



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:04 AM UTC

PDB ID : 7CU2 / pdb_00007cu2
Title : CRYSTAL STRUCTURE OF STREPTOMYCES ALBOGRISEOLUS
FLAVIN-DEPENDENT TRYPTOPHAN 6-HALOGENASE THAL IN
COMPLEX WITH REDUCED FAD
Authors : Chitnumsub, P.; Jaruwat, A.; Phintha, A.; Chaiyen, P.
Deposited on : 2020-08-20
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 types of validation reports are described at

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

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

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

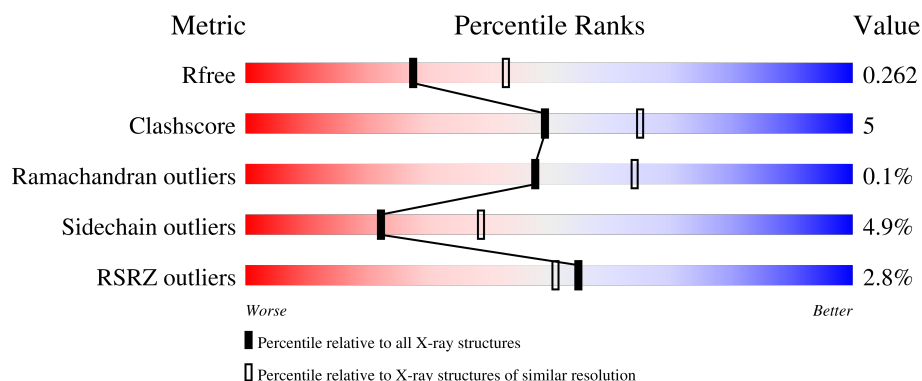
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 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	551	
1	B	551	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8798 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 Tryptophan 6-halogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	522	Total	C	N	O	S	0	0	0
			4160	2656	716	767	21			
1	B	520	Total	C	N	O	S	0	0	0
			4149	2650	714	764	21			

There are 40 discrepancies between the modelled and reference sequences:

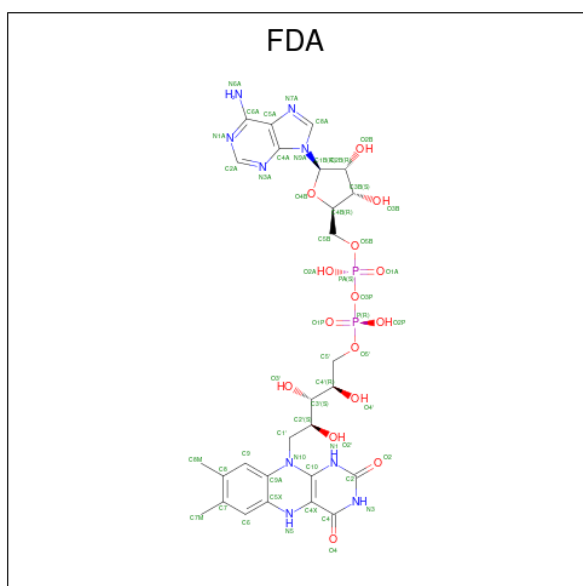
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP A1E280
A	-18	GLY	-	expression tag	UNP A1E280
A	-17	SER	-	expression tag	UNP A1E280
A	-16	SER	-	expression tag	UNP A1E280
A	-15	HIS	-	expression tag	UNP A1E280
A	-14	HIS	-	expression tag	UNP A1E280
A	-13	HIS	-	expression tag	UNP A1E280
A	-12	HIS	-	expression tag	UNP A1E280
A	-11	HIS	-	expression tag	UNP A1E280
A	-10	HIS	-	expression tag	UNP A1E280
A	-9	SER	-	expression tag	UNP A1E280
A	-8	SER	-	expression tag	UNP A1E280
A	-7	GLY	-	expression tag	UNP A1E280
A	-6	LEU	-	expression tag	UNP A1E280
A	-5	VAL	-	expression tag	UNP A1E280
A	-4	PRO	-	expression tag	UNP A1E280
A	-3	ARG	-	expression tag	UNP A1E280
A	-2	GLY	-	expression tag	UNP A1E280
A	-1	SER	-	expression tag	UNP A1E280
A	0	HIS	-	expression tag	UNP A1E280
B	-19	MET	-	expression tag	UNP A1E280
B	-18	GLY	-	expression tag	UNP A1E280
B	-17	SER	-	expression tag	UNP A1E280
B	-16	SER	-	expression tag	UNP A1E280
B	-15	HIS	-	expression tag	UNP A1E280

