



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 04:19 PM EDT

PDB ID : 4MOI / pdb_00004moi
Title : Pyranose 2-oxidase H450G/V546C double mutant with 3-fluorinated glucose
Authors : Tan, T.C.; Spadiut, O.; Gandini, R.; Haltrich, D.; Divne, C.
Deposited on : 2013-09-12
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

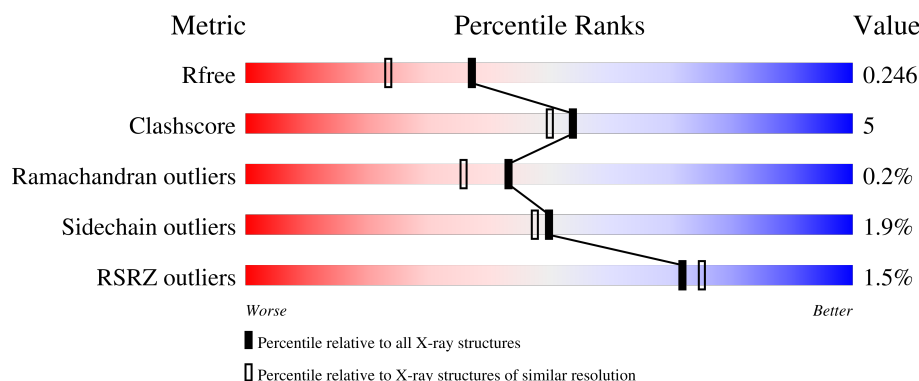
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	% 75% 15% • 9%
1	B	633	% 78% 13% 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9835 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
1	A	576	Total	C	N	O	S	0	0	0
			4535	2862	775	872	26			
1	B	576	Total	C	N	O	S	0	0	0
			4535	2862	775	872	26			

There are 28 discrepancies between the modelled and reference sequences:

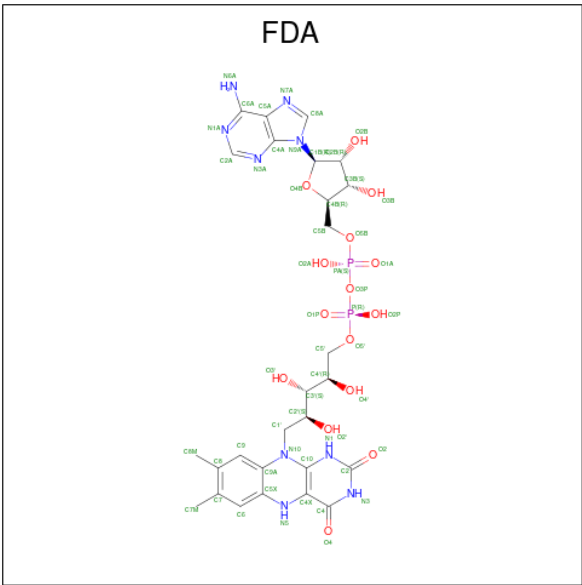
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	SER	SEE REMARK 999	UNP Q7ZA32
A	450	GLY	HIS	engineered mutation	UNP Q7ZA32
A	546	CYS	VAL	engineered mutation	UNP Q7ZA32
A	623	ALA	-	expression tag	UNP Q7ZA32
A	624	ALA	-	expression tag	UNP Q7ZA32
A	625	ALA	-	expression tag	UNP Q7ZA32
A	626	LEU	-	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	SEE REMARK 999	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
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

Continued on next page...

Continued from previous page...

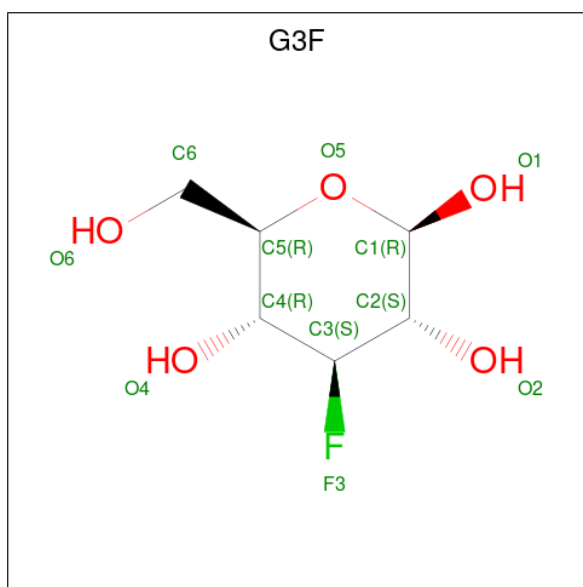
Chain	Residue	Modelled	Actual	Comment	Reference
B	631	HIS	-	expression tag	UNP Q7ZA32
B	632	HIS	-	expression tag	UNP Q7ZA32
B	633	HIS	-	expression tag	UNP Q7ZA32

- Molecule 2 is DIHYDROFLAVINE-ADENINE DINUCLEOTIDE (CCD ID: FDA) (formula: C₂₇H₃₅N₉O₁₅P₂).



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 3-deoxy-3-fluoro-beta-D-glucopyranose (CCD ID: G3F) (formula: C₆H₁₁FO₅).



