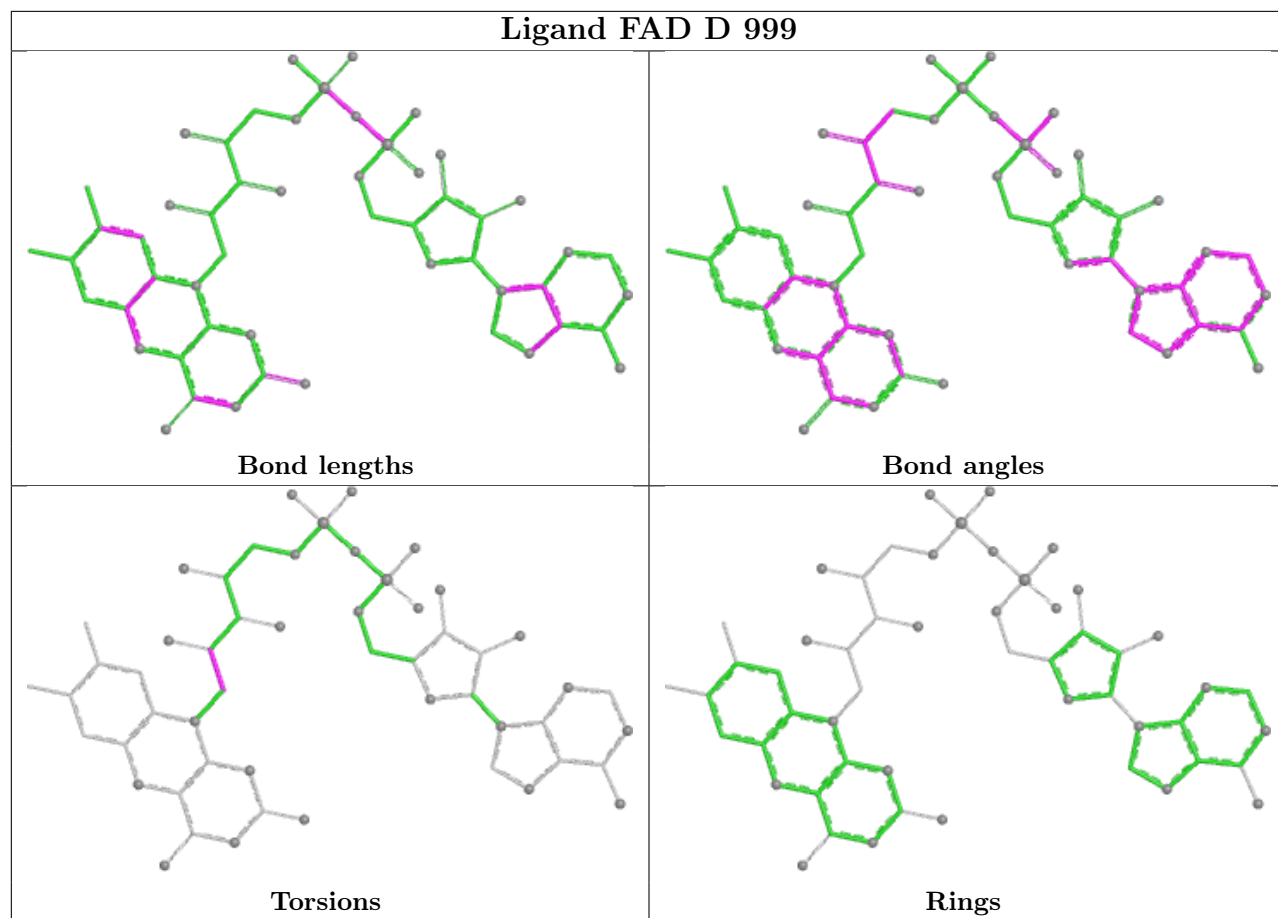


Ligand FAD C 999



Ligand B2Z B 888





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	560/658 (85%)	0.06	17 (3%)	52	55	15, 31, 57, 74	1 (0%)
1	B	539/658 (81%)	0.02	10 (1%)	66	69	17, 30, 53, 72	0
1	C	559/658 (84%)	-0.09	3 (0%)	87	88	14, 28, 50, 77	3 (0%)
1	D	564/658 (85%)	0.08	17 (3%)	52	55	16, 31, 57, 78	0
All	All	2222/2632 (84%)	0.02	47 (2%)	63	66	14, 30, 55, 78	4 (0%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	455	PHE	5.3
1	A	156	PRO	4.7
1	D	456	LYS	4.7
1	A	452	ILE	3.9
1	D	448	LYS	3.8
1	A	451	TYR	3.6
1	C	559	PHE	3.6
1	B	140	LEU	3.4
1	A	157	PRO	3.3
1	B	460	PRO	3.2
1	A	559	PHE	3.1
1	D	451	TYR	3.1
1	A	505[A]	TYR	3.0
1	D	450	PHE	3.0
1	C	455	PHE	2.9
1	A	457	GLY	2.9
1	B	159	ILE	2.9
1	D	559	PHE	2.9
1	B	243	TYR	2.8
1	A	586	ARG	2.7
1	A	140	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	522	TYR	2.7
1	D	452	ILE	2.6
1	D	506	LEU	2.5
1	A	443	PHE	2.5
1	A	447	LEU	2.5
1	A	201	MET	2.5
1	D	142	HIS	2.5
1	B	589	SER	2.4
1	D	454	LYS	2.4
1	A	81	GLY	2.4
