



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:52 PM UTC

PDB ID : 3FGC / pdb_00003fgc
Title : Crystal Structure of the Bacterial Luciferase:Flavin Complex Reveals the Basis of Intersubunit Communication
Authors : Campbell, Z.T.; Weichsel, A.; Montfort, W.R.; Baldwin, T.O.
Deposited on : 2008-12-05
Resolution : 2.30 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

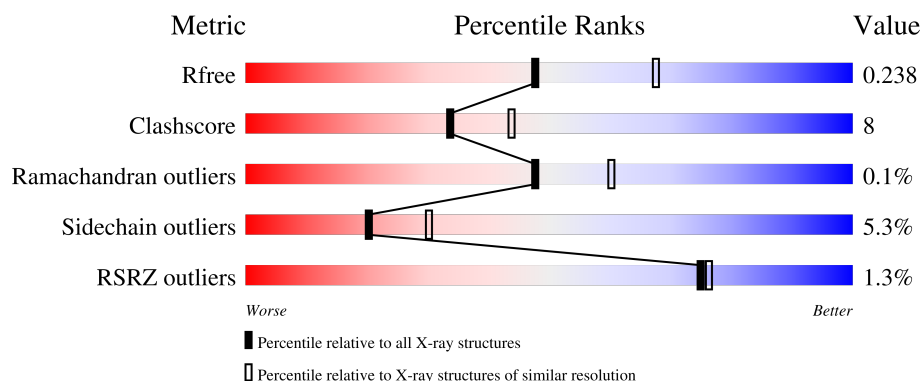
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	355	% 77% 20% ...
1	C	355	3% 79% 17% ..
2	B	332	83% 12% ..
2	D	332	% 81% 15% ..

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
4	PO4	A	356[B]	-	X	-	-
4	PO4	C	359	-	-	X	-
5	SO4	A	361	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11895 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 Alkanal monooxygenase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	349	Total	C	N	O	S	0	7	0
			2832	1797	471	546	18			
1	C	348	Total	C	N	O	S	0	11	0
			2849	1809	470	552	18			

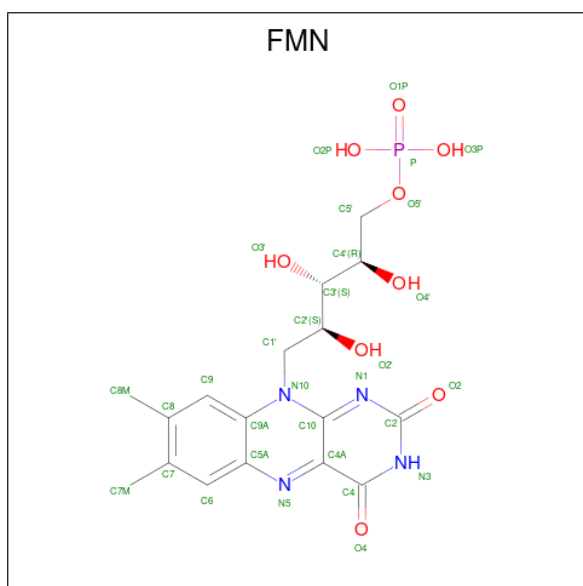
- Molecule 2 is a protein called Alkanal monooxygenase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	318	Total	C	N	O	S	0	5	0
			2550	1601	440	494	15			
2	D	325	Total	C	N	O	S	0	15	0
			2696	1695	465	521	15			

There are 16 discrepancies between the modelled and reference sequences:

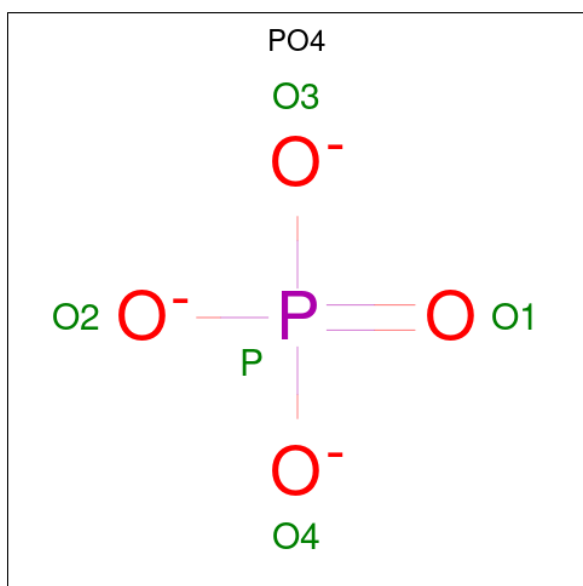
Chain	Residue	Modelled	Actual	Comment	Reference
B	325	LEU	-	expression tag	UNP P07739
B	326	GLU	-	expression tag	UNP P07739
B	327	HIS	-	expression tag	UNP P07739
B	328	HIS	-	expression tag	UNP P07739
B	329	HIS	-	expression tag	UNP P07739
B	330	HIS	-	expression tag	UNP P07739
B	331	HIS	-	expression tag	UNP P07739
B	332	HIS	-	expression tag	UNP P07739
D	325	LEU	-	expression tag	UNP P07739
D	326	GLU	-	expression tag	UNP P07739
D	327	HIS	-	expression tag	UNP P07739
D	328	HIS	-	expression tag	UNP P07739
D	329	HIS	-	expression tag	UNP P07739
D	330	HIS	-	expression tag	UNP P07739
D	331	HIS	-	expression tag	UNP P07739
D	332	HIS	-	expression tag	UNP P07739

