



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 03:22 am BST

PDB ID : 5NPU  
Title : Inferred ancestral pyruvate decarboxylase  
Authors : Buddrus, L.; Crennell, S.J.; Leak, D.J.; Danson, M.J.; Andrews, E.S.V.; Arcus, V.L.  
Deposited on : 2017-04-19  
Resolution : 3.50 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) 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 : 2.11  
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) : 2.11

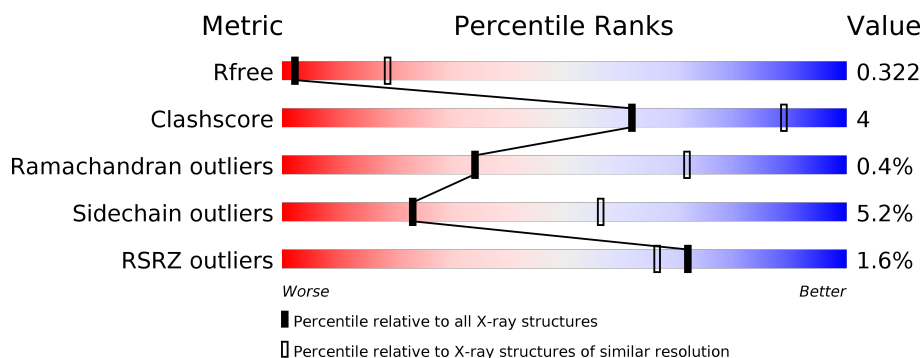
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	563	<div> <div>84%</div> <div>12%</div> <div>• •</div> </div>
1	B	563	<div> <div>%</div> <div>84%</div> <div>11%</div> <div>• •</div> </div>
1	C	563	<div> <div>3%</div> <div>80%</div> <div>16%</div> <div>• •</div> </div>
1	D	563	<div> <div>2%</div> <div>86%</div> <div>9%</div> <div>• •</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 33050 atoms, of which 16394 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.

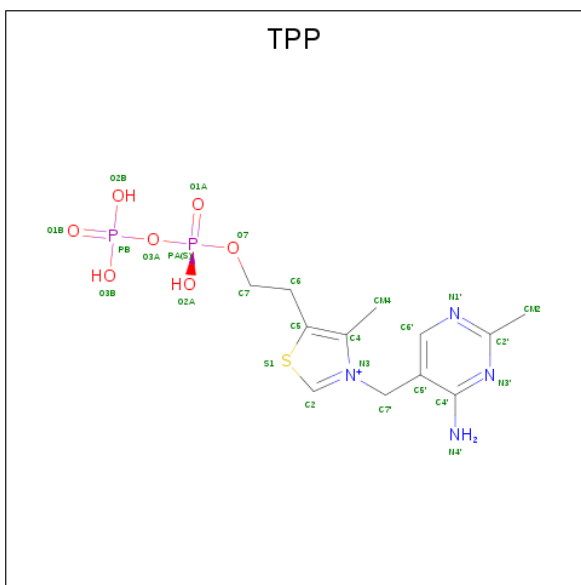
- Molecule 1 is a protein called ANC27.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	547	Total	C	H	N	O	S	0	0	0
			8235	2629	4089	713	785	19			
1	B	545	Total	C	H	N	O	S	0	0	0
			8213	2622	4080	711	781	19			
1	C	547	Total	C	H	N	O	S	0	0	0
			8232	2628	4089	713	783	19			
1	D	543	Total	C	H	N	O	S	0	0	0
			8180	2612	4062	709	778	19			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

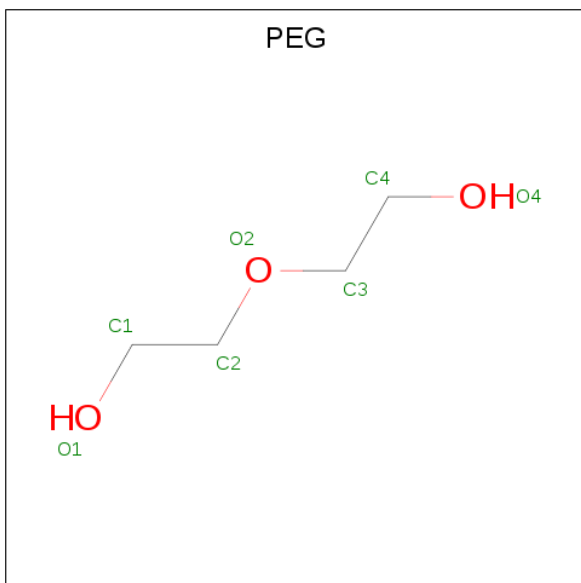
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

- Molecule 3 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: C<sub>12</sub>H<sub>19</sub>N<sub>4</sub>O<sub>7</sub>P<sub>2</sub>S).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total 42	C 12	H 16	N 4	O 7	P 2	S 1	0	0
3	B	1	Total 42	C 12	H 16	N 4	O 7	P 2	S 1	0	0
3	C	1	Total 42	C 12	H 16	N 4	O 7	P 2	S 1	0	0
3	D	1	Total 42	C 12	H 16	N 4	O 7	P 2	S 1	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $\text{C}_4\text{H}_{10}\text{O}_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	H	O	0	0
			17	4	10	3		