1	A	159	ILE	2.4
1	D	426	PHE	2.3
1	A	444	LEU	2.3
1	D	586	ARG	2.2
1	B	434	PRO	2.2
1	A	82	ILE	2.2
1	D	453	THR	2.2
1	B	426	PHE	2.1
1	D	199	GLU	2.1
1	C	457	GLY	2.1
1	D	81	GLY	2.1
1	B	199	GLU	2.1
1	D	139	ASN	2.1
1	D	460	PRO	2.0
1	A	456	LYS	2.0
1	B	81	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

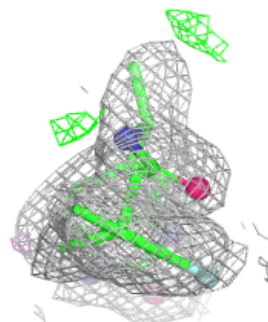
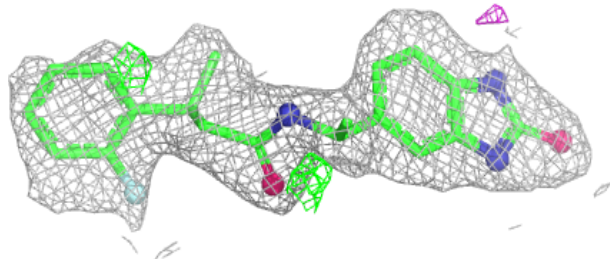
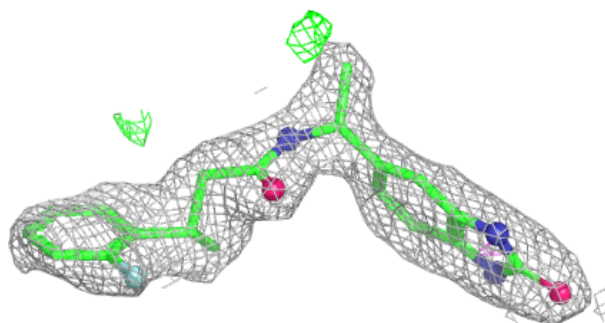
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	B2Z	B	888	25/25	0.89	0.12	33,38,58,70	0
4	SO4	D	1659	5/5	0.90	0.23	42,50,58,76	0
4	SO4	B	1659	5/5	0.91	0.16	51,52,58,63	0
2	B2Z	C	888	25/25	0.91	0.09	23,32,39,53	0
2	B2Z	A	888	25/25	0.92	0.11	30,34,57,65	0
4	SO4	A	1659	5/5	0.92	0.12	52,54,60,60	0
2	B2Z	D	888	25/25	0.93	0.10	31,38,51,56	0
4	SO4	C	1659	5/5	0.95	0.14	35,45,53,58	0
3	FAD	B	999	53/53	0.98	0.04	15,18,20,24	0
3	FAD	D	999	53/53	0.98	0.04	15,17,20,21	0
3	FAD	A	999	53/53	0.98	0.04	15,19,21,22	0
3	FAD	C	999	53/53	0.99	0.04	12,15,17,18	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.

