



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:09 AM UTC

PDB ID : 5HIN / pdb_00005hin
Title : Crystal structure of human dihydroorotate dehydrogenase (DHODH) with 18L compound
Authors : Huang, J.; Wu, D.; Lu, Q.; Yao, X.
Deposited on : 2016-01-12
Resolution : 1.60 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

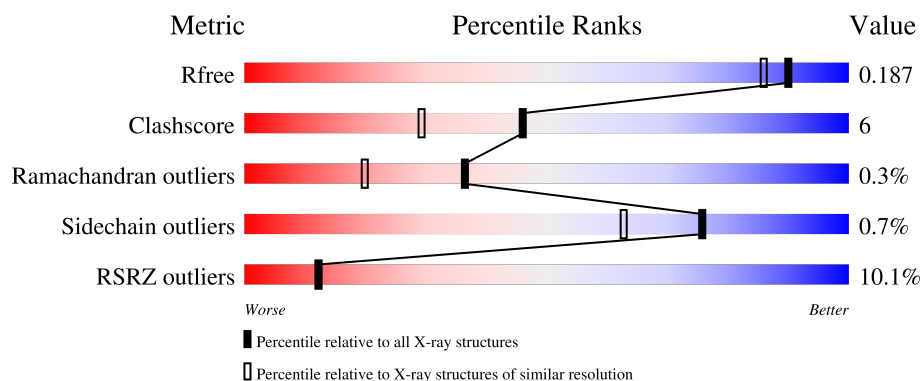
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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% 69% 21% 6%

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
6	ACT	A	410	-	X	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3100 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	365	Total	C	N	O	S	0	3	0
			2807	1760	519	524	4			

There are 23 discrepancies between the modelled and reference sequences:

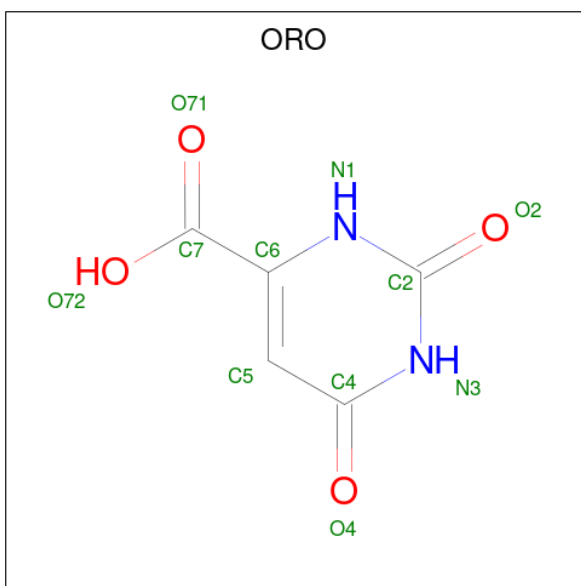
Chain	Residue	Modelled	Actual	Comment	Reference
A	7	MET	-	expression tag	UNP Q02127
A	8	GLY	-	expression tag	UNP Q02127
A	9	HIS	-	expression tag	UNP Q02127
A	10	HIS	-	expression tag	UNP Q02127
A	11	HIS	-	expression tag	UNP Q02127
A	12	HIS	-	expression tag	UNP Q02127
A	13	HIS	-	expression tag	UNP Q02127
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: $C_5H_4N_2O_4$).



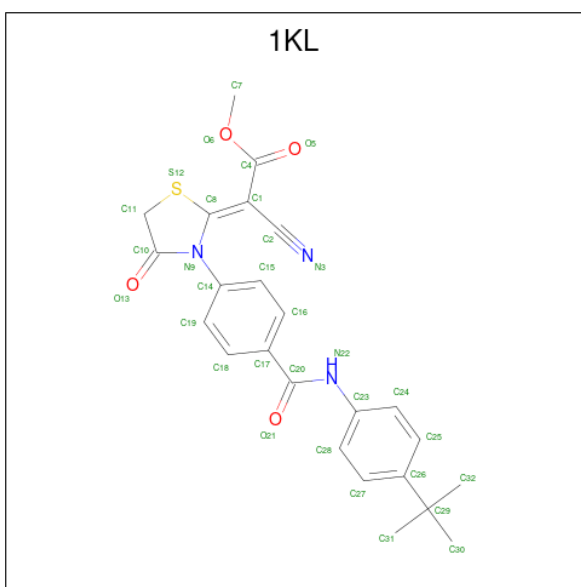
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			11	5	2	4		