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		

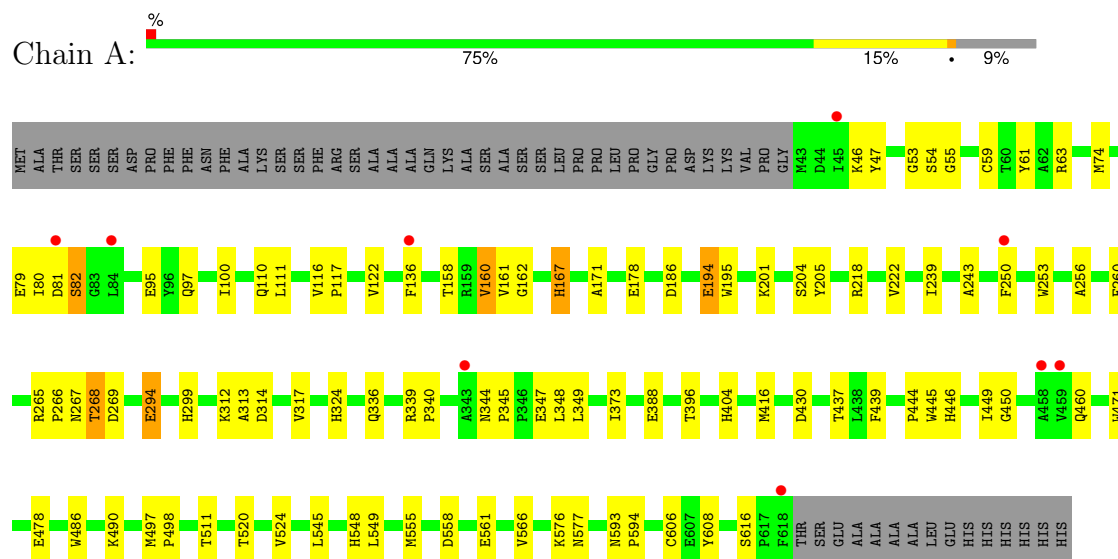
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	300	Total	O	0	0
			300	300		
4	B	335	Total	O	0	0
			335	335		

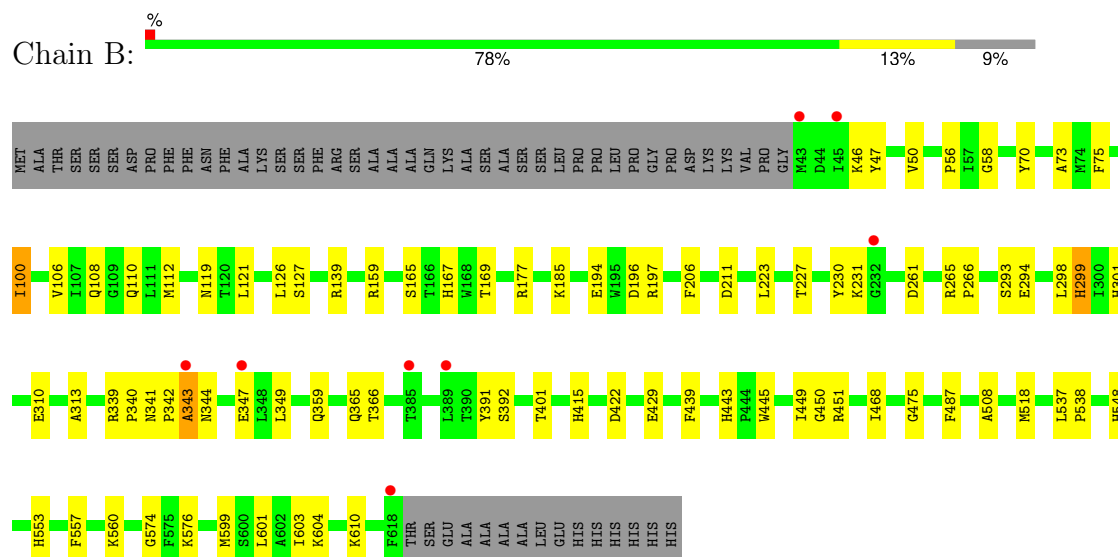
3 Residue-property plots [i](#)

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	101.50Å 101.50Å 238.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.88 – 1.90 45.88 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.88-1.90) 100.0 (45.88-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.196 , 0.245 0.203 , 0.246	Depositor DCC
R_{free} test set	2000 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å ²)	22.8	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 34.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9835	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.77 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6806e-04.*

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: G3F, 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	1.39	24/4650 (0.5%)	1.23	12/6321 (0.2%)
1	B	1.36	19/4650 (0.4%)	1.19	8/6321 (0.1%)
All	All	1.37	43/9300 (0.5%)	1.21	20/12642 (0.2%)

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	345	PRO	CA-C	7.09	1.56	1.52
1	B	443	HIS	CG-CD2	6.92	1.43	1.35
1	A	299	HIS	ND1-CE1	6.58	1.39	1.32
1	B	553	HIS	CG-CD2	6.36	1.42	1.35
1	A	117	PRO	N-CA	-6.34	1.40	1.47
1	B	443	HIS	ND1-CE1	6.29	1.38	1.32
1	B	127	SER	N-CA	-6.28	1.38	1.45
1	B	601	LEU	C-O	6.18	1.31	1.24
1	A	299	HIS	CG-CD2	5.98	1.42	1.35
1	A	437	THR	C-O	-5.92	1.17	1.24
1	B	391	TYR	C-O	-5.91	1.16	1.23
1	B	449	ILE	C-O	-5.78	1.17	1.24
1	B	75	PHE	CA-C	5.72	1.59	1.52
1	A	549	LEU	C-O	-5.64	1.17	1.23
1	B	415	HIS	CG-ND1	-5.63	1.32	1.38
1	A	446	HIS	CG-ND1	-5.62	1.32	1.38
1	B	261	ASP	CA-C	5.57	1.60	1.52
1	A	324	HIS	ND1-CE1	5.56	1.38	1.32
1	A	239	ILE	C-O	-5.51	1.18	1.25
1	A	594	PRO	C-O	-5.50	1.17	1.24
1	A	446	HIS	CD2-NE2	-5.46	1.31	1.37
1	A	80	ILE	C-O	-5.46	1.18	1.24
1	A	606	CYS	N-CA	5.46	1.53	1.46
1	B	301	HIS	CE1-NE2	5.44	1.38	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	195	TRP	NE1-CE2	-5.41	1.31	1.37
1	B	341	ASN	C-O	-5.41	1.20	1.25
1	B	450	GLY	C-O	-5.36	1.16	1.23
1	A	548	HIS	ND1-CE1	5.34	1.37	1.32
1	B	106	VAL	CA-CB	5.34	1.60	1.54
1	B	299	HIS	CG-ND1	-5.33	1.32	1.38
1	A	450	GLY	C-O	-5.30	1.16	1.23
1	A	222	VAL	C-O	-5.27	1.18	1.24
1	A	486	TRP	NE1-CE2	-5.23	1.31	1.37
1	A	171	ALA	CA-C	-5.14	1.46	1.52
1	A	167	HIS	C-O	-5.14	1.17	1.24
1	B	365	GLN	N-CA	-5.10	1.39	1.45
1	B	126	LEU	C-O	-5.10	1.17	1.23
1	A	446	HIS	CA-C	-5.09	1.46	1.52
1	A	160	VAL	C-O	5.08	1.29	1.23
1	B	415	HIS	ND1-CE1	5.02	1.37	1.32
1	A	498	PRO	C-O	5.01	1.29	1.23
1	B	553	HIS	ND1-CE1	5.01	1.37	1.32
1	A	260	PHE	N-CA	5.00	1.52	1.46

