Full wwPDB X-ray Structure Validation Report (i)

Sep 11, 2023 – 10:44 PM EDT

PDB ID	:	4MIF
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 (i) 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 (i)) were used in the production of this report:

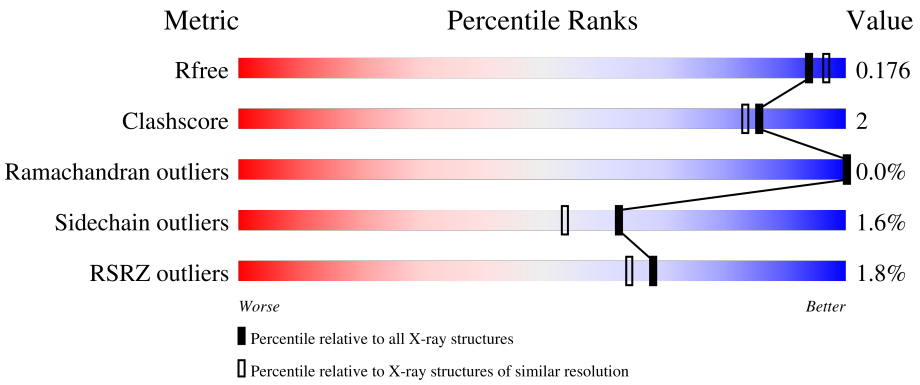
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (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 <=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	2% 83% 8% • 8%
1	B	620	2% 85% 8% • 6%
1	C	620	2% 84% 8% 8%
1	D	620	% 82% 9% • 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.

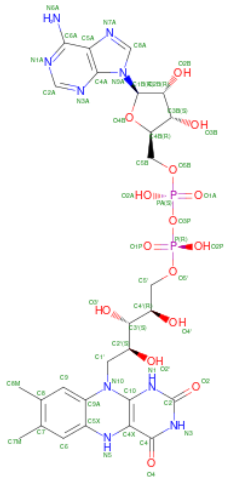
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Pyranose 2-oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	572	4542	2890	789	837	26	0	3	0
1	B	581	4593	2918	799	850	26	0	1	0
1	C	572	4529	2882	786	835	26	0	1	0
1	D	572	4539	2888	787	838	26	0	3	0

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

FDA



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

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is water.

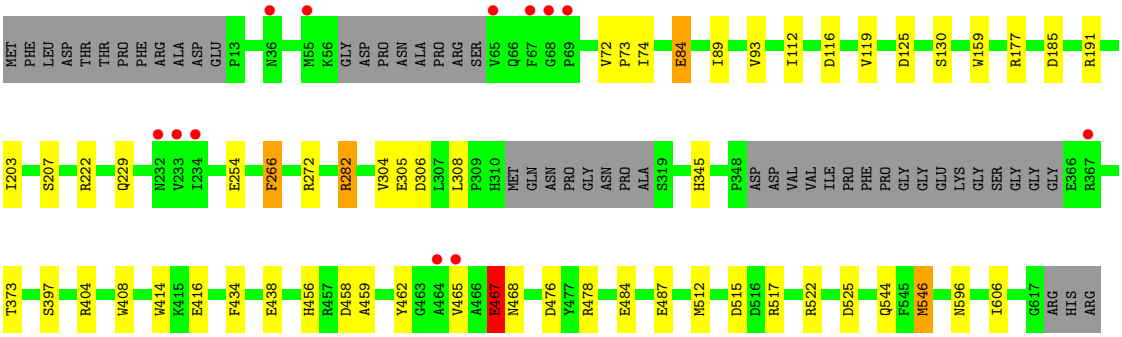
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	364	364	364	0	0
4	B	393	393	393	0	0
4	C	384	384	384	0	0
4	D	421	421	421	0	0

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.

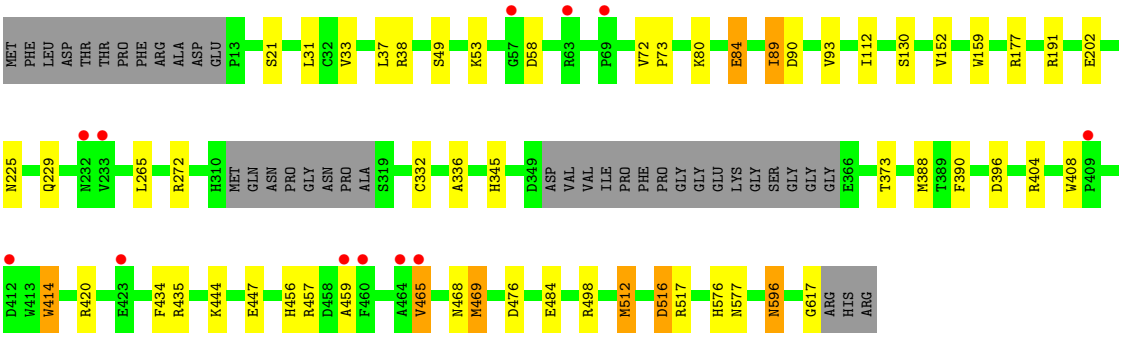
- Molecule 1: Pyranose 2-oxidase

Chain A:



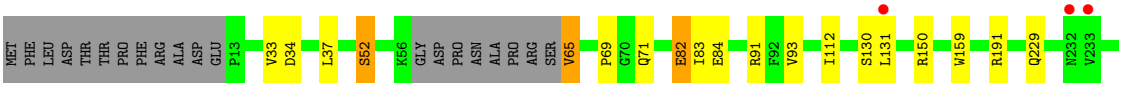
- Molecule 1: Pyranose 2-oxidase

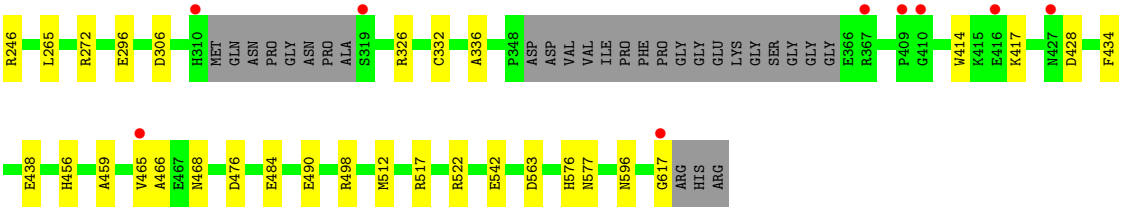
Chain B:



- Molecule 1: Pyranose 2-oxidase

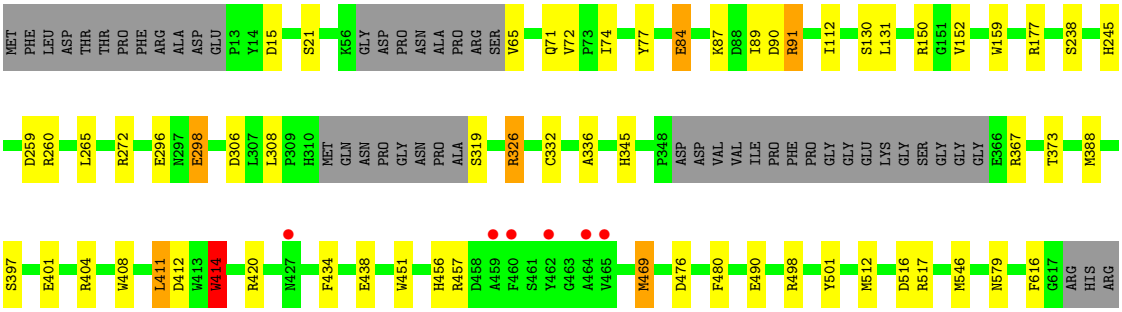
Chain C:





- Molecule 1: Pyranose 2-oxidase

Chain D:



4 Data and refinement statistics (i)

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) 99.9 (46.40-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.92 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.153 , 0.171 0.161 , 0.176	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 , 47.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	1.24	13/4674 (0.3%)	1.11	25/6358 (0.4%)
1	B	1.22	10/4722 (0.2%)	1.14	22/6427 (0.3%)
1	C	1.24	11/4655 (0.2%)	1.13	21/6333 (0.3%)
1	D	1.26	15/4671 (0.3%)	1.18	29/6355 (0.5%)
All	All	1.24	49/18722 (0.3%)	1.14	97/25473 (0.4%)

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	484	GLU	CD-OE1	11.72	1.38	1.25
1	D	438	GLU	CD-OE2	8.83	1.35	1.25
1	C	130	SER	CB-OG	8.41	1.53	1.42
1	C	484	GLU	CD-OE1	8.12	1.34	1.25
1	D	296	GLU	CD-OE1	8.04	1.34	1.25
1	B	447	GLU	CG-CD	7.35	1.62	1.51
1	C	296	GLU	CG-CD	7.20	1.62	1.51
1	B	484	GLU	CD-OE2	7.19	1.33	1.25
1	B	202	GLU	CD-OE2	6.95	1.33	1.25
1	A	438	GLU	CD-OE2	6.78	1.33	1.25
1	C	484	GLU	CD-OE2	6.56	1.32	1.25
1	A	416	GLU	CG-CD	6.47	1.61	1.51
1	A	484	GLU	CD-OE1	6.41	1.32	1.25
1	D	408	TRP	CD2-CE2	6.41	1.49	1.41
1	A	254	GLU	CD-OE2	6.40	1.32	1.25
1	D	77	TYR	CE1-CZ	-6.22	1.30	1.38
1	A	397	SER	CB-OG	-6.11	1.34	1.42
1	A	408	TRP	CD2-CE2	6.03	1.48	1.41
1	B	130	SER	CB-OG	6.03	1.50	1.42
1	A	266	PHE	CG-CD1	-5.91	1.29	1.38
1	A	130	SER	CB-OG	5.88	1.49	1.42
1	A	84	GLU	CD-OE1	5.85	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	451	TRP	CD2-CE2	5.83	1.48	1.41
1	C	490	GLU	CD-OE2	-5.81	1.19	1.25
1	A	416	GLU	CD-OE1	5.72	1.31	1.25
1	D	245	HIS	CG-CD2	5.65	1.45	1.35
1	D	501	TYR	CE2-CZ	-5.63	1.31	1.38
1	D	238	SER	CB-OG	-5.61	1.34	1.42
1	C	438	GLU	CD-OE1	5.60	1.31	1.25
1	B	49	SER	CB-OG	-5.56	1.35	1.42
1	C	484	GLU	CG-CD	5.49	1.60	1.51
1	C	542	GLU	CD-OE2	5.46	1.31	1.25
1	D	490	GLU	CG-CD	5.41	1.60	1.51
1	B	484	GLU	CG-CD	5.39	1.60	1.51
1	C	434	PHE	CG-CD2	-5.39	1.30	1.38
1	B	408	TRP	CD2-CE2	5.35	1.47	1.41
1	B	435	ARG	N-CA	5.35	1.57	1.46
1	D	414	TRP	CD2-CE2	5.34	1.47	1.41
1	B	457	ARG	C-O	5.31	1.33	1.23
1	D	401	GLU	CD-OE1	5.27	1.31	1.25
1	A	84	GLU	CG-CD	5.26	1.59	1.51
1	C	52	SER	CB-OG	-5.23	1.35	1.42
1	D	401	GLU	CG-CD	5.21	1.59	1.51
1	D	397	SER	CB-OG	-5.19	1.35	1.42
1	A	207	SER	CB-OG	5.16	1.49	1.42
1	D	130	SER	CB-OG	5.16	1.49	1.42
1	C	82	GLU	CG-CD	5.07	1.59	1.51
1	A	487	GLU	CD-OE2	5.04	1.31	1.25
1	D	90	ASP	CB-CG	5.00	1.62	1.51