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



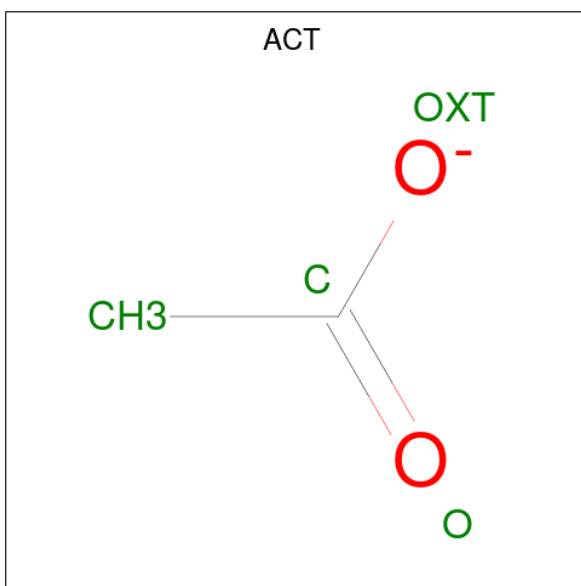
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is methyl (2Z)-(3-{4-[(4-tert-butylphenyl)carbamoyl]phenyl}-4-oxo-1,3-thiazolidi n-2-ylidene)(cyano)acetate (CCD ID: 1KL) (formula: C₂₄H₂₃N₃O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			32	24	3	4	1		

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2^-$).



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

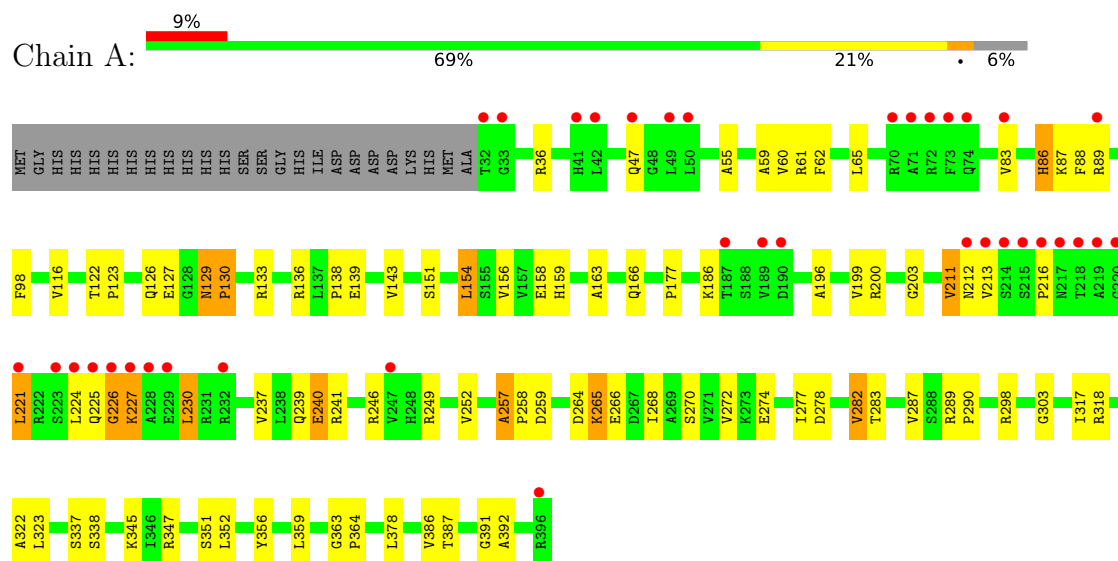
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	186	Total 186	O 186	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 (quinone), mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	90.73Å 90.73Å 122.63Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.56 – 1.60 28.56 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (28.56-1.60) 99.7 (28.56-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.97 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.163 , 0.182 0.167 , 0.187	Depositor DCC
R_{free} test set	2001 reflections (2.59%)	wwPDB-VP
Wilson B-factor (Å ²)	17.3	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 41.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3100	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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: 1KL, SO4, FMN, ACT, 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	1.85	54/2865 (1.9%)	1.70	46/3870 (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 (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	212	ASN	N-CA	-9.68	1.34	1.46
1	A	386	VAL	CA-C	-8.55	1.41	1.52
1	A	392	ALA	N-CA	7.63	1.55	1.46
1	A	55	ALA	N-CA	-7.56	1.37	1.46
1	A	83	VAL	CA-C	7.51	1.60	1.52
1	A	252	VAL	CA-CB	-7.37	1.45	1.54
1	A	211	VAL	CA-C	-7.32	1.43	1.52
1	A	257	ALA	N-CA	-7.07	1.35	1.45
1	A	323	LEU	CA-CB	-7.05	1.41	1.53
1	A	212	ASN	CA-C	-6.66	1.44	1.52
1	A	166	GLN	C-O	-6.65	1.16	1.24
1	A	116	VAL	N-CA	-6.57	1.38	1.46
1	A	282	VAL	C-O	-6.51	1.16	1.24
1	A	163	ALA	CA-CB	-6.47	1.42	1.53
1	A	130	PRO	C-O	6.47	1.31	1.23
1	A	246	ARG	C-O	6.42	1.31	1.24
1	A	359	LEU	N-CA	6.28	1.54	1.46
1	A	318	ARG	C-O	-6.20	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	126	GLN	C-O	-6.19	1.16	1.23
1	A	258	PRO	C-O	-6.04	1.16	1.24
1	A	230	LEU	CA-C	6.02	1.60	1.52
1	A	259	ASP	C-O	-6.02	1.16	1.24
1	A	133	ARG	NE-CZ	5.93	1.39	1.33
1	A	338	SER	N-CA	-5.84	1.38	1.45
1	A	274	GLU	CA-CB	-5.79	1.44	1.53
1	A	60	VAL	CA-C	5.76	1.60	1.52
1	A	154	LEU	C-O	-5.72	1.17	1.24
1	A	129	ASN	C-O	-5.68	1.16	1.23
1	A	212	ASN	CG-OD1	-5.59	1.12	1.23
1	A	303	GLY	CA-C	-5.55	1.46	1.52
1	A	356	TYR	C-O	-5.54	1.17	1.24
1	A	186	LYS	C-O	-5.46	1.17	1.24
1	A	317	ILE	CA-CB	-5.39	1.48	1.54
1	A	122	THR	CA-C	5.37	1.59	1.52
1	A	241	ARG	N-CA	-5.33	1.40	1.46
1	A	143	VAL	CA-C	-5.31	1.46	1.52
1	A	61	ARG	CA-C	-5.30	1.46	1.52
1	A	59	ALA	N-CA	-5.30	1.40	1.46
1	A	272	VAL	CA-CB	5.29	1.61	1.54
1	A	290	PRO	CA-C	-5.27	1.46	1.52
1	A	387	THR	CA-C	5.25	1.59	1.52
1	A	163	ALA	N-CA	5.22	1.53	1.46
1	A	130	PRO	CA-CB	5.21	1.60	1.53
1	A	391	GLY	C-N	-5.20	1.27	1.34
1	A	352	LEU	N-CA	-5.12	1.39	1.45
1	A	143	VAL	C-N	5.12	1.40	1.33
1	A	65	LEU	N-CA	5.12	1.52	1.46
1	A	337	SER	CB-OG	-5.11	1.31	1.42
1	A	264	ASP	C-O	5.11	1.30	1.24
1	A	133	ARG	C-N	-5.10	1.26	1.33
1	A	266	GLU	C-O	-5.09	1.18	1.24
1	A	138	PRO	C-O	-5.04	1.18	1.24
1	A	257	ALA	CA-CB	5.04	1.59	1.53
1	A	277	ILE	N-CA	5.04	1.52	1.46