- Molecule 3 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	1
			31	17	4	9	1		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	1
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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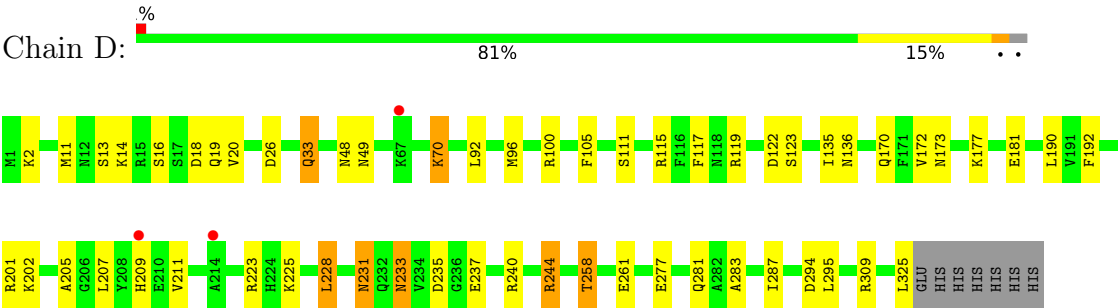
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	251	Total	O	0	21
			272	272		
6	B	218	Total	O	1	14
			233	233		
6	C	133	Total	O	0	10
			144	144		
6	D	179	Total	O	0	19
			198	198		

● Molecule 2: Alkanal monooxygenase beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.89Å 109.30Å 301.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.33 – 2.30 27.33 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (27.33-2.30) 99.8 (27.33-2.30)	Depositor EDS
R_{merge}	0.43	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.35 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.184 , 0.241 0.185 , 0.238	Depositor DCC
R_{free} test set	4385 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11895	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 2.39% 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: FMN, PO4, 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	1.21	10/2905 (0.3%)	1.12	2/3935 (0.1%)
1	C	1.00	2/2933 (0.1%)	1.04	2/3974 (0.1%)
2	B	1.14	1/2607 (0.0%)	1.04	1/3525 (0.0%)
2	D	1.09	5/2753 (0.2%)	1.01	0/3720
All	All	1.11	18/11198 (0.2%)	1.05	5/15154 (0.0%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	41	VAL	CA-CB	7.55	1.63	1.54
1	A	212	ALA	CA-CB	6.38	1.63	1.53
1	C	68	THR	N-CA	5.83	1.53	1.45
1	A	12	PRO	CA-C	5.76	1.56	1.52
1	A	339	SER	CA-C	5.73	1.60	1.52
1	C	76	ILE	CA-CB	5.73	1.60	1.54
1	A	348	MET	C-O	-5.65	1.18	1.24
2	D	20	VAL	CA-CB	5.44	1.61	1.54
1	A	260	ILE	CA-CB	5.42	1.61	1.54
1	A	60	ALA	CA-CB	5.36	1.61	1.53
2	D	13	SER	N-CA	5.29	1.52	1.46
2	D	228	LEU	C-O	-5.22	1.17	1.23
1	A	39	VAL	CA-CB	5.21	1.60	1.54
1	A	310	ILE	CA-CB	5.16	1.60	1.54
1	A	139	PHE	N-CA	5.13	1.52	1.46
2	D	135	ILE	CA-CB	5.09	1.60	1.54
2	D	258	THR	CA-CB	5.04	1.61	1.53
1	A	168	ALA	CA-CB	5.03	1.60	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	31	SER	N-CA-C	6.16	117.66	111.07
1	A	148	ASN	CA-C-N	5.42	128.30	120.38
1	A	148	ASN	C-N-CA	5.42	128.30	120.38
1	C	209	ASN	N-CA-C	5.33	117.09	111.28
2	B	248	GLU	N-CA-C	5.19	116.63	110.97

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	2832	0	2710	46	0
1	C	2849	0	2709	54	0
2	B	2550	0	2426	31	0
2	D	2696	0	2566	40	0
3	A	31	0	19	1	0
4	A	5	0	0	1	0
4	C	5	0	0	2	0
5	A	25	0	0	2	0
5	B	15	0	0	1	0
5	C	15	0	0	0	0
5	D	25	0	0	0	0
6	A	272	0	0	2	0
6	B	233	0	0	7	0
6	C	144	0	0	5	0
6	D	198	0	0	4	0
All	All	11895	0	10430	166	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 8.