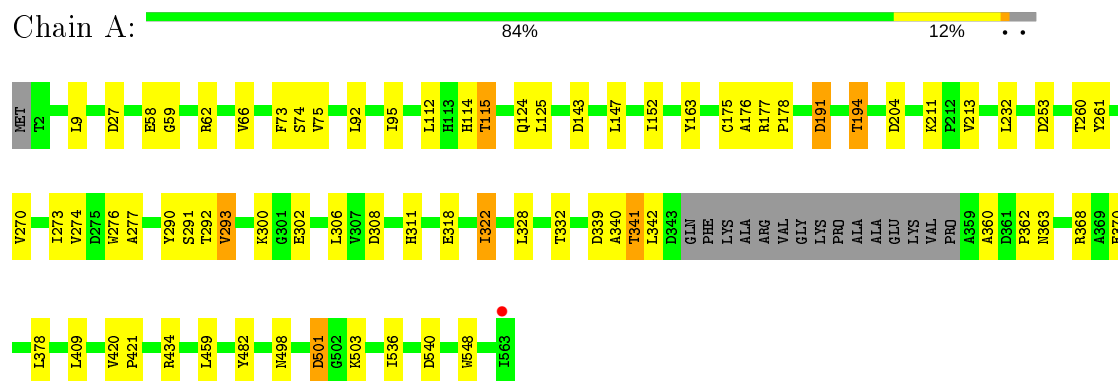
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			1	1		

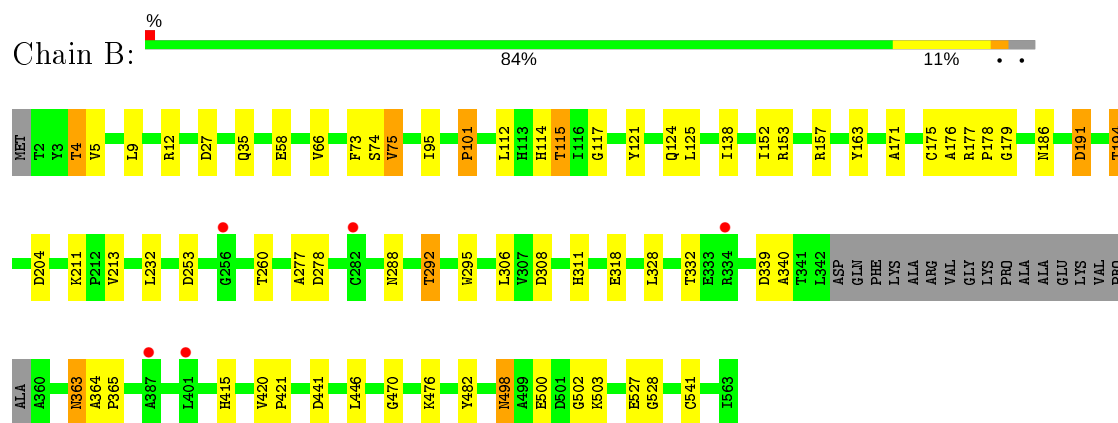
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

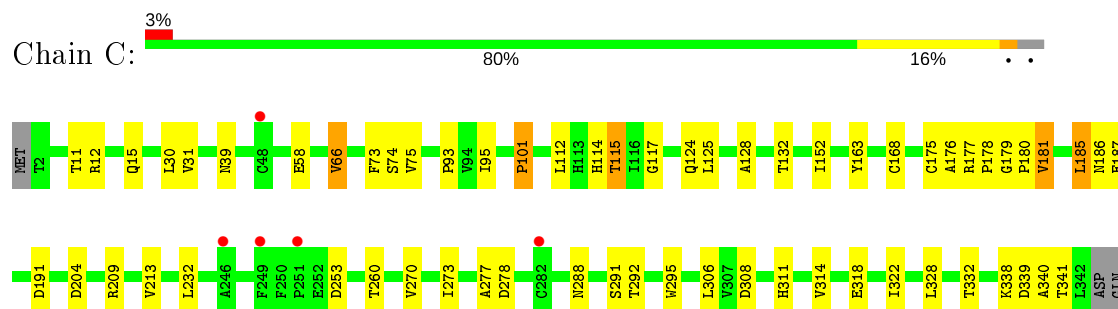
#### • Molecule 1: ANC27

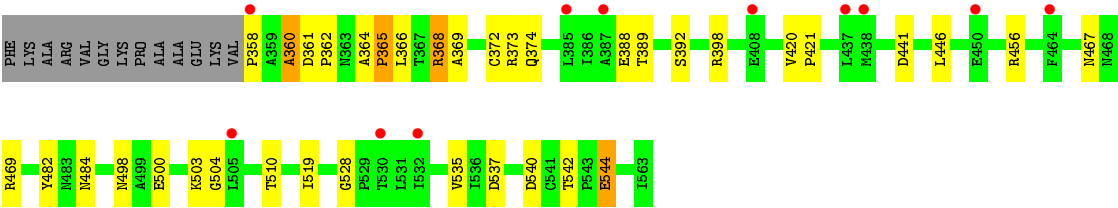


#### • Molecule 1: ANC27

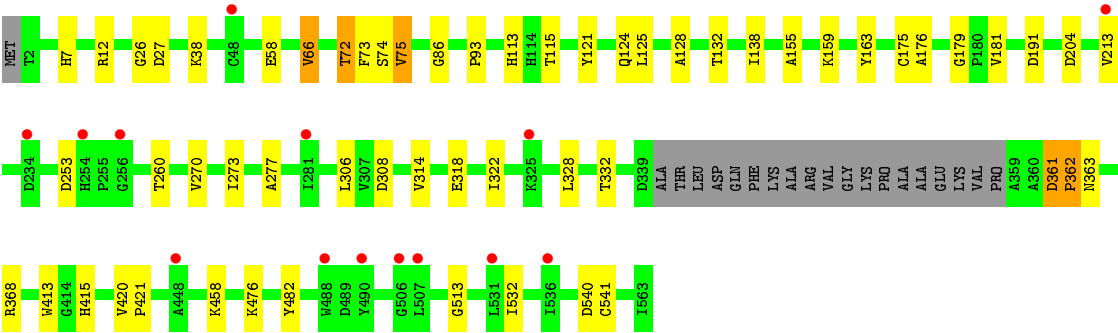
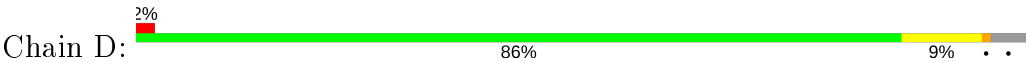


