



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 12:31 pm BST

PDB ID : 1TV5
Title : Plasmodium falciparum dihydroorotate dehydrogenase with a bound inhibitor
Authors : Hurt, D.E.; Widom, J.; Clardy, J.
Deposited on : 2004-06-27
Resolution : 2.40 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

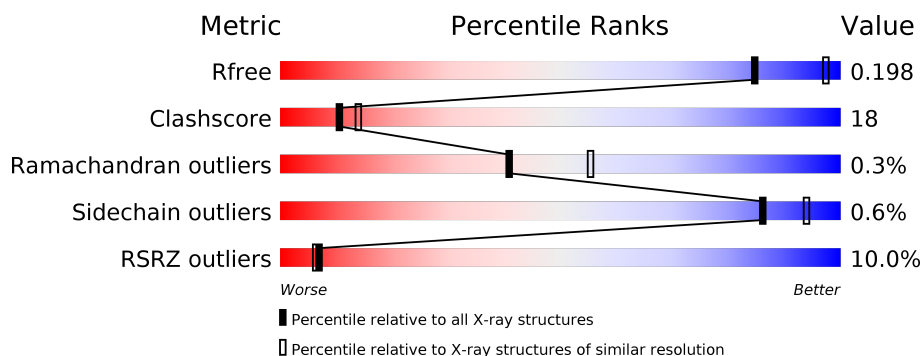
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 on 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	443	<div> <div>8%</div> <div>55%</div> <div>28%</div> <div>16%</div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3282 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 Dihydroorotate dehydrogenase homolog, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	371	2956	1893	493	554	16	0	2	0

There are 31 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	127	MET	-	INSERTION	UNP Q08210
A	128	ARG	-	INSERTION	UNP Q08210
A	129	GLY	-	INSERTION	UNP Q08210
A	130	SER	-	INSERTION	UNP Q08210
A	131	HIS	-	INSERTION	UNP Q08210
A	132	HIS	-	INSERTION	UNP Q08210
A	133	HIS	-	INSERTION	UNP Q08210
A	134	HIS	-	INSERTION	UNP Q08210
A	135	HIS	-	INSERTION	UNP Q08210
A	136	HIS	-	INSERTION	UNP Q08210
A	137	GLY	-	INSERTION	UNP Q08210
A	138	MET	-	INSERTION	UNP Q08210
A	139	ALA	-	INSERTION	UNP Q08210
A	140	SER	-	INSERTION	UNP Q08210
A	141	MET	-	INSERTION	UNP Q08210
A	142	THR	-	INSERTION	UNP Q08210
A	143	GLY	-	INSERTION	UNP Q08210
A	144	GLY	-	INSERTION	UNP Q08210
A	145	GLN	-	INSERTION	UNP Q08210
A	146	GLN	-	INSERTION	UNP Q08210
A	147	MET	-	INSERTION	UNP Q08210
A	148	GLY	-	INSERTION	UNP Q08210
A	149	ARG	-	INSERTION	UNP Q08210
A	150	ASP	-	INSERTION	UNP Q08210
A	151	LEU	-	INSERTION	UNP Q08210
A	152	TYR	-	INSERTION	UNP Q08210
A	153	ASP	-	INSERTION	UNP Q08210

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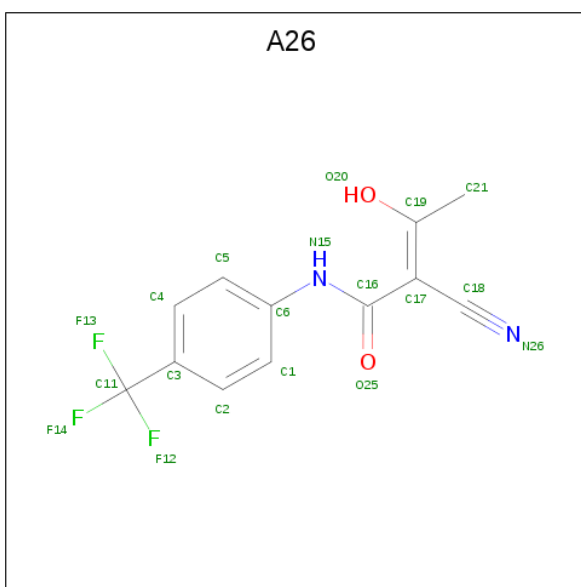
Chain	Residue	Modelled	Actual	Comment	Reference
A	154	ASP	-	INSERTION	UNP Q08210
A	155	ASP	-	INSERTION	UNP Q08210
A	156	ASP	-	INSERTION	UNP Q08210
A	157	LYS	-	INSERTION	UNP Q08210

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



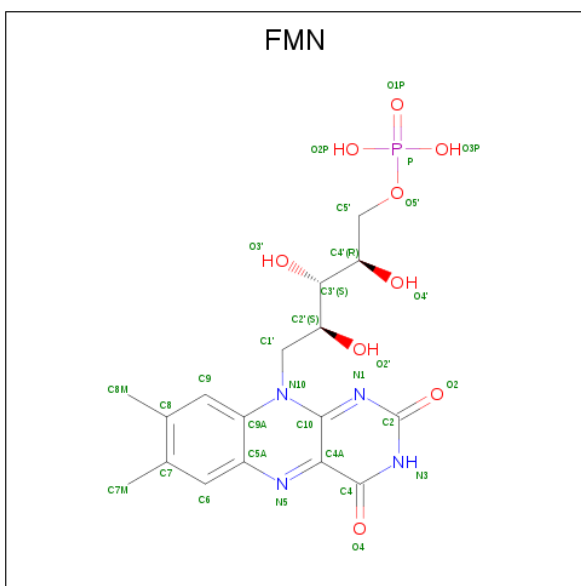
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is (2Z)-2-cyano-3-hydroxy-N-[4-(trifluoromethyl)phenyl]but-2-enamide (three-letter code: A26) (formula: C₁₂H₉F₃N₂O₂).