All (166) 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:10[B]:TYR:CD2	1:C:250[B]:TRP:HZ3	1.65	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10[B]:TYR:CD2	1:C:250[B]:TRP:CZ3	2.37	1.11
2:D:16:SER:OG	2:D:19[A]:GLN:HG3	1.57	1.04
2:D:181:GLU:HG3	2:D:211:VAL:HG21	1.41	0.98
2:B:173:ASN:ND2	2:B:193:ARG:HD2	1.81	0.96
2:B:181:GLU:HG3	2:B:211:VAL:HG21	1.47	0.95
1:A:6[A]:PHE:CE2	1:A:227:SER:HB2	2.02	0.94
1:A:112:LYS:HB3	1:A:260:ILE:HD11	1.48	0.93
1:A:6[A]:PHE:HE2	1:A:227:SER:HB2	1.38	0.88
1:C:10[B]:TYR:HD2	1:C:250[B]:TRP:HZ3	1.22	0.85
1:A:175[B]:GLU:CA	1:A:176:SER:N	2.42	0.82
1:C:282:LEU:HD13	1:C:283:LYS:H	1.47	0.79
2:D:205:ALA:O	2:D:209[B]:HIS:CD2	2.36	0.78
1:C:262:ASP:O	1:C:263:ASP:HB2	1.84	0.76
1:A:249:HIS:HE1	6:D:354:HOH:O	1.70	0.74
1:C:237:ASN:ND2	6:C:400:HOH:O	2.21	0.74
2:D:205:ALA:O	2:D:209[B]:HIS:HD2	1.71	0.74
2:B:173:ASN:HD21	2:B:193:ARG:HD2	1.54	0.72
1:C:107:ARG:HG3	6:C:380:HOH:O	1.90	0.72
1:A:175[B]:GLU:CA	1:A:175[B]:GLU:O	2.40	0.70
1:A:175[B]:GLU:O	1:A:176:SER:N	2.25	0.70
1:C:136[A]:LYS:HE2	6:C:422:HOH:O	1.92	0.68
1:C:32:GLU:HB2	1:C:69:LEU:HD13	1.77	0.67
1:A:175[B]:GLU:O	1:A:175[B]:GLU:CD	2.37	0.67
1:A:299:ASN:O	1:A:310:ILE:HD13	1.96	0.66
2:B:233:ASN:HD22	2:B:235:ASP:H	1.44	0.65
1:C:49:PHE:O	1:C:250[B]:TRP:CH2	2.49	0.65
2:D:16:SER:H	2:D:19[A]:GLN:HE21	1.47	0.62
1:C:23:ARG:NH2	1:C:331:GLY:O	2.33	0.62
1:C:10[B]:TYR:CD2	1:C:250[B]:TRP:CE3	2.88	0.61
1:C:282:LEU:CD1	1:C:283:LYS:H	2.13	0.61
1:C:21:MET:HE2	2:D:92:LEU:HD12	1.83	0.61
1:C:6[B]:PHE:CE2	1:C:227[B]:SER:HB2	2.36	0.60
2:B:252:ARG:HD2	6:B:353:HOH:O	2.01	0.60
1:C:271:ASP:O	1:C:275:GLY:CA	2.50	0.60
2:B:173:ASN:ND2	2:B:193:ARG:CD	2.61	0.60
2:D:181:GLU:HG3	2:D:211:VAL:CG2	2.24	0.60
2:D:277:GLU:HG2	2:D:281:GLN:NE2	2.18	0.59
1:C:8:LEU:HD13	1:C:250[B]:TRP:CZ2	2.37	0.59
2:D:244:ARG:NH2	2:D:261:GLU:OE2	2.36	0.58
2:B:231:ASN:C	2:B:231:ASN:HD22	2.11	0.57
1:C:107:ARG:NH1	4:C:359:PO4:O2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:PRO:HB2	1:C:73:THR:HG22	1.87	0.57
1:C:292:ILE:O	1:C:295[B]:SER:HB2	2.05	0.57
1:C:73:THR:O	1:C:104:GLY:HA3	2.04	0.56
2:B:233:ASN:ND2	2:B:235:ASP:H	2.03	0.56
1:C:233:ASP:O	1:C:303:THR:HA	2.06	0.56
1:C:271:ASP:O	1:C:275:GLY:HA2	2.05	0.56
2:B:111:SER:O	2:B:115[B]:ARG:HG3	2.05	0.56
2:D:172[A]:VAL:HG13	2:D:190:LEU:HD23	1.86	0.56
1:A:264:SER:HB2	5:A:361:SO4:O3	2.05	0.56
2:B:227:THR:HG22	2:B:296:LEU:HB2	1.87	0.56
1:C:3:PHE:CZ	1:C:348:MET:HG2	2.41	0.56
1:C:49:PHE:O	1:C:250[B]:TRP:CZ3	2.59	0.56
1:C:260:ILE:HG23	1:C:261:PHE:CD1	2.42	0.55
2:D:2:LYS:HG3	2:D:223:ARG:NH2	2.21	0.55
