



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:33 AM UTC

PDB ID : 6QII / pdb_00006qii
Title : Xenon derivatization of the F420-reducing [NiFe] hydrogenase complex from Methanosarcina barkeri
Authors : Ilina, Y.; Lorent, C.; Katz, S.; Jeoung, J.H.; Shima, S.; Horch, M.; Zebger, I.; Dobbek, H.
Deposited on : 2019-01-19
Resolution : 2.28 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

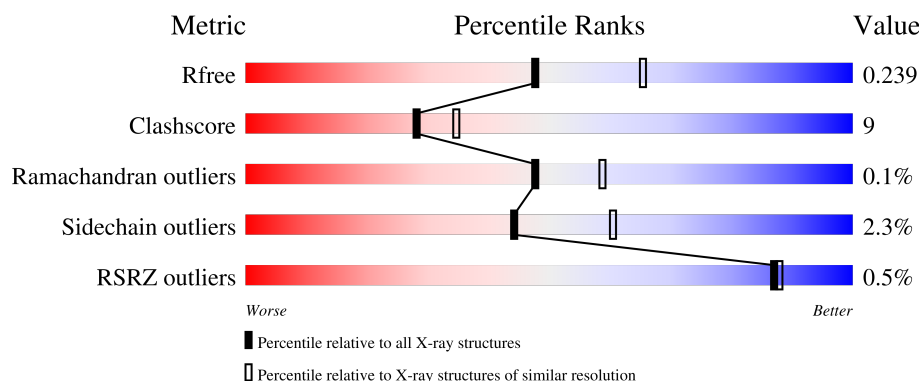
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	G	275	
2	A	437	
3	B	291	

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	SF4	G	302	-	-	X	-
5	144	G	304	-	-	X	-
7	XE	A	501	-	-	-	X
7	XE	G	310	-	-	-	X
8	BU3	G	312	-	-	X	-

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 8033 atoms, of which 82 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 Coenzyme F420 hydrogenase subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	253	Total	C	N	O	S	0	1	0
			1927	1210	325	369	23			

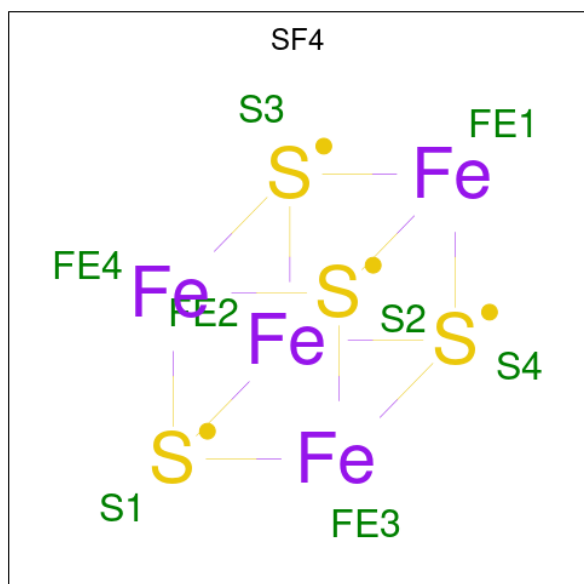
- Molecule 2 is a protein called Coenzyme F420 hydrogenase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	437	Total	C	N	O	S	0	2	0
			3412	2149	606	630	27			

- Molecule 3 is a protein called Coenzyme F420 hydrogenase subunit beta.

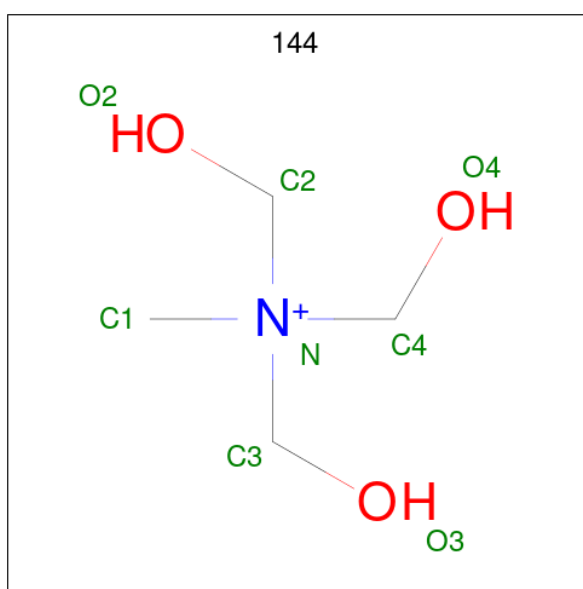
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	291	Total	C	N	O	S	0	3	0
			2286	1452	391	429	14			

