



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:07 AM UTC

PDB ID : 5CNS / pdb_00005cns
Title : Crystal structure of the dATP inhibited E. coli class Ia ribonucleotide reductase complex bound to CDP and dATP at 2.97 Angstroms resolution
Authors : Chen, P.Y.-T.; Zimanyi, C.M.; Funk, M.A.; Drennan, C.L.
Deposited on : 2015-07-18
Resolution : 2.98 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

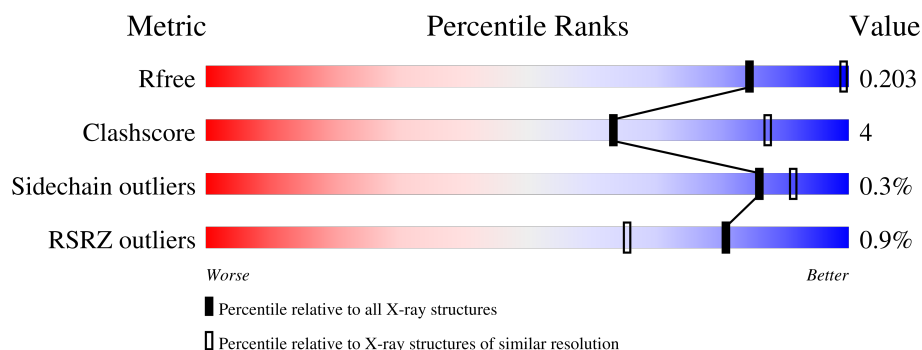
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.98 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	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

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	761	85%11%.
1	B	761	87%9%.
1	C	761	% 87%9%.
1	D	761	% 86%10%.
2	E	375	2% 84%10%6%
2	F	375	% 85%10%5%

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Mol	Chain	Length	Quality of chain
2	G	375	2% 83% 12% 5%
2	H	375	% 84% 11% 5%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 35406 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.

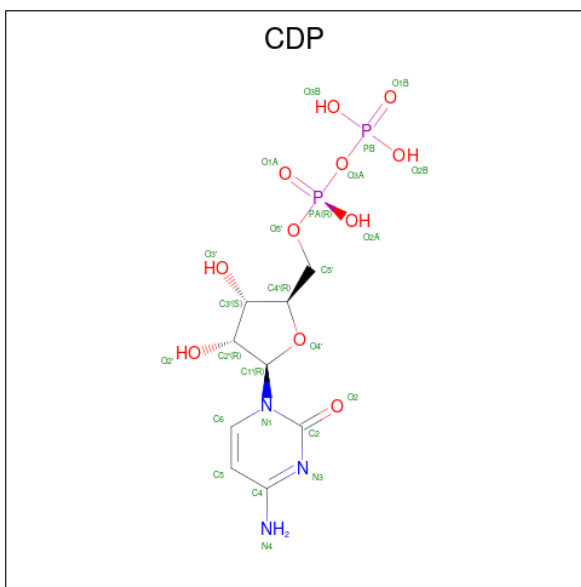
- Molecule 1 is a protein called Ribonucleoside-diphosphate reductase 1 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	732	Total	C	N	O	S	0	0	0
			5829	3703	1000	1102	24			
1	B	734	Total	C	N	O	S	0	0	0
			5843	3711	1003	1105	24			
1	C	732	Total	C	N	O	S	0	0	0
			5829	3703	1000	1102	24			
1	D	734	Total	C	N	O	S	0	0	0
			5843	3711	1003	1105	24			

- Molecule 2 is a protein called Ribonucleoside-diphosphate reductase 1 subunit beta.

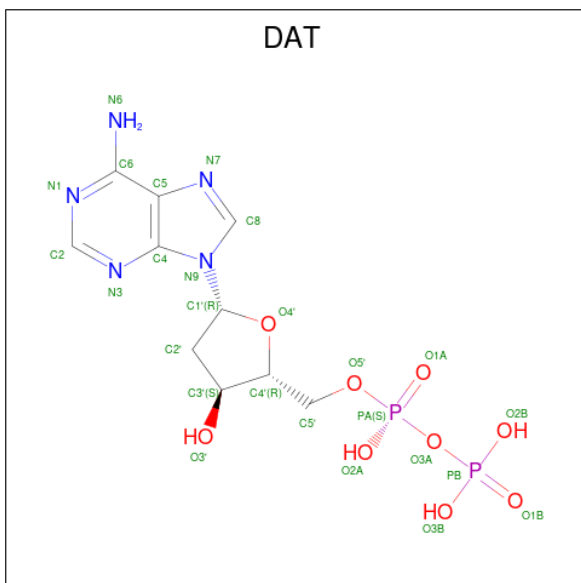
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	352	Total	C	N	O	S	0	0	0
			2866	1830	474	549	13			
2	F	357	Total	C	N	O	S	0	0	0
			2913	1858	481	561	13			
2	G	357	Total	C	N	O	S	0	0	0
			2906	1855	481	557	13			
2	H	355	Total	C	N	O	S	0	0	0
			2890	1846	478	553	13			

- Molecule 3 is CYTIDINE-5'-DIPHOSPHATE (CCD ID: CDP) (formula: $C_9H_{15}N_3O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			25	9	3	11	2		
3	B	1	Total	C	N	O	P	0	0
			25	9	3	11	2		
3	C	1	Total	C	N	O	P	0	0
			25	9	3	11	2		
3	D	1	Total	C	N	O	P	0	0
			25	9	3	11	2		

- Molecule 4 is 2'-DEOXYADENOSINE-5'-DIPHOSPHATE (CCD ID: DAT) (formula: $C_{10}H_{15}N_5O_9P_2$).

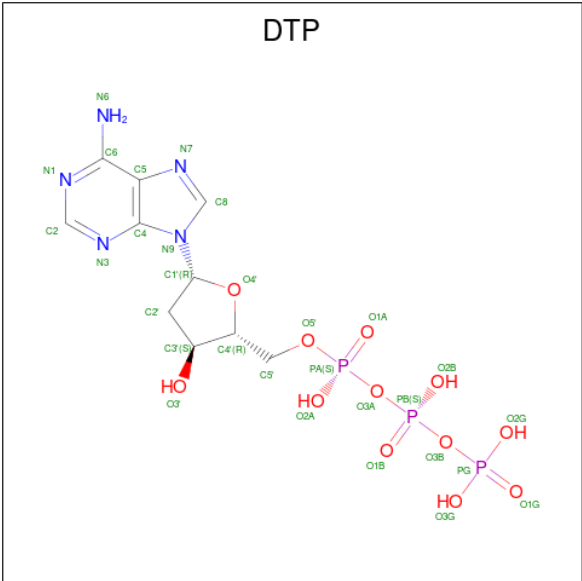


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			26	10	5	9	2		
4	B	1	Total	C	N	O	P	0	0
			26	10	5	9	2		
4	C	1	Total	C	N	O	P	0	0
			26	10	5	9	2		
4	D	1	Total	C	N	O	P	0	0
			26	10	5	9	2		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Mg	0	0
			2	2		
5	B	2	Total	Mg	0	0
			2	2		
5	C	2	Total	Mg	0	0
			2	2		
5	D	2	Total	Mg	0	0
			2	2		

- Molecule 6 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (CCD ID: DTP) (formula: C₁₀H₁₆N₅O₁₂P₃).



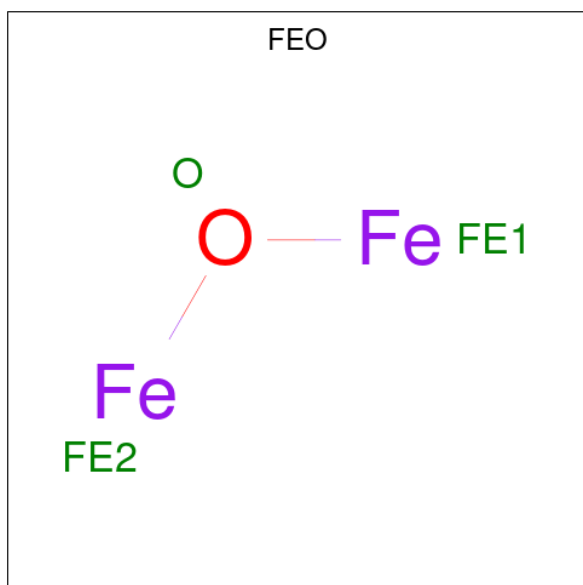
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
6	B	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
6	D	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

- Molecule 7 is MU-OXO-DIIRON (CCD ID: FEO) (formula: Fe_2O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	E	1	Total	Fe	O	0	0
			3	2	1		
7	F	1	Total	Fe	O	0	0
			3	2	1		
7	G	1	Total	Fe	O	0	0
			3	2	1		
7	H	1	Total	Fe	O	0	0
			3	2	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	41	Total	O	0	0
			41	41		
8	B	25	Total	O	0	0
			25	25		
8	C	12	Total	O	0	0
			12	12		

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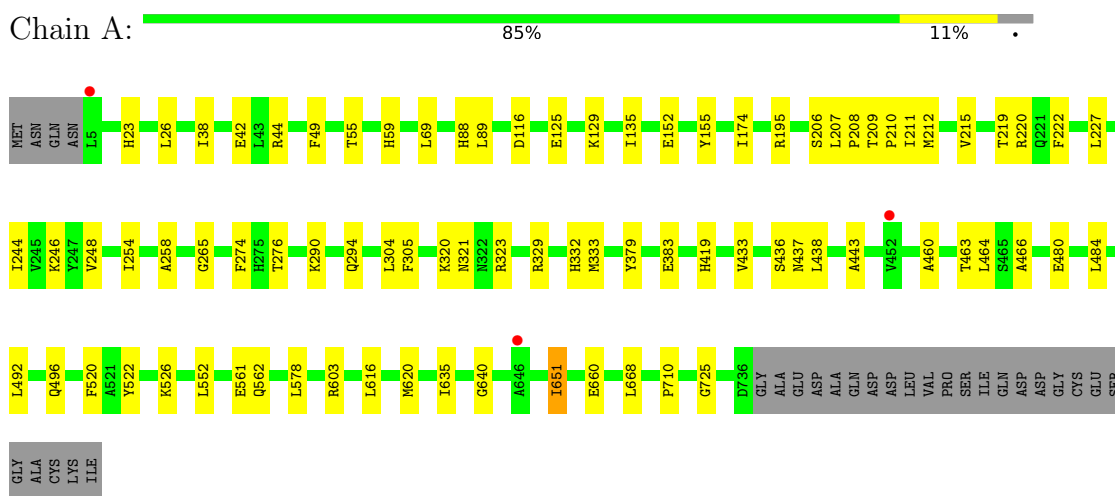
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	19	Total 19	O 19	0	0
8	E	9	Total 9	O 9	0	0
8	F	14	Total 14	O 14	0	0
8	G	14	Total 14	O 14	0	0
8	H	9	Total 9	O 9	0	0

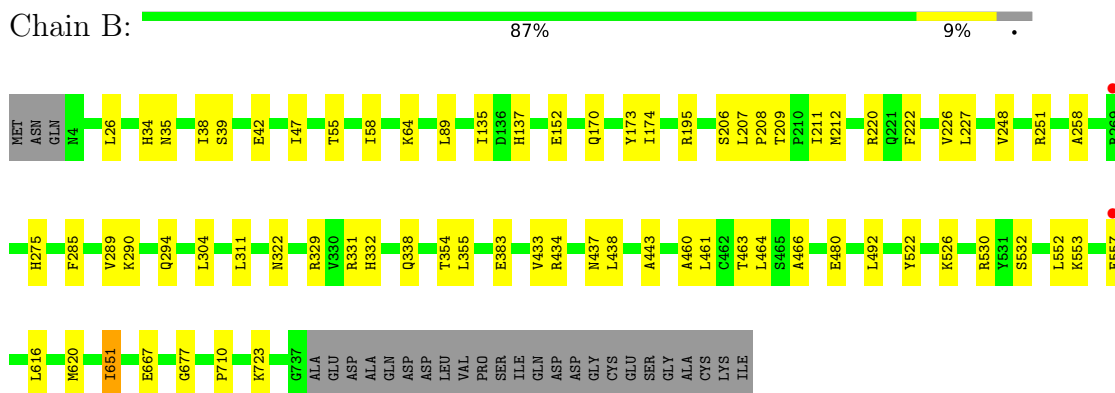
3 Residue-property plots

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.

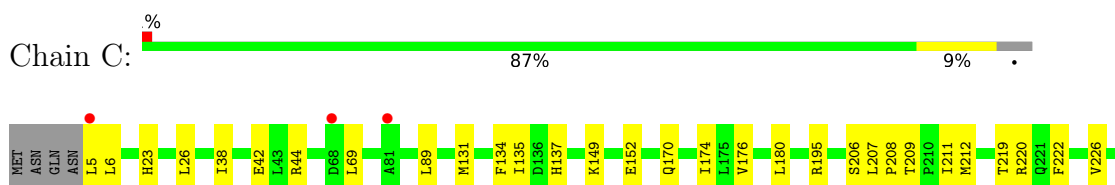
• Molecule 1: Ribonucleoside-diphosphate reductase 1 subunit alpha

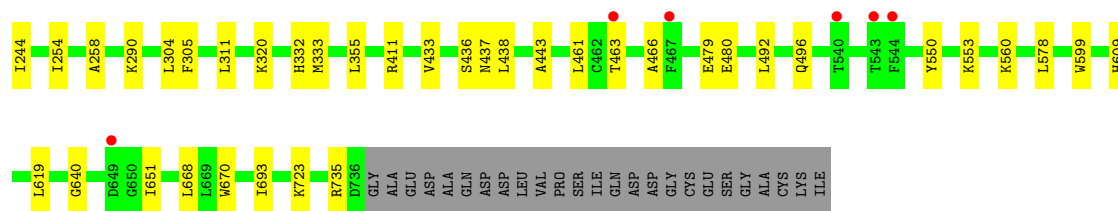


• Molecule 1: Ribonucleoside-diphosphate reductase 1 subunit alpha

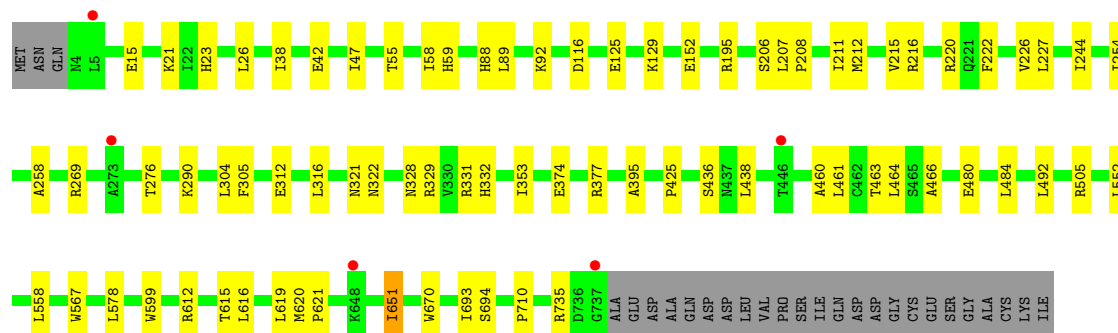
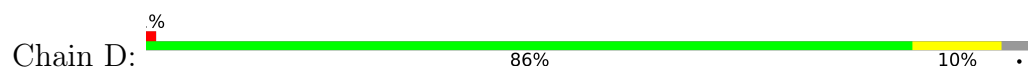


• Molecule 1: Ribonucleoside-diphosphate reductase 1 subunit alpha

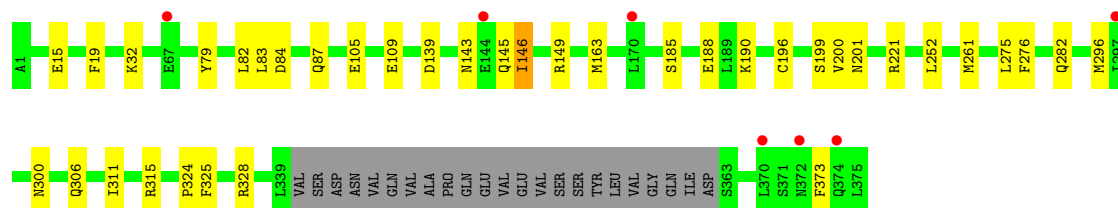
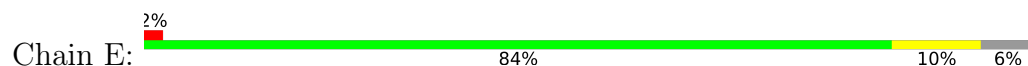




