



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 01:52 PM UTC

PDB ID : 5H2Z / pdb_00005h2z
Title : Crystal structure of Human Dihydroorotate Dehydrogenase (DHODH) with 7GF
Authors : Wu, D.; Huang, J.
Deposited on : 2016-10-19
Resolution : 1.58 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

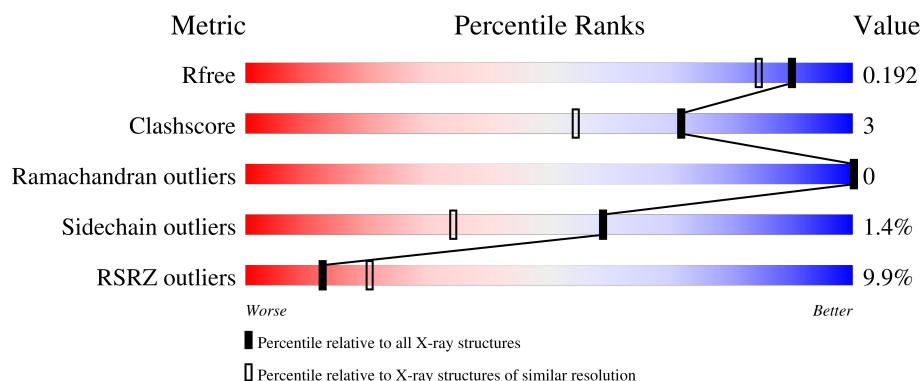
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.58 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	1094 (1.58-1.58)
Clashscore	190562	1105 (1.58-1.58)
Ramachandran outliers	187476	1082 (1.58-1.58)
Sidechain outliers	187428	1081 (1.58-1.58)
RSRZ outliers	180081	1094 (1.58-1.58)

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	390	9% 72% 18% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ORO	A	402	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	ACT	A	406	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 2998 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.

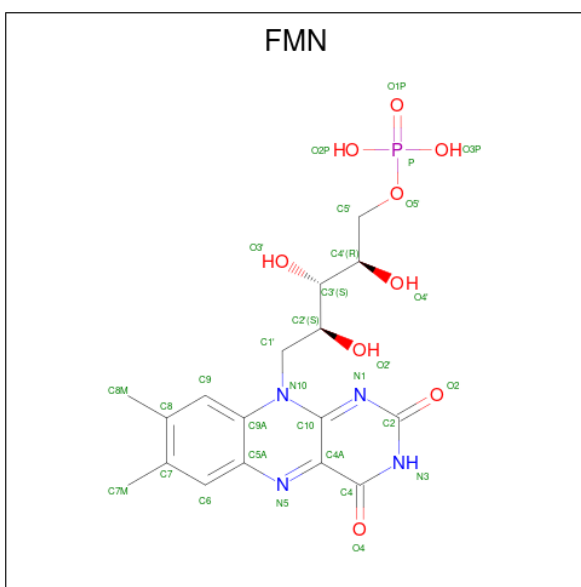
- Molecule 1 is a protein called Dihydroorotate dehydrogenase (quinone), mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	364	Total	C	N	O	S	0	1	0
			2784	1747	514	519	4			

There are 23 discrepancies between the modelled and reference sequences:

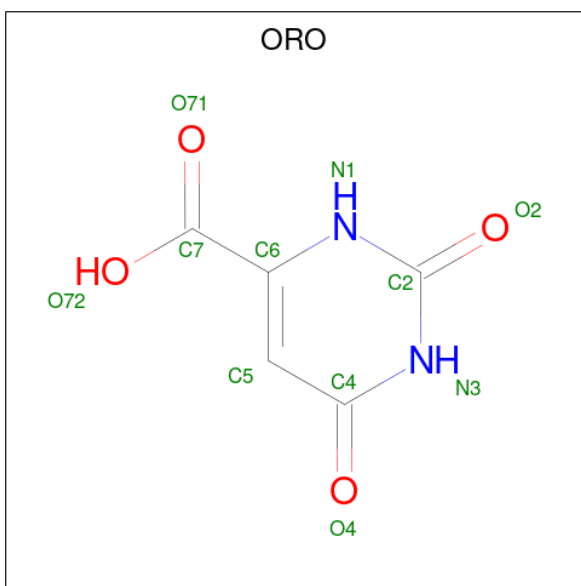
Chain	Residue	Modelled	Actual	Comment	Reference
A	7	MET	-	expression tag	UNP Q02127
A	8	GLY	-	expression tag	UNP Q02127
A	9	HIS	-	expression tag	UNP Q02127
A	10	HIS	-	expression tag	UNP Q02127
A	11	HIS	-	expression tag	UNP Q02127
A	12	HIS	-	expression tag	UNP Q02127
A	13	HIS	-	expression tag	UNP Q02127
A	14	HIS	-	expression tag	UNP Q02127
A	15	HIS	-	expression tag	UNP Q02127
A	16	HIS	-	expression tag	UNP Q02127
A	17	HIS	-	expression tag	UNP Q02127
A	18	HIS	-	expression tag	UNP Q02127
A	19	SER	-	expression tag	UNP Q02127
A	20	SER	-	expression tag	UNP Q02127
A	21	GLY	-	expression tag	UNP Q02127
A	22	HIS	-	expression tag	UNP Q02127
A	23	ILE	-	expression tag	UNP Q02127
A	24	ASP	-	expression tag	UNP Q02127
A	25	ASP	-	expression tag	UNP Q02127
A	26	ASP	-	expression tag	UNP Q02127
A	27	ASP	-	expression tag	UNP Q02127
A	28	LYS	-	expression tag	UNP Q02127
A	29	HIS	-	expression tag	UNP Q02127