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227	LYS	N-CA-C	11.58	135.46	110.80
1	A	203	GLY	CA-C-O	9.38	125.60	119.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	290	PRO	CA-C-O	7.46	129.78	121.43
1	A	268	ILE	O-C-N	-7.26	114.83	121.87
1	A	156	VAL	CA-C-O	6.92	128.51	121.17
1	A	303	GLY	O-C-N	-6.88	118.26	123.35
1	A	127	GLU	O-C-N	6.76	131.38	122.33
1	A	237	VAL	O-C-N	-6.51	115.55	121.87
1	A	60	VAL	O-C-N	6.36	128.04	121.87
1	A	364	PRO	N-CA-C	6.29	118.38	110.70
1	A	240	GLU	O-C-N	-6.29	115.46	122.12
1	A	130	PRO	CA-C-O	-6.28	114.27	121.56
1	A	290	PRO	O-C-N	-6.24	115.06	122.99
1	A	378	LEU	O-C-N	6.23	128.48	122.07
1	A	289	ARG	O-C-N	6.21	126.97	121.32
1	A	351	SER	N-CA-C	6.20	120.04	112.23
1	A	270	SER	O-C-N	5.96	128.29	122.09
1	A	62	PHE	CA-C-O	5.91	126.82	120.55
1	A	139	GLU	N-CA-C	-5.91	105.33	112.54
1	A	133	ARG	NE-CZ-NH1	-5.85	115.65	121.50
1	A	391	GLY	CA-C-O	-5.81	112.03	119.58
1	A	249	ARG	O-C-N	5.67	126.58	120.85
1	A	322	ALA	CA-C-N	5.61	128.36	120.28
1	A	322	ALA	C-N-CA	5.61	128.36	120.28
1	A	151	SER	O-C-N	5.54	129.89	123.41
1	A	86	HIS	N-CA-C	5.52	117.57	109.24
1	A	298	ARG	N-CA-C	5.50	118.79	111.75
1	A	282	VAL	CA-C-N	5.46	131.52	121.70
1	A	282	VAL	C-N-CA	5.46	131.52	121.70
1	A	239	GLN	N-CA-C	-5.45	105.24	111.07
1	A	386	VAL	CB-CA-C	-5.41	104.96	112.04
1	A	98	PHE	N-CA-C	-5.37	104.31	111.24
1	A	278	ASP	N-CA-C	5.35	119.53	112.89
1	A	36	ARG	N-CA-C	5.32	117.08	111.28
1	A	265	LYS	CG-CD-CE	-5.32	99.08	111.30
1	A	196	ALA	CA-C-O	-5.31	114.92	120.55
1	A	363	GLY	O-C-N	-5.30	116.47	121.77
1	A	199	VAL	O-C-N	5.29	127.09	121.91
1	A	87	LYS	CA-C-O	5.29	127.08	121.05
1	A	345	LYS	N-CA-C	5.25	117.08	111.36
1	A	226	GLY	CA-C-O	-5.17	116.18	122.75
1	A	363	GLY	CA-C-N	5.11	125.64	120.38
1	A	363	GLY	C-N-CA	5.11	125.64	120.38
1	A	347	ARG	CA-C-O	5.10	125.86	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	199	VAL	CA-C-O	-5.07	115.80	121.17
1	A	122	THR	CA-C-O	-5.02	115.69	120.97