- Molecule 4 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



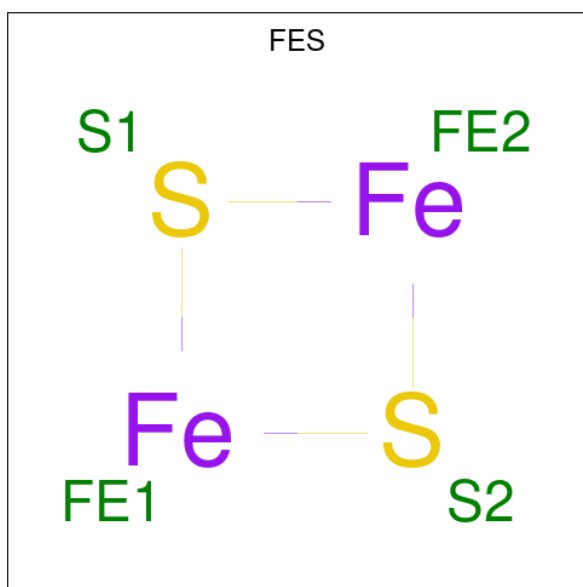
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	G	1	Total	Fe	S	0	0
			8	4	4		
4	G	1	Total	Fe	S	0	0
			8	4	4		
4	G	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 5 is TRIS-HYDROXYMETHYL-METHYL-AMMONIUM (CCD ID: 144) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	G	1	Total	C	N	O	0	0
			8	4	1	3		
5	A	1	Total	C	H	N	O	0
			20	4	12	1	3	

- Molecule 6 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).

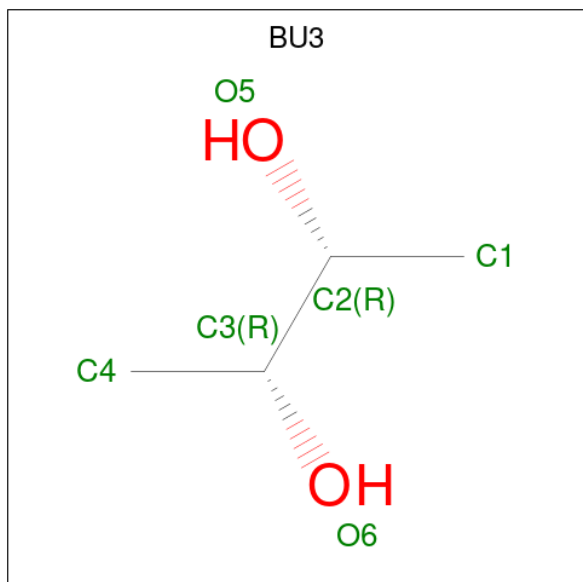


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	G	1	Total	Fe	S	0	0
			3	1	2		

- Molecule 7 is XENON (CCD ID: XE) (formula: Xe).

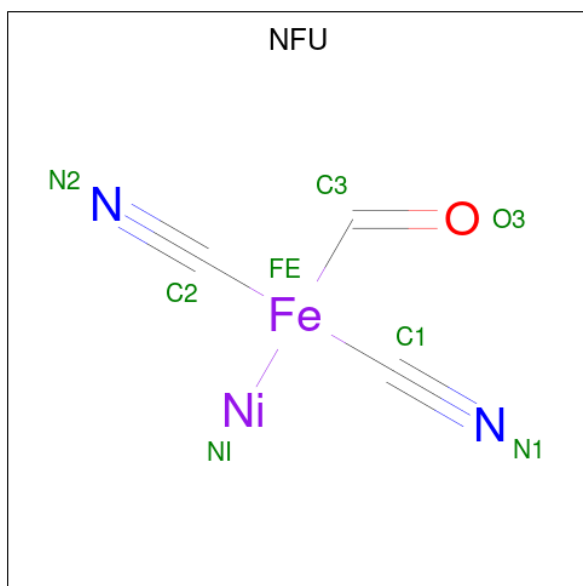
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	6	Total	Xe	1	0
			6	6		
7	A	1	Total	Xe	0	0
			1	1		

- Molecule 8 is (R,R)-2,3-BUTANEDIOL (CCD ID: BU3) (formula: C₄H₁₀O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	G	1	Total	C	H	O	0	0
			16	4	10	2		
8	G	1	Total	C	H	O	0	0
			16	4	10	2		
8	G	1	Total	C	H	O	0	0
			16	4	10	2		
8	B	1	Total	C	H	O	0	0
			16	4	10	2		
8	B	1	Total	C	H	O	0	0
			16	4	10	2		
8	B	1	Total	C	H	O	0	0
			16	4	10	2		
8	B	1	Total	C	H	O	0	0
			16	4	10	2		

- Molecule 9 is formyl[bis(hydrocyanato-1kappaC)]ironnickel(Fe-Ni) (CCD ID: NFU) (formula: C_3HFeN_2NiO).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
9	A	1	Total	C	Fe	N	Ni	O	0	0
			8	3	1	2	1	1		

- Molecule 10 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1	Total	Fe	0	0
			1	1		

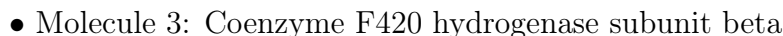
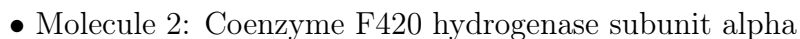
- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 11 | A | 1 | Total Mg
1 1 | 0 | 0 |

- # FAD

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

- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 13 | G | 33 | Total O
33 33 | 0 | 0 |
| 13 | A | 104 | Total O
104 104 | 0 | 0 |
| 13 | B | 26 | Total O
26 26 | 0 | 0 |