#### • Molecule 1: ANC27





● Molecule 1: ANC27



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.33Å 108.33Å 322.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	81.10 – 3.50 93.82 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (81.10-3.50) 99.5 (93.82-3.50)	Depositor EDS
$R_{merge}$	0.24	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.57 (at 3.49Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.246 , 0.319 0.247 , 0.322	Depositor DCC
$R_{free}$ test set	1360 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	68.6	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 57.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.045 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	33050	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MG, PEG, TPP

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	0.38	2/4238 (0.0%)	0.50	0/5775
1	B	0.29	0/4225	0.47	0/5757
1	C	0.30	0/4235	0.49	1/5771 (0.0%)
1	D	0.29	0/4210	0.46	0/5736
All	All	0.32	2/16908 (0.0%)	0.48	1/23039 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	459	LEU	C-N	9.25	1.51	1.34
1	A	92	LEU	C-N	-5.62	1.23	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	358	PRO	N-CA-CB	6.07	110.58	103.30

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	4146	4089	4089	39	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4133	4080	4080	37	0
1	C	4143	4089	4087	45	3
1	D	4118	4062	4062	24	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	26	16	16	0	0
3	B	26	16	16	2	0
3	C	26	16	16	1	0
3	D	26	16	16	1	0
4	C	7	10	10	0	0
5	A	1	0	0	0	0
All	All	16656	16394	16392	144	5