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	158	GLU	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	2807	0	2879	31	0
2	A	31	0	19	0	0
3	A	11	0	3	0	0
4	A	25	0	0	0	0
5	A	32	0	0	3	0
6	A	8	0	6	4	0
7	A	186	0	0	2	0
All	All	3100	0	2907	34	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 6.

All (34) 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:47:GLN:HG3	1:A:136:ARG:CZ	1.46	1.41
1:A:47:GLN:HG3	1:A:136:ARG:NH1	1.70	1.06
1:A:47:GLN:CG	1:A:136:ARG:CZ	2.35	1.03
1:A:47:GLN:HG3	1:A:136:ARG:NH2	1.92	0.84
1:A:47:GLN:CG	1:A:136:ARG:NH1	2.45	0.79
1:A:221:LEU:HD23	1:A:224:LEU:HD12	1.68	0.73
1:A:200:ARG:NH1	1:A:240:GLU:OE2	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:VAL:HA	1:A:221:LEU:HD21	1.74	0.69
1:A:47:GLN:CD	1:A:136:ARG:NE	2.53	0.67
1:A:226:GLY:O	1:A:230:LEU:HB2	1.96	0.64
5:A:408:1KL:S12	5:A:408:1KL:O5	2.57	0.62
1:A:200:ARG:HH11	1:A:240:GLU:CD	2.06	0.62
1:A:159:HIS:HD2	7:A:671:HOH:O	1.82	0.62
1:A:200:ARG:NH1	1:A:240:GLU:CD	2.57	0.62
1:A:216:PRO:HB3	1:A:287:VAL:CG1	2.33	0.59
1:A:226:GLY:O	1:A:230:LEU:CB	2.52	0.58
1:A:221:LEU:CD2	1:A:221:LEU:C	2.80	0.54
5:A:408:1KL:C14	5:A:408:1KL:C2	2.85	0.54
1:A:211:VAL:HG12	1:A:213:VAL:HG13	1.89	0.54
1:A:225:GLN:HE22	1:A:257:ALA:H	1.56	0.51
1:A:265:LYS:NZ	6:A:410:ACT:CH3	2.74	0.50
1:A:129:ASN:HB3	1:A:130:PRO:HD2	1.93	0.50
1:A:221:LEU:C	1:A:221:LEU:HD22	2.37	0.50
1:A:47:GLN:CD	1:A:136:ARG:CZ	2.84	0.48
1:A:265:LYS:HZ1	6:A:410:ACT:H1	1.78	0.48
1:A:86:HIS:HB3	7:A:537:HOH:O	2.14	0.47
1:A:221:LEU:CD2	1:A:221:LEU:O	2.63	0.47
1:A:123:PRO:HA	1:A:154:LEU:HG	1.98	0.46
1:A:265:LYS:NZ	6:A:410:ACT:H1	2.30	0.46
1:A:265:LYS:HZ1	6:A:410:ACT:CH3	2.29	0.45
1:A:282:VAL:HA	1:A:283:THR:HA	1.83	0.43
5:A:408:1KL:C2	5:A:408:1KL:C15	2.97	0.43
1:A:47:GLN:OE1	1:A:136:ARG:CD	2.68	0.42
1:A:88:PHE:CE2	1:A:177:PRO:HG2	2.57	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	367/390 (94%)	354 (96%)	12 (3%)	1 (0%)	36 20

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	227	LYS

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	299/317 (94%)	297 (99%)	2 (1%)	76 63

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

Mol	Chain	Res	Type
1	A	89	ARG
1	A	221	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	141	GLN
1	A	159	HIS
1	A	225	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 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	404	-	4,4,4	0.44	0	6,6,6	0.55	0
4	SO4	A	406	-	4,4,4	0.73	0	6,6,6	0.60	0
5	1KL	A	408	-	34,34,34	2.56	11 (32%)	43,49,49	2.05	12 (27%)
6	ACT	A	409	-	3,3,3	0.93	0	3,3,3	0.56	0
3	ORO	A	402	-	11,11,11	2.46	5 (45%)	14,15,15	1.61	3 (21%)
4	SO4	A	403	-	4,4,4	0.53	0	6,6,6	0.75	0
4	SO4	A	407	-	4,4,4	0.52	0	6,6,6	1.19	1 (16%)
2	FMN	A	401	-	33,33,33	1.63	9 (27%)	48,50,50	1.42	8 (16%)
4	SO4	A	405	-	4,4,4	0.79	0	6,6,6	0.81	0
6	ACT	A	410	-	3,3,3	1.96	1 (33%)	3,3,3	3.06	2 (66%)