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP A1E280
B	-13	HIS	-	expression tag	UNP A1E280
B	-12	HIS	-	expression tag	UNP A1E280
B	-11	HIS	-	expression tag	UNP A1E280
B	-10	HIS	-	expression tag	UNP A1E280
B	-9	SER	-	expression tag	UNP A1E280
B	-8	SER	-	expression tag	UNP A1E280
B	-7	GLY	-	expression tag	UNP A1E280
B	-6	LEU	-	expression tag	UNP A1E280
B	-5	VAL	-	expression tag	UNP A1E280
B	-4	PRO	-	expression tag	UNP A1E280
B	-3	ARG	-	expression tag	UNP A1E280
B	-2	GLY	-	expression tag	UNP A1E280
B	-1	SER	-	expression tag	UNP A1E280
B	0	HIS	-	expression tag	UNP A1E280

- Molecule 2 is DIHYDROFLAVINE-ADENINE DINUCLEOTIDE (CCD ID: FDA) (formula: $C_{27}H_{35}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



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

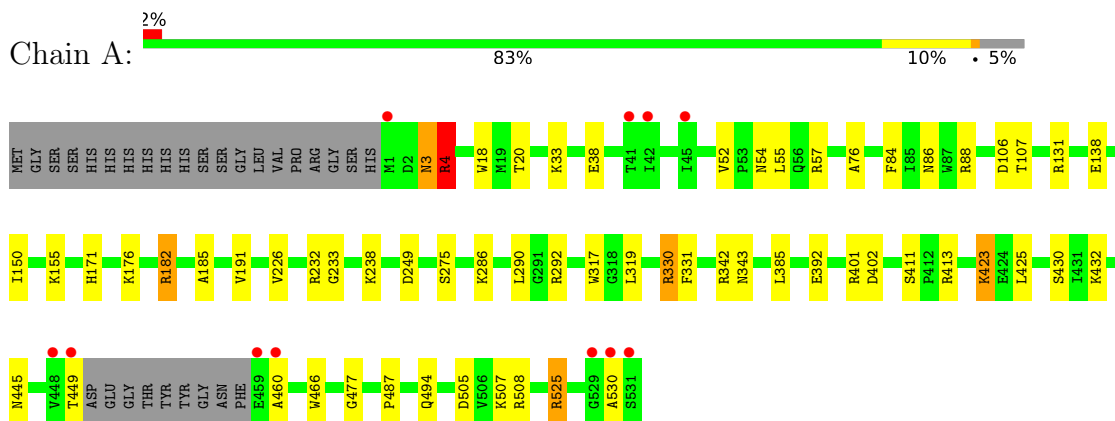
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	240	Total 240	O 240	0	0
3	B	143	Total 143	O 143	0	0

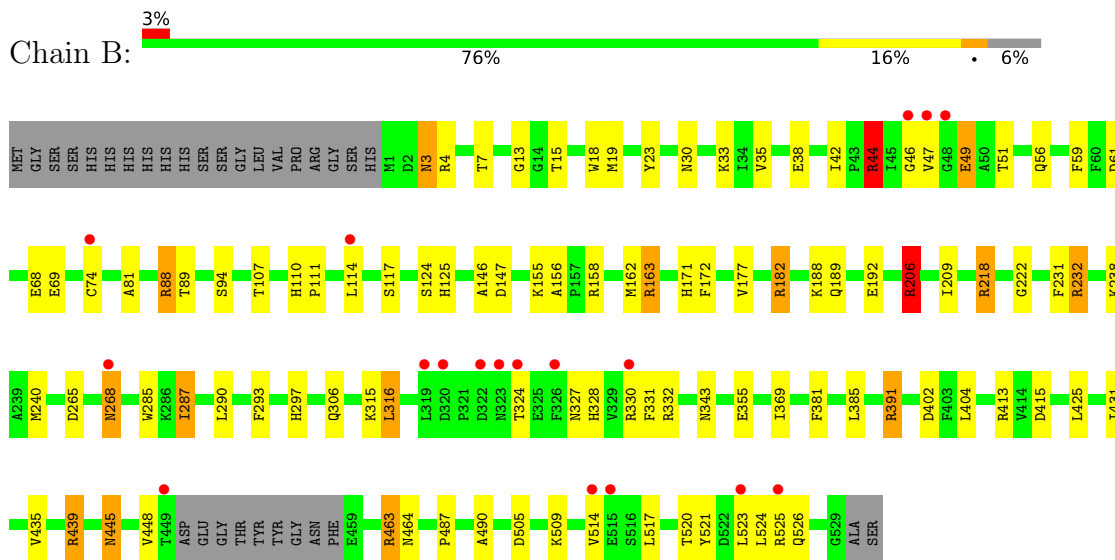
3 Residue-property plots [i](#)

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: Tryptophan 6-halogenase



- Molecule 1: Tryptophan 6-halogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.45Å 119.31Å 86.63Å 90.00° 104.37° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 20.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.2 (20.00-2.40) 96.2 (20.00-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.31 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.205 , 0.263 0.209 , 0.262	Depositor DCC
R_{free} test set	1905 reflections (4.54%)	wwPDB-VP
Wilson B-factor (Å ²)	22.2	Xtriage
Anisotropy	0.507	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8798	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% 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: FDA