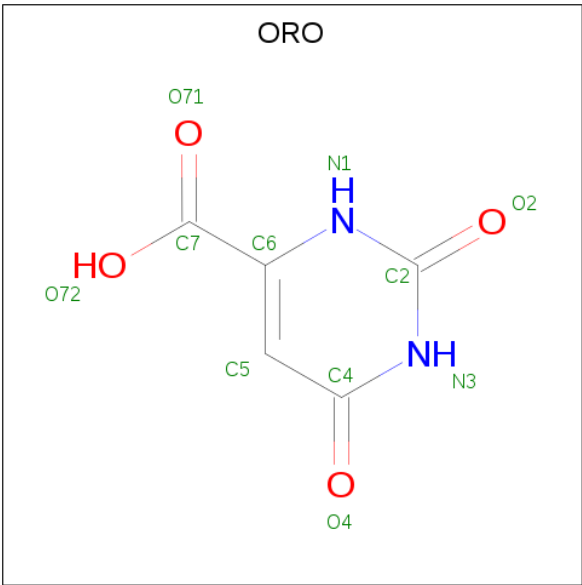
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			19	12	3	2	2		

- Molecule 4 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



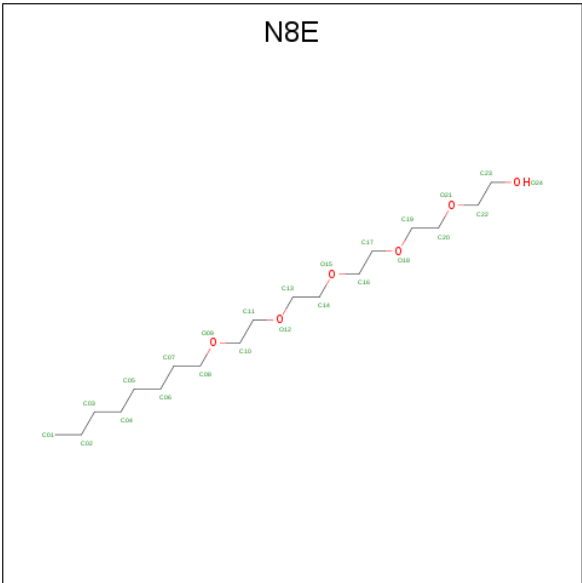
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 5 is OROTIC ACID (three-letter code: ORO) (formula: $C_5H_4N_2O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			11	5	2	4		

- Molecule 6 is 3,6,9,12,15-PENTAOXATRICOSAN-1-OL (three-letter code: N8E) (formula: C₁₈H₃₈O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			24	18	6		
6	A	1	Total	C	O	0	0
			24	18	6		

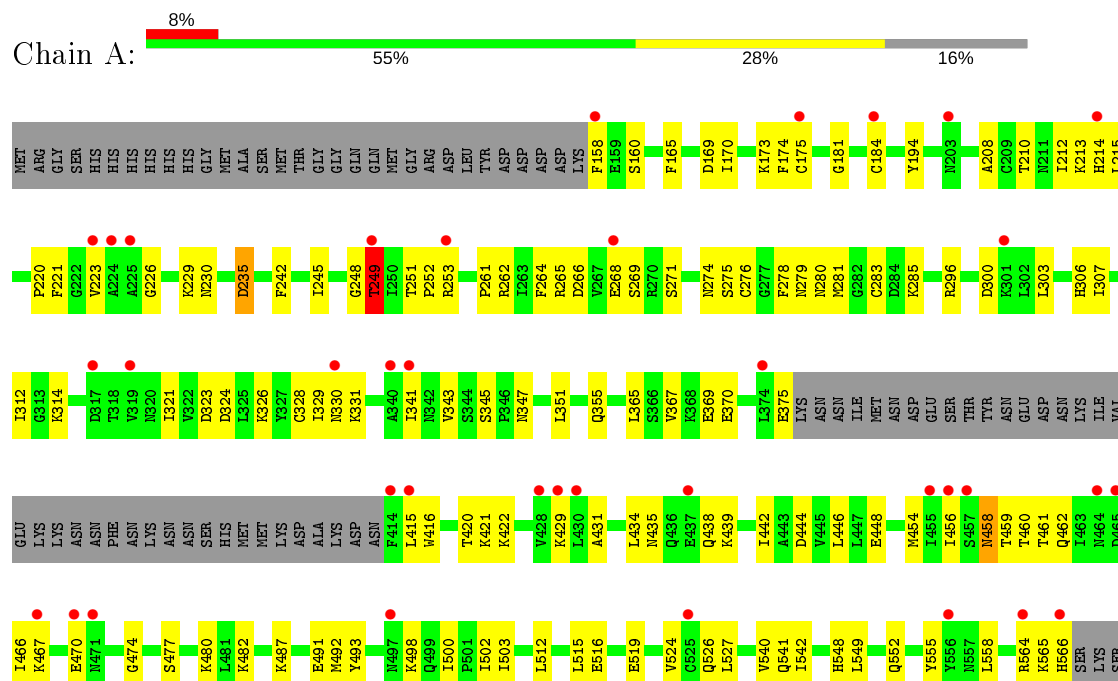
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	212	Total 212	O 212	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Dihydroorotate dehydrogenase homolog, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	105.43 Å 105.43 Å 276.63 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	33.48 – 2.40 33.48 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.3 (33.48-2.40) 97.9 (33.48-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.80 (at 2.39 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.201 , 0.243 0.197 , 0.198	Depositor DCC
R_{free} test set	1181 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	31.0	Xtriage
Anisotropy	0.400	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 53.8	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	3282	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.19% 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: N8E, FMN, SO4, A26, ORO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.36	0/3007	0.64	2/4048 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	THR	N-CA-C	-11.33	80.41	111.00
1	A	458	ASN	N-CA-C	-5.68	95.66	111.00