1:C:332:SER:O	1:C:336:ILE:HG13	2.06	0.55
2:B:213:GLN:NE2	6:B:417:HOH:O	2.39	0.55
2:D:26[A]:ASP:OD2	2:D:309:ARG:NH2	2.35	0.54
2:D:233:ASN:HD22	2:D:235:ASP:H	1.54	0.54
2:D:136:ASN:HD22	2:D:170:GLN:HE22	1.54	0.54
1:A:254:TYR:O	1:A:258:THR:HG23	2.08	0.54
1:A:148:ASN:O	1:A:152:LYS:HE2	2.08	0.53
2:B:1:MET:HE1	2:B:287:ILE:HG12	1.91	0.53
1:C:10[B]:TYR:CG	1:C:250[B]:TRP:CZ3	2.94	0.53
1:C:262:ASP:O	1:C:263:ASP:CB	2.56	0.53
1:A:6[A]:PHE:CZ	1:A:227:SER:HB2	2.42	0.52
1:C:228:TYR:CD1	1:C:300:PRO:HD3	2.45	0.52
2:D:237[A]:GLU:CD	2:D:240:ARG:HE	2.18	0.51
2:B:307:GLN:HG3	6:B:713:HOH:O	2.11	0.51
2:B:136:ASN:HD22	2:B:170:GLN:HE22	1.58	0.51
2:B:193:ARG:HG2	2:B:193:ARG:HH11	1.75	0.51
1:C:121:MET:O	1:C:121:MET:HG2	2.09	0.51
2:D:117:PHE:O	2:D:119:ARG:NH1	2.42	0.51
1:A:102:ARG:HD3	1:A:169:PRO:HG2	1.94	0.50
2:D:237[A]:GLU:OE2	2:D:240:ARG:NE	2.41	0.50
1:C:21:MET:CE	2:D:92:LEU:HD12	2.40	0.50
2:B:173:ASN:HD21	2:B:193:ARG:CD	2.23	0.50
1:C:49:PHE:O	1:C:250[B]:TRP:HH2	1.92	0.50
2:D:231:ASN:C	2:D:231:ASN:HD22	2.20	0.50
2:D:237[A]:GLU:HG3	6:D:414:HOH:O	2.12	0.49
1:C:12:PRO:HB2	1:C:13:PRO:HD2	1.94	0.49
1:C:221:LYS:NZ	6:C:738:HOH:O	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:33:GLN:HB2	6:B:705:HOH:O	2.13	0.49
2:B:173:ASN:HD22	2:B:191:VAL:HG13	1.78	0.49
2:D:177:LYS:HG2	2:D:207:LEU:HD22	1.95	0.49
1:A:260:ILE:HD13	1:A:261:PHE:H	1.78	0.48
1:A:175[B]:GLU:O	1:A:175[B]:GLU:OE1	2.30	0.48
2:D:287:ILE:HD11	2:D:295:LEU:HD22	1.96	0.48
1:A:229[A]:ILE:HG22	1:A:299:ASN:CG	2.39	0.48
1:C:21:MET:HE1	2:D:92:LEU:CD1	2.44	0.47
1:C:107:ARG:HD2	4:C:359:PO4:O3	2.15	0.47
1:C:240:LYS:NZ	6:C:400:HOH:O	2.39	0.47
1:C:327:PHE:HD2	1:C:339[B]:SER:OG	1.98	0.47
2:D:111:SER:OG	2:D:115[B]:ARG:NH2	2.47	0.47
2:D:244:ARG:HH22	2:D:261:GLU:CD	2.24	0.46
1:A:257:ALA:O	1:A:260:ILE:HD12	2.15	0.46
1:C:21:MET:CE	2:D:92:LEU:CD1	2.93	0.46
2:B:3:PHE:HA	2:B:295:LEU:O	2.16	0.46
1:A:175[B]:GLU:N	1:A:176:SER:N	2.61	0.46
2:B:193:ARG:NH2	6:B:426:HOH:O	2.45	0.46
1:A:21:MET:HB3	1:A:21:MET:HE3	1.64	0.46
1:A:86:GLN:O	1:A:90:VAL:HG23	2.16	0.46
1:A:260:ILE:HD12	1:A:260:ILE:H	1.81	0.46
2:D:225:LYS:HG3	2:D:294:ASP:HB2	1.97	0.45
2:B:92:LEU:HG	2:B:96:MET:HE2	1.98	0.45
1:A:23:ARG:NH1	6:A:383:HOH:O	2.49	0.45
2:B:145:HIS:ND1	5:B:335:SO4:O2	2.50	0.45
2:D:105:PHE:CZ	2:D:172[B]:VAL:HG22	2.52	0.45
1:A:8:LEU:HD13	1:A:250:TRP:CZ2	2.52	0.45
1:A:176:SER:N	4:A:356[B]:PO4:O3	2.50	0.44
1:A:194:TRP:CZ3	1:A:195:ILE:HG22	2.52	0.44
1:C:3:PHE:CE2	1:C:348:MET:HG2	2.52	0.44
1:A:215:HIS:HD2	6:A:586:HOH:O	2.00	0.44
2:D:33[A]:GLN:H	2:D:33[A]:GLN:HG2	1.53	0.44
1:A:114:PHE:CD2	1:A:119:THR:HG23	2.53	0.44
