



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 07:09 PM UTC

PDB ID : 4MIF / pdb_00004mif
Title : Pyranose 2-oxidase from Phanerochaete chrysosporium, wild type from natural source
Authors : Hassan, N.; Tan, T.C.; Spadiut, O.; Pisanelli, I.; Fusco, L.; Haltrich, D.; Peterbauer, C.; Divne, C.
Deposited on : 2013-08-31
Resolution : 1.80 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

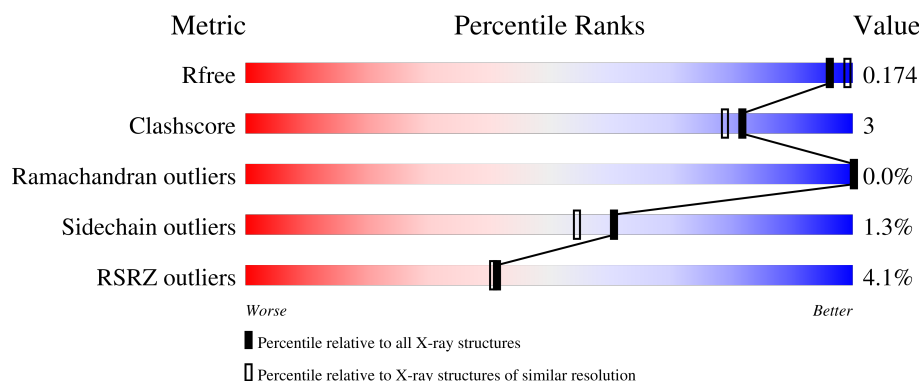
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	620	5% 82% 9% 8%
1	B	620	4% 83% 9% 6%
1	C	620	4% 83% 9% 8%
1	D	620	3% 81% 10% 8%

2 Entry composition (i)

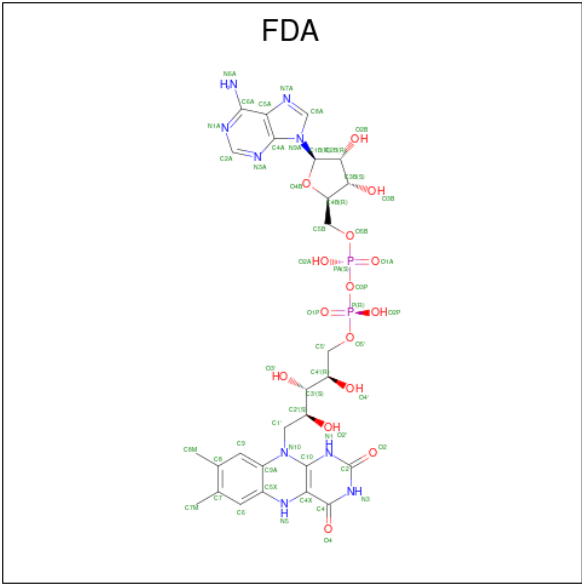
There are 4 unique types of molecules in this entry. The entry contains 19978 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	572	Total	C	N	O	S	0	3	0
			4542	2890	789	837	26			
1	B	581	Total	C	N	O	S	0	1	0
			4593	2918	799	850	26			
1	C	572	Total	C	N	O	S	0	1	0
			4529	2882	786	835	26			
1	D	572	Total	C	N	O	S	0	3	0
			4539	2888	787	838	26			

- 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
			53	27	9	15	2	
2	B	1	Total	C	N	O	P	0
			53	27	9	15	2	

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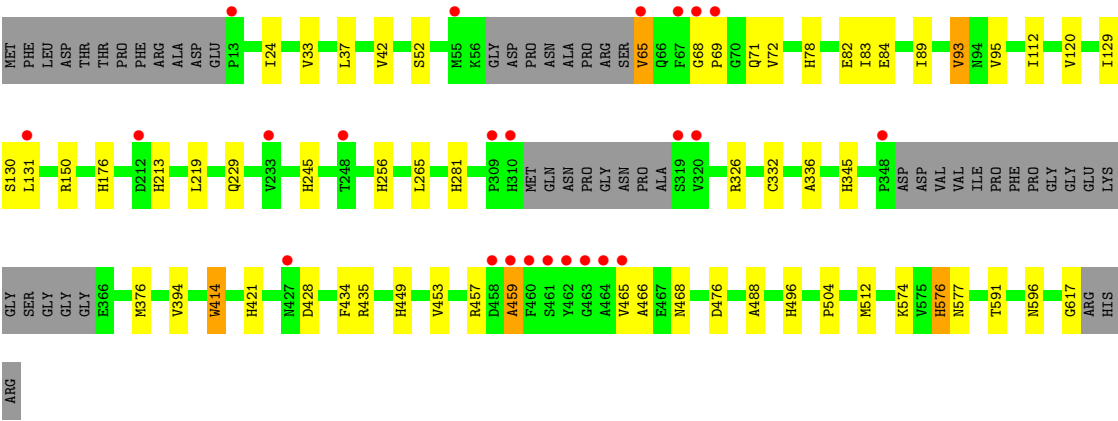
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

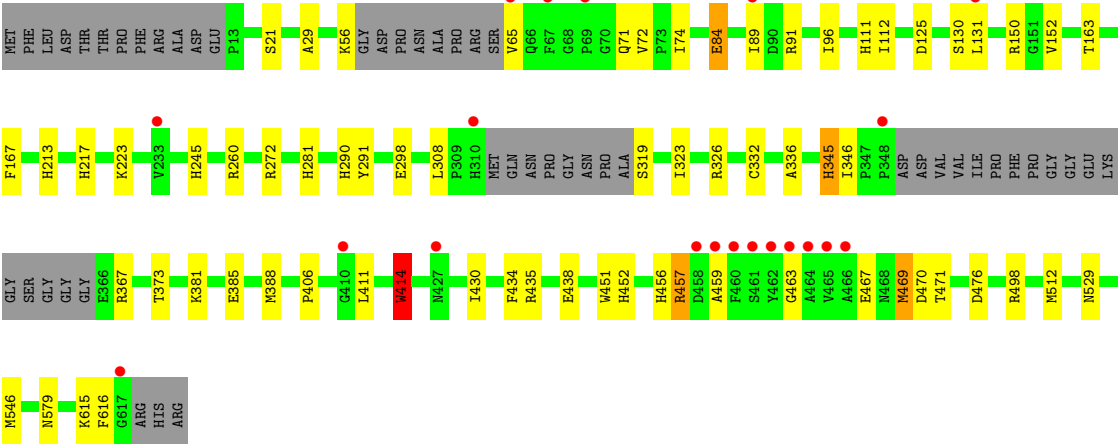
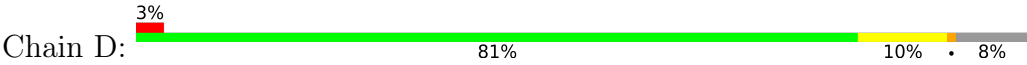
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	364	Total	O	0	0
			364	364		
4	B	393	Total	O	0	0
			393	393		
4	C	384	Total	O	0	0
			384	384		
4	D	421	Total	O	0	0
			421	421		



● Molecule 1: Pyranose 2-oxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	164.03Å 164.03Å 232.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.40 – 1.80 46.40 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.40-1.80) 99.0 (46.40-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.153 , 0.171 (Not available) , 0.174	Depositor DCC
R_{free} test set	1999 reflections (0.60%)	wwPDB-VP
Wilson B-factor (Å ²)	23.3	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	19978	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	1.57	23/4674 (0.5%)	1.26	17/6358 (0.3%)
1	B	1.55	27/4722 (0.6%)	1.27	14/6427 (0.2%)
1	C	1.56	29/4655 (0.6%)	1.28	15/6333 (0.2%)
1	D	1.59	32/4671 (0.7%)	1.30	20/6355 (0.3%)
All	All	1.57	111/18722 (0.6%)	1.28	66/25473 (0.3%)

