



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 09:00 PM UTC

PDB ID : 4MOR / pdb_00004mor
Title : Pyranose 2-oxidase H450G/V546C double mutant with 3-fluorinated galactose
Authors : Tan, T.C.; Spadiut, O.; Gandini, R.; Haltrich, D.; Divne, C.
Deposited on : 2013-09-12
Resolution : 1.50 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)
Xtrriage (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

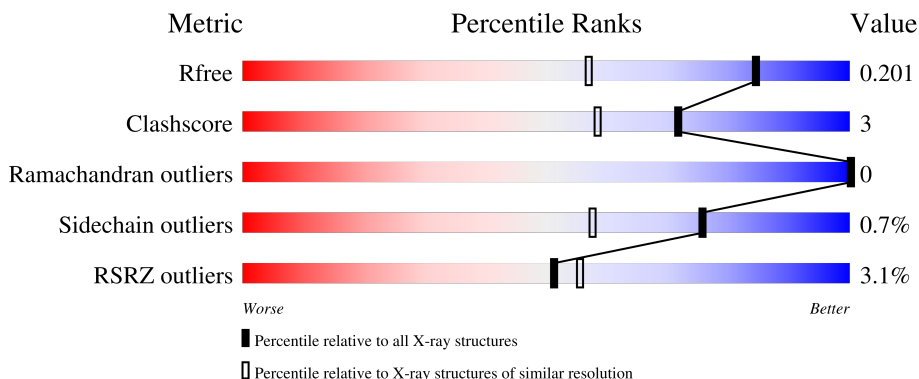
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	633	
1	B	633	
1	C	633	
1	D	633	

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
5	MES	B	804	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 21660 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 Pyranose 2-oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	576	4571	2890	775	879	27	0	8	0
1	B	576	4595	2905	781	882	27	0	10	0
1	C	573	4531	2862	772	872	25	0	4	0
1	D	576	4561	2881	775	879	26	0	5	0

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	SER	cloning artifact	UNP Q7ZA32
A	450	GLY	HIS	engineered mutation	UNP Q7ZA32
A	546	CYS	VAL	engineered mutation	UNP Q7ZA32
A	623	ALA	-	expression tag	UNP Q7ZA32
A	624	ALA	-	expression tag	UNP Q7ZA32
A	625	ALA	-	expression tag	UNP Q7ZA32
A	626	LEU	-	expression tag	UNP Q7ZA32
A	627	GLU	-	expression tag	UNP Q7ZA32
A	628	HIS	-	expression tag	UNP Q7ZA32
A	629	HIS	-	expression tag	UNP Q7ZA32
A	630	HIS	-	expression tag	UNP Q7ZA32
A	631	HIS	-	expression tag	UNP Q7ZA32
A	632	HIS	-	expression tag	UNP Q7ZA32
A	633	HIS	-	expression tag	UNP Q7ZA32
B	2	ALA	SER	cloning artifact	UNP Q7ZA32
B	450	GLY	HIS	engineered mutation	UNP Q7ZA32
B	546	CYS	VAL	engineered mutation	UNP Q7ZA32
B	623	ALA	-	expression tag	UNP Q7ZA32
B	624	ALA	-	expression tag	UNP Q7ZA32
B	625	ALA	-	expression tag	UNP Q7ZA32
B	626	LEU	-	expression tag	UNP Q7ZA32

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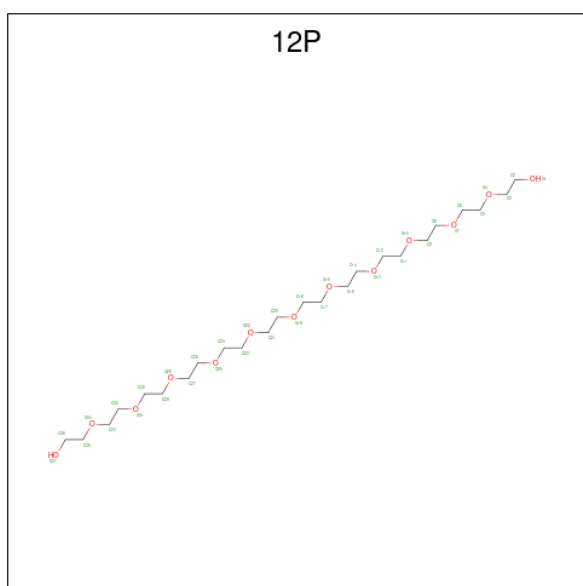
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Chain	Residue	Modelled	Actual	Comment	Reference
B	627	GLU	-	expression tag	UNP Q7ZA32
B	628	HIS	-	expression tag	UNP Q7ZA32
B	629	HIS	-	expression tag	UNP Q7ZA32
B	630	HIS	-	expression tag	UNP Q7ZA32
B	631	HIS	-	expression tag	UNP Q7ZA32
B	632	HIS	-	expression tag	UNP Q7ZA32
B	633	HIS	-	expression tag	UNP Q7ZA32
C	2	ALA	SER	cloning artifact	UNP Q7ZA32
C	450	GLY	HIS	engineered mutation	UNP Q7ZA32
C	546	CYS	VAL	engineered mutation	UNP Q7ZA32
C	623	ALA	-	expression tag	UNP Q7ZA32
C	624	ALA	-	expression tag	UNP Q7ZA32
C	625	ALA	-	expression tag	UNP Q7ZA32
C	626	LEU	-	expression tag	UNP Q7ZA32
C	627	GLU	-	expression tag	UNP Q7ZA32
C	628	HIS	-	expression tag	UNP Q7ZA32
C	629	HIS	-	expression tag	UNP Q7ZA32
C	630	HIS	-	expression tag	UNP Q7ZA32
C	631	HIS	-	expression tag	UNP Q7ZA32
C	632	HIS	-	expression tag	UNP Q7ZA32
C	633	HIS	-	expression tag	UNP Q7ZA32
D	2	ALA	SER	cloning artifact	UNP Q7ZA32
D	450	GLY	HIS	engineered mutation	UNP Q7ZA32
D	546	CYS	VAL	engineered mutation	UNP Q7ZA32
D	623	ALA	-	expression tag	UNP Q7ZA32
D	624	ALA	-	expression tag	UNP Q7ZA32
D	625	ALA	-	expression tag	UNP Q7ZA32
D	626	LEU	-	expression tag	UNP Q7ZA32
D	627	GLU	-	expression tag	UNP Q7ZA32
D	628	HIS	-	expression tag	UNP Q7ZA32
D	629	HIS	-	expression tag	UNP Q7ZA32
D	630	HIS	-	expression tag	UNP Q7ZA32
D	631	HIS	-	expression tag	UNP Q7ZA32
D	632	HIS	-	expression tag	UNP Q7ZA32
D	633	HIS	-	expression tag	UNP Q7ZA32

- Molecule 2 is DIHYDROFLAVINE-ADENINE DINUCLEOTIDE (CCD ID: FDA) (formula: $C_{27}H_{35}N_9O_{15}P_2$).

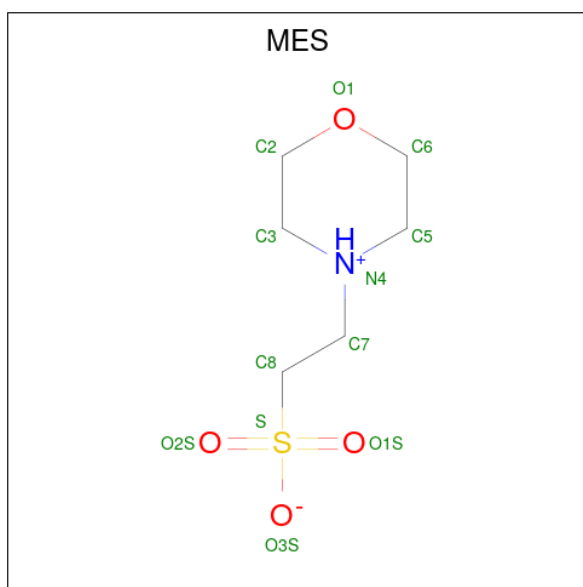
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	F	O	0	0
			12	6	1	5		
3	B	1	Total	C	F	O	0	0
			12	6	1	5		
3	C	1	Total	C	F	O	0	0
			12	6	1	5		
3	D	1	Total	C	F	O	0	0
			12	6	1	5		

- Molecule 4 is DODECAETHYLENE GLYCOL (CCD ID: 12P) (formula: $C_{24}H_{50}O_{13}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			15	10	5		
4	B	1	Total	C	O	0	0
			16	10	6		
4	C	1	Total	C	O	0	0
			11	8	3		
4	D	1	Total	C	O	0	0
			14	9	5		

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
5	B	1	12	6	1	4	1	0	0
5	D	1	12	6	1	4	1	0	0

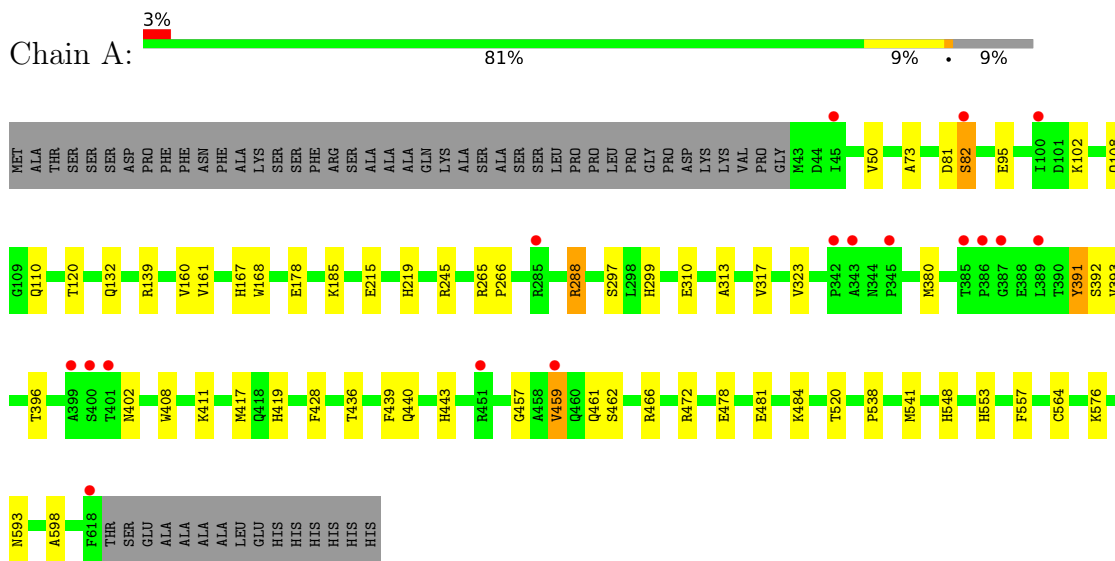
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	839	Total 839	O 839	0	0
6	B	847	Total 847	O 847	0	0
6	C	653	Total 653	O 653	0	0
6	D	723	Total 723	O 723	0	0