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	A	2956	0	2992	113	0
2	A	5	0	0	1	0
3	A	19	0	9	0	0
4	A	31	0	19	1	0
5	A	11	0	3	2	0
6	A	48	0	76	5	0
7	A	212	0	0	13	0
All	All	3282	0	3099	113	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 18.

All (113) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:LYS:O	1:A:248:GLY:HA2	1.77	0.83
1:A:249:THR:O	1:A:249:THR:HG22	1.81	0.79
1:A:323:ASP:HA	1:A:326:LYS:HE2	1.65	0.79
1:A:213:LYS:HE3	7:A:1125:HOH:O	1.82	0.79
1:A:223:VAL:HG22	1:A:245:ILE:HG13	1.65	0.76
1:A:355:GLN:HE22	1:A:431:ALA:H	1.34	0.76
1:A:174:PHE:HB2	6:A:1005:N8E:H071	1.73	0.70
1:A:454:MET:HE2	1:A:456:ILE:HD11	1.72	0.69
1:A:158:PHE:HB3	1:A:165:PHE:HD1	1.58	0.68
1:A:223:VAL:CG2	1:A:245:ILE:HG13	2.24	0.67
1:A:365:LEU:O	1:A:369:GLU:HG3	1.97	0.65
1:A:512:LEU:O	1:A:516:GLU:HG3	1.95	0.65
1:A:444:ASP:O	1:A:448:GLU:HG3	1.97	0.65
1:A:454:MET:CE	1:A:456:ILE:HD11	2.29	0.63
1:A:355:GLN:NE2	1:A:431:ALA:H	1.96	0.62
1:A:312:ILE:HD13	1:A:328:CYS:CB	2.31	0.61
1:A:306:HIS:HE1	7:A:1150:HOH:O	1.83	0.61
1:A:460:THR:OG1	1:A:462:GLN:HG2	2.01	0.61
1:A:347:ASN:HD21	1:A:474:GLY:HA2	1.65	0.61
1:A:565:LYS:HE3	7:A:1146:HOH:O	2.01	0.60
1:A:235:ASP:OD1	1:A:296:ARG:HD2	2.02	0.59
1:A:210:THR:HG21	1:A:524:VAL:HG12	1.84	0.59
1:A:248:GLY:O	1:A:249:THR:HB	2.02	0.58
1:A:375:GLU:HG3	1:A:415:LEU:HD21	1.85	0.57
1:A:208:ALA:O	1:A:220:PRO:HD3	2.04	0.56
1:A:420:THR:HG22	1:A:422:LYS:HB2	1.88	0.56
1:A:454:MET:HE1	1:A:492:MET:HB3	1.88	0.56
1:A:442:ILE:O	1:A:446:LEU:HG	2.06	0.56
1:A:345:SER:HB3	1:A:351:LEU:HD23	1.88	0.55
1:A:435:ASN:OD1	1:A:438:GLN:HG3	2.05	0.55
1:A:268:GLU:HG3	1:A:269:SER:N	2.22	0.55
1:A:312:ILE:HD13	1:A:328:CYS:HB2	1.88	0.55
1:A:169:ASP:HB3	6:A:1004:N8E:H142	1.90	0.54
1:A:329:ILE:HD11	1:A:367:VAL:HG13	1.90	0.54
1:A:375:GLU:HB2	1:A:416:TRP:HZ2	1.72	0.54
1:A:271:SER:OG	1:A:480:LYS:HG2	2.08	0.54
1:A:251:THR:H	1:A:280:ASN:HD21	1.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:LEU:HG	1:A:307:ILE:HD13	1.91	0.52
1:A:223:VAL:HG22	1:A:245:ILE:CG1	2.37	0.52
1:A:555:TYR:CE2	1:A:564:ARG:HD3	2.45	0.51
1:A:300:ASP:C	7:A:1028:HOH:O	2.49	0.51
1:A:331:LYS:HD2	7:A:1138:HOH:O	2.09	0.51
1:A:555:TYR:HE2	1:A:564:ARG:HD3	1.75	0.51
1:A:312:ILE:HD13	1:A:328:CYS:HB3	1.92	0.51
1:A:420:THR:CG2	1:A:422:LYS:HB2	2.41	0.51
1:A:170:ILE:HG22	6:A:1005:N8E:H072	1.93	0.50
1:A:467:LYS:O	1:A:470:GLU:HG3	2.12	0.50
1:A:552:GLN:NE2	7:A:1046:HOH:O	2.44	0.50
1:A:268:GLU:HG3	1:A:269:SER:H	1.76	0.50
1:A:459:THR:HG22	1:A:477:SER:OG	2.12	0.49
1:A:173:LYS:HE3	6:A:1004:N8E:H071	1.94	0.49
1:A:249:THR:CG2	1:A:249:THR:O	2.54	0.49
1:A:303:LEU:HA	1:A:306:HIS:CD2	2.47	0.49
1:A:461:THR:HG22	1:A:461:THR:O	2.12	0.49
1:A:456:ILE:HG12	1:A:502:ILE:HG23	1.94	0.49