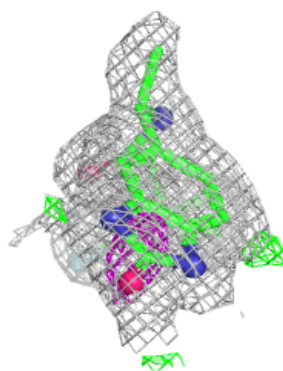
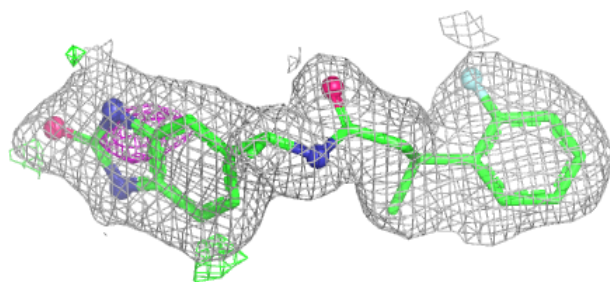
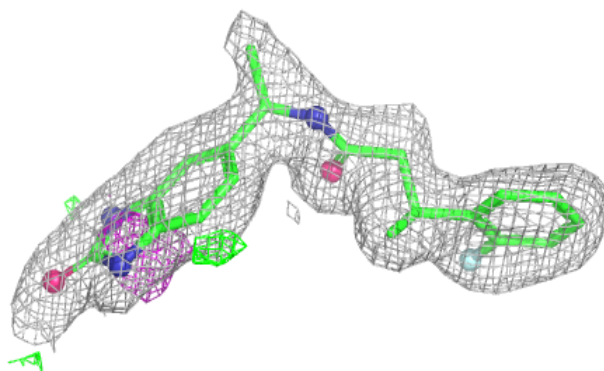
Electron density around B2Z B 888:

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

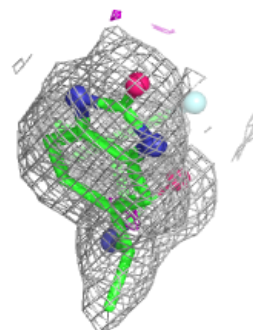
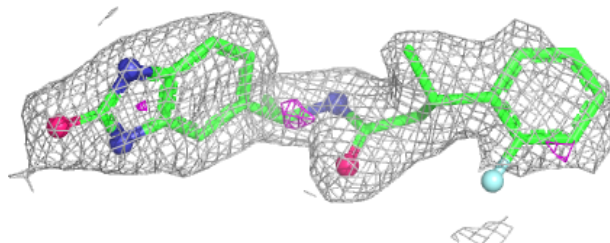
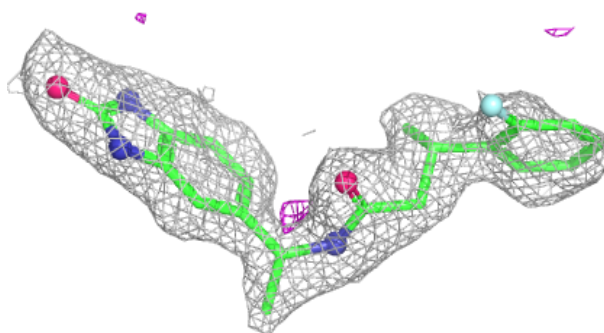


Electron density around B2Z C 888:

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

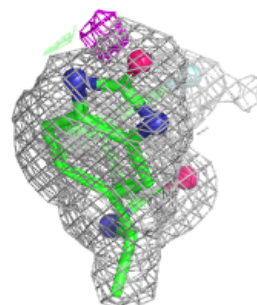
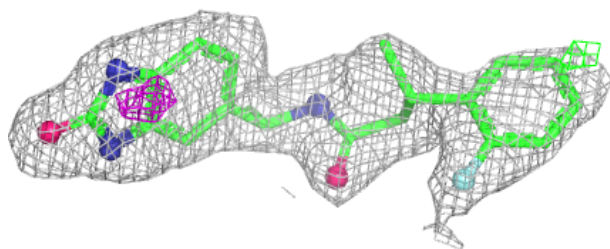
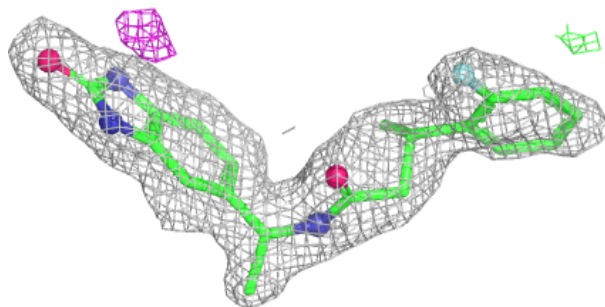
**Electron density around B2Z A 888:**