- Molecule 2 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P).



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

- Molecule 3 is OROTIC ACID (CCD ID: ORO) (formula: $C_5H_4N_2O_4$).



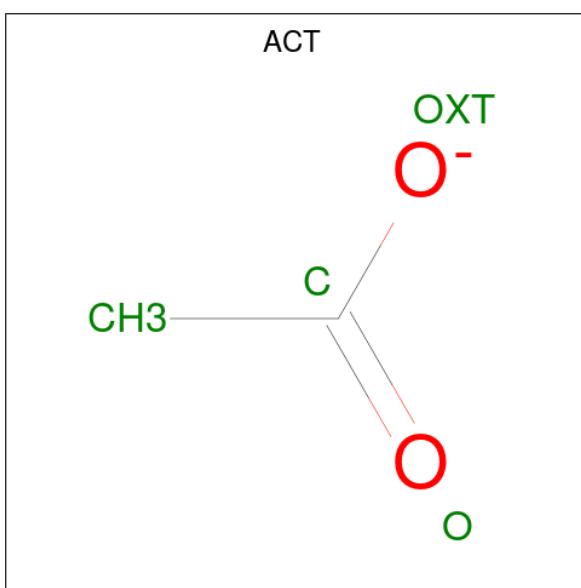
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			11	5	2	4		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



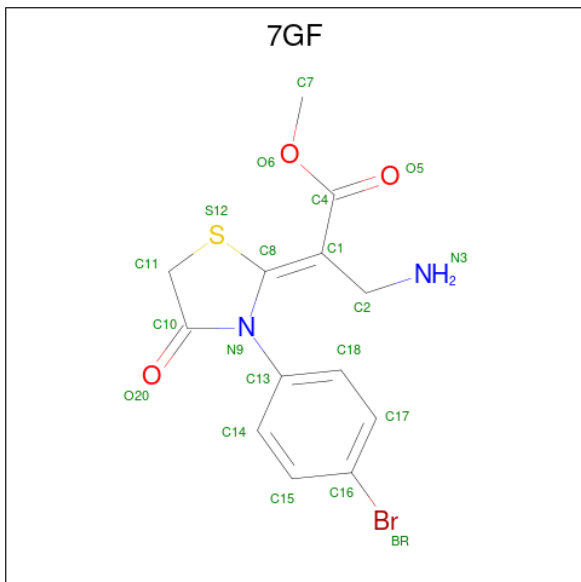
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

- Molecule 6 is methyl (2Z)-3-azanyl-2-[3-(4-bromophenyl)-4-oxidanylidene-1,3-thiazolidin-2-ylidene]propanoate (CCD ID: 7GF) (formula: C₁₃H₁₃BrN₂O₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	Br	C	N	O	S	0	0
			20	1	13	2	3	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	134	Total	O	0	0
			134	134		