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 (144) 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:D:361:ASP:O	1:D:363:ASN:N	2.12	0.82
1:A:74:SER:OG	1:A:114:HIS:O	2.02	0.77
1:A:368:ARG:NE	1:A:540:ASP:O	2.19	0.76
1:D:175:CYS:SG	1:D:176:ALA:N	2.62	0.72
1:D:368:ARG:NE	1:D:540:ASP:O	2.24	0.71
1:C:15:GLN:HB3	1:C:181:VAL:HG11	1.73	0.71
1:D:124:GLN:NE2	1:D:163:TYR:OH	2.27	0.68
1:B:175:CYS:SG	1:B:176:ALA:N	2.68	0.66
1:A:501:ASP:N	1:A:501:ASP:OD1	2.25	0.66
1:A:175:CYS:SG	1:A:176:ALA:N	2.71	0.64
1:C:175:CYS:SG	1:C:176:ALA:N	2.71	0.63
1:B:364:ALA:HB1	1:B:365:PRO:HD2	1.79	0.63
1:D:12:ARG:NH1	1:D:179:GLY:O	2.32	0.61
1:C:74:SER:OG	1:C:114:HIS:O	2.14	0.60
1:A:293:VAL:O	1:A:293:VAL:HG13	2.02	0.60
1:B:124:GLN:NE2	1:B:163:TYR:OH	2.35	0.59
1:C:366:LEU:HD22	1:C:510:THR:O	2.02	0.59
1:B:476:LYS:NZ	1:B:541:CYS:SG	2.67	0.58
1:B:74:SER:OG	1:B:114:HIS:O	2.18	0.57
1:C:124:GLN:NE2	1:C:163:TYR:OH	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:420:VAL:HB	1:D:421:PRO:HD3	1.87	0.56
1:A:124:GLN:NE2	1:A:163:TYR:OH	2.39	0.56
1:C:388:GLU:OE1	1:C:389:THR:N	2.38	0.56
1:A:420:VAL:HB	1:A:421:PRO:HD3	1.88	0.55
1:A:293:VAL:HG23	1:A:548:TRP:CD1	2.41	0.55
1:A:73:PHE:O	1:A:75:VAL:N	2.38	0.55
1:B:73:PHE:O	1:B:75:VAL:N	2.38	0.55
1:C:544:GLU:OE1	1:C:544:GLU:N	2.41	0.53
1:D:361:ASP:HB2	1:D:362:PRO:HD3	1.91	0.53
1:D:476:LYS:NZ	1:D:541:CYS:SG	2.70	0.52
1:B:191:ASP:OD2	1:B:194:THR:OG1	2.28	0.52
1:B:288:ASN:O	1:B:292:THR:HG23	2.11	0.51
1:C:420:VAL:HB	1:C:421:PRO:HD3	1.91	0.51
1:A:300:LYS:NZ	1:A:302:GLU:OE2	2.44	0.51
1:C:360:ALA:O	1:C:362:PRO:HD3	2.11	0.50
1:C:368:ARG:HH12	1:C:372:CYS:HB3	1.76	0.50
1:A:213:VAL:CG2	1:A:277:ALA:CB	2.89	0.50
1:C:498:ASN:OD1	1:C:504:GLY:N	2.45	0.50
1:A:232:LEU:HA	1:A:332:THR:HG22	1.93	0.49
1:C:364:ALA:HB1	1:C:365:PRO:HD2	1.95	0.49
1:B:503:LYS:HD2	1:B:527:GLU:HG2	1.94	0.49
1:C:270:VAL:O	1:C:273:ILE:HG22	2.12	0.49
1:B:420:VAL:HB	1:B:421:PRO:HD3	1.95	0.48
1:C:292:THR:HG23	1:C:295:TRP:H	1.78	0.48
1:C:361:ASP:OD1	1:C:364:ALA:HB3	2.14	0.48
1:C:73:PHE:O	1:C:75:VAL:N	2.46	0.48
1:D:415:HIS:CD2	3:D:602:TPP:HM21	2.48	0.48
1:A:328:LEU:O	1:A:332:THR:HG23	2.13	0.48
1:B:4:THR:OG1	1:B:5:VAL:N	2.46	0.48
1:C:177:ARG:HG3	1:C:178:PRO:HD2	1.96	0.48
1:C:537:ASP:HB3	1:C:540:ASP:HB3	1.94	0.48
1:D:74:SER:N	1:D:124:GLN:OE1	2.42	0.48
1:D:26:GLY:HA3	1:D:72:THR:OG1	2.14	0.48
1:D:73:PHE:O	1:D:75:VAL:N	2.45	0.48
1:C:185:LEU:CD1	1:C:185:LEU:N	2.77	0.48
1:B:35:GLN:NE2	1:B:171:ALA:O	2.47	0.47
1:A:112:LEU:O	1:A:115:THR:CG2	2.62	0.47
1:A:62:ARG:NH1	1:A:409:LEU:O	2.40	0.47
1:A:261:TYR:CE1	1:A:274:VAL:HG21	2.49	0.47
1:C:369:ALA:O	1:C:373:ARG:HG2	2.15	0.47
1:B:115:THR:HG23	1:B:117:GLY:H	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:THR:HG22	1:C:39:ASN:HD22	1.79	0.46
1:D:128:ALA:O	1:D:132:THR:HG22	2.15	0.46
1:A:339:ASP:OD2	1:A:341:THR:N	2.48	0.46
1:C:328:LEU:O	1:C:332:THR:HG23	2.16	0.46
1:A:360:ALA:HB3	1:A:370:GLU:OE1	2.16	0.46
1:C:273:ILE:HD11	1:C:340:ALA:O	2.15	0.46
1:B:339:ASP:OD1	1:B:340:ALA:N	2.47	0.46
1:C:366:LEU:H	1:C:366:LEU:HD23	1.80	0.46
1:D:138:ILE:HG13	1:D:138:ILE:O	2.16	0.46
1:D:362:PRO:HB3	1:D:513:GLY:CA	2.46	0.46
1:B:498:ASN:HD21	1:B:503:LYS:CA	2.29	0.45
1:A:191:ASP:OD2	1:A:194:THR:OG1	2.35	0.45
1:A:232:LEU:CA	1:A:332:THR:HG22	2.47	0.45
1:A:339:ASP:OD2	1:A:340:ALA:N	2.50	0.45
1:A:368:ARG:NE	1:A:536:ILE:HD12	2.31	0.45
1:D:27:ASP:OD2	1:D:113:HIS:NE2	2.49	0.45
1:A:211:LYS:HG3	1:A:276:TRP:HZ3	1.82	0.45
1:A:194:THR:HG23	1:C:180:PRO:HG2	1.99	0.45
1:C:288:ASN:O	1:C:292:THR:HG22	2.17	0.45
1:D:155:ALA:O	1:D:159:LYS:N	2.48	0.45
1:B:153:ARG:O	1:B:157:ARG:HG3	2.16	0.45
1:B:328:LEU:O	1:B:332:THR:HG23	2.17	0.45
1:B:503:LYS:O	1:B:528:GLY:HA3	2.17	0.44
1:C:232:LEU:HA	1:C:332:THR:HG22	2.00	0.44
1:C:368:ARG:NH1	1:C:369:ALA:HA	2.32	0.44
1:B:74:SER:N	1:B:124:GLN:OE1	2.41	0.44
1:D:361:ASP:HB2	1:D:362:PRO:CD	2.47	0.44
1:A:177:ARG:HG3	1:A:178:PRO:HD2	2.00	0.44
1:B:74:SER:OG	1:B:75:VAL:N	2.51	0.44
1:D:7:HIS:NE2	1:D:38:LYS:HD3	2.33	0.44
1:B:213:VAL:CG2	1:B:277:ALA:CB	2.95	0.44
1:B:498:ASN:ND2	1:B:502:GLY:C	2.71	0.44
1:B:232:LEU:HA	1:B:332:THR:HG22	2.00	0.43
1:C:101:PRO:HB3	1:C:112:LEU:CD1	2.48	0.43
1:A:74:SER:N	1:A:124:GLN:OE1	2.43	0.43
1:C:115:THR:HG23	1:C:117:GLY:H	1.84	0.43
1:A:270:VAL:O	1:A:273:ILE:HG22	2.18	0.43
1:B:415:HIS:CD2	3:B:602:TPP:HM21	2.53	0.43
1:B:27:ASP:N	1:B:27:ASP:OD1	2.52	0.43
1:A:293:VAL:O	1:A:293:VAL:CG1	2.66	0.43
1:B:446:LEU:CD2	3:B:602:TPP:HM23	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:PRO:O	1:A:363:ASN:HB3	2.19	0.43
1:B:12:ARG:NH1	1:B:179:GLY:O	2.49	0.43
1:B:363:ASN:ND2	1:B:363:ASN:O	2.40	0.43
1:C:374:GLN:HG3	1:C:519:ILE:CD1	2.49	0.43
1:D:270:VAL:O	1:D:273:ILE:HG22	2.18	0.43
1:D:86:GLY:HA2	1:D:413:TRP:CG	2.54	0.43
1:C:95:ILE:HD13	1:C:152:ILE:HG12	2.01	0.42
1:C:15:GLN:OE1	1:C:181:VAL:HG13	2.19	0.42
1:B:278:ASP:OD1	1:B:278:ASP:N	2.52	0.42
1:C:66:VAL:HA	1:C:93:PRO:HG2	2.01	0.42
1:B:177:ARG:HG3	1:B:178:PRO:HD2	2.02	0.42
1:B:95:ILE:HD13	1:B:152:ILE:HG12	2.02	0.42
1:D:213:VAL:CG2	1:D:277:ALA:CB	2.97	0.42
1:D:328:LEU:O	1:D:332:THR:HG23	2.19	0.42
1:A:143:ASP:HB3	1:A:147:LEU:HD13	2.02	0.42
1:B:138:ILE:HG13	1:B:138:ILE:O	2.20	0.41
1:A:292:THR:O	1:A:293:VAL:HG12	2.19	0.41
1:B:292:THR:OG1	1:B:295:TRP:HA	2.20	0.41
1:A:95:ILE:HD13	1:A:152:ILE:HG12	2.02	0.41
1:B:73:PHE:O	1:B:74:SER:OG	2.39	0.41
1:C:128:ALA:O	1:C:132:THR:HG22	2.20	0.41
1:C:368:ARG:HH21	1:C:398:ARG:NE	2.18	0.41
1:C:209:ARG:O	1:C:338:LYS:HE3	2.19	0.41
1:C:441:ASP:HB3	1:C:467:ASN:HA	2.03	0.41
1:C:366:LEU:HD11	1:C:535:VAL:O	2.21	0.41
1:C:213:VAL:CG2	1:C:277:ALA:CB	2.98	0.41
1:D:66:VAL:HA	1:D:93:PRO:HG2	2.03	0.41
1:A:147:LEU:N	1:A:147:LEU:HD12	2.35	0.41
1:B:441:ASP:OD2	1:B:470:GLY:N	2.54	0.41
1:B:101:PRO:HB3	1:B:112:LEU:CD1	2.51	0.41
1:C:446:LEU:CD2	3:C:602:TPP:HM23	2.50	0.40
1:C:503:LYS:O	1:C:528:GLY:HA3	2.21	0.40
1:A:59:GLY:O	1:A:62:ARG:N	2.47	0.40
1:A:112:LEU:O	1:A:115:THR:HG23	2.21	0.40
1:A:498:ASN:OD1	1:A:503:LYS:N	2.55	0.40
1:B:211:LYS:HD2	1:B:340:ALA:CB	2.52	0.40
1:C:31:VAL:HG11	1:C:168:CYS:O	2.20	0.40
1:A:378:LEU:O	1:A:434:ARG:NH1	2.54	0.40
1:C:278:ASP:N	1:C:278:ASP:OD1	2.53	0.40
1:A:143:ASP:HB3	1:A:147:LEU:CD1	2.52	0.40
1:A:322:ILE:HD13	1:A:322:ILE:N	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:ARG:NH1	1:C:179:GLY:O	2.54	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:469:ARG:HE	1:C:500:GLU:OE2[6_554]	1.50	0.10
1:C:456:ARG:HH22	1:C:484:ASN:O[6_554]	1.52	0.08
1:A:27:ASP:OD2	1:A:290:TYR:HH[6_554]	1.53	0.07
1:C:456:ARG:NH2	1:C:484:ASN:O[6_554]	2.14	0.06
1:A:27:ASP:OD2	1:A:290:TYR:OH[6_554]	2.17	0.03