1:C:247:LEU:HD22	1:C:292:ILE:HD12	2.00	0.44
1:C:250[B]:TRP:CE3	1:C:250[B]:TRP:HA	2.52	0.44
1:C:32:GLU:HA	1:C:36:PHE:O	2.18	0.43
2:D:11:MET:O	2:D:48:ASN:HB3	2.18	0.43
1:A:73:THR:O	1:A:104:GLY:HA3	2.18	0.43
2:B:115[B]:ARG:NH1	6:B:376:HOH:O	2.51	0.43
2:D:92:LEU:HG	2:D:96:MET:HE2	1.99	0.43
1:C:149[B]:GLU:H	1:C:149[B]:GLU:CD	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:MET:HE3	1:C:192:LEU:HD21	2.01	0.43
2:B:1:MET:HE3	2:B:292:ALA:O	2.18	0.43
2:B:1:MET:HA	2:B:293:ALA:O	2.19	0.43
1:A:265:ASP:HB3	5:A:361:SO4:O4	2.19	0.43
2:D:192:PHE:HB3	2:D:201:ARG:HD2	2.01	0.43
2:B:181:GLU:HG2	2:B:211:VAL:HG11	2.00	0.43
1:A:236:SER:HB2	1:A:303:THR:HG23	2.00	0.43
1:C:250[A]:TRP:CZ3	1:C:292:ILE:HD13	2.54	0.43
1:A:181:GLU:O	1:A:185:GLU:HG3	2.19	0.42
1:C:6[B]:PHE:CE2	1:C:324:CYS:HB3	2.54	0.42
1:A:140:ASN:ND2	1:A:166:GLY:HA2	2.34	0.42
1:C:10[B]:TYR:CE2	1:C:250[B]:TRP:CE3	3.07	0.42
1:A:176:SER:N	3:A:3402[A]:FMN:O3P	2.52	0.42
1:A:251:TYR:O	1:A:255:VAL:HG23	2.19	0.42
2:D:49:ASN:ND2	6:D:701:HOH:O	2.51	0.42
2:B:184:ALA:HA	2:B:208:TYR:CE2	2.55	0.42
2:B:181:GLU:HG3	2:B:211:VAL:CG2	2.34	0.42
1:A:11:GLN:HB3	1:A:48:GLU:HB2	2.02	0.42
2:D:136:ASN:ND2	2:D:170:GLN:HE22	2.17	0.41
2:D:70[B]:LYS:HG2	2:D:100:ARG:O	2.20	0.41
1:C:353:GLU:H	1:C:353:GLU:HG2	1.62	0.41
2:B:9:ASN:ND2	6:B:549[A]:HOH:O	2.53	0.41
2:D:228:LEU:HD11	2:D:283:ALA:HA	2.02	0.41
1:A:233:ASP:O	1:A:303:THR:HA	2.20	0.41
2:B:305:LYS:O	2:B:309:ARG:HG2	2.21	0.41
1:C:127:LEU:HD23	1:C:127:LEU:HA	1.92	0.41
2:D:223:ARG:NH2	2:D:294:ASP:OD1	2.46	0.41
1:A:13:PRO:O	2:D:202[A]:LYS:HD2	2.20	0.41
1:A:114:PHE:HD2	1:A:119:THR:HG23	1.86	0.41
1:A:228:TYR:CD1	1:A:300:PRO:HD3	2.56	0.41
1:A:259:LYS:O	1:A:262:ASP:HB2	2.21	0.41
1:C:170:VAL:O	1:C:189:PRO:HD2	2.21	0.41
1:A:38:THR:HA	1:A:70:ASN:O	2.21	0.40
1:C:10[B]:TYR:CE2	1:C:250[B]:TRP:CZ3	3.04	0.40
2:D:33[B]:GLN:HE21	2:D:33[B]:GLN:HB3	1.79	0.40
2:D:244:ARG:HD2	6:D:632:HOH:O	2.20	0.40
1:A:70:ASN:HD22	1:A:100:ARG:HB3	1.86	0.40
1:A:194:TRP:HB3	1:A:227:SER:O	2.20	0.40
1:A:219:VAL:HA	1:A:222:ILE:HD12	2.02	0.40
1:C:107:ARG:HG3	1:C:107:ARG:H	1.62	0.40
1:A:233:ASP:HB3	1:A:239:ALA:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:119:ARG:HG3	2:B:127:LEU:HD21	2.04	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	352/355 (99%)	346 (98%)	6 (2%)	0	100	100
1	C	355/355 (100%)	339 (96%)	15 (4%)	1 (0%)	36	46
2	B	321/332 (97%)	315 (98%)	6 (2%)	0	100	100
2	D	338/332 (102%)	329 (97%)	9 (3%)	0	100	100
All	All	1366/1374 (99%)	1329 (97%)	36 (3%)	1 (0%)	48	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	282	LEU

