



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:46 AM UTC

PDB ID : 4IGH / pdb_00004igh
Title : High resolution crystal structure of human dihydroorotate dehydrogenase bound with 4-quinoline carboxylic acid analog
Authors : Deng, X.; Das, P.; Fontoura, B.M.A.; Phillips, M.A.; De Brabander, J.K.
Deposited on : 2012-12-17
Resolution : 1.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

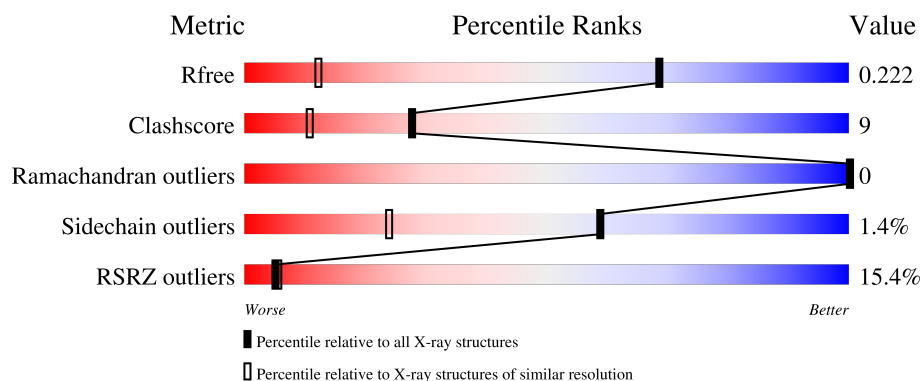
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1553 (1.30-1.30)
Clashscore	190562	1595 (1.30-1.30)
Ramachandran outliers	187476	1551 (1.30-1.30)
Sidechain outliers	187428	1551 (1.30-1.30)
RSRZ outliers	180081	1549 (1.30-1.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	372	15% 55% 36% 5%

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	502	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GOL	A	506	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6321 atoms, of which 3039 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.

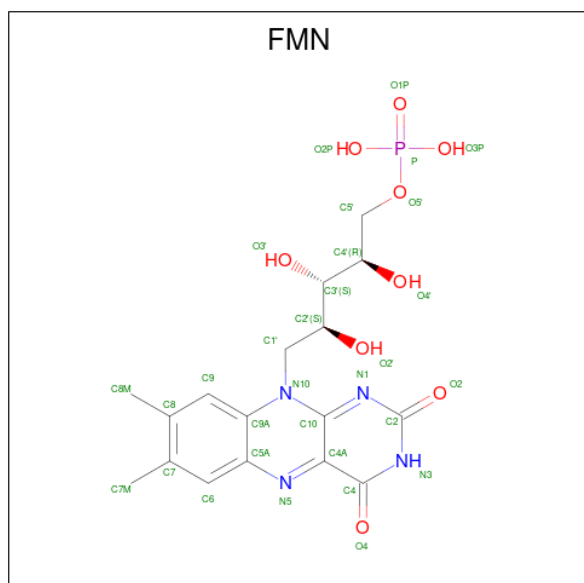
- Molecule 1 is a protein called Dihydroorotate dehydrogenase (quinone), mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	356	5830	1804	2950	530	542	4	853	22	0

There are 8 discrepancies between the modelled and reference sequences:

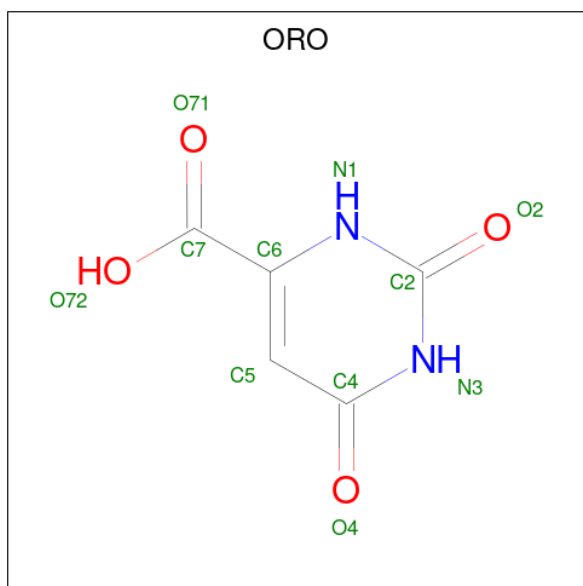
Chain	Residue	Modelled	Actual	Comment	Reference
A	397	LEU	-	expression tag	UNP Q02127
A	398	GLU	-	expression tag	UNP Q02127
A	399	HIS	-	expression tag	UNP Q02127
A	400	HIS	-	expression tag	UNP Q02127
A	401	HIS	-	expression tag	UNP Q02127
A	402	HIS	-	expression tag	UNP Q02127
A	403	HIS	-	expression tag	UNP Q02127
A	404	HIS	-	expression tag	UNP Q02127

- Molecule 2 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



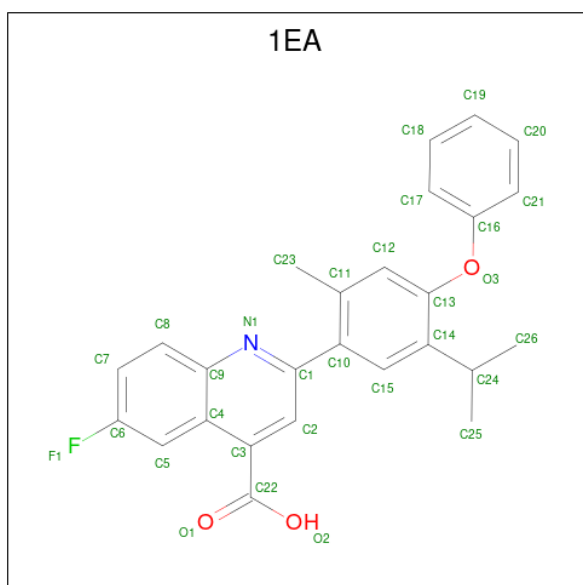
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	
			50	17	19	4	9	1	
								9	0