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	0.89	2/4271 (0.0%)	1.05	4/5796 (0.1%)
1	B	0.83	0/4260	1.05	2/5781 (0.0%)
All	All	0.86	2/8531 (0.0%)	1.05	6/11577 (0.1%)

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	8
1	B	0	11
All	All	0	19

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	460	ALA	N-CA	5.49	1.53	1.46
1	A	343	ASN	N-CA	5.11	1.52	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	330	ARG	CB-CA-C	5.52	119.24	110.19
1	B	94	SER	CA-C-N	5.23	124.73	119.19
1	B	94	SER	C-N-CA	5.23	124.73	119.19
1	A	331	PHE	CA-CB-CG	5.15	118.95	113.80
1	A	52	VAL	CA-C-N	5.12	124.91	119.28
1	A	52	VAL	C-N-CA	5.12	124.91	119.28

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	131	ARG	Sidechain
1	A	182	ARG	Sidechain
1	A	292	ARG	Sidechain
1	A	342	ARG	Sidechain
1	A	4	ARG	Sidechain
1	A	401	ARG	Sidechain
1	A	413	ARG	Sidechain
1	A	525	ARG	Sidechain
1	B	182	ARG	Sidechain
1	B	206	ARG	Sidechain
1	B	330	ARG	Sidechain
1	B	332	ARG	Sidechain
1	B	391	ARG	Sidechain
1	B	4	ARG	Sidechain
1	B	439	ARG	Sidechain
1	B	44	ARG	Sidechain
1	B	463	ARG	Sidechain
1	B	525	ARG	Sidechain
1	B	88	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	4160	0	4036	32	0
1	B	4149	0	4026	60	0
2	A	53	0	33	1	0
2	B	53	0	33	1	0
3	A	240	0	0	5	0
3	B	143	0	0	6	0
All	All	8798	0	8128	89	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 5.