- Molecule 1: Coenzyme F420 hydrogenase subunit gamma



4 Data and refinement statistics

Property	Value	Source
Space group	F 2 3	Depositor
Cell constants a, b, c, α , β , γ	236.71Å 236.71Å 236.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.55 – 2.28 45.55 – 2.28	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.55-2.28) 100.0 (45.55-2.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 2.27Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.176 , 0.227 0.194 , 0.239	Depositor DCC
R_{free} test set	1073 reflections (2.14%)	wwPDB-VP
Wilson B-factor (Å ²)	57.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 39.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.029 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8033	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FES, MG, FAD, XE, NFU, 144, FE, SF4, BU3

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	G	0.48	0/1959	0.63	0/2647
2	A	0.63	2/3493 (0.1%)	0.72	1/4747 (0.0%)
3	B	0.60	0/2333	0.75	0/3148
All	All	0.59	2/7785 (0.0%)	0.71	1/10542 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	382	SER	C-O	-5.26	1.17	1.24
2	A	14	GLU	C-O	-5.07	1.17	1.24

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	12	ARG	CB-CA-C	5.37	119.06	111.86

There are no chirality outliers.

There are no planarity outliers.

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	G	1927	0	1912	47	0
2	A	3412	0	3389	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2286	0	2321	42	0
4	B	8	0	0	0	0
4	G	24	0	0	2	0
5	A	8	12	12	0	0
5	G	8	0	12	9	0
6	G	3	0	0	0	0
7	A	1	0	0	1	0
7	G	6	0	0	2	0
8	B	24	40	40	4	0
8	G	18	30	30	6	0
9	A	8	0	0	1	0
10	A	1	0	0	0	0
11	A	1	0	0	0	0
12	B	53	0	31	1	0
13	A	104	0	0	3	0
13	B	26	0	0	0	0
13	G	33	0	0	1	0
All	All	7951	82	7747	138	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 (138) 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)
5:G:304:144:C2	5:G:304:144:N	1.67	1.51
3:B:11:VAL:HG12	3:B:12:THR:HG23	1.48	0.92
1:G:46:ILE:HD11	2:A:139:MET:HE2	1.58	0.86
5:G:304:144:C2	5:G:304:144:C1	2.54	0.85
1:G:142:ILE:HG23	1:G:151:LEU:HD23	1.60	0.81
5:G:304:144:C2	5:G:304:144:C3	2.58	0.80
1:G:153:ARG:HH11	8:G:312:BU3:H12	1.47	0.80
1:G:89:ASP:OD1	5:G:304:144:H13	1.86	0.76
1:G:153:ARG:NH1	8:G:312:BU3:H12	2.02	0.74
3:B:7:LEU:CD1	3:B:256:LEU:HD11	2.16	0.74
5:G:304:144:H42	2:A:9:PRO:HD3	1.69	0.73
5:G:304:144:C2	5:G:304:144:C4	2.66	0.72
1:G:153:ARG:NH1	8:G:312:BU3:O6	2.24	0.71
1:G:206:MET:O	1:G:206:MET:HG2	1.89	0.71
3:B:137:PHE:CD2	3:B:213:GLY:HA3	2.29	0.67
2:A:301:VAL:HG13	2:A:408:PRO:HG3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:46:ILE:HD11	2:A:139:MET:CE	2.25	0.66
7:G:314:XE:XE	2:A:108:LEU:HD11	2.74	0.65
1:G:166:ASN:OD1	1:G:168:GLU:HB3	1.96	0.65
1:G:258:GLU:OE2	3:B:229:LYS:HG3	1.97	0.65
3:B:125:ASP:OD1	8:B:304:BU3:H41	1.98	0.64
1:G:49:LEU:HD21	7:G:307:XE:XE	2.76	0.62
1:G:80:CYS:HB2	1:G:129:TYR:CE2	2.36	0.61
2:A:148:ILE:HG23	2:A:186:LEU:HB3	1.82	0.60
2:A:403:THR:HG22	2:A:436:ALA:HB2	1.84	0.60
2:A:332:HIS:O	2:A:336:GLN:HG2	2.02	0.60
3:B:163:LYS:HB2	3:B:177:GLU:HG2	1.82	0.60
3:B:9:LYS:O	3:B:9:LYS:HG2	1.99	0.60
1:G:258:GLU:O	1:G:262:GLU:HG3	2.02	0.59
1:G:172:LEU:HD13	8:G:313:BU3:H2	1.87	0.56
3:B:18:SER:O	3:B:24:LEU:HD11	2.06	0.56
3:B:89:LEU:HD23	3:B:123:MET:CE	2.36	0.55
1:G:249:PHE:CZ	3:B:111:GLN:HB3	2.41	0.55
3:B:2:ILE:HG22	3:B:3:GLU:N	2.20	0.55
2:A:148:ILE:HG21	2:A:190:CYS:HB2	1.88	0.55
2:A:221:ILE:HD12	2:A:420:GLN:HB2	1.88	0.55
1:G:154:ASN:HD21	8:G:312:BU3:H11	1.71	0.54
2:A:24:ASN:HB2	13:A:616:HOH:O	2.06	0.54
2:A:205:ILE:HD13	2:A:332:HIS:HB3	1.87	0.54
2:A:201:MET:O	2:A:205:ILE:HG13	2.09	0.53
1:G:253:VAL:HG13	1:G:260:ILE:HD13	1.91	0.52
2:A:88[B]:THR:HG22	13:A:687:HOH:O	2.09	0.52
5:G:304:144:C4	2:A:9:PRO:HD3	2.39	0.51
2:A:401:VAL:CG1	2:A:402:PRO:HD2	2.41	0.51
2:A:35:LEU:HD22	2:A:293:PRO:HB3	1.93	0.51
2:A:252:TRP:CE2	2:A:384:ILE:HD13	2.46	0.51
3:B:20:ASP:CG	3:B:23:ILE:HG13	2.36	0.51
1:G:176:TYR:O	1:G:179:PRO:HD2	2.11	0.51
2:A:8:SER:HB2	2:A:18:LYS:HB2	1.92	0.51