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	90.88Å 90.88Å 123.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.40 – 1.58 36.40 – 1.58	Depositor EDS
% Data completeness (in resolution range)	99.9 (36.40-1.58) 99.9 (36.40-1.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 1.58Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.170 , 0.186 0.182 , 0.192	Depositor DCC
R_{free} test set	4024 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	21.1	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 40.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2998	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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: ACT, FMN, ORO, 7GF, 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	1.97	61/2833 (2.2%)	1.79	45/3830 (1.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	266	GLU	CD-OE1	13.74	1.51	1.25
1	A	136	ARG	CZ-NH2	-9.90	1.20	1.33
1	A	200	ARG	CD-NE	-9.13	1.33	1.46
1	A	211	VAL	CA-C	-8.61	1.42	1.52
1	A	266	GLU	CG-CD	8.27	1.72	1.52
1	A	246	ARG	C-O	8.11	1.33	1.24
1	A	359	LEU	N-CA	7.97	1.56	1.46
1	A	99	ASP	N-CA	7.63	1.57	1.46
1	A	203	GLY	C-N	7.49	1.41	1.34
1	A	81	VAL	CA-CB	7.16	1.65	1.54
1	A	65	LEU	N-CA	7.04	1.55	1.46
1	A	359	LEU	CA-C	-6.94	1.43	1.52
1	A	325	GLN	CA-C	-6.70	1.43	1.53
1	A	361	PHE	N-CA	-6.65	1.37	1.46
1	A	212	ASN	CA-C	-6.56	1.44	1.52
1	A	177	PRO	N-CA	-6.46	1.39	1.47
1	A	379	LYS	N-CA	6.43	1.54	1.46
1	A	130	PRO	C-O	6.43	1.31	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	147	TYR	C-O	6.37	1.31	1.24
1	A	312	LEU	N-CA	-6.23	1.38	1.46
1	A	212	ASN	CA-CB	6.20	1.60	1.52
1	A	290	PRO	CA-C	-6.15	1.45	1.52
1	A	145	ASN	C-N	6.10	1.41	1.33
1	A	160	ARG	CZ-NH1	6.02	1.41	1.32
1	A	118	ILE	CA-C	-6.01	1.47	1.52
1	A	136	ARG	CD-NE	-5.95	1.38	1.46
1	A	199	VAL	CA-CB	5.94	1.61	1.54
1	A	241	ARG	CA-CB	5.94	1.62	1.53
1	A	129	ASN	C-N	5.91	1.41	1.33
1	A	287	VAL	CA-CB	-5.88	1.47	1.54
1	A	242	ASP	CA-C	5.85	1.60	1.52
1	A	315	GLN	CA-C	-5.77	1.44	1.52
1	A	143	VAL	C-N	5.75	1.40	1.33
1	A	386	VAL	CA-C	-5.74	1.45	1.52
1	A	55	ALA	N-CA	-5.73	1.39	1.46
1	A	322	ALA	CA-C	-5.69	1.45	1.52
1	A	160	ARG	CZ-NH2	-5.68	1.26	1.33
1	A	138	PRO	CA-C	5.62	1.61	1.52
1	A	237	VAL	C-O	5.59	1.30	1.24
1	A	312	LEU	CB-CG	-5.58	1.42	1.53
1	A	392	ALA	N-CA	5.55	1.53	1.46
1	A	342	ALA	CA-C	5.55	1.59	1.52
1	A	246	ARG	CD-NE	5.44	1.53	1.46
1	A	289	ARG	N-CA	-5.41	1.40	1.46
1	A	127	GLU	C-O	-5.38	1.17	1.24
1	A	278	ASP	N-CA	-5.36	1.39	1.46
1	A	281	ILE	CA-C	5.36	1.59	1.52
1	A	154	LEU	C-O	-5.32	1.17	1.24
1	A	173	GLU	C-O	5.31	1.30	1.24
1	A	213	VAL	CA-C	5.30	1.59	1.52
1	A	207	ASP	C-O	5.28	1.30	1.24
1	A	389	ALA	N-CA	5.26	1.53	1.46
1	A	235	THR	CA-C	5.26	1.59	1.52
1	A	232	ARG	C-O	5.25	1.30	1.24
1	A	332	GLY	CA-C	-5.25	1.48	1.52
1	A	236	LYS	CA-CB	-5.12	1.45	1.53
1	A	58	LEU	C-N	5.06	1.40	1.33
1	A	103	GLU	C-O	5.06	1.30	1.24
1	A	238	LEU	N-CA	-5.05	1.40	1.46
1	A	133	ARG	NE-CZ	5.05	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	252	VAL	CA-CB	-5.02	1.47	1.54