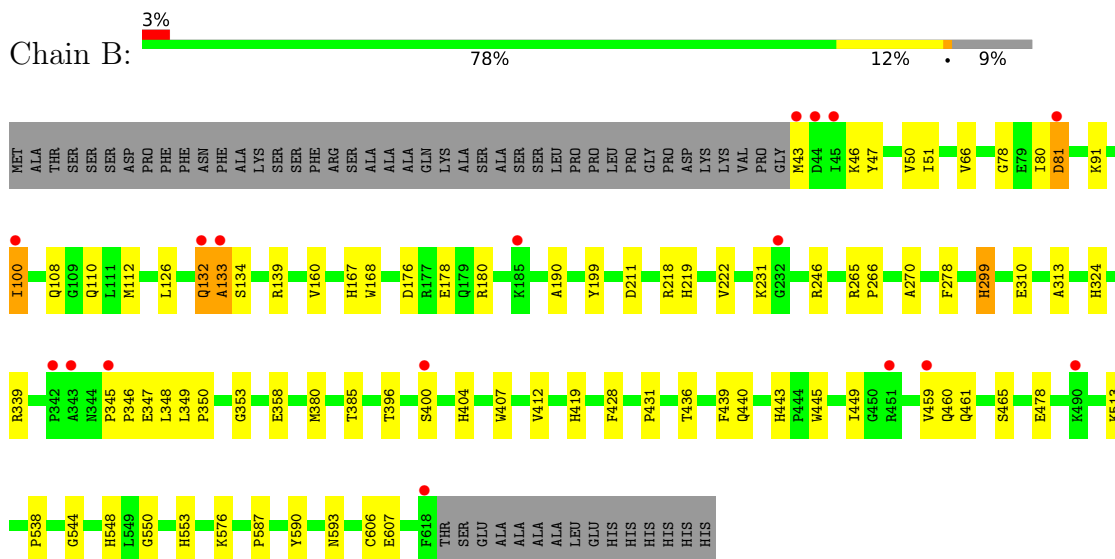
3 Residue-property plots i

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: Pyranose 2-oxidase



- Molecule 1: Pyranose 2-oxidase



- Molecule 1: Pyranose 2-oxidase

4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	100.24Å 102.47Å 137.84Å 90.00° 91.09° 90.00°	Depositor
Resolution (Å)	49.33 – 1.50 49.33 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.33-1.50) 99.7 (49.33-1.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.156 , 0.198 0.166 , 0.201	Depositor DCC
R_{free} test set	1107 reflections (0.25%)	wwPDB-VP
Wilson B-factor (Å ²)	16.7	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.016 for -k,-h,-l 0.012 for k,h,-l 0.022 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	21660	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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: 12P, FDA, 2H5, MES

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.59	35/4710 (0.7%)	1.30	13/6403 (0.2%)
1	B	1.64	46/4746 (1.0%)	1.38	26/6449 (0.4%)
1	C	1.41	18/4658 (0.4%)	1.18	10/6333 (0.2%)
1	D	1.48	25/4694 (0.5%)	1.21	6/6381 (0.1%)
All	All	1.53	124/18808 (0.7%)	1.27	55/25566 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	D	0	1
All	All	0	3

All (124) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	132	GLN	C-O	12.22	1.37	1.24
1	B	299	HIS	CG-CD2	10.04	1.46	1.35
1	A	82	SER	N-CA	9.81	1.58	1.46
1	B	380	MET	SD-CE	-8.92	1.57	1.79
1	A	443	HIS	CG-CD2	8.69	1.45	1.35
1	B	78	GLY	N-CA	8.50	1.52	1.44
1	D	349	LEU	N-CA	8.48	1.52	1.46
1	A	478	GLU	CD-OE1	8.45	1.41	1.25
1	B	478	GLU	CD-OE1	8.31	1.41	1.25
1	A	299	HIS	CG-CD2	8.23	1.45	1.35
1	B	139	ARG	CD-NE	-8.23	1.34	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	132[A]	GLN	C-O	8.23	1.33	1.23
1	B	132[B]	GLN	C-O	8.23	1.33	1.23
1	B	132[C]	GLN	C-O	8.23	1.33	1.23
1	B	443	HIS	CE1-NE2	7.89	1.40	1.32
1	B	222	VAL	CA-C	7.87	1.63	1.52
1	B	443	HIS	CG-CD2	7.82	1.44	1.35
1	C	349	LEU	N-CA	7.61	1.51	1.46
1	D	299	HIS	CG-CD2	7.51	1.44	1.35
1	B	51	ILE	C-O	7.29	1.32	1.24
1	D	443	HIS	CG-CD2	7.27	1.43	1.35
1	B	80	ILE	C-O	-7.25	1.16	1.24
1	D	553	HIS	CA-CB	7.12	1.58	1.53
1	B	299	HIS	ND1-CE1	6.91	1.39	1.32
1	D	80	ILE	C-O	-6.84	1.17	1.24
1	A	443	HIS	ND1-CE1	6.78	1.39	1.32
1	D	478	GLU	CD-OE2	6.59	1.37	1.25
1	A	317	VAL	C-O	6.58	1.31	1.24
1	C	219	HIS	CE1-NE2	6.58	1.39	1.32
1	A	297	SER	CA-C	-6.50	1.44	1.52
1	A	299	HIS	ND1-CE1	6.44	1.39	1.32
1	A	402	ASN	N-CA	6.41	1.54	1.46
1	B	219	HIS	CE1-NE2	6.40	1.39	1.32
1	C	349	LEU	C-O	6.39	1.27	1.23
1	A	520	THR	N-CA	-6.34	1.38	1.46
1	B	353	GLY	C-O	-6.33	1.15	1.24
1	B	180	ARG	CZ-NH2	-6.30	1.25	1.33
1	A	288	ARG	C-O	6.24	1.31	1.23
1	A	95	GLU	N-CA	-6.19	1.38	1.46
1	B	349	LEU	N-CA	6.17	1.50	1.46
1	B	431	PRO	N-CA	6.17	1.54	1.47
1	C	64	GLU	C-O	6.15	1.31	1.24
1	D	308	ARG	C-O	6.09	1.31	1.23
1	D	75	PHE	C-O	6.06	1.31	1.24
1	B	168	TRP	N-CA	6.05	1.54	1.45
1	A	160	VAL	CA-CB	6.00	1.61	1.55
1	B	548	HIS	ND1-CE1	5.99	1.38	1.32
1	D	260	PHE	C-O	5.99	1.30	1.23
1	B	133	ALA	CA-C	-5.97	1.45	1.52
1	B	553	HIS	CG-CD2	5.97	1.42	1.35
1	B	324	HIS	ND1-CE1	5.91	1.38	1.32
1	B	440	GLN	C-O	-5.89	1.18	1.24
1	A	310	GLU	CA-CB	5.83	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	161	VAL	N-CA	5.83	1.53	1.46
1	B	219	HIS	CG-CD2	5.82	1.42	1.35
1	A	120	THR	N-CA	5.82	1.52	1.46
1	A	459	VAL	C-O	-5.80	1.18	1.24
1	B	445	TRP	NE1-CE2	-5.79	1.31	1.37
1	A	553	HIS	ND1-CE1	5.79	1.38	1.32
1	B	81	ASP	CA-C	5.78	1.60	1.52
1	C	299	HIS	CG-CD2	5.78	1.42	1.35
1	A	457	GLY	N-CA	5.76	1.50	1.44
1	B	46	LYS	N-CA	5.76	1.53	1.46
1	A	598	ALA	CA-C	-5.75	1.45	1.52
1	C	51	ILE	C-O	5.74	1.30	1.24
1	C	117	PRO	C-O	5.73	1.30	1.23
1	D	270	ALA	N-CA	5.72	1.52	1.46
1	B	412	VAL	C-O	5.66	1.30	1.24
1	B	587	PRO	N-CA	5.64	1.52	1.47
1	D	132	GLN	N-CA	5.58	1.53	1.46
1	D	279	PRO	C-O	5.56	1.30	1.23
1	A	168	TRP	N-CA	5.55	1.53	1.45
1	A	245	ARG	CZ-NH1	5.53	1.40	1.32
1	D	134	SER	N-CA	5.52	1.53	1.46
1	D	482	GLU	CD-OE2	5.51	1.35	1.25
1	D	361	LEU	CA-C	5.49	1.59	1.52
1	D	44	ASP	N-CA	5.48	1.52	1.45
1	B	407	TRP	CA-CB	5.44	1.61	1.53
1	D	371	GLU	C-O	5.44	1.30	1.24
1	D	218	ARG	CD-NE	-5.44	1.38	1.46
1	B	400	SER	CA-CB	5.43	1.61	1.53
1	B	449	ILE	C-O	-5.42	1.18	1.24
1	A	541	MET	N-CA	5.42	1.52	1.45
1	B	199	TYR	C-O	-5.40	1.17	1.24
1	C	443	HIS	CG-CD2	5.36	1.41	1.35
1	C	404	HIS	CD2-NE2	-5.35	1.31	1.37
1	C	408	TRP	C-O	5.34	1.30	1.24
1	C	108	GLN	C-O	5.33	1.30	1.24
1	A	440	GLN	CD-NE2	-5.27	1.22	1.33
1	B	396	THR	N-CA	5.27	1.52	1.46
1	C	256	ALA	N-CA	5.27	1.52	1.46
1	A	391	TYR	C-O	5.26	1.30	1.23
1	C	460	GLN	CA-C	5.26	1.59	1.52
1	D	500	PRO	C-O	5.26	1.29	1.23
1	A	132	GLN	N-CA	5.25	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	100	ILE	N-CA	5.25	1.53	1.46
1	A	323	VAL	C-O	5.24	1.29	1.24
1	C	449	ILE	C-O	-5.23	1.18	1.24
1	D	81	ASP	CB-CG	-5.22	1.39	1.52
1	B	339	ARG	CZ-NH2	5.21	1.40	1.33
1	D	218	ARG	NE-CZ	5.20	1.38	1.33
1	D	415	HIS	ND1-CE1	5.19	1.37	1.32
1	D	508	ALA	C-O	5.19	1.31	1.23
1	B	400	SER	CB-OG	5.18	1.52	1.42
1	C	316	TYR	C-O	5.15	1.29	1.24
1	A	564	CYS	C-O	5.15	1.30	1.24
1	C	407	TRP	N-CA	5.15	1.52	1.46
1	C	161	VAL	CA-C	5.14	1.58	1.52
1	A	299	HIS	CE1-NE2	5.13	1.37	1.32
1	C	82	SER	N-CA	5.13	1.52	1.46
1	B	590	TYR	N-CA	5.13	1.52	1.45
1	A	459	VAL	N-CA	5.12	1.52	1.46
1	B	550	GLY	CA-C	-5.11	1.47	1.52
1	D	349	LEU	CA-CB	5.10	1.56	1.52
1	B	270	ALA	N-CA	5.09	1.52	1.46
1	A	419	HIS	CA-C	-5.09	1.46	1.53
1	A	219	HIS	CG-CD2	5.08	1.41	1.35
1	B	211	ASP	CG-OD1	5.08	1.35	1.25
1	A	548	HIS	ND1-CE1	5.08	1.37	1.32
1	B	246	ARG	C-O	5.07	1.30	1.24
1	A	466	ARG	N-CA	5.06	1.52	1.46
1	B	404	HIS	CA-CB	5.05	1.60	1.54
1	A	310	GLU	CD-OE2	5.00	1.34	1.25
1	B	419	HIS	CG-CD2	5.00	1.41	1.35