All (89) 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:B:290:LEU:HD13	1:B:524:LEU:HB3	1.54	0.88
1:A:425:LEU:HD12	3:A:876:HOH:O	1.81	0.81
1:A:411:SER:O	1:A:423:LYS:HE2	1.83	0.78
1:B:44:ARG:NH2	3:B:701:HOH:O	2.20	0.74
1:B:47:VAL:HG12	1:B:327:ASN:HD22	1.57	0.70
1:A:185:ALA:HB1	1:A:191:VAL:HG21	1.73	0.69
1:A:411:SER:O	1:A:423:LYS:CE	2.40	0.68
1:B:44:ARG:NH2	1:B:44:ARG:HG3	2.10	0.67
1:B:56:GLN:NE2	1:B:61:ASP:OD1	2.31	0.64
1:B:19:MET:HG2	1:B:59:PHE:CZ	2.33	0.64
1:B:402:ASP:HB3	1:B:431:ILE:HB	1.80	0.62
1:B:306:GLN:OE1	1:B:328:HIS:CG	2.54	0.61
1:B:49:GLU:HG3	2:B:601:FDA:C4	2.31	0.59
1:B:265:ASP:HB3	1:B:521:TYR:CD1	2.36	0.59
1:B:44:ARG:HG3	1:B:44:ARG:HH21	1.67	0.56
1:B:435:VAL:O	1:B:439:ARG:HG2	2.06	0.56
1:B:38:GLU:HG2	3:B:701:HOH:O	2.05	0.56
1:B:156:ALA:HB1	1:B:523:LEU:HD22	1.88	0.56
1:B:18:TRP:CZ2	1:B:182:ARG:HG3	2.41	0.56
1:B:445:ASN:HD21	1:B:464:ASN:HB3	1.72	0.55
1:A:150:ILE:HG23	1:A:155:LYS:HB2	1.88	0.54
1:A:487:PRO:HG2	1:B:385:LEU:HD11	1.88	0.54
1:B:33:LYS:HE2	1:B:35:VAL:HG22	1.89	0.54
1:A:18:TRP:CE2	1:A:182:ARG:HG3	2.43	0.53
1:A:4:ARG:CD	1:B:490:ALA:HB1	2.38	0.53
1:B:290:LEU:HD13	1:B:524:LEU:CB	2.32	0.53
1:B:425:LEU:HD12	3:B:806:HOH:O	2.09	0.52
1:B:44:ARG:HH21	1:B:44:ARG:CG	2.22	0.51
1:A:275:SER:HB2	1:A:286:LYS:HB3	1.91	0.51
1:B:47:VAL:HG12	1:B:327:ASN:ND2	2.25	0.50
1:B:463:ARG:NH1	3:B:712:HOH:O	2.43	0.50
1:A:138:GLU:OE2	1:A:507:LYS:NZ	2.30	0.50
1:B:13:GLY:HA3	1:B:38:GLU:HG3	1.94	0.50
1:A:185:ALA:HB1	1:A:191:VAL:CG2	2.42	0.49
2:A:601:FDA:H5'1	3:A:719:HOH:O	2.13	0.49
1:A:86:ASN:HA	1:A:106:ASP:OD2	2.13	0.49
1:B:268:ASN:H	1:B:268:ASN:HD22	1.59	0.49
1:B:189:GLN:NE2	1:B:189:GLN:HA	2.27	0.49
1:A:385:LEU:HD11	1:B:487:PRO:HG2	1.95	0.47
1:B:74:CYS:HB3	3:B:797:HOH:O	2.13	0.47
1:B:171:HIS:CD2	1:B:287:ILE:HG23	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:ARG:HD3	1:B:163:ARG:HA	1.81	0.47
1:A:88:ARG:HD2	1:A:477:GLY:O	2.15	0.46
1:B:51:THR:HB	3:B:751:HOH:O	2.15	0.46
1:A:525:ARG:HD3	1:A:530:ALA:HB3	1.96	0.46
1:B:81:ALA:HB2	1:B:111:PRO:HA	1.97	0.46
1:A:76:ALA:HA	1:A:171:HIS:O	2.16	0.46
1:A:290:LEU:HD22	3:A:899:HOH:O	2.16	0.45
1:A:249:ASP:N	1:A:249:ASP:OD1	2.47	0.45
1:B:445:ASN:ND2	1:B:464:ASN:HB3	2.31	0.45
1:A:191:VAL:CG2	3:A:762:HOH:O	2.64	0.45
1:A:232:ARG:O	1:A:233:GLY:C	2.59	0.44
1:B:18:TRP:CE2	1:B:182:ARG:HG3	2.52	0.44
1:B:155:LYS:NZ	1:B:517:LEU:O	2.48	0.44
1:B:23:TYR:HB3	1:B:369:ILE:HG21	2.00	0.44
1:B:343:ASN:HA	1:B:381:PHE:CE1	2.52	0.44
1:B:231:PHE:CZ	1:B:331:PHE:HB2	2.53	0.44
1:A:18:TRP:CZ2	1:A:182:ARG:HG3	2.53	0.44
1:B:268:ASN:H	1:B:268:ASN:ND2	2.16	0.44
1:B:124:SER:OG	1:B:125:HIS:HD2	2.01	0.44
1:A:402:ASP:OD2	1:A:430:SER:OG	2.31	0.43
1:B:315:LYS:O	1:B:316:LEU:C	2.61	0.43
1:A:4:ARG:HD3	1:B:490:ALA:HB1	1.99	0.43
1:B:110:HIS:CD2	1:B:110:HIS:C	2.96	0.43
1:A:449:THR:O	1:A:449:THR:HG22	2.18	0.43
1:B:88:ARG:NH2	1:B:107:THR:N	2.67	0.43
1:B:285:TRP:CD1	1:B:287:ILE:HG13	2.53	0.43
1:B:343:ASN:HB2	1:B:381:PHE:CZ	2.54	0.43
1:A:3:ASN:HD22	1:A:3:ASN:HA	1.63	0.42
1:B:192:GLU:OE2	1:B:218:ARG:NH2	2.44	0.42
1:A:54:ASN:O	1:A:55:LEU:C	2.60	0.42
1:B:146:ALA:O	1:B:147:ASP:C	2.63	0.42
1:B:293:PHE:O	1:B:293:PHE:CD1	2.72	0.42
1:B:158:ARG:HD3	1:B:162:MET:HE3	2.01	0.42
1:B:7:THR:HB	1:B:222:GLY:HA2	2.01	0.42
1:A:33:LYS:CE	3:A:807:HOH:O	2.67	0.41
1:B:172:PHE:CE1	1:B:177:VAL:HG21	2.54	0.41
1:A:505:ASP:OD1	1:A:508:ARG:NH2	2.53	0.41
1:B:3:ASN:HD22	1:B:3:ASN:HA	1.68	0.41
1:B:290:LEU:CD1	1:B:524:LEU:HB3	2.37	0.41
1:B:206:ARG:H	1:B:206:ARG:HG3	1.67	0.41
1:B:209:ILE:CD1	1:B:240:MET:HE2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:ARG:H	1:B:232:ARG:HG3	1.68	0.41
1:B:89:THR:O	1:B:413:ARG:HD2	2.21	0.41
1:A:317:TRP:HB2	1:A:319:LEU:HG	2.02	0.40
1:B:171:HIS:CG	1:B:287:ILE:HG23	2.55	0.40
1:A:445:ASN:ND2	1:A:466:TRP:O	2.53	0.40
1:A:20:THR:HG21	1:A:226:VAL:HG11	2.03	0.40
1:A:84:PHE:O	1:A:107:THR:HA	2.21	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	518/551 (94%)	501 (97%)	17 (3%)	0	100	100
1	B	516/551 (94%)	494 (96%)	21 (4%)	1 (0%)	43	58
All	All	1034/1102 (94%)	995 (96%)	38 (4%)	1 (0%)	48	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	46	GLY

