



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 21, 2024 – 04:19 pm GMT

PDB ID : 8REQ
Title : Crystal structure of reduced ThyX-Y91F mutant
Authors : Pecqueur, L.; Hamdane, D.
Deposited on : 2023-12-12
Resolution : 1.94 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

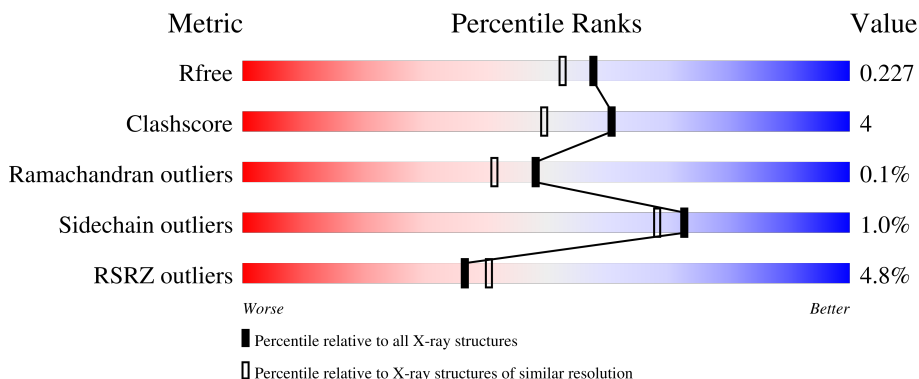
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.94 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}	164625	1306 (1.94-1.94)
Clashscore	180529	1400 (1.94-1.94)
Ramachandran outliers	177936	1387 (1.94-1.94)
Sidechain outliers	177891	1387 (1.94-1.94)
RSRZ outliers	164620	1306 (1.94-1.94)

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	232	 6% 86% 7% 6%
1	B	232	 4% 89% 7% 7%
1	C	232	 5% 87% 8% 5%
1	D	232	 4% 84% 10% 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
4	PEG	A	303	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7686 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 Flavin-dependent thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	217	Total 1770	C 1156	N 296	O 313	S 5	0	4	0
1	B	216	Total 1764	C 1152	N 302	O 305	S 5	0	0	0
1	C	220	Total 1784	C 1163	N 302	O 313	S 6	0	0	0
1	D	218	Total 1795	C 1172	N 304	O 313	S 6	0	1	0

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	initiating methionine	UNP Q9WYT0
A	-10	GLY	-	expression tag	UNP Q9WYT0
A	-9	SER	-	expression tag	UNP Q9WYT0
A	-8	ASP	-	expression tag	UNP Q9WYT0
A	-7	LYS	-	expression tag	UNP Q9WYT0
A	-6	ILE	-	expression tag	UNP Q9WYT0
A	-5	HIS	-	expression tag	UNP Q9WYT0
A	-4	HIS	-	expression tag	UNP Q9WYT0
A	-3	HIS	-	expression tag	UNP Q9WYT0
A	-2	HIS	-	expression tag	UNP Q9WYT0
A	-1	HIS	-	expression tag	UNP Q9WYT0
A	0	HIS	-	expression tag	UNP Q9WYT0
A	91	PHE	TYR	engineered mutation	UNP Q9WYT0
B	-11	MET	-	initiating methionine	UNP Q9WYT0
B	-10	GLY	-	expression tag	UNP Q9WYT0
B	-9	SER	-	expression tag	UNP Q9WYT0
B	-8	ASP	-	expression tag	UNP Q9WYT0
B	-7	LYS	-	expression tag	UNP Q9WYT0
B	-6	ILE	-	expression tag	UNP Q9WYT0
B	-5	HIS	-	expression tag	UNP Q9WYT0
B	-4	HIS	-	expression tag	UNP Q9WYT0

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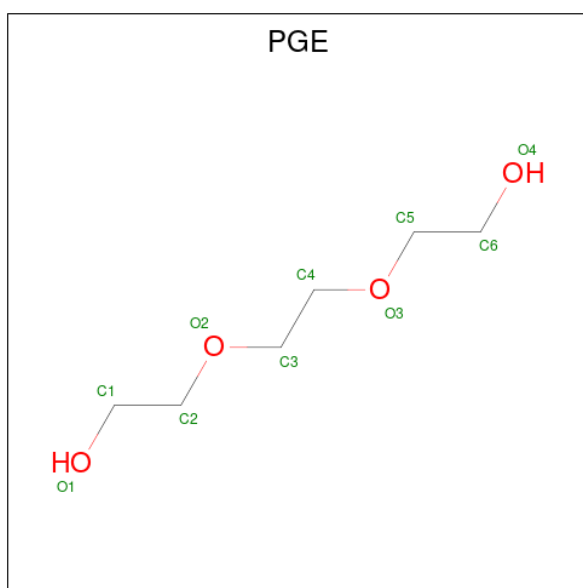
Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	HIS	-	expression tag	UNP Q9WYT0
B	-2	HIS	-	expression tag	UNP Q9WYT0
B	-1	HIS	-	expression tag	UNP Q9WYT0
B	0	HIS	-	expression tag	UNP Q9WYT0
B	91	PHE	TYR	engineered mutation	UNP Q9WYT0
C	-11	MET	-	initiating methionine	UNP Q9WYT0
C	-10	GLY	-	expression tag	UNP Q9WYT0
C	-9	SER	-	expression tag	UNP Q9WYT0
C	-8	ASP	-	expression tag	UNP Q9WYT0
C	-7	LYS	-	expression tag	UNP Q9WYT0
C	-6	ILE	-	expression tag	UNP Q9WYT0
C	-5	HIS	-	expression tag	UNP Q9WYT0
C	-4	HIS	-	expression tag	UNP Q9WYT0
C	-3	HIS	-	expression tag	UNP Q9WYT0
C	-2	HIS	-	expression tag	UNP Q9WYT0
C	-1	HIS	-	expression tag	UNP Q9WYT0
C	0	HIS	-	expression tag	UNP Q9WYT0
C	91	PHE	TYR	engineered mutation	UNP Q9WYT0
D	-11	MET	-	initiating methionine	UNP Q9WYT0
D	-10	GLY	-	expression tag	UNP Q9WYT0
D	-9	SER	-	expression tag	UNP Q9WYT0
D	-8	ASP	-	expression tag	UNP Q9WYT0
D	-7	LYS	-	expression tag	UNP Q9WYT0
D	-6	ILE	-	expression tag	UNP Q9WYT0
D	-5	HIS	-	expression tag	UNP Q9WYT0
D	-4	HIS	-	expression tag	UNP Q9WYT0
D	-3	HIS	-	expression tag	UNP Q9WYT0
D	-2	HIS	-	expression tag	UNP Q9WYT0
D	-1	HIS	-	expression tag	UNP Q9WYT0
D	0	HIS	-	expression tag	UNP Q9WYT0
D	91	PHE	TYR	engineered mutation	UNP Q9WYT0

- Molecule 2 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	8	5		
2	C	1	Total	C	O	0	0
			13	8	5		

- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



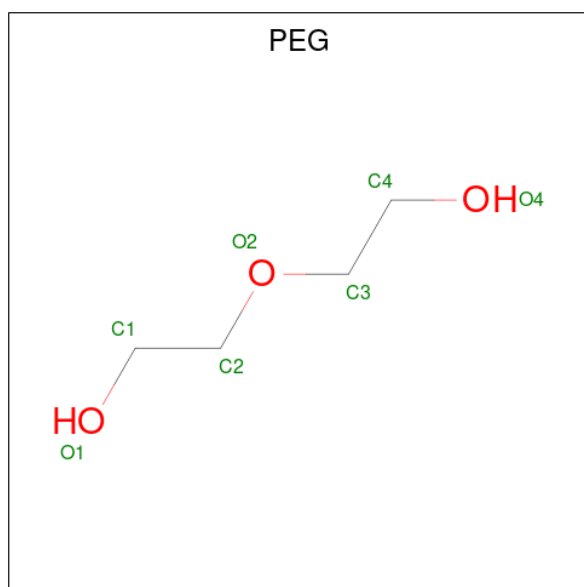
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			10	6	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			10	6	4		
3	D	1	Total	C	O	0	0
			10	6	4		
3	D	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