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	82	SER	CB-CA-C	-9.76	94.22	110.72
1	B	380	MET	CG-SD-CE	-9.19	80.67	100.90
1	B	180	ARG	CA-C-N	-9.08	111.41	120.31
1	B	180	ARG	C-N-CA	-9.08	111.41	120.31
1	B	139	ARG	NE-CZ-NH2	-8.32	111.71	119.20
1	A	81	ASP	CA-C-N	8.24	135.46	122.60
1	A	81	ASP	C-N-CA	8.24	135.46	122.60
1	D	345	PRO	CA-C-N	-7.94	111.83	119.85
1	D	345	PRO	C-N-CA	-7.94	111.83	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	139	ARG	NE-CZ-NH1	7.65	129.15	121.50
1	A	82	SER	CA-CB-OG	7.57	126.23	111.10
1	B	139	ARG	NE-CZ-NH1	7.55	129.05	121.50
1	B	459	VAL	N-CA-CB	7.53	119.38	110.95
1	B	139	ARG	CD-NE-CZ	6.97	134.16	124.40
1	B	66	VAL	N-CA-C	-6.75	103.94	110.42
1	C	82	SER	CB-CA-C	-6.63	99.35	110.56
1	B	324	HIS	N-CA-C	6.53	119.39	111.82
1	A	459	VAL	N-CA-CB	6.28	117.98	110.95
1	D	139	ARG	NE-CZ-NH2	-6.20	113.62	119.20
1	D	459	VAL	N-CA-CB	6.16	117.25	110.53
1	C	81	ASP	CA-C-N	6.14	132.47	122.65
1	C	81	ASP	C-N-CA	6.14	132.47	122.65
1	A	139	ARG	NE-CZ-NH1	6.06	127.56	121.50
1	B	428	PHE	N-CA-C	5.96	118.55	111.33
1	A	472	ARG	NE-CZ-NH2	5.92	124.52	119.20
1	A	139	ARG	NE-CZ-NH2	-5.81	113.97	119.20
1	C	66	VAL	N-CA-C	-5.79	104.86	110.42
1	B	478	GLU	CG-CD-OE2	-5.73	105.22	118.40
1	C	82	SER	CA-CB-OG	5.72	122.54	111.10
1	B	400	SER	CA-C-O	5.60	126.68	120.63
1	A	478	GLU	CG-CD-OE2	-5.60	105.53	118.40
1	B	345	PRO	CA-C-N	-5.55	114.25	119.85
1	B	345	PRO	C-N-CA	-5.55	114.25	119.85
1	B	478	GLU	CG-CD-OE1	5.47	130.99	118.40
1	C	430	ASP	CA-C-N	-5.45	114.63	120.03
1	C	430	ASP	C-N-CA	-5.45	114.63	120.03
1	B	218	ARG	NH1-CZ-NH2	-5.41	112.27	119.30
1	C	459	VAL	N-CA-CB	5.39	116.99	110.95
1	B	190	ALA	N-CA-C	-5.39	105.49	111.36
1	B	218	ARG	NE-CZ-NH1	5.30	126.80	121.50
1	A	380	MET	CG-SD-CE	-5.24	89.38	100.90
1	B	160	VAL	O-C-N	-5.23	118.42	122.97
1	C	582	GLY	CA-C-O	5.23	126.31	121.76
1	A	81	ASP	O-C-N	5.20	127.76	122.09
1	D	478	GLU	CG-CD-OE2	5.19	130.34	118.40
1	B	428	PHE	CA-C-N	-5.18	114.94	122.86
1	B	428	PHE	C-N-CA	-5.18	114.94	122.86
1	B	576	LYS	CD-CE-NZ	5.18	128.47	111.90
1	A	428	PHE	CA-C-N	-5.15	114.90	122.83
1	A	428	PHE	C-N-CA	-5.15	114.90	122.83
1	B	134	SER	N-CA-CB	5.13	118.45	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	139	ARG	CG-CD-NE	-5.13	100.72	112.00
1	C	412	VAL	N-CA-C	-5.12	105.72	110.53
1	B	606	CYS	N-CA-C	5.10	117.50	111.33
1	B	465	SER	N-CA-C	5.09	118.26	111.75

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	436	THR	Peptide
1	B	436	THR	Peptide
1	D	436	THR	Peptide

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	4571	0	4438	33	0
1	B	4595	0	4473	43	0
1	C	4531	0	4384	24	0
1	D	4561	0	4418	16	0
2	A	53	0	32	1	0
2	B	53	0	32	1	0
2	C	53	0	32	3	0
2	D	53	0	32	2	0
3	A	12	0	10	1	0
3	B	12	0	11	1	0
3	C	12	0	11	1	0
3	D	12	0	11	1	0
4	A	15	0	18	0	0
4	B	16	0	21	0	0
4	C	11	0	12	1	0
4	D	14	0	16	0	0
5	B	12	0	13	14	0
5	D	12	0	13	0	0
6	A	839	0	0	7	0
6	B	847	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	653	0	0	5	0
6	D	723	0	0	3	0
All	All	21660	0	17977	119	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (119) 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:133:ALA:CB	5:B:804:MES:H71	1.44	1.43
1:B:133:ALA:HB3	5:B:804:MES:C7	1.59	1.32
1:A:393:VAL:N	1:A:417[B]:MET:HE3	1.56	1.18
1:B:133:ALA:CB	5:B:804:MES:C7	2.24	1.07
1:B:126:LEU:HD12	1:B:132[A]:GLN:CG	1.87	1.05
1:B:126:LEU:HD12	1:B:132[A]:GLN:HG3	1.43	0.98
1:A:393:VAL:HG23	1:A:417[B]:MET:CE	1.96	0.94
1:A:393:VAL:H	1:A:417[B]:MET:HE3	1.36	0.90
1:D:110:GLN:HE21	1:D:167:HIS:HD1	1.24	0.85
1:B:126:LEU:CD1	1:B:132[A]:GLN:CG	2.55	0.84
1:A:393:VAL:HG23	1:A:417[B]:MET:HE2	1.57	0.82
1:B:133:ALA:HB2	5:B:804:MES:H71	1.58	0.81
1:A:110:GLN:HE21	1:A:167:HIS:HD1	1.26	0.81
1:B:110:GLN:HE21	1:B:167:HIS:HD1	1.27	0.80
1:B:133:ALA:HB2	5:B:804:MES:O1S	1.81	0.80
1:A:393:VAL:N	1:A:417[B]:MET:CE	2.44	0.79
1:C:110:GLN:HE21	1:C:167:HIS:HD1	1.34	0.76
1:A:462[B]:SER:OG	5:B:804:MES:H61	1.88	0.73
1:B:133:ALA:HB3	5:B:804:MES:H71	0.77	0.73
1:B:126:LEU:CD1	1:B:132[A]:GLN:HG2	2.17	0.72
1:A:393:VAL:HG23	1:A:417[B]:MET:HE3	1.72	0.72
4:C:803:12P:C5	6:C:1322:HOH:O	2.37	0.71
1:C:101:ASP:HB2	6:C:1375:HOH:O	1.92	0.69
2:D:801:FDA:N5	3:D:802:2H5:H1	2.08	0.68
1:A:538:PRO:HG2	1:C:538:PRO:HG2	1.78	0.65
1:B:133:ALA:HB2	5:B:804:MES:C8	2.27	0.65
1:A:82:SER:HB2	6:A:1064:HOH:O	1.97	0.64
1:B:126:LEU:HD12	1:B:132[A]:GLN:HG2	1.70	0.64
1:B:133:ALA:HB2	5:B:804:MES:S	2.37	0.64
1:B:133:ALA:HB2	5:B:804:MES:C7	2.21	0.64
1:A:396[A]:THR:HG23	6:A:1717:HOH:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:LYS:NZ	6:A:1563:HOH:O	2.30	0.63
1:B:81:ASP:OD1	1:B:81:ASP:C	2.37	0.62
1:C:285:ARG:HD2	6:C:1433:HOH:O	1.97	0.62
1:A:50[A]:VAL:HG13	1:A:313:ALA:HB2	1.81	0.61
1:B:460:GLN:NE2	6:B:1617:HOH:O	2.33	0.60
2:C:801:FDA:N5	3:C:802:2H5:H1	2.17	0.60
1:B:50[B]:VAL:HG23	1:B:313:ALA:HB2	1.84	0.59
1:D:81:ASP:OD1	1:D:81:ASP:C	2.41	0.59
2:B:801:FDA:N5	3:B:802:2H5:H1	2.18	0.58
1:B:126:LEU:HD12	1:B:132[C]:GLN:HG3	1.85	0.58
1:B:108:GLN:NE2	6:B:1292:HOH:O	2.38	0.57
1:C:82:SER:HB2	6:C:1036:HOH:O	2.03	0.57
1:B:133:ALA:CB	5:B:804:MES:C8	2.83	0.56
1:A:393:VAL:H	1:A:417[B]:MET:CE	2.14	0.55
1:A:50[B]:VAL:HG22	1:A:73:ALA:HB3	1.87	0.55
1:C:299:HIS:CD2	1:C:310:GLU:HG3	2.42	0.55
1:B:299:HIS:CD2	1:B:310:GLU:HG3	2.42	0.55
1:D:388:GLU:CB	1:D:390:THR:HG22	2.36	0.55
1:A:392:SER:C	1:A:417[B]:MET:HE3	2.30	0.54
1:A:393:VAL:CG2	1:A:417[B]:MET:HE3	2.38	0.54
1:B:43[B]:MET:HG3	1:B:278:PHE:CE1	2.42	0.54
1:D:388:GLU:HB3	1:D:390:THR:HG22	1.90	0.54
1:B:299:HIS:NE2	1:B:310:GLU:HG2	2.23	0.54
1:A:393:VAL:CA	1:A:417[B]:MET:HE3	2.36	0.53
1:A:393:VAL:CB	1:A:417[B]:MET:HE3	2.39	0.53
1:A:288:ARG:NH1	6:A:1412:HOH:O	2.42	0.52
1:B:347:GLU:HG3	6:B:1386:HOH:O	2.07	0.52
1:C:459:VAL:HG13	1:C:461:GLN:HE21	1.74	0.52
1:D:462[C]:SER:OG	6:D:1477:HOH:O	2.20	0.51
1:C:215:GLU:O	1:C:411:LYS:NZ	2.44	0.50
1:A:462[B]:SER:HG	5:B:804:MES:H61	1.77	0.50
1:B:132[C]:GLN:HE21	5:B:804:MES:H31	1.76	0.50
1:B:108:GLN:HG2	6:B:1611:HOH:O	2.11	0.50
1:B:347:GLU:HG2	1:B:348:LEU:HG	1.94	0.49
1:B:538:PRO:HG2	1:D:538:PRO:HG2	1.95	0.49
1:A:459:VAL:HG13	1:A:461:GLN:HE21	1.78	0.49
1:C:299:HIS:NE2	1:C:310:GLU:HG2	2.27	0.49
1:A:178:GLU:CD	1:A:439:PHE:HE1	2.21	0.48
1:C:299:HIS:NE2	1:C:310:GLU:CG	2.77	0.48
1:D:108:GLN:NE2	6:D:1052:HOH:O	2.37	0.47
1:A:481[B]:GLU:OE2	1:A:484:LYS:NZ	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:VAL:CG2	1:A:417[B]:MET:CE	2.81	0.46
1:C:265:ARG:HA	1:C:266:PRO:C	2.41	0.46
2:A:801:FDA:N5	3:A:802:2H5:H1	2.30	0.46
1:D:214:LYS:HG3	1:D:215:GLU:HG3	1.98	0.46
1:B:513:LYS:NZ	6:B:1442:HOH:O	2.48	0.46
1:B:346:PRO:HG2	1:B:350:PRO:HA	1.98	0.46
1:C:404:HIS:HB3	1:C:405:PRO:HD2	1.98	0.46
1:B:176:ASP:OD2	1:B:178:GLU:OE2	2.34	0.46
1:C:459:VAL:HG13	1:C:461:GLN:NE2	2.32	0.45
1:A:265:ARG:HA	1:A:266:PRO:C	2.42	0.45
1:C:218:ARG:HG3	1:C:430:ASP:OD2	2.16	0.45
1:A:576:LYS:NZ	6:A:1593:HOH:O	2.50	0.44
1:A:392:SER:CA	1:A:417[B]:MET:HE1	2.47	0.44
1:B:299:HIS:NE2	1:B:310:GLU:CG	2.80	0.44
1:C:47:TYR:O	1:C:313:ALA:HA	2.17	0.44
1:C:91:LYS:HD2	1:C:100:ILE:HD11	2.00	0.44
1:C:218:ARG:HD2	6:C:932:HOH:O	2.18	0.44
1:C:81:ASP:OD1	1:C:81:ASP:C	2.59	0.44
1:B:178:GLU:CD	1:B:439:PHE:HE1	2.26	0.43
1:C:169:THR:H	2:C:801:FDA:HN5	1.66	0.43
1:D:218:ARG:HG3	1:D:430:ASP:OD2	2.18	0.43
1:A:108:GLN:NE2	6:A:1372:HOH:O	2.35	0.43
1:B:91:LYS:HD2	1:B:100:ILE:HD11	1.99	0.43
1:C:169:THR:HB	2:C:801:FDA:O4	2.18	0.43
1:D:132:GLN:HG2	6:D:1613:HOH:O	2.18	0.43
1:A:392:SER:C	1:A:417[B]:MET:CE	2.89	0.43
1:B:126:LEU:CD1	1:B:132[A]:GLN:CD	2.91	0.43
1:D:178:GLU:CD	1:D:439:PHE:HE1	2.27	0.43
1:D:459:VAL:HG13	1:D:461:GLN:HE21	1.84	0.43
1:A:215:GLU:O	1:A:411:LYS:NZ	2.50	0.43
1:B:133:ALA:HB3	5:B:804:MES:H72	1.81	0.43
1:D:346:PRO:HG2	1:D:350:PRO:HA	2.00	0.42
1:A:391:TYR:CE2	1:A:417[B]:MET:HE2	2.54	0.42
1:B:358:GLU:HG2	1:B:544:GLY:HA2	2.02	0.42
1:B:91:LYS:CE	6:B:1710:HOH:O	2.68	0.42
1:A:185:LYS:HG2	1:A:557:PHE:CE2	2.55	0.42
1:D:388:GLU:HB2	1:D:390:THR:HG22	2.01	0.41
1:B:607:GLU:HG3	6:B:1254:HOH:O	2.20	0.41
1:C:548:HIS:CD2	1:C:594:PRO:HD2	2.55	0.41
1:C:346:PRO:HG2	1:C:350:PRO:HA	2.02	0.41
1:B:47:TYR:O	1:B:313:ALA:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:ARG:HA	1:B:266:PRO:C	2.46	0.41
1:C:47:TYR:CE2	1:C:73:ALA:HB2	2.55	0.41
1:C:178:GLU:CD	1:C:439:PHE:HE1	2.29	0.41
1:D:169:THR:H	2:D:801:FDA:HN5	1.68	0.41
1:D:185:LYS:HG2	1:D:557:PHE:CZ	2.56	0.40
6:A:1377:HOH:O	1:B:461:GLN:HG3	2.20	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	582/633 (92%)	569 (98%)	13 (2%)	0	100	100
1	B	585/633 (92%)	573 (98%)	12 (2%)	0	100	100
1	C	575/633 (91%)	562 (98%)	13 (2%)	0	100	100
1	D	580/633 (92%)	566 (98%)	14 (2%)	0	100	100
All	All	2322/2532 (92%)	2270 (98%)	52 (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	511/547 (93%)	509 (100%)	2 (0%)	84	71
1	B	515/547 (94%)	510 (99%)	5 (1%)	68	45
1	C	504/547 (92%)	500 (99%)	4 (1%)	73	54
1	D	509/547 (93%)	505 (99%)	4 (1%)	73	54
All	All	2039/2188 (93%)	2024 (99%)	15 (1%)	76	57