1:A:466:ILE:HD11	1:A:480:LYS:HG3	1.94	0.49
1:A:482:LYS:HE2	7:A:1217:HOH:O	2.11	0.49
1:A:194:TYR:OH	2:A:1006:SO4:O2	2.29	0.48
1:A:158:PHE:HB3	1:A:165:PHE:CD1	2.44	0.48
1:A:210:THR:CG2	1:A:524:VAL:HG12	2.44	0.48
1:A:420:THR:O	1:A:421:LYS:HB2	2.15	0.47
1:A:503:ILE:HG13	1:A:524:VAL:CG2	2.44	0.47
1:A:540:VAL:HG23	1:A:541:GLN:N	2.30	0.47
1:A:212:ILE:O	1:A:213:LYS:HB2	2.16	0.46
1:A:226:GLY:HA3	4:A:1002:FMN:N5	2.30	0.46
1:A:170:ILE:CG2	6:A:1005:N8E:H072	2.45	0.46
1:A:160:SER:HA	1:A:165:PHE:CG	2.51	0.46
1:A:253:ARG:HD3	7:A:1188:HOH:O	2.16	0.45
1:A:375:GLU:HB2	1:A:416:TRP:CZ2	2.52	0.45
1:A:434:LEU:O	1:A:439:LYS:HE3	2.16	0.45
1:A:512:LEU:HA	1:A:549:LEU:CD2	2.46	0.45
1:A:262:ARG:HD2	1:A:276:CYS:HA	1.99	0.45
1:A:281:MET:HE3	1:A:285:LYS:HG3	1.99	0.45
1:A:326:LYS:HD2	7:A:1084:HOH:O	2.16	0.44
1:A:515:LEU:O	1:A:519:GLU:HG3	2.17	0.44
1:A:242:PHE:HE2	1:A:527:LEU:HD12	1.81	0.44
1:A:229:LYS:HA	1:A:248:GLY:HA2	1.99	0.44
1:A:261:PRO:HG2	1:A:264:PHE:HZ	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:MET:HE1	1:A:492:MET:HG3	2.00	0.43
1:A:278:PHE:CE2	5:A:1003:ORO:H5	2.52	0.43
1:A:230:ASN:CG	1:A:281:MET:HG3	2.39	0.43
1:A:175[A]:CYS:HG	1:A:184[A]:CYS:HG	0.92	0.43
1:A:429:LYS:HE2	1:A:458:ASN:HA	2.01	0.43
1:A:283:CYS:SG	1:A:331:LYS:HB2	2.59	0.43
1:A:275:SER:HA	1:A:347:ASN:CG	2.39	0.43
1:A:341:ILE:CD1	1:A:367:VAL:HG21	2.49	0.42
1:A:283:CYS:SG	1:A:328:CYS:HA	2.59	0.42
1:A:278:PHE:HE2	5:A:1003:ORO:H5	1.84	0.42
1:A:420:THR:HG22	1:A:422:LYS:CB	2.48	0.42
1:A:493:TYR:CE2	1:A:498:LYS:HG2	2.55	0.42
1:A:558:LEU:C	1:A:558:LEU:HD23	2.40	0.42
1:A:221:PHE:CZ	1:A:542:ILE:HG12	2.55	0.42
1:A:323:ASP:CA	1:A:326:LYS:HE2	2.44	0.42
1:A:266:ASP:OD1	1:A:268:GLU:HG3	2.19	0.42
1:A:229:LYS:HD3	1:A:279:ASN:O	2.20	0.42
1:A:487:LYS:O	1:A:491:GLU:HG3	2.18	0.42
1:A:214:HIS:HB2	7:A:1197:HOH:O	2.21	0.41
1:A:341:ILE:HG22	1:A:343:VAL:HG13	2.00	0.41
1:A:548:HIS:HB3	7:A:1046:HOH:O	2.21	0.41
1:A:565:LYS:O	1:A:566:HIS:C	2.59	0.41
1:A:274:ASN:O	1:A:474:GLY:HA3	2.20	0.41
1:A:303:LEU:HB2	7:A:1028:HOH:O	2.20	0.41
1:A:446:LEU:HB3	1:A:500:ILE:HD13	2.03	0.41
1:A:249:THR:HG21	1:A:278:PHE:CE2	2.55	0.41
1:A:213:LYS:NZ	7:A:1143:HOH:O	2.54	0.41
1:A:181:GLY:HA2	1:A:265:ARG:NH1	2.36	0.41
1:A:323:ASP:O	1:A:326:LYS:HG2	2.20	0.41
1:A:454:MET:HE1	1:A:492:MET:CB	2.48	0.41
1:A:330:ASN:ND2	1:A:370:GLU:OE2	2.43	0.40
1:A:314:LYS:HB3	1:A:321:ILE:HG13	2.03	0.40
1:A:252:PRO:HG2	1:A:324:ASP:HA	2.03	0.40
1:A:503:ILE:CG2	1:A:526:GLN:HG3	2.52	0.40
1:A:215:LEU:HA	1:A:215:LEU:HD12	1.98	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	369/443 (83%)	348 (94%)	20 (5%)	1 (0%)	41	55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	249	THR