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	512	MET	CG-SD-CE	-14.91	76.34	100.20
1	C	498	ARG	NE-CZ-NH1	11.31	125.96	120.30
1	C	191	ARG	NE-CZ-NH1	10.54	125.57	120.30
1	D	476	ASP	CB-CG-OD2	-10.23	109.09	118.30
1	D	91	ARG	NE-CZ-NH1	9.63	125.11	120.30
1	B	476	ASP	CB-CG-OD2	-9.44	109.81	118.30
1	B	404	ARG	NE-CZ-NH2	-8.91	115.85	120.30
1	B	434	PHE	C-N-CA	-8.82	99.66	121.70
1	B	498	ARG	NE-CZ-NH1	8.81	124.70	120.30
1	C	91	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	D	91	ARG	NE-CZ-NH2	-8.77	115.92	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	512	MET	CG-SD-CE	-8.75	86.19	100.20
1	D	265	LEU	CB-CG-CD2	8.34	125.18	111.00
1	A	476	ASP	CB-CG-OD1	8.31	125.78	118.30
1	C	517	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	B	517	ARG	NE-CZ-NH1	8.17	124.39	120.30
1	D	546	MET	CG-SD-CE	-8.16	87.15	100.20
1	A	476	ASP	CB-CG-OD2	-8.15	110.97	118.30
1	D	404[A]	ARG	NE-CZ-NH2	-8.05	116.27	120.30
1	D	404[B]	ARG	NE-CZ-NH2	-8.05	116.27	120.30
1	A	116	ASP	CB-CG-OD2	7.99	125.49	118.30
1	C	476	ASP	CB-CG-OD2	-7.58	111.47	118.30
1	D	434	PHE	C-N-CA	-7.49	102.98	121.70
1	C	434	PHE	C-N-CA	-7.45	103.07	121.70
1	B	498	ARG	NE-CZ-NH2	-7.43	116.58	120.30
1	A	434	PHE	C-N-CA	-7.40	103.20	121.70
1	B	512	MET	CG-SD-CE	-7.26	88.58	100.20
1	C	522	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	D	326	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	D	512	MET	CG-SD-CE	-6.74	89.42	100.20
1	D	84	GLU	CA-CB-CG	6.69	128.12	113.40
1	A	222	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	D	388	MET	CG-SD-CE	-6.61	89.63	100.20
1	D	498	ARG	CG-CD-NE	6.60	125.65	111.80
1	C	246	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	C	191	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	A	517	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	D	177	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	B	58	ASP	CB-CG-OD1	6.38	124.04	118.30
1	C	498	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	B	80	LYS	CD-CE-NZ	6.33	126.27	111.70
1	C	306	ASP	CB-CG-OD1	6.33	123.99	118.30
1	B	177	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	D	259	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	B	53	LYS	CD-CE-NZ	-6.20	97.45	111.70
1	B	516	ASP	CB-CG-OD1	-6.05	112.86	118.30
1	A	478	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	D	498	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	A	458	ASP	CB-CG-OD2	5.99	123.69	118.30
1	D	420	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	D	498	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	A	191[A]	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	A	191[B]	ARG	NE-CZ-NH1	5.81	123.21	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	411	LEU	CB-CG-CD1	-5.77	101.19	111.00
1	A	306	ASP	CB-CG-OD1	5.75	123.47	118.30
1	C	476	ASP	CB-CA-C	-5.74	98.92	110.40
1	D	326	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	B	38	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	C	417	LYS	CD-CE-NZ	-5.68	98.64	111.70
1	A	522	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	D	516	ASP	CB-CG-OD1	-5.59	113.27	118.30
1	C	246	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	177	ARG	NE-CZ-NH2	-5.57	117.51	120.30
1	B	31	LEU	CB-CG-CD2	5.57	120.48	111.00
1	C	563	ASP	CB-CG-OD1	5.57	123.31	118.30
1	B	388	MET	CG-SD-CE	-5.53	91.35	100.20
1	A	525	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	D	298	GLU	OE1-CD-OE2	5.45	129.84	123.30
1	D	469	MET	CG-SD-CE	-5.45	91.49	100.20
1	D	87	LYS	CD-CE-NZ	5.40	124.12	111.70
1	A	467	GLU	N-CA-CB	5.40	120.32	110.60
1	D	517	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	D	306	ASP	CB-CG-OD2	-5.35	113.49	118.30
1	D	480	PHE	CB-CG-CD1	5.34	124.54	120.80
1	B	469	MET	CG-SD-CE	-5.34	91.66	100.20
1	A	546	MET	CG-SD-CE	-5.32	91.69	100.20
1	C	130	SER	CB-CA-C	5.31	120.18	110.10
1	C	34	ASP	CB-CG-OD1	5.27	123.05	118.30
1	B	420	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	C	428	ASP	CB-CG-OD2	-5.26	113.57	118.30
1	A	125	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	A	282	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	D	15	ASP	CB-CG-OD1	-5.20	113.62	118.30
1	A	404[A]	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	A	404[B]	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	B	38	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	A	185	ASP	CB-CG-OD1	5.14	122.93	118.30
1	A	84	GLU	CA-CB-CG	5.14	124.70	113.40
1	B	476	ASP	CB-CG-OD1	5.13	122.92	118.30
1	D	438	GLU	CG-CD-OE2	5.13	128.56	118.30
1	A	119	VAL	CG1-CB-CG2	5.11	119.08	110.90
1	B	390	PHE	CB-CG-CD1	-5.08	117.25	120.80
1	B	84	GLU	CB-CA-C	-5.06	100.28	110.40
1	C	191	ARG	CD-NE-CZ	5.06	130.68	123.60
1	C	272	ARG	NE-CZ-NH2	-5.05	117.78	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	515	ASP	CB-CG-OD2	5.02	122.82	118.30
1	B	457	ARG	O-C-N	5.02	130.72	122.70

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	25	0
1	B	4593	0	4479	28	0
1	C	4529	0	4424	14	0
1	D	4539	0	4434	21	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	1	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	81	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 2.

All (81) 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: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	0.74
1:A:93:VAL:HG23	1:A:459:ALA:HB1	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:326:ARG:NH2	1:D:616:PHE:O	2.22	0.71
1:A:544:GLN:HG3	1:A:546:MET:HE3	1.71	0.70
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: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: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:A:544:GLN:HG3	1:A:546:MET:HE1	1.94	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:ILE:CD1	1:A:266:PHE:HB2	2.47	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:B:89:ILE:HG23	1:B:90:ASP:N	2.31	0.44
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: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: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:D:298:GLU:HG2	1:D:579[B]:ASN:ND2	2.34	0.42
1:A:282:ARG:O	1:A:304:VAL:HA	2.20	0.41
1:B:414:TRP:CD1	1:B:414:TRP:C	2.94	0.41
1:D:71:GLN:HG2	4:D:1275:HOH:O	2.21	0.41
1:B:93:VAL:CG2	1:B:459:ALA:C	2.89	0.41
1:D:411:LEU:HD23	1:D:414:TRP:CE3	2.56	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:B:512:MET:HE3	1:B:516:ASP:HB3	2.02	0.40
1:A:93:VAL:CG2	1:A:459:ALA:C	2.90	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 (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	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%)	47	33
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 (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	495/529 (94%)	487 (98%)	8 (2%)	62	54
1	B	500/529 (94%)	492 (98%)	8 (2%)	62	54
1	C	493/529 (93%)	486 (99%)	7 (1%)	67	59
1	D	495/529 (94%)	486 (98%)	9 (2%)	59	48
All	All	1983/2116 (94%)	1951 (98%)	32 (2%)	62	54

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	159	TRP
1	A	229	GLN
1	A	272	ARG
1	A	305	GLU
1	A	308	LEU
1	A	414	TRP
1	A	456	HIS
1	A	467	GLU
1	B	84	GLU
1	B	89	ILE
1	B	159	TRP
1	B	414	TRP
1	B	456	HIS
1	B	465	VAL
1	B	469	MET
1	B	596	ASN
1	C	52	SER
1	C	65	VAL
1	C	159	TRP
1	C	326	ARG
1	C	414	TRP
1	C	456	HIS
1	C	596	ASN
1	D	65	VAL
1	D	89	ILE
1	D	159	TRP
1	D	260	ARG
1	D	319	SER
1	D	367	ARG
1	D	412	ASP
1	D	414	TRP
1	D	456	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	229	GLN
1	B	111	HIS
1	B	572	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	A	801	1	52,58,58	2.20	14 (26%)	60,89,89	2.08	16 (26%)
2	FDA	C	801	1	52,58,58	1.41	10 (19%)	60,89,89	2.05	13 (21%)
2	FDA	D	801	1	52,58,58	1.96	9 (17%)	60,89,89	2.29	20 (33%)
2	FDA	B	801	1	52,58,58	1.55	9 (17%)	60,89,89	2.56	24 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FDA	A	801	1	-	1/30/50/50	0/6/6/6
2	FDA	C	801	1	-	2/30/50/50	0/6/6/6
2	FDA	D	801	1	-	2/30/50/50	0/6/6/6
2	FDA	B	801	1	-	2/30/50/50	0/6/6/6

