



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:16 PM UTC

PDB ID : 4ZCS / pdb_00004zcs
Title : Crystal structure of the C-terminal catalytic domain of Plasmodium falciparum CTP:phosphocholine cytidyltransferase in complex with CDP-choline
Authors : Guca, E.; Hoh, F.; Guichou, J.-F.; Cerdan, R.
Deposited on : 2015-04-16
Resolution : 2.45 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

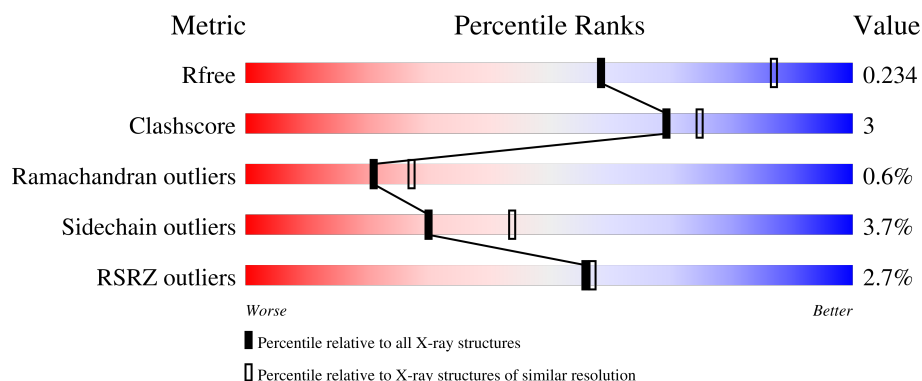
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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.



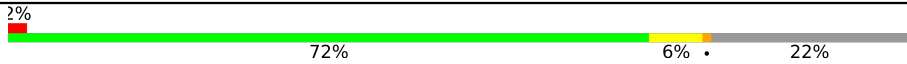
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	180	71% 7% • 22%
1	B	180	2% 69% 8% • 22%
1	C	180	2% 66% 9% • 24%
1	D	180	5% 67% 8% •• 23%
1	E	180	• 68% 9% • 22%

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Mol	Chain	Length	Quality of chain
1	F	180	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: a small red segment at the beginning labeled '2%', a large green segment in the middle labeled '72%', and a small yellow segment at the end labeled '6%'. A grey segment follows the yellow one, labeled '22%'. The total length of the bar represents 100%.

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7377 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 Choline-phosphate cytidylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	1	0
			1154	744	193	214	3			
1	C	137	Total	C	N	O	S	0	0	0
			1107	714	184	206	3			
1	E	141	Total	C	N	O	S	0	0	0
			1149	740	192	214	3			
1	B	140	Total	C	N	O	S	0	0	0
			1132	733	187	209	3			
1	D	139	Total	C	N	O	S	0	0	0
			1128	727	187	211	3			
1	F	141	Total	C	N	O	S	0	0	0
			1142	738	186	215	3			

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	578	GLY	-	expression tag	UNP Q8IEE9
A	579	HIS	-	expression tag	UNP Q8IEE9
A	580	MET	-	expression tag	UNP Q8IEE9
A	?	-	LYS	deletion	UNP Q8IEE9
A	?	-	LYS	deletion	UNP Q8IEE9
A	?	-	LYS	deletion	UNP Q8IEE9
A	?	-	LYS	deletion	UNP Q8IEE9
A	?	-	LYS	deletion	UNP Q8IEE9
A	?	-	LYS	deletion	UNP Q8IEE9
A	?	-	SER	deletion	UNP Q8IEE9
A	?	-	LYS	deletion	UNP Q8IEE9
A	?	-	GLY	deletion	UNP Q8IEE9
A	?	-	LYS	deletion	UNP Q8IEE9
A	?	-	SER	deletion	UNP Q8IEE9
A	?	-	PHE	deletion	UNP Q8IEE9
A	?	-	SER	deletion	UNP Q8IEE9
A	?	-	PHE	deletion	UNP Q8IEE9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASP	deletion	UNP Q8IEE9
A	?	-	GLU	deletion	UNP Q8IEE9
A	?	-	GLU	deletion	UNP Q8IEE9
A	?	-	ASN	deletion	UNP Q8IEE9
C	578	GLY	-	expression tag	UNP Q8IEE9
C	579	HIS	-	expression tag	UNP Q8IEE9
C	580	MET	-	expression tag	UNP Q8IEE9
C	?	-	LYS	deletion	UNP Q8IEE9
C	?	-	LYS	deletion	UNP Q8IEE9
C	?	-	LYS	deletion	UNP Q8IEE9
C	?	-	LYS	deletion	UNP Q8IEE9
C	?	-	LYS	deletion	UNP Q8IEE9
C	?	-	LYS	deletion	UNP Q8IEE9
C	?	-	SER	deletion	UNP Q8IEE9
C	?	-	LYS	deletion	UNP Q8IEE9
C	?	-	GLY	deletion	UNP Q8IEE9
C	?	-	LYS	deletion	UNP Q8IEE9
C	?	-	SER	deletion	UNP Q8IEE9
C	?	-	PHE	deletion	UNP Q8IEE9
C	?	-	SER	deletion	UNP Q8IEE9
C	?	-	PHE	deletion	UNP Q8IEE9
C	?	-	ASP	deletion	UNP Q8IEE9
C	?	-	GLU	deletion	UNP Q8IEE9
C	?	-	GLU	deletion	UNP Q8IEE9
C	?	-	ASN	deletion	UNP Q8IEE9
E	578	GLY	-	expression tag	UNP Q8IEE9
E	579	HIS	-	expression tag	UNP Q8IEE9
E	580	MET	-	expression tag	UNP Q8IEE9
E	?	-	LYS	deletion	UNP Q8IEE9
E	?	-	LYS	deletion	UNP Q8IEE9
E	?	-	LYS	deletion	UNP Q8IEE9
E	?	-	LYS	deletion	UNP Q8IEE9
E	?	-	LYS	deletion	UNP Q8IEE9
E	?	-	LYS	deletion	UNP Q8IEE9
E	?	-	SER	deletion	UNP Q8IEE9
E	?	-	LYS	deletion	UNP Q8IEE9
E	?	-	GLY	deletion	UNP Q8IEE9
E	?	-	LYS	deletion	UNP Q8IEE9
E	?	-	SER	deletion	UNP Q8IEE9
E	?	-	PHE	deletion	UNP Q8IEE9
E	?	-	SER	deletion	UNP Q8IEE9
E	?	-	PHE	deletion	UNP Q8IEE9