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	349	LEU	CB-CA-C	-8.52	105.15	111.20
1	B	508	ALA	N-CA-C	-7.88	100.72	110.41
1	A	396	THR	CA-C-N	-7.68	111.85	119.76
1	A	396	THR	C-N-CA	-7.68	111.85	119.76
1	A	116	VAL	CA-C-N	-7.31	113.28	120.52
1	A	116	VAL	C-N-CA	-7.31	113.28	120.52
1	A	268	THR	CB-CA-C	-6.47	100.04	110.79
1	B	560	LYS	N-CA-C	6.42	118.16	111.03
1	A	324	HIS	N-CA-C	6.28	120.15	112.23
1	B	58	GLY	N-CA-C	-6.02	105.51	112.73
1	A	616	SER	CA-C-N	-5.88	113.88	119.76
1	A	616	SER	C-N-CA	-5.88	113.88	119.76
1	B	422	ASP	CA-C-N	-5.80	114.27	121.00
1	B	422	ASP	C-N-CA	-5.80	114.27	121.00
1	A	55	GLY	CA-C-N	5.42	124.93	119.19
1	A	55	GLY	C-N-CA	5.42	124.93	119.19
1	B	366	THR	N-CA-C	5.25	118.14	109.85
1	B	46	LYS	N-CA-C	5.06	117.66	109.06
1	A	497	MET	CA-C-N	-5.03	114.58	119.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	497	MET	C-N-CA	-5.03	114.58	119.76

There are no chirality outliers.

There are no planarity outliers.