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	801	FDA	C6-C5X	7.13	1.50	1.39
2	A	801	FDA	C2A-N3A	6.60	1.42	1.32
2	A	801	FDA	C5'-C4'	6.39	1.60	1.51
2	D	801	FDA	C5'-C4'	6.30	1.60	1.51
2	A	801	FDA	C6-C5X	5.40	1.47	1.39
2	D	801	FDA	C2A-N3A	5.15	1.40	1.32
2	A	801	FDA	C7M-C7	4.46	1.60	1.51
2	B	801	FDA	C4X-C4	4.44	1.53	1.42
2	C	801	FDA	C5'-C4'	4.13	1.57	1.51
2	B	801	FDA	C5X-C9A	-3.64	1.36	1.40
2	A	801	FDA	C8M-C8	3.46	1.57	1.51
2	D	801	FDA	O2-C2	3.41	1.30	1.23
2	B	801	FDA	O2-C2	3.36	1.30	1.23
2	D	801	FDA	C7M-C7	3.36	1.57	1.51
2	C	801	FDA	C6-C5X	3.25	1.44	1.39
2	A	801	FDA	C4X-C4	3.16	1.50	1.42
2	A	801	FDA	C5A-C4A	-3.02	1.32	1.40
2	C	801	FDA	C4X-C4	2.90	1.49	1.42
2	A	801	FDA	C4'-C3'	-2.90	1.48	1.53
2	C	801	FDA	C2-N3	-2.81	1.32	1.37
2	B	801	FDA	C5'-C4'	2.80	1.55	1.51
2	B	801	FDA	C6-C5X	2.76	1.43	1.39
2	B	801	FDA	C7M-C7	2.64	1.56	1.51
2	A	801	FDA	O3B-C3B	-2.63	1.36	1.43
2	B	801	FDA	C8M-C8	2.57	1.56	1.51
2	A	801	FDA	O2-C2	2.47	1.28	1.23
2	A	801	FDA	C5X-N5	-2.43	1.35	1.39
2	C	801	FDA	C9A-N10	2.39	1.45	1.41
2	C	801	FDA	C5X-N5	-2.35	1.35	1.39
2	D	801	FDA	C5X-C9A	-2.34	1.37	1.40
2	D	801	FDA	C2B-C3B	-2.29	1.47	1.53
2	A	801	FDA	C4X-N5	2.26	1.40	1.35
2	B	801	FDA	C5A-C4A	-2.26	1.35	1.40
2	C	801	FDA	O2-C2	2.19	1.28	1.23
2	A	801	FDA	C2-N1	-2.18	1.33	1.37
2	D	801	FDA	C8A-N7A	2.14	1.38	1.34
2	C	801	FDA	O4B-C4B	-2.12	1.40	1.45
2	A	801	FDA	C9-C8	2.11	1.42	1.39
2	C	801	FDA	C2-N1	-2.10	1.33	1.37
2	D	801	FDA	C10-N10	-2.09	1.34	1.38
2	C	801	FDA	C7M-C7	2.05	1.55	1.51
2	B	801	FDA	C6A-C5A	-2.02	1.35	1.43

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	801	FDA	C4-N3-C2	8.93	139.20	126.34
2	B	801	FDA	O4-C4-N3	8.43	136.28	120.12
2	A	801	FDA	O4-C4-N3	7.40	134.31	120.12
2	C	801	FDA	C5A-C6A-N6A	7.30	131.44	120.35
2	D	801	FDA	O4-C4-N3	6.68	132.92	120.12
2	D	801	FDA	N3A-C2A-N1A	-6.67	118.26	128.68
2	A	801	FDA	N3A-C2A-N1A	-6.38	118.71	128.68
2	D	801	FDA	C4-N3-C2	6.05	135.05	126.34
2	B	801	FDA	N3A-C2A-N1A	-5.94	119.40	128.68
2	C	801	FDA	O4-C4-N3	5.73	131.11	120.12
2	A	801	FDA	O4-C4-C4X	-5.34	115.01	127.24
2	D	801	FDA	C2A-N1A-C6A	4.85	127.05	118.75
2	C	801	FDA	C5'-C4'-C3'	-4.63	103.25	112.20
2	C	801	FDA	C4-N3-C2	4.20	132.38	126.34
2	D	801	FDA	C5'-C4'-C3'	-4.12	104.25	112.20
2	C	801	FDA	O4-C4-C4X	-4.08	117.89	127.24
2	B	801	FDA	C2A-N1A-C6A	3.90	125.43	118.75
2	A	801	FDA	C2A-N1A-C6A	3.89	125.40	118.75
2	D	801	FDA	C6-C7-C8	3.75	125.04	119.67
2	B	801	FDA	O4-C4-C4X	-3.68	118.80	127.24
2	C	801	FDA	C5A-C6A-N1A	-3.64	112.10	120.35
2	D	801	FDA	C9A-C5X-N5	3.64	124.42	119.56
2	A	801	FDA	C4-N3-C2	3.55	131.45	126.34
2	B	801	FDA	C5A-C6A-N6A	3.49	125.66	120.35
2	D	801	FDA	O4-C4-C4X	-3.48	119.25	127.24
2	B	801	FDA	C5A-C6A-N1A	-3.30	112.88	120.35
2	B	801	FDA	C6-C5X-C9A	-3.22	116.28	119.67
2	A	801	FDA	O4B-C1B-C2B	-3.21	102.23	106.93
2	B	801	FDA	C5'-C4'-C3'	-3.13	106.15	112.20
2	B	801	FDA	O2'-C2'-C3'	3.11	116.66	109.10
2	B	801	FDA	N3-C2-N1	-3.10	110.82	115.80
2	D	801	FDA	C9-C8-C7	-2.95	115.44	119.67
2	A	801	FDA	C5'-C4'-C3'	-2.94	106.52	112.20
2	C	801	FDA	O2A-PA-O1A	2.80	126.09	112.24
2	A	801	FDA	O4'-C4'-C3'	2.77	115.83	109.10
2	C	801	FDA	O3B-C3B-C4B	2.74	118.97	111.05
2	B	801	FDA	C9A-C5X-N5	2.72	123.20	119.56
2	B	801	FDA	O5'-C5'-C4'	-2.72	102.11	109.36
2	D	801	FDA	O4'-C4'-C3'	2.71	115.69	109.10
2	D	801	FDA	C5X-C6-C7	-2.69	114.36	120.01
2	A	801	FDA	C3B-C2B-C1B	2.67	104.99	100.98
2	B	801	FDA	C4X-C4-N3	-2.66	104.38	112.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	801	FDA	O4B-C1B-C2B	-2.59	103.14	106.93
2	A	801	FDA	C7M-C7-C6	-2.58	114.72	119.49
2	C	801	FDA	O2B-C2B-C3B	2.55	120.07	111.82
2	A	801	FDA	O2P-P-O1P	2.55	124.83	112.24
2	D	801	FDA	C7M-C7-C6	-2.54	114.80	119.49
2	B	801	FDA	C1'-N10-C9A	2.53	124.73	120.51
2	D	801	FDA	C5A-C6A-N1A	-2.50	114.69	120.35
2	D	801	FDA	C4'-C3'-C2'	-2.45	108.26	113.36
2	D	801	FDA	N6A-C6A-N1A	2.42	123.59	118.57
2	A	801	FDA	C5A-C6A-N6A	2.41	124.01	120.35
2	B	801	FDA	C9-C8-C7	-2.40	116.22	119.67
2	C	801	FDA	O4'-C4'-C3'	2.35	114.83	109.10
2	B	801	FDA	C3B-C2B-C1B	2.29	104.43	100.98
2	C	801	FDA	C7M-C7-C8	-2.28	116.06	120.74
2	A	801	FDA	C5A-C6A-N1A	-2.26	115.22	120.35
2	B	801	FDA	O4'-C4'-C3'	2.24	114.53	109.10
2	D	801	FDA	O2'-C2'-C3'	2.22	114.50	109.10
2	C	801	FDA	C4-C4X-N5	2.21	122.67	116.63
2	A	801	FDA	O2A-PA-O1A	2.16	122.93	112.24
2	C	801	FDA	C2A-N1A-C6A	2.15	122.44	118.75
2	B	801	FDA	C9A-C9-C8	2.14	123.61	119.30
2	B	801	FDA	C5X-N5-C4X	-2.11	116.04	121.02
2	B	801	FDA	O4'-C4'-C5'	2.08	114.59	109.92
2	D	801	FDA	O5'-C5'-C4'	-2.07	103.83	109.36
2	D	801	FDA	C6-C5X-C9A	-2.07	117.49	119.67
2	A	801	FDA	C9A-C5X-N5	2.06	122.32	119.56
2	D	801	FDA	O2A-PA-O1A	2.06	122.42	112.24
2	B	801	FDA	O2-C2-N3	2.06	125.70	121.82
2	A	801	FDA	C6-C7-C8	2.05	122.60	119.67
2	D	801	FDA	O2P-P-O1P	2.04	122.32	112.24
2	B	801	FDA	O2A-PA-O1A	2.03	122.27	112.24