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	438/462 (95%)	427 (98%)	11 (2%)	42	64
1	B	437/462 (95%)	405 (93%)	32 (7%)	13	22
All	All	875/924 (95%)	832 (95%)	43 (5%)	22	39

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	4	ARG
1	A	38	GLU
1	A	57	ARG
1	A	176	LYS
1	A	238	LYS
1	A	330	ARG
1	A	392	GLU
1	A	423	LYS
1	A	432	LYS
1	A	494	GLN
1	B	3	ASN
1	B	15	THR
1	B	30	ASN
1	B	42	ILE
1	B	44	ARG
1	B	49	GLU
1	B	68	GLU
1	B	69	GLU
1	B	114	LEU
1	B	117	SER
1	B	163	ARG
1	B	188	LYS
1	B	206	ARG
1	B	218	ARG
1	B	232	ARG
1	B	238	LYS
1	B	268	ASN
1	B	287	ILE
1	B	297	HIS
1	B	316	LEU
1	B	324	THR
1	B	355	GLU
1	B	391	ARG
1	B	404	LEU

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Mol	Chain	Res	Type
1	B	415	ASP
1	B	445	ASN
1	B	448	VAL
1	B	505	ASP
1	B	509	LYS
1	B	514	VAL
1	B	520	THR
1	B	526	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	125	HIS
1	A	133	GLN
1	A	139	ASN
1	A	193	HIS
1	A	328	HIS
1	B	3	ASN
1	B	125	HIS
1	B	133	GLN
1	B	139	ASN
1	B	189	GLN
1	B	268	ASN
1	B	327	ASN
1	B	445	ASN
1	B	484	ASN
1	B	526	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

2 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	FDA	A	601	-	57,58,58	2.07	15 (26%)	78,89,89	1.82	22 (28%)
2	FDA	B	601	-	57,58,58	1.81	11 (19%)	78,89,89	1.81	16 (20%)

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	FDA	A	601	-	-	5/34/50/50	0/6/6/6
2	FDA	B	601	-	-	4/34/50/50	0/6/6/6

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FDA	C5X-C9A	9.37	1.50	1.40
2	B	601	FDA	C5X-C9A	7.82	1.49	1.40
2	A	601	FDA	C5A-C4A	5.23	1.48	1.39
2	B	601	FDA	C5X-N5	-4.21	1.32	1.39
2	B	601	FDA	C5A-C4A	3.79	1.45	1.39
2	A	601	FDA	PA-O3P	3.76	1.63	1.59
2	A	601	FDA	C5A-N7A	-3.69	1.32	1.39
2	B	601	FDA	C5A-N7A	-3.59	1.32	1.39
2	A	601	FDA	P-O3P	3.56	1.63	1.59
2	A	601	FDA	C8A-N7A	3.45	1.38	1.31
2	B	601	FDA	C8-C7	3.37	1.49	1.40
2	B	601	FDA	C10-N10	3.35	1.44	1.38
2	A	601	FDA	C2-N1	-3.03	1.32	1.37
2	B	601	FDA	C4X-C4	2.65	1.49	1.41
2	A	601	FDA	C6-C5X	2.63	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	FDA	C4A-N9A	-2.58	1.32	1.37
2	B	601	FDA	C5A-C6A	2.57	1.48	1.41
2	A	601	FDA	C4A-N9A	-2.42	1.32	1.37
2	A	601	FDA	C4X-C4	2.36	1.48	1.41
2	A	601	FDA	C4'-C3'	-2.34	1.49	1.53
2	A	601	FDA	C10-N1	-2.33	1.33	1.37
2	A	601	FDA	C8-C7	2.22	1.46	1.40
2	B	601	FDA	C2-N3	2.21	1.41	1.37
2	A	601	FDA	C5X-N5	-2.21	1.36	1.39
2	B	601	FDA	C8A-N7A	2.19	1.35	1.31
2	A	601	FDA	C1'-C2'	-2.06	1.49	1.52