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	408	TRP
1	A	593	ASN
1	B	112	MET
1	B	231	LYS
1	B	385[A]	THR
1	B	385[B]	THR
1	B	593	ASN
1	C	82	SER
1	C	312	LYS
1	C	496	ASN
1	C	593	ASN
1	D	385	THR
1	D	576	LYS
1	D	593	ASN
1	D	611	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	ASN
1	A	105	ASN
1	A	257	ASN
1	A	344	ASN
1	A	365	GLN
1	A	461	GLN
1	A	496	ASN
1	A	611	GLN
1	B	108	GLN
1	B	224	ASN
1	B	257	ASN
1	B	365	GLN

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Mol	Chain	Res	Type
1	B	419	HIS
1	B	461	GLN
1	C	257	ASN
1	C	331	ASN
1	C	344	ASN
1	C	419	HIS
1	C	461	GLN
1	D	257	ASN
1	D	419	HIS
1	D	440	GLN
1	D	461	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](#)

14 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	MES	B	804	-	12,12,12	1.91	3 (25%)	15,16,16	2.99	7 (46%)
3	2H5	A	802	-	12,12,12	2.39	3 (25%)	17,17,17	1.51	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FDA	D	801	1	57,58,58	1.42	9 (15%)	78,89,89	2.38	28 (35%)
5	MES	D	804	-	12,12,12	2.03	2 (16%)	15,16,16	1.38	1 (6%)
3	2H5	C	802	-	12,12,12	1.46	2 (16%)	17,17,17	1.66	3 (17%)
2	FDA	A	801	1	57,58,58	1.86	10 (17%)	78,89,89	1.74	16 (20%)
2	FDA	C	801	1	57,58,58	1.74	10 (17%)	78,89,89	1.86	24 (30%)
3	2H5	D	802	-	12,12,12	1.11	1 (8%)	17,17,17	2.18	4 (23%)
4	12P	A	803	-	14,14,36	0.67	0	13,13,35	1.23	3 (23%)
4	12P	B	803	-	15,15,36	0.66	0	14,14,35	0.71	0
4	12P	C	803	-	10,10,36	1.47	3 (30%)	9,9,35	2.51	3 (33%)
4	12P	D	803	-	13,13,36	0.66	0	12,12,35	0.76	0
3	2H5	B	802	-	12,12,12	1.32	2 (16%)	17,17,17	1.29	2 (11%)
2	FDA	B	801	1	57,58,58	1.76	12 (21%)	78,89,89	1.95	23 (29%)

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	MES	B	804	-	-	0/6/14/14	0/1/1/1
3	2H5	A	802	-	-	0/2/22/22	0/1/1/1
2	FDA	D	801	1	-	0/34/50/50	0/6/6/6
5	MES	D	804	-	-	0/6/14/14	0/1/1/1
3	2H5	C	802	-	-	0/2/22/22	0/1/1/1
2	FDA	A	801	1	-	0/34/50/50	0/6/6/6
2	FDA	C	801	1	-	2/34/50/50	0/6/6/6
3	2H5	D	802	-	-	0/2/22/22	0/1/1/1
4	12P	A	803	-	-	0/12/12/34	-
4	12P	B	803	-	-	0/13/13/34	-
4	12P	C	803	-	-	3/8/8/34	-
4	12P	D	803	-	-	0/11/11/34	-
3	2H5	B	802	-	-	0/2/22/22	0/1/1/1
2	FDA	B	801	1	-	1/34/50/50	0/6/6/6

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	FDA	PA-O3P	8.41	1.68	1.59
2	B	801	FDA	P-O3P	7.22	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	FDA	P-O3P	5.77	1.65	1.59
5	D	804	MES	C8-S	-5.38	1.70	1.77
3	A	802	2H5	C3-C2	-5.20	1.47	1.52
3	A	802	2H5	C3-C4	-4.52	1.48	1.52
2	C	801	FDA	C8A-N9A	-4.47	1.29	1.37
5	B	804	MES	C8-S	-4.22	1.71	1.77
2	C	801	FDA	PA-O3P	4.17	1.64	1.59
2	B	801	FDA	C2B-C3B	-4.09	1.42	1.53
2	A	801	FDA	C5A-C4A	3.91	1.46	1.39
2	C	801	FDA	C1'-C2'	-3.77	1.47	1.52
3	A	802	2H5	C4-C5	3.59	1.60	1.53
2	C	801	FDA	C9-C8	3.57	1.44	1.39
2	B	801	FDA	C9-C9A	3.52	1.45	1.39
2	C	801	FDA	C7M-C7	3.52	1.57	1.51
2	D	801	FDA	PA-O3P	3.49	1.63	1.59
2	A	801	FDA	C5X-C9A	-3.46	1.36	1.40
2	D	801	FDA	O4B-C4B	-3.46	1.37	1.45
2	C	801	FDA	C6-C5X	3.42	1.44	1.39
2	D	801	FDA	C7M-C7	3.10	1.56	1.51
2	A	801	FDA	C2'-C3'	3.04	1.58	1.53
2	C	801	FDA	C4X-N5	3.03	1.41	1.35
5	B	804	MES	O2S-S	3.01	1.53	1.45
3	D	802	2H5	C4-C5	2.99	1.59	1.53
2	A	801	FDA	C4X-C4	2.95	1.50	1.41
2	D	801	FDA	C5X-C9A	-2.84	1.37	1.40
2	B	801	FDA	C2-N1	-2.83	1.32	1.37
3	B	802	2H5	C4-C5	2.81	1.59	1.53
2	D	801	FDA	C1B-N9A	-2.68	1.38	1.46
2	A	801	FDA	C10-N1	-2.68	1.32	1.37
4	C	803	12P	C8-C9	2.66	1.62	1.49
3	C	802	2H5	C3-C4	2.65	1.55	1.52
2	B	801	FDA	C8A-N9A	-2.61	1.33	1.37
3	B	802	2H5	C3-C4	-2.60	1.50	1.52
2	B	801	FDA	C4-N3	-2.51	1.34	1.38
2	B	801	FDA	O2-C2	2.46	1.28	1.23
2	D	801	FDA	C5X-N5	-2.44	1.35	1.39
2	D	801	FDA	C4'-C3'	2.43	1.57	1.53
4	C	803	12P	O10-C9	2.43	1.52	1.42
2	B	801	FDA	C9-C8	2.42	1.42	1.39
2	B	801	FDA	C5A-C4A	-2.42	1.34	1.39
2	B	801	FDA	C5X-C9A	-2.38	1.37	1.40
2	B	801	FDA	C7M-C7	2.32	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	802	2H5	F3-C3	-2.30	1.35	1.40
2	A	801	FDA	C4A-N9A	-2.25	1.33	1.37
5	D	804	MES	C5-N4	2.23	1.52	1.46
2	A	801	FDA	C4-N3	-2.15	1.34	1.38
2	C	801	FDA	O4'-C4'	-2.13	1.38	1.43
2	A	801	FDA	C8M-C8	2.12	1.55	1.51
2	D	801	FDA	C2-N1	-2.09	1.34	1.37
4	C	803	12P	O7-C8	2.08	1.51	1.42
2	A	801	FDA	O2'-C2'	-2.06	1.39	1.43
2	C	801	FDA	O2-C2	2.06	1.27	1.23
5	B	804	MES	C5-N4	2.02	1.52	1.46
2	D	801	FDA	C8A-N7A	2.02	1.35	1.31
2	B	801	FDA	C5A-C6A	-2.02	1.35	1.41