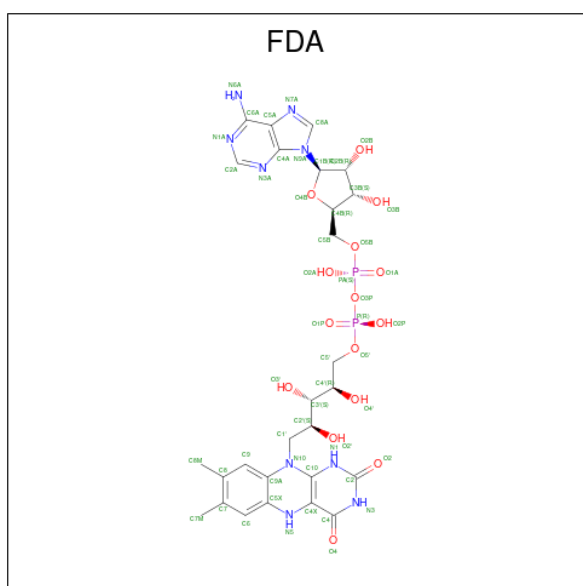
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		

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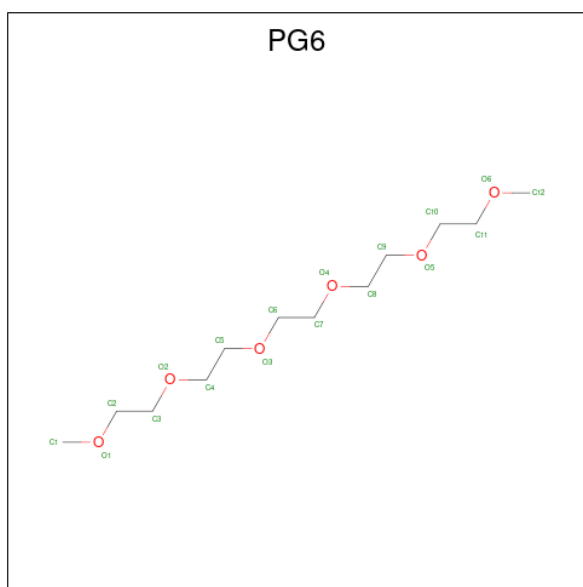
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is DIHYDROFLAVINE-ADENINE DINUCLEOTIDE (three-letter code: FDA) (formula: $C_{27}H_{35}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 6 is 1-(2-METHOXY-ETHOXY)-2-{2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHANE (three-letter code: PG6) (formula: $C_{12}H_{26}O_6$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	C O	0	0
			16	10 6		

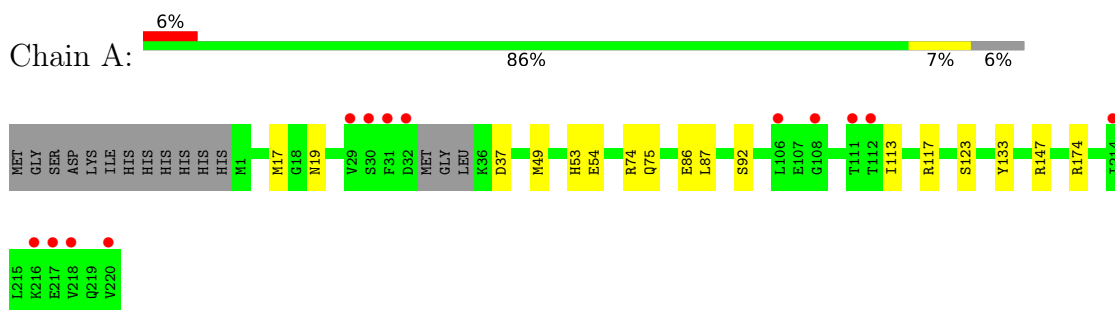
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	44	Total	O	0	1
			45	45		
7	B	51	Total	O	0	0
			51	51		
7	C	40	Total	O	0	0
			40	40		
7	D	49	Total	O	0	0
			49	49		

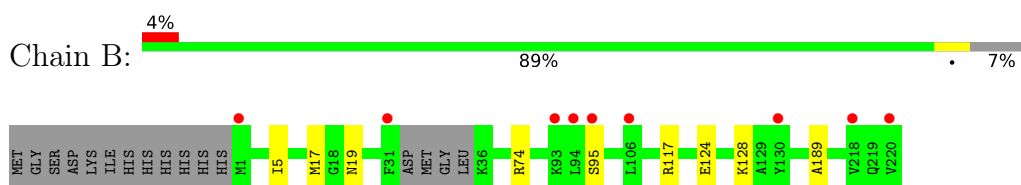
3 Residue-property plots [i](#)

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.

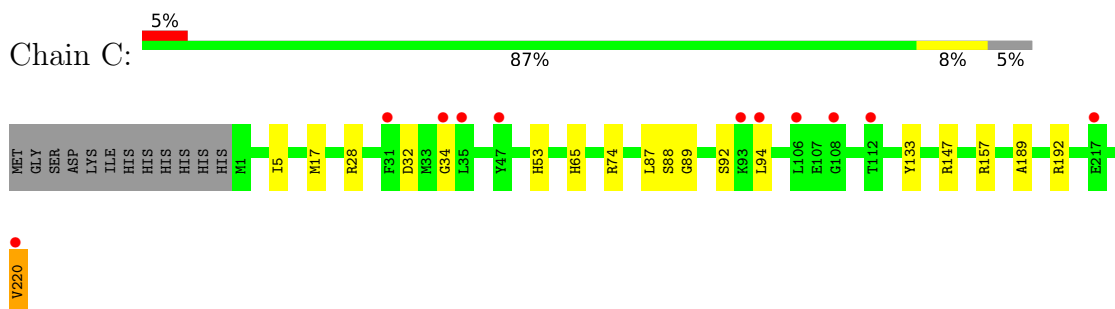
- Molecule 1: Flavin-dependent thymidylate synthase



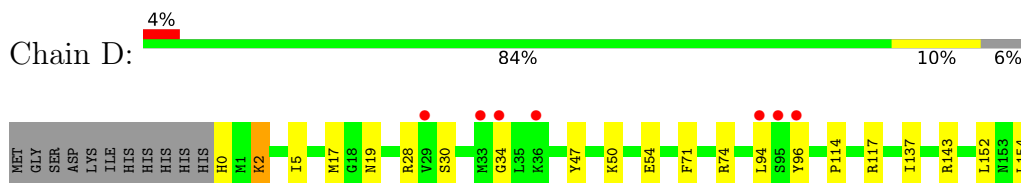
- Molecule 1: Flavin-dependent thymidylate synthase

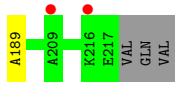


- Molecule 1: Flavin-dependent thymidylate synthase



- Molecule 1: Flavin-dependent thymidylate synthase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.02Å 117.09Å 141.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.58 – 1.94 38.58 – 1.94	Depositor EDS
% Data completeness (in resolution range)	99.5 (38.58-1.94) 99.5 (38.58-1.94)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 1.94Å)	Xtrriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.213 , 0.240 0.204 , 0.227	Depositor DCC
R_{free} test set	3388 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	41.7	Xtrriage
Anisotropy	0.088	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7686	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% 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: FDA, PG4, PG6, PGE, PEG

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	0.43	0/1818	0.58	0/2467
1	B	0.42	0/1812	0.56	0/2456
1	C	0.42	0/1833	0.58	0/2488
1	D	0.44	0/1848	0.58	0/2506
All	All	0.43	0/7311	0.58	0/9917

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1770	0	1707	18	0
1	B	1764	0	1722	7	0
1	C	1784	0	1728	19	0
1	D	1795	0	1754	21	0
2	A	13	0	18	0	0
2	C	13	0	18	1	0
3	A	10	0	14	1	0
3	B	20	0	28	1	0
3	D	20	0	28	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	28	0	40	12	0
4	C	14	0	20	0	0
4	D	42	0	60	2	0
5	A	53	0	33	1	0
5	B	53	0	33	0	0
5	C	53	0	33	0	0
5	D	53	0	33	1	0
6	C	16	0	20	3	0
7	A	45	0	0	1	0
7	B	51	0	0	2	0
7	C	40	0	0	0	0
7	D	49	0	0	1	0
All	All	7686	0	7289	61	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 4.