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	4535	0	4380	49	0
1	B	4535	0	4380	37	0
2	A	53	0	29	3	0
2	B	53	0	30	3	0
3	A	12	0	11	2	0
3	B	12	0	11	2	0
4	A	300	0	0	5	0
4	B	335	0	0	4	0
All	All	9835	0	8841	88	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 (88) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ILE:HG22	4:A:1064:HOH:O	1.62	0.99
1:B:342:PRO:O	1:B:343:ALA:HB3	1.73	0.89
1:B:342:PRO:O	1:B:343:ALA:CB	2.23	0.85
1:B:110:GLN:HE21	1:B:167:HIS:HD1	1.25	0.84
1:A:110:GLN:HE21	1:A:167:HIS:HD1	1.34	0.75
2:A:801:FDA:N5	3:A:802:G3F:H2	2.02	0.75
1:B:299:HIS:HE1	1:B:310:GLU:OE2	1.76	0.68
1:A:558:ASP:OD2	1:A:561:GLU:HG3	1.95	0.66
1:B:604:LYS:HE3	4:B:1066:HOH:O	1.94	0.66
1:A:100:ILE:HD11	4:A:959:HOH:O	1.99	0.63
1:B:100:ILE:HD12	1:B:100:ILE:O	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:HIS:HE1	4:A:1084:HOH:O	1.83	0.62
1:B:47:TYR:O	1:B:313:ALA:HA	2.00	0.61
1:A:97:GLN:HG3	1:A:250:PHE:CE2	2.37	0.60
1:B:299:HIS:CE1	1:B:310:GLU:OE2	2.56	0.59
1:B:223:LEU:O	1:B:227:THR:HG23	2.02	0.58
1:A:347:GLU:OE1	1:A:347:GLU:N	2.30	0.58
1:B:194:GLU:OE2	1:B:197:ARG:NH2	2.34	0.58
1:A:218:ARG:HG3	1:A:430:ASP:OD2	2.03	0.57
1:B:50:VAL:HG12	1:B:73:ALA:HB3	1.87	0.57
1:A:336:GLN:NE2	1:A:344:ASN:O	2.37	0.57
1:B:185:LYS:HB3	1:B:557:PHE:CE2	2.43	0.53
1:A:194:GLU:HA	1:A:194:GLU:OE1	2.08	0.53
1:A:81:ASP:N	1:A:81:ASP:OD1	2.38	0.53
1:A:167:HIS:CD2	2:A:801:FDA:HM73	2.44	0.52
1:A:449:ILE:HG12	1:A:471:TRP:CE3	2.45	0.51
2:A:801:FDA:C5X	3:A:802:G3F:H2	2.41	0.50
1:A:347:GLU:CD	1:A:348:LEU:H	2.20	0.50
1:B:265:ARG:HA	1:B:266:PRO:C	2.37	0.50
1:B:56:PRO:HD3	1:B:165:SER:HB3	1.93	0.50
1:A:46:LYS:HD3	1:A:312:LYS:CG	2.42	0.49
2:B:801:FDA:N5	3:B:802:G3F:H2	2.28	0.49
1:B:344:ASN:O	1:B:344:ASN:OD1	2.31	0.48
1:A:178:GLU:CD	1:A:439:PHE:HE1	2.22	0.47
1:B:169:THR:HG22	1:B:169:THR:O	2.15	0.47
1:A:79:GLU:C	1:A:161:VAL:HG23	2.39	0.47
1:B:548:HIS:CE1	3:B:802:G3F:HO2	2.30	0.47
1:B:445:TRP:CG	1:B:518:MET:HG3	2.50	0.47
1:A:47:TYR:O	1:A:313:ALA:HA	2.16	0.46
1:A:460:GLN:O	1:A:460:GLN:NE2	2.49	0.46
1:A:558:ASP:CG	1:A:561:GLU:HG3	2.41	0.45
1:A:339:ARG:O	1:A:340:PRO:C	2.58	0.45
1:B:159:ARG:HA	2:B:801:FDA:O2B	2.17	0.45
1:A:520:THR:O	1:A:524:VAL:HG23	2.16	0.45
1:B:211:ASP:OD1	1:B:211:ASP:C	2.59	0.45
1:A:388:GLU:OE1	1:A:388:GLU:HA	2.17	0.44
1:A:218:ARG:HD2	4:A:1001:HOH:O	2.18	0.44
1:A:444:PRO:HD2	1:A:445:TRP:CZ3	2.52	0.44
1:A:46:LYS:HD3	1:A:312:LYS:HG2	1.99	0.44
1:B:487:PHE:N	1:B:487:PHE:CD2	2.86	0.44
1:A:95:GLU:HG3	1:B:112:MET:HE2	2.00	0.44
1:B:599:MET:O	1:B:603:ILE:HG13	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:608:TYR:C	1:A:608:TYR:CD1	2.96	0.43
1:A:478:GLU:HG3	1:A:511:THR:OG1	2.18	0.43
1:B:293:SER:HA	1:B:574:GLY:O	2.19	0.43
1:B:294:GLU:OE2	1:B:576:LYS:HE3	2.17	0.43
1:A:158:THR:HG22	1:A:160:VAL:HG22	2.01	0.43
1:A:53:GLY:O	1:A:74:MET:HE2	2.19	0.43
1:A:201:LYS:O	1:A:204:SER:HB3	2.19	0.43
1:A:268:THR:OG1	1:A:269:ASP:N	2.51	0.43
1:B:169:THR:H	2:B:801:FDA:HN5	1.66	0.43
1:A:63:ARG:NE	1:A:205:TYR:CE1	2.87	0.43
1:A:294:GLU:OE2	1:A:576:LYS:HE3	2.19	0.43
1:A:347:GLU:CG	1:A:348:LEU:N	2.82	0.43
1:B:342:PRO:HD2	4:B:1194:HOH:O	2.19	0.43
1:B:537:LEU:HB3	1:B:538:PRO:HD2	2.00	0.43
1:A:267:ASN:O	1:A:268:THR:C	2.60	0.42
1:B:70:TYR:OH	1:B:610:LYS:HA	2.19	0.42
1:A:54:SER:O	1:A:162:GLY:HA2	2.20	0.42
1:A:61:TYR:CG	1:A:317:VAL:HG11	2.55	0.41
1:B:119:ASN:O	1:B:139:ARG:NH2	2.51	0.41
1:A:243:ALA:HB2	1:A:253:TRP:CE3	2.55	0.41
1:A:265:ARG:HA	1:A:266:PRO:C	2.46	0.41
1:B:169:THR:O	1:B:169:THR:CG2	2.68	0.41
1:B:230:TYR:O	1:B:231:LYS:C	2.63	0.41
1:B:177:ARG:HG3	4:B:1006:HOH:O	2.21	0.41
1:A:122:VAL:HG22	1:A:136:PHE:HZ	1.85	0.41
1:A:555:MET:HA	1:A:566:VAL:O	2.20	0.41
1:B:339:ARG:HA	1:B:340:PRO:HD3	1.95	0.41
1:B:359:GLN:HG2	1:B:475:GLY:O	2.20	0.41
1:A:347:GLU:CD	1:A:348:LEU:N	2.79	0.41
1:A:416:MET:HB3	1:A:416:MET:HE2	1.80	0.41
1:A:59:CYS:SG	1:A:256:ALA:HB1	2.61	0.41
1:A:111:LEU:HD23	1:A:111:LEU:HA	1.87	0.41
1:A:314:ASP:O	1:A:577:ASN:HB2	2.20	0.41
1:A:545:LEU:HD12	4:A:1031:HOH:O	2.20	0.40
1:B:196:ASP:HB2	4:B:1230:HOH:O	2.21	0.40
1:B:439:PHE:CD1	1:B:439:PHE:C	3.00	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	574/633 (91%)	551 (96%)	22 (4%)	1 (0%)	43	36
1	B	574/633 (91%)	559 (97%)	14 (2%)	1 (0%)	43	36
All	All	1148/1266 (91%)	1110 (97%)	36 (3%)	2 (0%)	43	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	SER
1	B	343	ALA

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	503/547 (92%)	495 (98%)	8 (2%)	55	54
1	B	503/547 (92%)	492 (98%)	11 (2%)	45	42
All	All	1006/1094 (92%)	987 (98%)	19 (2%)	50	47

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	SER
1	A	186	ASP
1	A	194	GLU
1	A	294	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	349	LEU
1	A	373	ILE
1	A	490	LYS
1	A	593	ASN
1	B	100	ILE
1	B	108	GLN
1	B	121	LEU
1	B	206	PHE
1	B	298	LEU
1	B	347	GLU
1	B	392	SER
1	B	401	THR
1	B	429	GLU
1	B	451	ARG
1	B	468	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	207	GLN
1	A	404	HIS
1	B	110	GLN
1	B	257	ASN
1	B	299	HIS
1	B	344	ASN

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

4 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
3	G3F	B	802	-	12,12,12	0.97	0	17,17,17	2.46	7 (41%)
2	FDA	B	801	1	57,58,58	1.75	9 (15%)	78,89,89	2.71	36 (46%)
3	G3F	A	802	-	12,12,12	1.17	2 (16%)	17,17,17	2.16	6 (35%)
2	FDA	A	801	1	57,58,58	1.74	12 (21%)	78,89,89	2.35	35 (44%)

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
3	G3F	B	802	-	-	0/2/22/22	0/1/1/1
2	FDA	B	801	1	-	4/34/50/50	0/6/6/6
3	G3F	A	802	-	-	0/2/22/22	0/1/1/1
2	FDA	A	801	1	-	3/34/50/50	0/6/6/6