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	FDA	C9A-C5X-N5	7.08	128.00	119.37
2	D	801	FDA	C5A-C4A-N9A	6.81	113.23	105.81
2	D	801	FDA	C4A-C5A-N7A	-6.74	102.87	110.58
5	B	804	MES	O3S-S-C8	6.00	117.74	106.00
4	C	803	12P	O7-C8-C9	5.69	136.29	110.35
5	B	804	MES	O1S-S-C8	5.30	114.74	106.73
2	C	801	FDA	C9A-C5X-N5	5.10	125.58	119.37
5	B	804	MES	O2S-S-C8	-5.02	99.15	106.73
3	D	802	2H5	F3-C3-C4	-4.90	104.57	108.81
2	C	801	FDA	C4A-N9A-C8A	4.89	110.87	105.74
2	D	801	FDA	C6A-C5A-C4A	4.54	123.37	117.18
3	D	802	2H5	C4-C3-C2	4.52	116.74	111.50
2	B	801	FDA	N3A-C2A-N1A	-4.47	121.81	128.58
2	A	801	FDA	C4A-C5A-N7A	-4.46	105.48	110.58
2	C	801	FDA	C2A-N1A-C6A	4.45	126.04	118.73
2	D	801	FDA	C5'-C4'-C3'	-4.40	103.91	112.22
2	A	801	FDA	C2B-C3B-C4B	4.29	110.89	102.61
2	A	801	FDA	N3A-C2A-N1A	-4.21	122.21	128.58
2	D	801	FDA	N3-C2-N1	4.18	122.31	115.74
5	D	804	MES	O2S-S-C8	4.08	112.89	106.73
2	A	801	FDA	C6A-C5A-N7A	4.06	139.91	132.09
2	D	801	FDA	C6-C5X-C9A	-4.01	115.41	119.80
2	B	801	FDA	C4A-C5A-N7A	-4.01	106.00	110.58
3	C	802	2H5	F3-C3-C2	-3.99	105.35	108.81
2	B	801	FDA	C6-C5X-N5	-3.98	112.84	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	FDA	C6A-C5A-C4A	3.81	122.37	117.18
2	D	801	FDA	C4-N3-C2	-3.80	121.13	126.37
4	C	803	12P	C9-O10-C11	3.77	129.77	113.26
2	C	801	FDA	N3A-C2A-N1A	-3.77	122.88	128.58
3	A	802	2H5	F3-C3-C2	-3.70	105.61	108.81
5	B	804	MES	O3S-S-O2S	-3.67	102.23	111.40
3	D	802	2H5	O5-C1-C2	3.66	116.73	110.30
2	D	801	FDA	C5X-N5-C4X	-3.63	112.69	121.08
2	D	801	FDA	C1'-N10-C9A	3.59	127.61	120.63
5	B	804	MES	O1-C6-C5	-3.59	104.05	111.77
3	D	802	2H5	O2-C2-C1	3.57	117.48	109.25
2	B	801	FDA	C6-C5X-C9A	3.53	123.66	119.80
2	B	801	FDA	C9-C9A-C5X	-3.52	115.04	119.95
2	A	801	FDA	O2P-P-O3P	-3.42	98.02	107.27
2	C	801	FDA	C6A-C5A-C4A	3.40	121.83	117.18
2	A	801	FDA	C1'-N10-C9A	3.35	127.14	120.63
2	A	801	FDA	C5A-C4A-N9A	3.34	109.45	105.81
2	C	801	FDA	O2-C2-N3	-3.32	115.97	121.86
2	C	801	FDA	C5X-N5-C4X	-3.23	113.63	121.08
2	B	801	FDA	C9A-C5X-N5	3.20	123.27	119.37
2	B	801	FDA	O4-C4-C4X	-3.17	119.61	127.26
2	D	801	FDA	C5A-N7A-C8A	3.17	108.43	103.45
2	D	801	FDA	C2B-C1B-N9A	3.14	121.09	113.30
2	D	801	FDA	C9-C8-C7	-3.07	115.18	119.69
2	B	801	FDA	C2A-N1A-C6A	3.04	123.73	118.73
2	B	801	FDA	C5A-C4A-N3A	-3.02	122.56	126.72
2	C	801	FDA	C6-C5X-N5	-3.00	114.54	119.76
2	B	801	FDA	C9-C9A-N10	2.98	125.86	121.85
2	B	801	FDA	C5A-N7A-C8A	2.94	108.06	103.45
2	C	801	FDA	N3-C2-N1	2.88	120.26	115.74
2	B	801	FDA	N9A-C8A-N7A	-2.87	109.86	113.94
2	B	801	FDA	C8M-C8-C7	2.85	126.57	120.76
2	B	801	FDA	C4-C4X-N5	2.81	123.56	116.37
3	C	802	2H5	C3-C2-C1	-2.77	106.39	110.84
2	D	801	FDA	C2A-N1A-C6A	2.73	123.22	118.73
2	C	801	FDA	C8M-C8-C7	2.73	126.34	120.76
2	B	801	FDA	C5A-C4A-N9A	2.73	108.79	105.81
2	B	801	FDA	C2B-C3B-C4B	2.71	107.84	102.61
2	A	801	FDA	C4A-N9A-C1B	2.67	132.89	126.63
2	D	801	FDA	C5A-C6A-N1A	-2.67	110.73	117.51
2	A	801	FDA	C2A-N1A-C6A	2.66	123.10	118.73
2	B	801	FDA	C8M-C8-C9	-2.66	114.89	119.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	FDA	O2A-PA-O1A	2.65	124.77	112.44
3	C	802	2H5	C3-C4-C5	-2.64	106.56	109.68
5	B	804	MES	O1-C2-C3	-2.63	106.10	111.77
2	D	801	FDA	O2'-C2'-C3'	2.63	115.40	109.25
2	C	801	FDA	C5A-C6A-N1A	-2.62	110.87	117.51
2	B	801	FDA	O2B-C2B-C3B	2.58	120.09	111.82
2	D	801	FDA	O2B-C2B-C3B	2.56	120.02	111.82
2	A	801	FDA	C5X-C9A-N10	2.52	120.86	118.01
2	A	801	FDA	C6-C7-C8	-2.51	116.00	119.69
2	C	801	FDA	C4A-C5A-N7A	-2.49	107.73	110.58
2	D	801	FDA	O3B-C3B-C4B	2.49	118.22	111.08
2	A	801	FDA	C5'-C4'-C3'	-2.48	107.54	112.22
4	A	803	12P	C9-O10-C11	-2.47	102.43	113.26
3	B	802	2H5	O4-C4-C3	2.46	114.18	109.63
2	D	801	FDA	C5A-C4A-N3A	-2.39	123.42	126.72
3	A	802	2H5	O5-C5-C4	-2.38	105.40	109.70
2	D	801	FDA	C9-C9A-N10	-2.37	118.66	121.85
2	C	801	FDA	O2A-PA-O1A	2.37	123.45	112.44
2	C	801	FDA	N6A-C6A-N1A	2.35	123.61	118.38
2	D	801	FDA	C3B-C2B-C1B	2.33	105.88	101.46
3	B	802	2H5	O2-C2-C3	-2.31	105.35	109.63
2	D	801	FDA	C4'-C3'-C2'	-2.31	109.72	113.57
2	A	801	FDA	C9A-C9-C8	2.31	123.87	119.22
2	D	801	FDA	N3A-C4A-N9A	-2.31	123.24	127.17
2	C	801	FDA	C9-C8-C7	-2.27	116.36	119.69
2	B	801	FDA	C3B-C2B-C1B	2.27	105.75	101.46
2	D	801	FDA	O3'-C3'-C2'	2.25	114.05	108.93
4	C	803	12P	C14-O13-C12	2.23	120.89	113.06
2	C	801	FDA	C5A-C4A-N9A	-2.23	103.38	105.81
2	A	801	FDA	C9-C8-C7	-2.21	116.45	119.69
2	D	801	FDA	C5A-C6A-N6A	2.20	128.74	123.29
2	C	801	FDA	O2P-P-O3P	-2.20	101.32	107.27
4	A	803	12P	C3-O4-C5	2.20	120.76	113.06
2	C	801	FDA	O3P-PA-O1A	-2.19	104.11	110.70
2	B	801	FDA	C4X-C4-N3	2.19	118.14	112.13
2	C	801	FDA	O4B-C1B-N9A	2.16	112.24	108.09
5	B	804	MES	C5-N4-C3	2.14	113.46	108.84
2	A	801	FDA	O2A-PA-O3P	2.13	113.04	107.27
2	C	801	FDA	C2B-C1B-N9A	2.12	118.57	113.30
2	D	801	FDA	N9A-C8A-N7A	-2.12	110.93	113.94
2	C	801	FDA	N9A-C8A-N7A	-2.11	110.95	113.94
2	A	801	FDA	C6A-C5A-C4A	-2.08	114.33	117.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	FDA	O4-C4-C4X	-2.07	122.28	127.26
2	C	801	FDA	C5A-N7A-C8A	2.07	106.70	103.45
2	B	801	FDA	C5'-C4'-C3'	-2.06	108.33	112.22
2	B	801	FDA	O2-C2-N1	2.06	125.53	121.86
2	C	801	FDA	O2B-C2B-C3B	2.05	118.37	111.82
4	A	803	12P	O10-C11-C12	-2.03	101.08	110.35
2	C	801	FDA	N3A-C4A-N9A	2.03	130.62	127.17

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	803	12P	O7-C8-C9-O10
2	C	801	FDA	PA-O3P-P-O5'
4	C	803	12P	C8-C9-O10-C11
4	C	803	12P	C5-C6-O7-C8
2	C	801	FDA	O4B-C4B-C5B-O5B
2	B	801	FDA	O4B-C4B-C5B-O5B