All (61) 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:C:92:SER:HB2	1:D:30:SER:O	1.49	1.11
1:D:54:GLU:HG2	4:D:302:PEG:H22	1.41	1.00
1:A:17:MET:HB2	1:B:17:MET:HB2	1.53	0.89
1:C:17:MET:HB2	1:D:17:MET:HB2	1.59	0.84
1:A:174:ARG:HH12	4:A:305:PEG:H41	1.51	0.74
1:D:152:LEU:HD13	3:D:309:PGE:H42	1.70	0.74
1:C:147:ARG:HB3	2:C:302:PG4:H31	1.75	0.69
1:C:65:HIS:NE2	1:C:157:ARG:NH1	2.42	0.68
1:A:54:GLU:HG2	4:A:306:PEG:H12	1.77	0.66
4:A:303:PEG:H31	1:D:74:ARG:HA	1.80	0.64
1:C:87:LEU:CD2	1:C:94:LEU:HD22	2.28	0.64
1:A:53:HIS:HA	3:A:302:PGE:H32	1.80	0.63
1:B:5:ILE:HD11	1:B:189:ALA:HB2	1.81	0.62
1:A:174:ARG:HH12	4:A:305:PEG:C4	2.12	0.62
1:D:71:PHE:HB2	3:D:309:PGE:H5	1.83	0.61
1:C:87:LEU:HD21	1:C:94:LEU:HD22	1.84	0.59
1:D:94:LEU:HD11	1:D:154:LEU:HD11	1.83	0.59
1:C:28:ARG:HD2	1:C:34:GLY:O	2.02	0.59
1:D:114:PRO:HD2	1:D:117:ARG:HG3	1.85	0.58
1:A:74:ARG:HE	4:A:303:PEG:C4	2.16	0.58
5:A:304:FDA:H2'	6:C:301:PG6:H101	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:47:TYR:HD1	3:D:301:PGE:H3	1.69	0.56
1:D:28:ARG:HD2	1:D:34:GLY:O	2.06	0.56
1:C:133:TYR:CE1	1:C:147:ARG:HG3	2.42	0.55
1:A:147:ARG:HB3	3:D:309:PGE:H3	1.89	0.54
1:A:74:ARG:HE	4:A:303:PEG:H41	1.72	0.53
1:C:133:TYR:HE1	1:C:147:ARG:HG3	1.74	0.53
1:A:133:TYR:CE1	1:A:147:ARG:HG3	2.44	0.53
1:C:5:ILE:HD11	1:C:189:ALA:HB2	1.93	0.51
1:B:124:GLU:HG2	1:B:128:LYS:HE2	1.94	0.49
1:B:74:ARG:HG2	1:C:74:ARG:NE	2.28	0.49
1:A:74:ARG:HH21	4:A:303:PEG:H42	1.77	0.49
1:D:5:ILE:HD11	1:D:189:ALA:HB2	1.95	0.48
1:C:87:LEU:HD23	1:C:94:LEU:HD22	1.94	0.48
1:B:74:ARG:HG2	1:C:74:ARG:HE	1.80	0.46
1:D:50:LYS:HZ3	3:D:301:PGE:H6	1.80	0.46
1:A:133:TYR:HE1	1:A:147:ARG:HG3	1.80	0.46
4:A:303:PEG:O1	1:D:74:ARG:HD2	2.16	0.46
1:C:53:HIS:ND1	6:C:301:PG6:H61	2.31	0.46
1:C:53:HIS:ND1	6:C:301:PG6:H51	2.30	0.45
1:A:19:ASN:HB2	7:A:412:HOH:O	2.16	0.45
1:D:19:ASN:HB2	7:D:408:HOH:O	2.15	0.45
1:D:163:ASN:ND2	4:D:305:PEG:H41	2.31	0.45
1:A:74:ARG:HE	4:A:303:PEG:H42	1.81	0.44
1:A:49:MET:SD	4:A:306:PEG:H11	2.58	0.43
3:B:302:PGE:H22	5:D:303:FDA:H2'	1.99	0.43
1:C:192:ARG:HD3	1:C:220:VAL:OXT	2.17	0.43
1:D:2:LYS:HE3	1:D:2:LYS:HB3	1.91	0.43
1:C:32:ASP:OD1	1:D:157:ARG:NH2	2.34	0.42
1:D:50:LYS:NZ	3:D:301:PGE:H6	2.34	0.42
1:B:19:ASN:HB2	7:B:416:HOH:O	2.20	0.41
1:A:113:ILE:HD12	1:A:117:ARG:HB3	2.02	0.41
1:C:89:GLY:O	1:C:147:ARG:HD2	2.20	0.41
1:C:88:SER:O	1:C:92:SER:HB3	2.19	0.41
1:D:137:ILE:HD11	1:D:143:ARG:HA	2.02	0.41
1:D:152:LEU:CD1	3:D:309:PGE:H42	2.46	0.41
1:A:75:GLN:HG2	4:A:305:PEG:H42	2.03	0.41
1:A:92:SER:HB3	4:A:307:PEG:H31	2.03	0.41
1:D:74:ARG:HH12	3:D:309:PGE:H2	1.85	0.41
1:B:74:ARG:HD3	7:B:448:HOH:O	2.20	0.40
1:A:86:GLU:HG2	1:A:87:LEU:N	2.37	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	213/232 (92%)	208 (98%)	4 (2%)	1 (0%)	25	15
1	B	212/232 (91%)	208 (98%)	4 (2%)	0	100	100
1	C	218/232 (94%)	213 (98%)	5 (2%)	0	100	100
1	D	217/232 (94%)	211 (97%)	6 (3%)	0	100	100
All	All	860/928 (93%)	840 (98%)	19 (2%)	1 (0%)	48	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	ASP

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	180/207 (87%)	179 (99%)	1 (1%)	84	83
1	B	180/207 (87%)	178 (99%)	2 (1%)	70	64
1	C	182/207 (88%)	181 (100%)	1 (0%)	86	86
1	D	185/207 (89%)	182 (98%)	3 (2%)	58	49
All	All	727/828 (88%)	720 (99%)	7 (1%)	73	68

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	SER
1	B	95	SER
1	B	117	ARG
1	C	220	VAL
1	D	0	HIS
1	D	2	LYS
1	D	96	TYR

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

Mol	Chain	Res	Type
1	C	85	ASN
1	D	43	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