3:B:79:ARG:HH21	3:B:79:ARG:HG2	1.76	0.51
2:A:13:LEU:HD12	2:A:13:LEU:N	2.26	0.50
2:A:78:MET:O	2:A:82:ILE:HG12	2.11	0.50
1:G:69:GLU:HG2	1:G:96:LYS:HD2	1.94	0.49
3:B:203:TYR:HD2	3:B:204:VAL:HG13	1.77	0.49
3:B:81:ASN:HA	3:B:142:PHE:O	2.12	0.49
2:A:109:HIS:O	2:A:113:ILE:HG12	2.13	0.49
3:B:14:VAL:HG21	3:B:246:THR:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:68:ILE:HD12	2:A:68:ILE:N	2.28	0.49
2:A:65:ILE:C	2:A:67:PRO:HD3	2.37	0.49
1:G:121:HIS:O	1:G:121:HIS:HD2	1.96	0.48
2:A:13:LEU:C	2:A:13:LEU:CD1	2.87	0.48
2:A:213:PHE:CD2	2:A:220:GLN:HG2	2.48	0.48
3:B:39:TYR:CZ	3:B:43:GLU:HG3	2.47	0.48
2:A:62:VAL:HG21	2:A:399:MET:HE1	1.96	0.47
1:G:32:THR:O	1:G:32:THR:HG22	2.14	0.47
1:G:165:GLY:O	1:G:170:LYS:HE3	2.14	0.47
3:B:91:GLU:OE2	3:B:95:SER:HB3	2.14	0.47
2:A:401:VAL:HG11	2:A:435:CYS:HB3	1.96	0.47
3:B:107:CYS:O	3:B:111:GLN:HG3	2.15	0.47
3:B:15:SER:HB2	3:B:249:ILE:CD1	2.45	0.47
2:A:430:ASP:N	2:A:431:PRO:HD3	2.29	0.47
1:G:34:CYS:SG	1:G:104:GLY:HA3	2.55	0.46
1:G:131:PRO:HG2	1:G:188:THR:HB	1.98	0.46
1:G:65:ARG:O	5:G:304:144:H41	2.15	0.46
1:G:206:MET:CE	1:G:246:ARG:HG3	2.45	0.46
2:A:2:THR:HA	2:A:23:VAL:O	2.16	0.46
2:A:21:LEU:HD12	2:A:419:TRP:HB2	1.98	0.46
1:G:69:GLU:HG2	1:G:96:LYS:CD	2.47	0.45
3:B:249:ILE:HD12	3:B:249:ILE:HA	1.71	0.45
1:G:24:GLY:HA3	1:G:70:MET:SD	2.57	0.45
2:A:403:THR:CG2	2:A:436:ALA:HB2	2.47	0.45
1:G:154:ASN:OD1	1:G:264:ILE:HD13	2.15	0.45
2:A:14:GLU:HB3	2:A:432:CYS:HA	1.99	0.45
3:B:4:ASP:HB3	3:B:7:LEU:H	1.81	0.45
3:B:36:LEU:HD13	3:B:210:ILE:HD12	1.99	0.45
2:A:380:ARG:HD2	9:A:502:NFU:C1	2.47	0.45
1:G:154:ASN:HD21	8:G:312:BU3:C1	2.30	0.45
1:G:192:PHE:HB2	4:G:302:SF4:S4	2.56	0.45
1:G:42:ASN:HB3	2:A:143:VAL:CG1	2.47	0.45
5:G:304:144:C3	5:G:304:144:O2	2.65	0.44
3:B:114:ARG:NH1	3:B:209:ASP:OD1	2.49	0.44
2:A:263:TRP:HA	2:A:294:GLN:HG2	1.99	0.44
1:G:42:ASN:ND2	13:G:403:HOH:O	2.51	0.44
3:B:4:ASP:CB	3:B:7:LEU:HB2	2.48	0.44
2:A:68:ILE:HD12	2:A:68:ILE:H	1.82	0.44
2:A:13:LEU:HD12	2:A:13:LEU:H	1.83	0.44
3:B:79:ARG:HD2	8:B:306:BU3:H2	2.00	0.44
2:A:214:VAL:HG13	2:A:223:LEU:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:133:GLN:HB3	2:A:134:PRO:HA	2.00	0.43
1:G:162:LEU:O	1:G:162:LEU:HG	2.17	0.43
1:G:26:VAL:HB	1:G:75:VAL:HG22	2.01	0.43
3:B:111:GLN:HG2	3:B:207:LEU:HD12	2.00	0.43
3:B:34:THR:OG1	12:B:302:FAD:O2A	2.35	0.43
3:B:79:ARG:HD2	8:B:306:BU3:C1	2.48	0.42
3:B:171[A]:LYS:HD2	3:B:173:TRP:CZ2	2.54	0.42
3:B:275:GLU:HA	3:B:278:LYS:HD2	2.01	0.42
1:G:121:HIS:O	1:G:121:HIS:CD2	2.72	0.42
2:A:151:THR:O	2:A:155:ILE:HG13	2.19	0.42
2:A:269:GLU:OE2	2:A:290:LYS:HD3	2.19	0.42
3:B:4:ASP:HB3	3:B:7:LEU:HB2	2.02	0.42
3:B:226:ILE:HD12	3:B:226:ILE:N	2.34	0.42
2:A:213:PHE:CE2	2:A:220:GLN:HG2	2.55	0.42
1:G:55:LEU:HD12	1:G:55:LEU:HA	1.92	0.42
2:A:13:LEU:C	2:A:13:LEU:HD13	2.45	0.41
2:A:342:CYS:O	2:A:346:ILE:HG13	2.20	0.41
3:B:137:PHE:CD1	3:B:204:VAL:HA	2.55	0.41
1:G:242:GLY:C	3:B:121:ILE:HD12	2.45	0.41
1:G:258:GLU:HA	8:B:305:BU3:H41	2.02	0.41
2:A:34:TRP:CH2	2:A:431:PRO:HB3	2.56	0.41
3:B:39:TYR:OH	3:B:237:LYS:HE3	2.20	0.41
1:G:70:MET:O	1:G:97:SER:HA	2.20	0.41
1:G:161:LEU:O	1:G:170:LYS:HG2	2.21	0.41
2:A:328:THR:HG23	2:A:428:ALA:HB2	2.03	0.41
1:G:206:MET:HE3	1:G:206:MET:HB3	1.65	0.41
1:G:215:CYS:HA	4:G:302:SF4:S1	2.60	0.41
2:A:408:PRO:O	2:A:412:ARG:HD2	2.20	0.41
3:B:269:LYS:HB2	3:B:269:LYS:HE2	1.90	0.41
1:G:206:MET:SD	1:G:208:CYS:HB3	2.60	0.41
3:B:186:LEU:HA	3:B:186:LEU:HD23	1.78	0.41
1:G:153:ARG:HD2	1:G:268:LEU:HD11	2.03	0.41
2:A:16:HIS:HA	13:A:605:HOH:O	2.20	0.41
2:A:111:ILE:HD13	7:A:501:XE:XE	2.99	0.41
3:B:277:ARG:HB3	3:B:286:LEU:HB2	2.02	0.40
1:G:206:MET:CE	1:G:246:ARG:CG	2.99	0.40
3:B:200:CYS:O	3:B:270:ASN:ND2	2.36	0.40
1:G:178:LYS:N	1:G:179:PRO:HD2	2.36	0.40
3:B:7:LEU:HD13	3:B:256:LEU:HD11	2.00	0.40
3:B:83:SER:O	3:B:85:GLN:N	2.55	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	G	252/275 (92%)	237 (94%)	14 (6%)	1 (0%)	30	36
2	A	437/437 (100%)	422 (97%)	15 (3%)	0	100	100
3	B	292/291 (100%)	275 (94%)	17 (6%)	0	100	100
All	All	981/1003 (98%)	934 (95%)	46 (5%)	1 (0%)	48	59