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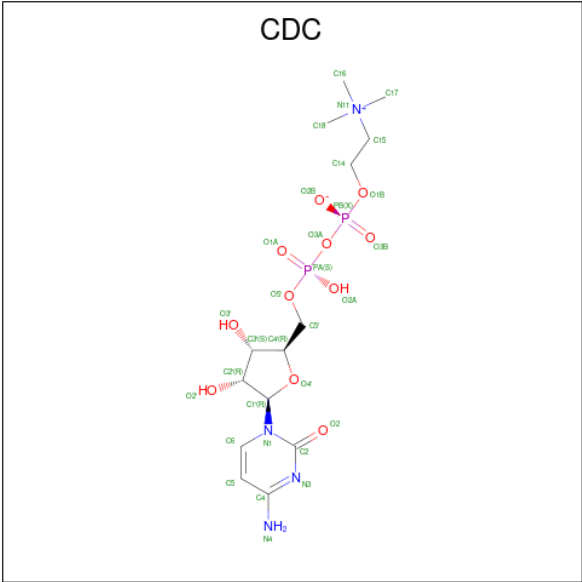
Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	ASP	deletion	UNP Q8IEE9
E	?	-	GLU	deletion	UNP Q8IEE9
E	?	-	GLU	deletion	UNP Q8IEE9
E	?	-	ASN	deletion	UNP Q8IEE9
B	578	GLY	-	expression tag	UNP Q8IEE9
B	579	HIS	-	expression tag	UNP Q8IEE9
B	580	MET	-	expression tag	UNP Q8IEE9
B	?	-	LYS	deletion	UNP Q8IEE9
B	?	-	LYS	deletion	UNP Q8IEE9
B	?	-	LYS	deletion	UNP Q8IEE9
B	?	-	LYS	deletion	UNP Q8IEE9
B	?	-	LYS	deletion	UNP Q8IEE9
B	?	-	LYS	deletion	UNP Q8IEE9
B	?	-	SER	deletion	UNP Q8IEE9
B	?	-	LYS	deletion	UNP Q8IEE9
B	?	-	GLY	deletion	UNP Q8IEE9
B	?	-	LYS	deletion	UNP Q8IEE9
B	?	-	SER	deletion	UNP Q8IEE9
B	?	-	PHE	deletion	UNP Q8IEE9
B	?	-	SER	deletion	UNP Q8IEE9
B	?	-	PHE	deletion	UNP Q8IEE9
B	?	-	ASP	deletion	UNP Q8IEE9
B	?	-	GLU	deletion	UNP Q8IEE9
B	?	-	GLU	deletion	UNP Q8IEE9
B	?	-	ASN	deletion	UNP Q8IEE9
D	578	GLY	-	expression tag	UNP Q8IEE9
D	579	HIS	-	expression tag	UNP Q8IEE9
D	580	MET	-	expression tag	UNP Q8IEE9
D	?	-	LYS	deletion	UNP Q8IEE9
D	?	-	LYS	deletion	UNP Q8IEE9
D	?	-	LYS	deletion	UNP Q8IEE9
D	?	-	LYS	deletion	UNP Q8IEE9
D	?	-	LYS	deletion	UNP Q8IEE9
D	?	-	LYS	deletion	UNP Q8IEE9
D	?	-	SER	deletion	UNP Q8IEE9
D	?	-	LYS	deletion	UNP Q8IEE9
D	?	-	GLY	deletion	UNP Q8IEE9
D	?	-	LYS	deletion	UNP Q8IEE9
D	?	-	SER	deletion	UNP Q8IEE9
D	?	-	PHE	deletion	UNP Q8IEE9
D	?	-	SER	deletion	UNP Q8IEE9
D	?	-	PHE	deletion	UNP Q8IEE9

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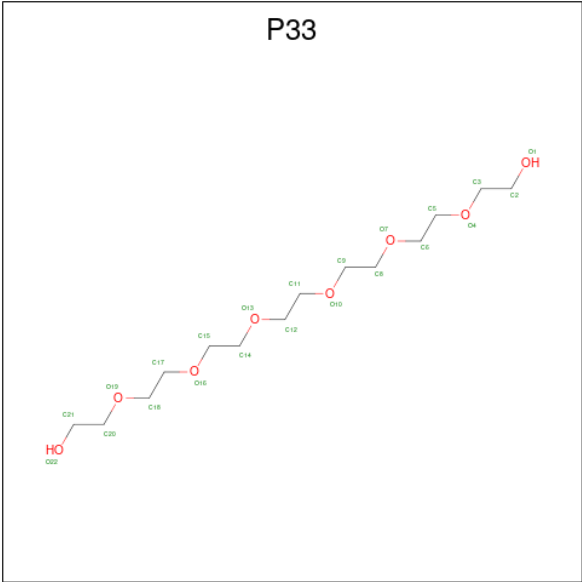
Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	ASP	deletion	UNP Q8IEE9
D	?	-	GLU	deletion	UNP Q8IEE9
D	?	-	GLU	deletion	UNP Q8IEE9
D	?	-	ASN	deletion	UNP Q8IEE9
F	578	GLY	-	expression tag	UNP Q8IEE9
F	579	HIS	-	expression tag	UNP Q8IEE9
F	580	MET	-	expression tag	UNP Q8IEE9
F	?	-	LYS	deletion	UNP Q8IEE9
F	?	-	LYS	deletion	UNP Q8IEE9
F	?	-	LYS	deletion	UNP Q8IEE9
F	?	-	LYS	deletion	UNP Q8IEE9
F	?	-	LYS	deletion	UNP Q8IEE9
F	?	-	LYS	deletion	UNP Q8IEE9
F	?	-	SER	deletion	UNP Q8IEE9
F	?	-	LYS	deletion	UNP Q8IEE9
F	?	-	GLY	deletion	UNP Q8IEE9
F	?	-	LYS	deletion	UNP Q8IEE9
F	?	-	SER	deletion	UNP Q8IEE9
F	?	-	PHE	deletion	UNP Q8IEE9
F	?	-	SER	deletion	UNP Q8IEE9
F	?	-	PHE	deletion	UNP Q8IEE9
F	?	-	ASP	deletion	UNP Q8IEE9
F	?	-	GLU	deletion	UNP Q8IEE9
F	?	-	GLU	deletion	UNP Q8IEE9
F	?	-	ASN	deletion	UNP Q8IEE9

- Molecule 2 is [2-CYTIDYLATE-O'-PHOSPHONYLOXYL]-ETHYL-TRIMETHYL-AMMONIUM (CCD ID: CDC) (formula: C₁₄H₂₆N₄O₁₁P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	14	4	11	2		
2	C	1	Total	C	N	O	P	0	0
			31	14	4	11	2		
2	E	1	Total	C	N	O	P	0	0
			31	14	4	11	2		
2	B	1	Total	C	N	O	P	0	0
			31	14	4	11	2		
2	D	1	Total	C	N	O	P	0	0
			31	14	4	11	2		
2	F	1	Total	C	N	O	P	0	0
			31	14	4	11	2		

- Molecule 3 is 3,6,9,12,15,18-HEXA OXAICOSANE-1,20-DIOL (CCD ID: P33) (formula: C₁₄H₃₀O₈).



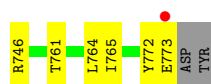
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			22	14	8		
3	D	1	Total	C	O	0	0
			16	10	6		

- Molecule 4 is water.

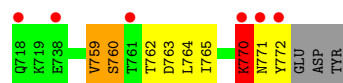
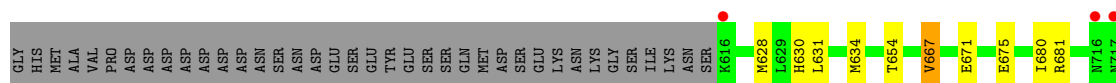
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	54	Total	O	0	0
			54	54		
4	C	51	Total	O	0	0
			51	51		
4	E	80	Total	O	0	0
			80	80		
4	B	53	Total	O	0	0
			53	53		
4	D	59	Total	O	0	0
			59	59		
4	F	44	Total	O	0	0
			44	44		

- Molecule 1: Choline-phosphate cytidyltransferase

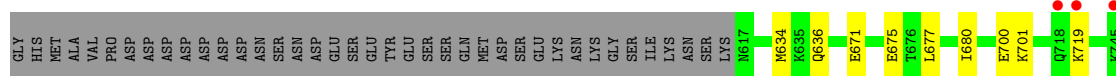




- Molecule 1: Choline-phosphate cytidylyltransferase



- Molecule 1: Choline-phosphate cytidylyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	114.63Å 149.13Å 175.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	113.67 – 2.45 113.67 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.6 (113.67-2.45) 99.6 (113.67-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.32	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.181 , 0.234 0.188 , 0.234	Depositor DCC
R_{free} test set	2808 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	40.8	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 28.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7377	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.13% 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: CDC, P33