All (111) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	435	ARG	N-CA	9.38	1.57	1.46
1	D	245	HIS	CE1-NE2	8.92	1.41	1.32
1	D	245	HIS	CG-CD2	8.65	1.45	1.35
1	C	345	HIS	ND1-CE1	8.59	1.41	1.32
1	B	457	ARG	C-O	8.11	1.33	1.23
1	D	245	HIS	ND1-CE1	7.94	1.40	1.32
1	B	595	ALA	CA-C	7.83	1.63	1.53
1	C	95	VAL	N-CA	-7.77	1.37	1.46
1	D	463	GLY	C-O	7.76	1.30	1.23
1	D	345	HIS	ND1-CE1	7.36	1.40	1.32
1	B	388	MET	SD-CE	-7.33	1.61	1.79
1	A	430	ILE	N-CA	-7.22	1.40	1.46
1	C	245	HIS	ND1-CE1	7.18	1.39	1.32
1	C	512	MET	SD-CE	-7.17	1.61	1.79
1	D	130	SER	CA-C	-7.04	1.44	1.52
1	B	484	GLU	CD-OE1	6.95	1.38	1.25
1	D	434	PHE	C-N	-6.91	1.25	1.33
1	A	405	ASN	CA-C	-6.71	1.45	1.52
1	C	496	HIS	ND1-CE1	6.63	1.39	1.32
1	B	274	ARG	C-O	-6.62	1.14	1.24
1	D	459	ALA	CA-C	6.60	1.60	1.52
1	B	472	ARG	N-CA	-6.56	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	176	HIS	CE1-NE2	6.55	1.39	1.32
1	D	96	ILE	N-CA	-6.49	1.39	1.46
1	D	470	ASP	CA-C	-6.47	1.44	1.52
1	A	281	HIS	ND1-CE1	6.34	1.38	1.32
1	C	459	ALA	C-O	6.33	1.31	1.23
1	D	281	HIS	CG-CD2	6.33	1.42	1.35
1	B	111	HIS	ND1-CE1	6.32	1.38	1.32
1	D	323	ILE	C-O	-6.32	1.17	1.24
1	D	435	ARG	N-CA	6.31	1.53	1.46
1	C	78	HIS	ND1-CE1	6.22	1.38	1.32
1	C	281	HIS	ND1-CE1	6.20	1.38	1.32
1	A	175	PRO	C-O	-6.19	1.16	1.24
1	A	204	ILE	CA-C	6.18	1.61	1.52
1	C	256	HIS	ND1-CE1	6.14	1.38	1.32
1	A	435	ARG	N-CA	6.13	1.53	1.46
1	B	281	HIS	ND1-CE1	6.13	1.38	1.32
1	A	346	ILE	CA-C	6.02	1.57	1.53
1	A	47	ALA	CA-C	-5.98	1.45	1.52
1	D	290	HIS	CE1-NE2	5.98	1.38	1.32
1	D	430	ILE	CA-C	5.97	1.58	1.53
1	A	546	MET	SD-CE	-5.88	1.64	1.79
1	B	572	HIS	ND1-CE1	5.86	1.38	1.32
1	B	456	HIS	ND1-CE1	5.85	1.38	1.32
1	A	465	VAL	CA-CB	5.83	1.61	1.54
1	B	463	GLY	C-O	5.75	1.29	1.23
1	A	281	HIS	CG-CD2	5.72	1.42	1.35
1	A	100	LEU	N-CA	5.70	1.52	1.46
1	A	434	PHE	C-N	-5.67	1.25	1.33
1	B	555	ALA	CA-C	-5.63	1.45	1.52
1	B	576	HIS	N-CA	5.62	1.52	1.46
1	A	408	TRP	NE1-CE2	-5.60	1.31	1.37
1	B	450	PRO	CA-C	5.57	1.58	1.53
1	C	72	VAL	C-O	-5.57	1.17	1.24
1	C	576	HIS	ND1-CE1	5.55	1.38	1.32
1	C	120	VAL	CA-CB	5.54	1.61	1.54
1	C	574	LYS	C-O	5.53	1.30	1.24
1	C	130	SER	CB-OG	5.52	1.53	1.42
1	B	347	PRO	CA-C	5.51	1.57	1.52
1	A	449	HIS	ND1-CE1	5.50	1.38	1.32
1	D	471	THR	CA-CB	5.49	1.62	1.53
1	D	451	TRP	NE1-CE2	-5.48	1.31	1.37
1	A	213	HIS	ND1-CE1	5.46	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	421	HIS	ND1-CE1	5.46	1.38	1.32
1	B	450	PRO	CA-CB	-5.43	1.48	1.53
1	B	94	ASN	CG-ND2	-5.43	1.21	1.33
1	B	45	GLY	N-CA	5.42	1.51	1.45
1	A	583	VAL	C-O	5.42	1.30	1.23
1	C	394	VAL	CA-CB	-5.42	1.47	1.54
1	B	503	MET	CA-C	5.40	1.59	1.52
1	D	414	TRP	N-CA	5.38	1.52	1.46
1	C	504	PRO	CA-C	-5.38	1.46	1.52
1	D	452	HIS	CE1-NE2	5.37	1.38	1.32
1	B	250	PRO	C-O	-5.36	1.17	1.24
1	C	213	HIS	ND1-CE1	5.33	1.37	1.32
1	B	459	ALA	C-O	5.32	1.30	1.23
1	A	217	HIS	CE1-NE2	5.32	1.37	1.32
1	A	245	HIS	CE1-NE2	5.31	1.37	1.32
1	D	476	ASP	CG-OD2	5.29	1.35	1.25
1	D	467	GLU	N-CA	5.29	1.53	1.46
1	A	45	GLY	C-O	5.29	1.28	1.23
1	C	421	HIS	ND1-CE1	5.28	1.37	1.32
1	D	438	GLU	CD-OE2	5.27	1.35	1.25
1	D	456	HIS	CE1-NE2	5.27	1.37	1.32
1	D	291	TYR	CA-CB	5.27	1.60	1.53
1	C	435	ARG	N-CA	5.25	1.51	1.46
1	D	29	ALA	CA-CB	5.23	1.61	1.53
1	A	439	PRO	N-CA	-5.22	1.40	1.47
1	B	340	VAL	N-CA	5.20	1.52	1.46
1	C	42	VAL	N-CA	-5.20	1.40	1.46
1	B	105	ILE	N-CA	5.18	1.51	1.46
1	C	488	ALA	CA-C	5.18	1.59	1.52
1	D	217	HIS	CG-CD2	5.15	1.41	1.35
1	C	376	MET	N-CA	5.13	1.52	1.46
1	B	390	PHE	CA-C	-5.12	1.46	1.52
1	D	381	LYS	C-O	-5.12	1.17	1.23
1	A	453	VAL	C-O	5.11	1.29	1.24
1	D	111	HIS	ND1-CE1	5.11	1.37	1.32
1	B	245	HIS	CG-CD2	5.10	1.41	1.35
1	C	457	ARG	N-CA	-5.10	1.39	1.46
1	C	345	HIS	CG-ND1	-5.10	1.32	1.38
1	C	449	HIS	ND1-CE1	5.09	1.37	1.32
1	D	345	HIS	CG-CD2	5.08	1.41	1.35
1	D	163	THR	C-O	5.08	1.29	1.24
1	C	457	ARG	C-O	5.06	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	278	LEU	CA-C	5.05	1.59	1.52
1	C	453	VAL	C-O	5.05	1.29	1.24
1	D	457	ARG	C-O	5.04	1.29	1.23
1	D	529	ASN	CG-ND2	-5.01	1.22	1.33
1	C	93	VAL	CA-C	-5.00	1.46	1.52

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	434	PHE	CA-C-N	-15.16	99.66	122.86
1	B	434	PHE	C-N-CA	-15.16	99.66	122.86
1	D	434	PHE	CA-C-N	-12.89	102.98	122.83
1	D	434	PHE	C-N-CA	-12.89	102.98	122.83
1	A	434	PHE	CA-C-N	-12.85	103.20	122.86
1	A	434	PHE	C-N-CA	-12.85	103.20	122.86
1	C	434	PHE	CA-C-N	-12.83	103.07	122.83
1	C	434	PHE	C-N-CA	-12.83	103.07	122.83
1	C	512	MET	CG-SD-CE	-11.16	76.34	100.90
1	D	84	GLU	CA-CB-CG	7.01	128.12	114.10
1	B	124	LEU	CA-C-N	-6.98	111.71	122.60
1	B	124	LEU	C-N-CA	-6.98	111.71	122.60
1	A	467	GLU	N-CA-CB	6.72	120.32	110.57
1	A	512	MET	CG-SD-CE	-6.68	86.19	100.90
1	C	68	GLY	CA-C-N	6.46	127.91	119.84
1	C	68	GLY	C-N-CA	6.46	127.91	119.84
1	D	125	ASP	N-CA-C	6.29	120.70	112.89
1	D	546	MET	CG-SD-CE	-6.25	87.15	100.90
1	D	498	ARG	CG-CD-NE	6.21	125.65	112.00
1	B	84	GLU	CB-CA-C	-6.12	100.28	110.68
1	B	457	ARG	O-C-N	6.11	130.72	123.33
1	C	591	THR	CA-C-N	-6.10	116.86	122.29
1	C	591	THR	C-N-CA	-6.10	116.86	122.29
1	A	346	ILE	CA-C-O	6.00	122.48	119.12
1	B	234	ILE	CB-CA-C	-5.94	102.91	111.34
1	D	84	GLU	N-CA-C	-5.91	104.18	111.33
1	B	24	ILE	CB-CG1-CD1	5.81	126.00	113.80
1	A	308	LEU	CA-C-N	-5.78	114.02	120.14
1	A	308	LEU	C-N-CA	-5.78	114.02	120.14
1	A	476	ASP	CA-CB-CG	5.77	118.37	112.60
1	C	476	ASP	CB-CA-C	-5.71	98.92	109.37
1	A	490	GLU	N-CA-C	5.68	117.81	109.24
1	C	130	SER	CB-CA-C	5.66	120.18	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	346	ILE	N-CA-C	5.63	112.69	107.56
1	A	471	THR	N-CA-C	5.62	118.17	111.71
1	B	512	MET	CG-SD-CE	-5.60	88.58	100.90
1	D	406	PRO	CA-C-N	-5.53	114.07	120.04
1	D	406	PRO	C-N-CA	-5.53	114.07	120.04
1	D	463	GLY	O-C-N	5.52	127.02	122.71
1	B	64	SER	N-CA-C	5.43	117.74	110.35
1	D	476	ASP	CA-CB-CG	5.38	117.98	112.60
1	C	129	ILE	CA-C-N	-5.38	114.87	122.94
1	C	129	ILE	C-N-CA	-5.38	114.87	122.94
1	A	495	GLN	N-CA-C	5.33	117.09	111.28
1	B	476	ASP	CB-CA-C	-5.32	100.50	109.50
1	A	84	GLU	CA-CB-CG	5.30	124.70	114.10
1	A	471	THR	CA-C-O	5.29	126.08	120.10
1	D	56	LYS	CA-C-O	-5.29	111.81	120.80
1	D	213	HIS	CA-CB-CG	-5.27	108.53	113.80
1	B	462	TYR	CA-CB-CG	-5.27	104.41	113.90
1	D	385	GLU	CB-CG-CD	5.27	121.56	112.60
1	A	53	LYS	CA-C-N	-5.23	114.53	119.76
1	A	53	LYS	C-N-CA	-5.23	114.53	119.76
1	D	223	LYS	N-CA-C	-5.23	105.66	111.36
1	D	512	MET	CG-SD-CE	-5.22	89.42	100.90
1	B	133	LYS	CB-CG-CD	5.19	123.24	111.30
1	C	24	ILE	CB-CG1-CD1	5.18	124.67	113.80
1	A	467	GLU	CA-CB-CG	-5.16	103.77	114.10
1	C	219	LEU	N-CA-C	-5.14	105.57	111.07
1	B	476	ASP	CA-CB-CG	5.14	117.74	112.60
1	A	434	PHE	N-CA-C	5.13	116.87	111.28
1	D	388	MET	CG-SD-CE	-5.12	89.63	100.90
1	D	167	PHE	N-CA-C	5.12	117.64	109.96
1	C	428	ASP	CA-C-N	-5.06	114.61	119.87
1	C	428	ASP	C-N-CA	-5.06	114.61	119.87
1	D	615	LYS	N-CA-C	5.04	117.88	111.69