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	58	CYS

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	G	216/234 (92%)	215 (100%)	1 (0%)	81	89
2	A	369/367 (100%)	363 (98%)	6 (2%)	55	71
3	B	249/246 (101%)	236 (95%)	13 (5%)	21	28
All	All	834/847 (98%)	814 (98%)	20 (2%)	44	59

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	206	MET
2	A	13	LEU

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Mol	Chain	Res	Type
2	A	35	LEU
2	A	104	HIS
2	A	225	LYS
2	A	255	THR
2	A	261	ARG
3	B	4	ASP
3	B	9	LYS
3	B	14	VAL
3	B	22	GLU
3	B	42[A]	GLU
3	B	42[B]	GLU
3	B	79	ARG
3	B	140	GLU
3	B	249	ILE
3	B	261	LYS
3	B	275	GLU
3	B	279	THR
3	B	287	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	121	HIS
2	A	249	ASN
2	A	376	ASN
2	A	383	ASN
3	B	271	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

Of 25 ligands modelled in this entry, 9 are monoatomic - leaving 16 for Mogul analysis.

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
8	BU3	B	304	-	4,5,5	0.82	0	6,6,6	0.95	0
4	SF4	G	303	1	0,12,12	-	-	-	-	-
8	BU3	G	311	-	4,5,5	0.60	0	6,6,6	0.48	0
8	BU3	B	306	-	4,5,5	0.79	0	6,6,6	0.38	0
12	FAD	B	302	-	58,58,58	2.72	24 (41%)	85,89,89	2.66	28 (32%)
4	SF4	G	301	1	0,12,12	-	-	-	-	-
4	SF4	B	303	3	0,12,12	-	-	-	-	-
8	BU3	B	305	-	4,5,5	0.86	0	6,6,6	0.42	0
9	NFU	A	502	2	2,7,7	2.53	1 (50%)	-	-	-
5	144	G	304	-	1,7,7	1.58	0	3,9,9	0.14	0
5	144	A	505	-	1,7,7	0.75	0	3,9,9	0.15	0
8	BU3	G	312	-	4,5,5	0.82	0	6,6,6	0.71	0
4	SF4	G	302	1	0,12,12	-	-	-	-	-
8	BU3	G	313	-	4,5,5	0.73	0	6,6,6	0.34	0
8	BU3	B	301	-	4,5,5	0.76	0	6,6,6	0.46	0
6	FES	G	305	1	0,2,4	-	-	-	-	-