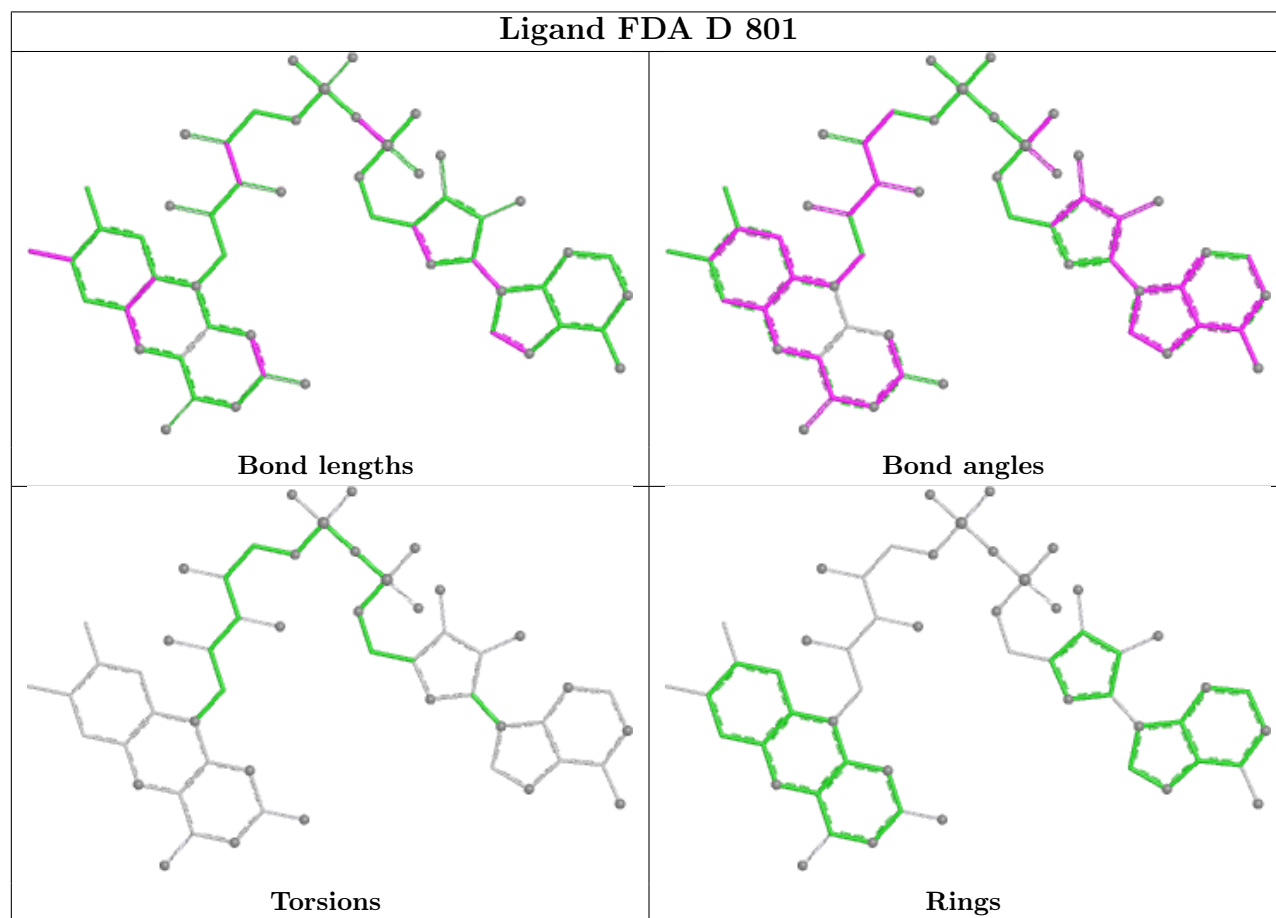
There are no ring outliers.

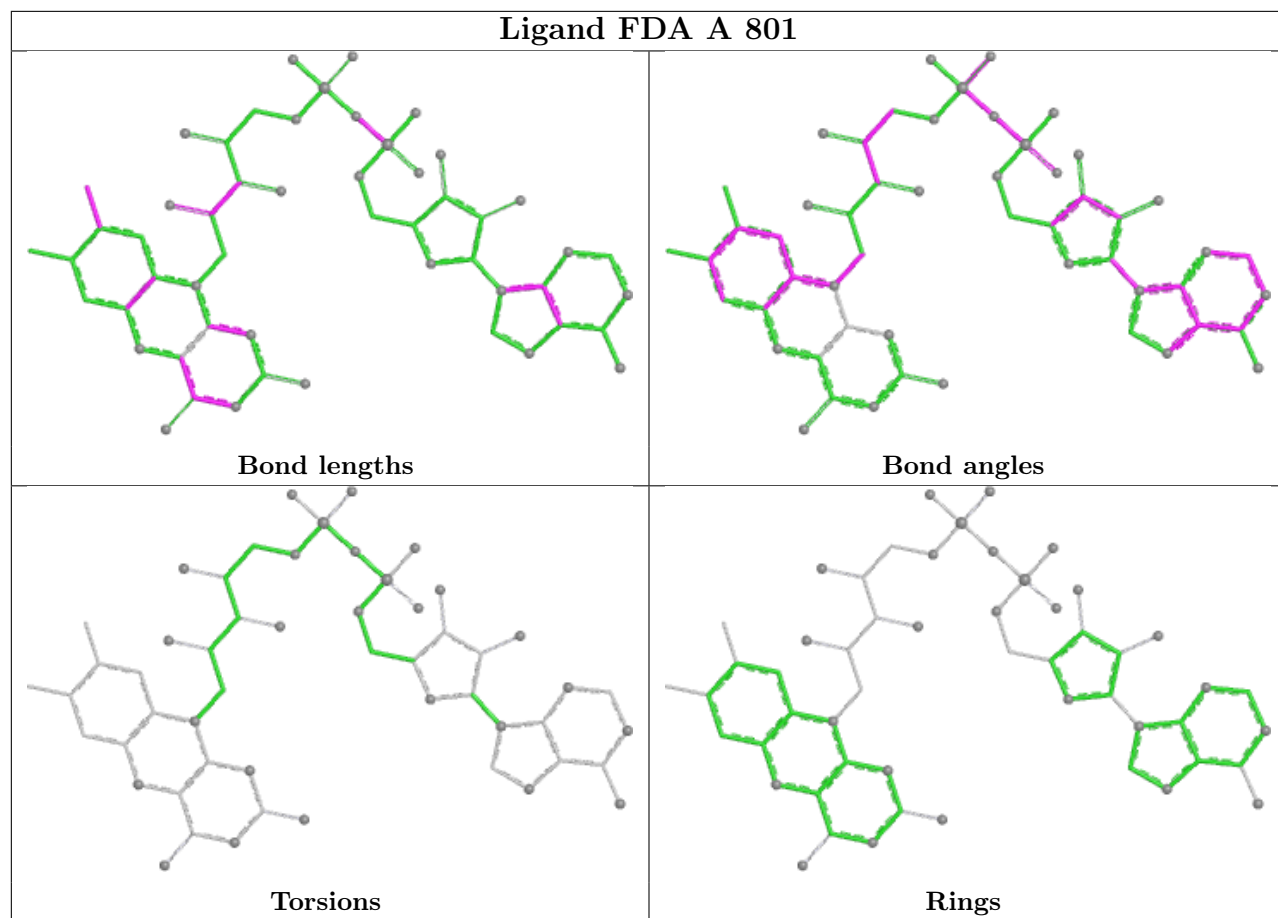
10 monomers are involved in 22 short contacts:

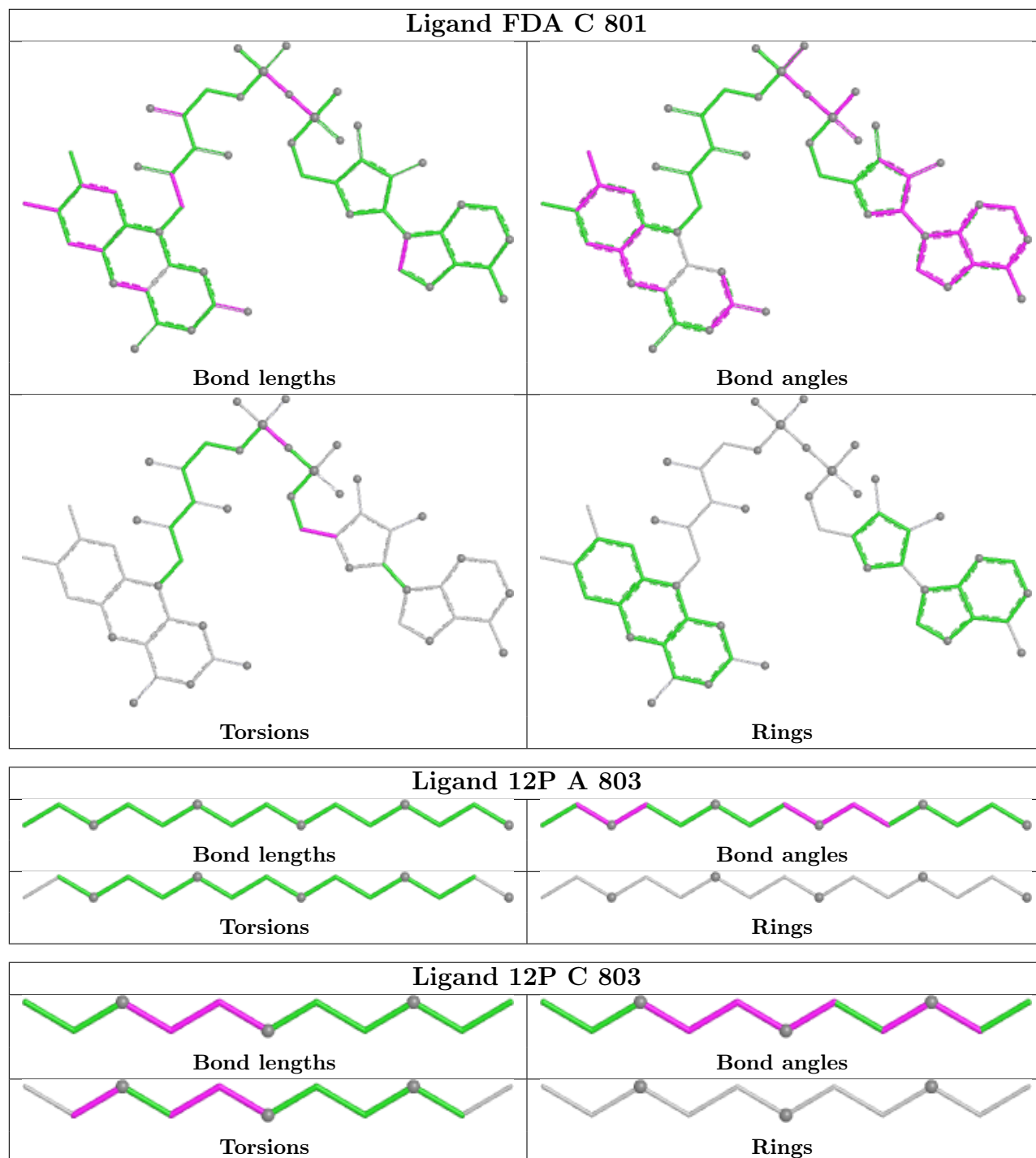
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	804	MES	14	0
3	A	802	2H5	1	0
2	D	801	FDA	2	0
3	C	802	2H5	1	0
2	A	801	FDA	1	0
2	C	801	FDA	3	0
3	D	802	2H5	1	0
4	C	803	12P	1	0
3	B	802	2H5	1	0
2	B	801	FDA	1	0