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	305/303 (101%)	285 (93%)	20 (7%)	15	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	308/303 (102%)	292 (95%)	16 (5%)	21	31
2	B	273/282 (97%)	260 (95%)	13 (5%)	23	35
2	D	290/282 (103%)	275 (95%)	15 (5%)	21	31
All	All	1176/1170 (100%)	1112 (95%)	64 (5%)	20	29

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ARG
1	A	42	LEU
1	A	47	THR
1	A	98	LYS
1	A	123	ASN
1	A	131	TRP
1	A	175[A]	GLU
1	A	175[B]	GLU
1	A	195	ILE
1	A	205	LEU
1	A	260	ILE
1	A	266	GLN
1	A	283	LYS
1	A	290	ARG
1	A	291	ARG
1	A	292	ILE
1	A	293	ASP
1	A	310	ILE
1	A	341	LYS
1	A	353	GLU
2	B	1	MET
2	B	13	SER
2	B	18	ASP
2	B	31	VAL
2	B	37	ASP
2	B	95	GLN
2	B	173	ASN
2	B	213	GLN
2	B	231	ASN
2	B	233	ASN
2	B	258	THR
2	B	262	GLN
2	B	318	ASN

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Mol	Chain	Res	Type
1	C	9	THR
1	C	29	LYS
1	C	54	ASN
1	C	107	ARG
1	C	131	TRP
1	C	205	LEU
1	C	229	ILE
1	C	232	VAL
1	C	260	ILE
1	C	268	LYS
1	C	276	GLN
1	C	281	VAL
1	C	282	LEU
1	C	292	ILE
1	C	334	GLU
1	C	353	GLU
2	D	14	LYS
2	D	18	ASP
2	D	33[A]	GLN
2	D	33[B]	GLN
2	D	70[A]	LYS
2	D	70[B]	LYS
2	D	122[A]	ASP
2	D	122[B]	ASP
2	D	123	SER
2	D	173	ASN
2	D	231	ASN
2	D	233	ASN
2	D	244	ARG
2	D	258	THR
2	D	325	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	70	ASN
1	A	95	GLN
1	A	123	ASN
1	A	140	ASN
1	A	204	GLN
1	A	234	HIS

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Mol	Chain	Res	Type
1	A	249	HIS
1	A	273	ASN
1	A	344	GLN
2	B	9	ASN
2	B	95	GLN
2	B	124	GLN
2	B	170	GLN
2	B	173	ASN
2	B	213	GLN
2	B	231	ASN
2	B	233	ASN
2	B	262	GLN
2	B	318	ASN
1	C	26	ASN
1	C	70	ASN
1	C	86	GLN
1	C	123	ASN
1	C	140	ASN
1	C	150	HIS
1	C	204	GLN
1	C	237	ASN
1	C	256	ASN
1	C	313	GLN
1	C	322	ASN
1	C	344	GLN
2	D	49	ASN
2	D	95	GLN
2	D	124	GLN
2	D	136	ASN
2	D	173	ASN
2	D	213	GLN
2	D	231	ASN
2	D	233	ASN
2	D	257	ASN
2	D	262	GLN
2	D	281	GLN
2	D	307	GLN
2	D	308	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

19 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	$\# Z > 2$
5	SO4	C	358	-	4,4,4	0.22	0	6,6,6	0.43	0
4	PO4	A	356[B]	-	4,4,4	4.03	4 (100%)	6,6,6	0.96	0
5	SO4	D	333	-	4,4,4	0.26	0	6,6,6	0.49	0
5	SO4	C	357	-	4,4,4	0.34	0	6,6,6	0.50	0
4	PO4	C	359	-	4,4,4	1.45	0	6,6,6	1.85	2 (33%)
5	SO4	B	335	-	4,4,4	0.36	0	6,6,6	0.64	0
5	SO4	B	334	-	4,4,4	0.55	0	6,6,6	0.56	0
5	SO4	A	357	-	4,4,4	0.17	0	6,6,6	0.84	0
5	SO4	C	356	-	4,4,4	0.28	0	6,6,6	0.73	0
5	SO4	A	358	-	4,4,4	0.31	0	6,6,6	0.59	0
5	SO4	A	361	-	4,4,4	0.28	0	6,6,6	0.48	0
5	SO4	B	333	-	4,4,4	0.20	0	6,6,6	0.70	0
5	SO4	A	359	-	4,4,4	0.38	0	6,6,6	0.26	0
5	SO4	D	335	-	4,4,4	0.49	0	6,6,6	0.74	0
5	SO4	D	337	-	4,4,4	0.35	0	6,6,6	0.64	0
5	SO4	A	360	-	4,4,4	0.40	0	6,6,6	0.41	0
5	SO4	D	336	-	4,4,4	0.43	0	6,6,6	0.81	0
3	FMN	A	3402[A]	-	33,33,33	1.28	4 (12%)	48,50,50	1.66	11 (22%)
5	SO4	D	334	-	4,4,4	0.27	0	6,6,6	0.40	0

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
3	FMN	A	3402[A]	-	-	8/18/18/18	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	356[B]	PO4	P-O2	-4.65	1.41	1.54
4	A	356[B]	PO4	P-O3	-4.56	1.41	1.54
3	A	3402[A]	FMN	C4A-N5	4.15	1.39	1.30
4	A	356[B]	PO4	P-O4	-4.02	1.42	1.54
4	A	356[B]	PO4	P-O1	-2.54	1.44	1.50
3	A	3402[A]	FMN	C10-N1	2.50	1.38	1.33
3	A	3402[A]	FMN	C1'-N10	2.06	1.52	1.47
3	A	3402[A]	FMN	C1'-C2'	2.02	1.55	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3402[A]	FMN	C4'-C3'-C2'	4.05	120.31	113.57
3	A	3402[A]	FMN	C4-N3-C2	-3.12	120.09	125.64
3	A	3402[A]	FMN	C4A-C10-N10	3.07	120.88	116.48
3	A	3402[A]	FMN	C4A-C4-N3	3.00	120.89	113.25
3	A	3402[A]	FMN	C10-C4A-N5	-2.91	118.86	124.81
3	A	3402[A]	FMN	C10-N1-C2	2.88	123.09	116.85
4	C	359	PO4	O4-P-O2	2.86	116.81	107.91
3	A	3402[A]	FMN	C4A-C10-N1	-2.86	117.58	124.59
4	C	359	PO4	O4-P-O1	-2.54	101.96	110.95
3	A	3402[A]	FMN	C9A-C5A-N5	-2.36	119.95	122.45
3	A	3402[A]	FMN	O3'-C3'-C4'	-2.33	103.63	108.93
3	A	3402[A]	FMN	C5A-N5-C4A	2.31	121.83	118.09
3	A	3402[A]	FMN	C4-C4A-N5	2.26	121.33	118.21