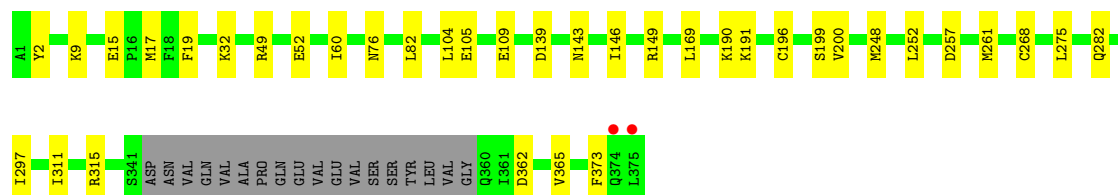
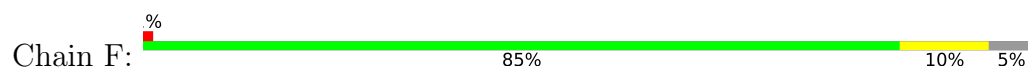
• Molecule 1: Ribonucleoside-diphosphate reductase 1 subunit alpha



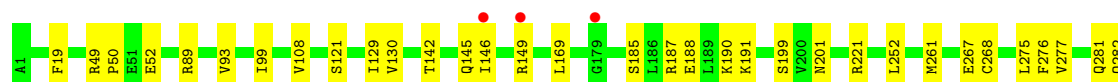
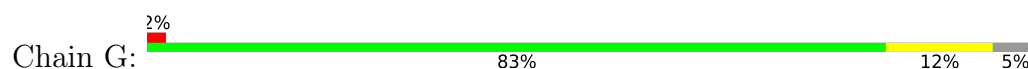
• Molecule 2: Ribonucleoside-diphosphate reductase 1 subunit beta

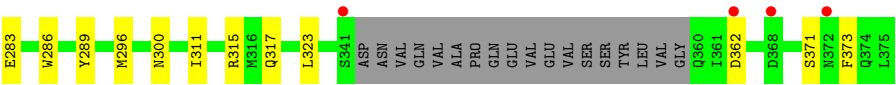


• Molecule 2: Ribonucleoside-diphosphate reductase 1 subunit beta

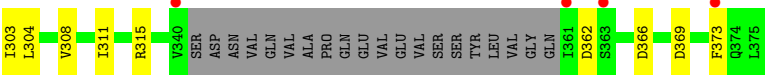
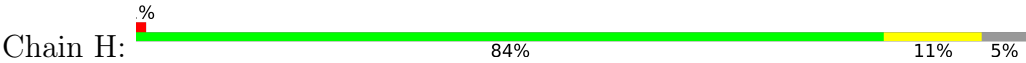


• Molecule 2: Ribonucleoside-diphosphate reductase 1 subunit beta





● Molecule 2: Ribonucleoside-diphosphate reductase 1 subunit beta



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	274.15Å 157.83Å 164.25Å 90.00° 118.82° 90.00°	Depositor
Resolution (Å)	49.48 – 2.98 49.48 – 2.98	Depositor EDS
% Data completeness (in resolution range)	98.2 (49.48-2.98) 98.2 (49.48-2.98)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 2.96Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.190 , 0.214 (Not available) , 0.203	Depositor DCC
R_{free} test set	6187 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	58.9	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 14.3	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	0.94	EDS
Total number of atoms	35406	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CDP, MG, DTP, DAT, FEO

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	0.15	0/5957	0.36	0/8070
1	B	0.14	0/5971	0.34	0/8088
1	C	0.12	0/5957	0.33	0/8070
1	D	0.13	0/5971	0.33	0/8088
2	E	0.12	0/2930	0.30	0/3976
2	F	0.15	0/2977	0.33	0/4039
2	G	0.16	0/2970	0.35	0/4030
2	H	0.13	0/2954	0.31	0/4009
All	All	0.14	0/35687	0.34	0/48370

There are no bond length outliers.

There are no bond angle outliers.

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	5829	0	5750	54	0
1	B	5843	0	5763	46	0
1	C	5829	0	5750	42	0
1	D	5843	0	5763	52	0
2	E	2866	0	2777	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	2913	0	2826	26	0
2	G	2906	0	2820	29	0
2	H	2890	0	2805	24	0
3	A	25	0	12	1	0
3	B	25	0	12	3	0
3	C	25	0	12	3	0
3	D	25	0	12	1	0
4	A	26	0	12	1	0
4	B	26	0	12	1	0
4	C	26	0	12	0	0
4	D	26	0	12	3	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
6	A	30	0	12	0	0
6	B	30	0	12	1	0
6	C	30	0	12	0	0
6	D	30	0	12	1	0
7	E	3	0	0	0	0
7	F	3	0	0	0	0
7	G	3	0	0	0	0
7	H	3	0	0	0	0
8	A	41	0	0	2	0
8	B	25	0	0	0	0
8	C	12	0	0	0	0
8	D	19	0	0	1	0
8	E	9	0	0	0	0
8	F	14	0	0	1	0
8	G	14	0	0	0	0
8	H	9	0	0	0	0
All	All	35406	0	34398	279	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 4.

All (279) 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)
2:G:149:ARG:HD3	2:G:282:GLN:HB3	1.63	0.80
1:A:207:LEU:HB2	1:A:212:MET:HE2	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:ALA:HB3	1:A:304:LEU:HD21	1.70	0.73
1:B:26:LEU:HB3	1:B:38:ILE:HD12	1.71	0.71
1:D:258:ALA:HB3	1:D:304:LEU:HD21	1.73	0.70
1:A:26:LEU:HB3	1:A:38:ILE:HD12	1.73	0.70
1:D:26:LEU:HB3	1:D:38:ILE:HD12	1.73	0.70
1:C:26:LEU:HB3	1:C:38:ILE:HD12	1.73	0.70
1:B:258:ALA:HB3	1:B:304:LEU:HD21	1.74	0.68
1:B:207:LEU:HB2	1:B:212:MET:HE2	1.76	0.68
1:A:321:ASN:OD1	1:A:329:ARG:NH2	2.26	0.68
1:D:322:ASN:HA	1:D:331:ARG:HE	1.59	0.67
1:B:710:PRO:HA	2:H:362:ASP:HB3	1.75	0.67
1:D:206:SER:HB3	1:D:466:ALA:HB3	1.76	0.67
1:C:258:ALA:HB3	1:C:304:LEU:HD21	1.77	0.67
1:A:49:PHE:HE1	2:F:297:ILE:HD11	1.59	0.66
1:B:222:PHE:CD2	1:B:492:LEU:HD11	2.32	0.65
2:H:82:LEU:HD22	2:H:146:ILE:HG23	1.79	0.65
1:A:227:LEU:HB2	1:A:460:ALA:HB3	1.80	0.63
1:C:206:SER:HB3	1:C:466:ALA:HB3	1.80	0.63
2:F:82:LEU:HD22	2:F:146:ILE:HG23	1.81	0.62
2:H:131:ASN:OD1	2:H:131:ASN:N	2.33	0.61
1:A:195:ARG:HH21	1:A:480:GLU:CD	2.09	0.61
1:A:222:PHE:CD2	1:A:492:LEU:HD11	2.36	0.61
1:C:437:ASN:ND2	3:C:801:CDP:O3'	2.32	0.61
1:C:438:LEU:HD23	3:C:801:CDP:H2'	1.83	0.59
1:C:208:PRO:HD2	1:C:211:ILE:HD12	1.84	0.59
1:C:320:LYS:HD3	1:C:333:MET:O	2.01	0.59
2:G:199:SER:HA	2:G:275:LEU:HD21	1.84	0.59
1:C:195:ARG:NH2	1:C:480:GLU:OE2	2.20	0.59
2:E:82:LEU:HD22	2:E:146:ILE:HG23	1.85	0.59
1:D:438:LEU:HD23	3:D:801:CDP:H2'	1.84	0.58
2:E:221:ARG:HH11	2:E:296:MET:HE3	1.68	0.58
1:A:710:PRO:HA	2:F:362:ASP:HB3	1.84	0.58
1:A:290:LYS:HE3	1:A:332:HIS:HB3	1.85	0.57
1:C:222:PHE:CD2	1:C:492:LEU:HD11	2.39	0.57
1:B:206:SER:HB3	1:B:466:ALA:HB3	1.86	0.57
1:C:479:GLU:OE2	1:C:553:LYS:NZ	2.33	0.57
1:D:710:PRO:HA	2:G:362:ASP:HB3	1.86	0.57
2:G:317:GLN:HB2	2:G:323:LEU:HD21	1.86	0.57
1:B:222:PHE:HD2	1:B:492:LEU:HD11	1.68	0.57
1:B:438:LEU:HD23	3:B:801:CDP:H2'	1.86	0.57
2:E:145:GLN:O	2:E:149:ARG:NH2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:VAL:HG11	1:A:443:ALA:HB1	1.87	0.56
1:D:195:ARG:HB3	1:D:484:LEU:HD21	1.88	0.56
1:D:226:VAL:HG22	1:D:461:LEU:HD22	1.86	0.56
1:B:433:VAL:HG11	1:B:443:ALA:HB1	1.87	0.56
2:F:199:SER:HA	2:F:275:LEU:HD21	1.86	0.56
1:A:116:ASP:OD2	1:A:220:ARG:NH2	2.34	0.56
1:D:207:LEU:HD12	1:D:212:MET:HE3	1.88	0.56
1:D:619:LEU:HB2	1:D:693:ILE:HG23	1.87	0.56
1:C:207:LEU:HB2	1:C:212:MET:HE3	1.88	0.56
1:B:42:GLU:HB3	2:H:297:ILE:HG23	1.88	0.55
2:G:221:ARG:HH11	2:G:296:MET:HE3	1.71	0.55
1:D:290:LYS:HE3	1:D:332:HIS:HB3	1.89	0.55
1:B:195:ARG:HH11	1:B:480:GLU:CD	2.14	0.55
1:A:438:LEU:HD23	3:A:801:CDP:H2'	1.88	0.55
1:D:463:THR:HG21	1:D:492:LEU:HD23	1.89	0.54
1:D:328:ASN:O	1:D:329:ARG:NH1	2.37	0.54
1:D:125:GLU:HG2	1:D:129:LYS:HE2	1.90	0.54
1:D:222:PHE:CD2	1:D:492:LEU:HD11	2.43	0.53
1:B:437:ASN:ND2	3:B:801:CDP:O3'	2.42	0.53
1:B:463:THR:HG21	1:B:492:LEU:HD23	1.90	0.53
1:A:320:LYS:HD3	1:A:333:MET:O	2.09	0.53
1:D:552:LEU:HD23	1:D:616:LEU:HD12	1.90	0.53
2:G:277:VAL:O	2:G:281:GLN:HG2	2.09	0.53
2:F:60:ILE:HD12	2:F:60:ILE:H	1.73	0.53
2:F:191:LYS:HG3	2:F:268:CYS:SG	2.48	0.53
1:B:173:TYR:HE1	1:B:212:MET:HE1	1.74	0.53
1:A:244:ILE:HG12	1:A:254:ILE:HG21	1.91	0.52
1:D:23:HIS:CD2	2:G:300:ASN:HD22	2.26	0.52
2:G:187:ARG:NH2	2:G:267:GLU:OE2	2.28	0.52
2:F:9:LYS:HD2	2:G:142:THR:CG2	2.39	0.52
1:B:55:THR:HG21	4:B:802:DAT:O2B	2.09	0.52
1:C:5:LEU:HD12	1:C:6:LEU:HD12	1.91	0.52
1:D:195:ARG:NH2	1:D:480:GLU:OE2	2.42	0.52
1:B:226:VAL:HG22	1:B:461:LEU:HD22	1.91	0.52
2:H:252:LEU:HD22	2:H:261:MET:HG2	1.91	0.52
1:B:135:ILE:HD11	1:B:174:ILE:HG21	1.92	0.51
1:A:59:HIS:HD2	1:A:88:HIS:HB2	1.75	0.51
1:C:44:ARG:HG3	1:C:69:LEU:HD21	1.92	0.51
2:G:191:LYS:HG3	2:G:268:CYS:SG	2.50	0.51
1:C:23:HIS:CD2	2:E:300:ASN:HD22	2.29	0.51
2:H:191:LYS:HG3	2:H:268:CYS:SG	2.50	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:199:SER:HA	2:H:275:LEU:HD21	1.92	0.51
1:D:208:PRO:HD2	1:D:211:ILE:HD12	1.91	0.51
1:A:208:PRO:HD2	1:A:211:ILE:HD12	1.93	0.50
1:A:660:GLU:H	1:A:660:GLU:CD	2.19	0.50
2:E:149:ARG:HD3	2:E:282:GLN:HB3	1.92	0.50
2:G:252:LEU:HD22	2:G:261:MET:HG2	1.94	0.49
1:A:89:LEU:HD11	1:A:152:GLU:HB3	1.95	0.49
1:C:433:VAL:HG11	1:C:443:ALA:HB1	1.92	0.49
2:G:149:ARG:NH2	2:G:283:GLU:OE2	2.46	0.49
1:C:320:LYS:HE2	1:C:411:ARG:HB2	1.93	0.49
1:B:285:PHE:O	1:B:289:VAL:HG23	2.13	0.49
2:F:149:ARG:HD3	2:F:282:GLN:HB3	1.95	0.49
2:G:129:ILE:HG13	2:G:130:VAL:HG13	1.95	0.49
1:A:321:ASN:HD22	1:A:323:ARG:NH2	2.11	0.49
1:A:578:LEU:HD11	1:A:603:ARG:HB2	1.95	0.49
2:E:306:GLN:HG2	2:E:328:ARG:HH12	1.78	0.48
2:F:196:CYS:O	2:F:200:VAL:HG23	2.13	0.48
1:A:463:THR:HG21	1:A:492:LEU:HD23	1.95	0.48
1:A:222:PHE:HD2	1:A:492:LEU:HD11	1.76	0.48
1:B:553:LYS:O	1:B:557:GLU:HG2	2.13	0.48
1:C:226:VAL:HG22	1:C:461:LEU:HD22	1.94	0.48
1:A:208:PRO:HB2	1:A:210:PRO:HD2	1.95	0.48
1:B:290:LYS:HE3	1:B:332:HIS:HB3	1.95	0.48
1:B:723:LYS:HE2	2:H:373:PHE:CZ	2.48	0.48
1:B:227:LEU:HB2	1:B:460:ALA:HB3	1.96	0.48
1:C:220:ARG:HB3	1:C:496:GLN:HA	1.94	0.48
1:C:560:LYS:HE2	1:C:609:HIS:CE1	2.49	0.48
1:B:195:ARG:NH1	1:B:480:GLU:OE2	2.31	0.47
1:B:552:LEU:HD23	1:B:616:LEU:HD12	1.95	0.47
1:A:135:ILE:HD11	1:A:174:ILE:HG21	1.95	0.47
2:F:104:LEU:HD11	2:F:248:MET:HE2	1.95	0.47
2:G:185:SER:HB3	2:G:188:GLU:HB2	1.97	0.47
1:C:149:LYS:NZ	1:C:152:GLU:OE1	2.36	0.47
2:F:311:ILE:O	2:F:315:ARG:HG2	2.14	0.47
1:A:552:LEU:HD23	1:A:616:LEU:HD12	1.96	0.47
1:D:88:HIS:NE2	1:D:92:LYS:HE3	2.30	0.47
1:D:505:ARG:HG2	1:D:567:TRP:HH2	1.78	0.47
2:E:15:GLU:O	2:E:32:LYS:NZ	2.38	0.47
1:B:89:LEU:HD11	1:B:152:GLU:HB3	1.96	0.47
1:D:374:GLU:OE2	1:D:377:ARG:NH2	2.34	0.47
1:D:425:PRO:HG3	1:D:615:THR:HG22	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:149:ARG:NH1	2:G:286:TRP:HB2	2.30	0.46
1:A:640:GLY:HA2	1:A:668:LEU:HD13	1.97	0.46
1:C:135:ILE:HD11	1:C:174:ILE:HG21	1.97	0.46
1:D:220:ARG:HA	1:D:222:PHE:CZ	2.50	0.46
2:G:311:ILE:O	2:G:315:ARG:HG2	2.16	0.46
1:A:520:PHE:HB3	1:A:635:ILE:HA	1.97	0.46
2:E:252:LEU:HD22	2:E:261:MET:HG2	1.96	0.46
2:G:145:GLN:HG3	2:G:289:TYR:CE1	2.50	0.46
1:C:137:HIS:HA	1:C:170:GLN:HG3	1.97	0.46
1:D:464:LEU:HB3	1:D:620:MET:HE2	1.98	0.46
2:H:84:ASP:HA	2:H:87:GLN:HB2	1.98	0.46
1:A:248:VAL:O	1:A:294:GLN:HA	2.16	0.45
1:A:651:ILE:H	1:A:651:ILE:HG13	1.56	0.45
1:D:55:THR:HG21	4:D:802:DAT:O1B	2.15	0.45
1:D:116:ASP:OD2	1:D:220:ARG:NH2	2.41	0.45
1:A:206:SER:HB3	1:A:466:ALA:HB3	1.98	0.45
1:A:329:ARG:HD3	1:A:329:ARG:HA	1.72	0.45
1:B:208:PRO:HD2	1:B:211:ILE:HD12	1.98	0.45
1:C:311:LEU:HA	1:C:355:LEU:HB3	1.97	0.45
1:A:59:HIS:CD2	1:A:88:HIS:HB2	2.52	0.45
1:A:55:THR:HG21	4:A:802:DAT:O1B	2.16	0.45
1:B:532:SER:HA	1:B:677:GLY:HA3	1.97	0.45
1:D:23:HIS:ND1	1:D:42:GLU:OE2	2.45	0.45
1:B:530:ARG:HB3	1:B:667:GLU:OE2	2.16	0.45
1:C:290:LYS:HE3	1:C:332:HIS:HB3	1.99	0.45
1:D:89:LEU:HD11	1:D:152:GLU:HB3	1.99	0.45
2:E:199:SER:HA	2:E:275:LEU:HD21	1.99	0.45
1:C:463:THR:HG21	1:C:492:LEU:HD23	1.98	0.44
1:C:723:LYS:HE2	2:E:373:PHE:CZ	2.52	0.44
1:D:244:ILE:HG12	1:D:254:ILE:HG21	2.00	0.44
2:E:201:ASN:HD22	2:E:276:PHE:HZ	1.65	0.44
2:G:49:ARG:O	2:G:52:GLU:HG2	2.18	0.44
1:A:522:TYR:CZ	1:A:526:LYS:HD3	2.53	0.44
1:D:651:ILE:H	1:D:651:ILE:HG13	1.50	0.44
2:E:84:ASP:HA	2:E:87:GLN:HB2	1.99	0.44
2:F:143:ASN:HB3	2:F:146:ILE:HB	1.99	0.44
2:H:163:MET:HB3	2:H:189:LEU:HD13	2.00	0.44
2:H:311:ILE:O	2:H:315:ARG:HG2	2.17	0.44
1:A:44:ARG:HG3	1:A:69:LEU:HD21	1.99	0.44
2:F:169:LEU:HD12	2:G:169:LEU:HD12	1.99	0.44
2:G:371:SER:C	2:G:373:PHE:H	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:THR:OG1	3:C:801:CDP:O2B	2.32	0.44
2:E:139:ASP:O	2:E:143:ASN:HB2	2.18	0.44
2:G:19:PHE:CE2	2:G:190:LYS:HG2	2.53	0.44
1:D:505:ARG:HG2	1:D:567:TRP:CH2	2.53	0.44
2:E:105:GLU:O	2:E:109:GLU:HG3	2.17	0.44
2:H:201:ASN:HD22	2:H:276:PHE:HZ	1.66	0.44
1:B:338:GLN:NE2	1:B:434:ARG:O	2.48	0.44
1:B:354:THR:OG1	1:B:383:GLU:OE2	2.29	0.44
1:D:211:ILE:HA	1:D:215:VAL:HG23	2.00	0.44
2:F:2:TYR:CE2	2:G:93:VAL:HG11	2.53	0.44
1:B:311:LEU:HA	1:B:355:LEU:HB3	2.00	0.43
1:A:23:HIS:ND1	1:A:42:GLU:OE2	2.47	0.43
1:A:561:GLU:HG2	1:A:562:GLN:HG3	2.00	0.43
1:B:251:ARG:HA	1:B:294:GLN:HG2	2.00	0.43
1:C:479:GLU:HB2	1:C:550:TYR:CE1	2.53	0.43
1:B:47:ILE:HD11	1:B:58:ILE:HG12	2.00	0.43
1:C:23:HIS:ND1	1:C:42:GLU:OE2	2.48	0.43
2:E:19:PHE:CE2	2:E:190:LYS:HG2	2.53	0.43
1:B:522:TYR:CZ	1:B:526:LYS:HD3	2.54	0.43
1:C:578:LEU:HD13	1:C:599:TRP:HE3	1.84	0.43
2:E:149:ARG:HG2	2:E:282:GLN:OE1	2.19	0.43
1:D:305:PHE:CZ	1:D:436:SER:HB3	2.54	0.43
2:G:50:PRO:HG3	2:G:121:SER:HB3	2.00	0.43
2:H:139:ASP:O	2:H:143:ASN:HB2	2.18	0.43
1:B:39:SER:HB2	2:H:303:ILE:HD13	2.00	0.43
1:B:64:LYS:HE3	1:B:64:LYS:HB3	1.73	0.43
1:B:275:HIS:CD2	6:B:804:DTP:H1'	2.53	0.43
1:C:219:THR:HG21	1:D:269:ARG:NH1	2.34	0.43
2:F:19:PHE:CE2	2:F:190:LYS:HG2	2.53	0.43
1:A:305:PHE:CZ	1:A:436:SER:HB3	2.54	0.43
1:A:211:ILE:HA	1:A:215:VAL:HG23	2.00	0.43
1:A:419:HIS:CD2	1:A:725:GLY:HA2	2.54	0.43
1:D:47:ILE:HD11	1:D:58:ILE:HG12	1.99	0.43
1:D:227:LEU:HB2	1:D:460:ALA:HB3	2.01	0.43
1:D:558:LEU:HD23	1:D:612:ARG:HG2	2.01	0.43
2:E:196:CYS:O	2:E:200:VAL:HG23	2.19	0.43
2:H:196:CYS:O	2:H:200:VAL:HG23	2.19	0.42
2:H:227:ASN:O	2:H:231:ILE:HG12	2.19	0.42
2:F:17:MET:H	2:F:257:ASP:CG	2.27	0.42
1:A:265:GLY:HA2	1:A:274:PHE:CZ	2.55	0.42
1:A:464:LEU:HB3	1:A:620:MET:HE2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:ARG:HA	1:C:222:PHE:CZ	2.53	0.42
1:D:312:GLU:O	1:D:316:LEU:HG	2.19	0.42
2:F:49:ARG:O	2:F:52:GLU:HG2	2.19	0.42
1:B:248:VAL:O	1:B:294:GLN:HA	2.19	0.42
2:E:185:SER:HB3	2:E:188:GLU:HB2	2.01	0.42
2:E:311:ILE:O	2:E:315:ARG:HG2	2.19	0.42
2:F:15:GLU:O	2:F:32:LYS:NZ	2.40	0.42
1:D:621:PRO:HD3	1:D:694:SER:OG	2.18	0.42
1:B:34:HIS:CD2	1:B:35:ASN:HB2	2.54	0.42
1:C:305:PHE:CZ	1:C:436:SER:HB3	2.54	0.42
1:D:59:HIS:HB2	4:D:802:DAT:H4'	2.01	0.42
1:D:207:LEU:HB2	1:D:212:MET:HE3	2.01	0.42
1:D:353:ILE:HG13	1:D:395:ALA:HB2	2.00	0.42
2:H:16:PRO:O	2:H:100:SER:OG	2.35	0.42
1:B:322:ASN:HA	1:B:331:ARG:HE	1.84	0.42
1:B:329:ARG:HG3	1:B:331:ARG:NH2	2.35	0.42
1:C:207:LEU:HD12	1:C:212:MET:HE3	2.00	0.42
1:C:244:ILE:HG12	1:C:254:ILE:HG21	2.01	0.42
1:D:578:LEU:HD13	1:D:599:TRP:HE3	1.85	0.42
2:H:366:ASP:OD2	2:H:369:ASP:HB2	2.19	0.42
2:H:80:GLN:HB3	2:H:122:TYR:CZ	2.55	0.42
2:H:163:MET:HB3	2:H:163:MET:HE2	1.96	0.42
1:A:195:ARG:HB3	1:A:484:LEU:HD21	2.00	0.42
1:A:379:TYR:O	1:A:383:GLU:HG3	2.20	0.42
2:H:111:TRP:O	2:H:115:GLU:HG2	2.19	0.42
1:A:220:ARG:HA	1:A:222:PHE:CZ	2.55	0.41
1:A:276:THR:HB	8:A:917:HOH:O	2.20	0.41
1:C:640:GLY:HA2	1:C:668:LEU:HD13	2.01	0.41
1:D:21:LYS:HD2	4:D:802:DAT:N7	2.35	0.41
1:A:155:TYR:HE1	1:A:209:THR:HG23	1.85	0.41
1:B:137:HIS:HA	1:B:170:GLN:HG3	2.00	0.41
1:C:670:TRP:CE2	1:C:735:ARG:HG3	2.55	0.41
2:F:252:LEU:HD22	2:F:261:MET:HG2	2.02	0.41
1:A:246:LYS:HD3	1:A:246:LYS:HA	1.94	0.41
2:G:99:ILE:HD11	2:G:108:VAL:HG21	2.02	0.41
1:C:131:MET:HA	1:C:134:PHE:CD2	2.56	0.41
2:F:76:ASN:OD1	8:F:601:HOH:O	2.21	0.41
1:B:651:ILE:H	1:B:651:ILE:HG13	1.61	0.41
1:D:670:TRP:CE2	1:D:735:ARG:HG3	2.56	0.41
1:A:437:ASN:HB2	8:A:916:HOH:O	2.21	0.41
1:C:176:VAL:O	1:C:180:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:GLU:HG2	1:A:129:LYS:HE2	2.03	0.41
1:D:329:ARG:HD3	1:D:329:ARG:HA	1.93	0.41
1:B:464:LEU:HB3	1:B:620:MET:HE2	2.03	0.41
1:C:89:LEU:HD21	1:C:152:GLU:HB2	2.02	0.41
2:E:163:MET:HE2	2:E:163:MET:HB3	1.98	0.41
2:E:324:PRO:HG2	2:E:325:PHE:CD2	2.56	0.41
2:F:139:ASP:O	2:F:143:ASN:HB2	2.20	0.41
2:G:201:ASN:HD22	2:G:276:PHE:HZ	1.69	0.41
1:A:42:GLU:HB3	2:F:297:ILE:HG23	2.03	0.41
1:A:49:PHE:CE1	2:F:297:ILE:HD11	2.48	0.41
1:D:276:THR:HB	8:D:905:HOH:O	2.20	0.41
2:E:79:TYR:O	2:E:83:LEU:HG	2.21	0.41
2:G:149:ARG:HH12	2:G:286:TRP:CG	2.38	0.41
2:H:304:LEU:O	2:H:308:VAL:HG23	2.21	0.41
1:C:619:LEU:HB2	1:C:693:ILE:HG23	2.03	0.41
1:D:276:THR:OG1	6:D:804:DTP:H2	2.21	0.41
2:H:19:PHE:CE2	2:H:190:LYS:HG2	2.57	0.41
1:D:215:VAL:O	1:D:216:ARG:HB3	2.22	0.40
2:G:221:ARG:NH1	2:G:296:MET:HE3	2.35	0.40
2:H:198:MET:HG3	2:H:272:CYS:SG	2.61	0.40
1:A:220:ARG:HB3	1:A:496:GLN:HA	2.04	0.40
1:B:209:THR:OG1	3:B:801:CDP:O1B	2.34	0.40
1:B:220:ARG:HA	1:B:222:PHE:CZ	2.56	0.40
1:D:15:GLU:OE2	1:D:21:LYS:NZ	2.45	0.40
2:F:149:ARG:HG2	2:F:282:GLN:OE1	2.21	0.40
1:C:180:LEU:CD2	1:C:492:LEU:HD13	2.52	0.40
2:F:105:GLU:CD	2:G:89:ARG:HE	2.29	0.40
1:D:321:ASN:OD1	1:D:329:ARG:NE	2.54	0.40
2:E:79:TYR:CZ	2:E:83:LEU:HD11	2.56	0.40
2:F:105:GLU:O	2:F:109:GLU:HG3	2.22	0.40
2:G:252:LEU:HB3	2:G:261:MET:HG2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