24 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	$\# Z > 2$
5	FDA	D	303	-	52,58,58	0.64	0	60,89,89	0.87	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FDA	A	304	-	52,58,58	0.64	0	60,89,89	0.78	2 (3%)
4	PEG	D	308	-	6,6,6	0.23	0	5,5,5	0.20	0
4	PEG	D	305	-	6,6,6	0.45	0	5,5,5	0.47	0
3	PGE	D	309	-	9,9,9	0.14	0	8,8,8	0.29	0
4	PEG	A	303	-	6,6,6	0.29	0	5,5,5	0.21	0
2	PG4	C	302	-	12,12,12	0.19	0	11,11,11	0.23	0
4	PEG	A	306	-	6,6,6	0.20	0	5,5,5	0.15	0
4	PEG	D	306	-	6,6,6	0.17	0	5,5,5	0.09	0
4	PEG	C	305	-	6,6,6	0.11	0	5,5,5	0.13	0
4	PEG	D	302	-	6,6,6	0.21	0	5,5,5	0.14	0
2	PG4	A	301	-	12,12,12	0.20	0	11,11,11	0.11	0
5	FDA	C	303	-	52,58,58	0.64	0	60,89,89	0.80	2 (3%)
3	PGE	B	302	-	9,9,9	0.20	0	8,8,8	0.15	0
4	PEG	A	305	-	6,6,6	0.23	0	5,5,5	0.12	0
4	PEG	D	307	-	6,6,6	0.10	0	5,5,5	0.19	0
4	PEG	D	304	-	6,6,6	0.15	0	5,5,5	0.15	0
4	PEG	A	307	-	6,6,6	0.27	0	5,5,5	0.20	0
3	PGE	B	301	-	9,9,9	0.18	0	8,8,8	0.10	0
4	PEG	C	304	-	6,6,6	0.20	0	5,5,5	0.06	0
3	PGE	A	302	-	9,9,9	0.21	0	8,8,8	0.18	0
6	PG6	C	301	-	15,15,17	0.24	0	14,14,16	0.12	0
3	PGE	D	301	-	9,9,9	0.20	0	8,8,8	0.19	0
5	FDA	B	303	-	52,58,58	0.61	0	60,89,89	0.79	2 (3%)

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	FDA	D	303	-	-	2/30/50/50	0/6/6/6
5	FDA	A	304	-	-	1/30/50/50	0/6/6/6
4	PEG	D	308	-	-	1/4/4/4	-
4	PEG	D	305	-	-	2/4/4/4	-
3	PGE	D	309	-	-	6/7/7/7	-
4	PEG	A	303	-	-	3/4/4/4	-
2	PG4	C	302	-	-	5/10/10/10	-
4	PEG	A	306	-	-	2/4/4/4	-
4	PEG	D	306	-	-	1/4/4/4	-
4	PEG	C	305	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	D	302	-	-	1/4/4/4	-
2	PG4	A	301	-	-	2/10/10/10	-
5	FDA	C	303	-	-	2/30/50/50	0/6/6/6
3	PGE	B	302	-	-	5/7/7/7	-
4	PEG	A	305	-	-	3/4/4/4	-
4	PEG	D	307	-	-	1/4/4/4	-
4	PEG	D	304	-	-	1/4/4/4	-
4	PEG	A	307	-	-	3/4/4/4	-
3	PGE	B	301	-	-	4/7/7/7	-
4	PEG	C	304	-	-	2/4/4/4	-
3	PGE	A	302	-	-	5/7/7/7	-
6	PG6	C	301	-	-	6/13/13/15	-
3	PGE	D	301	-	-	3/7/7/7	-
5	FDA	B	303	-	-	2/30/50/50	0/6/6/6

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	303	FDA	O5'-C5'-C4'	-2.71	102.13	109.36
5	B	303	FDA	C5A-C6A-N6A	2.52	124.18	120.35
5	D	303	FDA	C5A-C6A-N6A	2.28	123.82	120.35
5	C	303	FDA	C4-C4X-N5	2.16	122.53	116.63
5	B	303	FDA	C4-C4X-N5	2.10	122.36	116.63
5	D	303	FDA	C4'-C3'-C2'	2.08	117.68	113.36
5	D	303	FDA	C4-C4X-N5	2.05	122.23	116.63
5	A	304	FDA	C5A-C6A-N6A	2.04	123.45	120.35
5	A	304	FDA	C4-C4X-N5	2.02	122.14	116.63
5	C	303	FDA	O5'-C5'-C4'	-2.02	103.98	109.36

There are no chirality outliers.

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	303	FDA	O4'-C4'-C5'-O5'
4	D	304	PEG	O1-C1-C2-O2
3	D	301	PGE	O3-C5-C6-O4
2	A	301	PG4	O2-C3-C4-O3

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Mol	Chain	Res	Type	Atoms
3	A	302	PGE	O1-C1-C2-O2
4	A	305	PEG	O1-C1-C2-O2
4	A	305	PEG	O2-C3-C4-O4
4	A	307	PEG	O2-C3-C4-O4
4	C	304	PEG	O2-C3-C4-O4
3	B	301	PGE	O3-C5-C6-O4
4	D	302	PEG	O2-C3-C4-O4
4	D	305	PEG	C4-C3-O2-C2
4	D	308	PEG	O2-C3-C4-O4
3	A	302	PGE	O2-C3-C4-O3
3	D	309	PGE	O3-C5-C6-O4
4	D	305	PEG	O2-C3-C4-O4
5	B	303	FDA	C3'-C4'-C5'-O5'
2	C	302	PG4	O1-C1-C2-O2
3	A	302	PGE	O3-C5-C6-O4
3	B	301	PGE	O1-C1-C2-O2
3	B	302	PGE	O3-C5-C6-O4
4	A	306	PEG	O2-C3-C4-O4
2	C	302	PG4	O2-C3-C4-O3
4	A	303	PEG	O1-C1-C2-O2
4	D	306	PEG	O1-C1-C2-O2
3	B	301	PGE	C3-C4-O3-C5
2	C	302	PG4	C4-C3-O2-C2
3	D	309	PGE	C1-C2-O2-C3
3	D	301	PGE	C1-C2-O2-C3
4	A	303	PEG	C4-C3-O2-C2
4	A	306	PEG	C1-C2-O2-C3
6	C	301	PG6	C6-C7-O4-C8
4	A	307	PEG	O1-C1-C2-O2
2	C	302	PG4	C5-C6-O4-C7
3	B	302	PGE	C4-C3-O2-C2
3	B	302	PGE	O1-C1-C2-O2
4	C	305	PEG	O2-C3-C4-O4
4	A	305	PEG	C4-C3-O2-C2
4	C	304	PEG	C4-C3-O2-C2
6	C	301	PG6	C7-C6-O3-C5
3	B	302	PGE	C6-C5-O3-C4
4	C	305	PEG	C4-C3-O2-C2
4	D	307	PEG	O2-C3-C4-O4
3	D	309	PGE	C4-C3-O2-C2
3	D	309	PGE	C3-C4-O3-C5
3	D	309	PGE	C6-C5-O3-C4

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Mol	Chain	Res	Type	Atoms
4	A	307	PEG	C1-C2-O2-C3
3	A	302	PGE	C3-C4-O3-C5
3	B	301	PGE	C6-C5-O3-C4
5	A	304	FDA	O4'-C4'-C5'-O5'
5	C	303	FDA	O4'-C4'-C5'-O5'
5	D	303	FDA	O4'-C4'-C5'-O5'
2	C	302	PG4	O3-C5-C6-O4
3	D	301	PGE	C3-C4-O3-C5
6	C	301	PG6	C11-C10-O5-C9
6	C	301	PG6	C4-C5-O3-C6
3	D	309	PGE	O2-C3-C4-O3
3	B	302	PGE	C1-C2-O2-C3
6	C	301	PG6	O2-C4-C5-O3
5	C	303	FDA	C5'-O5'-P-O1P
5	D	303	FDA	C5'-O5'-P-O1P
4	A	303	PEG	C1-C2-O2-C3
3	A	302	PGE	C6-C5-O3-C4
2	A	301	PG4	O3-C5-C6-O4
6	C	301	PG6	O4-C8-C9-O5