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	1.30	2/1181 (0.2%)	1.21	5/1600 (0.3%)
1	B	1.26	2/1156 (0.2%)	1.20	3/1568 (0.2%)
1	C	1.23	2/1130 (0.2%)	1.14	3/1534 (0.2%)
1	D	1.14	1/1152 (0.1%)	1.16	3/1564 (0.2%)
1	E	1.25	1/1173 (0.1%)	1.07	1/1590 (0.1%)
1	F	1.06	0/1167	1.04	1/1586 (0.1%)
All	All	1.21	8/6959 (0.1%)	1.14	16/9442 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	E	0	1
All	All	0	2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	675	GLU	C-O	-6.07	1.17	1.24
1	B	622	ALA	CA-C	-6.06	1.45	1.52
1	A	671	GLU	CA-C	5.66	1.60	1.52
1	B	675	GLU	N-CA	5.56	1.53	1.46
1	E	772	TYR	CA-C	5.44	1.59	1.52
1	A	772	TYR	CA-C	5.19	1.59	1.52
1	C	648	THR	N-CA	-5.13	1.40	1.46
1	C	637	LEU	C-O	-5.12	1.17	1.24

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	698	PHE	N-CA-C	6.12	117.62	111.07
1	C	681	ARG	N-CA-C	6.01	118.62	111.71
1	D	759	VAL	N-CA-C	-5.78	101.77	108.82
1	F	700	GLU	N-CA-C	-5.78	100.42	109.25
1	A	768	ILE	CB-CA-C	-5.60	104.81	111.97
1	A	772	TYR	CA-C-N	5.51	130.12	121.08
1	A	772	TYR	C-N-CA	5.51	130.12	121.08
1	E	650	ILE	N-CA-C	-5.48	100.44	108.11
1	D	667	VAL	CB-CA-C	-5.40	104.85	112.14
1	B	710	ASP	CA-C-N	5.39	128.26	120.38
1	B	710	ASP	C-N-CA	5.39	128.26	120.38
1	C	765	ILE	CB-CA-C	-5.28	105.01	112.14
1	A	772	TYR	CB-CA-C	5.26	120.88	110.42
1	D	631	LEU	N-CA-CB	-5.15	102.33	110.06
1	A	617	ASN	N-CA-C	5.12	117.12	109.59
1	C	648	THR	N-CA-C	-5.01	100.12	108.34

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	770	LYS	Peptide
1	E	715	ALA	Peptide

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	1154	0	1162	6	0
1	B	1132	0	1127	10	0
1	C	1107	0	1103	11	0
1	D	1128	0	1121	13	0
1	E	1149	0	1151	9	0
1	F	1142	0	1122	6	0
2	A	31	0	25	1	0
2	B	31	0	25	3	0
2	C	31	0	25	4	0
2	D	31	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	31	0	25	3	0
2	F	31	0	25	3	0
3	B	22	0	30	1	0
3	D	16	0	20	0	0
4	A	54	0	0	0	0
4	B	53	0	0	1	0
4	C	51	0	0	0	0
4	D	59	0	0	3	0
4	E	80	0	0	1	0
4	F	44	0	0	0	0
All	All	7377	0	6986	49	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 (49) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:624:GLY:HA2	2:C:801:CDC:H142	1.70	0.72
1:A:761:THR:HG23	1:B:761:THR:HG23	1.75	0.69
1:E:761:THR:HG23	1:F:761:THR:HG23	1.75	0.68
1:E:639:GLN:HE22	1:E:754:GLN:H	1.42	0.68
1:D:681:ARG:NH2	4:D:902:HOH:O	2.26	0.67
1:E:617:ASN:ND2	4:E:901:HOH:O	2.30	0.64
1:D:630:HIS:CD2	1:D:760:SER:HA	2.36	0.61
1:B:654:THR:HG21	2:B:801:CDC:H172	1.83	0.60
1:D:760:SER:OG	4:D:901:HOH:O	2.17	0.59
1:C:628:MET:HG2	1:D:764:LEU:HD13	1.87	0.56
1:C:740:ILE:HD11	2:C:801:CDC:H173	1.88	0.55
1:E:624:GLY:HA2	2:E:801:CDC:H141	1.87	0.55
1:E:765:ILE:CG1	1:F:765:ILE:HG13	2.39	0.52
1:E:765:ILE:HG12	1:F:765:ILE:HG13	1.92	0.52
2:F:801:CDC:O1B	2:F:801:CDC:H163	2.11	0.51
1:D:763:ASP:HB2	4:D:901:HOH:O	2.12	0.49
1:C:628:MET:O	1:C:629:LEU:C	2.57	0.48
1:F:773:GLU:H	1:F:773:GLU:CD	2.20	0.48
1:E:710:ASP:HA	1:E:753:THR:O	2.14	0.47
1:C:768:ILE:HG12	1:D:667:VAL:HG22	1.96	0.47
1:A:765:ILE:HG13	1:B:765:ILE:HG13	1.96	0.47
1:B:623:ASP:OD2	2:B:801:CDC:H162	2.15	0.46
1:C:716:ASN:HD21	1:C:719:LYS:HB2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:765:ILE:HG13	1:B:765:ILE:CG1	2.45	0.45
1:C:741:TYR:OH	2:C:801:CDC:H152	2.16	0.45
1:C:765:ILE:HG13	1:D:765:ILE:CD1	2.46	0.45
2:C:801:CDC:C16	2:C:801:CDC:O1B	2.65	0.45
1:D:634:MET:HG2	1:D:680:ILE:HD12	1.99	0.45
1:A:771:ASN:O	1:A:773:GLU:N	2.51	0.43
2:A:801:CDC:O1B	2:A:801:CDC:H183	2.17	0.43
2:E:801:CDC:H163	2:E:801:CDC:O1B	2.18	0.43
2:F:801:CDC:O1B	2:F:801:CDC:C16	2.66	0.43
1:B:675:GLU:HG2	4:B:923:HOH:O	2.19	0.43
1:D:654:THR:HG21	2:D:801:CDC:H162	2.00	0.43
1:F:636:GLN:HG3	2:F:801:CDC:H1'	2.01	0.42
1:A:628:MET:HG2	1:B:764:LEU:HD13	2.01	0.42
1:C:716:ASN:HD22	1:C:716:ASN:C	2.27	0.42
1:E:746:ARG:HD2	1:B:681:ARG:NH1	2.35	0.42
1:C:765:ILE:HG13	1:D:765:ILE:HG13	2.01	0.42
1:B:772:TYR:O	1:B:773:GLU:CB	2.68	0.41
1:B:685:GLU:OE1	3:B:802:P33:O4	2.38	0.41
1:E:636:GLN:HG3	2:E:801:CDC:H1'	2.03	0.41
1:A:635:LYS:HE2	1:A:756:THR:HG21	2.03	0.41
1:D:759:VAL:O	1:D:760:SER:CB	2.69	0.41
1:C:651:VAL:HG21	1:C:683:VAL:HG22	2.01	0.40
2:B:801:CDC:H142	2:B:801:CDC:H173	1.76	0.40
1:D:771:ASN:O	1:D:772:TYR:HB2	2.20	0.40
1:F:634:MET:HG2	1:F:680:ILE:HD12	2.03	0.40
1:D:628:MET:CE	1:D:667:VAL:HG21	2.51	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	140/180 (78%)	136 (97%)	3 (2%)	1 (1%)	18	24
1	B	138/180 (77%)	134 (97%)	3 (2%)	1 (1%)	18	24
1	C	135/180 (75%)	131 (97%)	4 (3%)	0	100	100
1	D	137/180 (76%)	130 (95%)	5 (4%)	2 (2%)	8	7
1	E	139/180 (77%)	135 (97%)	4 (3%)	0	100	100
1	F	139/180 (77%)	135 (97%)	3 (2%)	1 (1%)	18	24
All	All	828/1080 (77%)	801 (97%)	22 (3%)	5 (1%)	21	27