There are no protein backbone outliers to report in this entry.

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	627/651 (96%)	625 (100%)	2 (0%)	86	91
1	B	628/651 (96%)	627 (100%)	1 (0%)	87	92
1	C	627/651 (96%)	626 (100%)	1 (0%)	87	92
1	D	628/651 (96%)	627 (100%)	1 (0%)	87	92
2	E	314/340 (92%)	313 (100%)	1 (0%)	86	91
2	F	321/340 (94%)	319 (99%)	2 (1%)	78	88
2	G	319/340 (94%)	318 (100%)	1 (0%)	86	91
2	H	317/340 (93%)	316 (100%)	1 (0%)	86	91
All	All	3781/3964 (95%)	3771 (100%)	10 (0%)	86	91

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	219	THR
1	A	651	ILE
1	B	651	ILE
1	C	651	ILE
1	D	651	ILE
2	E	146	ILE
2	F	365	VAL
2	F	373	PHE
2	G	146	ILE
2	H	131	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	A	137	HIS
1	A	250	GLN
1	A	630	ASN

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Mol	Chain	Res	Type
1	B	34	HIS
1	B	630	ASN
1	C	34	HIS
1	C	40	GLN
1	C	250	GLN
1	C	453	ASN
1	C	609	HIS
1	C	630	ASN
1	C	733	ASN
1	D	170	GLN
1	D	453	ASN
1	D	630	ASN
1	D	696	ASN
1	D	733	ASN
2	E	124	HIS
2	E	201	ASN
2	E	247	HIS
2	F	124	HIS
2	F	306	GLN
2	G	247	HIS
2	H	80	GLN
2	H	124	HIS
2	H	143	ASN
2	H	201	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 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
3	CDP	D	801	-	25,26,26	0.90	1 (4%)	38,40,40	0.91	0
7	FEO	G	501	2,8	0,2,2	-	-	-	-	-
3	CDP	B	801	-	25,26,26	0.91	1 (4%)	38,40,40	0.94	0
7	FEO	F	501	2,8	0,2,2	-	-	-	-	-
4	DAT	B	802	5	27,28,28	1.50	5 (18%)	41,43,43	1.79	9 (21%)
6	DTP	D	804	5	31,32,32	1.55	8 (25%)	46,50,50	1.80	11 (23%)
4	DAT	C	802	5	27,28,28	1.51	5 (18%)	41,43,43	1.80	9 (21%)
7	FEO	E	501	2,8	0,2,2	-	-	-	-	-
4	DAT	D	802	5	27,28,28	1.47	5 (18%)	41,43,43	1.86	9 (21%)
6	DTP	B	804	5	31,32,32	1.52	6 (19%)	46,50,50	1.79	11 (23%)
6	DTP	C	804	5	31,32,32	1.53	7 (22%)	46,50,50	1.72	9 (19%)
3	CDP	C	801	-	25,26,26	0.88	1 (4%)	38,40,40	0.91	0
7	FEO	H	501	2,8	0,2,2	-	-	-	-	-
3	CDP	A	801	-	25,26,26	0.92	1 (4%)	38,40,40	0.89	0
4	DAT	A	802	5	27,28,28	1.48	5 (18%)	41,43,43	1.86	10 (24%)
6	DTP	A	804	5	31,32,32	1.61	8 (25%)	46,50,50	1.77	10 (21%)

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	CDP	D	801	-	-	4/16/32/32	0/2/2/2
3	CDP	B	801	-	-	5/16/32/32	0/2/2/2
4	DAT	B	802	5	-	5/16/28/28	0/3/3/3
6	DTP	D	804	5	-	3/22/34/34	0/3/3/3
4	DAT	C	802	5	-	2/16/28/28	0/3/3/3
4	DAT	D	802	5	-	2/16/28/28	0/3/3/3
6	DTP	B	804	5	-	3/22/34/34	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	DTP	C	804	5	-	5/22/34/34	0/3/3/3
3	CDP	C	801	-	-	6/16/32/32	0/2/2/2
3	CDP	A	801	-	-	3/16/32/32	0/2/2/2
4	DAT	A	802	5	-	5/16/28/28	0/3/3/3
6	DTP	A	804	5	-	4/22/34/34	0/3/3/3