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



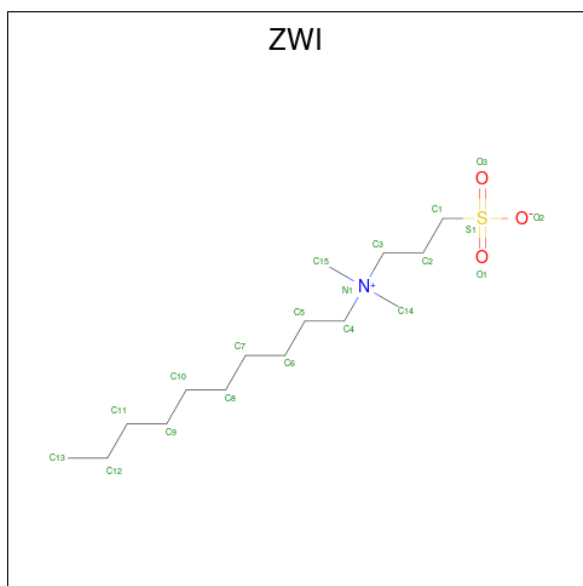
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O		
			14	5	3	2	4		
								0	0

- Molecule 4 is 6-fluoro-2-[2-methyl-4-phenoxy-5-(propan-2-yl)phenyl]quinoline-4-carboxylic acid (CCD ID: 1EA) (formula: $C_{26}H_{22}FNO_3$).



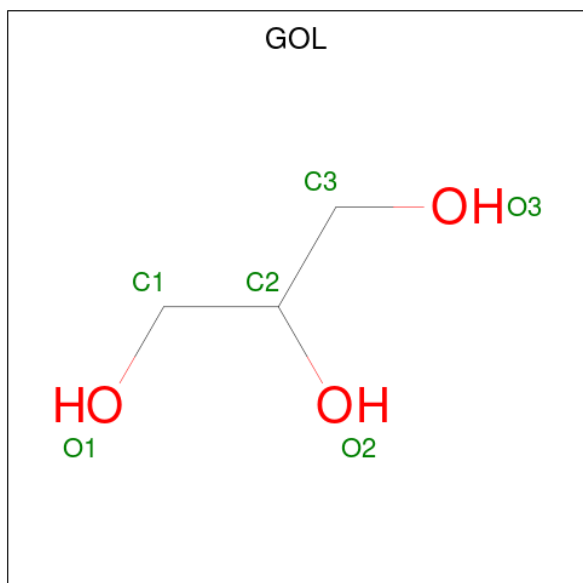
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	H	N	O	
			50	26	1	19	1	3	
								6	0

- Molecule 5 is 3-[decyl(dimethyl)ammonio]propane-1-sulfonate (CCD ID: ZWI) (formula: $C_{15}H_{33}NO_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	S	
			53	15	33	1	3	1	
								9	0

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	1	0
			13	3	7	3		
6	A	1	Total	C	H	O	2	0
			14	3	8	3		

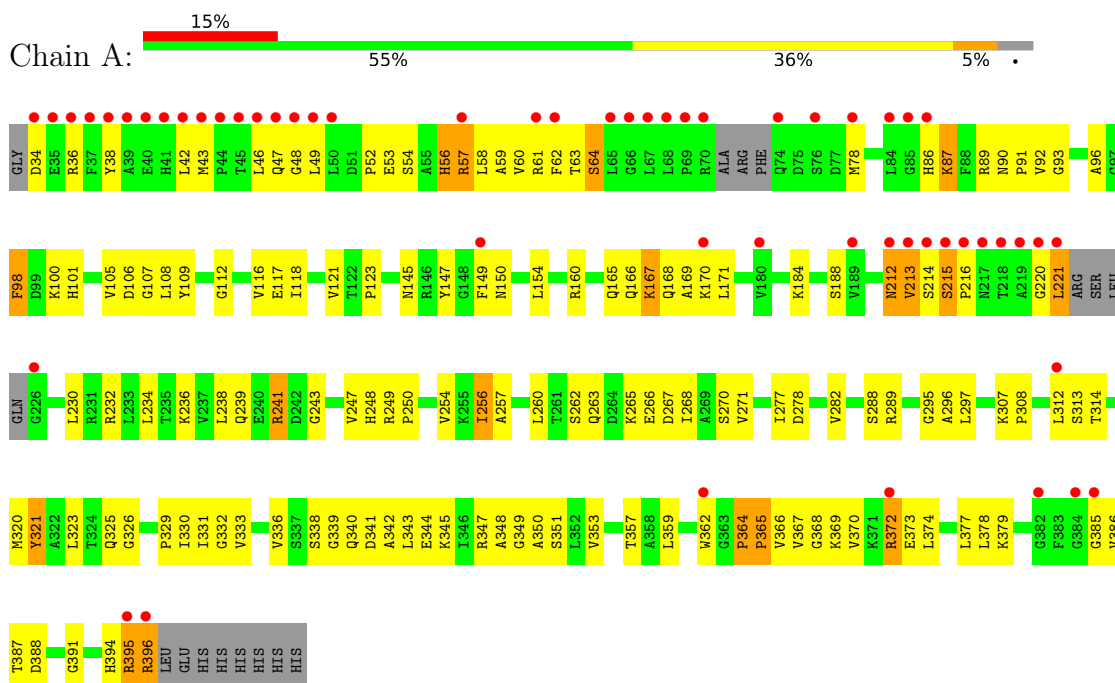
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	297	Total	O	0	0
			297	297		

3 Residue-property plots

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	90.79Å 90.79Å 122.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	78.62 – 1.30 78.62 – 1.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (78.62-1.30) 99.6 (78.62-1.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 1.22Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.138 , 0.148 0.214 , 0.222	Depositor DCC
R_{free} test set	5186 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å ²)	12.2	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.46 , 57.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.016 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6321	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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: FMN, 1EA, GOL, ORO, ZWI

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	2.05	134/2944 (4.6%)	1.28	17/3974 (0.4%)