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	3402[A]	FMN	C2'-C3'-C4'-C5'
3	A	3402[A]	FMN	C3'-C4'-C5'-O5'
3	A	3402[A]	FMN	C5'-O5'-P-O1P
3	A	3402[A]	FMN	C5'-O5'-P-O2P

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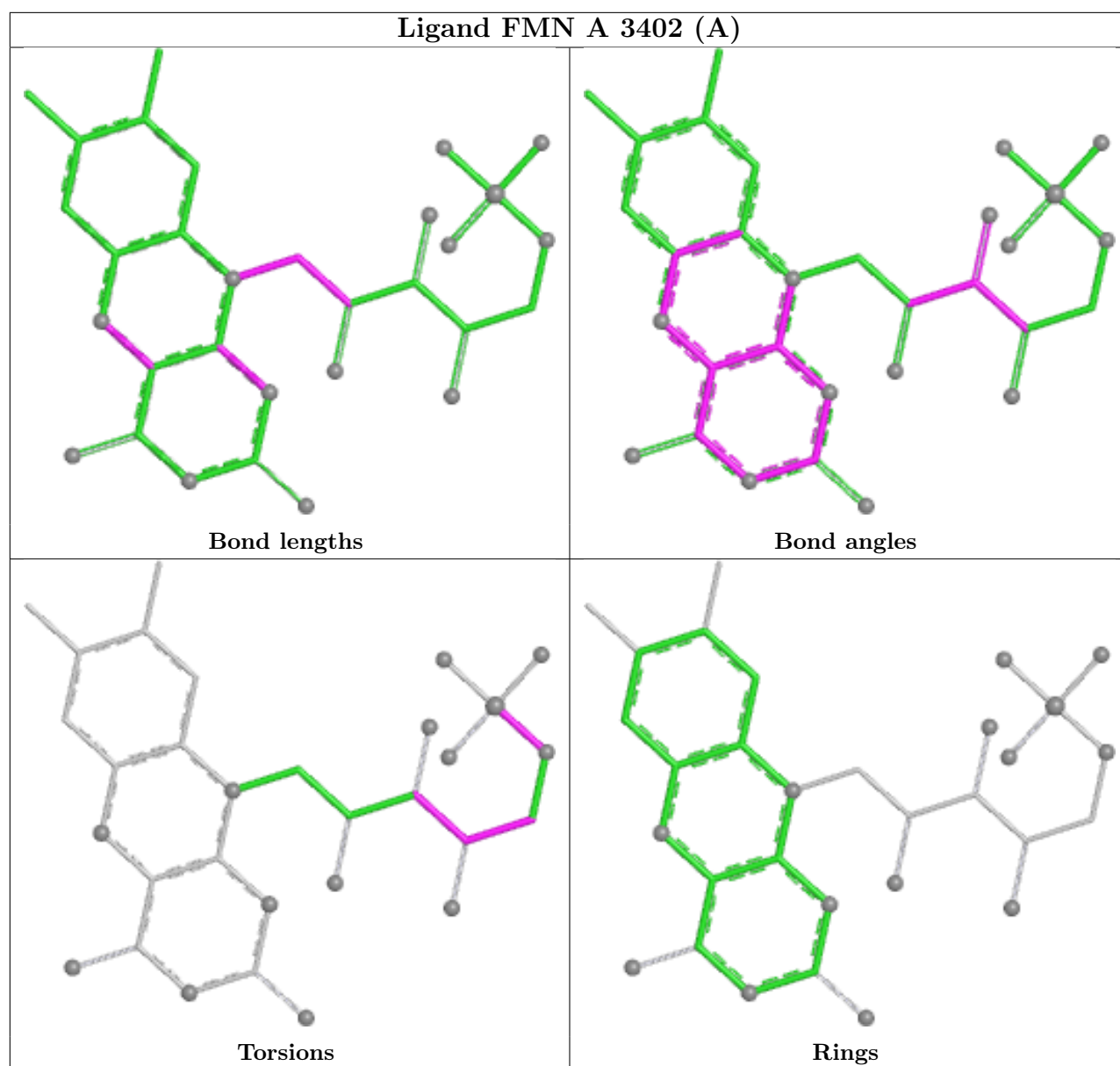
Mol	Chain	Res	Type	Atoms
3	A	3402[A]	FMN	O3'-C3'-C4'-C5'
3	A	3402[A]	FMN	O3'-C3'-C4'-O4'
3	A	3402[A]	FMN	C2'-C3'-C4'-O4'
3	A	3402[A]	FMN	C5'-O5'-P-O3P

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	356[B]	PO4	1	0
4	C	359	PO4	2	0
5	B	335	SO4	1	0
5	A	361	SO4	2	0
3	A	3402[A]	FMN	1	0