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	330/393 (84%)	328 (99%)	2 (1%)	86	94

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	235	ASP
1	A	249	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	214	HIS
1	A	280	ASN
1	A	306	HIS

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Mol	Chain	Res	Type
1	A	320	ASN
1	A	330	ASN
1	A	347	ASN
1	A	355	GLN
1	A	548	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

6 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	$\# Z > 2$
6	N8E	A	1004	-	23,23,23	0.38	0	22,22,22	0.64	0
3	A26	A	1001	-	19,19,19	2.47	5 (26%)	27,27,27	2.14	7 (25%)
2	SO4	A	1006	-	4,4,4	1.93	2 (50%)	6,6,6	0.97	0
4	FMN	A	1002	-	31,33,33	2.30	8 (25%)	40,50,50	2.61	9 (22%)
5	ORO	A	1003	-	6,11,11	2.52	2 (33%)	3,15,15	4.69	2 (66%)
6	N8E	A	1005	-	23,23,23	0.44	0	22,22,22	0.87	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
6	N8E	A	1004	-	-	2/21/21/21	-
6	N8E	A	1005	-	-	5/21/21/21	-
4	FMN	A	1002	-	-	1/18/18/18	0/3/3/3
3	A26	A	1001	-	-	0/20/20/20	0/1/1/1
5	ORO	A	1003	-	-	0/0/4/4	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1002	FMN	C4A-C10	9.53	1.48	1.38
3	A	1001	A26	F14-C11	-6.40	1.09	1.32
4	A	1002	FMN	C9A-N10	4.18	1.44	1.38
5	A	1003	ORO	C4-N3	4.04	1.40	1.33
5	A	1003	ORO	C6-N1	3.87	1.40	1.34
3	A	1001	A26	C5-C6	3.86	1.45	1.39
3	A	1001	A26	F12-C11	-3.75	1.19	1.32
3	A	1001	A26	C2-C3	3.61	1.45	1.39
3	A	1001	A26	C17-C16	3.61	1.52	1.46
4	A	1002	FMN	C4-C4A	3.24	1.46	1.41
4	A	1002	FMN	C2-N3	3.18	1.44	1.38
2	A	1006	SO4	O1-S	3.15	1.63	1.46
4	A	1002	FMN	C6-C5A	2.55	1.45	1.41
4	A	1002	FMN	C8-C7	2.22	1.46	1.40
2	A	1006	SO4	O3-S	-2.19	1.29	1.47
4	A	1002	FMN	O3'-C3'	2.05	1.47	1.43
4	A	1002	FMN	C5A-N5	2.05	1.38	1.35

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1002	FMN	C4-N3-C2	12.19	125.43	115.14
5	A	1003	ORO	C5-C4-N3	-7.48	115.34	124.08
4	A	1002	FMN	C4-C4A-C10	-6.40	115.72	119.95
3	A	1001	A26	C18-C17-C19	5.57	125.16	118.75
4	A	1002	FMN	C4A-C4-N3	-4.84	116.82	123.43
3	A	1001	A26	F14-C11-F12	4.57	122.49	105.72
3	A	1001	A26	O25-C16-C17	-4.43	115.81	120.83
4	A	1002	FMN	C4A-C10-N10	-3.50	116.70	120.30
5	A	1003	ORO	C4-C5-C6	2.90	118.60	116.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	A26	F14-C11-C3	-2.83	106.71	112.93
3	A	1001	A26	F13-C11-C3	-2.68	107.05	112.93
4	A	1002	FMN	C10-C4A-N5	2.65	123.09	121.26
4	A	1002	FMN	C4A-N5-C5A	2.29	119.06	116.77
4	A	1002	FMN	C4-C4A-N5	2.27	121.19	118.60
3	A	1001	A26	F14-C11-F13	-2.26	97.43	105.72
3	A	1001	A26	C18-C17-C16	-2.15	114.63	119.15
4	A	1002	FMN	C5A-C9A-N10	-2.10	116.19	117.72
4	A	1002	FMN	C1'-N10-C9A	2.03	119.89	118.29

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1005	N8E	O12-C13-C14-O15
6	A	1004	N8E	C06-C07-C08-O09
6	A	1005	N8E	O15-C16-C17-O18
4	A	1002	FMN	C4'-C5'-O5'-P
6	A	1005	N8E	C10-C11-O12-C13
6	A	1005	N8E	C20-C19-O18-C17
6	A	1004	N8E	C07-C08-O09-C10
6	A	1005	N8E	C11-C10-O09-C08