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
5	1KL	A	408	-	-	2/28/43/43	0/3/3/3
3	ORO	A	402	-	-	4/4/4/4	0/1/1/1
2	FMN	A	401	-	-	5/18/18/18	0/3/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	408	1KL	C10-N9	-6.42	1.31	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	408	1KL	C1-C8	-6.08	1.29	1.39
5	A	408	1KL	C2-C1	-5.98	1.30	1.43
5	A	408	1KL	C11-S12	-4.45	1.74	1.80
5	A	408	1KL	C11-C10	3.77	1.56	1.50
3	A	402	ORO	C4-N3	-3.71	1.32	1.38
2	A	401	FMN	C9A-C5A	3.56	1.46	1.41
3	A	402	ORO	O72-C7	-3.53	1.21	1.30
3	A	402	ORO	C2-N3	-3.36	1.31	1.37
5	A	408	1KL	C14-N9	3.32	1.49	1.44
3	A	402	ORO	C6-N1	-3.20	1.31	1.38
3	A	402	ORO	C2-N1	-3.09	1.32	1.37
5	A	408	1KL	C2-N3	2.99	1.20	1.14
5	A	408	1KL	O13-C10	2.90	1.29	1.23
5	A	408	1KL	C23-N22	-2.90	1.35	1.41
5	A	408	1KL	C8-N9	-2.76	1.34	1.39
6	A	410	ACT	OXT-C	2.76	1.43	1.30
2	A	401	FMN	C5A-N5	-2.70	1.34	1.39
2	A	401	FMN	C4-N3	-2.61	1.34	1.38
2	A	401	FMN	O2-C2	-2.41	1.19	1.24
2	A	401	FMN	C2-N3	-2.39	1.33	1.39
5	A	408	1KL	C16-C17	-2.26	1.36	1.39
2	A	401	FMN	C6-C7	-2.19	1.36	1.39
2	A	401	FMN	C2-N1	-2.02	1.32	1.36
2	A	401	FMN	P-O1P	-2.02	1.44	1.50
2	A	401	FMN	C8-C7	2.01	1.45	1.40

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	408	1KL	O13-C10-N9	7.50	131.81	124.03
6	A	410	ACT	O-C-CH3	-4.58	103.75	122.53
2	A	401	FMN	C4-C4A-N5	4.02	123.76	118.21
5	A	408	1KL	C14-N9-C10	-4.00	116.08	123.17
5	A	408	1KL	C24-C25-C26	3.72	126.30	121.17
5	A	408	1KL	O13-C10-C11	-3.32	116.86	123.64
5	A	408	1KL	C27-C28-C23	3.32	124.12	120.30
3	A	402	ORO	C4-N3-C2	-3.05	122.59	125.55
2	A	401	FMN	C10-N1-C2	3.04	123.44	116.85
5	A	408	1KL	C27-C26-C25	-2.99	113.57	118.03
5	A	408	1KL	C25-C26-C29	2.89	127.38	121.47
3	A	402	ORO	N3-C2-N1	2.84	120.20	115.74
2	A	401	FMN	C9A-C5A-N5	-2.72	119.57	122.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	410	ACT	OXT-C-CH3	2.62	126.06	115.05
2	A	401	FMN	O4-C4-C4A	-2.58	119.72	126.53
5	A	408	1KL	C2-C1-C8	2.51	127.70	122.02
5	A	408	1KL	O6-C4-C1	2.48	115.81	111.47
2	A	401	FMN	C6-C5A-N5	2.43	122.48	118.44
5	A	408	1KL	C10-C11-S12	-2.17	104.45	107.56
5	A	408	1KL	C28-C23-C24	-2.15	116.18	119.04
2	A	401	FMN	O4'-C4'-C3'	2.15	114.28	109.25
2	A	401	FMN	C4A-C10-N1	-2.15	119.33	124.59
3	A	402	ORO	C6-N1-C2	-2.13	120.37	122.65
4	A	407	SO4	O3-S-O2	-2.12	98.45	109.56
5	A	408	1KL	C32-C29-C30	-2.10	102.11	108.36
2	A	401	FMN	C5A-N5-C4A	2.01	121.33	118.09

There are no chirality outliers.

All (11) 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
3	A	402	ORO	C5-C6-C7-O72
2	A	401	FMN	C2'-C3'-C4'-O4'
2	A	401	FMN	O3'-C3'-C4'-O4'
2	A	401	FMN	O3'-C3'-C4'-C5'
3	A	402	ORO	C5-C6-C7-O71
2	A	401	FMN	C2'-C3'-C4'-C5'
2	A	401	FMN	C4'-C5'-O5'-P
5	A	408	1KL	C25-C26-C29-C30
5	A	408	1KL	C27-C26-C29-C30