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	ARG	NE-CZ-NH2	-14.77	105.90	119.20
1	A	136	ARG	NE-CZ-NH1	14.39	135.89	121.50
1	A	266	GLU	CG-CD-OE2	-11.09	92.88	118.40
1	A	36	ARG	N-CA-C	7.35	119.29	111.28
1	A	268	ILE	CA-C-O	7.29	128.53	120.95
1	A	136	ARG	CD-NE-CZ	7.14	134.40	124.40
1	A	199	VAL	O-C-N	7.05	128.82	121.91
1	A	160	ARG	NE-CZ-NH2	6.97	125.47	119.20
1	A	98	PHE	N-CA-C	-6.92	102.96	111.40
1	A	266	GLU	CA-CB-CG	6.91	127.91	114.10
1	A	290	PRO	CA-C-O	6.88	129.14	121.43
1	A	378	LEU	O-C-N	6.66	129.18	122.12
1	A	364	PRO	N-CA-C	6.48	118.60	110.70
1	A	266	GLU	O-C-N	6.38	128.88	122.12
1	A	106	ASP	N-CA-C	6.36	118.21	111.28
1	A	235	THR	O-C-N	6.34	128.84	122.12
1	A	130	PRO	CA-C-O	-6.34	114.21	121.56
1	A	289	ARG	O-C-N	6.20	126.96	121.32
1	A	237	VAL	O-C-N	-6.12	115.92	121.91
1	A	266	GLU	OE1-CD-OE2	5.97	137.23	122.90
1	A	290	PRO	O-C-N	-5.92	115.47	122.99
1	A	324	THR	O-C-N	-5.90	115.26	122.34
1	A	198	GLY	CA-C-O	5.83	126.76	120.75
1	A	127	GLU	O-C-N	5.77	130.43	122.46
1	A	129	ASN	O-C-N	-5.74	115.10	121.53
1	A	242	ASP	O-C-N	5.71	130.08	122.43
1	A	231	ARG	O-C-N	5.69	127.93	122.07
1	A	268	ILE	O-C-N	-5.67	116.37	121.87
1	A	32	THR	CA-C-N	5.65	126.21	119.94
1	A	32	THR	C-N-CA	5.65	126.21	119.94
1	A	235	THR	CA-C-O	-5.56	114.65	120.55
1	A	249	ARG	O-C-N	5.42	126.28	121.19
1	A	298	ARG	NE-CZ-NH1	-5.39	116.11	121.50
1	A	202	LEU	CA-C-O	5.29	124.96	119.14
1	A	160	ARG	NH1-CZ-NH2	-5.29	112.42	119.30
1	A	227	LYS	N-CA-C	5.29	117.47	111.02
1	A	129	ASN	CA-C-O	5.23	126.74	120.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	282	VAL	CA-C-N	5.17	131.01	121.70
1	A	282	VAL	C-N-CA	5.17	131.01	121.70
1	A	58	LEU	CD1-CG-CD2	5.16	122.15	110.80
1	A	240	GLU	O-C-N	-5.09	116.83	122.07
1	A	272	VAL	CG1-CB-CG2	5.05	121.92	110.80
1	A	165	GLN	O-C-N	-5.05	116.87	122.07
1	A	387	THR	N-CA-C	5.03	117.42	111.33
1	A	196	ALA	O-C-N	5.02	127.44	122.12

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	245	ARG	Sidechain

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	2784	0	2850	17	0
2	A	31	0	19	0	0
3	A	11	0	3	1	0
4	A	10	0	0	0	0
5	A	8	0	6	3	0
6	A	20	0	0	2	0
7	A	134	0	0	1	0
All	All	2998	0	2878	19	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 (19) 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:261:THR:OG1	5:A:406:ACT:H2	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:GLN:HE22	1:A:318:ARG:HE	1.33	0.77
1:A:145:ASN:OD1	3:A:402:ORO:H5	1.87	0.74
1:A:32:THR:HB	1:A:72:ARG:NH1	2.11	0.65
1:A:200:ARG:HH11	1:A:240:GLU:CD	2.06	0.64
1:A:200:ARG:NH1	1:A:240:GLU:CD	2.61	0.58
6:A:407:7GF:O5	6:A:407:7GF:S12	2.63	0.57
1:A:200:ARG:NH1	1:A:240:GLU:OE1	2.38	0.57
1:A:315:GLN:NE2	1:A:318:ARG:HE	2.03	0.54
1:A:173:GLU:HG3	7:A:573:HOH:O	2.10	0.51
1:A:224:LEU:HD23	1:A:229:GLU:OE1	2.12	0.49
1:A:189:VAL:O	1:A:189:VAL:HG12	2.13	0.49
1:A:261:THR:HG1	5:A:406:ACT:H2	1.75	0.48
1:A:160:ARG:HH21	5:A:405:ACT:H3	1.80	0.47
6:A:407:7GF:C13	6:A:407:7GF:C2	2.94	0.46
1:A:192:ALA:HB1	1:A:236:LYS:HD3	1.98	0.45
1:A:123:PRO:HA	1:A:154:LEU:HG	1.99	0.44
1:A:32:THR:HB	1:A:72:ARG:CZ	2.49	0.42
1:A:129:ASN:HB3	1:A:130:PRO:HD2	2.03	0.41

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	363/390 (93%)	353 (97%)	10 (3%)	0	100 100

There are no Ramachandran outliers to report.

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	295/317 (93%)	291 (99%)	4 (1%)	59 34

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	LEU
1	A	78	MET
1	A	247	VAL
1	A	272	VAL

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

Mol	Chain	Res	Type
1	A	86	HIS
1	A	141	GLN
1	A	239	GLN
1	A	294	GLN
1	A	315	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 ⓘ

7 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	SO4	A	403	-	4,4,4	0.88	0	6,6,6	1.03	0
2	FMN	A	401	-	33,33,33	1.89	6 (18%)	48,50,50	2.01	16 (33%)
4	SO4	A	404	-	4,4,4	1.07	0	6,6,6	1.00	0
5	ACT	A	405	-	3,3,3	0.91	0	3,3,3	1.28	0
5	ACT	A	406	-	3,3,3	0.59	0	3,3,3	0.20	0
6	7GF	A	407	-	20,21,21	3.11	11 (55%)	22,29,29	3.15	12 (54%)
3	ORO	A	402	-	11,11,11	2.48	5 (45%)	14,15,15	3.32	9 (64%)