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	4

All (134) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	64[A]	SER	N-CA	17.20	1.68	1.46
1	A	64[B]	SER	N-CA	17.20	1.68	1.46
1	A	62	PHE	N-CA	11.54	1.60	1.46
1	A	295	GLY	C-O	-10.64	1.12	1.23
1	A	342	ALA	C-O	-10.00	1.12	1.24
1	A	64[A]	SER	CA-C	9.90	1.66	1.52
1	A	64[B]	SER	CA-C	9.90	1.66	1.52
1	A	168	GLN	C-O	-8.80	1.13	1.24
1	A	370	VAL	C-O	-8.50	1.14	1.24
1	A	330	ILE	C-O	-8.17	1.15	1.24
1	A	367	VAL	C-O	-8.11	1.15	1.24
1	A	230	LEU	CA-C	8.01	1.63	1.52
1	A	59	ALA	C-O	-7.58	1.15	1.24
1	A	366	VAL	C-O	-7.49	1.15	1.24
1	A	372	ARG	C-O	-7.48	1.15	1.24
1	A	58	LEU	C-O	-7.47	1.15	1.24
1	A	345	LYS	C-O	-7.41	1.15	1.24
1	A	333	VAL	C-O	-7.40	1.15	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	101	HIS	CG-ND1	-7.30	1.30	1.38
1	A	101	HIS	CD2-NE2	-7.18	1.29	1.37
1	A	339	GLY	C-O	-7.14	1.15	1.23
1	A	106	ASP	C-O	-7.11	1.15	1.24
1	A	263	GLN	C-O	-7.11	1.15	1.24
1	A	332	GLY	C-O	-7.08	1.15	1.23
1	A	357	THR	C-O	-7.05	1.15	1.24
1	A	277	ILE	C-O	-6.91	1.16	1.24
1	A	98	PHE	C-O	-6.80	1.16	1.24
1	A	374	LEU	C-O	-6.79	1.16	1.24
1	A	353	VAL	C-O	-6.78	1.16	1.23
1	A	331	ILE	C-O	-6.77	1.16	1.24
1	A	313[A]	SER	C-O	-6.77	1.16	1.24
1	A	313[B]	SER	C-O	-6.77	1.16	1.24
1	A	243	GLY	C-O	-6.77	1.15	1.23
1	A	340	GLN	C-O	-6.75	1.16	1.24
1	A	86	HIS	CG-ND1	-6.72	1.30	1.38
1	A	238	LEU	C-O	-6.68	1.16	1.24
1	A	296	ALA	C-O	-6.68	1.15	1.24
1	A	329	PRO	C-O	-6.64	1.16	1.23
1	A	385	GLY	C-O	-6.63	1.16	1.23
1	A	260	LEU	C-O	-6.62	1.15	1.23
1	A	60	VAL	CA-C	6.61	1.61	1.52
1	A	248	HIS	CD2-NE2	-6.59	1.30	1.37
1	A	54	SER	C-O	-6.53	1.16	1.24
1	A	165	GLN	C-O	-6.50	1.16	1.24
1	A	368	GLY	C-O	-6.48	1.16	1.23
1	A	307	LYS	C-O	-6.45	1.18	1.24
1	A	267	ASP	C-O	-6.44	1.16	1.24
1	A	270	SER	C-O	-6.41	1.16	1.24
1	A	373	GLU	C-O	-6.38	1.16	1.24
1	A	266	GLU	C-O	-6.38	1.16	1.24
1	A	320	MET	C-O	-6.36	1.16	1.24
1	A	369	LYS	C-O	-6.29	1.16	1.24
1	A	108	LEU	C-O	-6.27	1.16	1.24
1	A	394	HIS	CG-ND1	-6.27	1.31	1.38
1	A	348	ALA	C-O	-6.24	1.16	1.24
1	A	171	LEU	C-O	-6.24	1.16	1.24
1	A	386	VAL	C-O	-6.22	1.16	1.24
1	A	278	ASP	C-O	-6.22	1.16	1.24
1	A	105	VAL	C-O	-6.21	1.17	1.24
1	A	271	VAL	C-O	-6.21	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	160	ARG	CB-CG	-6.20	1.33	1.52
1	A	268	ILE	C-O	-6.17	1.17	1.24
1	A	241	ARG	C-O	-6.16	1.17	1.24
1	A	343	LEU	C-O	-6.14	1.17	1.24
1	A	365	PRO	C-O	-6.14	1.16	1.24
1	A	257	ALA	C-O	-6.13	1.16	1.23
1	A	121	VAL	C-O	-6.05	1.17	1.24
1	A	117	GLU	C-O	-6.03	1.17	1.24
1	A	308	PRO	C-O	-6.03	1.16	1.24
1	A	326	GLY	C-O	-5.99	1.15	1.23
1	A	378	LEU	C-O	-5.98	1.17	1.24
1	A	254	VAL	C-O	-5.97	1.17	1.24
1	A	265	LYS	C-O	-5.97	1.17	1.24
1	A	282	VAL	C-O	-5.89	1.17	1.24
1	A	341	ASP	C-O	-5.88	1.17	1.24
1	A	215	SER	C-N	5.87	1.40	1.34
1	A	167	LYS	C-O	-5.85	1.17	1.24
1	A	57	ARG	C-O	-5.85	1.17	1.24
1	A	170	LYS	C-O	-5.83	1.17	1.24
1	A	56	HIS	CD2-NE2	-5.80	1.31	1.37
1	A	91	PRO	C-O	-5.77	1.17	1.23
1	A	387	THR	C-O	-5.75	1.17	1.24
1	A	43	MET	C-O	-5.75	1.16	1.24
1	A	216	PRO	N-CD	5.72	1.55	1.47
1	A	351	SER	C-O	-5.71	1.16	1.24
1	A	344	GLU	C-O	-5.71	1.17	1.24
1	A	87	LYS	C-O	-5.69	1.17	1.24
1	A	256	ILE	C-O	-5.68	1.17	1.23
1	A	323	LEU	C-O	-5.66	1.17	1.24
1	A	86	HIS	C-O	-5.65	1.17	1.24
1	A	391	GLY	C-O	-5.59	1.16	1.23
1	A	118	ILE	C-O	-5.58	1.17	1.23
1	A	350	ALA	C-O	-5.56	1.17	1.24
1	A	250	PRO	C-O	-5.54	1.17	1.23
1	A	364	PRO	C-O	-5.49	1.18	1.24
1	A	239	GLN	C-O	-5.47	1.17	1.24
1	A	321	TYR	C-O	-5.46	1.17	1.24
1	A	100	LYS	C-O	-5.46	1.17	1.24
1	A	377	LEU	C-O	-5.46	1.17	1.24
1	A	53	GLU	C-O	-5.45	1.17	1.24
1	A	48	GLY	C-O	-5.42	1.17	1.23
1	A	289	ARG	C-O	-5.42	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	247	VAL	C-O	-5.42	1.17	1.24
1	A	93	GLY	C-O	-5.42	1.16	1.23
1	A	314	THR	C-O	-5.40	1.17	1.24
1	A	312[A]	LEU	C-O	-5.39	1.17	1.24
1	A	312[B]	LEU	C-O	-5.39	1.17	1.24
1	A	109	TYR	C-O	-5.37	1.17	1.24
1	A	347[A]	ARG	C-O	-5.37	1.17	1.24
1	A	347[B]	ARG	C-O	-5.37	1.17	1.24
1	A	92	VAL	C-O	-5.35	1.18	1.24
1	A	312[A]	LEU	N-CA	5.33	1.52	1.46
1	A	312[B]	LEU	N-CA	5.33	1.52	1.46
1	A	248	HIS	CG-ND1	-5.32	1.32	1.38
1	A	169	ALA	C-O	-5.32	1.17	1.24
1	A	297	LEU	C-O	-5.30	1.17	1.24
1	A	338	SER	C-O	-5.29	1.17	1.23
1	A	38	TYR	C-O	-5.28	1.18	1.24
1	A	116	VAL	C-O	-5.28	1.18	1.24
1	A	359	LEU	C-O	-5.20	1.17	1.24
1	A	52	PRO	C-O	-5.20	1.17	1.24
1	A	107	GLY	C-O	-5.15	1.17	1.23
1	A	249	ARG	C-O	-5.14	1.17	1.24
1	A	262	SER	C-O	-5.13	1.18	1.24
1	A	112	GLY	C-O	-5.10	1.17	1.24
1	A	166	GLN	C-O	-5.09	1.18	1.24
1	A	234	LEU	C-O	-5.08	1.18	1.24
1	A	60	VAL	C-O	-5.06	1.18	1.24
1	A	336	VAL	C-O	-5.05	1.18	1.24
1	A	96	ALA	C-O	-5.04	1.17	1.23
1	A	325	GLN	C-O	-5.04	1.16	1.23
1	A	349	GLY	C-O	-5.03	1.17	1.23
1	A	288	SER	C-O	-5.03	1.17	1.23
1	A	90	ASN	C-O	-5.03	1.19	1.24