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	718	GLN
1	D	760	SER
1	F	701	LYS
1	D	770	LYS
1	A	772	TYR

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	126/164 (77%)	124 (98%)	2 (2%)	55	69
1	B	120/164 (73%)	117 (98%)	3 (2%)	42	56
1	C	119/164 (73%)	112 (94%)	7 (6%)	18	26
1	D	122/164 (74%)	119 (98%)	3 (2%)	42	56
1	E	125/164 (76%)	118 (94%)	7 (6%)	19	27
1	F	122/164 (74%)	117 (96%)	5 (4%)	27	40
All	All	734/984 (75%)	707 (96%)	27 (4%)	30	44

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	666	VAL
1	A	767	ARG
1	C	675	GLU
1	C	677	LEU
1	C	697	GLU
1	C	716	ASN
1	C	719	LYS
1	C	760	SER
1	C	761	THR
1	E	645	GLU
1	E	661	LEU
1	E	665	GLN
1	E	703	LYS
1	E	754	GLN
1	E	765	ILE
1	E	769	LEU
1	B	675	GLU
1	B	700	GLU
1	B	746	ARG
1	D	671	GLU
1	D	762	THR
1	D	770	LYS
1	F	671	GLU
1	F	675	GLU
1	F	677	LEU
1	F	719	LYS
1	F	773	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	617	ASN
1	C	665	GLN
1	C	716	ASN
1	C	717	ASN
1	C	754	GLN
1	E	639	GLN
1	E	665	GLN
1	B	665	GLN
1	D	617	ASN
1	D	717	ASN
1	D	754	GLN
1	F	665	GLN

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 ⓘ

8 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	P33	B	802	-	21,21,21	0.91	0	20,20,20	0.74	0
2	CDC	F	801	-	32,32,32	2.16	6 (18%)	46,49,49	1.25	2 (4%)
2	CDC	E	801	-	32,32,32	1.68	7 (21%)	46,49,49	1.35	6 (13%)
2	CDC	C	801	-	32,32,32	1.45	7 (21%)	46,49,49	1.24	5 (10%)
2	CDC	B	801	-	32,32,32	1.61	4 (12%)	46,49,49	1.66	11 (23%)
3	P33	D	802	-	15,15,21	1.16	0	14,14,20	1.04	1 (7%)
2	CDC	A	801	-	32,32,32	1.60	6 (18%)	46,49,49	1.12	4 (8%)
2	CDC	D	801	-	32,32,32	2.15	8 (25%)	46,49,49	1.48	5 (10%)

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	P33	B	802	-	-	13/19/19/19	-
2	CDC	F	801	-	-	3/24/40/40	0/2/2/2
2	CDC	E	801	-	-	0/24/40/40	0/2/2/2
2	CDC	C	801	-	-	3/24/40/40	0/2/2/2
2	CDC	B	801	-	-	5/24/40/40	0/2/2/2
3	P33	D	802	-	-	9/13/13/19	-
2	CDC	A	801	-	-	3/24/40/40	0/2/2/2
2	CDC	D	801	-	-	3/24/40/40	0/2/2/2

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	801	CDC	PB-O3A	7.23	1.67	1.59
2	D	801	CDC	PB-O3A	6.36	1.66	1.59
2	D	801	CDC	PA-O3A	-6.02	1.53	1.59
2	B	801	CDC	PA-O3A	-5.73	1.53	1.59
2	F	801	CDC	C2-N3	4.93	1.46	1.36
2	D	801	CDC	C2-N1	-4.91	1.29	1.40
2	A	801	CDC	PA-O3A	-4.19	1.55	1.59
2	A	801	CDC	C2-N1	-3.99	1.31	1.40
2	C	801	CDC	C2-N1	-3.96	1.31	1.40
2	F	801	CDC	PA-O3A	-3.76	1.55	1.59
2	E	801	CDC	PB-O3A	3.64	1.63	1.59
2	E	801	CDC	O4'-C4'	3.46	1.52	1.45
2	E	801	CDC	PA-O3A	3.36	1.63	1.59
2	B	801	CDC	C2-N1	-3.30	1.33	1.40
2	B	801	CDC	O1B-C14	-3.19	1.32	1.44
2	D	801	CDC	C5-C4	-3.05	1.35	1.42
2	A	801	CDC	C4-N3	2.98	1.40	1.34
2	E	801	CDC	C6-N1	2.88	1.44	1.38
2	E	801	CDC	C2-N1	-2.76	1.34	1.40
2	F	801	CDC	C2-N1	-2.75	1.34	1.40
2	F	801	CDC	C5-C4	-2.67	1.36	1.42
2	C	801	CDC	PB-O1B	-2.46	1.49	1.59
2	C	801	CDC	C4-N3	2.45	1.39	1.34
2	B	801	CDC	C5-C4	-2.37	1.37	1.42
2	D	801	CDC	O2'-C2'	-2.29	1.37	1.43
2	E	801	CDC	C2-N3	2.27	1.40	1.36
2	E	801	CDC	C6-C5	2.24	1.40	1.35
2	C	801	CDC	PA-O2A	-2.22	1.45	1.55
2	C	801	CDC	PA-O1A	-2.22	1.43	1.50
2	F	801	CDC	C6-C5	2.20	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	CDC	O4'-C4'	2.18	1.49	1.45
2	A	801	CDC	C6-C5	2.13	1.40	1.35
2	C	801	CDC	C5-C4	-2.10	1.38	1.42
2	D	801	CDC	PB-O2B	2.06	1.64	1.55
2	A	801	CDC	PA-O1A	-2.02	1.43	1.50
2	D	801	CDC	C3'-C2'	-2.01	1.47	1.53
2	D	801	CDC	C6-C5	2.01	1.39	1.35
2	C	801	CDC	C2'-C1'	2.01	1.59	1.53

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	CDC	O3A-PA-O1A	-5.78	93.30	110.70
2	D	801	CDC	O2A-PA-O3A	3.86	117.70	107.27
2	B	801	CDC	C14-C15-N11	-3.74	103.81	115.82
2	F	801	CDC	O3A-PA-O1A	-3.68	99.64	110.70
2	B	801	CDC	O3A-PA-O1A	-3.63	99.79	110.70
2	E	801	CDC	O3A-PA-O1A	-3.58	99.92	110.70
2	B	801	CDC	O4'-C4'-C5'	-3.47	98.21	109.33
2	A	801	CDC	O3A-PA-O1A	-3.43	100.39	110.70
2	E	801	CDC	C4-N3-C2	3.29	125.45	120.26
2	B	801	CDC	O2-C2-N3	-3.16	117.35	122.33
2	B	801	CDC	O4'-C1'-C2'	-3.12	99.93	106.62
2	E	801	CDC	O4'-C1'-N1	3.07	115.31	108.36
2	D	801	CDC	O1B-PB-O3B	3.04	120.97	108.94
2	B	801	CDC	O2B-PB-O3A	-2.98	99.22	107.27
2	A	801	CDC	O1B-PB-O3B	2.84	120.20	108.94
2	C	801	CDC	O2-C2-N1	2.74	124.28	118.90
2	C	801	CDC	C4-N3-C2	2.68	124.48	120.26
2	F	801	CDC	N4-C4-N3	2.61	122.58	117.91
2	D	801	CDC	C5-C4-N3	-2.59	116.95	121.32
2	D	801	CDC	C4-N3-C2	2.54	124.27	120.26
2	C	801	CDC	O2-C2-N3	-2.54	118.32	122.33
2	E	801	CDC	O2-C2-N1	2.52	123.83	118.90
2	E	801	CDC	C5-C4-N4	2.48	124.98	120.63
2	C	801	CDC	O3A-PA-O1A	-2.43	103.40	110.70
2	C	801	CDC	O2B-PB-O1B	-2.42	96.58	107.57
2	B	801	CDC	O4'-C1'-N1	2.27	113.49	108.36
2	A	801	CDC	N4-C4-N3	2.19	121.82	117.91
2	B	801	CDC	C1'-N1-C2	2.15	123.19	118.44
3	D	802	P33	C9-O10-C11	2.10	122.44	113.26
2	B	801	CDC	PB-O1B-C14	-2.09	111.33	121.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	CDC	N4-C4-N3	2.07	121.62	117.91
2	A	801	CDC	O4'-C4'-C5'	2.07	115.96	109.33
2	E	801	CDC	O2-C2-N3	-2.06	119.08	122.33
2	B	801	CDC	C1'-N1-C6	-2.06	116.38	120.78