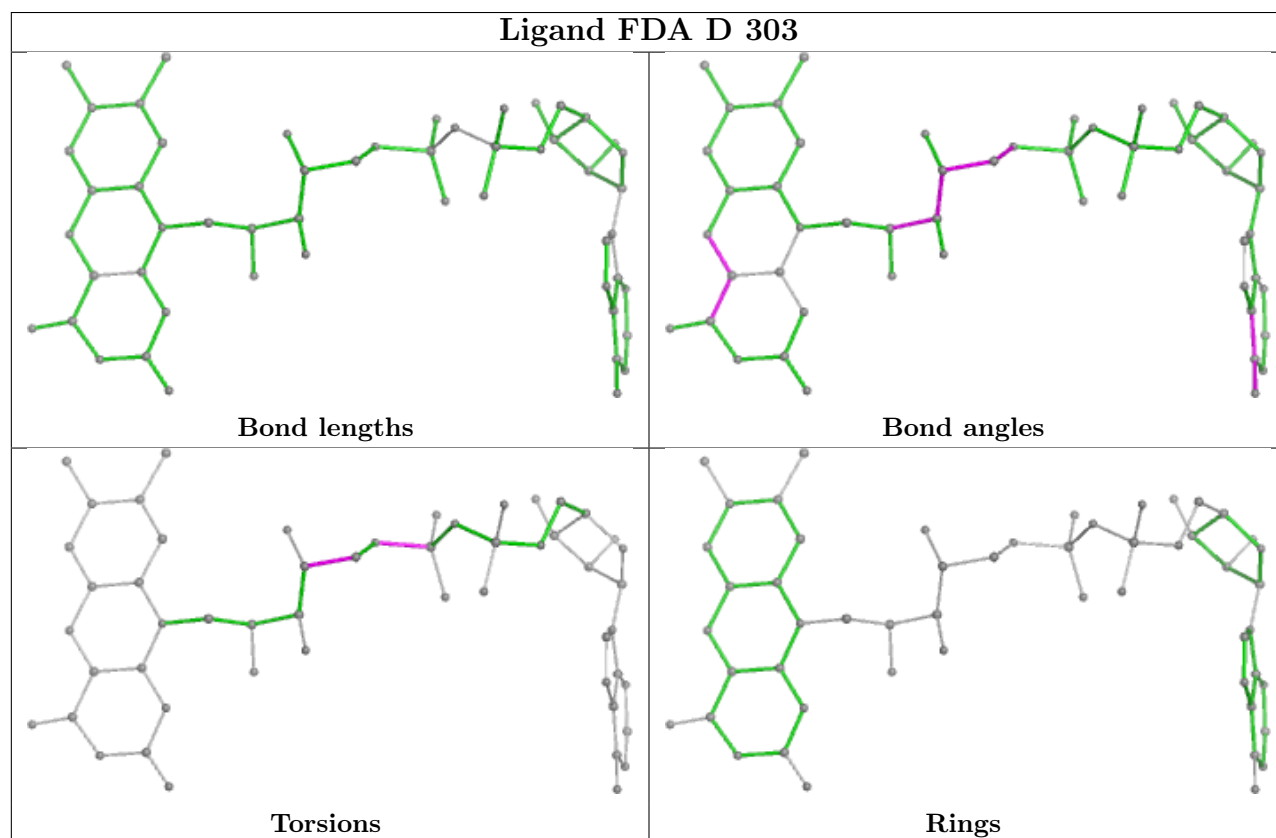
There are no ring outliers.

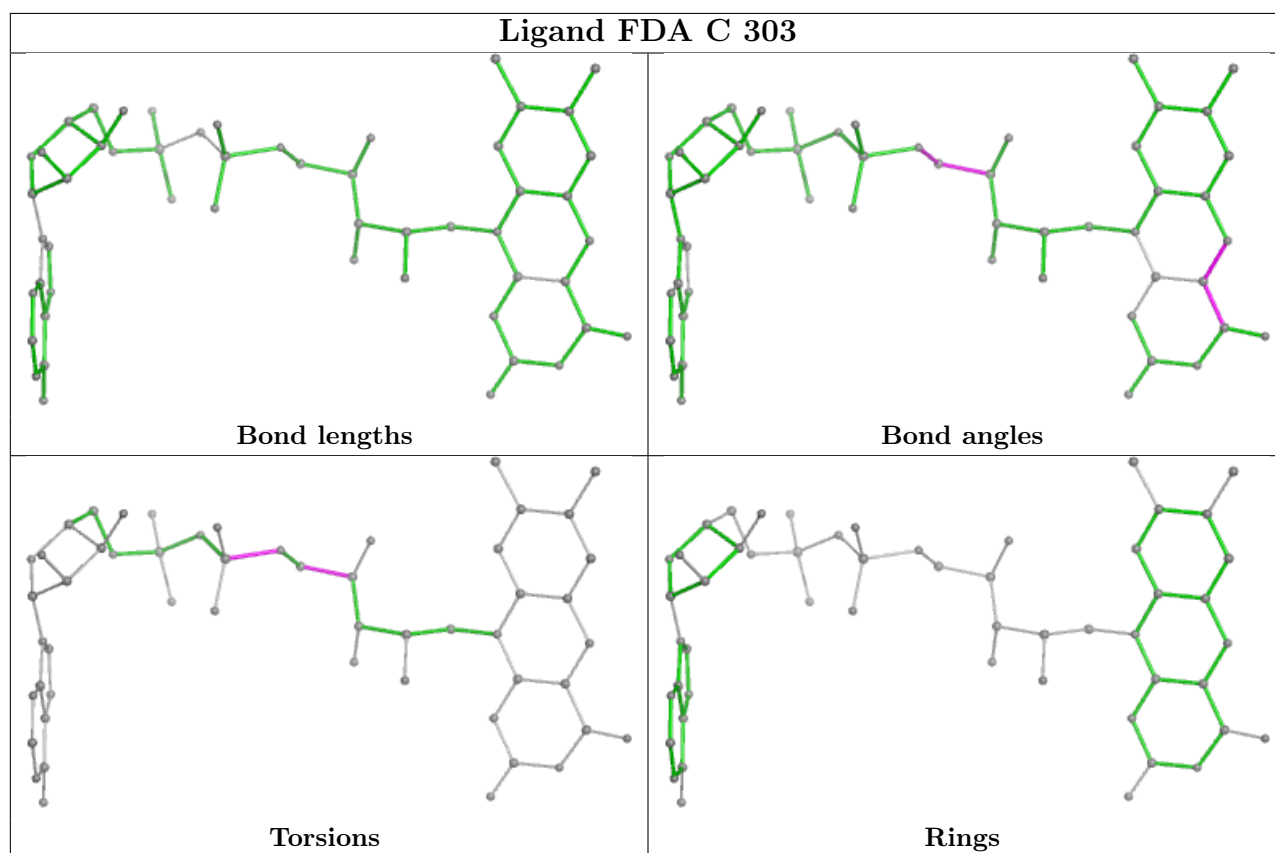
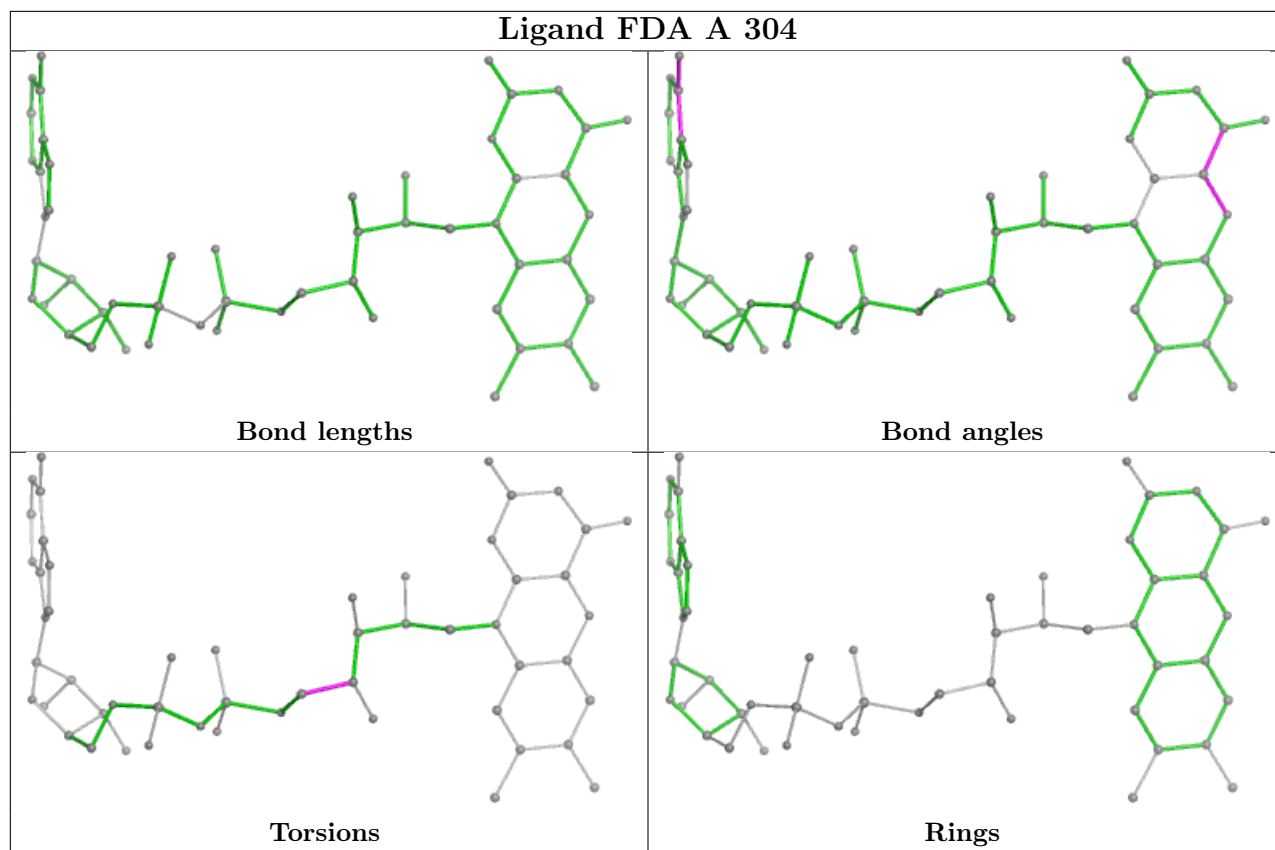
14 monomers are involved in 28 short contacts:

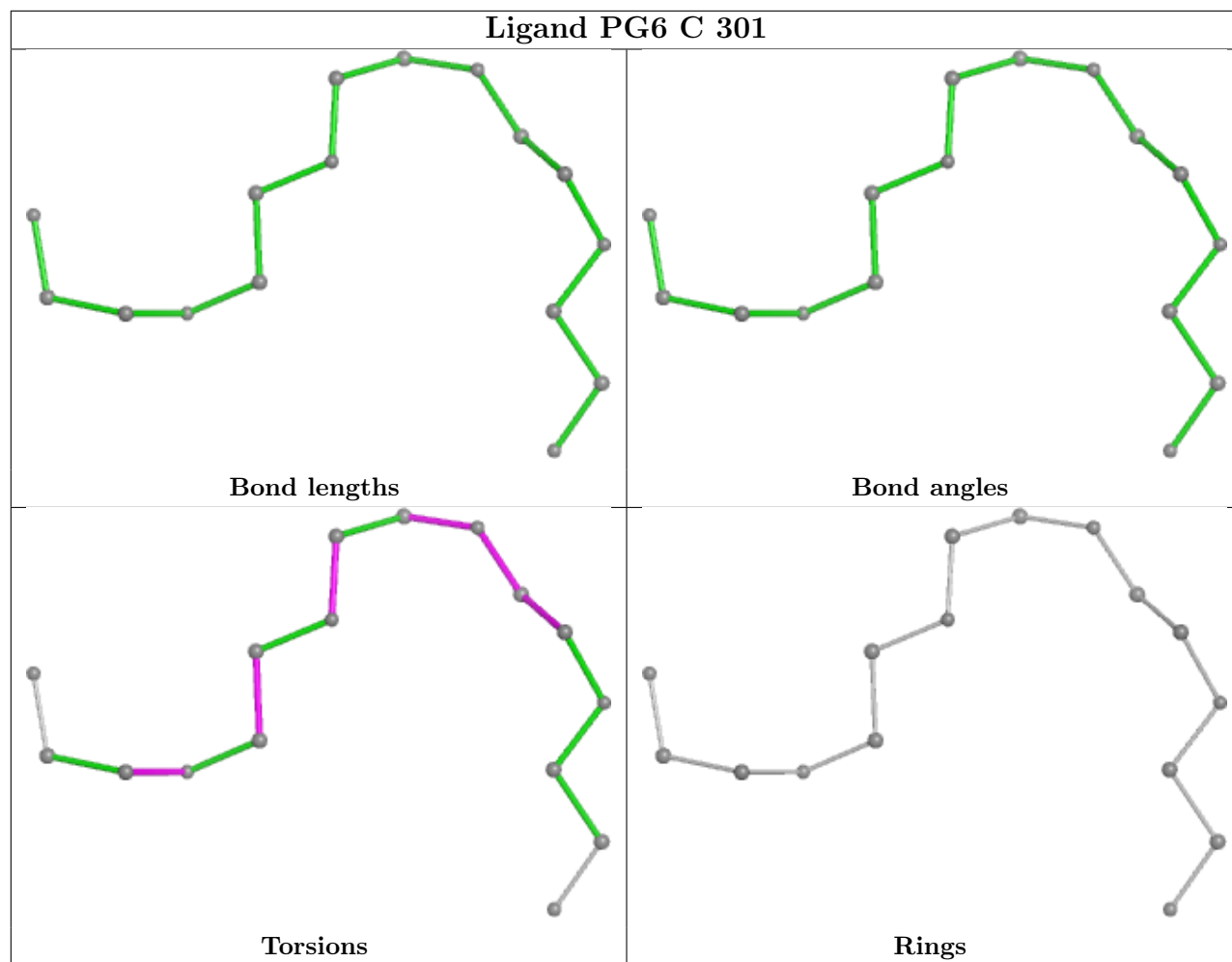
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	303	FDA	1	0
5	A	304	FDA	1	0
4	D	305	PEG	1	0
3	D	309	PGE	5	0
4	A	303	PEG	6	0
2	C	302	PG4	1	0
4	A	306	PEG	2	0
4	D	302	PEG	1	0
3	B	302	PGE	1	0
4	A	305	PEG	3	0
4	A	307	PEG	1	0
3	A	302	PGE	1	0
6	C	301	PG6	3	0
3	D	301	PGE	3	0