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	804	DTP	C5-C4	4.77	1.47	1.39
4	C	802	DAT	C5-C4	4.74	1.47	1.39
6	C	804	DTP	C5-C4	4.73	1.47	1.39
6	D	804	DTP	C5-C4	4.71	1.47	1.39
4	B	802	DAT	C5-C4	4.70	1.47	1.39
4	A	802	DAT	C5-C4	4.66	1.47	1.39
6	A	804	DTP	C5-C4	4.63	1.47	1.39
4	D	802	DAT	C5-C4	4.56	1.47	1.39
6	A	804	DTP	PB-O3B	3.22	1.63	1.59
6	A	804	DTP	PB-O3A	2.99	1.62	1.59
6	B	804	DTP	C5-C6	2.96	1.49	1.41
4	D	802	DAT	C5-C6	2.87	1.49	1.41
6	A	804	DTP	PA-O3A	2.86	1.62	1.59
6	D	804	DTP	PB-O3B	2.83	1.62	1.59
6	C	804	DTP	C5-C6	2.80	1.48	1.41
4	C	802	DAT	C5-C6	2.80	1.48	1.41
6	D	804	DTP	C5-C6	2.79	1.48	1.41
4	A	802	DAT	C5-C6	2.78	1.48	1.41
4	B	802	DAT	C5-C6	2.73	1.48	1.41
6	A	804	DTP	C5-C6	2.70	1.48	1.41
4	C	802	DAT	PA-O3A	2.67	1.62	1.59
6	B	804	DTP	PB-O3B	2.61	1.62	1.59
3	A	801	CDP	PA-O3A	2.58	1.62	1.59
4	A	802	DAT	PA-O3A	2.58	1.62	1.59
4	B	802	DAT	PA-O3A	2.58	1.62	1.59
6	C	804	DTP	PA-O3A	2.54	1.62	1.59
6	B	804	DTP	C8-N7	2.54	1.36	1.31
4	A	802	DAT	C8-N7	2.53	1.36	1.31
4	D	802	DAT	PA-O3A	2.53	1.62	1.59
6	D	804	DTP	PB-O3A	2.51	1.62	1.59
6	D	804	DTP	PA-O3A	2.50	1.62	1.59
4	C	802	DAT	C8-N7	2.44	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	804	DTP	PB-O3A	2.43	1.62	1.59
6	C	804	DTP	PB-O3B	2.42	1.62	1.59
6	C	804	DTP	C8-N7	2.40	1.36	1.31
4	B	802	DAT	C8-N7	2.39	1.36	1.31
6	A	804	DTP	C8-N7	2.38	1.36	1.31
6	D	804	DTP	C8-N7	2.37	1.36	1.31
4	D	802	DAT	C8-N7	2.35	1.36	1.31
6	B	804	DTP	PB-O3A	2.31	1.62	1.59
4	B	802	DAT	C5-N7	-2.23	1.35	1.39
3	D	801	CDP	PA-O3A	2.23	1.61	1.59
4	C	802	DAT	C5-N7	-2.20	1.35	1.39
4	D	802	DAT	C5-N7	-2.18	1.35	1.39
6	A	804	DTP	C5-N7	-2.17	1.35	1.39
3	C	801	CDP	PA-O3A	2.17	1.61	1.59
3	B	801	CDP	PA-O3A	2.16	1.61	1.59
6	C	804	DTP	C5-N7	-2.15	1.35	1.39
4	A	802	DAT	C5-N7	-2.13	1.35	1.39
6	D	804	DTP	C5-N7	-2.13	1.35	1.39
6	A	804	DTP	C4-N9	-2.01	1.33	1.37
6	D	804	DTP	C4-N9	-2.00	1.33	1.37
6	B	804	DTP	PA-O3A	2.00	1.61	1.59

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	802	DAT	C5-C4-N3	-5.75	118.81	126.72
4	D	802	DAT	C5-C4-N3	-5.63	118.97	126.72
6	C	804	DTP	C5-C4-N3	-5.60	119.00	126.72
4	B	802	DAT	C5-C4-N3	-5.59	119.03	126.72
4	A	802	DAT	C5-C4-N3	-5.57	119.04	126.72
6	B	804	DTP	C5-C4-N3	-5.56	119.06	126.72
6	D	804	DTP	C5-C4-N3	-5.50	119.15	126.72
6	A	804	DTP	C5-C4-N3	-5.50	119.15	126.72
6	C	804	DTP	N3-C4-N9	4.44	134.72	127.17
6	A	804	DTP	N3-C4-N9	4.41	134.68	127.17
4	B	802	DAT	N3-C4-N9	4.41	134.67	127.17
4	C	802	DAT	N3-C4-N9	4.38	134.62	127.17
4	D	802	DAT	N3-C4-N9	4.31	134.50	127.17
4	A	802	DAT	N3-C4-N9	4.30	134.48	127.17
6	D	804	DTP	N3-C4-N9	4.29	134.47	127.17
6	B	804	DTP	N3-C4-N9	4.23	134.37	127.17
4	D	802	DAT	C4-C5-N7	-3.82	106.21	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	804	DTP	C2-N3-C4	3.75	120.99	111.83
4	C	802	DAT	C4-C5-N7	-3.71	106.34	110.58
6	C	804	DTP	C2-N3-C4	3.70	120.86	111.83
4	A	802	DAT	C2-N3-C4	3.68	120.82	111.83
4	D	802	DAT	C2-N3-C4	3.68	120.81	111.83
6	B	804	DTP	C4-C5-N7	-3.66	106.39	110.58
4	C	802	DAT	C2-N3-C4	3.65	120.75	111.83
4	B	802	DAT	C2-N3-C4	3.62	120.67	111.83
6	A	804	DTP	C2-N3-C4	3.61	120.64	111.83
6	D	804	DTP	C2-N3-C4	3.61	120.64	111.83
4	A	802	DAT	C4-C5-N7	-3.60	106.46	110.58
4	B	802	DAT	C4-C5-N7	-3.55	106.53	110.58
6	D	804	DTP	C4-C5-N7	-3.53	106.55	110.58
6	C	804	DTP	C4-C5-N7	-3.49	106.59	110.58
4	A	802	DAT	N3-C2-N1	-3.38	123.46	128.58
6	B	804	DTP	N3-C2-N1	-3.36	123.50	128.58
6	A	804	DTP	C4-C5-N7	-3.34	106.76	110.58
6	C	804	DTP	N3-C2-N1	-3.33	123.55	128.58
6	D	804	DTP	N3-C2-N1	-3.28	123.61	128.58
4	B	802	DAT	N3-C2-N1	-3.27	123.63	128.58
6	A	804	DTP	N3-C2-N1	-3.25	123.66	128.58
4	D	802	DAT	N3-C2-N1	-3.22	123.70	128.58
4	C	802	DAT	N3-C2-N1	-3.16	123.80	128.58
6	A	804	DTP	C4-N9-C8	2.93	108.82	105.74
4	A	802	DAT	C4-N9-C8	2.85	108.73	105.74
4	D	802	DAT	C4-N9-C8	2.85	108.73	105.74
6	C	804	DTP	C4-N9-C8	2.83	108.71	105.74
4	D	802	DAT	C5-N7-C8	2.80	107.85	103.45
4	B	802	DAT	C4-N9-C8	2.76	108.64	105.74
6	D	804	DTP	C4-N9-C8	2.75	108.62	105.74
6	B	804	DTP	C4-N9-C8	2.74	108.62	105.74
4	C	802	DAT	C5-N7-C8	2.65	107.62	103.45
4	B	802	DAT	C5-N7-C8	2.59	107.51	103.45
4	A	802	DAT	C5-N7-C8	2.58	107.50	103.45
4	C	802	DAT	C4-N9-C8	2.55	108.42	105.74
6	C	804	DTP	C5-N7-C8	2.53	107.43	103.45
6	B	804	DTP	C5-N7-C8	2.53	107.42	103.45
6	B	804	DTP	C6-C5-N7	2.49	136.90	132.09
6	D	804	DTP	C5-N7-C8	2.48	107.34	103.45
6	A	804	DTP	C5-N7-C8	2.45	107.30	103.45
4	D	802	DAT	C6-C5-N7	2.44	136.80	132.09
6	D	804	DTP	O2B-PB-O3A	2.44	113.86	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	804	DTP	O2B-PB-O3A	2.38	113.71	107.27
4	A	802	DAT	C6-C5-N7	2.35	136.62	132.09
4	D	802	DAT	N9-C8-N7	-2.29	110.68	113.94
6	C	804	DTP	C6-C5-N7	2.27	136.46	132.09
4	C	802	DAT	C6-C5-N7	2.26	136.46	132.09
6	D	804	DTP	C6-C5-N7	2.26	136.44	132.09
6	B	804	DTP	O2B-PB-O3B	2.20	113.23	107.27
4	A	802	DAT	N9-C8-N7	-2.20	110.82	113.94
6	A	804	DTP	C6-C5-N7	2.17	136.27	132.09
4	B	802	DAT	C6-C5-N7	2.16	136.25	132.09
6	A	804	DTP	N9-C8-N7	-2.10	110.95	113.94
6	C	804	DTP	N9-C8-N7	-2.07	110.99	113.94
6	B	804	DTP	N9-C8-N7	-2.07	111.00	113.94
4	B	802	DAT	N9-C8-N7	-2.06	111.01	113.94
4	A	802	DAT	O2A-PA-O3A	2.05	112.81	107.27
6	D	804	DTP	O2B-PB-O3B	2.05	112.81	107.27
4	C	802	DAT	N9-C8-N7	-2.03	111.05	113.94
6	A	804	DTP	O2B-PB-O3A	2.02	112.75	107.27
6	D	804	DTP	N9-C8-N7	-2.00	111.10	113.94

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	801	CDP	C5'-O5'-PA-O3A
3	A	801	CDP	C5'-O5'-PA-O2A
3	B	801	CDP	C5'-O5'-PA-O3A
3	B	801	CDP	C5'-O5'-PA-O1A
3	B	801	CDP	C5'-O5'-PA-O2A
3	C	801	CDP	C5'-O5'-PA-O3A
3	C	801	CDP	C5'-O5'-PA-O1A
3	C	801	CDP	C5'-O5'-PA-O2A
3	D	801	CDP	C5'-O5'-PA-O3A
3	D	801	CDP	C5'-O5'-PA-O1A
4	A	802	DAT	C5'-O5'-PA-O1A
4	B	802	DAT	C5'-O5'-PA-O2A
6	A	804	DTP	PB-O3B-PG-O3G
6	C	804	DTP	C5'-O5'-PA-O1A
6	C	804	DTP	C5'-O5'-PA-O3A
3	C	801	CDP	O4'-C4'-C5'-O5'
4	A	802	DAT	C3'-C4'-C5'-O5'
4	A	802	DAT	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
4	C	802	DAT	O4'-C4'-C5'-O5'
4	C	802	DAT	C3'-C4'-C5'-O5'
3	C	801	CDP	C3'-C4'-C5'-O5'
6	A	804	DTP	PB-O3B-PG-O1G
6	B	804	DTP	PB-O3B-PG-O2G
3	D	801	CDP	O4'-C4'-C5'-O5'
4	B	802	DAT	PB-O3A-PA-O1A
6	A	804	DTP	PA-O3A-PB-O2B
6	B	804	DTP	PA-O3A-PB-O2B
6	D	804	DTP	PA-O3A-PB-O1B
3	A	801	CDP	C5'-O5'-PA-O1A
3	D	801	CDP	C5'-O5'-PA-O2A
4	A	802	DAT	C5'-O5'-PA-O2A
4	A	802	DAT	C5'-O5'-PA-O3A
4	B	802	DAT	C5'-O5'-PA-O1A
4	B	802	DAT	C5'-O5'-PA-O3A
6	C	804	DTP	C5'-O5'-PA-O2A
6	D	804	DTP	PA-O3A-PB-O2B
3	B	801	CDP	O4'-C4'-C5'-O5'
3	B	801	CDP	PB-O3A-PA-O2A
3	C	801	CDP	PB-O3A-PA-O2A
4	D	802	DAT	PB-O3A-PA-O1A
4	D	802	DAT	PB-O3A-PA-O2A
6	A	804	DTP	PA-O3A-PB-O1B
6	D	804	DTP	PB-O3A-PA-O1A
4	B	802	DAT	PB-O3A-PA-O2A
6	B	804	DTP	PA-O3A-PB-O1B
6	C	804	DTP	PG-O3B-PB-O2B
6	C	804	DTP	PB-O3A-PA-O2A

There are no ring outliers.

9 monomers are involved in 15 short contacts:

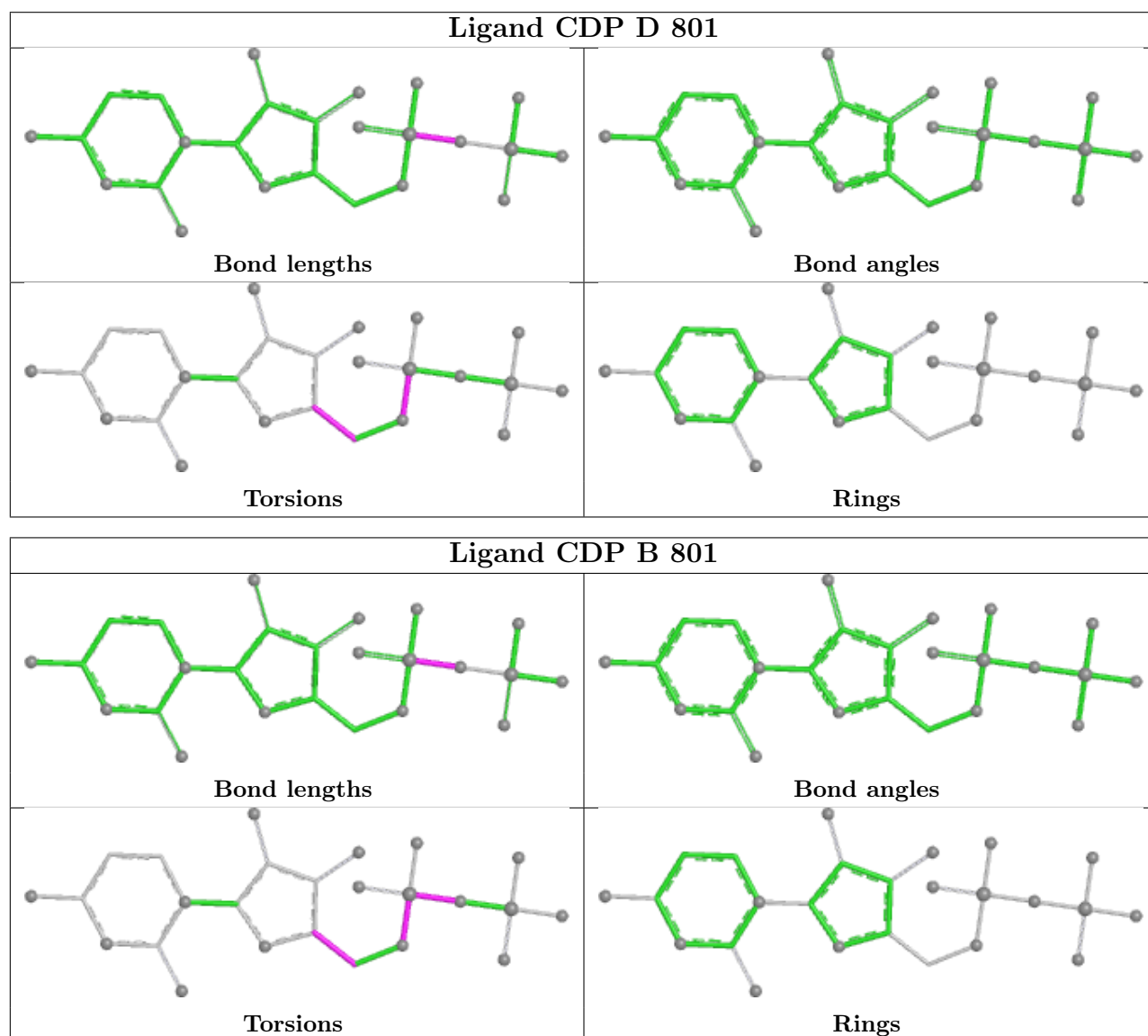
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	801	CDP	1	0
3	B	801	CDP	3	0
4	B	802	DAT	1	0
6	D	804	DTP	1	0
4	D	802	DAT	3	0
6	B	804	DTP	1	0
3	C	801	CDP	3	0
3	A	801	CDP	1	0