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	543/563 (96%)	507 (93%)	36 (7%)	0	100	100
1	B	541/563 (96%)	502 (93%)	37 (7%)	2 (0%)	34	72
1	C	543/563 (96%)	501 (92%)	38 (7%)	4 (1%)	22	61
1	D	539/563 (96%)	498 (92%)	39 (7%)	2 (0%)	34	72
All	All	2166/2252 (96%)	2008 (93%)	150 (7%)	8 (0%)	34	72

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	361	ASP
1	C	186	ASN
1	D	362	PRO
1	B	186	ASN
1	C	360	ALA

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Mol	Chain	Res	Type
1	B	101	PRO
1	C	365	PRO
1	C	101	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	427/439 (97%)	406 (95%)	21 (5%)	25	59
1	B	426/439 (97%)	404 (95%)	22 (5%)	23	56
1	C	426/439 (97%)	400 (94%)	26 (6%)	18	51
1	D	424/439 (97%)	404 (95%)	20 (5%)	26	60
All	All	1703/1756 (97%)	1614 (95%)	89 (5%)	23	56

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	58	GLU
1	A	66	VAL
1	A	115	THR
1	A	125	LEU
1	A	191	ASP
1	A	194	THR
1	A	204	ASP
1	A	253	ASP
1	A	260	THR
1	A	291	SER
1	A	293	VAL
1	A	306	LEU
1	A	308	ASP
1	A	311	HIS
1	A	318	GLU
1	A	322	ILE
1	A	341	THR