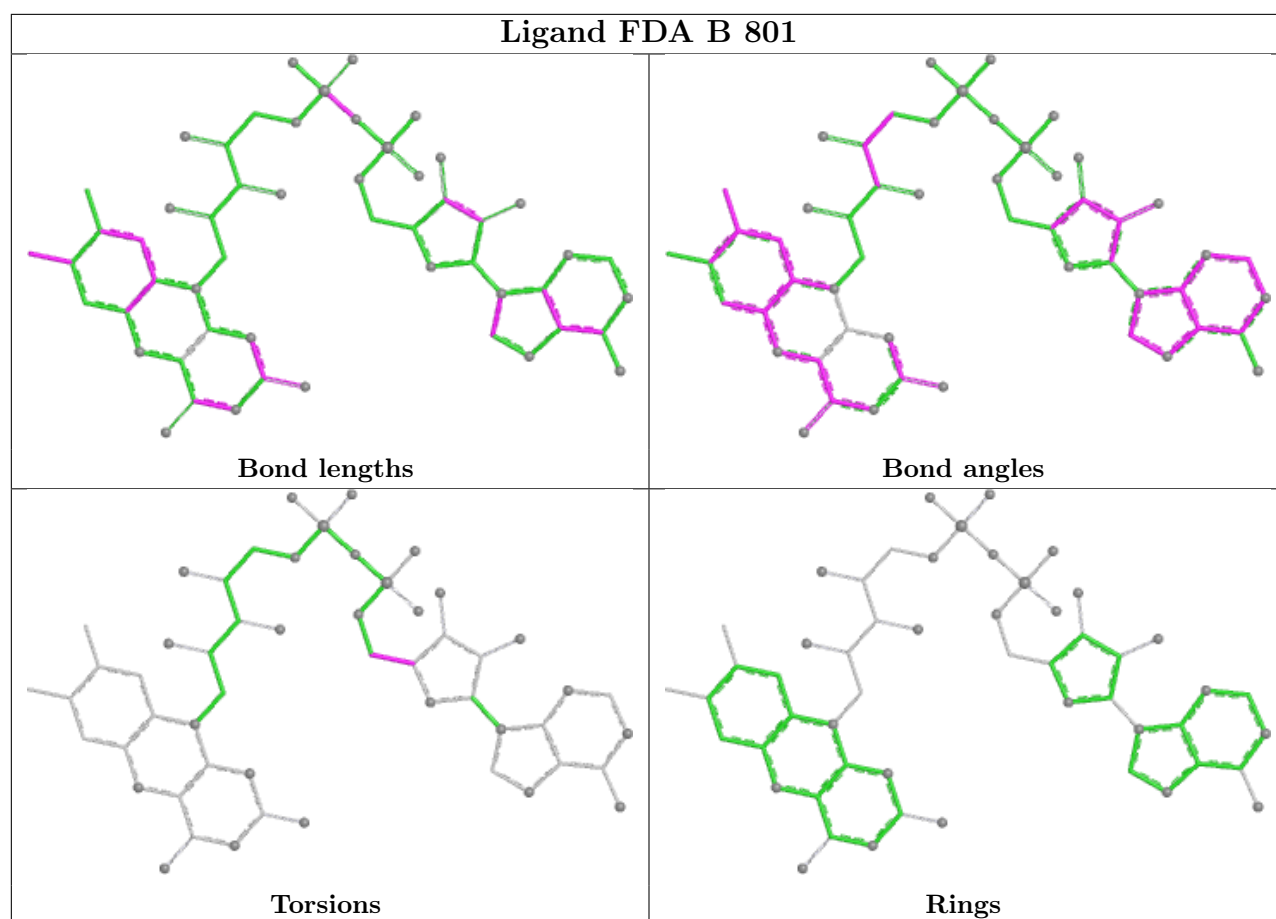
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	576/633 (90%)	-0.15	17 (2%) 52 56	10, 19, 35, 61	8 (1%)
1	B	576/633 (90%)	-0.17	17 (2%) 52 56	10, 18, 33, 63	10 (1%)
1	C	573/633 (90%)	0.28	19 (3%) 49 53	11, 27, 47, 75	4 (0%)
1	D	576/633 (90%)	0.07	19 (3%) 49 53	11, 23, 43, 94	5 (0%)
All	All	2301/2532 (90%)	0.01	72 (3%) 51 55	10, 22, 41, 94	27 (1%)

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	389	LEU	5.4
1	D	45	ILE	5.0
1	B	45	ILE	4.7
1	A	82	SER	4.0
1	C	618	PHE	4.0
1	B	618	PHE	3.9
1	D	44	ASP	3.8
1	C	291	LEU	3.6
1	C	343	ALA	3.5
1	A	343	ALA	3.4
1	A	400	SER	3.4
1	D	343	ALA	3.3
1	B	345	PRO	3.3
1	C	82	SER	3.3
1	A	45	ILE	3.2
1	B	343	ALA	3.2
1	B	132[A]	GLN	3.2
1	A	618	PHE	3.1
1	D	383	ARG	3.1
1	B	133	ALA	3.1
1	D	81	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	342	PRO	2.9
1	B	400	SER	2.9
1	D	459	VAL	2.9
1	B	43[A]	MET	2.9
1	D	618	PHE	2.9
1	A	389	LEU	2.9
1	D	390	THR	2.8
1	C	459	VAL	2.8
1	D	342	PRO	2.8
1	A	451	ARG	2.8
1	B	232	GLY	2.7
1	D	345	PRO	2.7
1	C	342	PRO	2.6
1	B	185	LYS	2.6
1	D	576	LYS	2.6
1	A	387	GLY	2.6
1	A	401	THR	2.6
1	C	451	ARG	2.6
1	D	185	LYS	2.6
1	C	188	ALA	2.6
1	C	345	PRO	2.6
1	D	385	THR	2.5
1	C	398	GLY	2.5
1	C	385	THR	2.5
1	D	82	SER	2.4
1	B	100	ILE	2.4
1	B	342	PRO	2.4
1	A	100	ILE	2.4
1	C	614	THR	2.3
1	C	346	PRO	2.3
1	B	81	ASP	2.3
1	B	451	ARG	2.3
1	A	459	VAL	2.3
1	A	399	ALA	2.2
1	A	345	PRO	2.2
1	A	386	PRO	2.2
1	A	385	THR	2.2
1	B	44	ASP	2.2
1	D	490	LYS	2.2
1	C	81	ASP	2.1
1	C	615	PRO	2.1
1	C	617	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	133	ALA	2.1
1	B	490	LYS	2.1
1	C	185	LYS	2.1
1	D	285	ARG	2.0
1	D	43	MET	2.0
1	A	285	ARG	2.0
1	C	290	ALA	2.0
1	B	459	VAL	2.0
1	C	309	PHE	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](#)

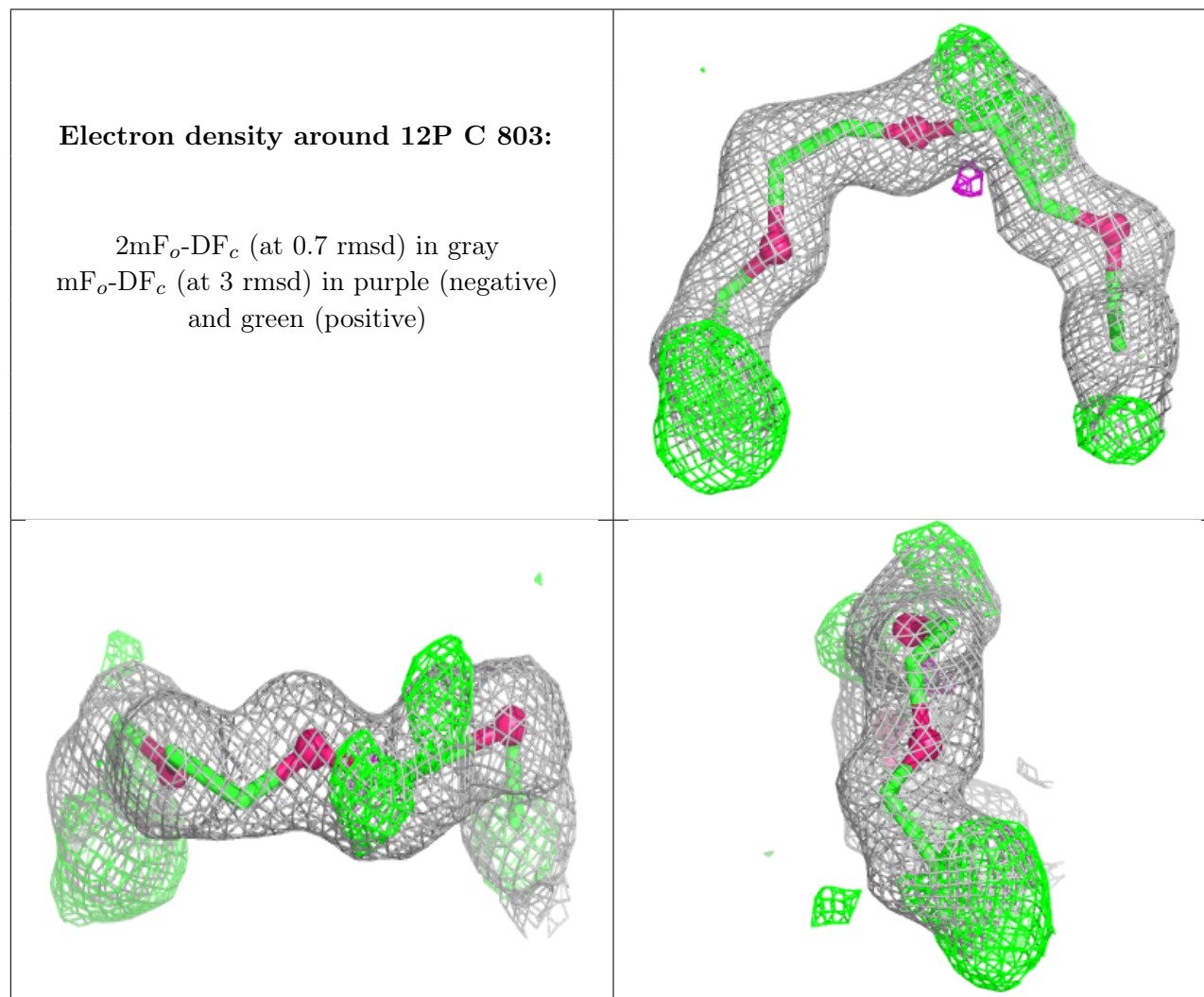
There are no oligosaccharides in this entry.

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.