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	387	THR	O-C-N	9.56	132.26	122.12
1	A	395	ARG	N-CA-C	7.82	124.90	113.40
1	A	388[A]	ASP	CA-C-O	7.20	128.23	119.38
1	A	388[B]	ASP	CA-C-O	7.20	128.23	119.38
1	A	49	LEU	N-CA-C	7.03	119.97	111.82
1	A	64[A]	SER	CA-C-O	6.97	127.98	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64[B]	SER	CA-C-O	6.97	127.98	120.10
1	A	232	ARG	NE-CZ-NH1	6.31	127.81	121.50
1	A	60	VAL	N-CA-C	-6.25	104.24	110.62
1	A	215	SER	CA-C-N	-6.20	113.35	120.04
1	A	215	SER	C-N-CA	-6.20	113.35	120.04
1	A	394	HIS	CA-C-N	6.12	133.36	123.93
1	A	394	HIS	C-N-CA	6.12	133.36	123.93
1	A	278	ASP	N-CA-C	5.19	117.02	111.36
1	A	42	LEU	N-CA-C	5.18	116.61	111.07
1	A	47	GLN	CA-CB-CG	5.14	124.37	114.10
1	A	220	GLY	N-CA-C	5.00	121.04	115.08

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	212[A]	ASN	Mainchain
1	A	213[A]	VAL	Peptide,Mainchain
1	A	213[B]	VAL	Mainchain

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	2880	2950	2929	54	0
2	A	31	19	19	0	0
3	A	11	3	3	1	0
4	A	31	19	20	2	0
5	A	20	33	33	0	0
6	A	12	15	16	4	0
7	A	297	0	0	7	0
All	All	3282	3039	3020	54	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 (54) 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:149[A]:PHE:CZ	1:A:215:SER:HB2	1.91	1.05
1:A:149[A]:PHE:HZ	1:A:215:SER:HB2	1.17	1.05
1:A:149[A]:PHE:CZ	1:A:215:SER:CB	2.50	0.94
1:A:46:LEU:HD13	4:A:503:1EA:H251	1.53	0.91
1:A:149[A]:PHE:HZ	1:A:215:SER:CB	1.90	0.84
1:A:213[A]:VAL:HG22	1:A:214:SER:HB3	1.59	0.83
1:A:213[A]:VAL:CG2	1:A:214:SER:HB3	2.09	0.83
1:A:150:ASN:HD21	6:A:506:GOL:H12	1.47	0.79
1:A:149[A]:PHE:CE1	1:A:215:SER:CB	2.66	0.78
1:A:46:LEU:HD13	4:A:503:1EA:C25	2.15	0.76
1:A:87:LYS:NZ	1:A:89[A]:ARG:HG2	2.02	0.74
1:A:145:ASN:OD1	3:A:502:ORO:H5	1.91	0.70
1:A:149[A]:PHE:CE1	1:A:215:SER:OG	2.47	0.67
1:A:61[B]:ARG:HD2	7:A:714:HOH:O	1.95	0.67
1:A:184[B]:LYS:HE2	1:A:188[B]:SER:HB3	1.76	0.67
1:A:57:ARG:CZ	6:A:506:GOL:O3	2.43	0.66
1:A:213[A]:VAL:O	1:A:221:LEU:HG	1.96	0.65
1:A:34:ASP:N	7:A:870:HOH:O	2.29	0.65
1:A:213[B]:VAL:HG22	1:A:213[B]:VAL:O	2.01	0.60
1:A:150:ASN:ND2	6:A:506:GOL:H12	2.16	0.60
1:A:149[A]:PHE:HE1	1:A:215:SER:OG	1.85	0.58
1:A:56:HIS:HD2	1:A:147:TYR:OH	1.88	0.56
1:A:236:LYS:HE3	7:A:769:HOH:O	2.05	0.55
1:A:154:LEU:HD21	7:A:871:HOH:O	2.07	0.54
1:A:213[A]:VAL:HG23	1:A:214:SER:HB3	1.89	0.52
1:A:61[B]:ARG:HA	1:A:61[B]:ARG:NE	2.25	0.52
1:A:57:ARG:NE	6:A:506:GOL:O3	2.44	0.51
1:A:362:TRP:HE3	7:A:728:HOH:O	1.94	0.50
1:A:213[A]:VAL:HG23	1:A:214:SER:CA	2.41	0.50
1:A:123:PRO:HA	1:A:154:LEU:HG	1.95	0.49
1:A:396:ARG:HD2	1:A:396:ARG:C	2.38	0.49
1:A:56:HIS:HE1	1:A:98:PHE:O	1.96	0.47
1:A:213[B]:VAL:HG22	1:A:221:LEU:O	2.16	0.47
1:A:149[A]:PHE:HE1	1:A:215:SER:CB	2.23	0.46
1:A:241:ARG:HD2	1:A:241:ARG:C	2.41	0.46
1:A:213[A]:VAL:HG22	1:A:256:ILE:HA	1.97	0.46
1:A:321:TYR:OH	1:A:396:ARG:HD3	2.17	0.45
1:A:149[A]:PHE:CZ	1:A:215:SER:HB3	2.50	0.44
1:A:213[B]:VAL:O	1:A:213[B]:VAL:HG13	2.18	0.44
1:A:56:HIS:CD2	1:A:147:TYR:OH	2.70	0.43
1:A:213[A]:VAL:HG23	1:A:214:SER:CB	2.49	0.42
1:A:372:ARG:HG2	7:A:874:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149[A]:PHE:CE1	1:A:215:SER:HB3	2.54	0.42
1:A:167:LYS:NZ	7:A:837:HOH:O	2.52	0.42
1:A:396:ARG:C	1:A:396:ARG:CD	2.93	0.41
1:A:364:PRO:N	1:A:365:PRO:CD	2.84	0.41
1:A:78:MET:SD	1:A:379:LYS:HE3	2.60	0.41
1:A:63:THR:C	1:A:64[A]:SER:CA	2.75	0.41
1:A:213[B]:VAL:CG2	1:A:221:LEU:O	2.69	0.41
1:A:221:LEU:O	1:A:221:LEU:HD23	2.21	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	372/372 (100%)	365 (98%)	7 (2%)	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	310/302 (103%)	306 (99%)	4 (1%)	61	26