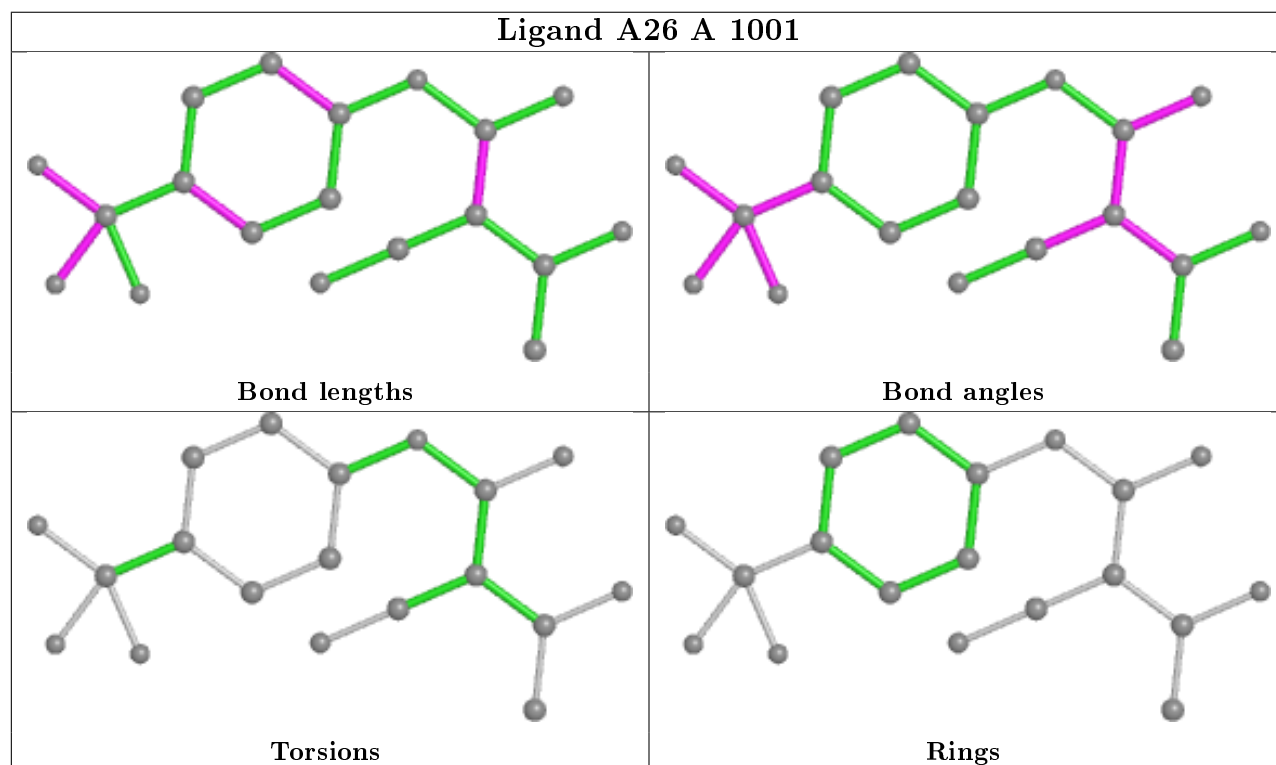
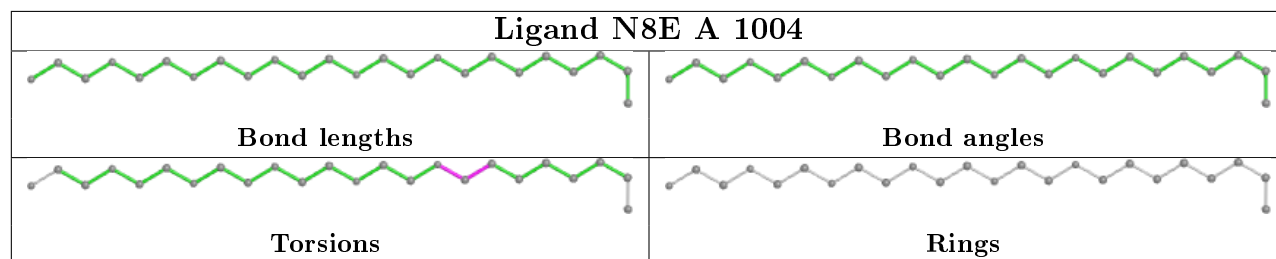
There are no ring outliers.