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	FDA	C5A-C4A-N3A	-5.86	118.64	126.72
2	B	601	FDA	C4-N3-C2	-5.19	119.23	126.37
2	B	601	FDA	C5A-C4A-N3A	-5.00	119.83	126.72
2	B	601	FDA	N3-C2-N1	4.61	122.99	115.74
2	B	601	FDA	C4A-C5A-N7A	-4.23	105.74	110.58
2	A	601	FDA	N3A-C4A-N9A	4.02	134.00	127.17
2	B	601	FDA	N3A-C2A-N1A	-3.99	122.55	128.58
2	A	601	FDA	C4-N3-C2	-3.76	121.19	126.37
2	B	601	FDA	C5A-N7A-C8A	3.55	109.03	103.45
2	B	601	FDA	N3A-C4A-N9A	3.49	133.10	127.17
2	B	601	FDA	C2A-N3A-C4A	3.44	120.24	111.83
2	A	601	FDA	C4A-C5A-N7A	-3.39	106.70	110.58
2	A	601	FDA	C4-C4X-N5	3.38	125.00	116.37
2	A	601	FDA	C4'-C3'-C2'	-3.30	108.08	113.57
2	B	601	FDA	O2-C2-N3	-3.28	116.03	121.86
2	A	601	FDA	N3-C2-N1	3.26	120.86	115.74
2	A	601	FDA	C2A-N3A-C4A	3.19	119.62	111.83
2	A	601	FDA	O4B-C1B-N9A	3.18	114.19	108.09
2	B	601	FDA	N9A-C8A-N7A	-3.16	109.45	113.94
2	A	601	FDA	C2B-C3B-C4B	-3.00	96.80	102.61
2	A	601	FDA	N3A-C2A-N1A	-2.84	124.28	128.58
2	B	601	FDA	C4A-N9A-C8A	2.82	108.70	105.74
2	A	601	FDA	C5'-C4'-C3'	-2.74	107.06	112.22
2	A	601	FDA	O4'-C4'-C5'	2.68	115.89	109.99
2	B	601	FDA	C2A-N1A-C6A	2.62	123.03	118.73
2	A	601	FDA	C6-C5X-N5	2.53	124.15	119.76
2	B	601	FDA	O4B-C1B-N9A	2.53	112.95	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	FDA	C5A-N7A-C8A	2.50	107.39	103.45
2	B	601	FDA	O3P-P-O1P	-2.37	103.58	110.70
2	B	601	FDA	C6A-C5A-N7A	2.34	136.61	132.09
2	B	601	FDA	O2P-P-O3P	2.33	113.56	107.27
2	A	601	FDA	O4B-C1B-C2B	-2.25	101.81	106.62
2	A	601	FDA	N6A-C6A-N1A	2.22	123.32	118.38
2	A	601	FDA	O4'-C4'-C3'	-2.18	104.15	109.25
2	A	601	FDA	C2A-N1A-C6A	2.14	122.24	118.73
2	A	601	FDA	O4-C4-N3	-2.10	116.17	120.11
2	A	601	FDA	O3'-C3'-C2'	2.09	113.68	108.93
2	A	601	FDA	N9A-C8A-N7A	-2.05	111.03	113.94

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FDA	N10-C1'-C2'-O2'
2	B	601	FDA	C2'-C3'-C4'-O4'
2	B	601	FDA	O3'-C3'-C4'-O4'
2	A	601	FDA	C2'-C3'-C4'-O4'
2	B	601	FDA	O3'-C3'-C4'-C5'
2	B	601	FDA	C2'-C3'-C4'-C5'
2	A	601	FDA	O3'-C3'-C4'-C5'
2	A	601	FDA	C2'-C3'-C4'-C5'
2	A	601	FDA	O3'-C3'-C4'-O4'

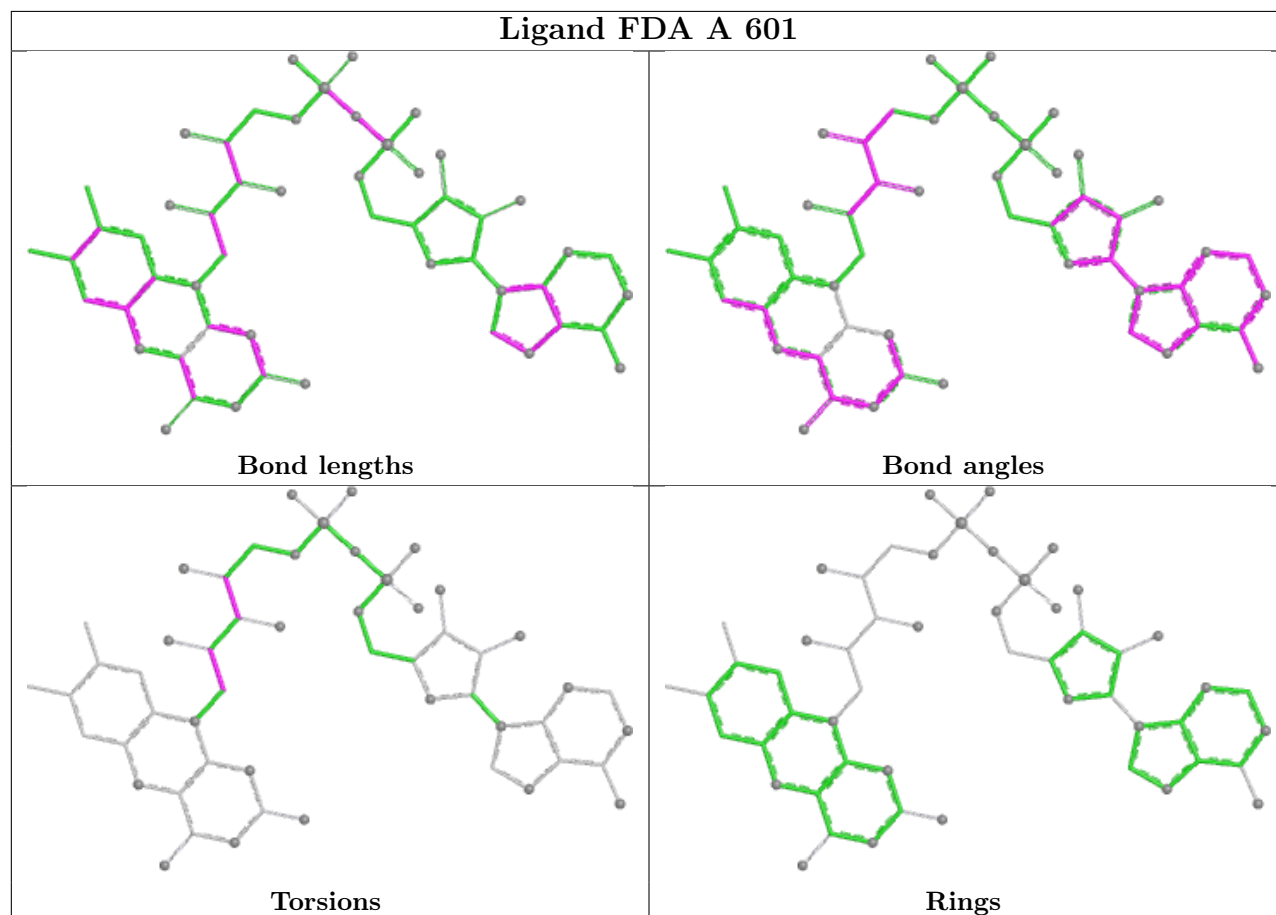
There are no ring outliers.