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



5.7 Other polymers [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	349/355 (98%)	-0.51	2 (0%) 85 86	9, 20, 36, 66	7 (2%)
1	C	348/355 (98%)	0.16	12 (3%) 48 50	12, 33, 56, 79	11 (3%)
2	B	318/332 (95%)	-0.51	1 (0%) 90 90	9, 21, 36, 49	5 (1%)
2	D	325/332 (97%)	-0.41	3 (0%) 81 82	10, 24, 39, 42	15 (4%)
All	All	1340/1374 (97%)	-0.31	18 (1%) 75 76	9, 24, 45, 79	38 (2%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	355	GLN	6.3
1	C	282	LEU	5.0
2	D	209[A]	HIS	4.5
1	A	175[A]	GLU	4.2
1	C	109	LEU	3.9
1	C	281	VAL	3.7
2	D	67[B]	LYS	3.4
1	C	283	LYS	3.3
1	C	136[A]	LYS	3.2
1	C	121	MET	2.8
1	C	149[A]	GLU	2.7
1	C	122	ASP	2.6
1	C	6[A]	PHE	2.5
1	C	275	GLY	2.4
2	B	258	THR	2.4
1	A	283	LYS	2.4
1	C	263	ASP	2.3
2	D	214	ALA	2.3

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](#)

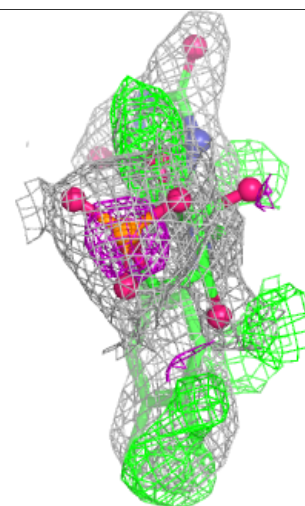
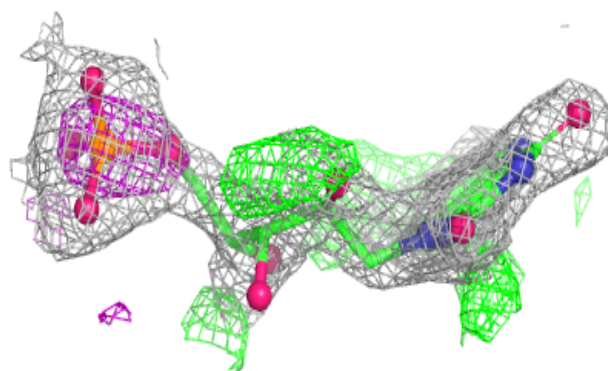
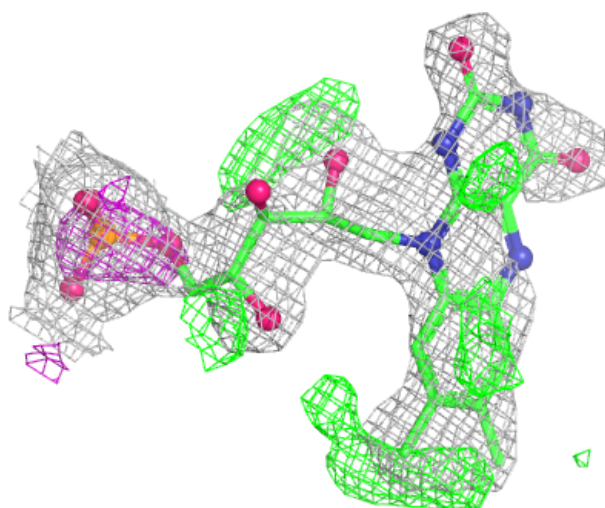
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
5	SO4	B	335	5/5	0.72	0.17	47,50,52,52	5
3	FMN	A	3402[A]	31/31	0.77	0.20	18,26,33,35	31
5	SO4	C	357	5/5	0.77	0.22	49,50,53,53	5
5	SO4	D	336	5/5	0.82	0.17	23,23,27,27	5
5	SO4	B	334	5/5	0.83	0.16	53,55,57,59	0
5	SO4	D	335	5/5	0.87	0.14	41,47,51,51	0
5	SO4	C	356	5/5	0.91	0.13	63,63,64,66	0
5	SO4	A	360	5/5	0.91	0.10	55,55,58,59	0
5	SO4	C	358	5/5	0.92	0.10	64,67,67,67	0
5	SO4	D	334	5/5	0.92	0.13	56,58,60,60	0
5	SO4	D	333	5/5	0.93	0.10	58,59,61,62	0
5	SO4	D	337	5/5	0.93	0.12	33,33,35,35	5
4	PO4	C	359	5/5	0.94	0.15	32,33,35,38	5
5	SO4	A	361	5/5	0.94	0.13	25,28,30,32	5
5	SO4	A	357	5/5	0.95	0.09	41,42,44,46	0
5	SO4	A	358	5/5	0.95	0.13	21,22,24,25	5
5	SO4	A	359	5/5	0.95	0.11	48,49,52,53	0
4	PO4	A	356[B]	5/5	0.98	0.12	20,20,20,20	5
5	SO4	B	333	5/5	0.98	0.07	35,38,40,40	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 FMN A 3402 (A):

$2mF_o-DF_c$ (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.