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
8	BU3	B	304	-	-	0/4/4/4	-
8	BU3	G	311	-	-	0/4/4/4	-
4	SF4	G	303	1	-	-	0/6/5/5
8	BU3	B	306	-	-	4/4/4/4	-
12	FAD	B	302	-	-	1/34/50/50	0/6/6/6
4	SF4	G	301	1	-	-	0/6/5/5
4	SF4	B	303	3	-	-	0/6/5/5
5	144	G	304	-	-	0/0/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	144	A	505	-	-	0/0/9/9	-
8	BU3	G	312	-	-	2/4/4/4	-
4	SF4	G	302	1	-	-	0/6/5/5
8	BU3	G	313	-	-	4/4/4/4	-
8	BU3	B	301	-	-	1/4/4/4	-
8	BU3	B	305	-	-	4/4/4/4	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	302	FAD	C6A-N6A	6.23	1.50	1.34
12	B	302	FAD	C2B-C1B	-5.94	1.34	1.53
12	B	302	FAD	C8A-N7A	5.91	1.43	1.31
12	B	302	FAD	O4B-C4B	-5.73	1.32	1.45
12	B	302	FAD	C4X-N5	5.56	1.42	1.30
12	B	302	FAD	O4B-C1B	5.30	1.54	1.42
12	B	302	FAD	C10-N1	5.04	1.43	1.33
12	B	302	FAD	C9A-N10	4.29	1.48	1.41
12	B	302	FAD	O2B-C2B	3.96	1.52	1.43
12	B	302	FAD	C10-N10	3.96	1.45	1.37
12	B	302	FAD	C2-N1	3.96	1.45	1.36
9	A	502	NFU	C1-N1	3.52	1.20	1.13
12	B	302	FAD	C5'-C4'	3.51	1.56	1.51
12	B	302	FAD	PA-O3P	3.15	1.62	1.59
12	B	302	FAD	C7M-C7	3.04	1.56	1.51
12	B	302	FAD	C4A-N3A	2.85	1.39	1.34
12	B	302	FAD	C8M-C8	2.79	1.56	1.51
12	B	302	FAD	O4-C4	-2.74	1.18	1.23
12	B	302	FAD	C4A-N9A	2.70	1.43	1.37
12	B	302	FAD	C4-N3	2.46	1.43	1.38
12	B	302	FAD	C2-N3	2.40	1.44	1.39
12	B	302	FAD	C5X-N5	2.36	1.43	1.39
12	B	302	FAD	C2A-N1A	2.35	1.38	1.33
12	B	302	FAD	O3'-C3'	-2.25	1.37	1.43
12	B	302	FAD	C2A-N3A	2.22	1.37	1.33

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	302	FAD	C7M-C7-C6	-11.53	99.25	119.57
12	B	302	FAD	C7M-C7-C8	9.51	140.18	120.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	302	FAD	N6A-C6A-N1A	-6.52	103.86	118.38
12	B	302	FAD	C5A-C4A-N3A	-6.48	117.80	126.72
12	B	302	FAD	C5A-C6A-N6A	5.30	136.40	123.29
12	B	302	FAD	N3A-C2A-N1A	-5.17	120.76	128.58
12	B	302	FAD	C2A-N3A-C4A	4.06	121.74	111.83
12	B	302	FAD	C4A-C5A-N7A	-4.00	106.01	110.58
12	B	302	FAD	N9A-C8A-N7A	-3.96	108.31	113.94
12	B	302	FAD	C5A-N7A-C8A	3.59	109.10	103.45
12	B	302	FAD	C4X-C10-N10	3.35	121.27	116.48
12	B	302	FAD	C5A-C4A-N9A	3.31	109.42	105.81
12	B	302	FAD	N3A-C4A-N9A	3.30	132.78	127.17
12	B	302	FAD	C10-N1-C2	2.97	123.28	116.85
12	B	302	FAD	O4B-C1B-N9A	-2.93	102.46	108.09
12	B	302	FAD	C3B-C2B-C1B	2.87	106.90	101.46
12	B	302	FAD	C5B-C4B-C3B	-2.82	105.07	115.21
12	B	302	FAD	C8M-C8-C7	-2.58	115.48	120.76
12	B	302	FAD	C4X-C4-N3	2.50	119.62	113.25
12	B	302	FAD	O4-C4-C4X	-2.47	120.00	126.53
12	B	302	FAD	C2B-C1B-N9A	2.44	119.38	113.30
12	B	302	FAD	C4-N3-C2	-2.41	121.36	125.64
12	B	302	FAD	O2-C2-N3	2.33	123.05	118.58
12	B	302	FAD	O2P-P-O3P	2.15	113.08	107.27
12	B	302	FAD	C8M-C8-C9	2.11	123.29	119.57
12	B	302	FAD	O2B-C2B-C3B	-2.10	105.09	111.82
12	B	302	FAD	C9A-N10-C10	-2.08	117.58	120.75
12	B	302	FAD	O3P-P-O1P	-2.02	104.62	110.70