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

Mol	Chain	Res	Type
1	A	36	ARG
1	A	221	LEU
1	A	395	ARG
1	A	396	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	HIS
1	A	166	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 [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	$\# Z > 2$
2	FMN	A	501	-	33,33,33	1.53	8 (24%)	48,50,50	1.42	8 (16%)
6	GOL	A	506	-	5,5,5	0.54	0	5,5,5	1.50	1 (20%)
4	1EA	A	503	-	34,34,34	2.63	12 (35%)	48,49,49	2.00	13 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GOL	A	505	-	5,5,5	1.26	0	5,5,5	2.25	2 (40%)
5	ZWI	A	504	-	19,19,19	2.22	1 (5%)	24,24,24	1.59	6 (25%)
3	ORO	A	502	-	11,11,11	1.85	4 (36%)	14,15,15	2.77	7 (50%)

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
2	FMN	A	501	-	-	5/18/18/18	0/3/3/3
6	GOL	A	506	-	-	1/4/4/4	-
4	1EA	A	503	-	-	2/16/16/16	0/4/4/4
6	GOL	A	505	-	-	1/4/4/4	-
5	ZWI	A	504	-	-	3/19/19/19	-
3	ORO	A	502	-	-	4/4/4/4	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	1EA	C25-C24	-10.63	1.29	1.53
5	A	504	ZWI	C1-S1	-8.94	1.65	1.77
4	A	503	1EA	C4-C9	3.95	1.48	1.42
4	A	503	1EA	F1-C6	-3.55	1.27	1.36
2	A	501	FMN	C5A-N5	-3.46	1.33	1.39
3	A	502	ORO	O72-C7	-3.35	1.21	1.30
4	A	503	1EA	C10-C11	3.34	1.46	1.40
4	A	503	1EA	O3-C16	-3.25	1.32	1.39
3	A	502	ORO	C6-N1	-3.16	1.32	1.38
4	A	503	1EA	C13-C14	3.01	1.45	1.39
4	A	503	1EA	C26-C24	-2.91	1.46	1.53
4	A	503	1EA	O2-C22	-2.78	1.22	1.30
2	A	501	FMN	C4-N3	-2.71	1.33	1.38
4	A	503	1EA	C18-C17	-2.70	1.34	1.38
2	A	501	FMN	C9A-C5A	2.68	1.45	1.41
2	A	501	FMN	C6-C7	-2.66	1.36	1.39
4	A	503	1EA	C3-C4	2.60	1.47	1.42
2	A	501	FMN	C2-N3	-2.49	1.33	1.39
2	A	501	FMN	C9-C9A	-2.37	1.35	1.39
3	A	502	ORO	C4-N3	-2.34	1.34	1.38
3	A	502	ORO	C5-C4	-2.33	1.37	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	1EA	C9-N1	-2.22	1.34	1.37
2	A	501	FMN	O2-C2	-2.21	1.20	1.24
4	A	503	1EA	C20-C21	-2.07	1.35	1.38
2	A	501	FMN	C4A-N5	2.02	1.35	1.30