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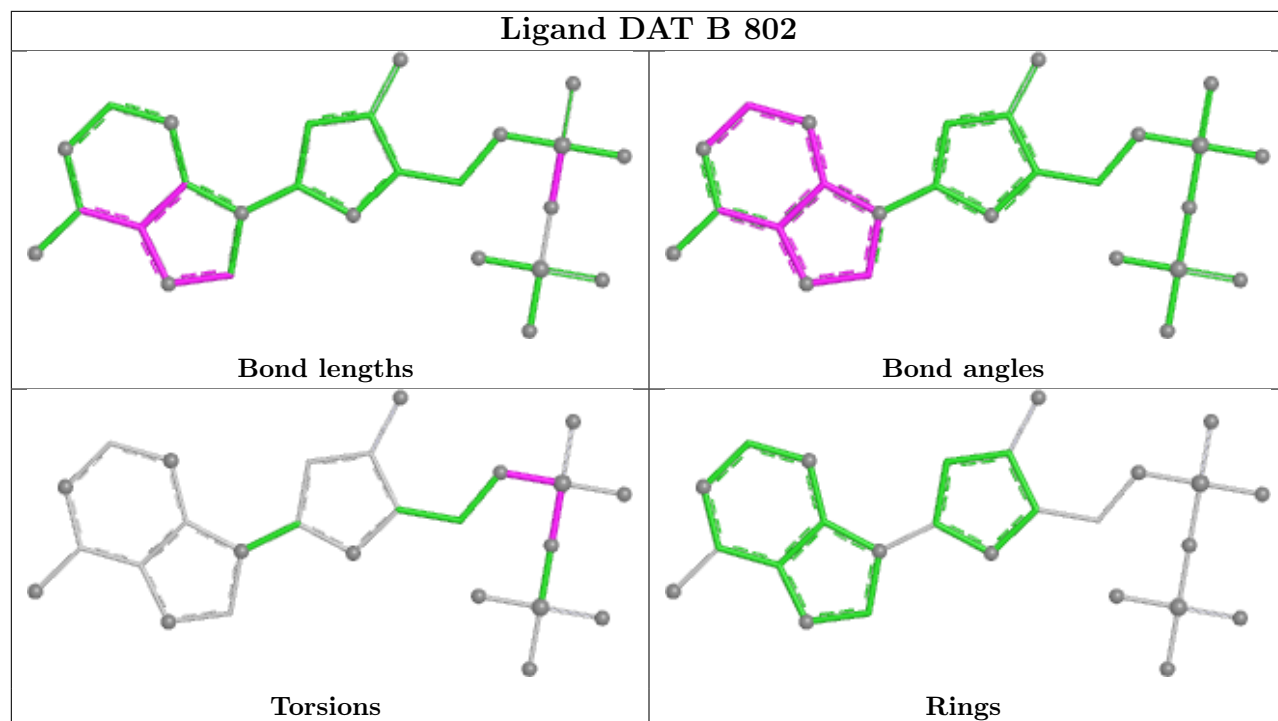
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	802	DAT	1	0

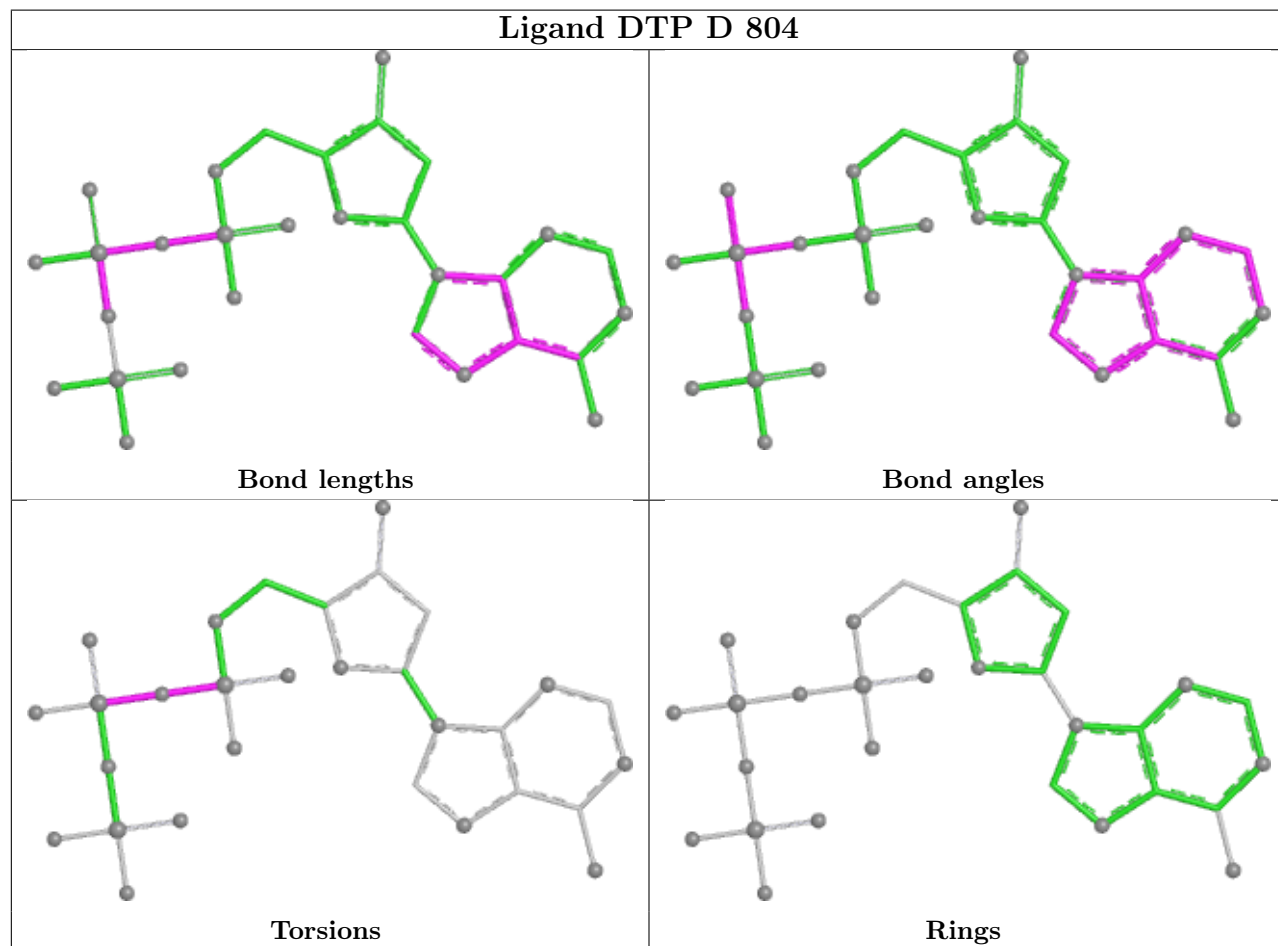
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