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	7GF	A	407	-	-	0/12/29/29	0/2/2/2
2	FMN	A	401	-	-	4/18/18/18	0/3/3/3
3	ORO	A	402	-	-	4/4/4/4	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	407	7GF	C2-C1	-6.99	1.30	1.50
6	A	407	7GF	C11-S12	-5.83	1.71	1.80
3	A	402	ORO	C2-N1	4.94	1.45	1.37
2	A	401	FMN	O4-C4	4.85	1.32	1.23
6	A	407	7GF	C2-N3	-4.67	1.20	1.48
2	A	401	FMN	C4-N3	-4.42	1.30	1.38
2	A	401	FMN	C6-C7	-4.25	1.33	1.39
6	A	407	7GF	O20-C10	3.78	1.31	1.23
6	A	407	7GF	C11-C10	3.73	1.56	1.50
6	A	407	7GF	BR-C16	3.53	1.97	1.90
2	A	401	FMN	C9A-C5A	3.42	1.46	1.41
3	A	402	ORO	C5-C4	-3.41	1.35	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	FMN	C5'-C4'	3.21	1.56	1.51
6	A	407	7GF	C17-C16	-3.01	1.32	1.38
3	A	402	ORO	C4-N3	-2.84	1.33	1.38
6	A	407	7GF	C10-N9	-2.84	1.36	1.40
6	A	407	7GF	C8-N9	-2.69	1.34	1.39
2	A	401	FMN	C4A-N5	2.61	1.36	1.30
6	A	407	7GF	C18-C17	2.55	1.42	1.38
6	A	407	7GF	C15-C14	2.44	1.42	1.38
3	A	402	ORO	O72-C7	-2.31	1.24	1.30
3	A	402	ORO	O71-C7	2.17	1.27	1.22

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	ORO	O4-C4-C5	-7.94	114.50	125.46
6	A	407	7GF	C17-C16-C15	6.31	130.91	121.33
6	A	407	7GF	C11-C10-N9	6.20	114.73	111.23
2	A	401	FMN	C4-C4A-N5	5.45	125.73	118.21
3	A	402	ORO	C5-C4-N3	5.16	121.66	115.24
6	A	407	7GF	C13-N9-C10	-5.15	114.04	123.17
6	A	407	7GF	C14-C15-C16	-4.89	113.33	119.18
6	A	407	7GF	C10-C11-S12	-4.23	101.50	107.56
3	A	402	ORO	C6-N1-C2	-4.12	118.24	122.65
2	A	401	FMN	C4-C4A-C10	-4.04	110.00	116.93
2	A	401	FMN	O4-C4-C4A	-3.82	116.45	126.53
2	A	401	FMN	C9A-N10-C10	3.75	126.46	120.75
6	A	407	7GF	BR-C16-C15	-3.67	114.30	119.30
6	A	407	7GF	BR-C16-C17	-3.64	114.33	119.30
2	A	401	FMN	C9-C9A-N10	3.59	126.69	121.85
2	A	401	FMN	C4A-C4-N3	3.40	121.92	113.25
3	A	402	ORO	C4-N3-C2	-3.19	122.46	125.55
2	A	401	FMN	C1'-N10-C9A	-3.15	114.51	120.63
3	A	402	ORO	O4-C4-N3	3.11	123.79	119.27
6	A	407	7GF	C18-C17-C16	-3.04	115.54	119.18
6	A	407	7GF	O5-C4-C1	-2.88	119.38	125.13
3	A	402	ORO	O2-C2-N3	-2.77	116.93	121.86
6	A	407	7GF	C2-C1-C8	2.77	127.04	120.36
2	A	401	FMN	C7M-C7-C6	2.72	124.37	119.57
2	A	401	FMN	C5A-C6-C7	2.71	125.84	120.83
2	A	401	FMN	C9A-C5A-N5	-2.69	119.60	122.45
3	A	402	ORO	O2-C2-N1	2.58	126.45	121.86
3	A	402	ORO	O72-C7-C6	2.48	119.61	114.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	FMN	C4A-C10-N10	-2.44	113.00	116.48
6	A	407	7GF	O6-C4-C1	2.40	116.17	112.27
6	A	407	7GF	C13-N9-C8	2.36	128.98	124.95
2	A	401	FMN	O4'-C4'-C3'	2.35	114.76	109.25
2	A	401	FMN	C10-N1-C2	2.33	121.89	116.85
3	A	402	ORO	O71-C7-C6	-2.27	116.41	121.01
2	A	401	FMN	C9-C9A-C5A	-2.22	116.11	120.03
2	A	401	FMN	O2-C2-N1	2.11	125.30	121.80
2	A	401	FMN	C6-C5A-N5	2.05	121.84	118.44