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Mol	Chain	Res	Type
1	A	342	LEU
1	A	482	TYR
1	A	501	ASP
1	B	4	THR
1	B	9	LEU
1	B	58	GLU
1	B	66	VAL
1	B	75	VAL
1	B	115	THR
1	B	121	TYR
1	B	125	LEU
1	B	191	ASP
1	B	194	THR
1	B	204	ASP
1	B	253	ASP
1	B	260	THR
1	B	292	THR
1	B	306	LEU
1	B	308	ASP
1	B	311	HIS
1	B	318	GLU
1	B	363	ASN
1	B	482	TYR
1	B	498	ASN
1	B	500	GLU
1	C	30	LEU
1	C	58	GLU
1	C	66	VAL
1	C	115	THR
1	C	125	LEU
1	C	181	VAL
1	C	185	LEU
1	C	187	GLU
1	C	191	ASP
1	C	204	ASP
1	C	253	ASP
1	C	260	THR
1	C	291	SER
1	C	306	LEU
1	C	308	ASP
1	C	311	HIS
1	C	314	VAL

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Mol	Chain	Res	Type
1	C	318	GLU
1	C	322	ILE
1	C	339	ASP
1	C	341	THR
1	C	368	ARG
1	C	392	SER
1	C	482	TYR
1	C	542	THR
1	C	544	GLU
1	D	58	GLU
1	D	66	VAL
1	D	72	THR
1	D	75	VAL
1	D	115	THR
1	D	121	TYR
1	D	125	LEU
1	D	181	VAL
1	D	191	ASP
1	D	204	ASP
1	D	253	ASP
1	D	260	THR
1	D	306	LEU
1	D	308	ASP
1	D	314	VAL
1	D	318	GLU
1	D	322	ILE
1	D	458	LYS
1	D	482	TYR
1	D	532	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	311	HIS
1	B	173	GLN
1	B	498	ASN
1	D	323	HIS

### 5.3.3 RNA ⓘ

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	TPP	C	602	2	22,27,27	1.47	4 (18%)	29,40,40	1.91	10 (34%)
3	TPP	D	602	2	22,27,27	1.56	5 (22%)	29,40,40	1.87	9 (31%)
4	PEG	C	603	-	6,6,6	0.51	0	5,5,5	0.28	0
3	TPP	A	602	2	22,27,27	1.69	5 (22%)	29,40,40	1.93	9 (31%)
3	TPP	B	602	2	22,27,27	1.62	6 (27%)	29,40,40	1.79	8 (27%)

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	TPP	C	602	2	-	1/16/17/17	0/2/2/2
3	TPP	D	602	2	-	2/16/17/17	0/2/2/2
4	PEG	C	603	-	-	0/4/4/4	-
3	TPP	A	602	2	-	1/16/17/17	0/2/2/2
3	TPP	B	602	2	-	1/16/17/17	0/2/2/2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	TPP	C4-N3	-4.92	1.35	1.39
3	B	602	TPP	C4-N3	-4.66	1.35	1.39
3	C	602	TPP	C4-N3	-4.17	1.36	1.39
3	D	602	TPP	C4-N3	-3.11	1.37	1.39
3	D	602	TPP	C6-C5	3.00	1.52	1.50
3	A	602	TPP	C5'-C4'	-2.57	1.38	1.42
3	D	602	TPP	C2'-N1'	2.57	1.38	1.34
3	B	602	TPP	C2'-N3'	2.41	1.38	1.34
3	A	602	TPP	C7'-N3	-2.40	1.44	1.48
3	D	602	TPP	C2'-N3'	2.32	1.38	1.34
3	B	602	TPP	C4'-N3'	2.32	1.38	1.35
3	D	602	TPP	C4'-N3'	2.29	1.38	1.35
3	A	602	TPP	C6-C5	-2.29	1.49	1.50
3	B	602	TPP	C2'-N1'	2.25	1.38	1.34
3	A	602	TPP	C2'-N1'	2.21	1.37	1.34
3	C	602	TPP	C2'-N3'	2.17	1.37	1.34
3	C	602	TPP	C2'-N1'	2.15	1.37	1.34
3	B	602	TPP	C7'-N3	-2.14	1.44	1.48
3	C	602	TPP	C7'-N3	-2.08	1.44	1.48
3	B	602	TPP	C5'-C4'	-2.03	1.39	1.42

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	602	TPP	C6-C5-C4	4.80	131.29	127.43
3	C	602	TPP	C5'-C7'-N3	-4.15	106.37	113.28
3	B	602	TPP	CM4-C4-N3	4.07	127.72	122.53
3	C	602	TPP	CM4-C4-N3	3.96	127.58	122.53
3	A	602	TPP	PA-O3A-PB	-3.78	119.85	132.83
3	C	602	TPP	C6-C5-C4	3.70	130.40	127.43
3	A	602	TPP	CM4-C4-N3	3.59	127.11	122.53
3	A	602	TPP	N1'-C2'-N3'	-3.47	119.57	125.54
3	D	602	TPP	N1'-C2'-N3'	-3.35	119.77	125.54
3	B	602	TPP	N1'-C2'-N3'	-3.33	119.81	125.54
3	D	602	TPP	CM2-C2'-N1'	3.33	120.80	117.14
3	A	602	TPP	C6-C5-C4	3.25	130.04	127.43
3	B	602	TPP	PA-O3A-PB	-3.21	121.81	132.83
3	D	602	TPP	CM4-C4-N3	3.10	126.49	122.53
3	A	602	TPP	C6'-C5'-C4'	3.00	119.81	115.72
3	C	602	TPP	N1'-C2'-N3'	-2.98	120.41	125.54
3	C	602	TPP	PA-O3A-PB	-2.97	122.63	132.83
3	A	602	TPP	CM2-C2'-N1'	2.80	120.22	117.14
3	A	602	TPP	C5'-C7'-N3	-2.77	108.67	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	602	TPP	PA-O3A-PB	-2.72	123.49	132.83
3	B	602	TPP	CM2-C2'-N1'	2.70	120.11	117.14
3	C	602	TPP	CM2-C2'-N1'	2.67	120.08	117.14
3	C	602	TPP	C6'-C5'-C4'	2.62	119.29	115.72
3	B	602	TPP	C5'-C7'-N3	-2.54	109.04	113.28
3	A	602	TPP	C6'-N1'-C2'	2.53	120.26	115.96
3	D	602	TPP	C6'-N1'-C2'	2.48	120.17	115.96
3	D	602	TPP	C6'-C5'-C4'	2.40	118.99	115.72
3	A	602	TPP	C5'-C6'-N1'	-2.35	119.90	123.82
3	B	602	TPP	C6'-C5'-C4'	2.35	118.92	115.72
3	B	602	TPP	CM4-C4-C5	-2.26	122.67	127.60
3	B	602	TPP	C6'-N1'-C2'	2.25	119.78	115.96
3	C	602	TPP	C6'-N1'-C2'	2.19	119.70	115.96
3	C	602	TPP	C5'-C6'-N1'	-2.12	120.28	123.82
3	D	602	TPP	C5'-C6'-N1'	-2.10	120.32	123.82
3	C	602	TPP	CM4-C4-C5	-2.02	123.17	127.60
3	D	602	TPP	C5'-C7'-N3	-2.02	109.91	113.28