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	4542	0	4441	32	0
1	B	4593	0	4479	29	0
1	C	4529	0	4424	15	0
1	D	4539	0	4434	23	0
2	A	53	0	31	1	0
2	B	53	0	32	1	0
2	C	53	0	32	1	0
2	D	53	0	32	1	0
3	B	1	0	0	0	0
4	A	364	0	0	2	0
4	B	393	0	0	4	0
4	C	384	0	0	1	0
4	D	421	0	0	2	0
All	All	19978	0	17905	92	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 (92) 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:544:GLN:HG3	1:A:546:MET:HE1	1.47	0.93
1:B:93:VAL:HG23	1:B:459:ALA:HB1	1.62	0.80
1:B:72:VAL:HG21	1:B:272:ARG:HH12	1.45	0.79
1:A:84:GLU:HG2	4:B:991:HOH:O	1.84	0.78
1:A:544:GLN:HG3	1:A:546:MET:CE	2.17	0.73
1:A:93:VAL:HG23	1:A:459:ALA:HB1	1.72	0.71
1:D:326:ARG:NH2	1:D:616:PHE:O	2.22	0.71
1:D:72:VAL:CG2	1:D:272:ARG:HH12	2.08	0.67
1:C:37:LEU:HD21	1:C:617:GLY:HA2	1.77	0.66
1:A:545:PHE:C	1:A:546:MET:HE2	2.21	0.66
1:B:191[A]:ARG:HG2	1:B:191[A]:ARG:NH1	2.09	0.65
1:D:457:ARG:NH2	4:D:1301:HOH:O	2.28	0.65
1:A:462:TYR:HB2	1:A:467:GLU:HB2	1.79	0.64
1:A:93:VAL:CG2	1:A:459:ALA:HB1	2.29	0.62
4:C:987:HOH:O	1:D:84:GLU:HG2	1.99	0.62
1:D:72:VAL:HG21	1:D:272:ARG:NH1	2.16	0.61
1:B:37:LEU:HD21	1:B:617:GLY:HA2	1.83	0.60
1:A:390:PHE:HB3	1:A:546:MET:HE3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191[A]:ARG:HG2	1:B:191[A]:ARG:HH11	1.69	0.57
1:A:468:ASN:HB2	1:B:112:ILE:HD11	1.86	0.57
1:A:112:ILE:HG23	1:B:465:VAL:HG23	1.88	0.56
1:D:72:VAL:HG23	1:D:272:ARG:HH12	1.70	0.55
1:B:93:VAL:HG23	1:B:459:ALA:CB	2.34	0.55
1:B:72:VAL:HG21	1:B:272:ARG:NH1	2.21	0.54
1:A:112:ILE:HD11	1:B:468:ASN:HB2	1.90	0.54
1:A:345:HIS:CD2	1:A:373:THR:HA	2.43	0.53
1:B:225:ASN:O	1:B:229:GLN:HG2	2.08	0.53
1:D:72:VAL:HG21	1:D:272:ARG:HH12	1.72	0.53
1:C:465:VAL:HG13	1:C:466:ALA:N	2.24	0.53
1:A:465:VAL:HG23	4:A:1217:HOH:O	2.09	0.52
1:C:93:VAL:HG23	1:C:459:ALA:HB1	1.93	0.51
1:C:229:GLN:HA	1:C:229:GLN:OE1	2.10	0.50
1:B:33:VAL:HG11	1:B:265:LEU:HD22	1.94	0.50
1:C:112:ILE:CD1	1:D:469:MET:HG2	2.42	0.50
1:B:89:ILE:O	1:B:89:ILE:HD12	2.12	0.49
1:B:444:LYS:CE	4:B:1249:HOH:O	2.61	0.48
1:C:33:VAL:HG11	1:C:265:LEU:HD22	1.96	0.48
1:A:89:ILE:HD12	1:A:89:ILE:O	2.14	0.47
1:B:388:MET:HE2	1:B:480:PHE:CE2	2.49	0.47
1:A:183:SER:OG	1:A:188:GLU:OE1	2.29	0.47
1:C:82:GLU:HG2	1:C:84:GLU:HG2	1.97	0.47
1:B:345:HIS:CD2	1:B:373:THR:HA	2.50	0.47
1:D:411:LEU:HD12	1:D:411:LEU:N	2.28	0.46
1:B:72:VAL:CG2	1:B:272:ARG:HH12	2.23	0.46
1:C:468:ASN:HB2	1:D:112:ILE:HD11	1.97	0.46
1:B:414:TRP:C	1:B:414:TRP:CD1	2.94	0.46
1:D:332:CYS:O	1:D:336:ALA:HB3	2.16	0.46
1:A:203:ILE:HD12	1:A:606:ILE:HD11	1.98	0.46
1:B:444:LYS:HE2	4:B:1249:HOH:O	2.16	0.46
1:B:576:HIS:O	1:B:577:ASN:HB2	2.16	0.45
1:A:74:ILE:CD1	1:A:266:PHE:HB2	2.47	0.45
1:B:93:VAL:CG2	1:B:459:ALA:C	2.89	0.45
1:A:93:VAL:CG2	1:A:459:ALA:C	2.90	0.45
1:C:414:TRP:C	1:C:414:TRP:CD1	2.95	0.45
1:B:396:ASP:OD2	4:B:1271:HOH:O	2.21	0.44
1:A:72:VAL:HG13	1:A:74:ILE:HD11	1.99	0.44
1:A:74:ILE:HD13	1:A:266:PHE:CB	2.46	0.44
1:A:546:MET:HE2	1:A:546:MET:N	2.33	0.44
1:B:89:ILE:HG23	1:B:90:ASP:N	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:150:ARG:HA	2:D:801:FDA:O2B	2.18	0.44
1:C:332:CYS:O	1:C:336:ALA:HB3	2.17	0.44
1:C:65:VAL:O	1:C:71:GLN:HG3	2.17	0.44
1:B:596:ASN:HB3	2:B:801:FDA:C2	2.48	0.44
1:A:93:VAL:CG2	1:A:459:ALA:CB	2.95	0.43
1:B:332:CYS:O	1:B:336:ALA:HB3	2.19	0.43
1:A:462:TYR:CB	1:A:467:GLU:HB2	2.46	0.43
1:D:469:MET:HE2	1:D:469:MET:HB3	1.81	0.43
1:A:93:VAL:HG22	1:A:459:ALA:CB	2.49	0.43
1:A:596:ASN:HB3	2:A:801:FDA:C2	2.48	0.43
1:B:21:SER:OG	1:B:152:VAL:HA	2.18	0.43
1:C:576:HIS:O	1:C:577:ASN:HB2	2.19	0.43
1:D:414:TRP:C	1:D:414:TRP:CD1	2.96	0.43
1:D:131:LEU:HD23	1:D:131:LEU:HA	1.84	0.42
1:A:73:PRO:HG3	1:B:73:PRO:HG3	2.02	0.42
1:B:191[A]:ARG:HH11	1:B:191[A]:ARG:CG	2.30	0.42
1:C:131:LEU:HA	1:C:131:LEU:HD12	1.74	0.42
1:D:72:VAL:HG13	1:D:74:ILE:HD11	2.00	0.42
1:A:74:ILE:HD13	1:A:266:PHE:HB2	2.01	0.42
1:A:158:HIS:CD2	1:A:158:HIS:C	2.98	0.42
1:D:298:GLU:HG2	1:D:579[B]:ASN:ND2	2.34	0.42
1:A:223:LYS:NZ	4:A:1183:HOH:O	2.51	0.41
1:A:282:ARG:O	1:A:304:VAL:HA	2.20	0.41
1:D:71:GLN:HG2	4:D:1275:HOH:O	2.21	0.41
1:B:469:MET:HB3	1:B:469:MET:HE2	1.59	0.41
1:D:411:LEU:HD23	1:D:414:TRP:CE3	2.56	0.41
1:A:65:VAL:O	1:A:66:GLN:C	2.64	0.41
1:C:150:ARG:HA	2:C:801:FDA:O2B	2.20	0.41
1:D:21:SER:OG	1:D:152:VAL:HA	2.21	0.41
1:D:84:GLU:OE2	1:D:91:ARG:NH1	2.53	0.41
1:A:249:ASP:OD1	1:A:249:ASP:C	2.65	0.40
1:C:83:ILE:HD11	1:D:308:LEU:HD23	2.02	0.40
1:D:345:HIS:CD2	1:D:373:THR:HA	2.57	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	567/620 (92%)	555 (98%)	12 (2%)	0	100	100
1	B	576/620 (93%)	569 (99%)	7 (1%)	0	100	100
1	C	565/620 (91%)	553 (98%)	11 (2%)	1 (0%)	43	31
1	D	567/620 (92%)	557 (98%)	10 (2%)	0	100	100
All	All	2275/2480 (92%)	2234 (98%)	40 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	69	PRO