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	ORO	N1-C6-C7-O71
3	A	402	ORO	N1-C6-C7-O72
2	A	401	FMN	O3'-C3'-C4'-O4'
2	A	401	FMN	C2'-C3'-C4'-O4'
2	A	401	FMN	O3'-C3'-C4'-C5'
2	A	401	FMN	C4'-C5'-O5'-P
3	A	402	ORO	C5-C6-C7-O71
3	A	402	ORO	C5-C6-C7-O72

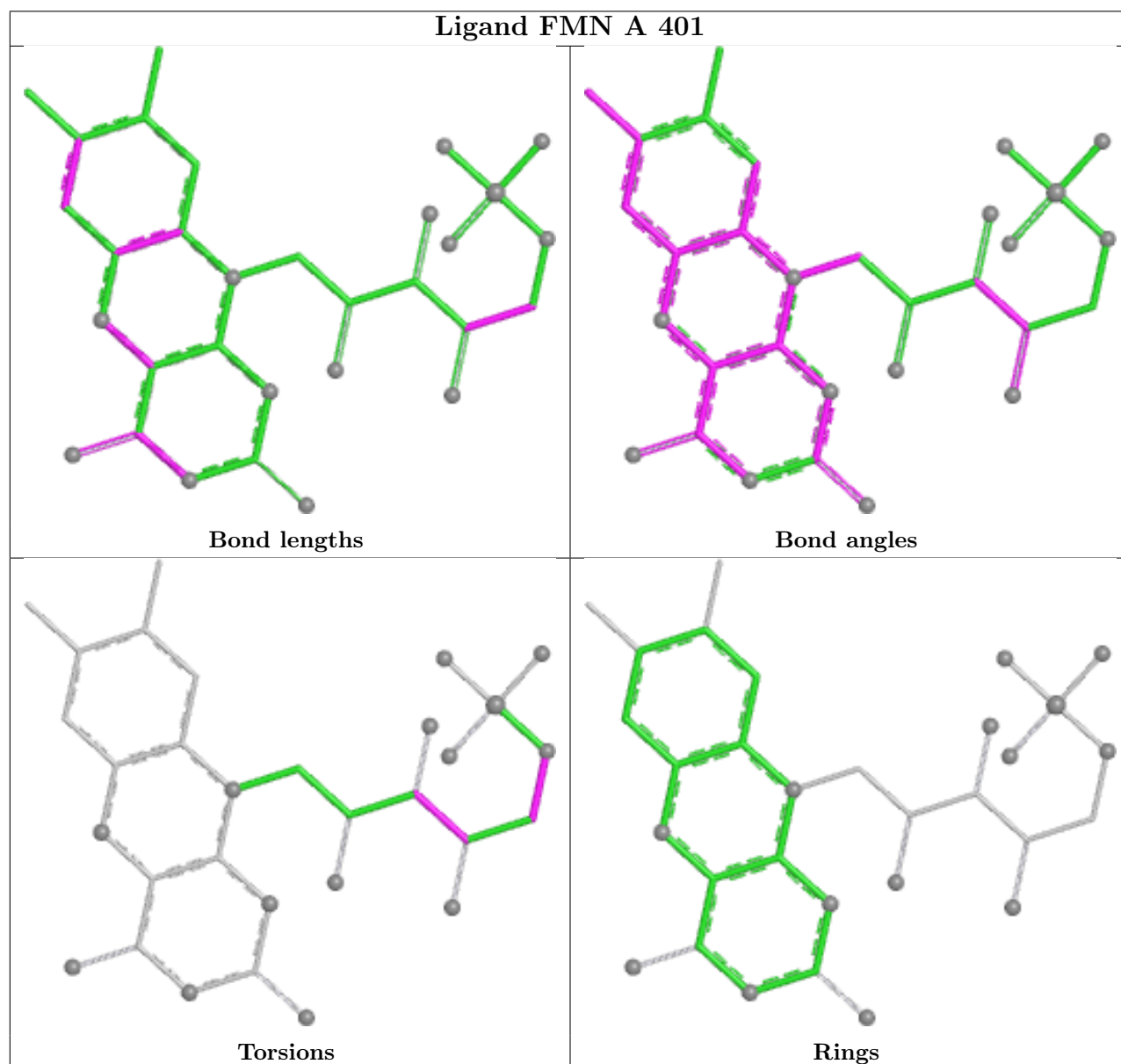
There are no ring outliers.