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	C	801	FDA	PA-O3P-P-O5'
2	D	801	FDA	PA-O3P-P-O5'
2	C	801	FDA	O4B-C4B-C5B-O5B
2	B	801	FDA	O4B-C4B-C5B-O5B
2	A	801	FDA	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
2	D	801	FDA	O4B-C4B-C5B-O5B

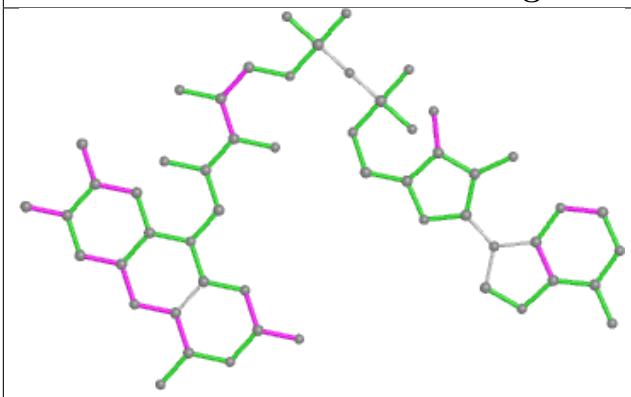
There are no ring outliers.

4 monomers are involved in 4 short contacts:

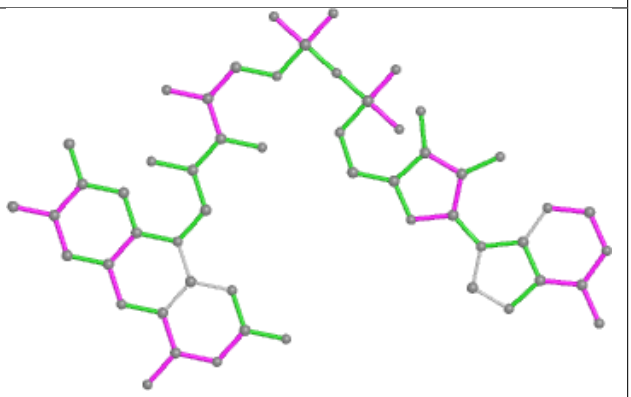
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	FDA	1	0
2	C	801	FDA	1	0
2	D	801	FDA	1	0
2	B	801	FDA	1	0

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 then 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.