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

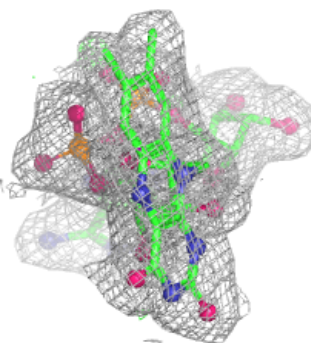
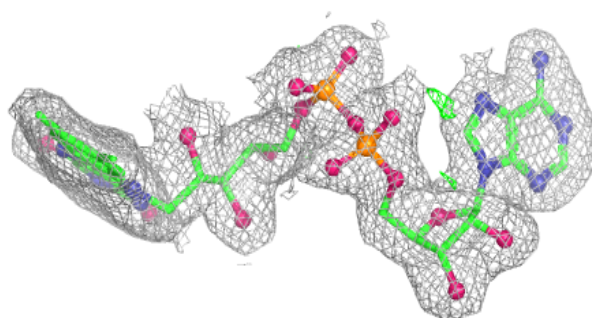
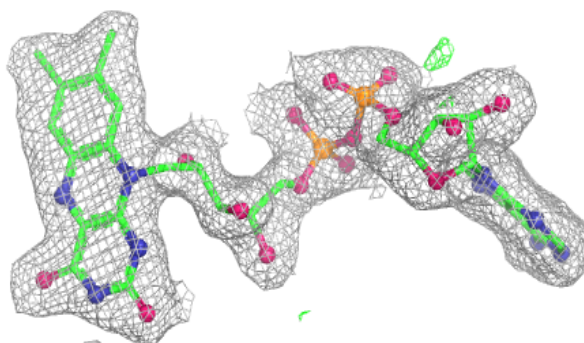


Electron density around B2Z D 888:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

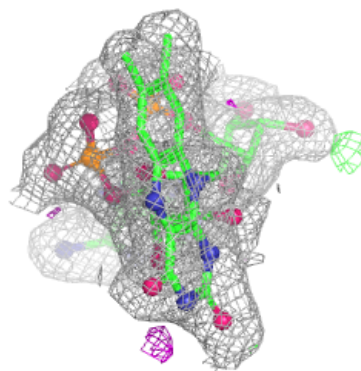
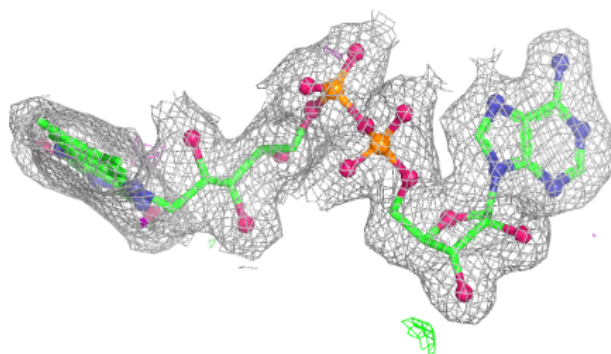
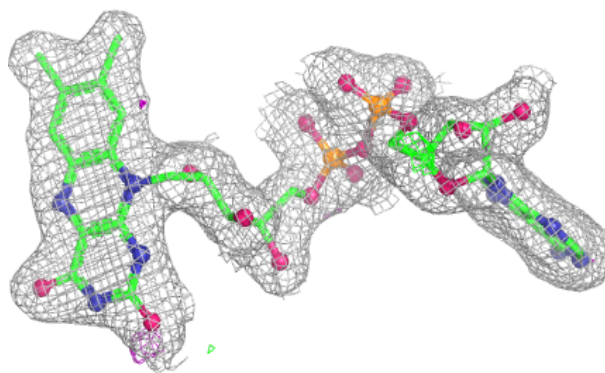
**Electron density around FAD B 999:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