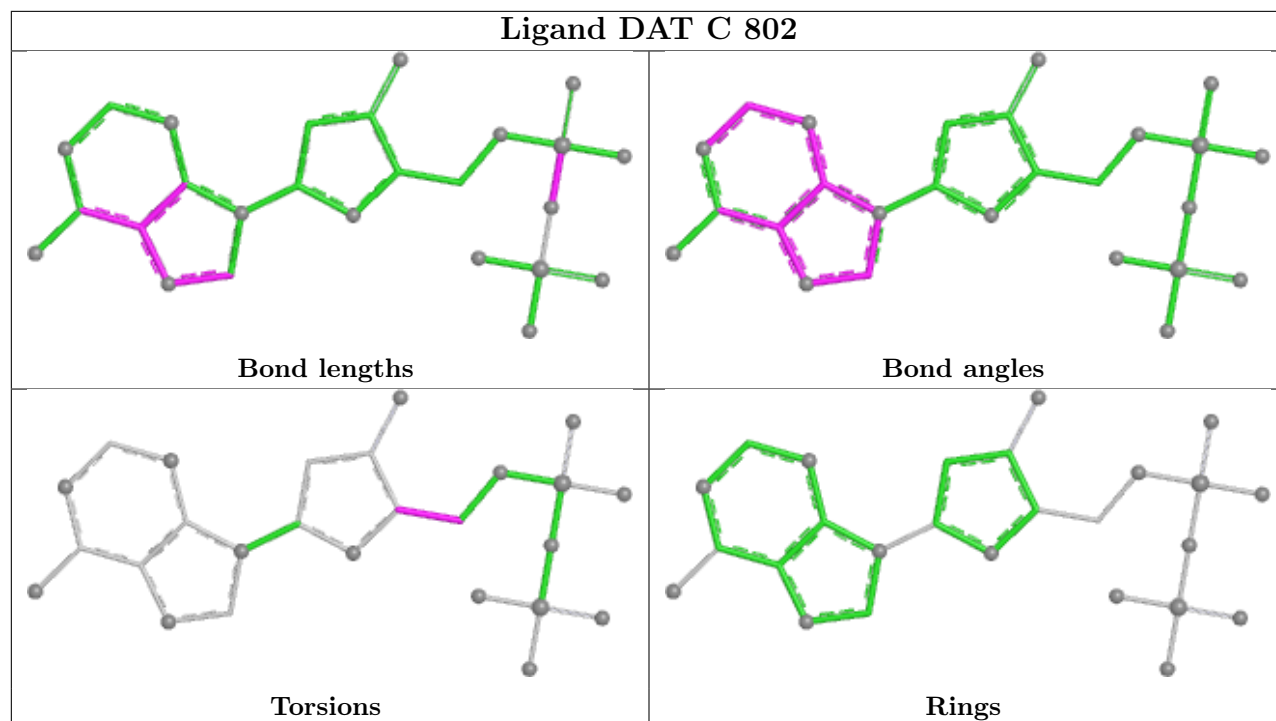
Ligand DAT B 802



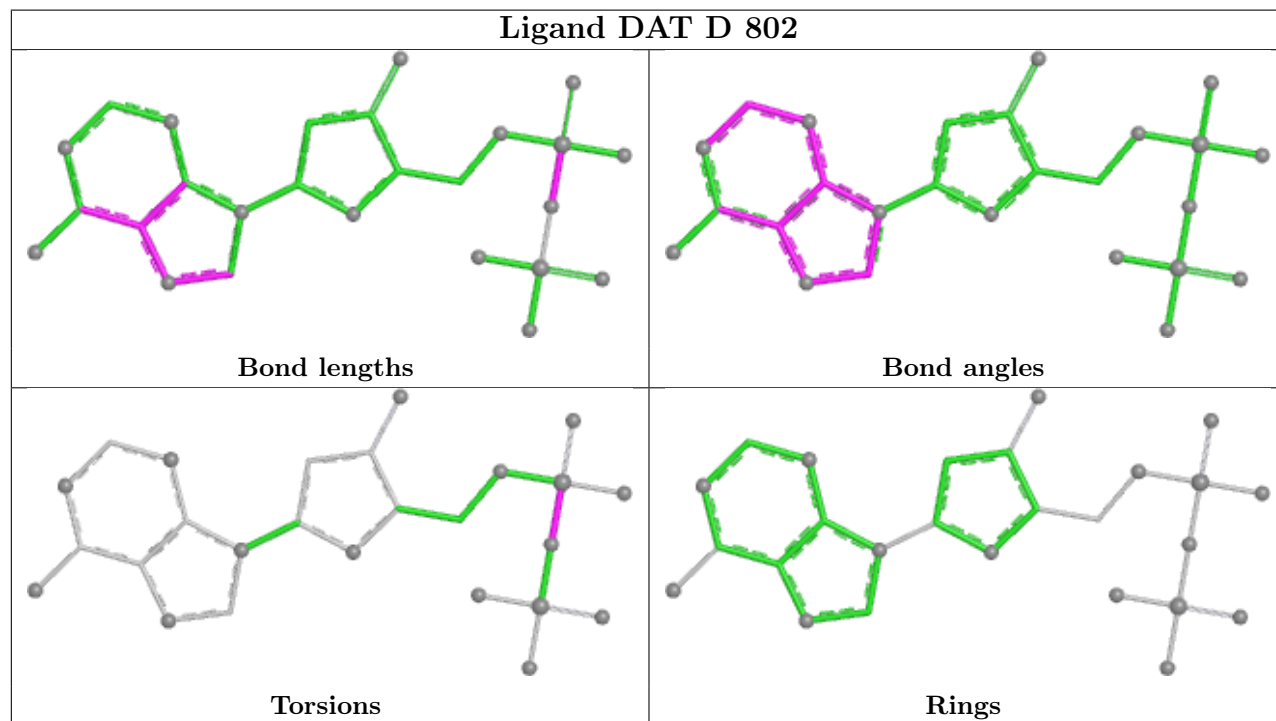
Ligand DTP D 804

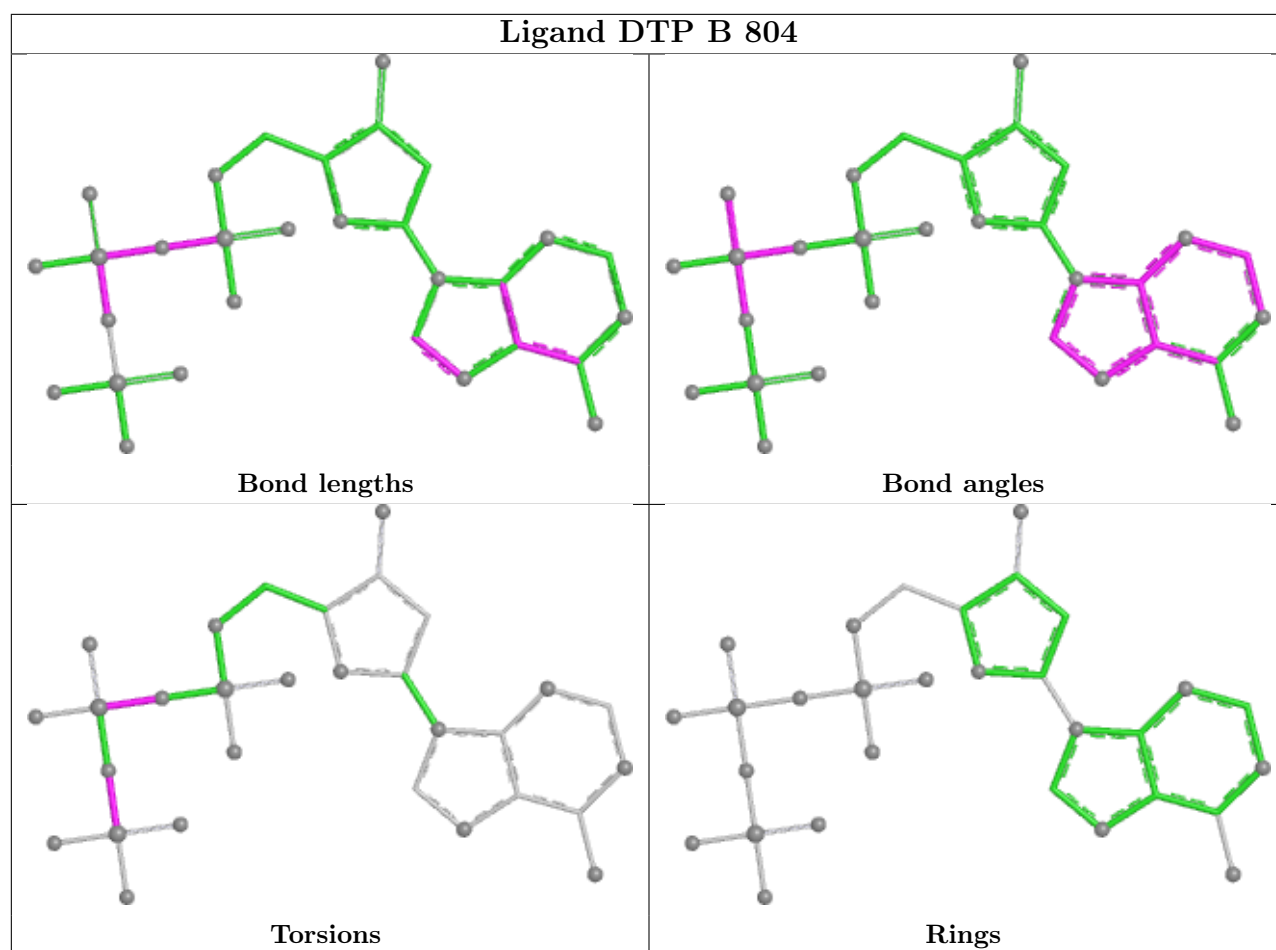


Ligand DAT C 802

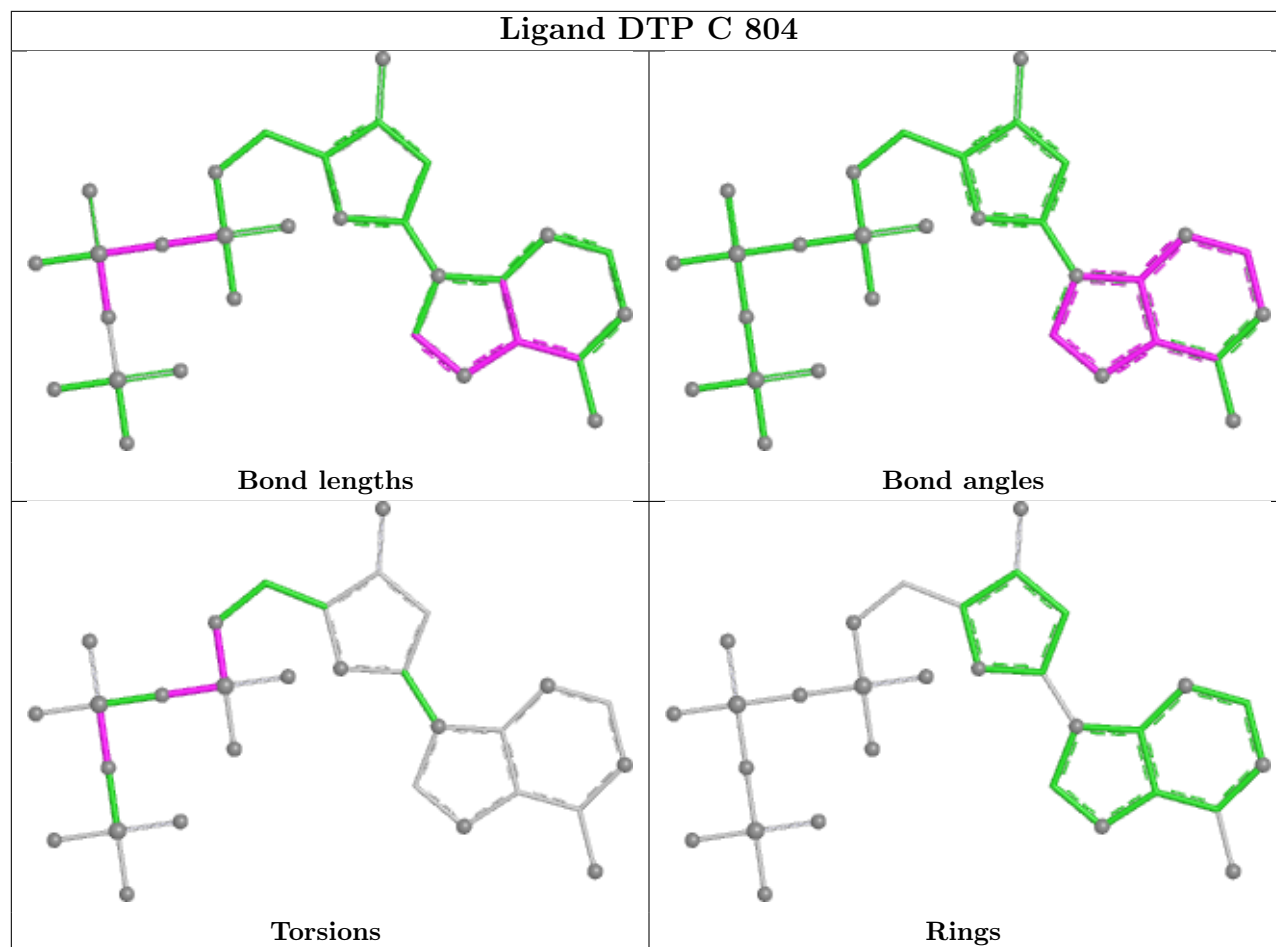


Ligand DAT D 802

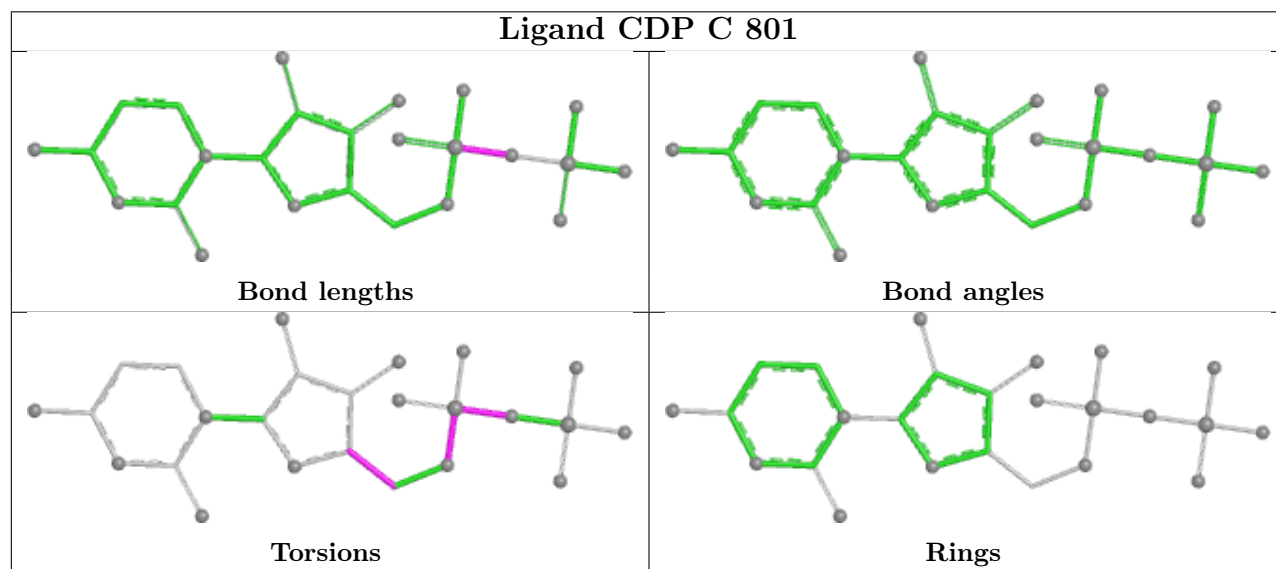


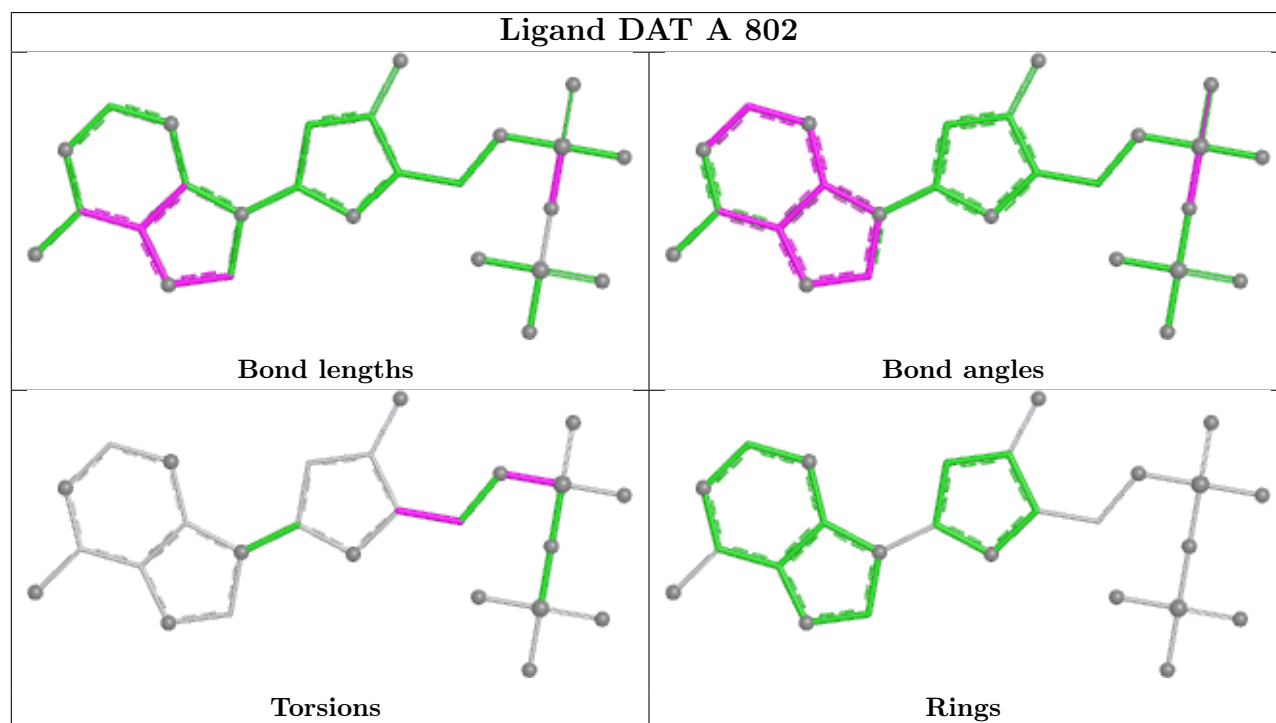
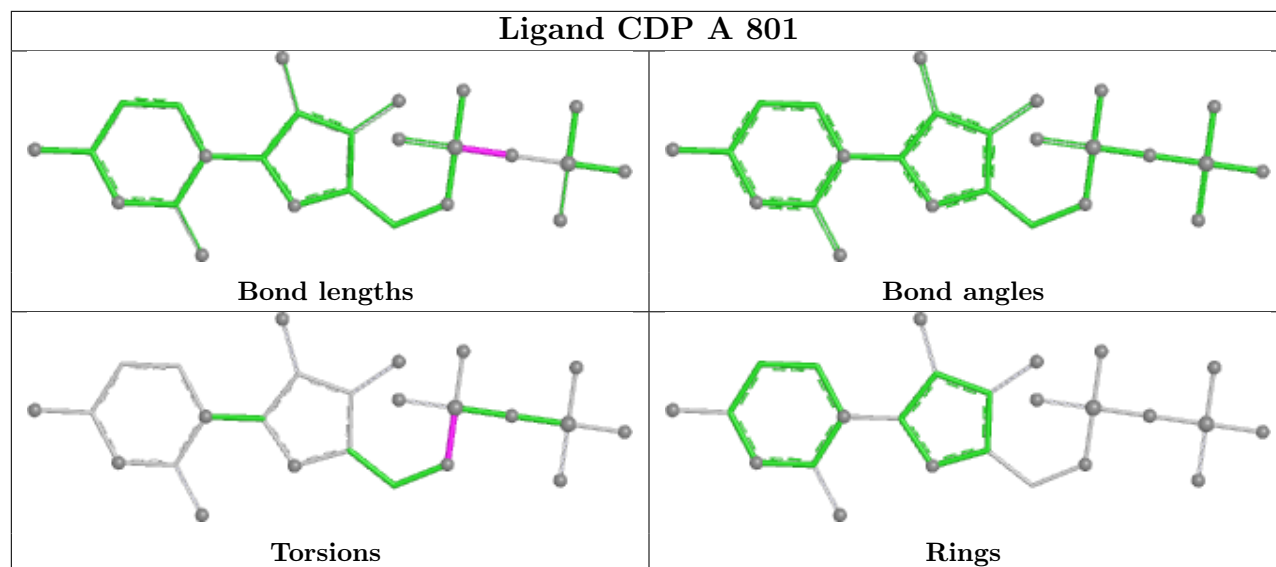


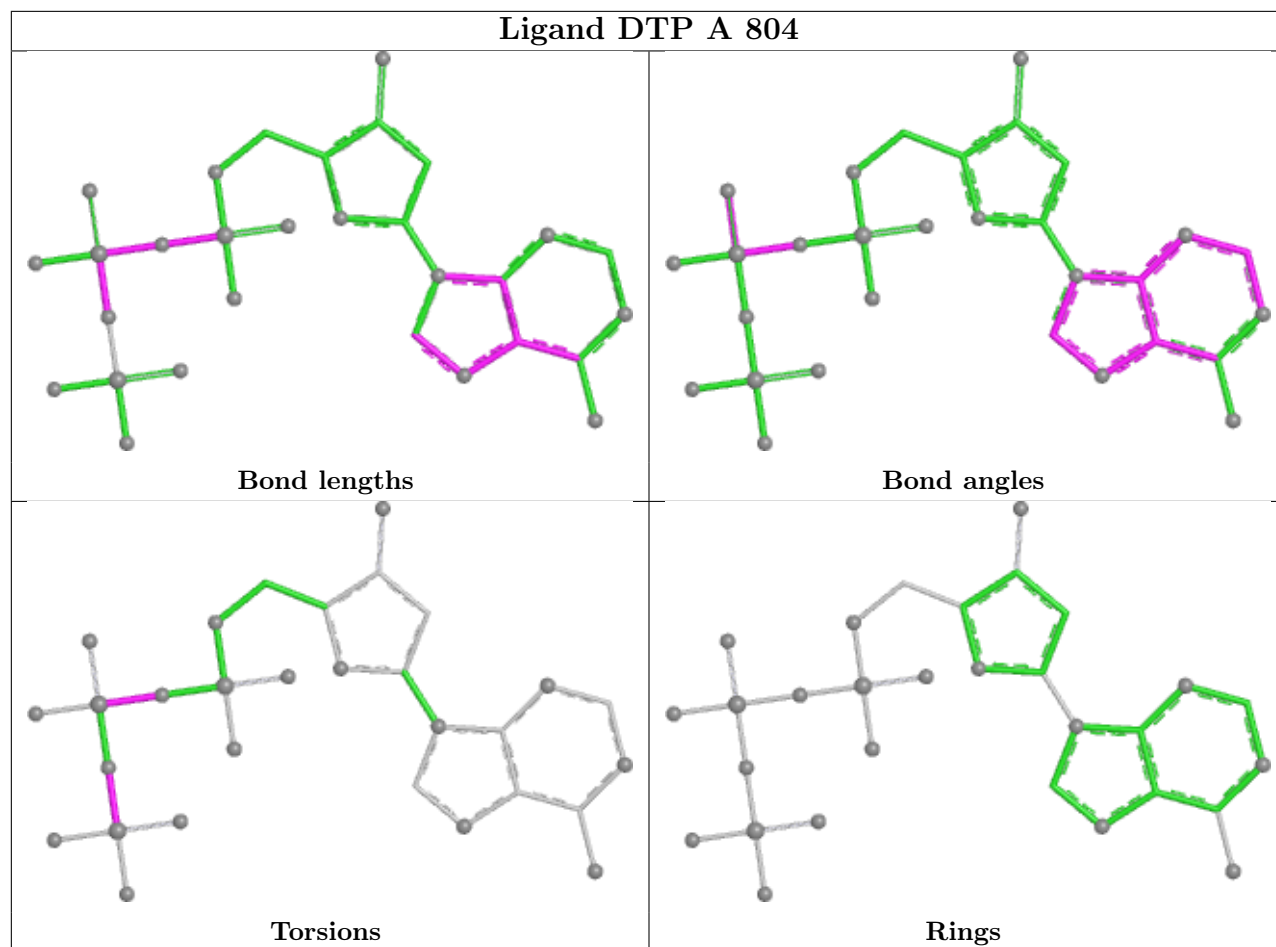
Ligand DTP C 804



Ligand CDP C 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 ⓘ

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	732/761 (96%)	-0.12	3 (0%) 88 79	37, 46, 66, 85	0
1	B	734/761 (96%)	-0.15	2 (0%) 90 82	38, 50, 65, 81	0
1	C	732/761 (96%)	0.38	9 (1%) 76 59	60, 73, 84, 93	0
1	D	734/761 (96%)	0.12	5 (0%) 84 70	47, 60, 76, 95	0
2	E	352/375 (93%)	0.31	7 (1%) 65 45	52, 67, 81, 103	0
2	F	357/375 (95%)	-0.18	2 (0%) 85 72	31, 43, 60, 81	0
2	G	357/375 (95%)	-0.13	7 (1%) 65 45	33, 46, 63, 85	0
2	H	355/375 (94%)	0.06	4 (1%) 78 61	48, 56, 76, 83	0
All	All	4353/4544 (95%)	0.04	39 (0%) 81 65	31, 56, 79, 103	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	5	LEU	4.7
2	E	374	GLN	3.4
1	A	5	LEU	3.0
1	B	557	GLU	3.0
1	C	543	THR	3.0
2	G	372	ASN	2.8
2	H	363	SER	2.7
2	H	340	VAL	2.7
2	G	149	ARG	2.7
2	G	368	ASP	2.6
1	C	540	THR	2.5
2	E	67	GLU	2.5
1	D	5	LEU	2.5
1	D	273	ALA	2.5
1	D	737	GLY	2.4
1	A	646	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
2	E	372	ASN	2.4
1	C	467	PHE	2.4
2	G	146	ILE	2.4
1	B	269	ARG	2.4
2	E	297	ILE	2.3
2	H	373	PHE	2.3
1	A	452	VAL	2.3
2	G	179	GLY	2.2
2	F	375	LEU	2.2
1	D	648	LYS	2.2
2	E	170	LEU	2.2
1	C	68	ASP	2.2
2	G	362	ASP	2.1
1	C	544	PHE	2.1
2	H	361	ILE	2.1
2	F	374	GLN	2.1
2	E	370	LEU	2.1
1	C	649	ASP	2.1
1	D	446	THR	2.1
1	C	81	ALA	2.1
2	G	341	SER	2.0
2	E	144	GLU	2.0
1	C	463	THR	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.