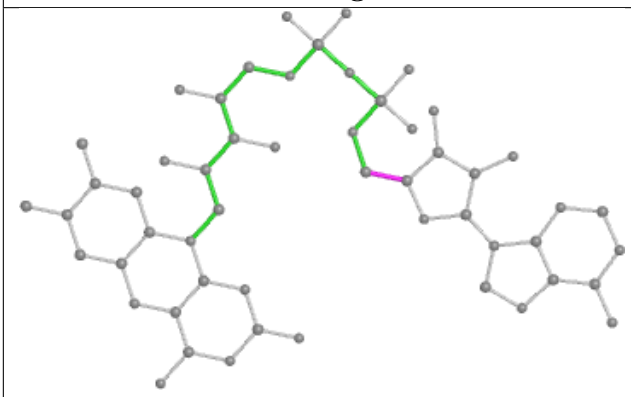
Ligand FDA A 801



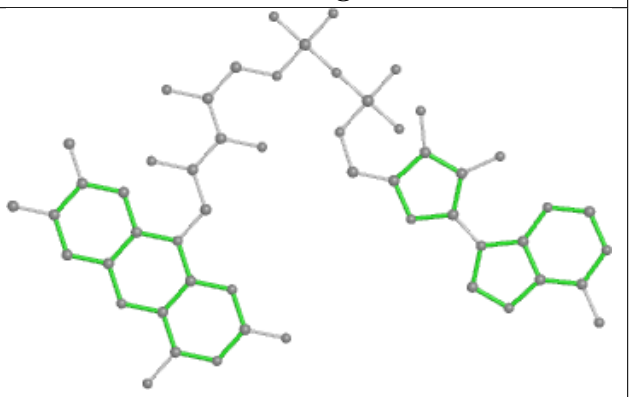
Bond lengths



Bond angles

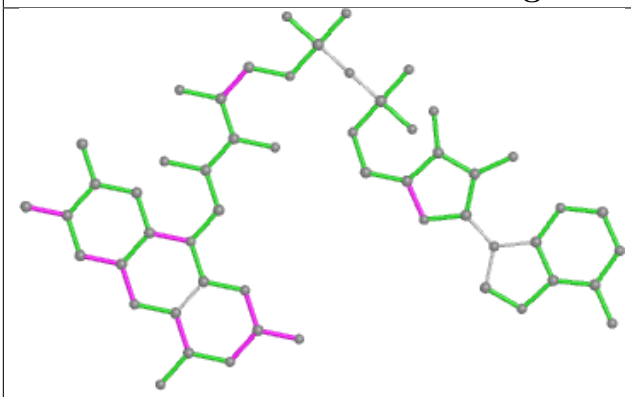


Torsions

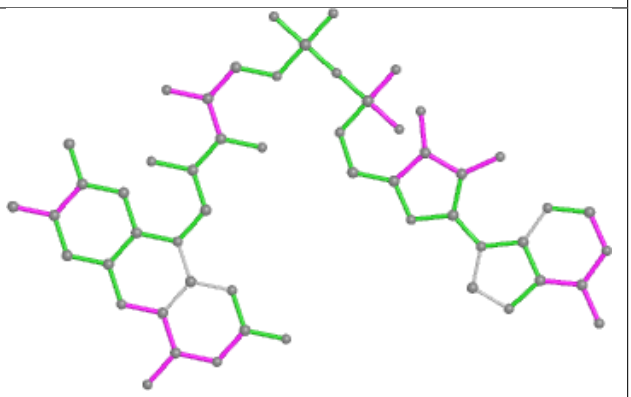


Rings

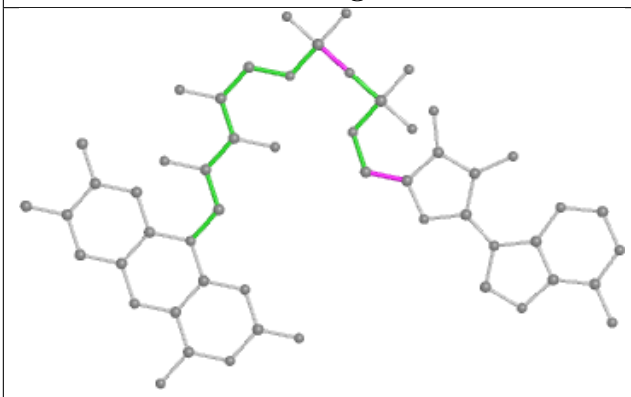
Ligand FDA C 801



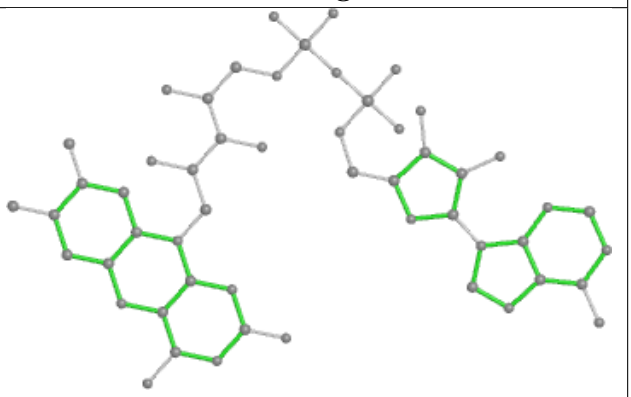
Bond lengths



Bond angles

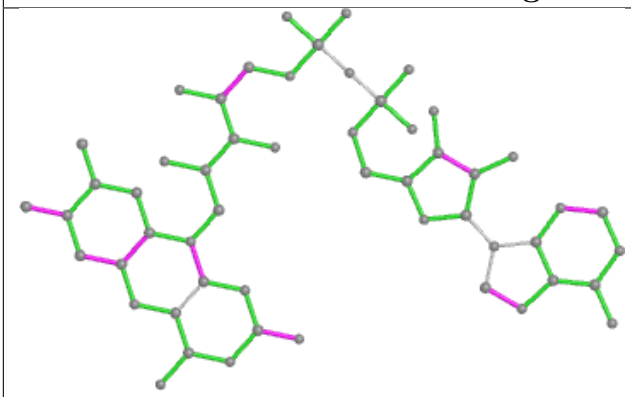


Torsions

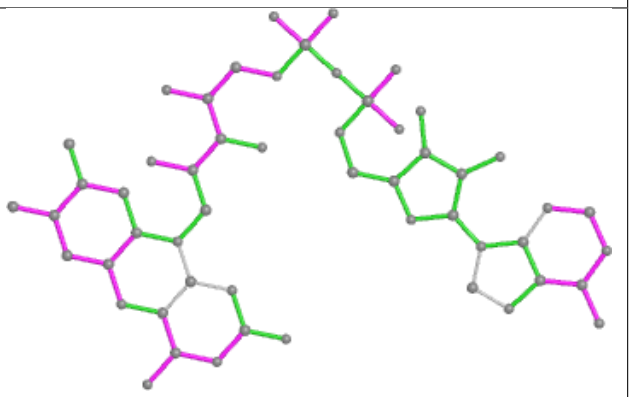


Rings

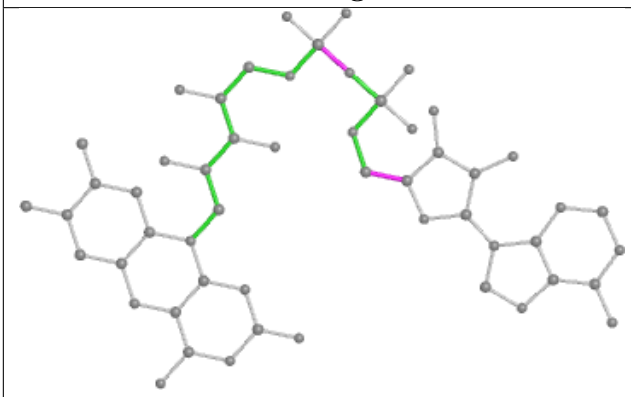
Ligand FDA D 801



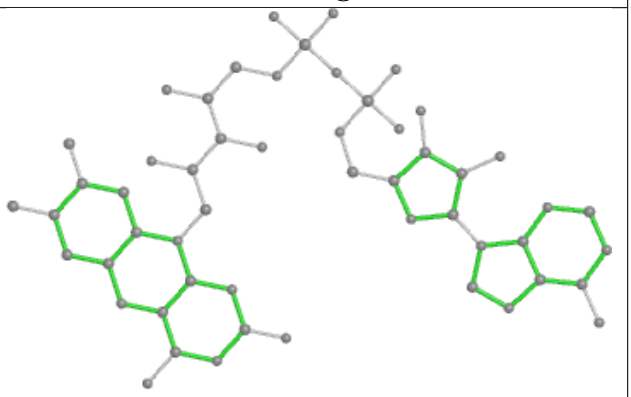
Bond lengths



Bond angles

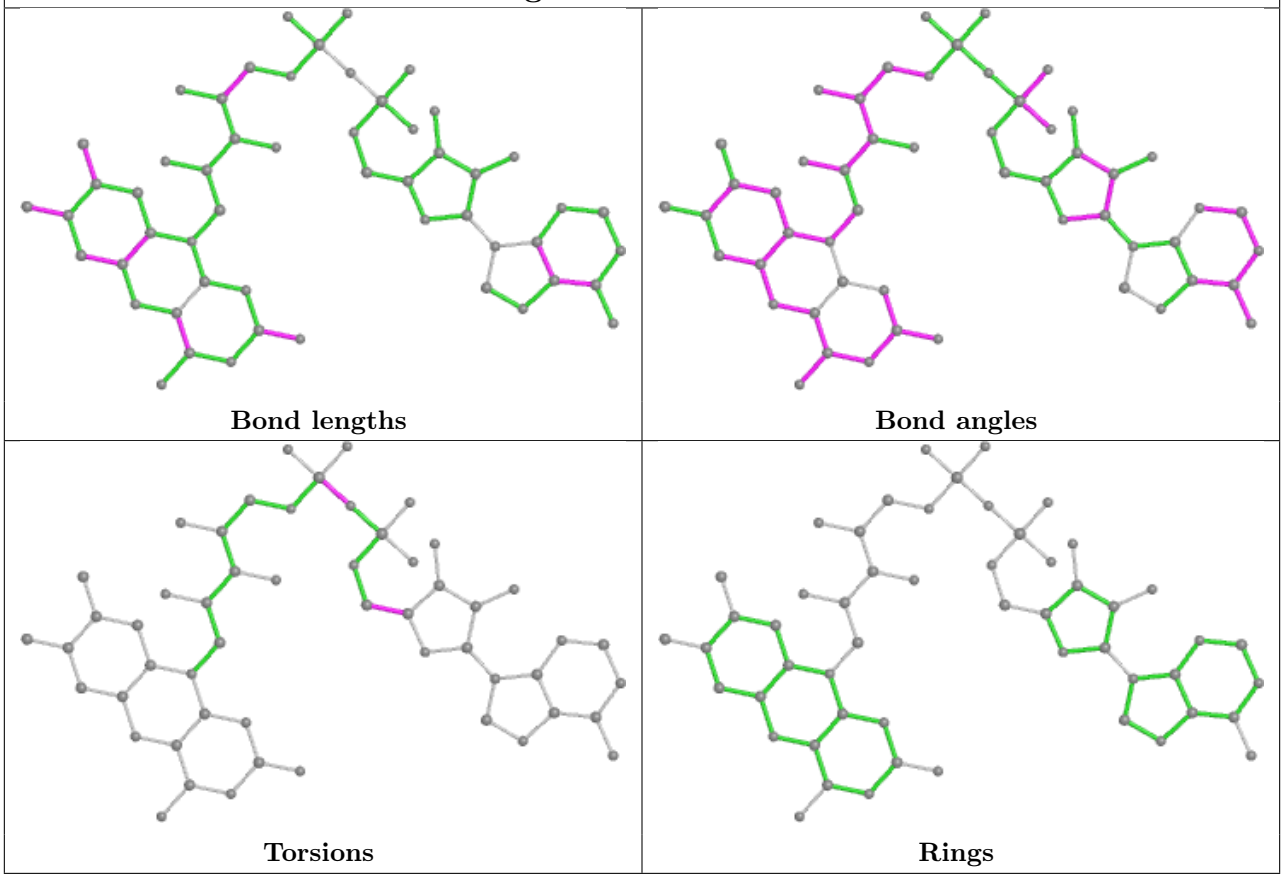


Torsions



Rings

Ligand FDA B 801



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	572/620 (92%)	-0.46	12 (2%)	63	59	18, 26, 53, 83	0
1	B	581/620 (93%)	-0.42	12 (2%)	63	59	17, 26, 50, 76	0
1	C	572/620 (92%)	-0.38	12 (2%)	63	59	18, 26, 52, 78	0
1	D	572/620 (92%)	-0.61	6 (1%)	82	80	17, 23, 47, 82	0