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	495/529 (94%)	487 (98%)	8 (2%)	55	47
1	B	500/529 (94%)	495 (99%)	5 (1%)	68	64
1	C	493/529 (93%)	487 (99%)	6 (1%)	63	57
1	D	495/529 (94%)	488 (99%)	7 (1%)	59	52
All	All	1983/2116 (94%)	1957 (99%)	26 (1%)	61	54

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	ILE
1	A	89	ILE
1	A	229	GLN
1	A	234	ILE
1	A	272	ARG
1	A	308	LEU
1	A	414	TRP
1	A	467	GLU
1	B	84	GLU
1	B	89	ILE
1	B	414	TRP
1	B	465	VAL
1	B	469	MET
1	C	52	SER
1	C	65	VAL
1	C	89	ILE
1	C	326	ARG
1	C	414	TRP
1	C	596	ASN
1	D	65	VAL
1	D	89	ILE
1	D	260	ARG
1	D	319	SER
1	D	367	ARG
1	D	414	TRP
1	D	469	MET

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	94	ASN
1	A	280	ASN
1	A	529	ASN
1	A	544	GLN
1	A	572	HIS
1	A	579	ASN
1	B	94	ASN
1	B	280	ASN
1	B	586	ASN
1	C	71	GLN
1	C	94	ASN
1	C	110	ASN
1	C	280	ASN

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Mol	Chain	Res	Type
1	C	392	GLN
1	C	486	GLN
1	C	572	HIS
1	C	586	ASN
1	D	94	ASN
1	D	110	ASN
1	D	111	HIS
1	D	392	GLN
1	D	572	HIS
1	D	586	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 ⓘ

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FDA	C	801	1	57,58,58	1.67	12 (21%)	78,89,89	2.01	25 (32%)
2	FDA	B	801	1	57,58,58	1.73	10 (17%)	78,89,89	2.59	30 (38%)
2	FDA	D	801	1	57,58,58	2.00	13 (22%)	78,89,89	2.37	25 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FDA	A	801	1	57,58,58	2.18	17 (29%)	78,89,89	2.16	21 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FDA	C	801	1	-	3/34/50/50	0/6/6/6
2	FDA	B	801	1	-	1/34/50/50	0/6/6/6
2	FDA	D	801	1	-	1/34/50/50	0/6/6/6
2	FDA	A	801	1	-	0/34/50/50	0/6/6/6

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	801	FDA	C6-C5X	7.04	1.50	1.39
2	A	801	FDA	C5'-C4'	6.64	1.60	1.51
2	D	801	FDA	C5'-C4'	6.55	1.60	1.51
2	C	801	FDA	PA-O3P	5.68	1.65	1.59
2	A	801	FDA	C6-C5X	5.34	1.47	1.39
2	B	801	FDA	P-O3P	5.24	1.65	1.59
2	A	801	FDA	C2A-N3A	4.96	1.42	1.33
2	A	801	FDA	C7M-C7	4.78	1.60	1.51
2	D	801	FDA	PA-O3P	4.60	1.64	1.59
2	A	801	FDA	P-O3P	4.41	1.64	1.59
2	C	801	FDA	C5'-C4'	4.29	1.57	1.51
2	C	801	FDA	P-O3P	-4.15	1.55	1.59
2	B	801	FDA	C4X-C4	3.98	1.53	1.41
2	B	801	FDA	C5X-C9A	-3.72	1.36	1.40
2	A	801	FDA	C8M-C8	3.71	1.57	1.51
2	D	801	FDA	C2A-N3A	3.64	1.40	1.33
2	D	801	FDA	C7M-C7	3.60	1.57	1.51
2	D	801	FDA	C8A-N7A	3.55	1.38	1.31
2	A	801	FDA	C5A-C4A	-3.44	1.32	1.39
2	D	801	FDA	O2-C2	3.38	1.30	1.23
2	B	801	FDA	O2-C2	3.33	1.30	1.23
2	C	801	FDA	C6-C5X	3.22	1.44	1.39
2	A	801	FDA	C4'-C3'	-3.09	1.48	1.53
2	B	801	FDA	C5'-C4'	2.90	1.55	1.51
2	C	801	FDA	C2-N3	-2.90	1.32	1.37
2	A	801	FDA	C4X-C4	2.88	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	FDA	C7M-C7	2.83	1.56	1.51
2	B	801	FDA	C8M-C8	2.75	1.56	1.51
2	B	801	FDA	C6-C5X	2.73	1.43	1.39
2	B	801	FDA	PA-O3P	2.68	1.62	1.59
2	C	801	FDA	C4X-C4	2.65	1.49	1.41
2	A	801	FDA	O3B-C3B	-2.49	1.36	1.43
2	A	801	FDA	O2-C2	2.45	1.28	1.23
2	A	801	FDA	C5X-N5	-2.45	1.35	1.39
2	A	801	FDA	C4X-N5	2.43	1.40	1.35
2	C	801	FDA	C9A-N10	2.41	1.45	1.41
2	D	801	FDA	C5X-C9A	-2.39	1.37	1.40
2	C	801	FDA	C5X-N5	-2.36	1.35	1.39
2	D	801	FDA	C2B-C3B	-2.32	1.47	1.53
2	B	801	FDA	C5A-C4A	-2.32	1.35	1.39
2	D	801	FDA	C10-N10	-2.31	1.34	1.38
2	A	801	FDA	C2-N1	-2.24	1.33	1.37
2	A	801	FDA	C9-C8	2.24	1.42	1.39
2	C	801	FDA	C7M-C7	2.20	1.55	1.51
2	C	801	FDA	O2-C2	2.17	1.28	1.23
2	A	801	FDA	C2'-C3'	2.17	1.57	1.53
2	C	801	FDA	C2-N1	-2.16	1.33	1.37
2	C	801	FDA	O4B-C4B	-2.13	1.40	1.45
2	D	801	FDA	C4X-N5	2.12	1.40	1.35
2	D	801	FDA	C5A-N7A	-2.11	1.35	1.39
2	A	801	FDA	PA-O3P	2.11	1.61	1.59
2	D	801	FDA	C1'-N10	2.10	1.52	1.47