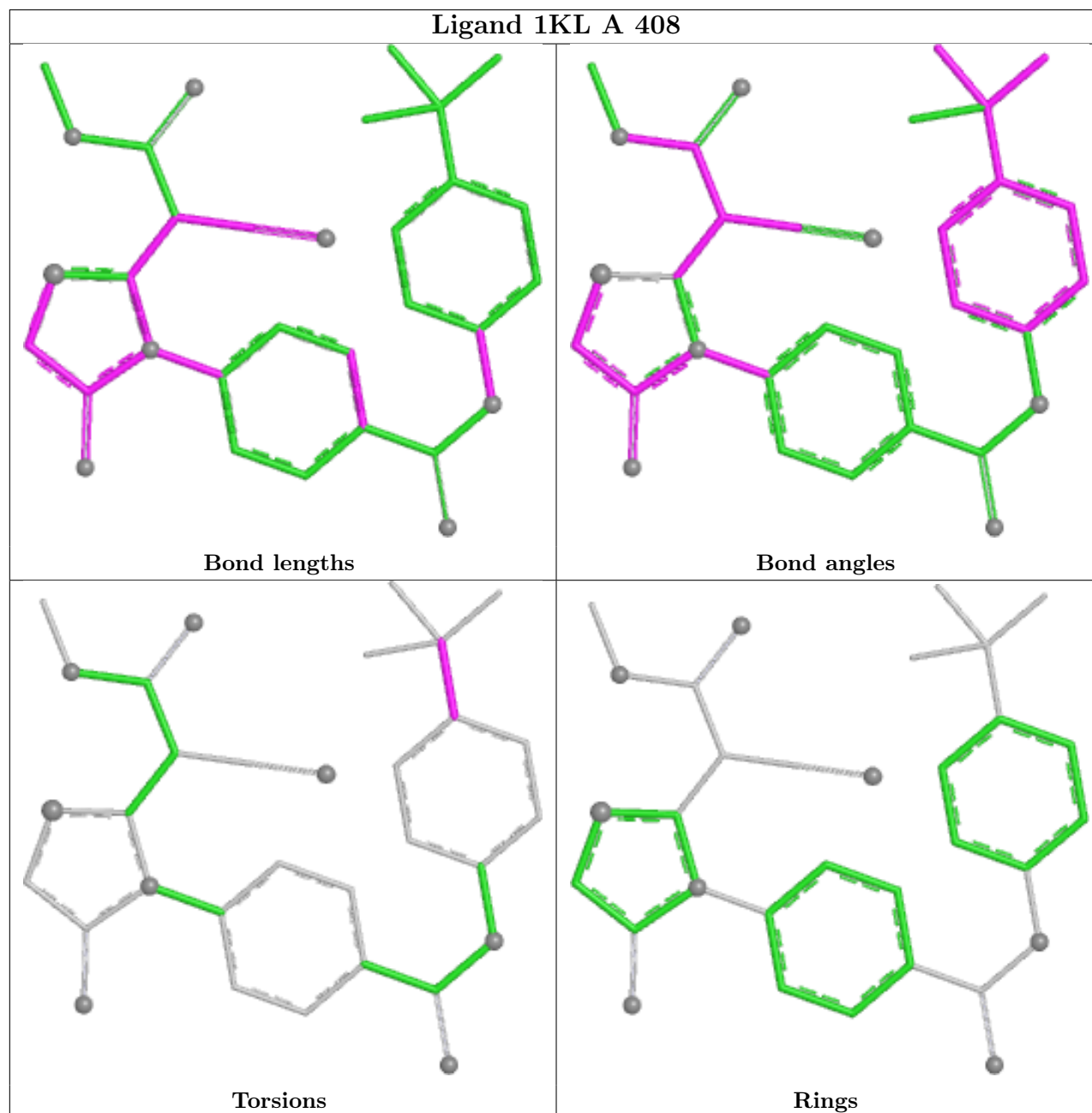
There are no ring outliers.