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	TPP	C4-C5-C6-C7
3	C	602	TPP	C4-C5-C6-C7
3	B	602	TPP	C4-C5-C6-C7
3	D	602	TPP	PB-O3A-PA-O2A
3	D	602	TPP	C4-C5-C6-C7

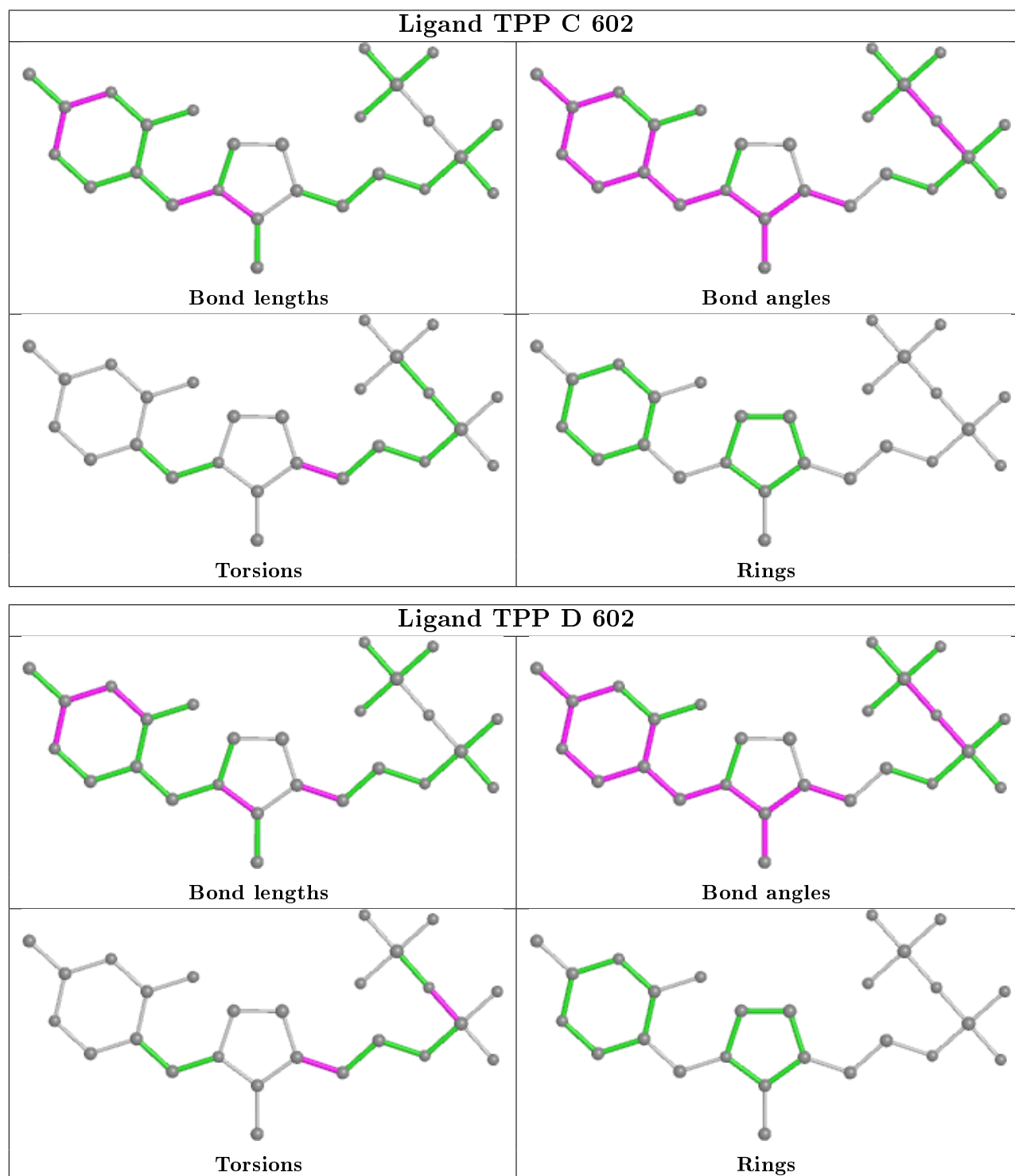
There are no ring outliers.