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	FDA	P-O3P	6.58	1.66	1.59
2	B	801	FDA	C8A-N9A	-6.50	1.26	1.37
2	A	801	FDA	PA-O3P	4.80	1.64	1.59
2	B	801	FDA	C8M-C8	4.22	1.58	1.51
2	B	801	FDA	C4X-C4	4.09	1.54	1.41
2	B	801	FDA	C2A-N1A	3.40	1.40	1.33
2	B	801	FDA	C2A-N3A	3.08	1.39	1.33
2	B	801	FDA	C5X-N5	-3.03	1.34	1.39
2	A	801	FDA	C4X-C4	2.90	1.50	1.41
2	B	801	FDA	O4B-C1B	2.67	1.48	1.42
2	A	801	FDA	O3B-C3B	-2.60	1.36	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	G3F	F3-C3	-2.55	1.35	1.40
2	A	801	FDA	P-O1P	-2.46	1.42	1.50
2	A	801	FDA	C8A-N7A	2.28	1.36	1.31
2	A	801	FDA	C1'-C2'	-2.28	1.49	1.52
2	A	801	FDA	C5A-N7A	-2.26	1.35	1.39
2	B	801	FDA	O4B-C4B	-2.21	1.40	1.45
2	A	801	FDA	C5X-N5	-2.17	1.36	1.39
2	A	801	FDA	C8A-N9A	-2.16	1.33	1.37
2	A	801	FDA	C2A-N3A	2.11	1.37	1.33
3	A	802	G3F	C3-C4	2.11	1.54	1.52
2	A	801	FDA	O2B-C2B	-2.10	1.37	1.43
2	B	801	FDA	P-O5'	2.02	1.67	1.59

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	FDA	C4A-N9A-C8A	8.65	114.82	105.74
2	B	801	FDA	C2B-C1B-N9A	7.34	131.54	113.30
2	A	801	FDA	C2B-C1B-N9A	6.99	130.67	113.30
2	B	801	FDA	N3A-C2A-N1A	-6.29	119.06	128.58
3	B	802	G3F	F3-C3-C4	-5.63	103.94	108.81
2	B	801	FDA	N3A-C4A-N9A	5.25	136.09	127.17
2	B	801	FDA	N9A-C8A-N7A	-5.23	106.52	113.94
3	A	802	G3F	F3-C3-C4	-5.22	104.30	108.81
2	A	801	FDA	O4-C4-C4X	-5.13	114.89	127.26
2	A	801	FDA	N3A-C2A-N1A	-4.65	121.54	128.58
2	B	801	FDA	O4-C4-N3	4.65	128.85	120.11
2	A	801	FDA	O2A-PA-O3P	4.44	119.27	107.27
2	B	801	FDA	O4B-C1B-N9A	4.25	116.25	108.09
2	A	801	FDA	O4B-C1B-N9A	4.24	116.22	108.09
2	A	801	FDA	N9A-C8A-N7A	-4.18	108.01	113.94
3	B	802	G3F	O5-C5-C4	4.14	117.15	109.70
2	B	801	FDA	O2B-C2B-C1B	4.13	124.32	110.10
2	B	801	FDA	O3B-C3B-C4B	4.12	122.92	111.08
2	B	801	FDA	O2A-PA-O3P	4.11	118.39	107.27
2	A	801	FDA	C4A-N9A-C8A	4.08	110.02	105.74
2	B	801	FDA	O4B-C4B-C3B	3.95	112.99	105.15
2	B	801	FDA	C5A-C4A-N3A	-3.91	121.34	126.72
3	B	802	G3F	C3-C2-C1	3.85	117.03	110.84
2	A	801	FDA	O2'-C2'-C3'	3.81	118.16	109.25
2	B	801	FDA	C5A-N7A-C8A	3.70	109.26	103.45
2	A	801	FDA	C6A-C5A-C4A	3.65	122.16	117.18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	FDA	O4-C4-C4X	-3.62	118.53	127.26
3	A	802	G3F	C3-C4-C5	3.58	113.92	109.68
3	B	802	G3F	O4-C4-C5	3.46	117.86	109.32
2	B	801	FDA	C6A-C5A-C4A	3.46	121.91	117.18
2	A	801	FDA	C5A-N7A-C8A	3.45	108.88	103.45
2	B	801	FDA	C2A-N1A-C6A	3.39	124.30	118.73
2	B	801	FDA	C4A-C5A-N7A	-3.38	106.72	110.58
2	A	801	FDA	O4B-C4B-C3B	3.36	111.82	105.15
2	A	801	FDA	O3B-C3B-C4B	3.33	120.66	111.08
3	A	802	G3F	F3-C3-C2	3.32	111.68	108.81
2	A	801	FDA	O4B-C4B-C5B	3.25	119.75	109.33
2	B	801	FDA	O2-C2-N1	-3.21	116.16	121.86
2	A	801	FDA	O2B-C2B-C1B	3.21	121.15	110.10
2	A	801	FDA	N6A-C6A-N1A	3.08	125.25	118.38
2	A	801	FDA	O2P-P-O1P	3.05	126.61	112.44
2	A	801	FDA	O3P-PA-O1A	-3.00	101.69	110.70
2	B	801	FDA	C5A-C4A-N9A	-2.98	102.56	105.81
2	A	801	FDA	C3B-C2B-C1B	2.98	107.09	101.46
2	B	801	FDA	C9-C8-C7	-2.86	115.50	119.69
2	A	801	FDA	C5A-C4A-N3A	-2.86	122.78	126.72
3	B	802	G3F	C4-C3-C2	-2.83	108.21	111.50
2	B	801	FDA	C5B-C4B-C3B	2.77	125.18	115.21
2	A	801	FDA	C2A-N1A-C6A	2.76	123.26	118.73
2	A	801	FDA	C4A-C5A-N7A	-2.73	107.46	110.58
2	A	801	FDA	O2B-C2B-C3B	2.73	120.56	111.82
3	B	802	G3F	O5-C5-C6	-2.72	99.70	106.44
3	A	802	G3F	C4-C3-C2	-2.68	108.39	111.50
2	B	801	FDA	O2'-C2'-C3'	2.67	115.50	109.25
2	B	801	FDA	C4B-O4B-C1B	-2.66	103.59	109.47
2	A	801	FDA	N3-C2-N1	2.65	119.90	115.74
2	A	801	FDA	N3A-C4A-N9A	2.59	131.57	127.17
2	A	801	FDA	O2-C2-N3	-2.55	117.32	121.86
2	B	801	FDA	O3P-PA-O1A	-2.55	103.03	110.70
2	B	801	FDA	O2P-P-O1P	2.52	124.18	112.44
2	B	801	FDA	N3-C2-N1	2.51	119.68	115.74
2	A	801	FDA	C5'-C4'-C3'	-2.50	107.50	112.22
2	B	801	FDA	O2P-P-O3P	-2.47	100.60	107.27
2	B	801	FDA	C8M-C8-C7	2.40	125.66	120.76
3	B	802	G3F	O4-C4-C3	-2.39	105.20	109.63
2	A	801	FDA	O2P-P-O3P	-2.34	100.95	107.27
2	B	801	FDA	C2A-N3A-C4A	2.31	117.48	111.83
2	B	801	FDA	O2B-C2B-C3B	2.29	119.15	111.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	FDA	C4A-N9A-C1B	-2.28	121.31	126.63
2	A	801	FDA	C5B-C4B-C3B	2.25	123.30	115.21
2	A	801	FDA	O2-C2-N1	-2.22	117.91	121.86
2	B	801	FDA	C5'-C4'-C3'	-2.19	108.08	112.22
2	A	801	FDA	C4B-O4B-C1B	-2.18	104.65	109.47
3	A	802	G3F	O2-C2-C3	2.14	113.58	109.63
3	A	802	G3F	O4-C4-C5	2.12	114.55	109.32
2	A	801	FDA	O2A-PA-O5B	-2.12	97.95	107.57
2	B	801	FDA	O3'-C3'-C2'	2.12	113.74	108.93
2	A	801	FDA	C9A-C9-C8	2.11	123.47	119.22
2	A	801	FDA	O4'-C4'-C3'	2.09	114.15	109.25
2	A	801	FDA	C2A-N3A-C4A	2.09	116.93	111.83
2	B	801	FDA	C7M-C7-C6	-2.05	115.96	119.57
2	B	801	FDA	C3B-C2B-C1B	2.05	105.34	101.46
2	B	801	FDA	O3'-C3'-C4'	-2.04	104.28	108.93
2	A	801	FDA	C6-C5X-C9A	-2.01	117.59	119.80