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	CDC	C14-O1B-PB-O3A
2	A	801	CDC	C14-O1B-PB-O3B
2	B	801	CDC	C14-O1B-PB-O2B
2	B	801	CDC	O1B-C14-C15-N11
2	D	801	CDC	C14-O1B-PB-O3A
2	D	801	CDC	C14-O1B-PB-O3B
2	F	801	CDC	C14-O1B-PB-O3A
2	F	801	CDC	C14-O1B-PB-O3B
3	B	802	P33	C21-C20-O19-C18
3	B	802	P33	O13-C14-C15-O16
3	B	802	P33	O10-C11-C12-O13
3	B	802	P33	O4-C5-C6-O7
3	D	802	P33	O13-C14-C15-O16
3	D	802	P33	O7-C8-C9-O10
3	B	802	P33	C2-C3-O4-C5
2	B	801	CDC	C14-C15-N11-C16
2	B	801	CDC	C14-C15-N11-C17
3	D	802	P33	O4-C5-C6-O7
2	B	801	CDC	C14-C15-N11-C18
2	C	801	CDC	C14-C15-N11-C16
3	B	802	P33	O7-C8-C9-O10
3	D	802	P33	O16-C17-C18-O19
3	D	802	P33	C18-C17-O16-C15
2	C	801	CDC	C14-C15-N11-C18
3	D	802	P33	C5-C6-O7-C8
3	B	802	P33	C11-C12-O13-C14
3	D	802	P33	C11-C12-O13-C14
3	B	802	P33	C12-C11-O10-C9
2	C	801	CDC	C14-C15-N11-C17
2	A	801	CDC	C14-O1B-PB-O2B
2	D	801	CDC	C14-O1B-PB-O2B
2	F	801	CDC	C14-O1B-PB-O2B
3	D	802	P33	C9-C8-O7-C6

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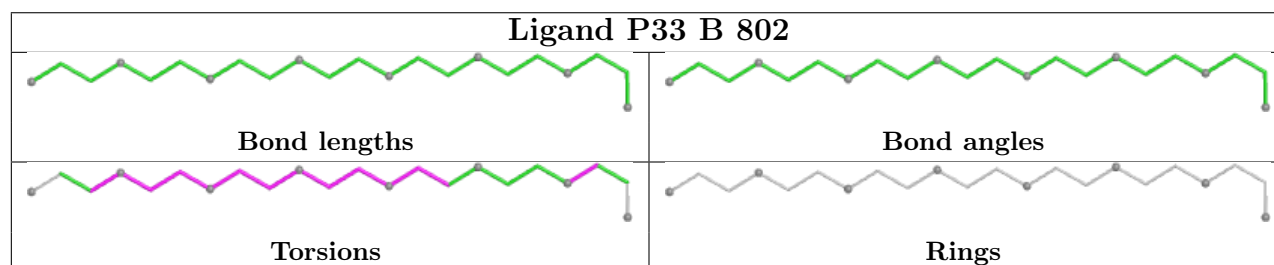
Mol	Chain	Res	Type	Atoms
3	B	802	P33	C15-C14-O13-C12
3	D	802	P33	C12-C11-O10-C9
3	B	802	P33	C5-C6-O7-C8
3	B	802	P33	C6-C5-O4-C3
3	B	802	P33	C9-C8-O7-C6
3	B	802	P33	C8-C9-O10-C11

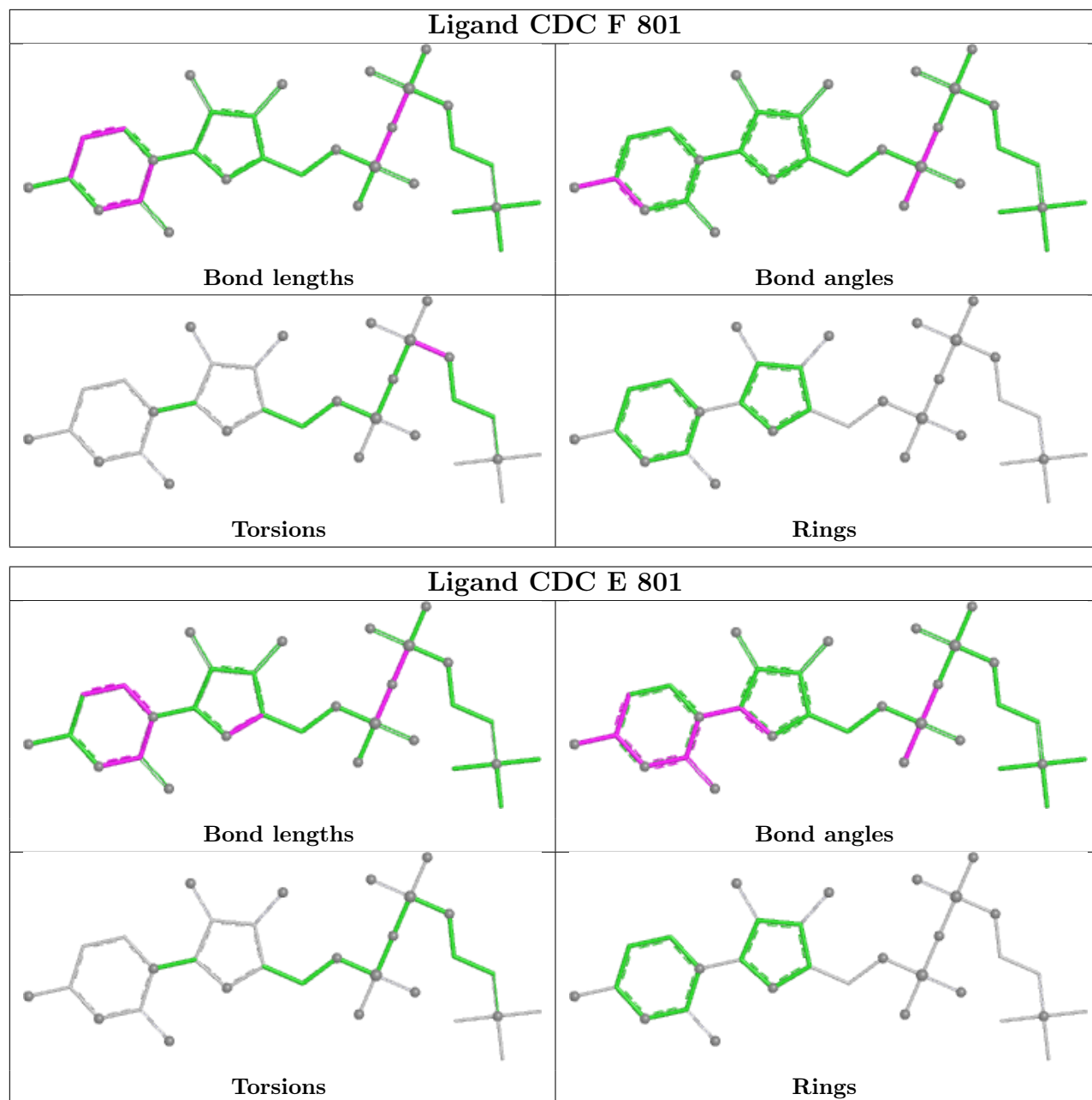
There are no ring outliers.