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	FDA	C4-N3-C2	9.32	139.20	126.37
2	B	801	FDA	O4-C4-N3	8.60	136.28	120.11
2	A	801	FDA	O4-C4-N3	7.55	134.31	120.11
2	D	801	FDA	N3A-C2A-N1A	-6.82	118.26	128.58
2	D	801	FDA	O4-C4-N3	6.81	132.92	120.11
2	A	801	FDA	N3A-C2A-N1A	-6.52	118.71	128.58
2	D	801	FDA	C4-N3-C2	6.31	135.05	126.37
2	D	801	FDA	C4A-N9A-C8A	6.13	112.17	105.74
2	D	801	FDA	N9A-C8A-N7A	-6.10	105.29	113.94
2	B	801	FDA	N3A-C2A-N1A	-6.07	119.40	128.58
2	A	801	FDA	N9A-C8A-N7A	-5.88	105.60	113.94
2	C	801	FDA	O4-C4-N3	5.85	131.11	120.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	FDA	C4A-N9A-C8A	5.55	111.57	105.74
2	B	801	FDA	N9A-C8A-N7A	-5.22	106.53	113.94
2	A	801	FDA	O4-C4-C4X	-5.08	115.01	127.26
2	D	801	FDA	C2A-N1A-C6A	5.06	127.05	118.73
2	C	801	FDA	C5'-C4'-C3'	-4.75	103.25	112.22
2	C	801	FDA	N9A-C8A-N7A	-4.67	107.31	113.94
2	C	801	FDA	C4-N3-C2	4.37	132.38	126.37
2	B	801	FDA	O4B-C1B-N9A	4.32	116.39	108.09
2	D	801	FDA	C5'-C4'-C3'	-4.22	104.25	112.22
2	A	801	FDA	C4A-N9A-C8A	4.18	110.13	105.74
2	D	801	FDA	C9A-C5X-N5	4.15	124.42	119.37
2	B	801	FDA	C2A-N1A-C6A	4.08	125.43	118.73
2	A	801	FDA	C2A-N1A-C6A	4.06	125.40	118.73
2	C	801	FDA	C6A-C5A-C4A	4.01	122.66	117.18
2	C	801	FDA	O4-C4-C4X	-3.89	117.89	127.26
2	A	801	FDA	O4B-C1B-N9A	3.84	115.47	108.09
2	C	801	FDA	O4B-C1B-N9A	3.78	115.35	108.09
2	A	801	FDA	C4-N3-C2	3.69	131.45	126.37
2	D	801	FDA	C6-C7-C8	3.64	125.04	119.69
2	A	801	FDA	C5A-N7A-C8A	3.57	109.06	103.45
2	B	801	FDA	O4-C4-C4X	-3.51	118.80	127.26
2	C	801	FDA	C4A-N9A-C8A	3.50	109.42	105.74
2	D	801	FDA	O4-C4-C4X	-3.32	119.25	127.26
2	C	801	FDA	C5A-N7A-C8A	3.31	108.65	103.45
2	C	801	FDA	C5A-C6A-N6A	3.30	131.44	123.29
2	B	801	FDA	C6-C5X-C9A	-3.22	116.28	119.80
2	B	801	FDA	C5'-C4'-C3'	-3.22	106.15	112.22
2	D	801	FDA	C4'-C3'-C2'	-3.19	108.26	113.57
2	B	801	FDA	O2'-C2'-C3'	3.16	116.66	109.25
2	B	801	FDA	C9A-C5X-N5	3.14	123.20	119.37
2	B	801	FDA	N3-C2-N1	-3.13	110.82	115.74
2	A	801	FDA	C5'-C4'-C3'	-3.02	106.52	112.22
2	B	801	FDA	C1B-N9A-C8A	-2.99	120.46	127.09
2	C	801	FDA	O2A-PA-O1A	2.93	126.09	112.44
2	B	801	FDA	C5A-N7A-C8A	2.90	108.01	103.45
2	D	801	FDA	C9-C8-C7	-2.89	115.44	119.69
2	B	801	FDA	C4X-C4-N3	-2.82	104.38	112.13
2	A	801	FDA	O4'-C4'-C3'	2.81	115.83	109.25
2	D	801	FDA	C5A-N7A-C8A	2.79	107.83	103.45
2	D	801	FDA	O4'-C4'-C3'	2.75	115.69	109.25
2	A	801	FDA	C7M-C7-C6	-2.75	114.72	119.57
2	C	801	FDA	O3B-C3B-C4B	2.75	118.97	111.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	FDA	C5A-C4A-N3A	-2.73	122.96	126.72
2	B	801	FDA	O5'-C5'-C4'	-2.72	102.11	109.36
2	D	801	FDA	C7M-C7-C6	-2.71	114.80	119.57
2	A	801	FDA	C6A-C5A-C4A	2.70	120.86	117.18
2	B	801	FDA	O3P-PA-O1A	-2.67	102.66	110.70
2	B	801	FDA	C6A-C5A-C4A	2.66	120.81	117.18
2	A	801	FDA	O2P-P-O1P	2.66	124.83	112.44
2	B	801	FDA	C4A-C5A-N7A	-2.64	107.57	110.58
2	D	801	FDA	C5X-C6-C7	-2.61	114.36	119.92
2	C	801	FDA	C5A-C4A-N3A	-2.61	123.13	126.72
2	D	801	FDA	C1B-N9A-C8A	-2.59	121.34	127.09
2	C	801	FDA	O2B-C2B-C3B	2.57	120.07	111.82
2	A	801	FDA	N3A-C4A-N9A	2.56	131.52	127.17
2	C	801	FDA	C4A-C5A-N7A	-2.50	107.72	110.58
2	C	801	FDA	C1B-N9A-C8A	-2.50	121.55	127.09
2	B	801	FDA	O2A-PA-O3P	2.49	114.00	107.27
2	C	801	FDA	C4-C4X-N5	2.46	122.67	116.37
2	A	801	FDA	C9A-C5X-N5	2.42	122.32	119.37
2	C	801	FDA	O4'-C4'-C3'	2.38	114.83	109.25
2	B	801	FDA	C9-C8-C7	-2.36	116.22	119.69
2	D	801	FDA	N6A-C6A-N1A	2.34	123.59	118.38
2	C	801	FDA	C7M-C7-C8	-2.30	116.06	120.76
2	B	801	FDA	O4'-C4'-C3'	2.26	114.53	109.25
2	C	801	FDA	C2A-N1A-C6A	2.26	122.44	118.73
2	A	801	FDA	O2A-PA-O1A	2.25	122.93	112.44
2	D	801	FDA	O2'-C2'-C3'	2.24	114.50	109.25
2	C	801	FDA	C2B-C1B-N9A	2.20	118.76	113.30
2	B	801	FDA	C9A-C9-C8	2.18	123.61	119.22
2	B	801	FDA	C5X-N5-C4X	-2.18	116.04	121.08
2	B	801	FDA	O2-C2-N3	2.16	125.70	121.86
2	D	801	FDA	O4B-C1B-N9A	2.15	112.22	108.09
2	C	801	FDA	C9A-C5X-N5	2.14	121.98	119.37
2	D	801	FDA	O2A-PA-O1A	2.14	122.42	112.44
2	B	801	FDA	C5X-C9A-N10	2.14	120.43	118.01
2	C	801	FDA	C5A-C6A-N1A	-2.13	112.10	117.51
2	D	801	FDA	O2P-P-O1P	2.12	122.32	112.44
2	D	801	FDA	O2P-P-O3P	-2.12	101.54	107.27
2	B	801	FDA	O2A-PA-O1A	2.11	122.27	112.44
2	B	801	FDA	C1'-N10-C9A	2.11	124.73	120.63
2	D	801	FDA	C6-C5X-C9A	-2.10	117.49	119.80
2	B	801	FDA	O4'-C4'-C5'	2.09	114.59	109.99
2	D	801	FDA	O5'-C5'-C4'	-2.07	103.83	109.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	FDA	O4B-C1B-C2B	-2.05	102.23	106.62
2	A	801	FDA	O2P-P-O3P	-2.05	101.74	107.27
2	C	801	FDA	C6-C5X-C9A	-2.04	117.56	119.80
2	A	801	FDA	C2A-N3A-C4A	2.03	116.79	111.83
2	C	801	FDA	O2P-P-O3P	-2.02	101.82	107.27

There are no chirality outliers.

All (5) torsion outliers are listed below:

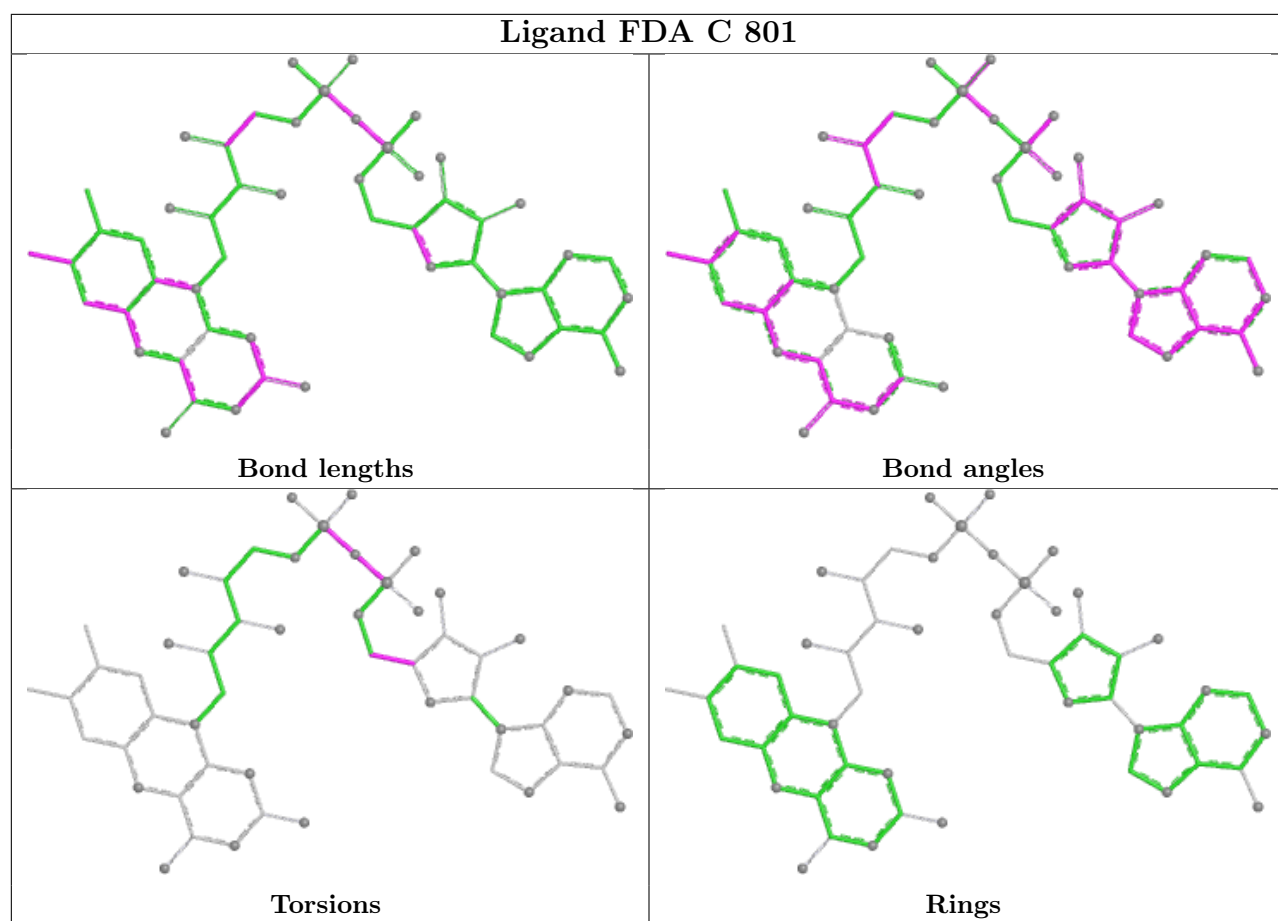
Mol	Chain	Res	Type	Atoms
2	B	801	FDA	PA-O3P-P-O5'
2	C	801	FDA	PA-O3P-P-O5'
2	D	801	FDA	PA-O3P-P-O5'
2	C	801	FDA	O4B-C4B-C5B-O5B
2	C	801	FDA	P-O3P-PA-O2A

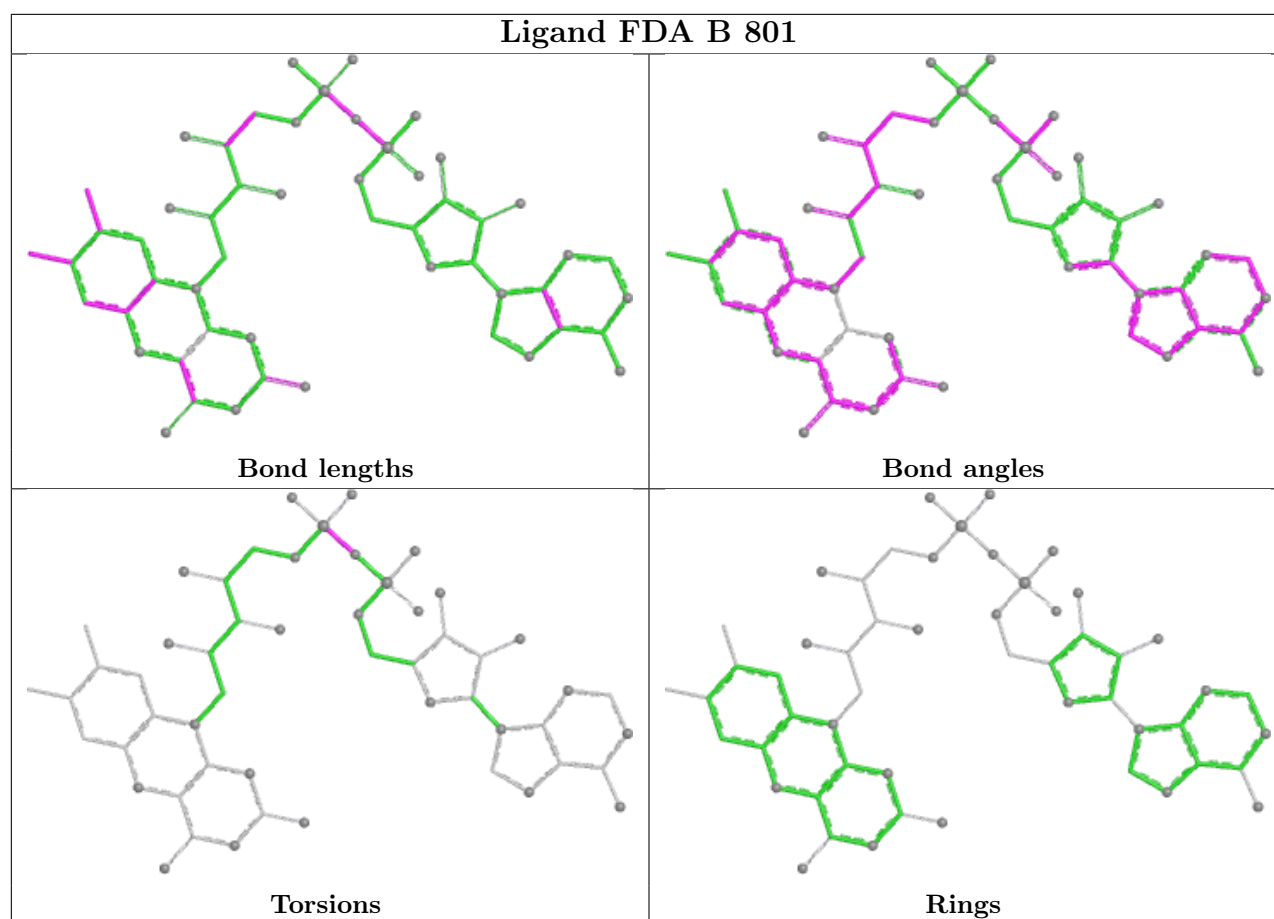
There are no ring outliers.

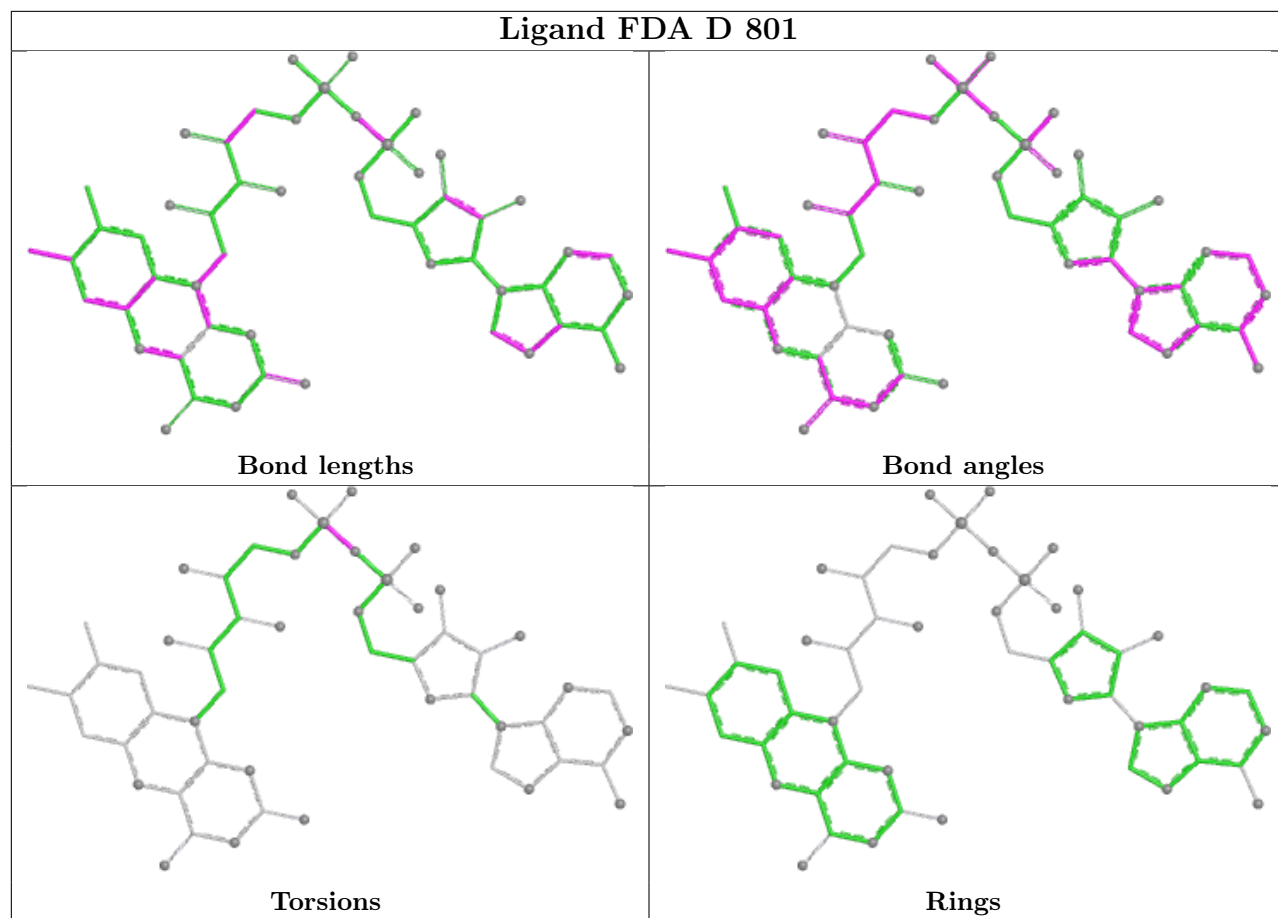
4 monomers are involved in 4 short contacts:

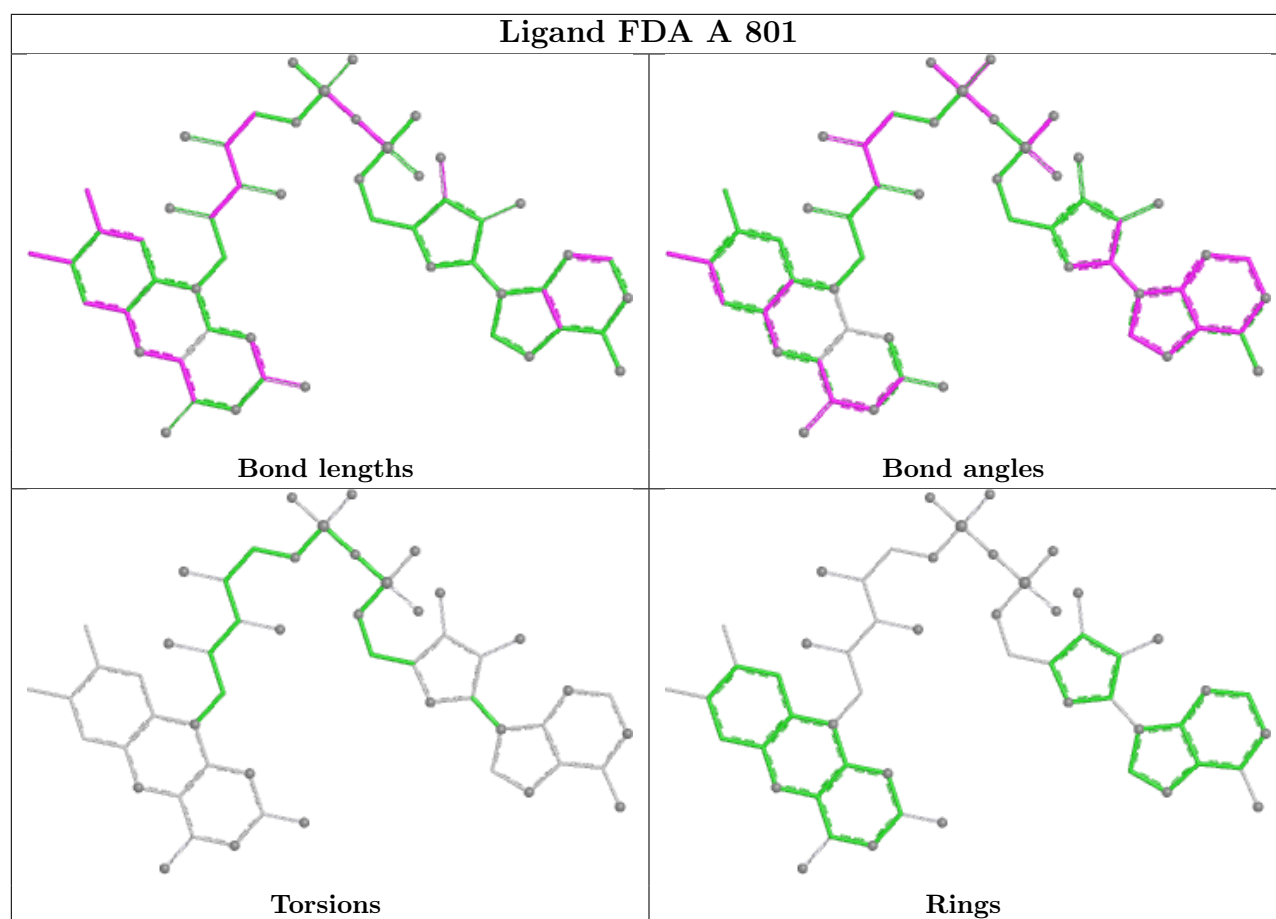
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	801	FDA	1	0
2	B	801	FDA	1	0
2	D	801	FDA	1	0
2	A	801	FDA	1	0

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	572/620 (92%)	-0.10	28 (4%) 35 33	15, 26, 53, 83	3 (0%)
1	B	581/620 (93%)	-0.21	22 (3%) 44 44	17, 26, 50, 76	1 (0%)
1	C	572/620 (92%)	-0.14	24 (4%) 40 40	18, 26, 52, 78	1 (0%)
1	D	572/620 (92%)	-0.27	20 (3%) 47 47	16, 23, 47, 82	3 (0%)
All	All	2297/2480 (92%)	-0.18	94 (4%) 41 41	15, 25, 51, 83	8 (0%)

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	464	ALA	8.2
1	A	465	VAL	8.2
1	D	465	VAL	7.5
1	D	460	PHE	6.0
1	A	460	PHE	5.6
1	B	459	ALA	5.5
1	D	65	VAL	5.4
1	B	460	PHE	5.4
1	D	462	TYR	5.4
1	D	464	ALA	5.2
1	B	465	VAL	5.2
1	C	465	VAL	5.2
1	A	459	ALA	5.1
1	D	466	ALA	5.0
1	C	131	LEU	4.8
1	A	462	TYR	4.4
1	C	69	PRO	4.4
1	C	462	TYR	4.4
1	A	65	VAL	4.3
1	A	458	ASP	4.3
1	D	459	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	462	TYR	4.0
1	A	55	MET	3.9
1	A	13	PRO	3.7
1	D	69	PRO	3.7
1	C	458	ASP	3.6
1	C	65	VAL	3.6
1	B	310	HIS	3.6
1	C	310	HIS	3.6
1	B	458	ASP	3.5
1	C	13	PRO	3.4
1	D	67	PHE	3.4
1	A	617	GLY	3.4
1	B	13	PRO	3.3
1	C	459	ALA	3.3
1	C	67	PHE	3.3
1	D	310	HIS	3.3
1	A	229	GLN	3.3
1	B	464	ALA	3.2
1	A	69	PRO	3.2
1	C	464	ALA	3.1
1	C	460	PHE	3.1
1	A	348	PRO	3.1
1	A	56	LYS	3.1
1	D	463	GLY	3.0
1	A	67	PHE	2.9
1	C	68	GLY	2.9
1	D	131	LEU	2.9
1	C	319	SER	2.9
1	D	461	SER	2.8
1	A	233	VAL	2.8
1	C	233	VAL	2.8
1	C	463	GLY	2.8
1	C	348	PRO	2.8
1	A	319	SER	2.7
1	B	233	VAL	2.7
1	A	131	LEU	2.7
1	C	320	VAL	2.6
1	D	617	GLY	2.6
1	D	427	ASN	2.6
1	A	231	GLU	2.5
1	A	466	ALA	2.5
1	A	310	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	55	MET	2.5
1	B	230	LYS	2.5
1	D	233	VAL	2.4
1	B	63	ARG	2.4
1	B	466	ALA	2.3
1	D	89	ILE	2.3
1	A	366	GLU	2.3
1	C	248	THR	2.3
1	C	461	SER	2.3
1	A	461	SER	2.2
1	A	230	LYS	2.2
1	A	232	ASN	2.2
1	D	458	ASP	2.2
1	A	463	GLY	2.2
1	B	229	GLN	2.1
1	B	461	SER	2.1
1	B	416	GLU	2.1
1	A	320	VAL	2.1
1	B	463	GLY	2.1
1	B	309	PRO	2.1
1	B	579	ASN	2.1
1	C	212	ASP	2.1
1	B	248	THR	2.0
1	D	410	GLY	2.0
1	B	232	ASN	2.0
1	B	320	VAL	2.0
1	C	309	PRO	2.0
1	C	427	ASN	2.0
1	B	409	PRO	2.0
1	D	348	PRO	2.0
1	A	38	ARG	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](#)