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	801	FDA	PA-O3P-P-O5'
2	A	801	FDA	PA-O3P-P-O5'
2	A	801	FDA	O4B-C4B-C5B-O5B
2	B	801	FDA	P-O3P-PA-O2A
2	A	801	FDA	P-O3P-PA-O2A
2	B	801	FDA	P-O3P-PA-O1A
2	B	801	FDA	O4B-C4B-C5B-O5B

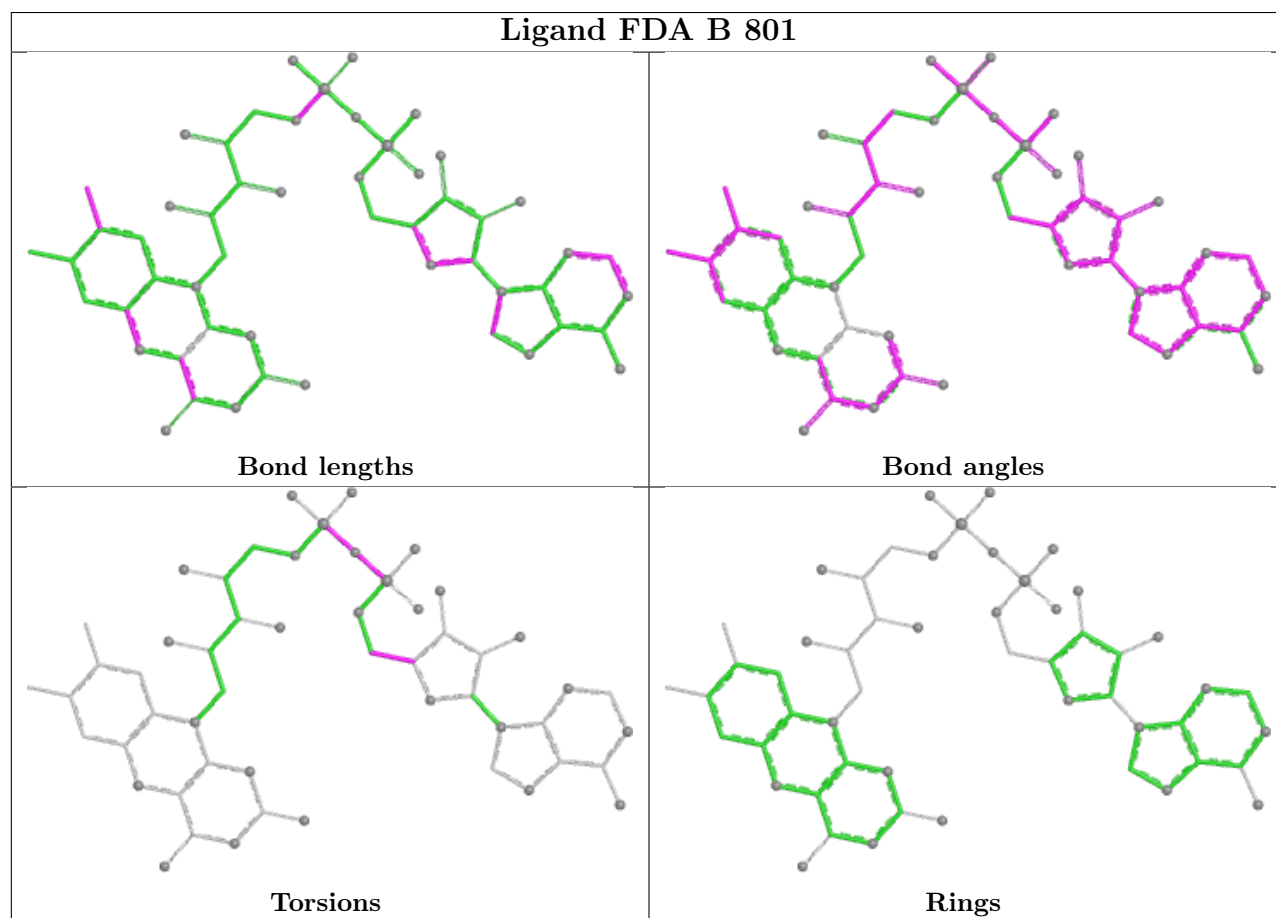
There are no ring outliers.