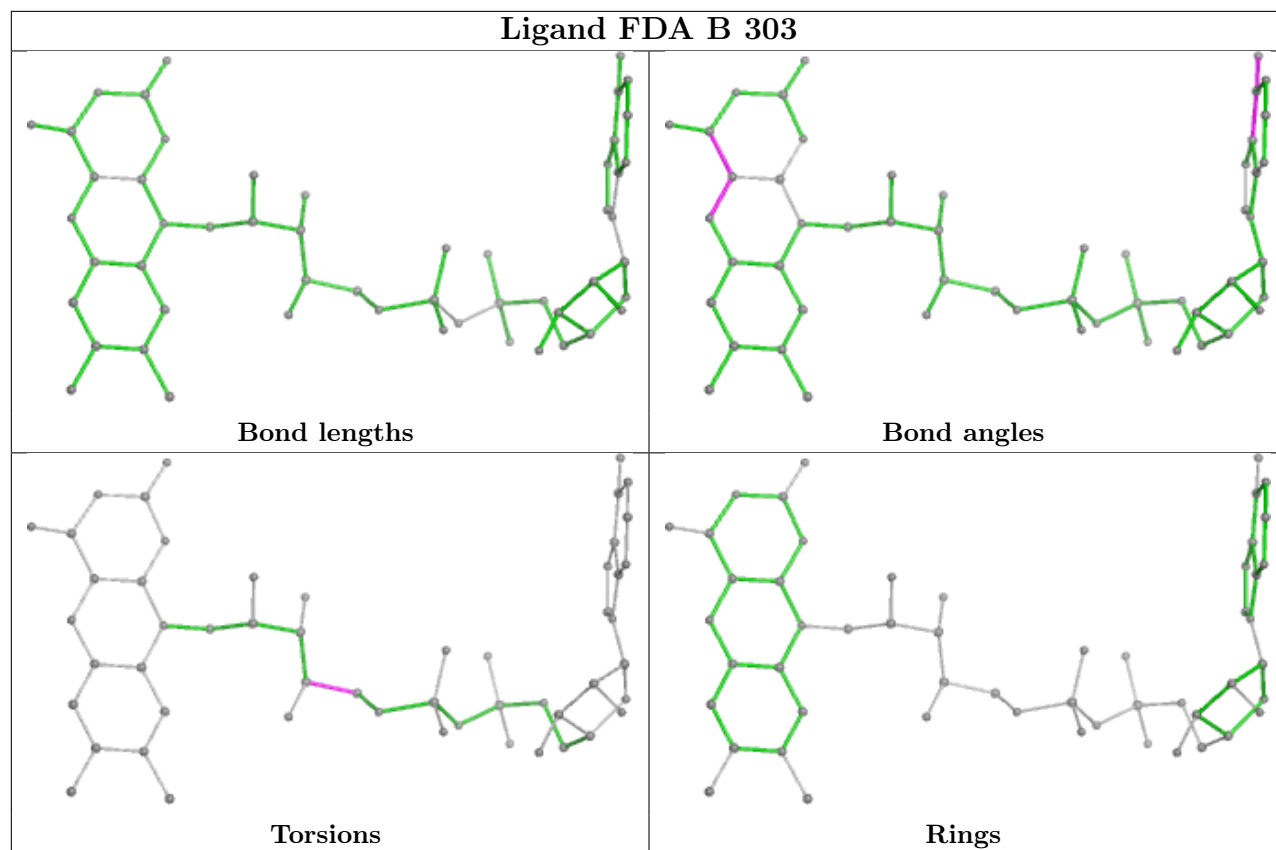
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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	217/232 (93%)	0.39	13 (5%) 29 31	32, 44, 69, 78	4 (1%)
1	B	216/232 (93%)	0.24	9 (4%) 41 46	32, 43, 63, 67	0
1	C	220/232 (94%)	0.40	11 (5%) 35 39	34, 46, 70, 78	0
1	D	218/232 (93%)	0.30	9 (4%) 42 46	33, 44, 67, 77	1 (0%)
All	All	871/928 (93%)	0.33	42 (4%) 36 40	32, 44, 67, 78	5 (0%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	32[A]	ASP	6.6
1	A	31[A]	PHE	5.7
1	A	29[A]	VAL	5.1
1	A	30[A]	SER	4.9
1	D	29[A]	VAL	4.6
1	D	96	TYR	3.9
1	D	34	GLY	3.4
1	C	112	THR	3.3
1	A	220	VAL	3.2
1	C	35	LEU	3.1
1	A	217	GLU	3.0
1	D	216	LYS	3.0
1	B	93	LYS	2.9
1	D	94	LEU	2.9
1	B	218	VAL	2.8
1	D	36	LYS	2.8
1	C	108	GLY	2.7
1	A	108	GLY	2.6
1	A	218	VAL	2.6
1	B	106	LEU	2.6
1	A	112	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	111	THR	2.4
1	C	217	GLU	2.4
1	B	130	TYR	2.4
1	A	214	ILE	2.4
1	D	33	MET	2.4
1	C	94	LEU	2.3
1	A	216	LYS	2.3
1	B	95	SER	2.3
1	C	93	LYS	2.2
1	B	31	PHE	2.2
1	B	94	LEU	2.2
1	B	1	MET	2.2
1	D	95	SER	2.2
1	B	220	VAL	2.1
1	C	34	GLY	2.1
1	C	31	PHE	2.1
1	A	106	LEU	2.1
1	C	106	LEU	2.0
1	C	47	TYR	2.0
1	C	220	VAL	2.0
1	D	209	ALA	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 monosaccharides 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
4	PEG	D	305	7/7	0.71	0.18	43,49,55,55	0
4	PEG	A	303	7/7	0.75	0.19	53,56,56,56	0

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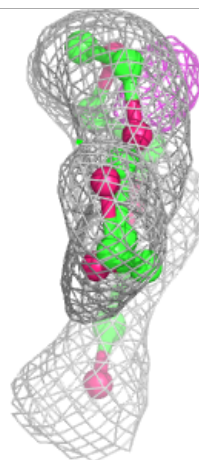
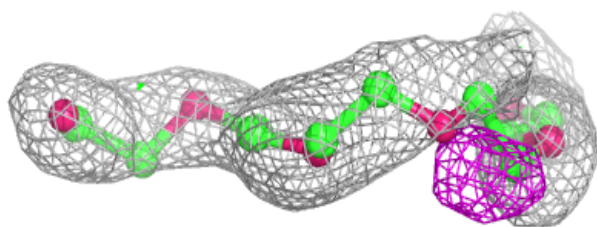
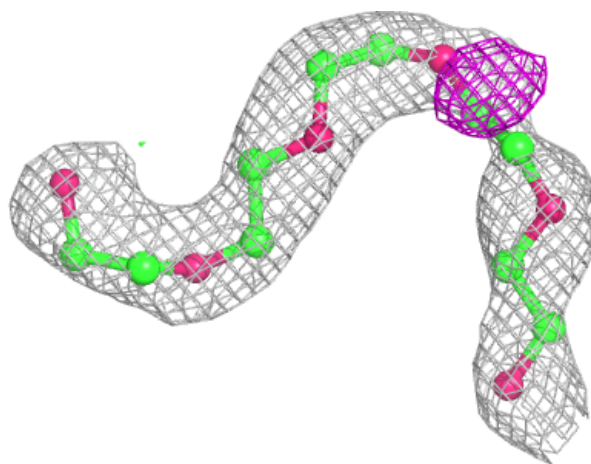
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PGE	B	301	10/10	0.77	0.16	80,82,82,82	0
4	PEG	A	305	7/7	0.78	0.18	53,55,56,57	0
2	PG4	C	302	13/13	0.78	0.18	63,66,71,71	0
4	PEG	C	305	7/7	0.79	0.17	69,70,72,73	0
3	PGE	B	302	10/10	0.79	0.20	67,68,69,69	0
4	PEG	C	304	7/7	0.82	0.13	61,63,65,65	0
4	PEG	D	306	7/7	0.83	0.18	61,61,63,63	0
6	PG6	C	301	16/18	0.83	0.17	66,68,73,73	0
4	PEG	D	302	7/7	0.84	0.19	73,74,75,75	0
4	PEG	A	307	7/7	0.85	0.14	68,70,70,70	0
4	PEG	D	308	7/7	0.87	0.11	55,57,61,61	0
3	PGE	A	302	10/10	0.87	0.14	66,67,67,67	0
2	PG4	A	301	13/13	0.88	0.13	64,65,66,66	0
3	PGE	D	301	10/10	0.88	0.12	63,64,64,64	0
4	PEG	A	306	7/7	0.89	0.17	73,73,74,74	0
4	PEG	D	307	7/7	0.89	0.10	58,58,59,59	0
4	PEG	D	304	7/7	0.90	0.13	60,60,61,62	0
3	PGE	D	309	10/10	0.90	0.14	62,62,63,64	0
5	FDA	B	303	53/53	0.96	0.07	32,37,42,43	0
5	FDA	C	303	53/53	0.96	0.07	34,39,42,43	0
5	FDA	D	303	53/53	0.96	0.07	31,36,46,46	0
5	FDA	A	304	53/53	0.96	0.07	33,36,40,41	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.