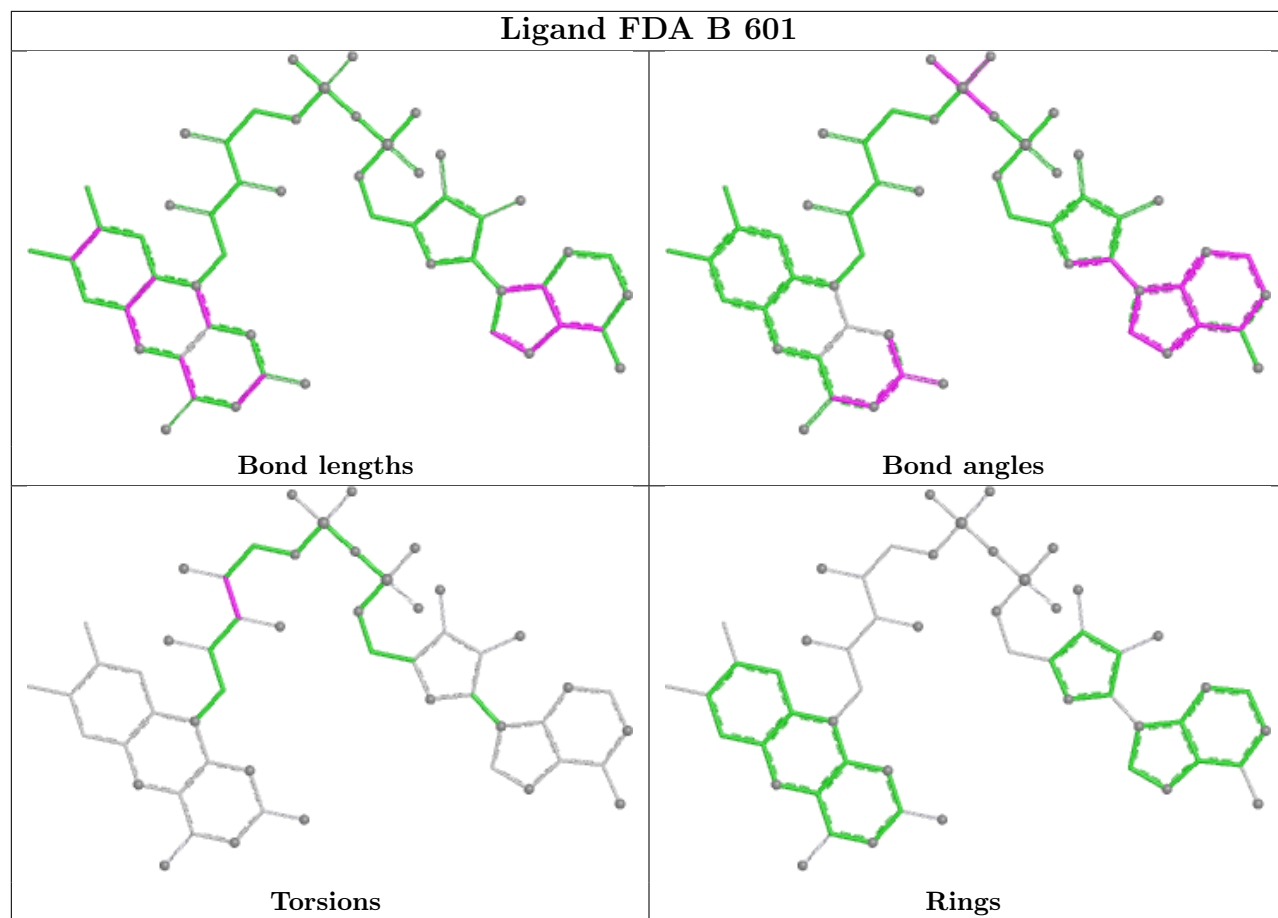
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	FDA	1	0
2	B	601	FDA	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	522/551 (94%)	-0.16	11 (2%) 63 59	8, 17, 37, 70	0
1	B	520/551 (94%)	0.27	18 (3%) 47 43	10, 27, 53, 77	0
All	All	1042/1102 (94%)	0.05	29 (2%) 55 51	8, 21, 49, 77	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	41	THR	5.6
1	A	42	ILE	3.9
1	A	531	SER	3.4
1	A	1	MET	3.4
1	A	448	VAL	3.4
1	B	324	THR	3.2
1	B	326	PHE	3.0
1	B	330	ARG	3.0
1	B	46	GLY	2.9
1	B	47	VAL	2.8
1	B	114	LEU	2.8
1	A	460	ALA	2.7
1	A	529	GLY	2.7
1	A	45	ILE	2.7
1	B	74	CYS	2.6
1	B	323	ASN	2.6
1	B	322	ASP	2.4
1	B	449	THR	2.3
1	B	514	VAL	2.3
1	A	530	ALA	2.2
1	B	268	ASN	2.2
1	B	48	GLY	2.2
1	B	515	GLU	2.2
1	B	525	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	320	ASP	2.1
1	B	319	LEU	2.1
1	A	459	GLU	2.1
1	B	523	LEU	2.0
1	A	449	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