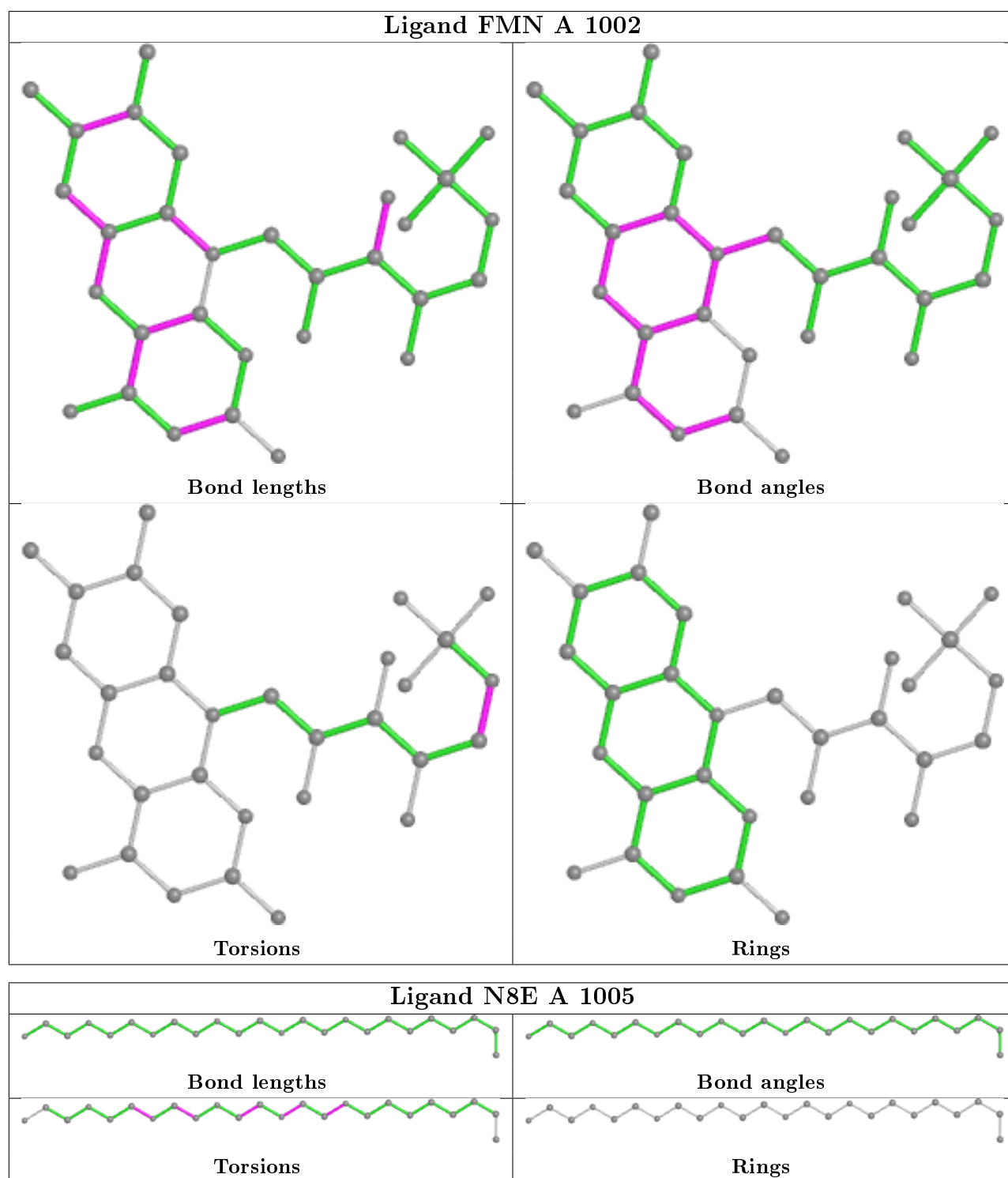
5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1004	N8E	2	0
2	A	1006	SO4	1	0
4	A	1002	FMN	1	0
5	A	1003	ORO	2	0
6	A	1005	N8E	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 ⓘ

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	371/443 (83%)	0.40	37 (9%) 7 6	19, 32, 53, 79	2 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	184[A]	CYS	14.8
1	A	414	PHE	6.6
1	A	158	PHE	6.2
1	A	175[A]	CYS	6.1
1	A	566	HIS	5.0
1	A	455	ILE	3.7
1	A	470	GLU	3.6
1	A	415	LEU	3.6
1	A	341	ILE	3.5
1	A	340	ALA	3.5
1	A	471	ASN	3.5
1	A	497	ASN	3.4
1	A	319	VAL	3.4
1	A	464	ASN	3.1
1	A	456	ILE	3.1
1	A	330	ASN	3.1
1	A	437	GLU	2.9
1	A	301	LYS	2.8
1	A	203	ASN	2.8
1	A	428	VAL	2.7
1	A	556	TYR	2.7
1	A	467	LYS	2.6
1	A	374	LEU	2.6
1	A	224	ALA	2.6
1	A	223	VAL	2.6
1	A	457	SER	2.5
1	A	214	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	253	ARG	2.5
1	A	430	LEU	2.4
1	A	465	ASP	2.3
1	A	525	CYS	2.3
1	A	429	LYS	2.2
1	A	564	ARG	2.2
1	A	225	ALA	2.1
1	A	317	ASP	2.1
1	A	268	GLU	2.0
1	A	249	THR	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 carbohydrates in this entry.

6.4 Ligands [i](#)

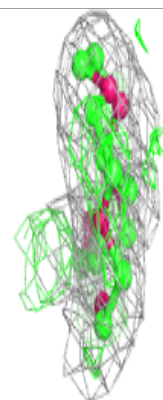
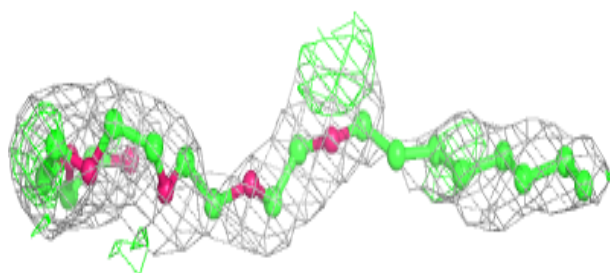
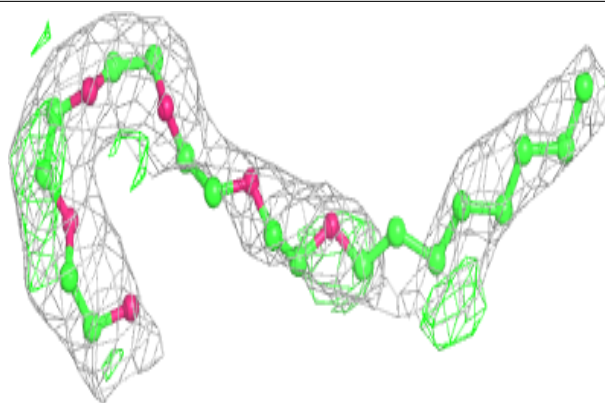
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	N8E	A	1005	24/24	0.60	0.37	86,92,94,94	0
6	N8E	A	1004	24/24	0.93	0.19	39,43,63,63	0
2	SO4	A	1006	5/5	0.95	0.31	30,30,30,30	5
3	A26	A	1001	19/19	0.96	0.15	19,25,33,33	0
5	ORO	A	1003	11/11	0.98	0.13	19,23,25,26	0
4	FMN	A	1002	31/31	0.98	0.20	18,21,24,24	0