All	All	2297/2480 (92%)	-0.47	42 (1%)	68	64	17, 25, 51, 83	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	464	ALA	6.5
1	A	464	ALA	6.4
1	A	465	VAL	5.9
1	B	63	ARG	5.9
1	D	465	VAL	5.5
1	A	232	ASN	4.5
1	A	69	PRO	4.2
1	C	232	ASN	3.9
1	B	232	ASN	3.8
1	B	465	VAL	3.8
1	C	410	GLY	3.6
1	C	367	ARG	3.5
1	C	233	VAL	3.3
1	B	409	PRO	3.2
1	C	319	SER	3.2
1	C	617	GLY	3.1
1	B	464	ALA	3.1
1	B	57	GLY	2.9
1	C	131	LEU	2.9
1	C	409	PRO	2.8
1	B	233	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	427	ASN	2.7
1	A	367	ARG	2.7
1	C	465	VAL	2.6
1	A	233	VAL	2.6
1	D	462	TYR	2.5
1	A	55	MET	2.5
1	A	65	VAL	2.5
1	D	460	PHE	2.4
1	C	427	ASN	2.3
1	A	67	PHE	2.2
1	B	459	ALA	2.2
1	C	310	HIS	2.2
1	A	234	ILE	2.2
1	A	36	ASN	2.2
1	A	68	GLY	2.2
1	B	69	PRO	2.1
1	C	416	GLU	2.1
1	B	412	ASP	2.1
1	D	459	ALA	2.1
1	B	460	PHE	2.0
1	B	423	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 monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	B	802	1/1	0.95	0.05	29,29,29,29	0
2	FDA	B	801	53/53	0.99	0.07	16,19,24,25	0