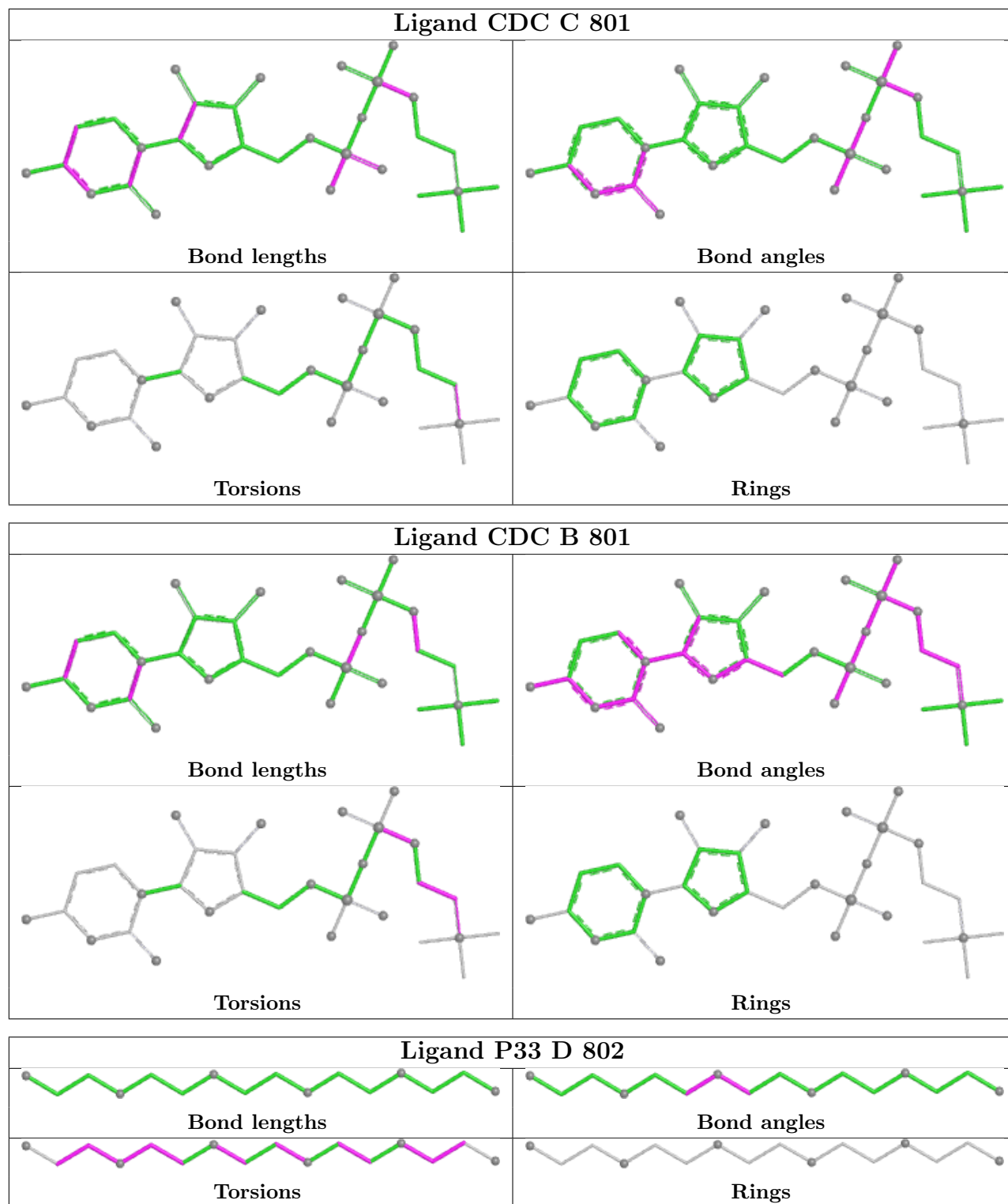
7 monomers are involved in 16 short contacts:

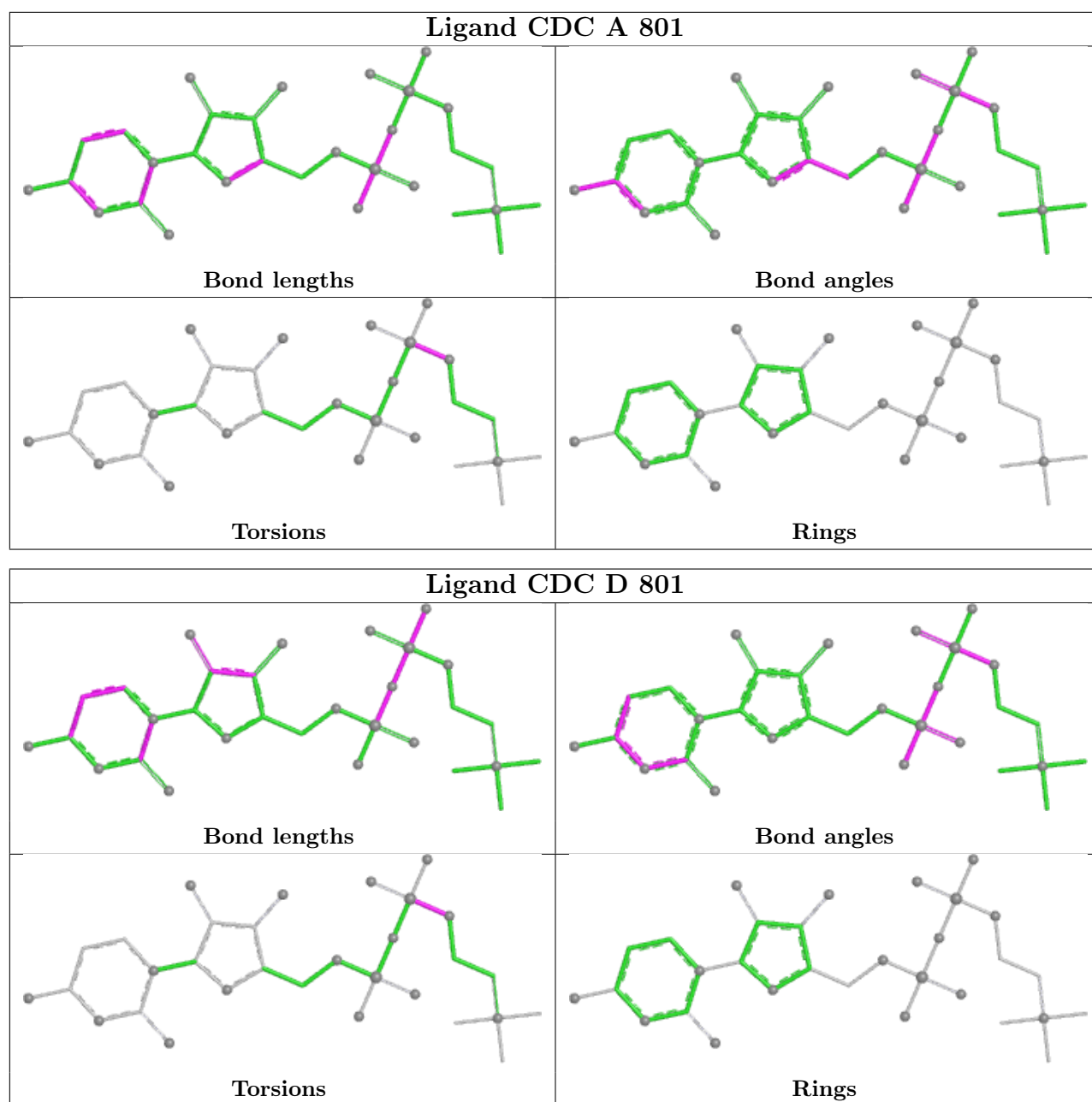
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	802	P33	1	0
2	F	801	CDC	3	0
2	E	801	CDC	3	0
2	C	801	CDC	4	0
2	B	801	CDC	3	0
2	A	801	CDC	1	0
2	D	801	CDC	1	0