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	G	312	BU3	C1-C2-C3-O6
8	G	313	BU3	O5-C2-C3-O6
8	G	313	BU3	C1-C2-C3-O6
8	G	313	BU3	O5-C2-C3-C4
8	B	301	BU3	C1-C2-C3-C4
8	B	305	BU3	C1-C2-C3-O6
8	B	305	BU3	O5-C2-C3-C4
8	B	305	BU3	C1-C2-C3-C4
8	B	306	BU3	C1-C2-C3-O6
8	B	306	BU3	O5-C2-C3-C4
8	B	306	BU3	C1-C2-C3-C4

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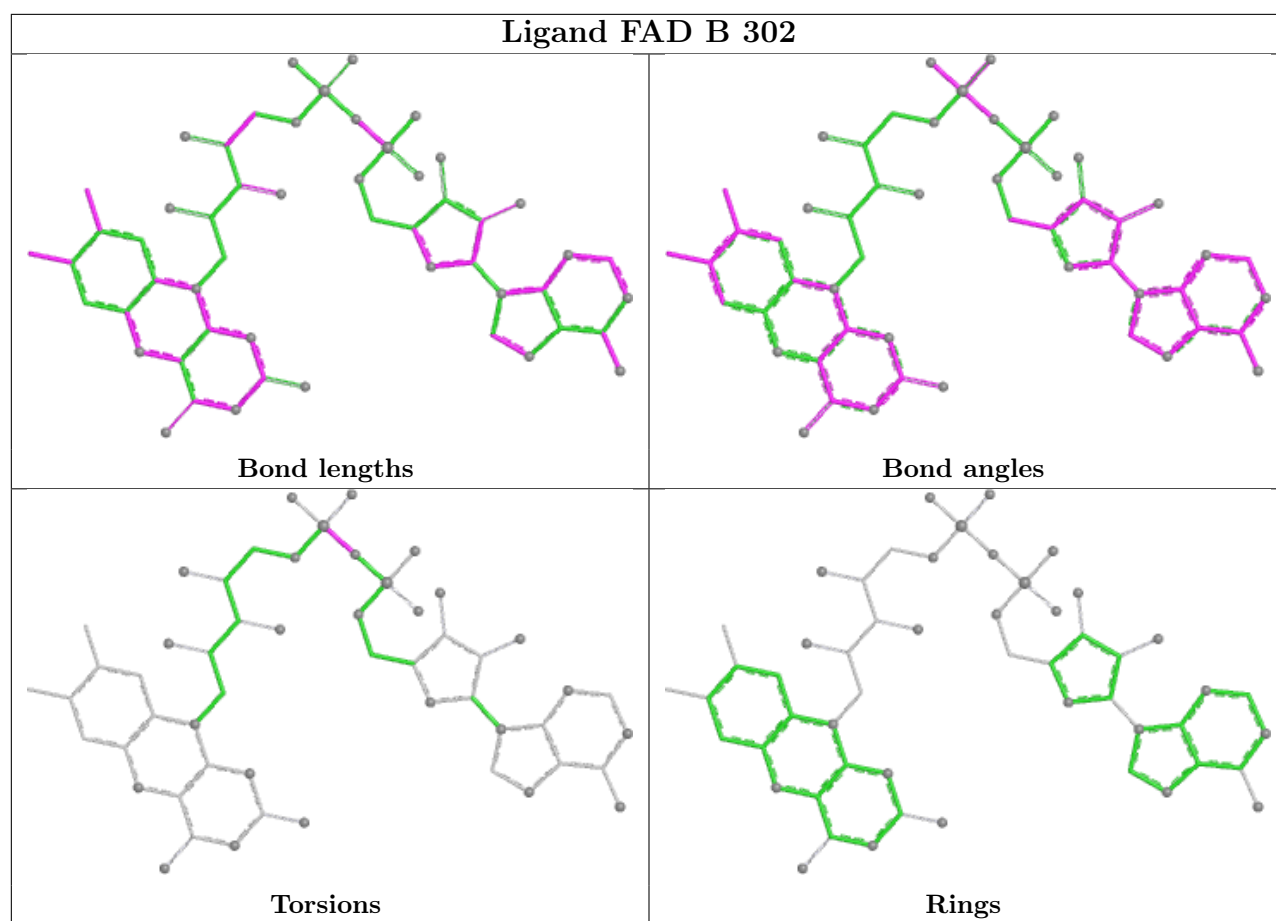
Mol	Chain	Res	Type	Atoms
8	G	313	BU3	C1-C2-C3-C4
8	G	312	BU3	O5-C2-C3-O6
8	B	305	BU3	O5-C2-C3-O6
8	B	306	BU3	O5-C2-C3-O6
12	B	302	FAD	PA-O3P-P-O2P

There are no ring outliers.