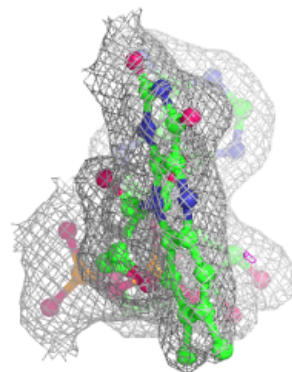
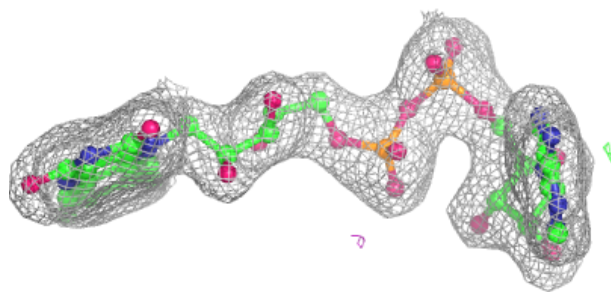
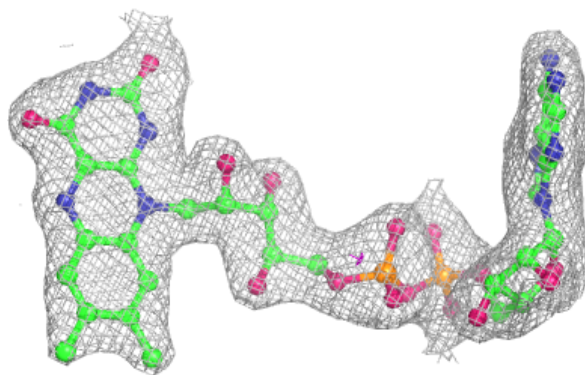
Electron density around PG6 C 301:

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

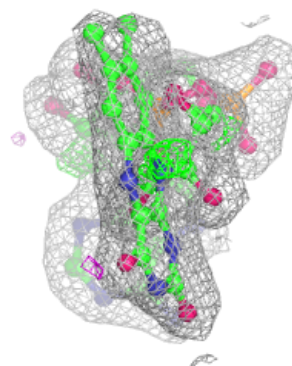
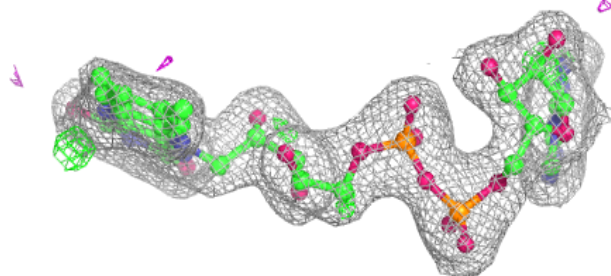
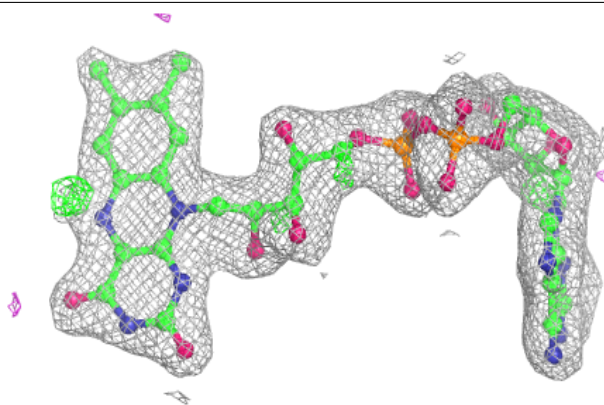


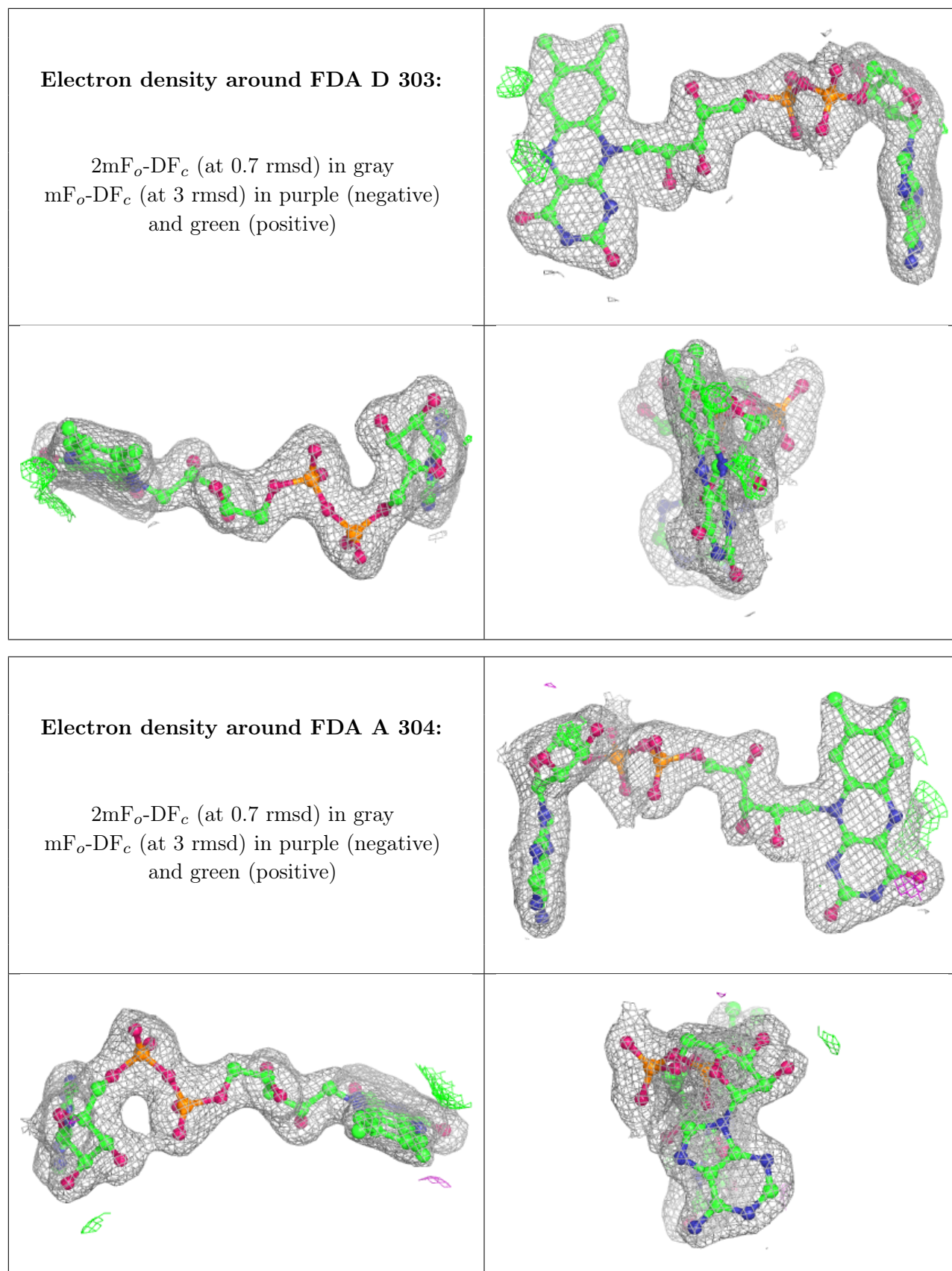
Electron density around FDA B 303:

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

**Electron density around FDA C 303:**

$2mF_o-DF_c$ (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.