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	141/180 (78%)	-0.29	1 (0%) 84 86	24, 35, 62, 92	3 (2%)
1	B	140/180 (77%)	-0.08	4 (2%) 53 55	26, 41, 74, 95	1 (0%)
1	C	137/180 (76%)	-0.16	3 (2%) 62 64	27, 39, 73, 119	1 (0%)
1	D	139/180 (77%)	0.18	9 (6%) 25 22	30, 44, 85, 119	0
1	E	141/180 (78%)	-0.33	2 (1%) 73 75	23, 35, 69, 88	1 (0%)
1	F	141/180 (78%)	0.14	4 (2%) 55 56	27, 49, 76, 108	0
All	All	839/1080 (77%)	-0.09	23 (2%) 56 57	23, 40, 76, 119	6 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	772	TYR	5.3
1	D	616	LYS	4.2
1	C	718	GLN	4.1
1	B	773	GLU	4.1
1	D	716	ASN	3.3
1	B	616	LYS	3.3
1	D	718	GLN	3.0
1	D	761	THR	2.9
1	E	774	ASP	2.9
1	B	718	GLN	2.8
1	B	717	ASN	2.6
1	E	718	GLN	2.5
1	D	770	LYS	2.5
1	F	718	GLN	2.3
1	C	770	LYS	2.3
1	F	746	ARG	2.3
1	A	718	GLN	2.2
1	D	738	GLU	2.2
1	D	771	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	719	LYS	2.2
1	C	738	GLU	2.2
1	F	745	LYS	2.1
1	D	717	ASN	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](#)

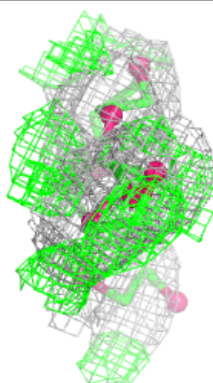
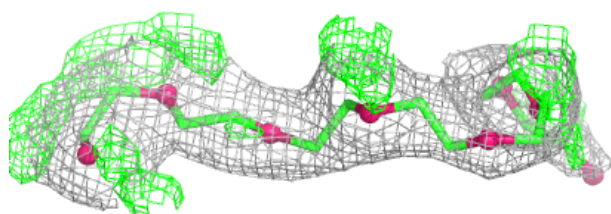
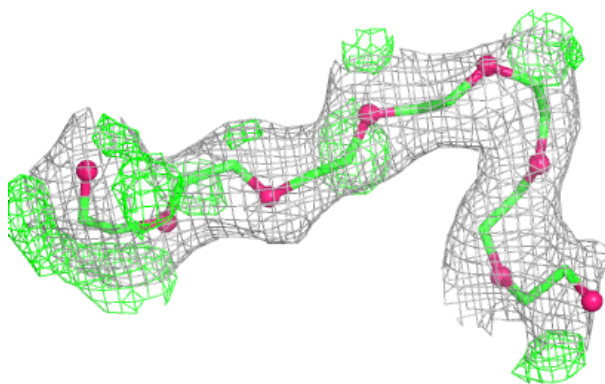
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	P33	B	802	22/22	0.82	0.20	61,85,97,101	0
3	P33	D	802	16/22	0.89	0.15	58,66,77,78	0
2	CDC	D	801	31/31	0.98	0.05	29,33,42,43	0
2	CDC	F	801	31/31	0.98	0.06	32,37,43,46	0
2	CDC	C	801	31/31	0.98	0.05	24,30,45,46	0
2	CDC	B	801	31/31	0.98	0.06	28,32,42,44	0
2	CDC	E	801	31/31	0.99	0.05	20,32,47,48	0
2	CDC	A	801	31/31	0.99	0.05	20,27,42,49	0

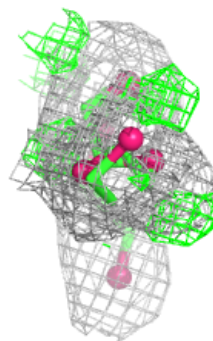
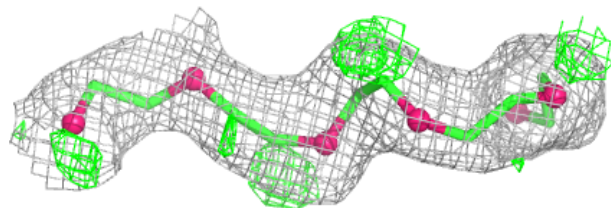
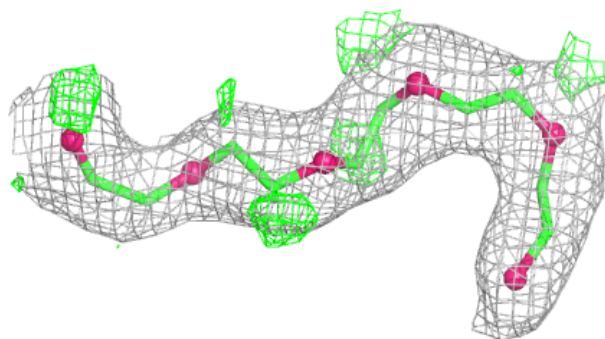
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around P33 B 802:

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

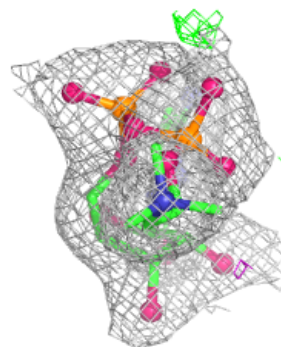
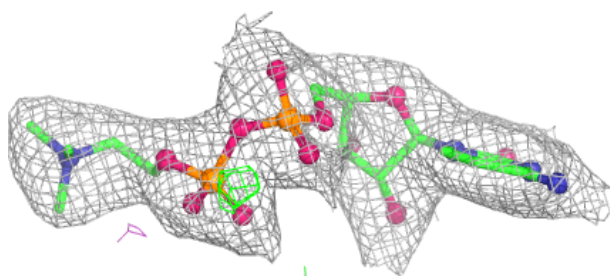
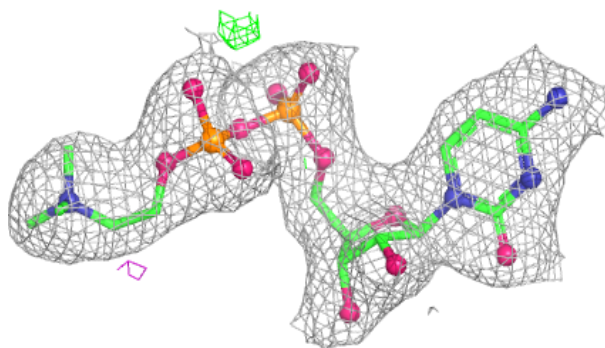
**Electron density around P33 D 802:**