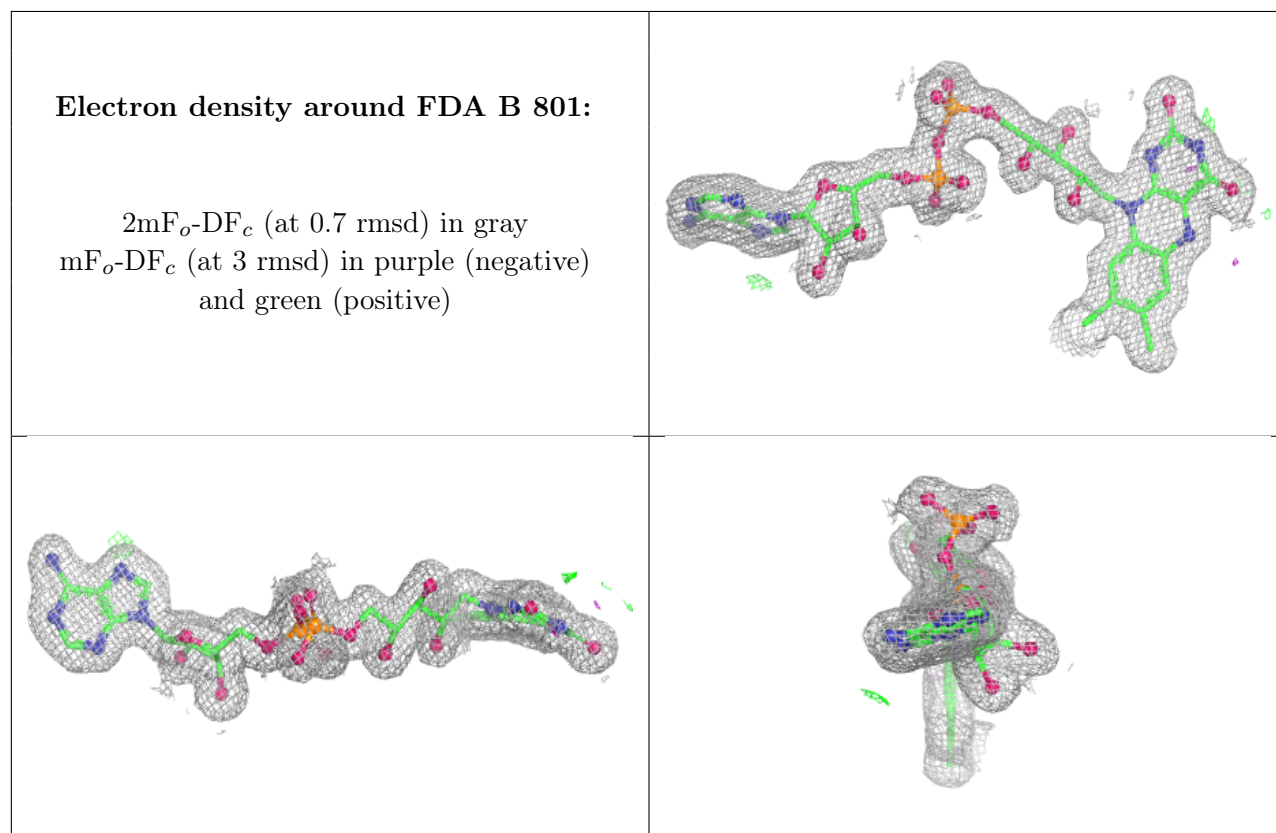
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

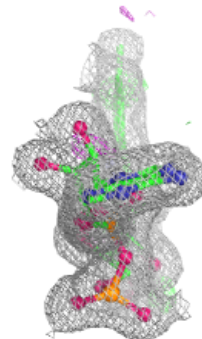
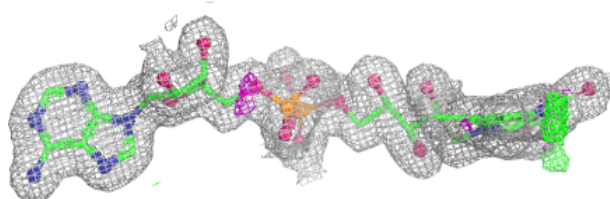
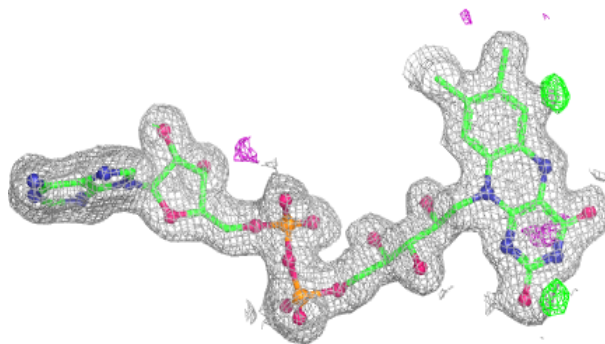
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	B	802	1/1	0.97	0.06	29,29,29,29	0
2	FDA	B	801	53/53	0.98	0.04	16,19,24,25	0
2	FDA	A	801	53/53	0.98	0.05	18,21,24,25	0
2	FDA	D	801	53/53	0.99	0.04	15,18,22,24	0
2	FDA	C	801	53/53	0.99	0.04	17,20,25,27	0

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.

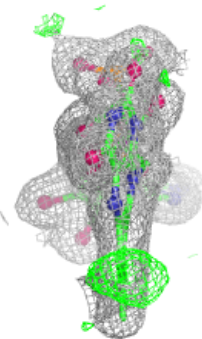
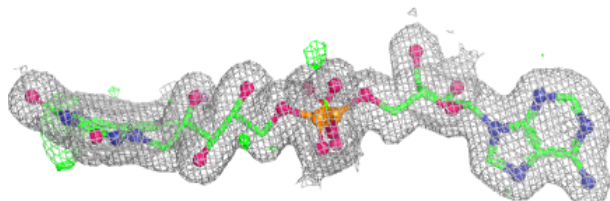
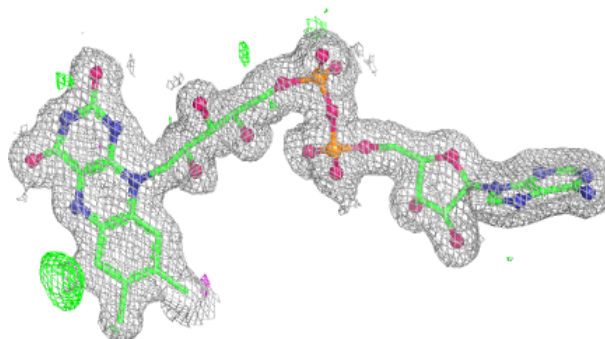


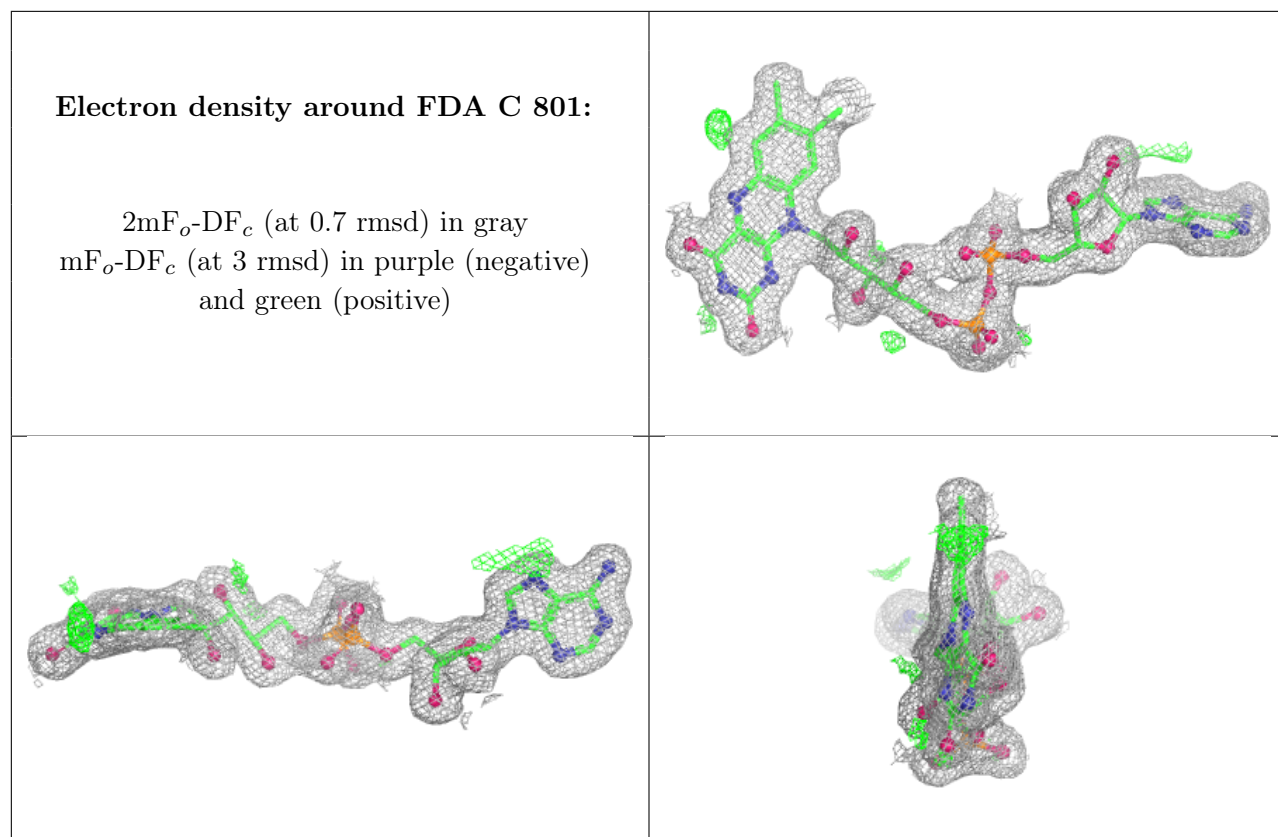
Electron density around FDA A 801:

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

**Electron density around FDA D 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.