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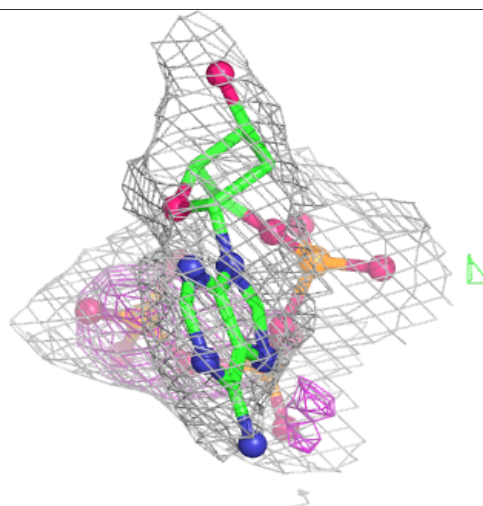
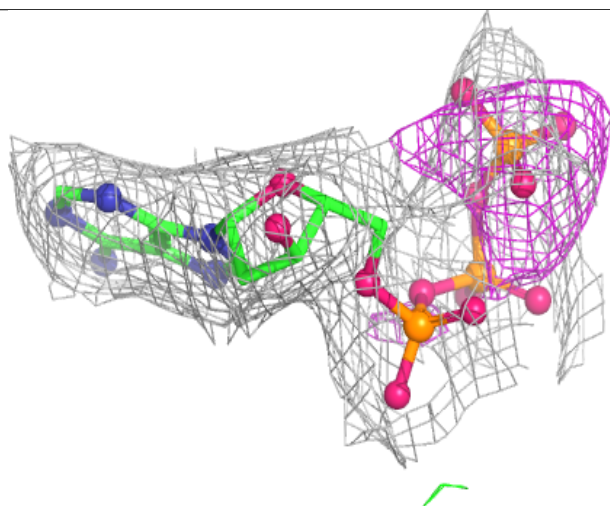
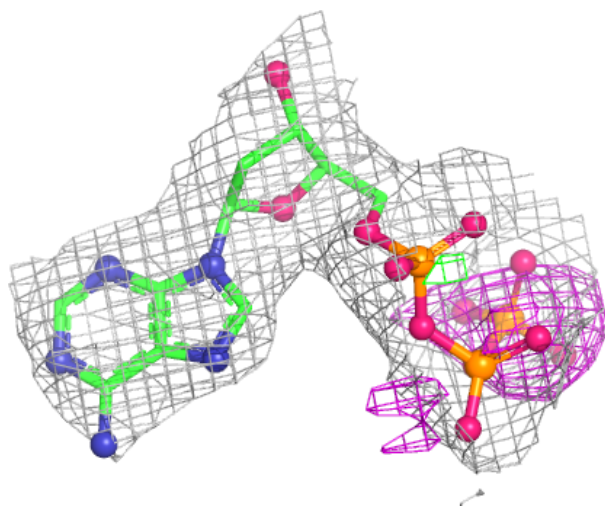
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	DTP	D	804	30/30	0.89	0.10	64,68,81,89	0
6	DTP	C	804	30/30	0.91	0.10	65,70,82,88	0
6	DTP	B	804	30/30	0.91	0.10	46,51,70,78	0
4	DAT	C	802	26/26	0.92	0.10	78,81,88,91	0
5	MG	A	805	1/1	0.92	0.09	52,52,52,52	0
6	DTP	A	804	30/30	0.92	0.09	44,46,59,66	0
4	DAT	A	802	26/26	0.93	0.09	65,73,82,83	0
4	DAT	D	802	26/26	0.94	0.09	68,74,76,79	0
3	CDP	C	801	25/25	0.94	0.08	65,66,66,67	0
5	MG	D	803	1/1	0.95	0.06	86,86,86,86	0
3	CDP	D	801	25/25	0.95	0.08	52,57,60,62	0
3	CDP	B	801	25/25	0.95	0.08	42,45,47,48	0
5	MG	A	803	1/1	0.95	0.07	79,79,79,79	0
4	DAT	B	802	26/26	0.95	0.08	52,55,57,60	0
5	MG	B	805	1/1	0.96	0.05	64,64,64,64	0
5	MG	D	805	1/1	0.96	0.06	76,76,76,76	0
3	CDP	A	801	25/25	0.97	0.07	41,43,45,46	0
5	MG	C	803	1/1	0.97	0.05	89,89,89,89	0
5	MG	C	805	1/1	0.97	0.09	79,79,79,79	0
5	MG	B	803	1/1	0.99	0.06	55,55,55,55	0
7	FEO	E	501	3/3	0.99	0.04	56,56,59,62	0
7	FEO	F	501	3/3	0.99	0.04	35,35,36,37	0
7	FEO	G	501	3/3	0.99	0.03	35,35,37,38	0
7	FEO	H	501	3/3	0.99	0.04	47,47,48,50	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.

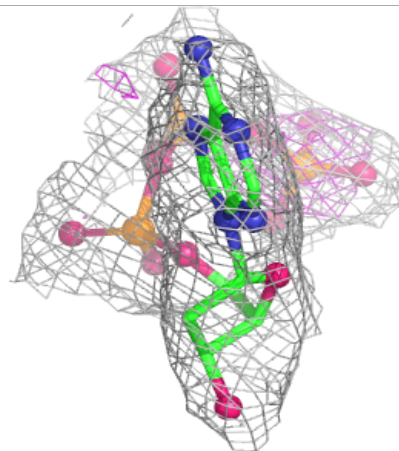
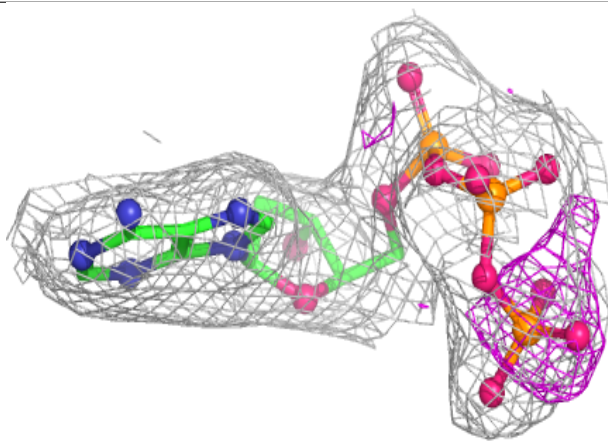
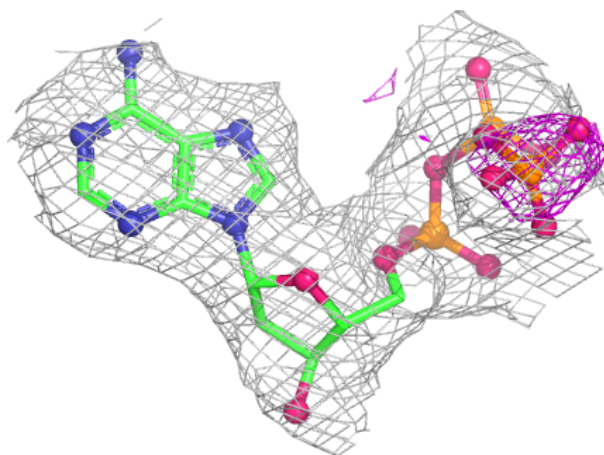
Electron density around DTP D 804:

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



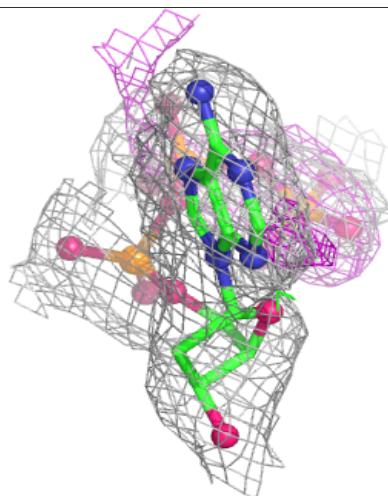
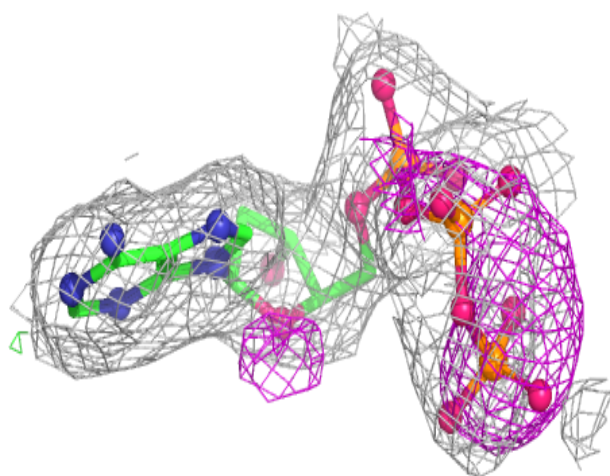
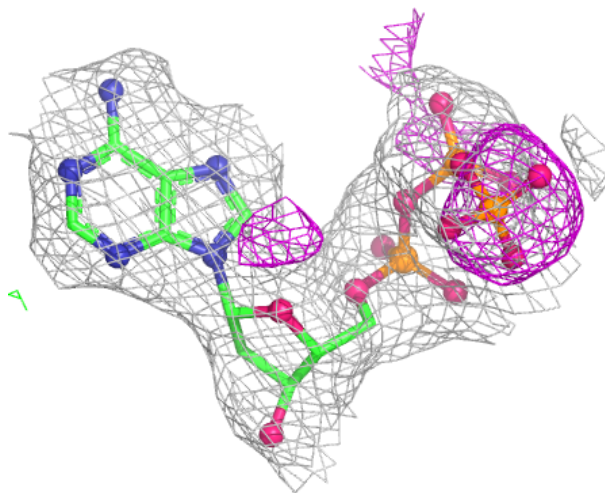
Electron density around DTP C 804:

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



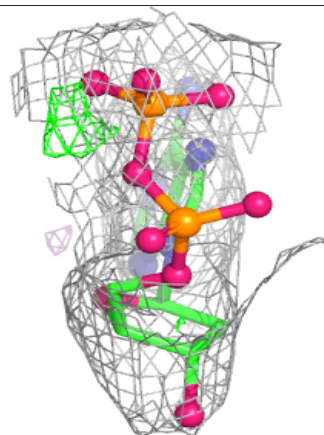
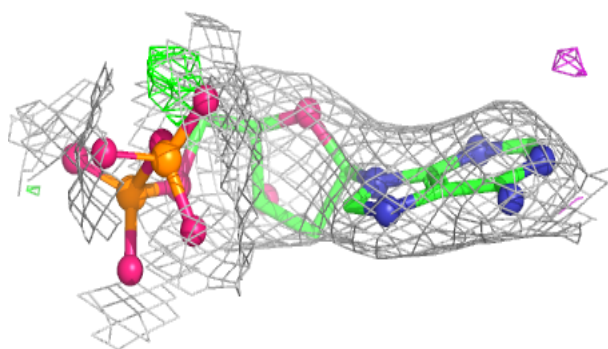
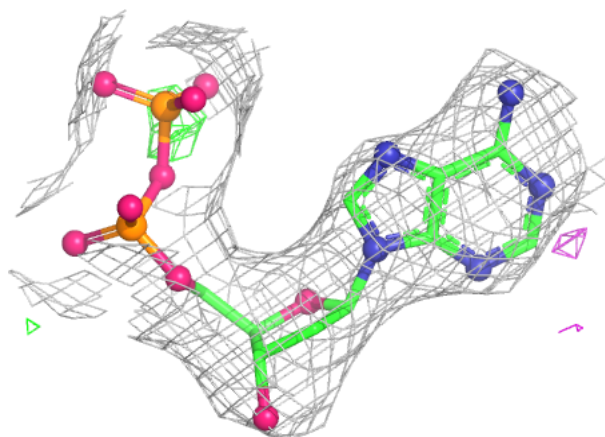
Electron density around DTP B 804:

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and green (positive)



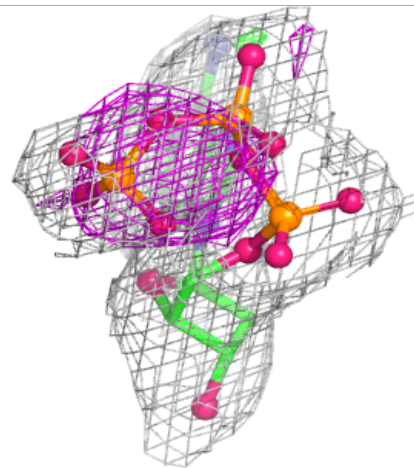
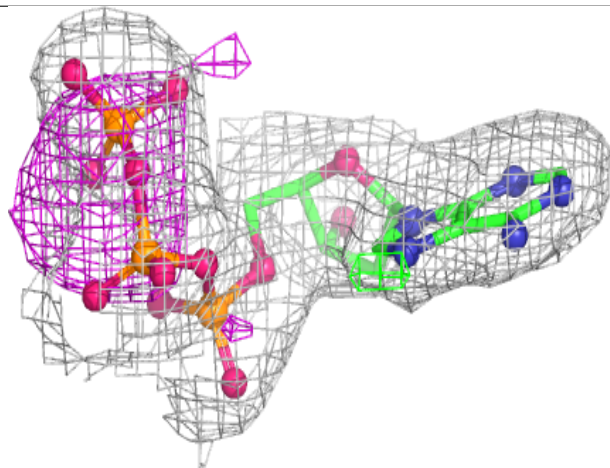
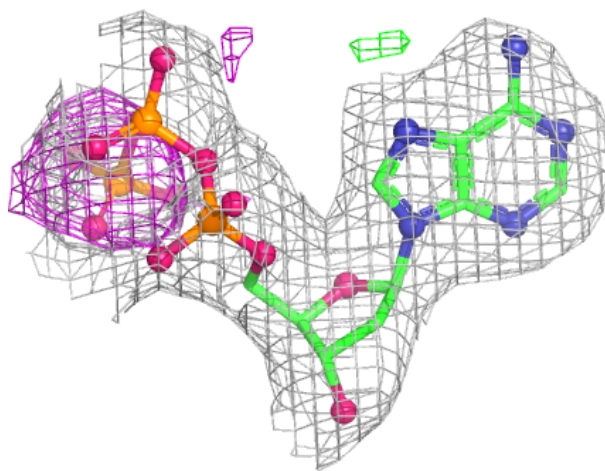
Electron density around DAT C 802:

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and green (positive)



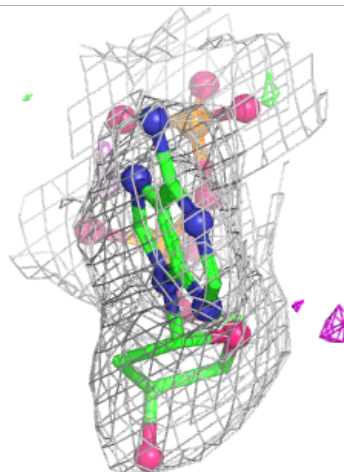
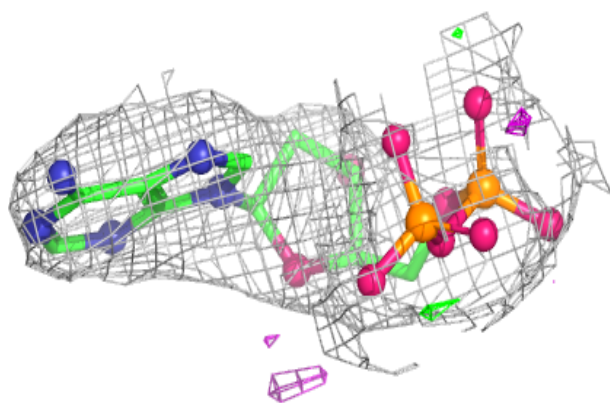
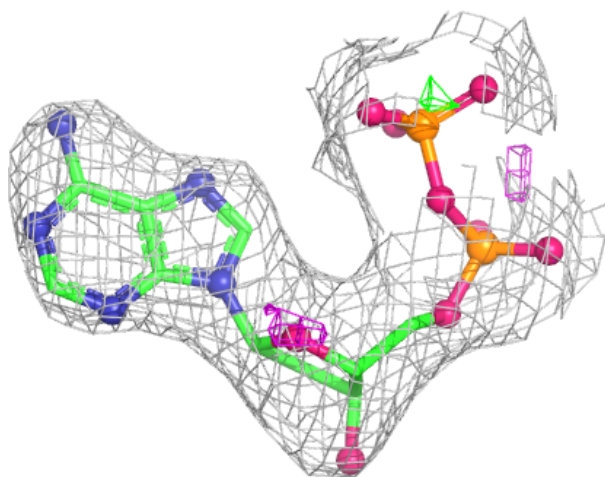
Electron density around DTP A 804:

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and green (positive)