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

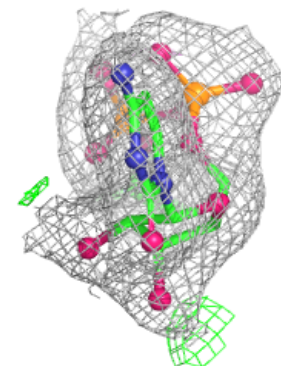
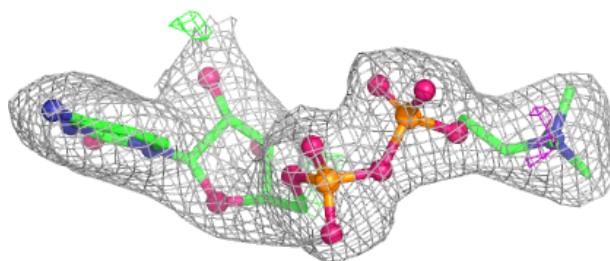
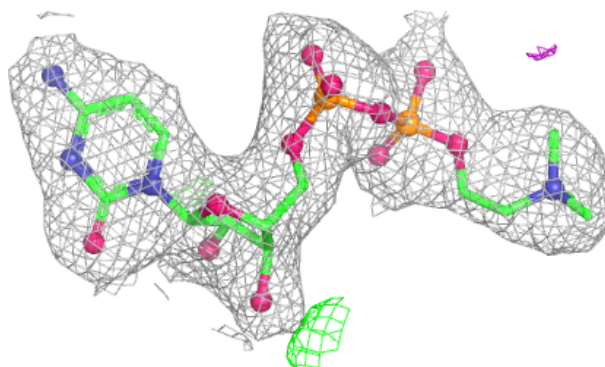


Electron density around CDC D 801:

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

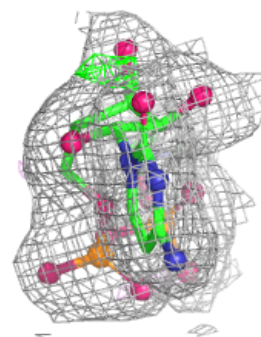
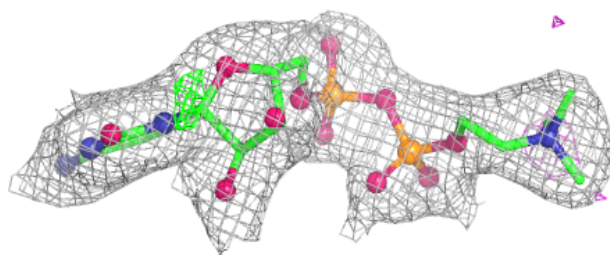
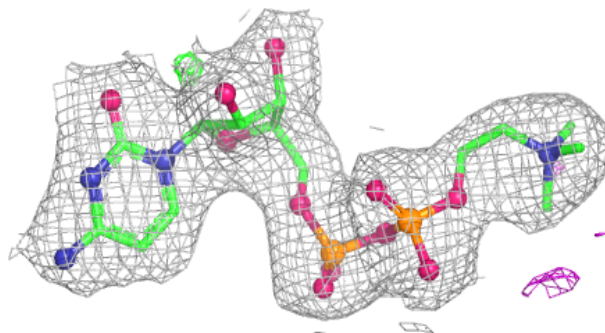
**Electron density around CDC F 801:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

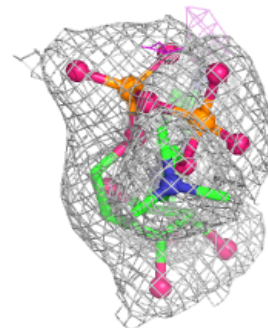
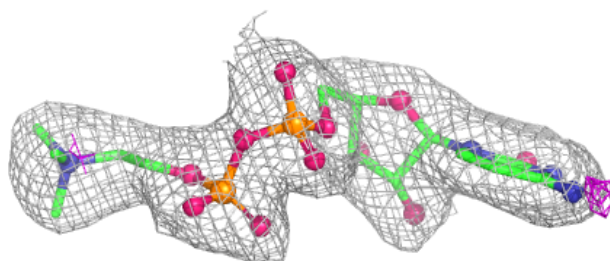
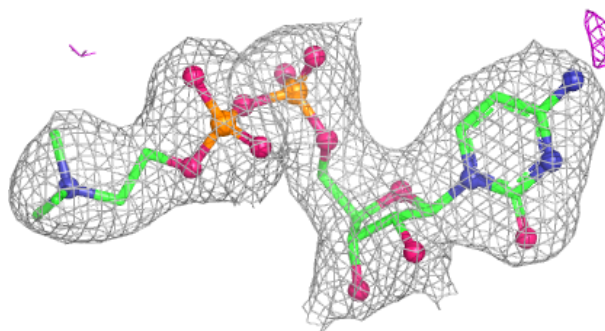


Electron density around CDC C 801:

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

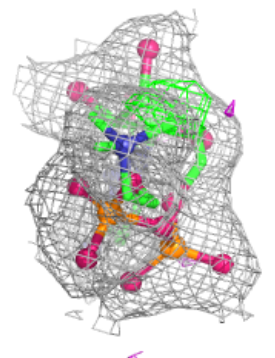
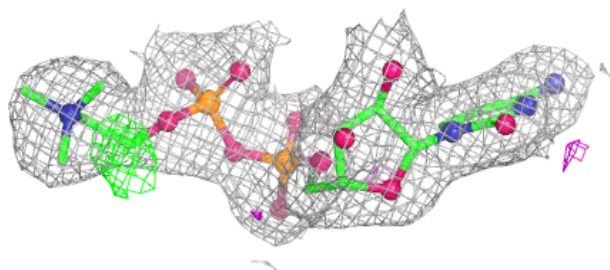
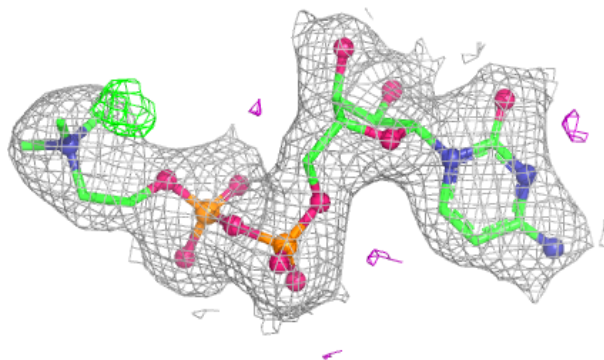
**Electron density around CDC B 801:**

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

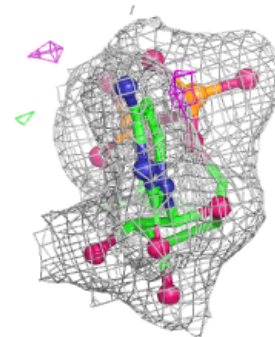
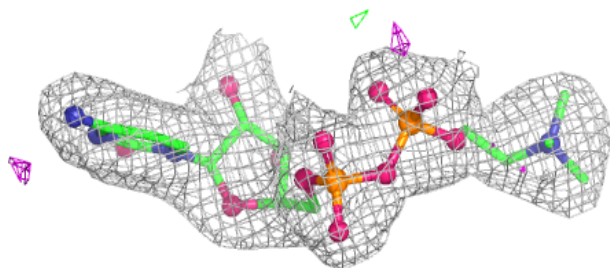
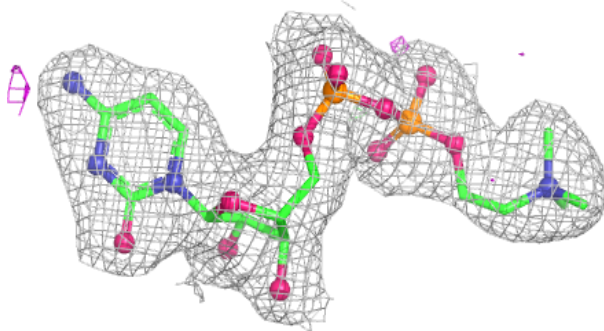


Electron density around CDC E 801:

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

**Electron density around CDC 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.