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	1EA	C25-C24-C14	8.33	126.08	111.71
3	A	502	ORO	O71-C7-C6	-4.56	111.75	121.01
2	A	501	FMN	C4-C4A-N5	4.37	124.24	118.21
3	A	502	ORO	C7-C6-N1	4.31	123.35	115.47
3	A	502	ORO	O4-C4-C5	-4.28	119.55	125.46
4	A	503	1EA	C25-C24-C26	4.01	118.49	110.23
5	A	504	ZWI	C4-C5-C6	3.63	126.43	110.81
3	A	502	ORO	O72-C7-C6	3.62	122.08	114.27
4	A	503	1EA	C13-C14-C24	3.53	126.30	120.94
6	A	505	GOL	O2-C2-C1	-3.51	94.65	109.18
6	A	505	GOL	C3-C2-C1	-3.46	99.10	111.80
4	A	503	1EA	C13-O3-C16	3.22	125.76	117.95
3	A	502	ORO	C4-N3-C2	-2.97	122.67	125.55
5	A	504	ZWI	O2-S1-C1	2.93	111.73	106.00
3	A	502	ORO	O2-C2-N3	-2.90	116.71	121.86
5	A	504	ZWI	C7-C6-C5	2.77	128.38	114.37
2	A	501	FMN	O4-C4-C4A	-2.73	119.33	126.53
6	A	506	GOL	O3-C3-C2	2.64	122.27	110.38
4	A	503	1EA	C2-C1-C10	-2.64	116.98	121.98
4	A	503	1EA	C15-C14-C24	-2.60	113.59	118.87
4	A	503	1EA	C6-C5-C4	2.59	120.79	118.75
4	A	503	1EA	O1-C22-C3	-2.51	115.78	122.31
2	A	501	FMN	C5A-C9A-N10	2.51	120.23	117.97
5	A	504	ZWI	O1-S1-O3	-2.42	105.94	113.82
4	A	503	1EA	C8-C9-C4	-2.42	116.53	119.13
2	A	501	FMN	C9A-C5A-N5	-2.42	119.89	122.45
4	A	503	1EA	C8-C7-C6	2.36	121.30	118.68
4	A	503	1EA	C12-C13-C14	-2.34	118.40	121.86
2	A	501	FMN	O2-C2-N1	-2.30	117.97	121.80
3	A	502	ORO	O4-C4-N3	2.30	122.61	119.27
4	A	503	1EA	C1-N1-C9	2.27	119.90	118.12
4	A	503	1EA	C7-C6-C5	-2.23	120.73	123.32
2	A	501	FMN	C9A-C9-C8	2.17	123.58	119.22
2	A	501	FMN	C4-C4A-C10	-2.16	113.23	116.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	504	ZWI	O3-S1-C1	-2.15	103.47	106.73
5	A	504	ZWI	C15-N1-C3	-2.15	103.64	109.49
2	A	501	FMN	C4A-C4-N3	2.05	118.48	113.25

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	ORO	N1-C6-C7-O71
3	A	502	ORO	N1-C6-C7-O72
4	A	503	1EA	C15-C14-C24-C26
4	A	503	1EA	C13-C14-C24-C26
2	A	501	FMN	C2'-C3'-C4'-O4'
6	A	506	GOL	C1-C2-C3-O3
6	A	505	GOL	O1-C1-C2-O2
5	A	504	ZWI	C8-C10-C9-C11
2	A	501	FMN	O3'-C3'-C4'-O4'
2	A	501	FMN	C2'-C3'-C4'-C5'
2	A	501	FMN	C4'-C5'-O5'-P
5	A	504	ZWI	C5-C6-C7-C8
2	A	501	FMN	O3'-C3'-C4'-C5'
5	A	504	ZWI	C4-C5-C6-C7
3	A	502	ORO	C5-C6-C7-O71
3	A	502	ORO	C5-C6-C7-O72

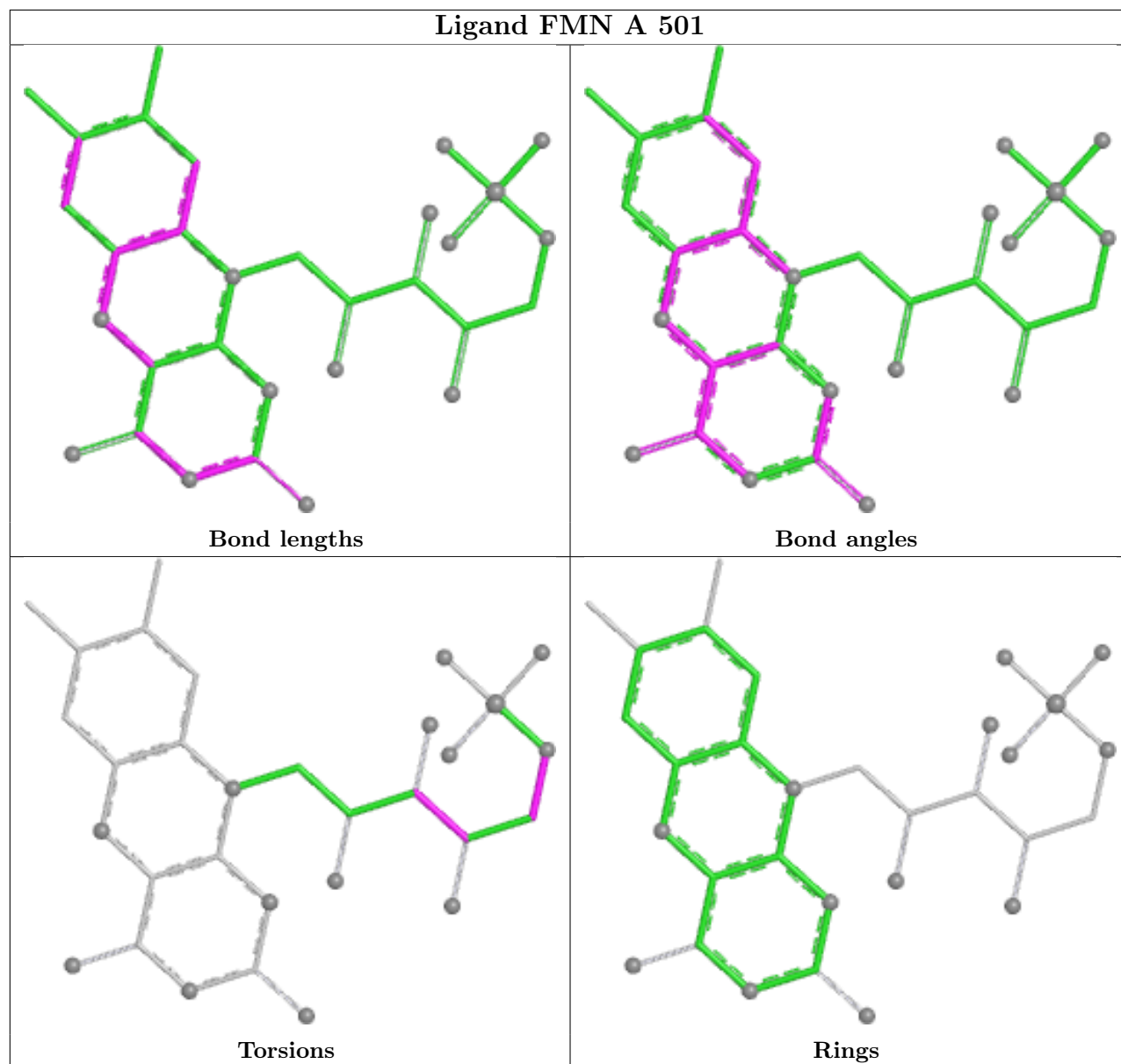
There are no ring outliers.