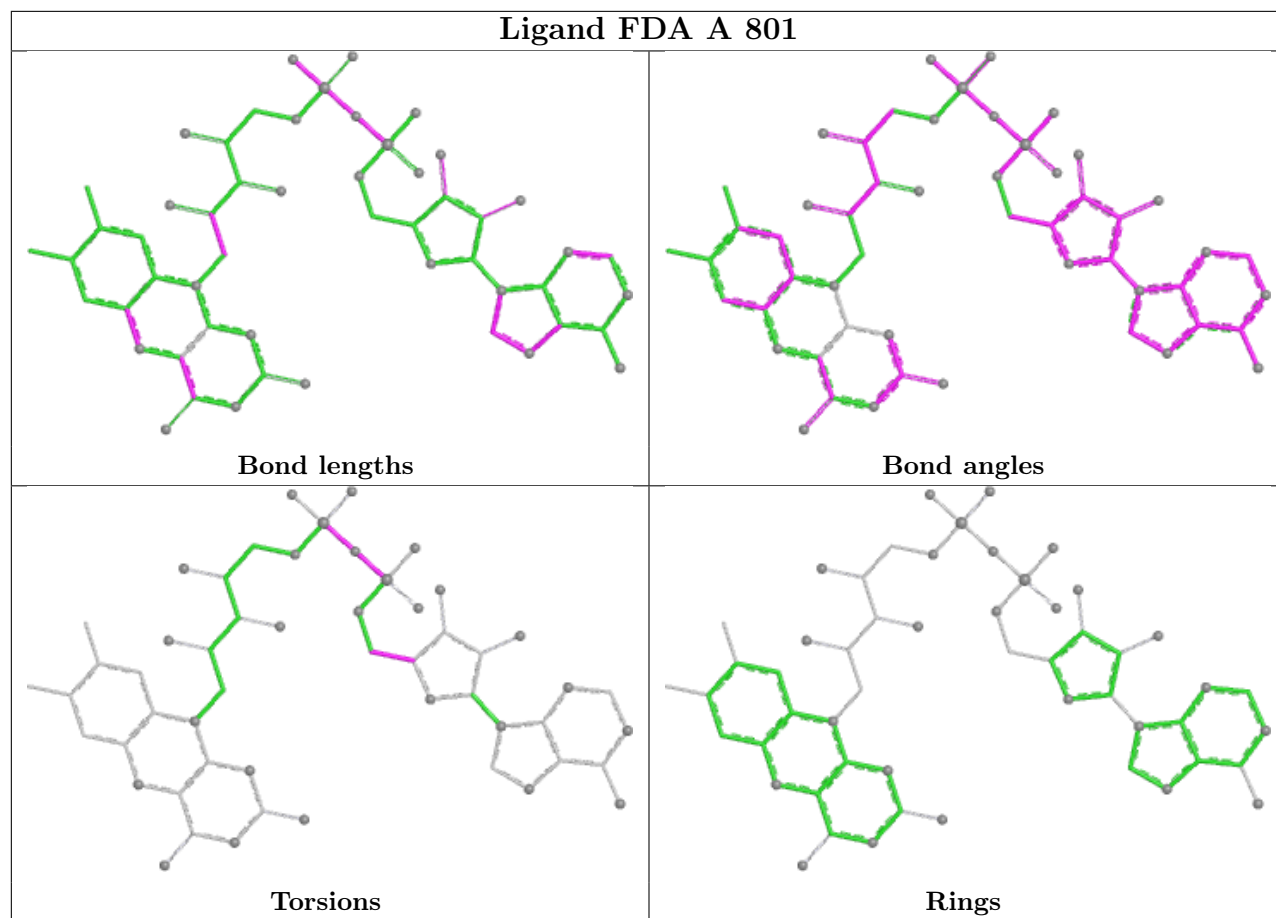
4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	802	G3F	2	0
2	B	801	FDA	3	0
3	A	802	G3F	2	0
2	A	801	FDA	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	0.14	9 (1%) 70 74	15, 26, 43, 66	0
1	B	576/633 (90%)	0.09	8 (1%) 73 76	15, 24, 42, 70	0
All	All	1152/1266 (90%)	0.11	17 (1%) 72 75	15, 25, 42, 70	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	618	PHE	4.9
1	B	343	ALA	3.9
1	A	459	VAL	3.8
1	A	343	ALA	3.5
1	B	45	ILE	3.2
1	B	618	PHE	2.9
1	A	45	ILE	2.9
1	B	232	GLY	2.8
1	A	81	ASP	2.5
1	B	385	THR	2.5
1	A	458	ALA	2.4
1	A	250	PHE	2.2
1	B	43	MET	2.1
1	A	136	PHE	2.0
1	A	84	LEU	2.0
1	B	389	LEU	2.0
1	B	347	GLU	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](#)