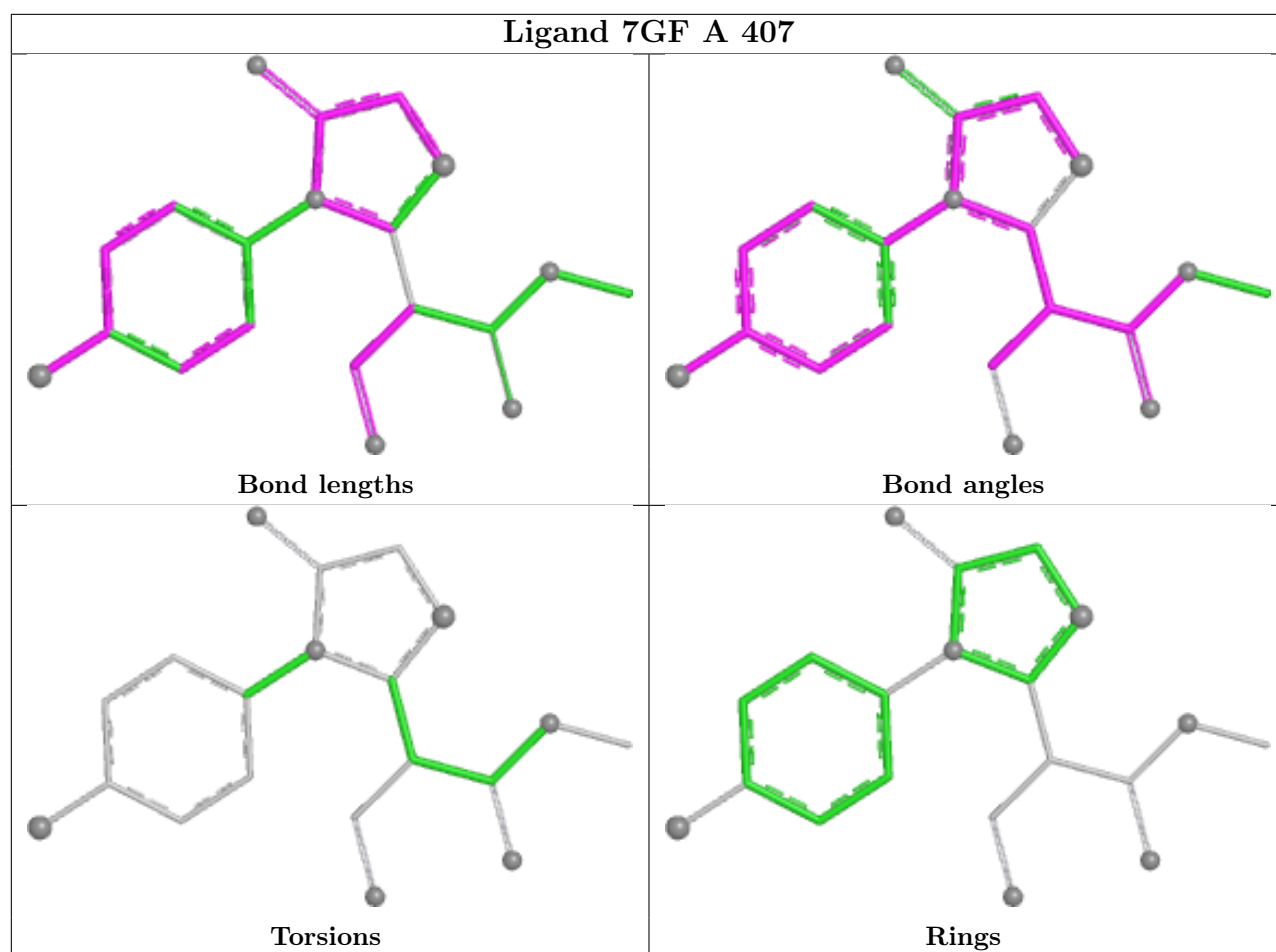
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	405	ACT	1	0
5	A	406	ACT	2	0
6	A	407	7GF	2	0
3	A	402	ORO	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	364/390 (93%)	0.52	36 (9%) 13 20	6, 21, 41, 86	12 (3%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	213	VAL	9.2
1	A	362	TRP	9.1
1	A	211	VAL	7.3
1	A	189	VAL	6.7
1	A	219	ALA	5.6
1	A	73	PHE	5.4
1	A	32	THR	5.3
1	A	226	GLY	5.0
1	A	224	LEU	5.0
1	A	72	ARG	4.5
1	A	134	VAL	4.2
1	A	225	GLN	4.0
1	A	212	ASN	3.8
1	A	70	ARG	3.6
1	A	228	ALA	3.5
1	A	71	ALA	3.3
1	A	223	SER	3.2
1	A	65	LEU	3.1
1	A	33	GLY	3.1
1	A	49	LEU	3.0
1	A	216	PRO	3.0
1	A	188	SER	2.9
1	A	187	THR	2.7
1	A	197	GLU	2.7
1	A	229	GLU	2.7
1	A	218	THR	2.7
1	A	247	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	74	GLN	2.6
1	A	313	SER	2.4
1	A	174	ASP	2.4
1	A	246	ARG	2.4
1	A	131	ARG	2.3
1	A	230	LEU	2.2
1	A	77	ASP	2.1
1	A	221	LEU	2.1
1	A	382	GLY	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](#)