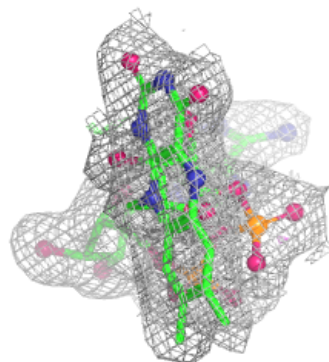
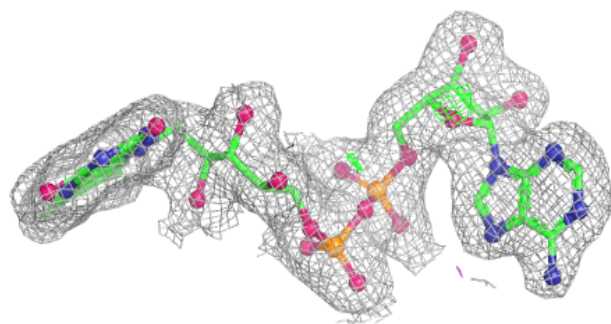
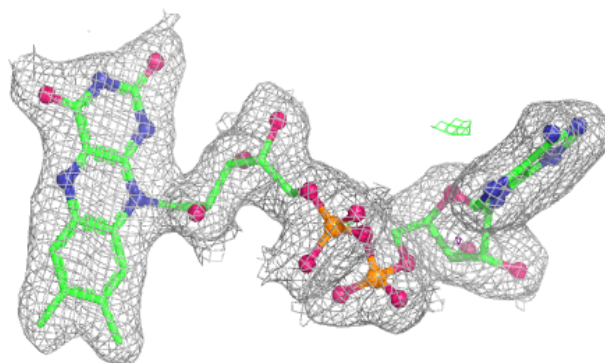


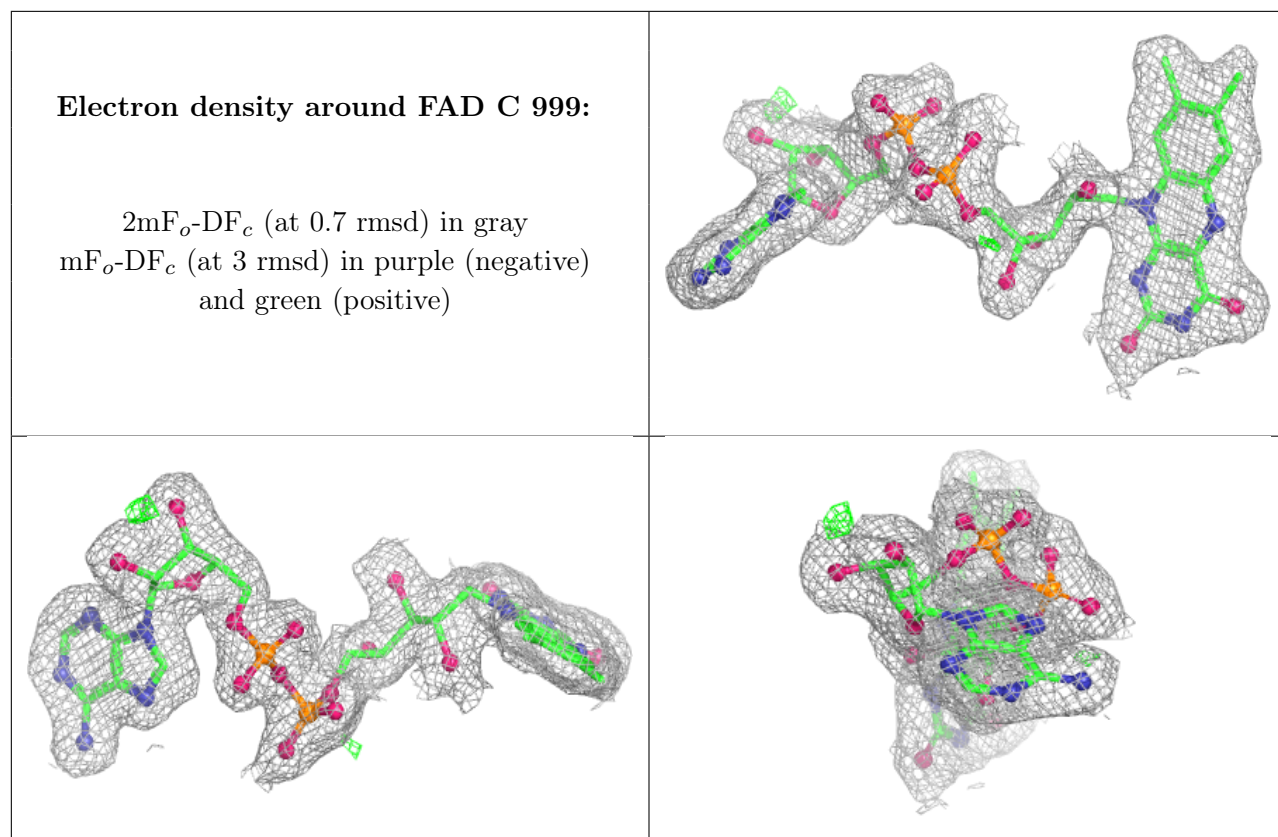
Electron density around FAD D 999:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around FAD A 999:**

$2mF_o-DF_c$ (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.