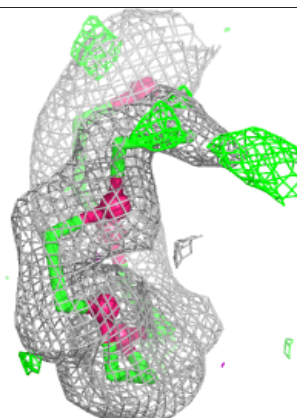
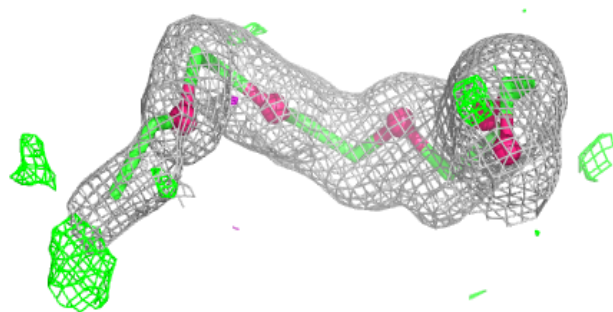
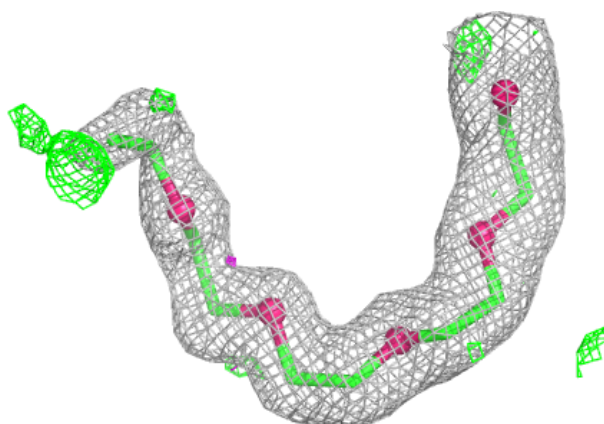
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	12P	C	803	11/37	0.83	0.16	27,31,34,35	0
5	MES	B	804	12/12	0.89	0.13	22,30,33,35	0
4	12P	D	803	14/37	0.90	0.12	24,30,40,42	0
4	12P	A	803	15/37	0.90	0.14	25,32,43,48	0
5	MES	D	804	12/12	0.94	0.10	28,31,40,42	0
4	12P	B	803	16/37	0.95	0.09	26,28,48,61	0
3	2H5	C	802	12/12	0.96	0.07	22,23,24,24	0
2	FDA	C	801	53/53	0.97	0.06	18,22,24,27	0
2	FDA	D	801	53/53	0.98	0.05	14,17,22,23	0
3	2H5	D	802	12/12	0.98	0.05	19,20,23,23	0
3	2H5	A	802	12/12	0.98	0.05	16,18,19,19	0
3	2H5	B	802	12/12	0.98	0.04	15,17,19,19	0
2	FDA	A	801	53/53	0.99	0.04	12,14,16,17	0
2	FDA	B	801	53/53	0.99	0.04	11,13,15,17	0

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

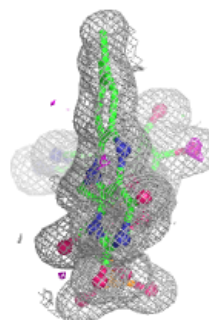
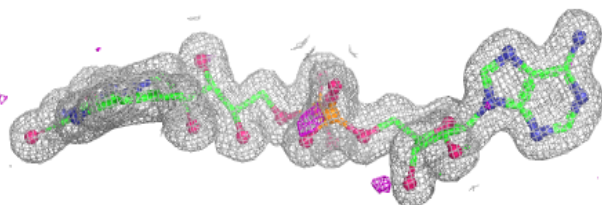
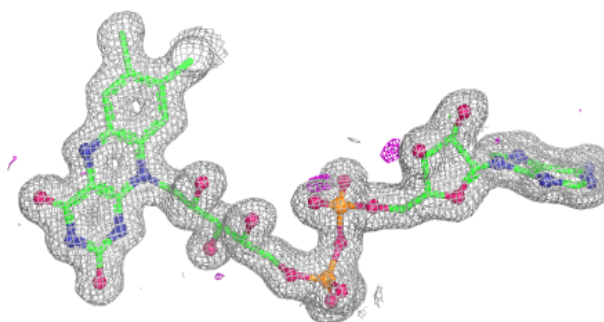


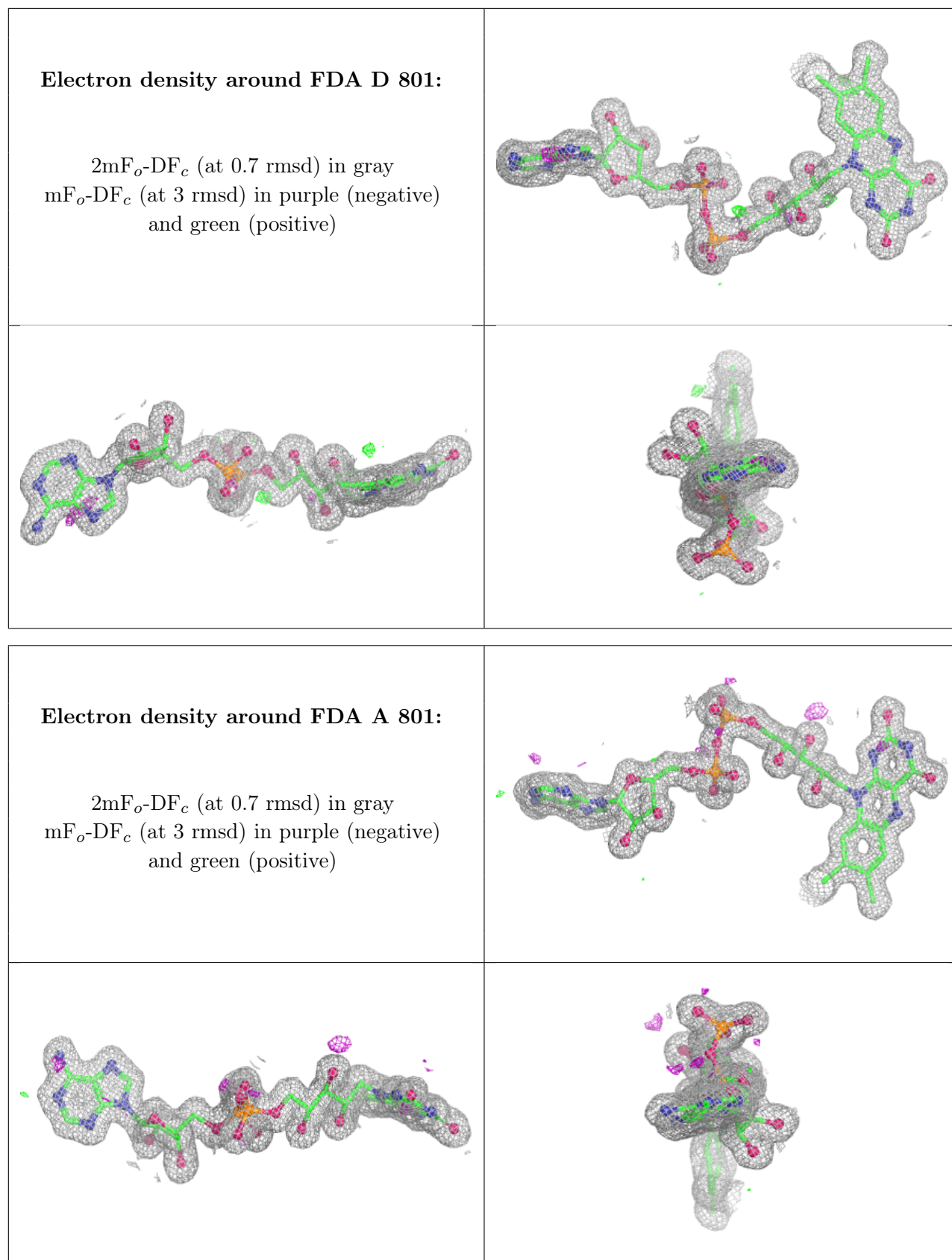
Electron density around 12P A 803:

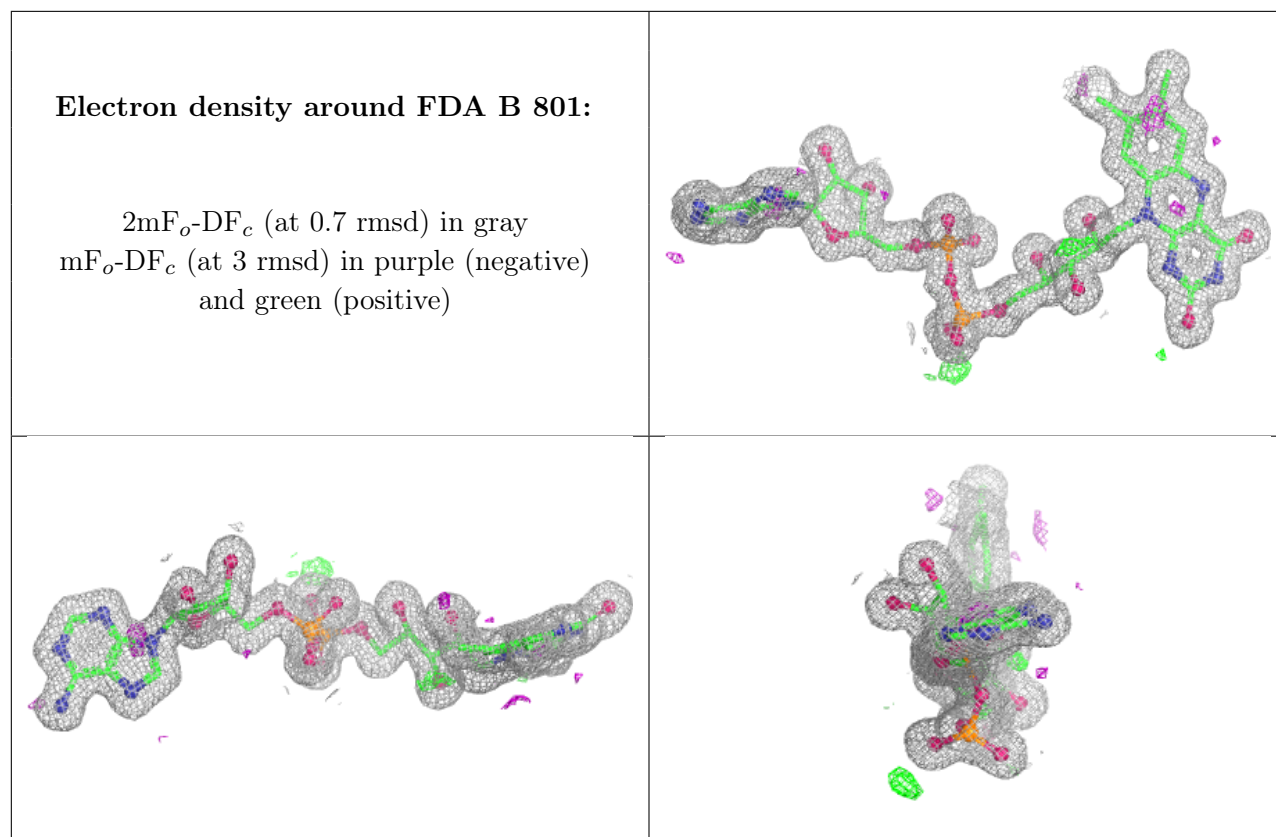
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around FDA C 801:**

$2mF_o-DF_c$ (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.