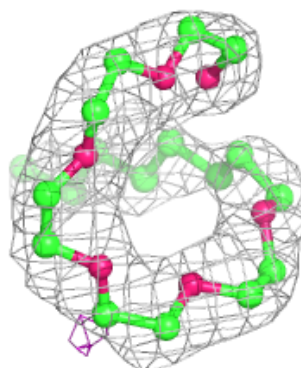
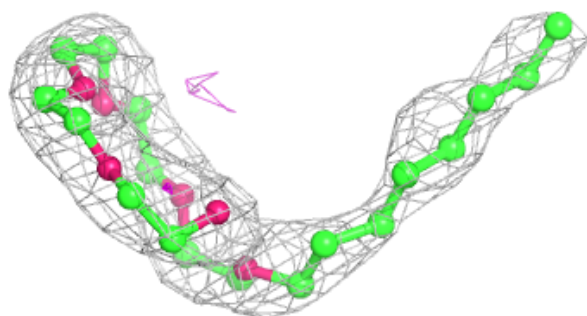
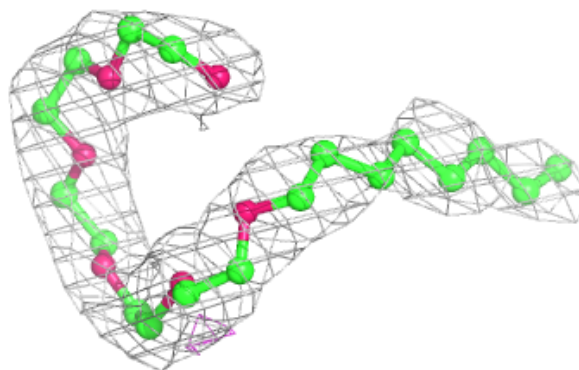
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around N8E A 1005:

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

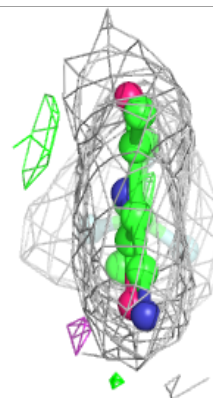
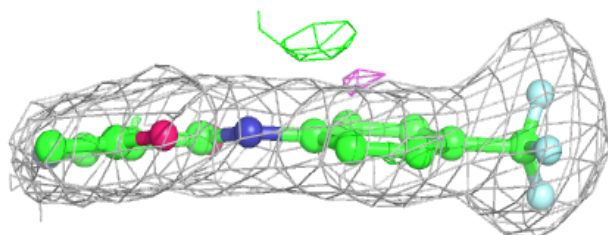
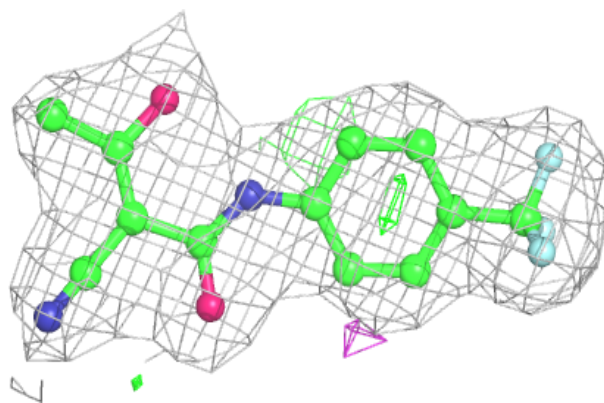
**Electron density around N8E A 1004:**

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

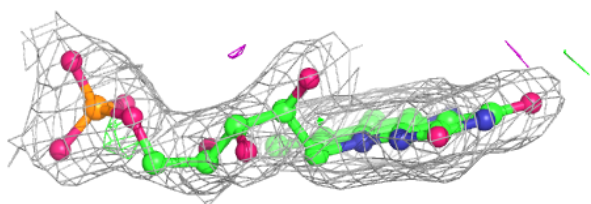
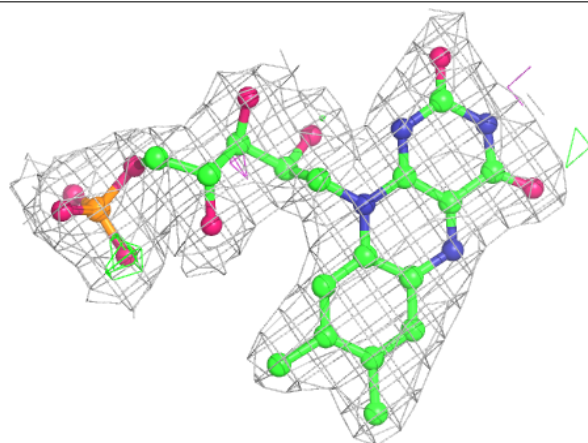


Electron density around A26 A 1001:

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

**Electron density around FMN A 1002:**

$2mF_o-DF_c$ (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.