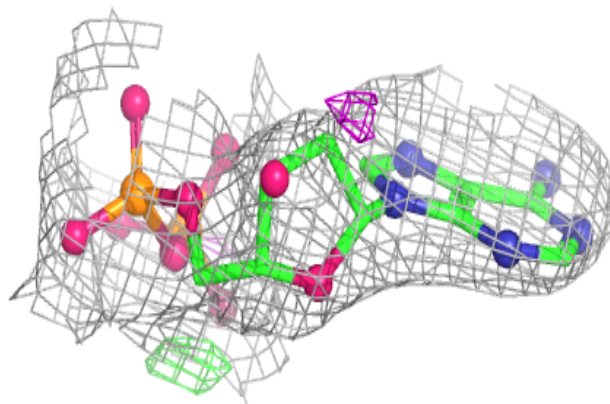
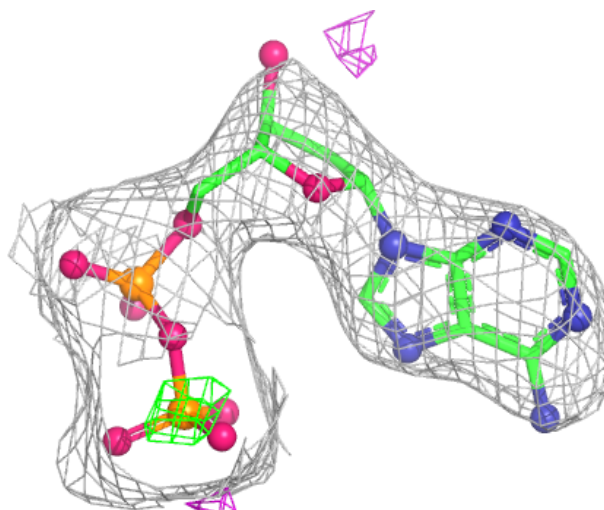
Electron density around DAT A 802:

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and green (positive)



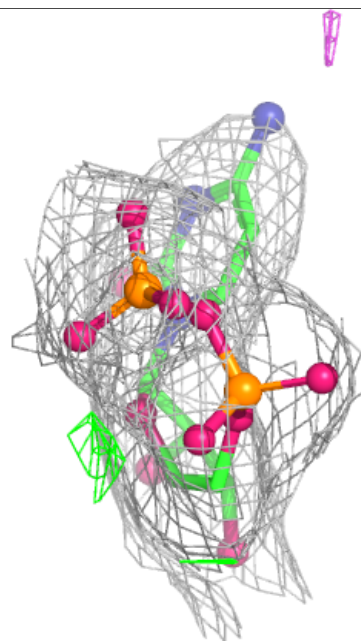
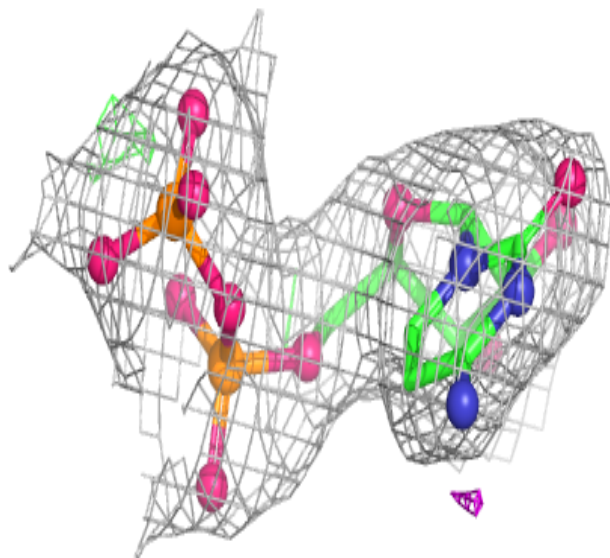
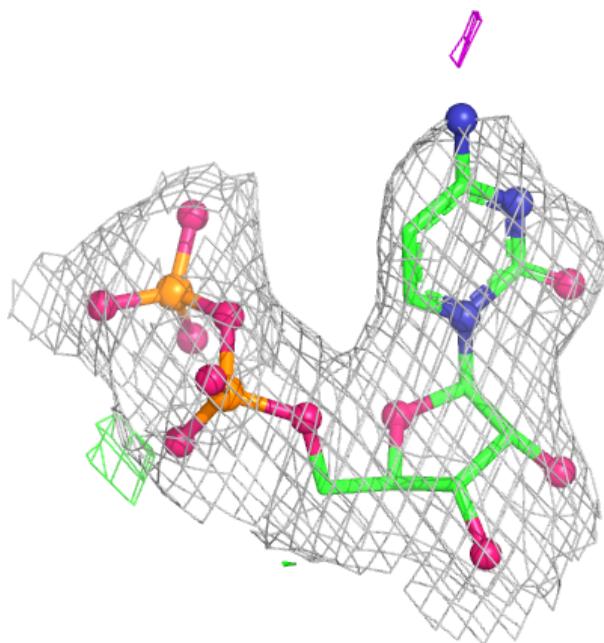
Electron density around DAT D 802:

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and green (positive)



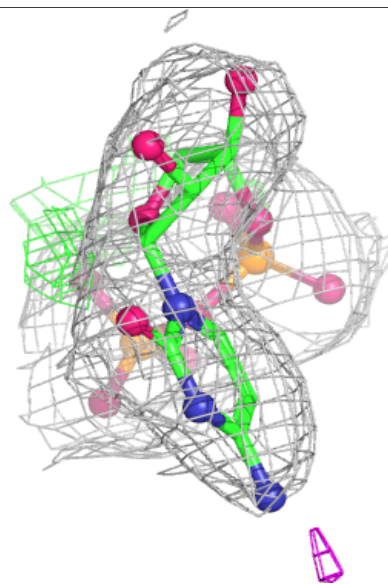
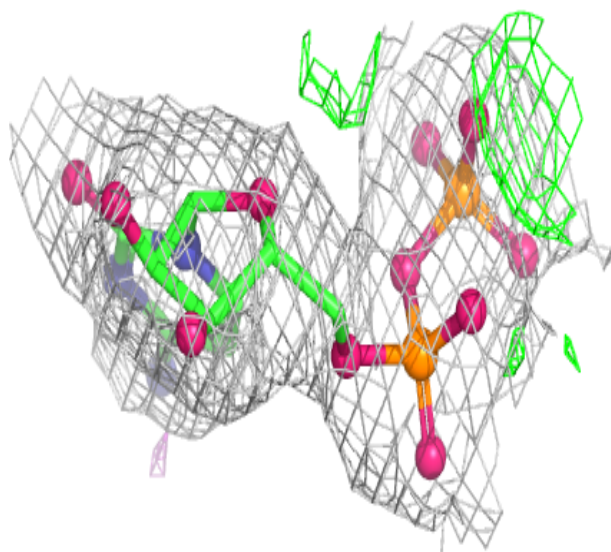
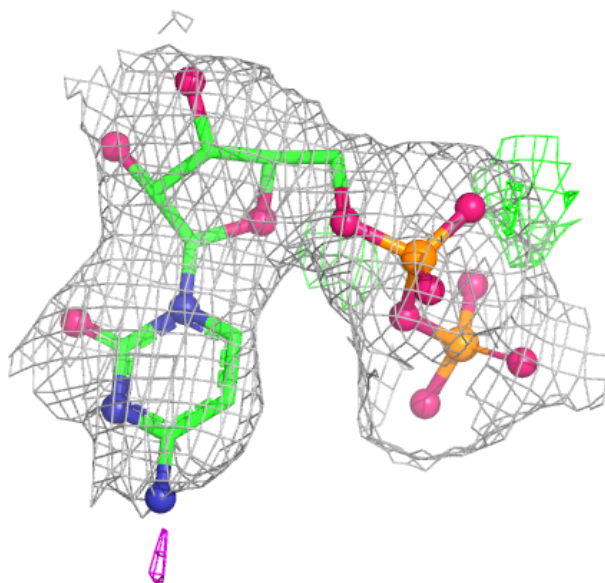
Electron density around CDP C 801:

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and green (positive)



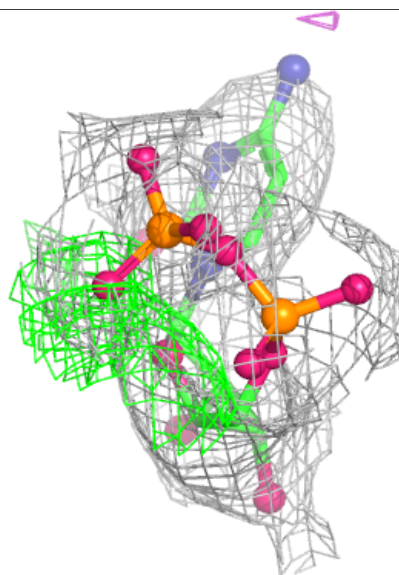
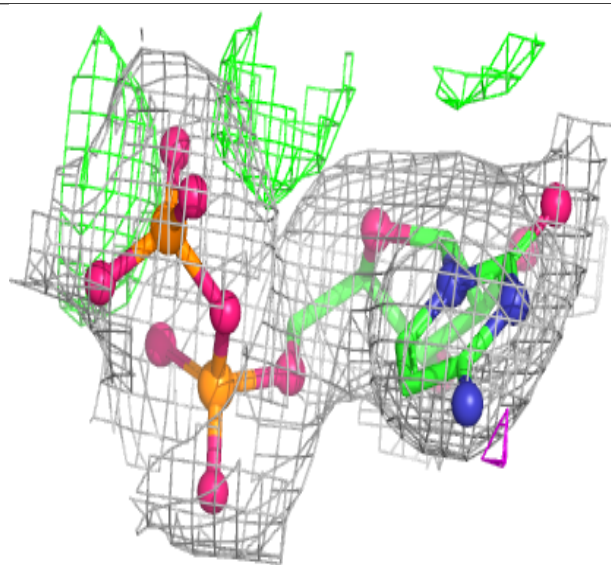
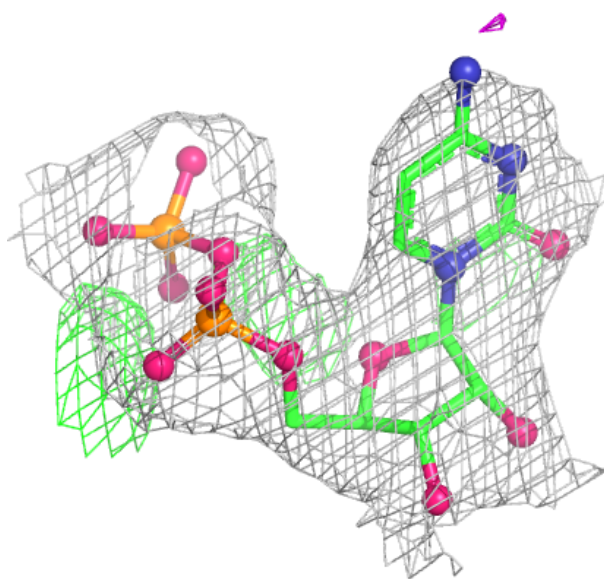
Electron density around CDP D 801:

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and green (positive)



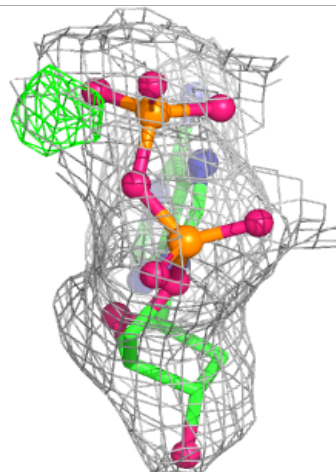
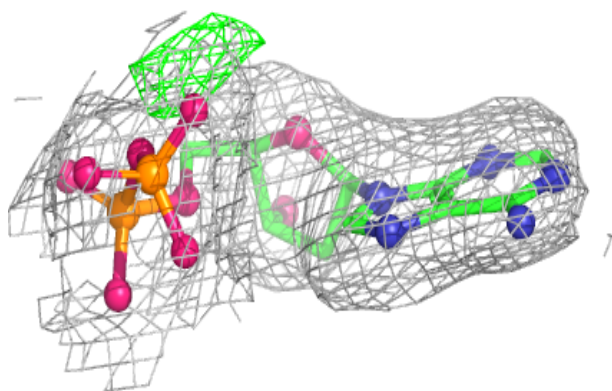
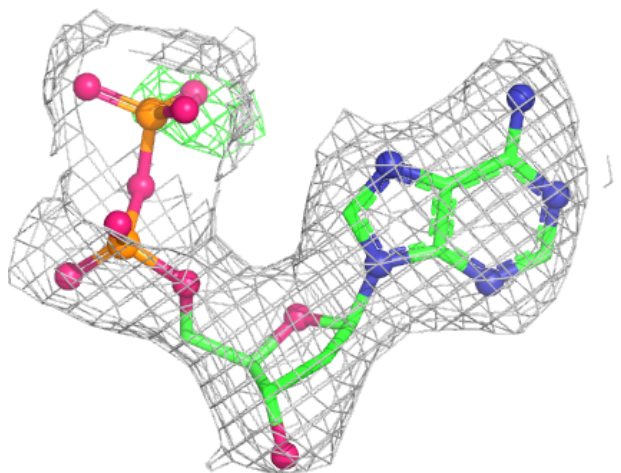
Electron density around CDP B 801:

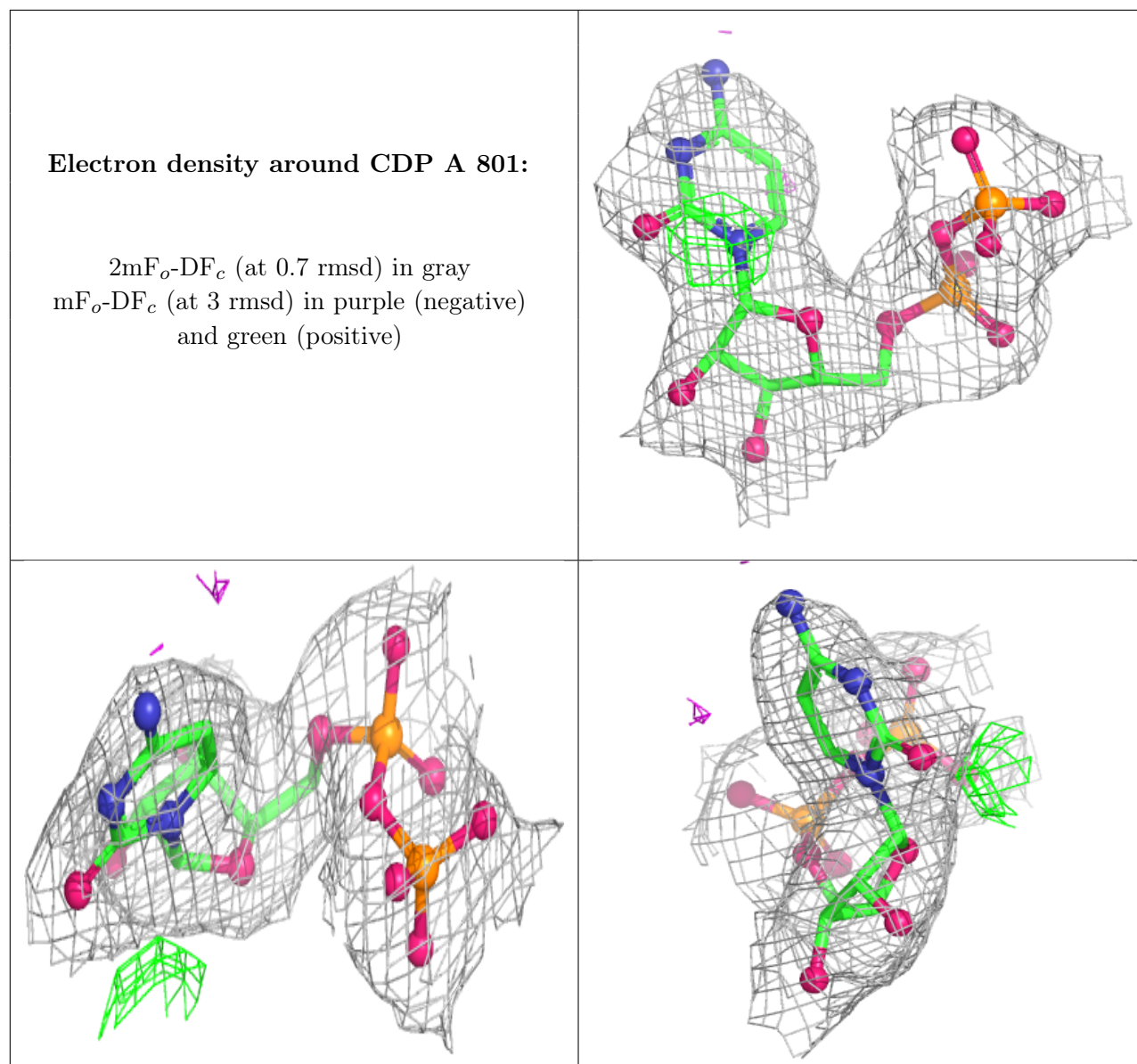
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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around DAT 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.