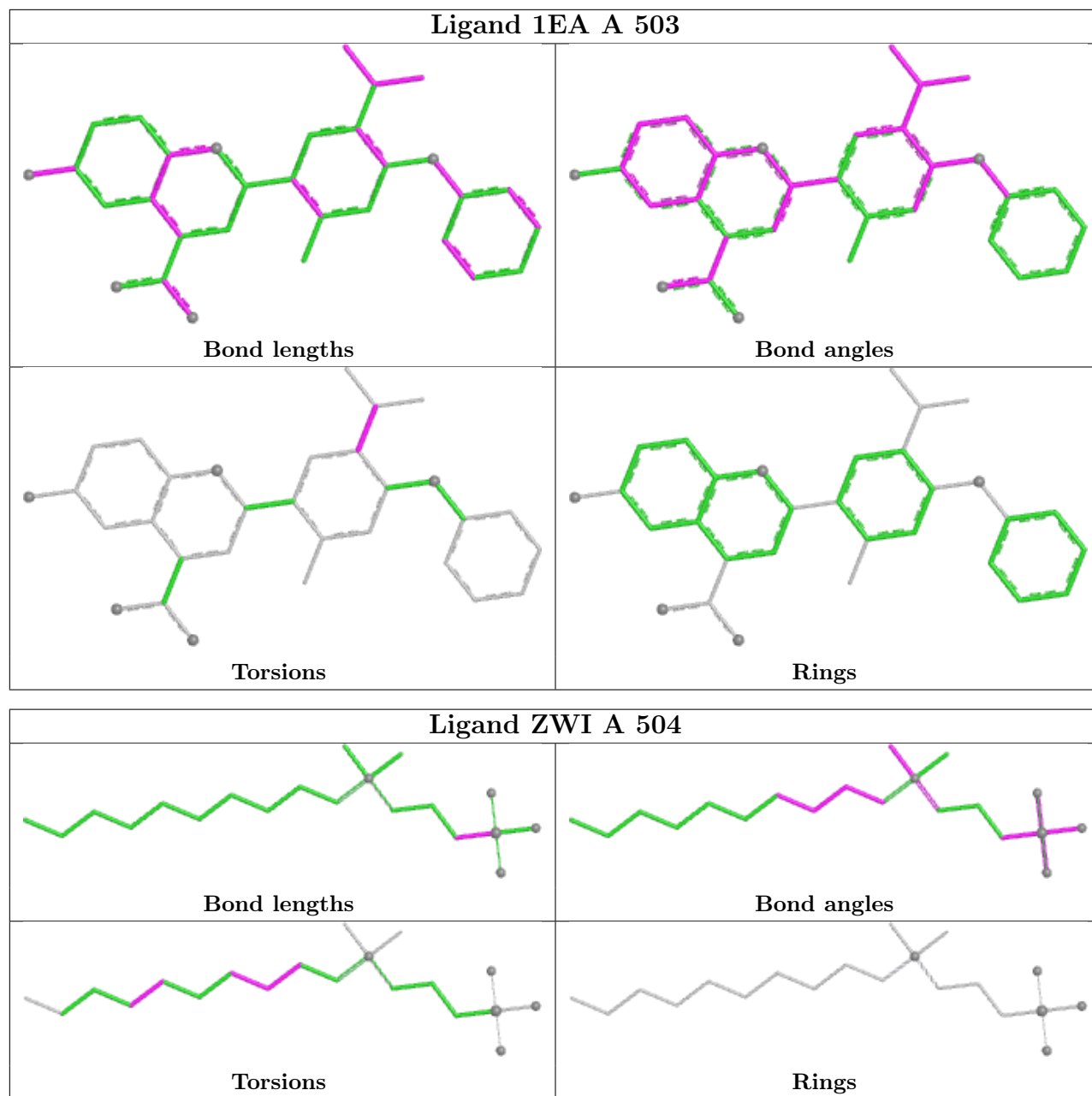
3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	506	GOL	4	0
4	A	503	1EA	2	0
3	A	502	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	356/372 (95%)	1.00	55 (15%) 5 5	3, 7, 24, 86	22 (6%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	213[A]	VAL	13.7
1	A	37	PHE	7.7
1	A	221	LEU	7.1
1	A	45	THR	7.0
1	A	46	LEU	7.0
1	A	189	VAL	6.6
1	A	84	LEU	6.2
1	A	218	THR	5.7
1	A	42	LEU	5.7
1	A	396	ARG	5.7
1	A	38	TYR	5.7
1	A	39	ALA	5.6
1	A	226	GLY	5.6
1	A	395	ARG	5.4
1	A	44	PRO	4.9
1	A	41	HIS	4.8
1	A	36	ARG	4.7
1	A	219	ALA	4.7
1	A	220	GLY	4.7
1	A	43	MET	4.5
1	A	68	LEU	4.5
1	A	215	SER	4.5
1	A	69	PRO	4.1
1	A	61[A]	ARG	4.0
1	A	217	ASN	3.8
1	A	212[A]	ASN	3.7
1	A	34	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	35	GLU	3.7
1	A	70	ARG	3.6
1	A	372	ARG	3.4
1	A	40	GLU	3.3
1	A	214	SER	3.3
1	A	149[A]	PHE	3.3
1	A	48	GLY	3.2
1	A	65	LEU	3.2
1	A	74	GLN	3.1
1	A	170	LYS	3.0
1	A	382	GLY	2.6
1	A	384	GLY	2.6
1	A	49	LEU	2.5
1	A	76	SER	2.4
1	A	67	LEU	2.4
1	A	47	GLN	2.4
1	A	66	GLY	2.4
1	A	86	HIS	2.3
1	A	85	GLY	2.2
1	A	78	MET	2.2
1	A	50	LEU	2.2
1	A	57	ARG	2.2
1	A	216	PRO	2.2
1	A	385	GLY	2.1
1	A	312[A]	LEU	2.1
1	A	180	VAL	2.1
1	A	62	PHE	2.0
1	A	362	TRP	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,