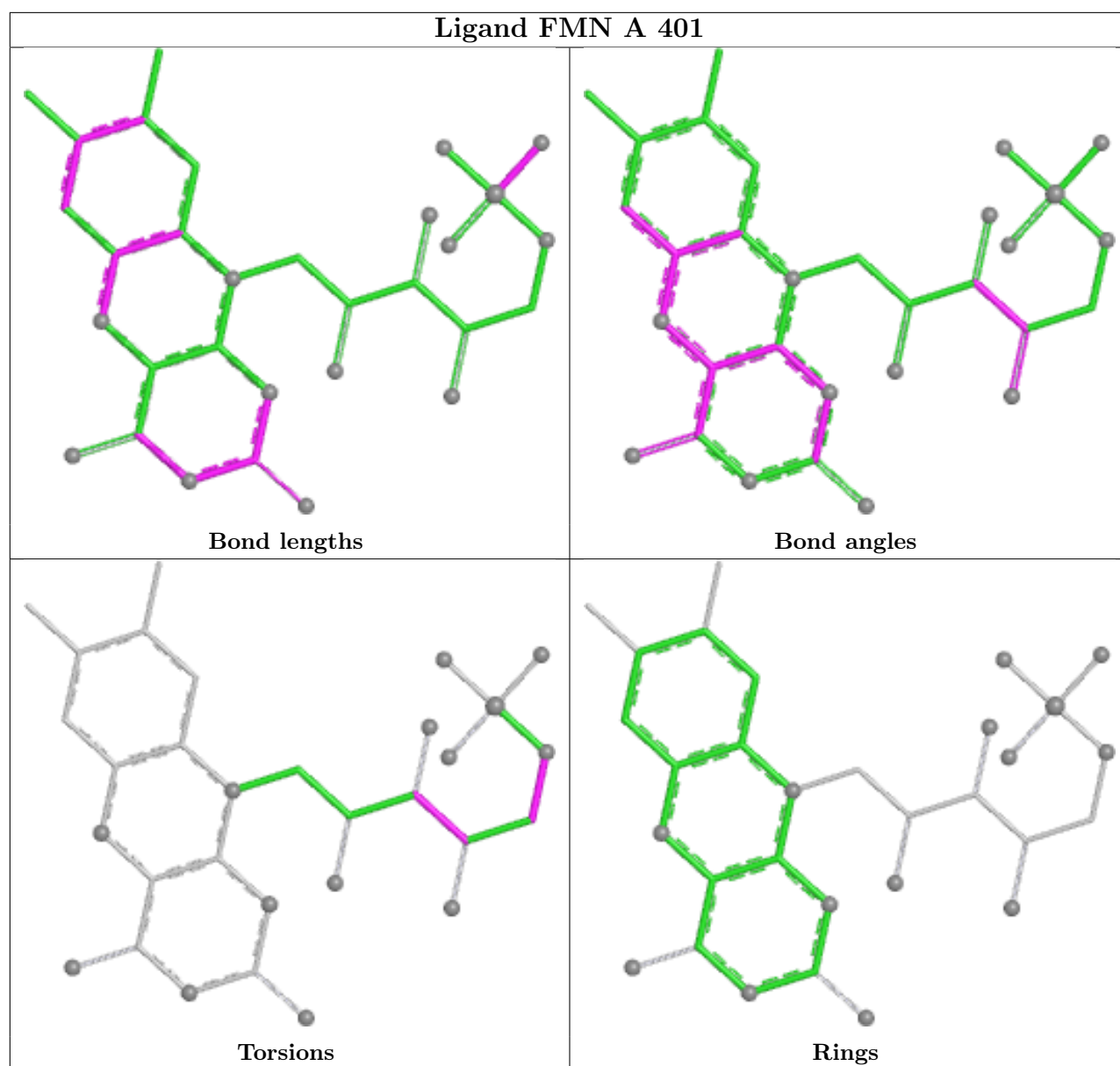
2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	408	1KL	3	0
6	A	410	ACT	4	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	365/390 (93%)	0.34	37 (10%)	12 12	5, 17, 41, 86	7 (1%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	213	VAL	8.1
1	A	226	GLY	7.2
1	A	223	SER	7.1
1	A	72	ARG	6.8
1	A	225	GLN	6.7
1	A	219	ALA	6.0
1	A	224	LEU	5.6
1	A	47	GLN	5.3
1	A	218	THR	5.1
1	A	189	VAL	5.0
1	A	32	THR	4.7
1	A	73	PHE	4.5
1	A	228	ALA	4.1
1	A	221	LEU	3.9
1	A	396	ARG	3.9
1	A	190	ASP	3.4
1	A	229	GLU	3.2
1	A	70	ARG	3.1
1	A	49	LEU	2.9
1	A	215	SER	2.7
1	A	74	GLN	2.7
1	A	247	VAL	2.6
1	A	212	ASN	2.6
1	A	232	ARG	2.6
1	A	41	HIS	2.5
1	A	71	ALA	2.5
1	A	33	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	214	SER	2.3
1	A	187	THR	2.3
1	A	217	ASN	2.2
1	A	50	LEU	2.2
1	A	220	GLY	2.2
1	A	216	PRO	2.2
1	A	42	LEU	2.1
1	A	83	VAL	2.0
1	A	89	ARG	2.0
1	A	227	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