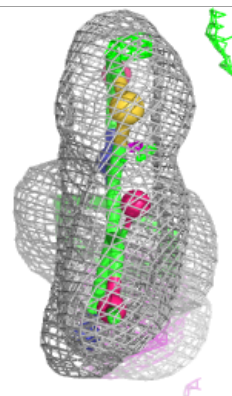
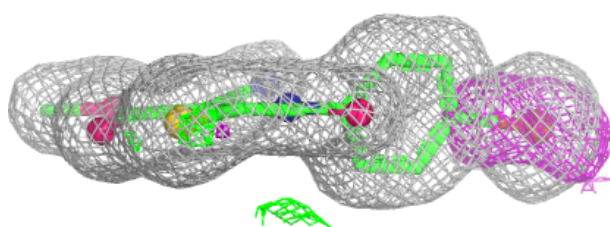
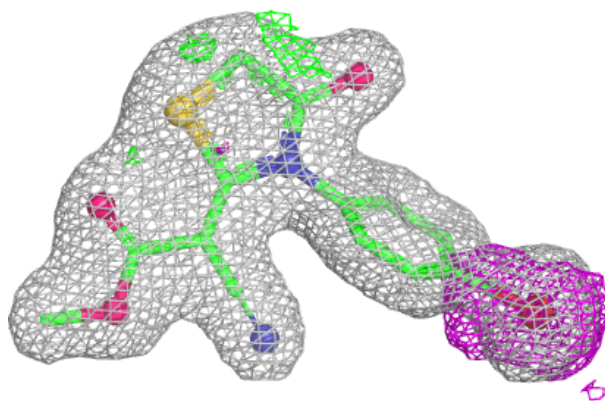
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	ACT	A	405	4/4	0.58	0.29	42,43,47,61	0
5	ACT	A	406	4/4	0.85	0.16	32,34,50,55	0
4	SO4	A	404	5/5	0.91	0.10	37,41,49,58	0
4	SO4	A	403	5/5	0.97	0.07	30,33,43,46	0
6	7GF	A	407	20/20	0.98	0.09	18,28,33,38	0
3	ORO	A	402	11/11	0.99	0.04	11,15,19,20	0
2	FMN	A	401	31/31	0.99	0.04	13,14,16,17	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.

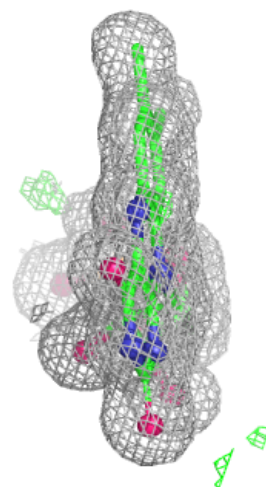
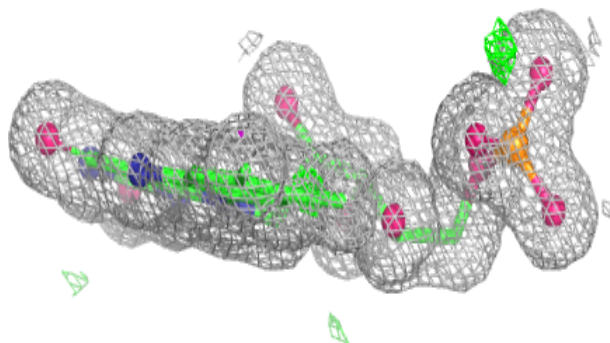
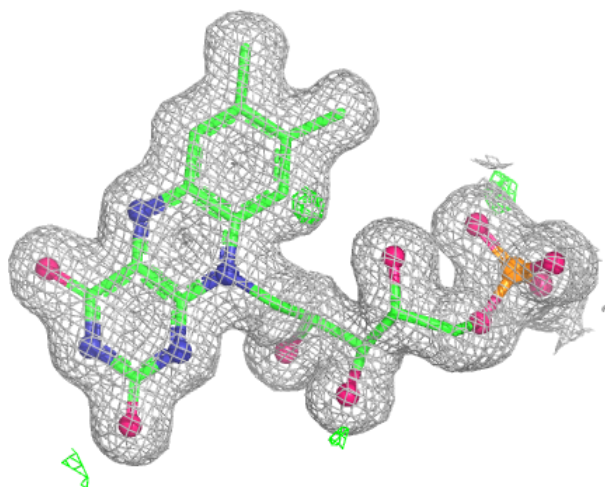
Electron density around 7GF A 407:

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



Electron density around FMN A 401:

$2mF_o-DF_c$ (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.