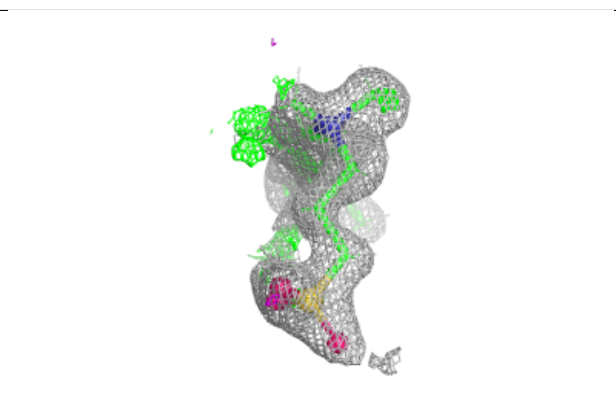
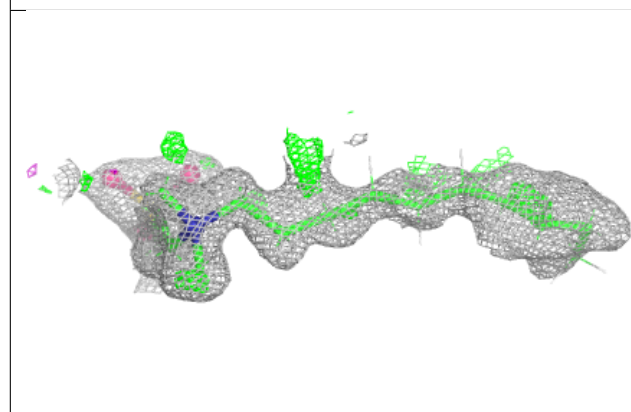
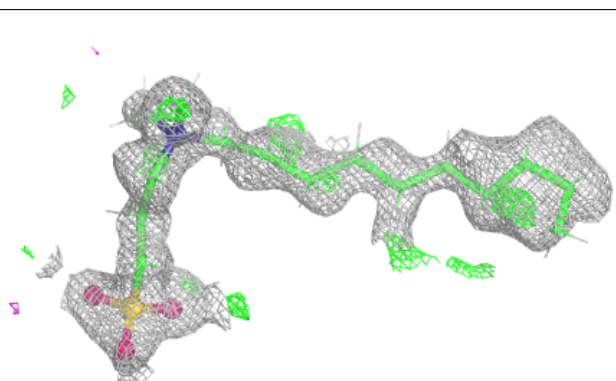
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	GOL	A	506	6/6	0.83	0.20	13,25,60,64	2
5	ZWI	A	504	20/20	0.85	0.18	14,34,62,103	9
6	GOL	A	505	6/6	0.94	0.12	11,26,35,55	1
3	ORO	A	502	11/11	0.95	0.10	7,9,12,12	0
4	1EA	A	503	31/31	0.96	0.10	10,18,32,33	6
2	FMN	A	501	31/31	0.96	0.10	7,8,18,18	9

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.

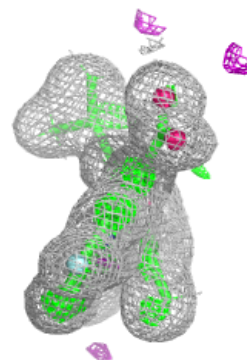
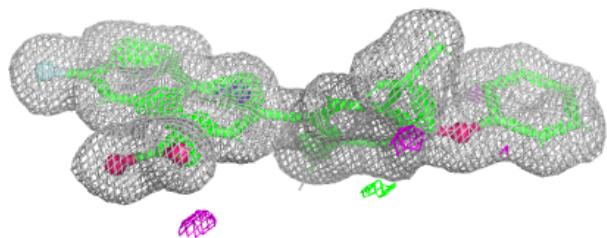
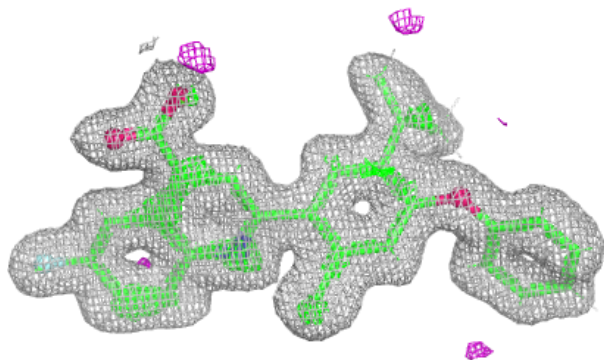
Electron density around ZWI A 504:

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



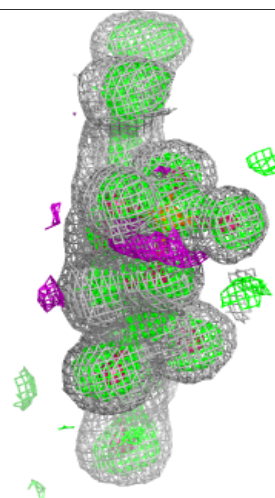
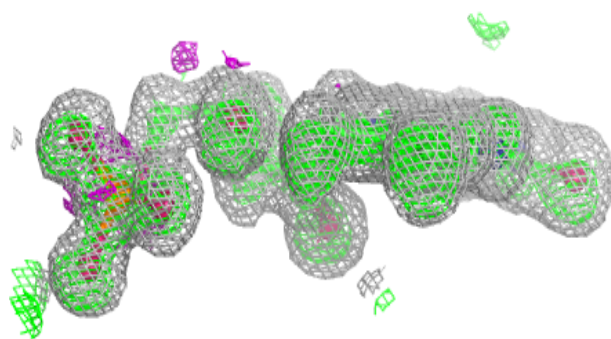
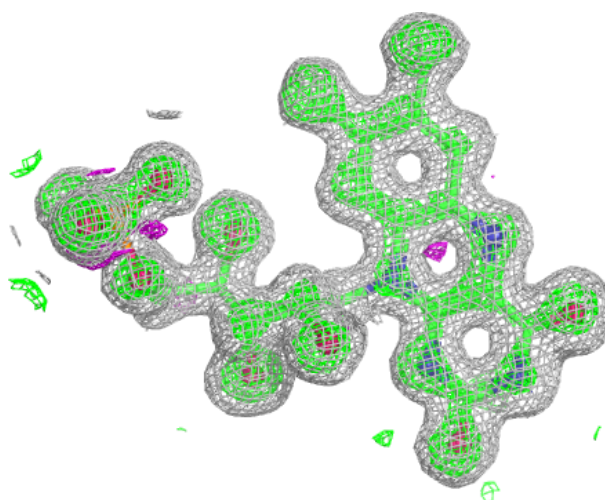
Electron density around 1EA A 503:

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



Electron density around FMN A 501:

$2mF_o-DF_c$ (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.