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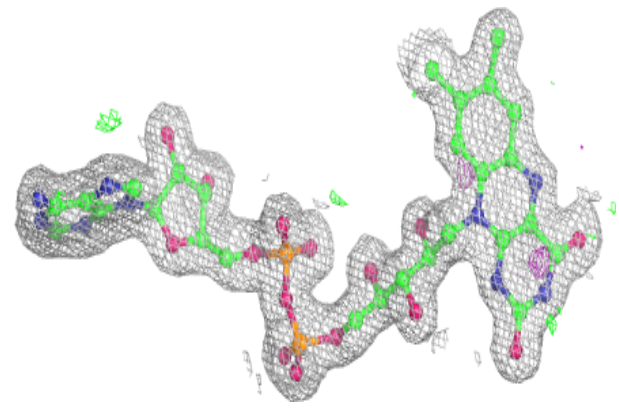
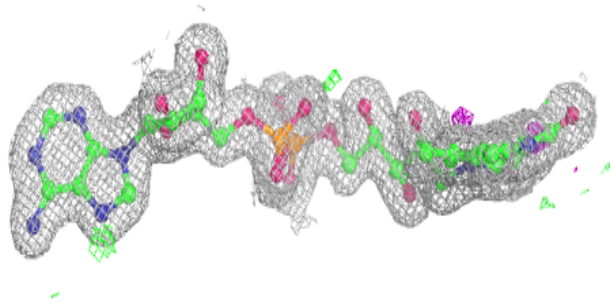
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FDA	C	801	53/53	0.99	0.09	17,20,25,27	0
2	FDA	D	801	53/53	0.99	0.07	15,18,22,24	0
2	FDA	A	801	53/53	0.99	0.07	18,21,24,25	0

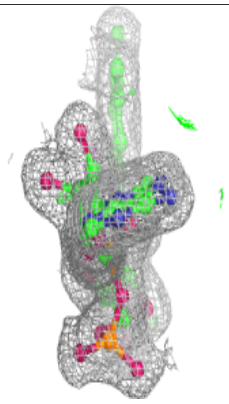
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FDA B 801:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

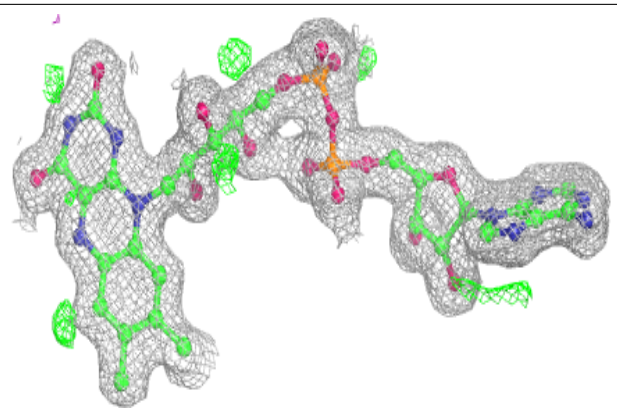


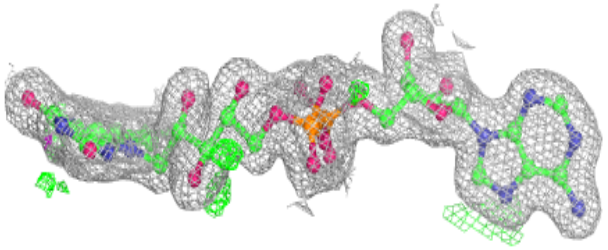


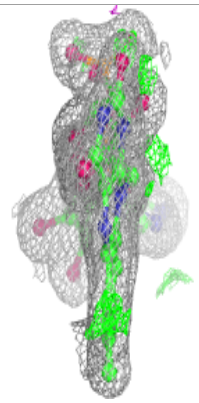


Electron density around FDA C 801:

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

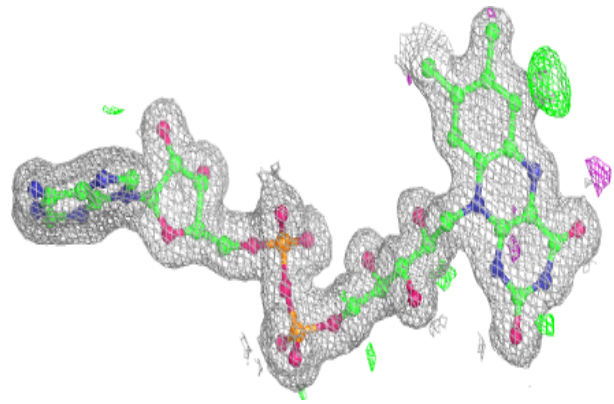


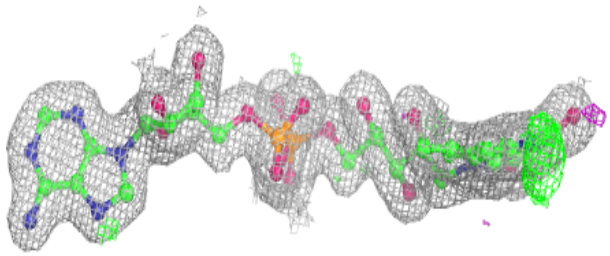


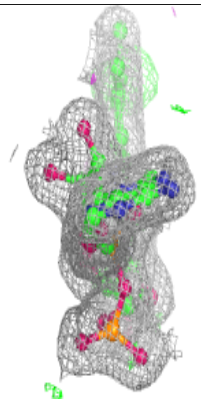


Electron density around FDA D 801:

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

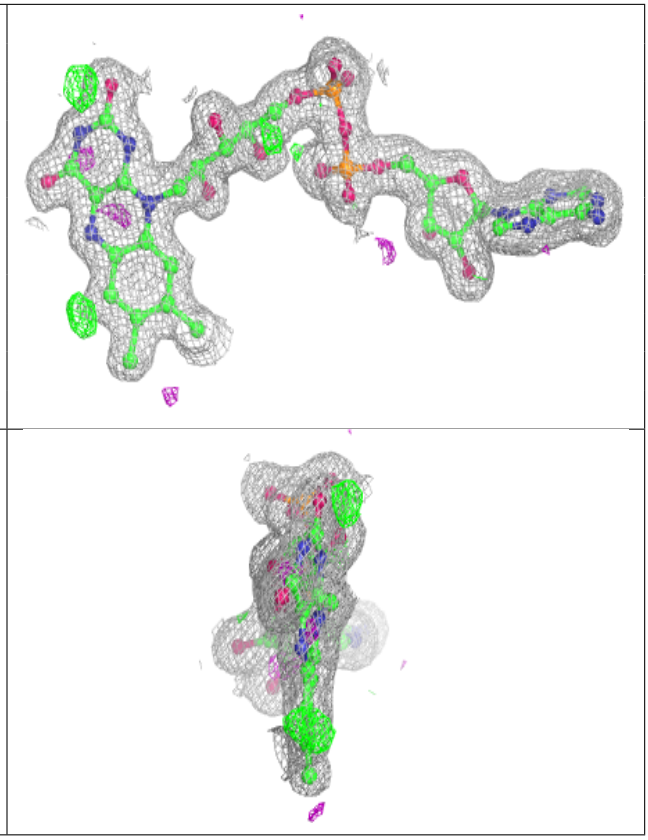






Electron density around FDA A 801:

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



6.5 Other polymers (i)

There are no such residues in this entry.