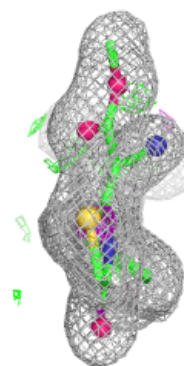
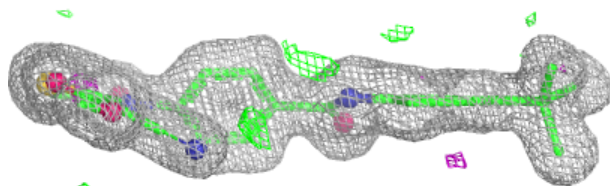
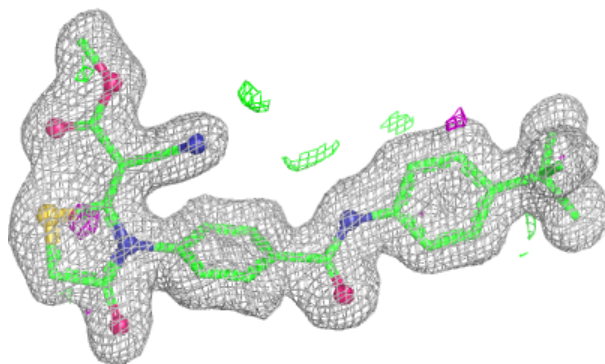
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	ACT	A	409	4/4	0.63	0.27	45,50,51,65	0
4	SO4	A	406	5/5	0.75	0.14	41,70,73,75	0
6	ACT	A	410	4/4	0.77	0.20	23,31,32,38	0
4	SO4	A	404	5/5	0.78	0.17	63,71,80,92	0
4	SO4	A	405	5/5	0.81	0.13	33,50,56,58	0
4	SO4	A	407	5/5	0.81	0.14	53,62,65,72	0
5	1KL	A	408	32/32	0.96	0.07	16,20,31,35	0
3	ORO	A	402	11/11	0.97	0.05	11,11,15,15	0
4	SO4	A	403	5/5	0.98	0.09	26,26,34,37	0
2	FMN	A	401	31/31	0.98	0.05	8,10,12,13	0

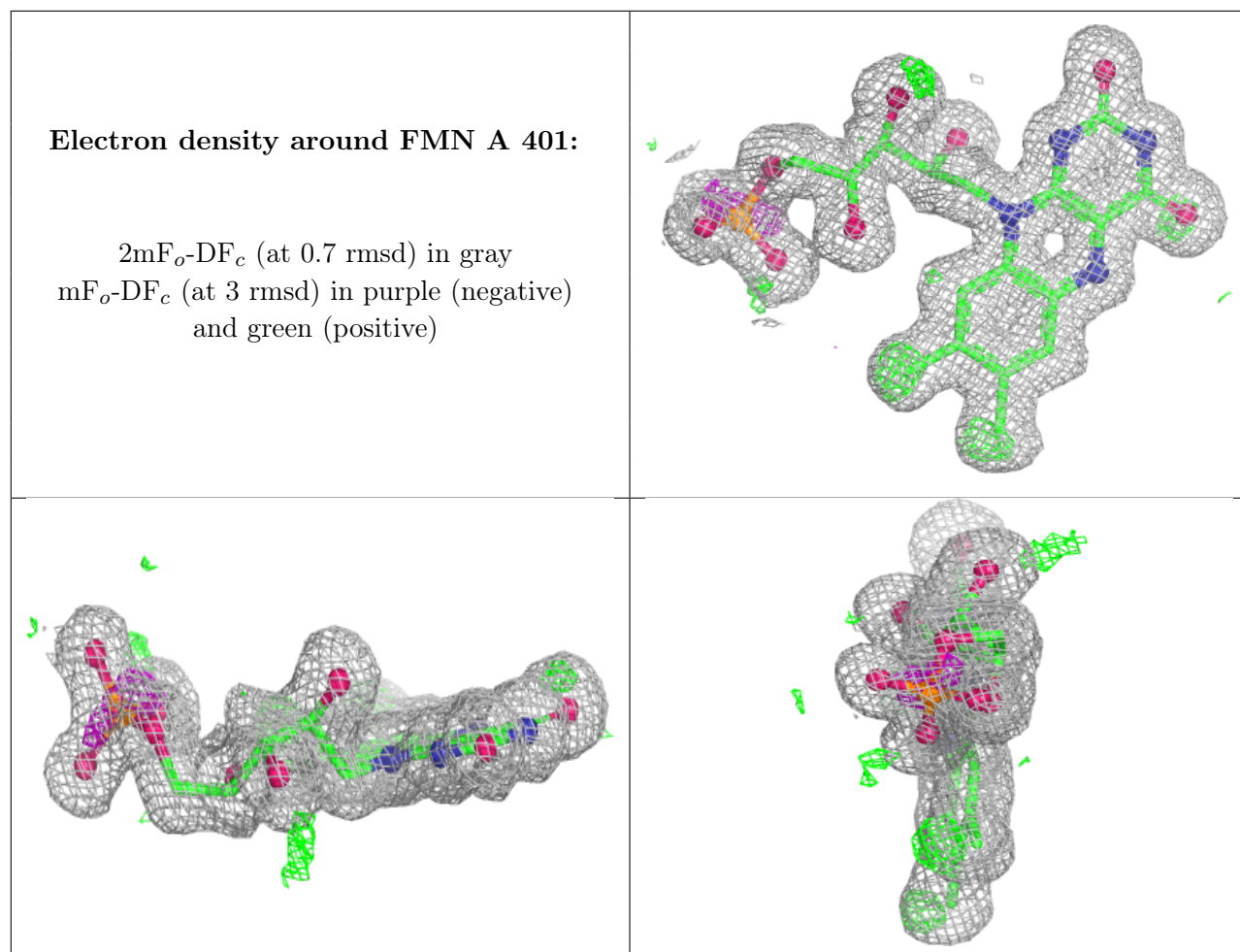
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

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 1KL A 408:

$2mF_o-DF_c$ (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.