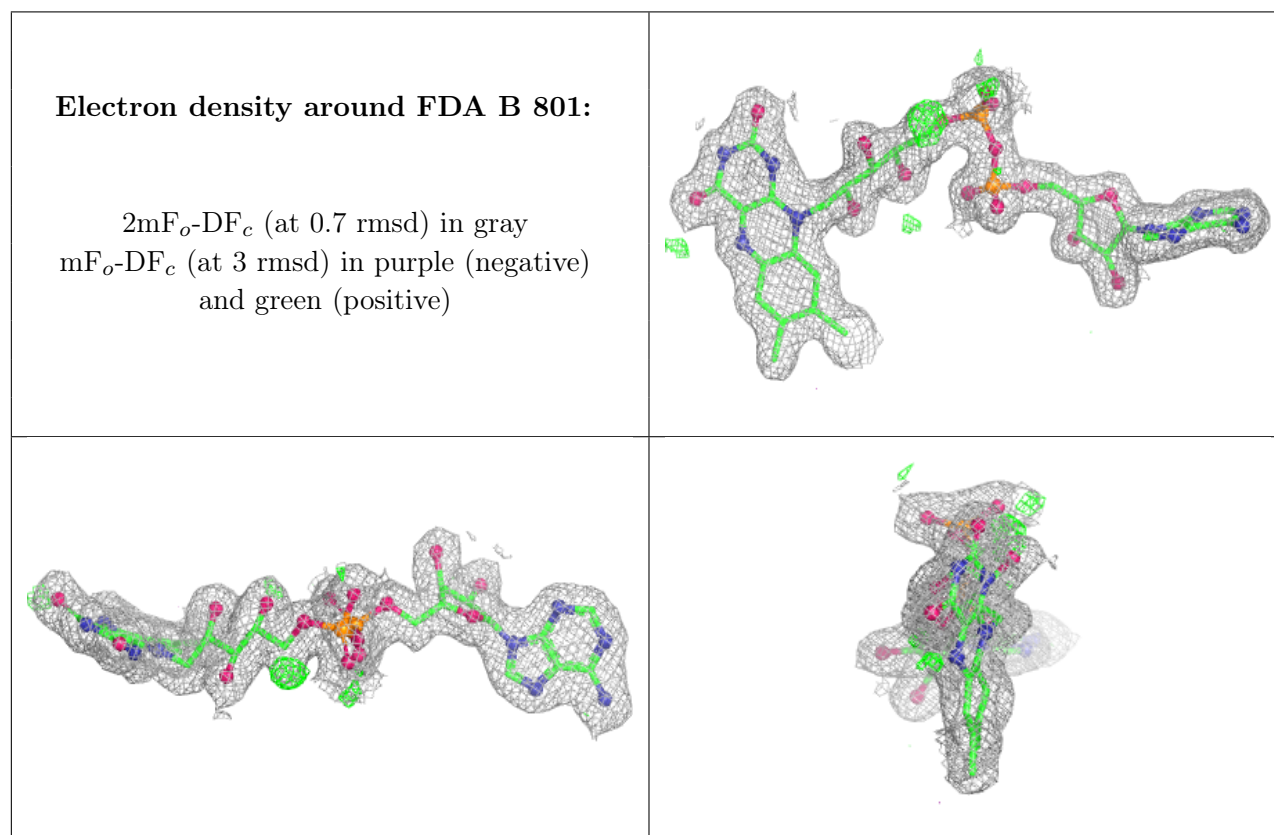
There are no oligosaccharides in this entry.

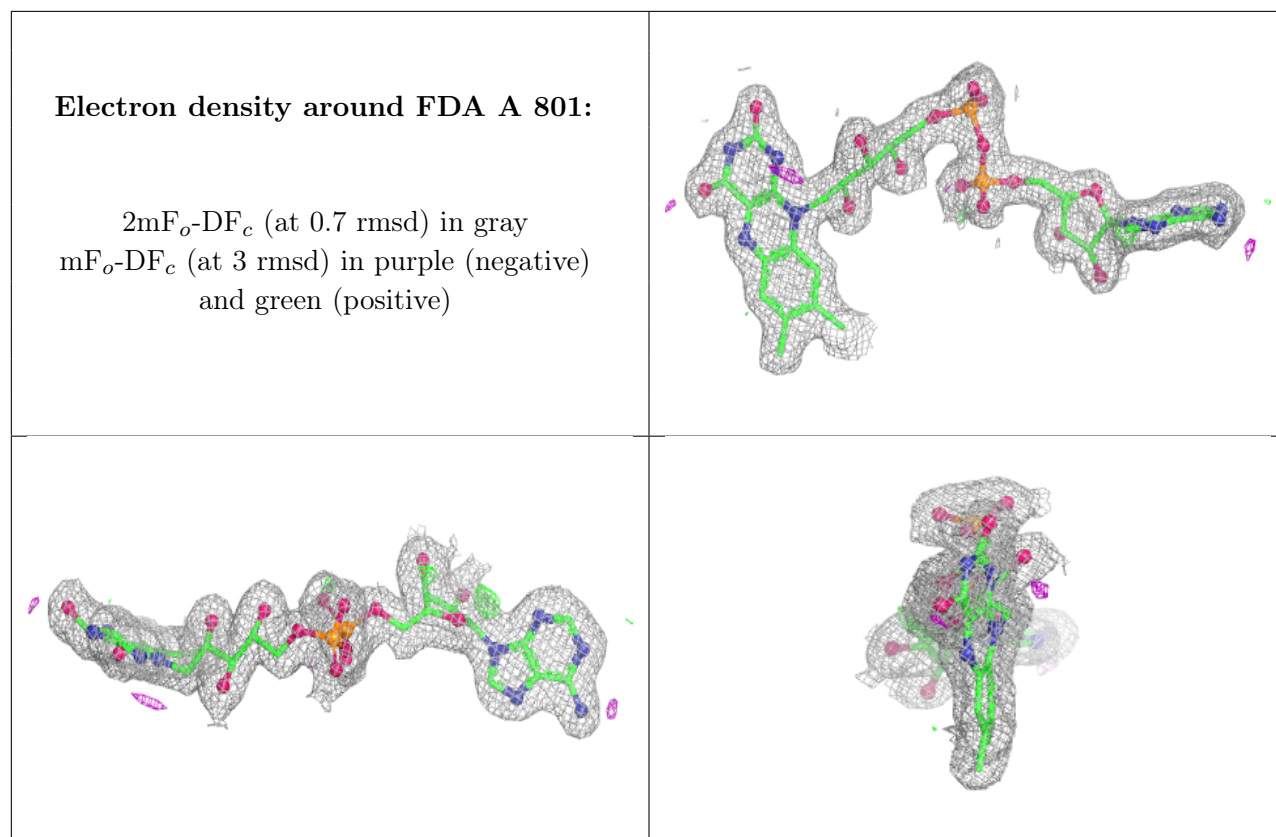
6.4 Ligands [i](#)

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
3	G3F	B	802	12/12	0.94	0.07	22,25,28,28	0
3	G3F	A	802	12/12	0.95	0.06	22,25,27,29	0
2	FDA	B	801	53/53	0.96	0.06	15,18,22,25	0
2	FDA	A	801	53/53	0.97	0.06	15,19,23,27	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.