9 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	304	BU3	1	0
8	B	306	BU3	2	0
12	B	302	FAD	1	0
8	B	305	BU3	1	0
9	A	502	NFU	1	0
5	G	304	144	9	0
8	G	312	BU3	5	0
4	G	302	SF4	2	0
8	G	313	BU3	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 [i](#)

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

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	G	253/275 (92%)	0.08	0 100 100	34, 61, 83, 107	1 (0%)
2	A	437/437 (100%)	-0.22	2 (0%) 87 88	25, 53, 72, 100	2 (0%)
3	B	291/291 (100%)	0.15	3 (1%) 79 81	31, 66, 86, 100	4 (1%)
All	All	981/1003 (97%)	-0.04	5 (0%) 87 88	25, 59, 82, 107	7 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	265	GLU	3.0
3	B	9	LYS	2.5
2	A	203	ASP	2.3
2	A	129	PHE	2.1
3	B	235	TRP	2.1

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](#)

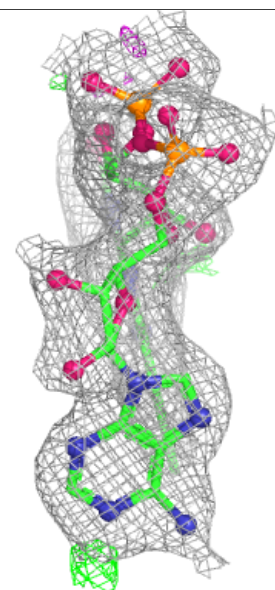
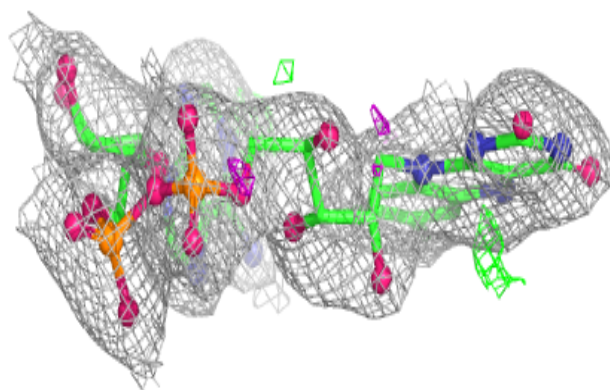
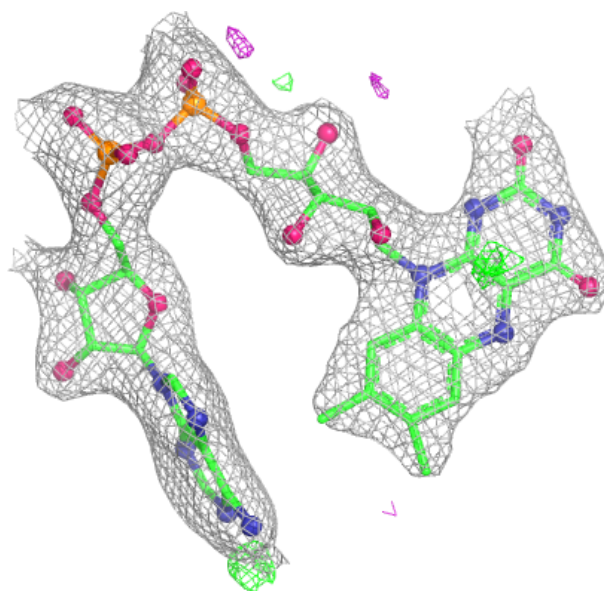
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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
7	XE	A	501	1/1	0.58	0.60	105,105,105,105	1
7	XE	G	310	1/1	0.71	0.44	126,126,126,126	1
8	BU3	B	301	6/6	0.73	0.28	50,50,50,50	0
8	BU3	G	312	6/6	0.74	0.19	71,85,93,95	16
8	BU3	B	304	6/6	0.77	0.17	73,88,100,103	0
8	BU3	B	306	6/6	0.78	0.20	50,50,50,50	0
8	BU3	G	311	6/6	0.80	0.16	62,79,95,102	0
7	XE	G	306	1/1	-	-	69,69,69,69	1
7	XE	G	307	1/1	0.81	0.37	89,89,89,89	1
8	BU3	G	313	6/6	0.85	0.14	80,104,113,113	0
7	XE	G	309	1/1	0.85	0.60	72,72,72,72	1
8	BU3	B	305	6/6	0.86	0.18	50,50,50,50	16
5	144	A	505	8/8	0.91	0.10	60,73,77,77	20
7	XE	G	314	1/1	0.91	0.27	72,72,72,72	1
11	MG	A	504	1/1	0.92	0.07	55,55,55,55	1
5	144	G	304	8/8	0.95	0.08	56,67,74,81	0
7	XE	G	308	1/1	0.96	0.29	69,69,69,69	1
4	SF4	G	302	8/8	0.97	0.06	44,49,55,56	0
4	SF4	B	303	8/8	0.97	0.09	58,63,66,72	0
10	FE	A	503	1/1	0.97	0.06	79,79,79,79	1
4	SF4	G	301	8/8	0.97	0.07	52,56,58,61	0
12	FAD	B	302	53/53	0.97	0.09	47,60,73,77	0
4	SF4	G	303	8/8	0.98	0.06	54,56,60,65	0
6	FES	G	305	3/4	0.98	0.06	47,47,50,57	2
9	NFU	A	502	8/8	0.99	0.10	49,53,58,63	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 302:

$2mF_o-DF_c$ (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.