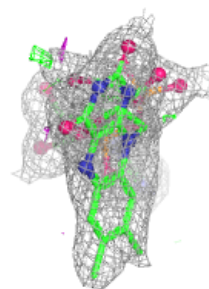
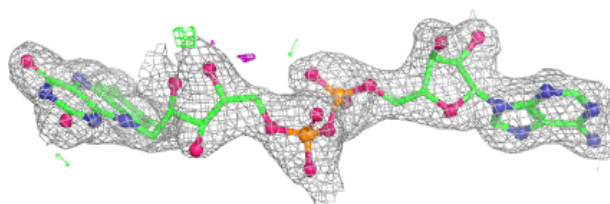
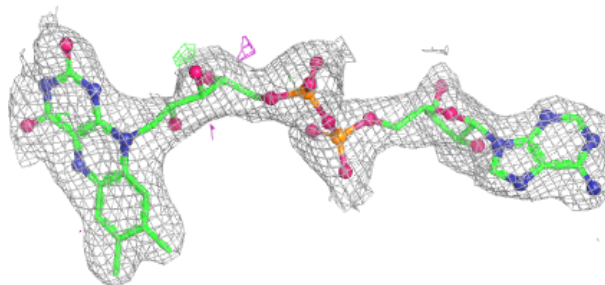
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FDA	B	601	53/53	0.95	0.07	17,24,30,35	0
2	FDA	A	601	53/53	0.96	0.07	10,14,16,18	0

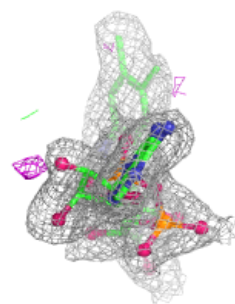
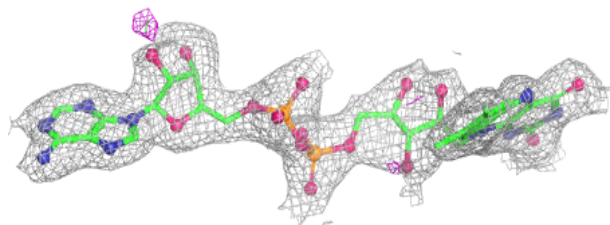
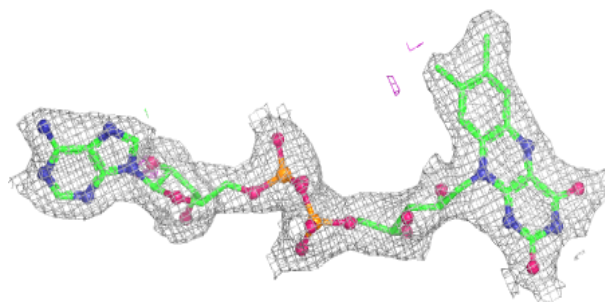
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FDA B 601:

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

**Electron density around FDA A 601:**

$2mF_o-DF_c$ (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.