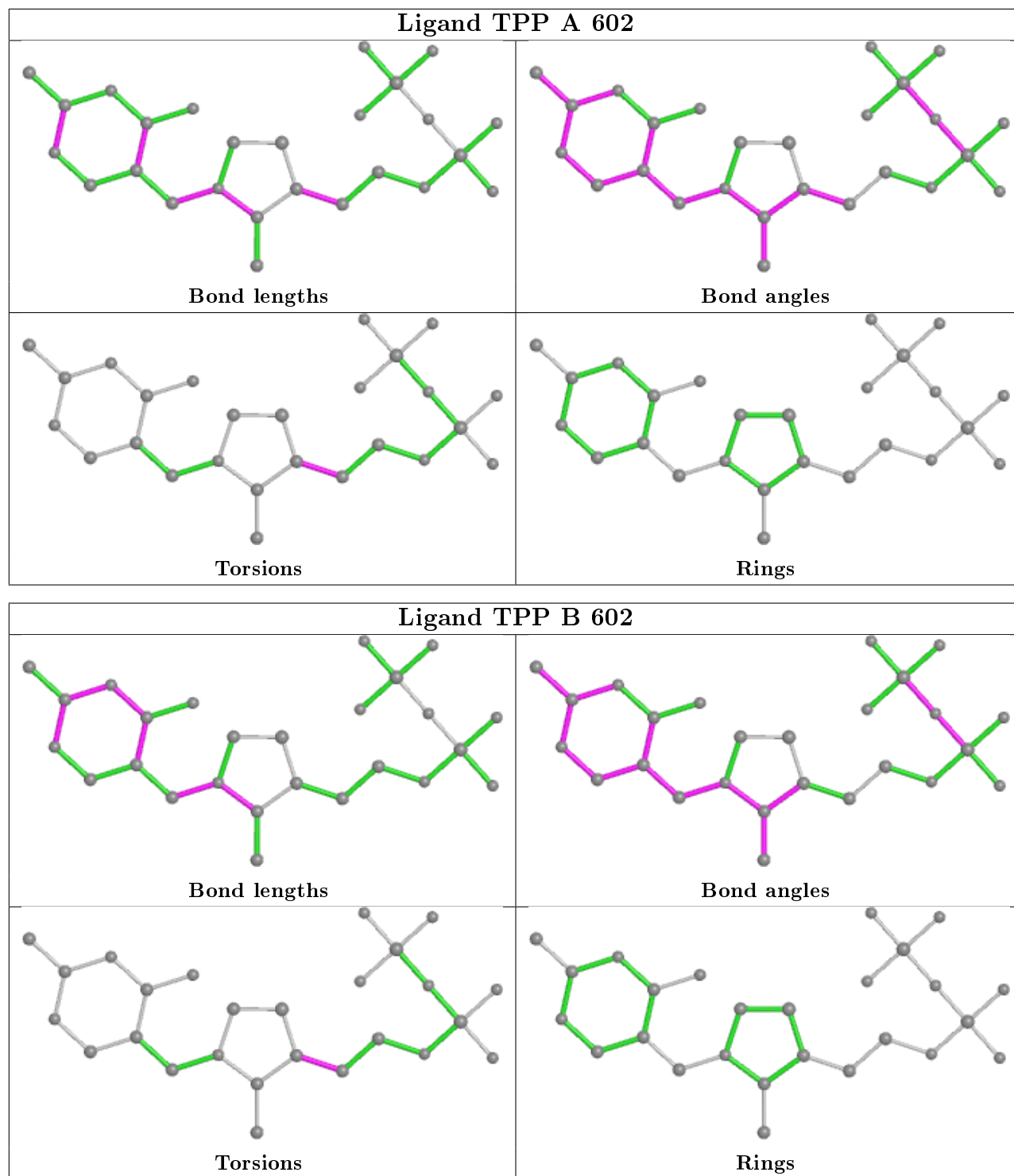
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	602	TPP	1	0
3	D	602	TPP	1	0
3	B	602	TPP	2	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 ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	547/563 (97%)	-0.23	1 (0%) 95 93	24, 49, 99, 141	0
1	B	545/563 (96%)	0.16	5 (0%) 84 79	37, 88, 144, 172	0
1	C	547/563 (97%)	0.29	16 (2%) 51 45	43, 99, 166, 190	0
1	D	543/563 (96%)	0.27	14 (2%) 56 49	51, 96, 149, 179	0
All	All	2182/2252 (96%)	0.12	36 (1%) 72 66	24, 83, 149, 190	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	387	ALA	5.1
1	C	251	PRO	4.6
1	D	507	LEU	4.1
1	C	505	LEU	3.9
1	C	530	THR	3.7
1	D	490	TYR	3.6
1	C	48	CYS	3.2
1	D	536	ILE	3.1
1	C	385	LEU	2.9
1	C	358	PRO	2.8
1	B	387	ALA	2.8
1	B	334	ARG	2.7
1	C	450	GLU	2.6
1	C	438	MET	2.6
1	D	48	CYS	2.5
1	B	256	GLY	2.5
1	C	408	GLU	2.5
1	D	254	HIS	2.5
1	C	246	ALA	2.4
1	C	249	PHE	2.4
1	D	213	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	563	ILE	2.3
1	D	506	GLY	2.3
1	B	282	CYS	2.2
1	B	401	LEU	2.2
1	C	532	ILE	2.2
1	C	282	CYS	2.2
1	D	256	GLY	2.2
1	C	464	PHE	2.2
1	D	488	TRP	2.1
1	C	437	LEU	2.1
1	D	531	LEU	2.1
1	D	281	ILE	2.1
1	D	325	LYS	2.1
1	D	234	ASP	2.0
1	D	448	ALA	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 carbohydrates 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, 95<sup>th</sup> 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.

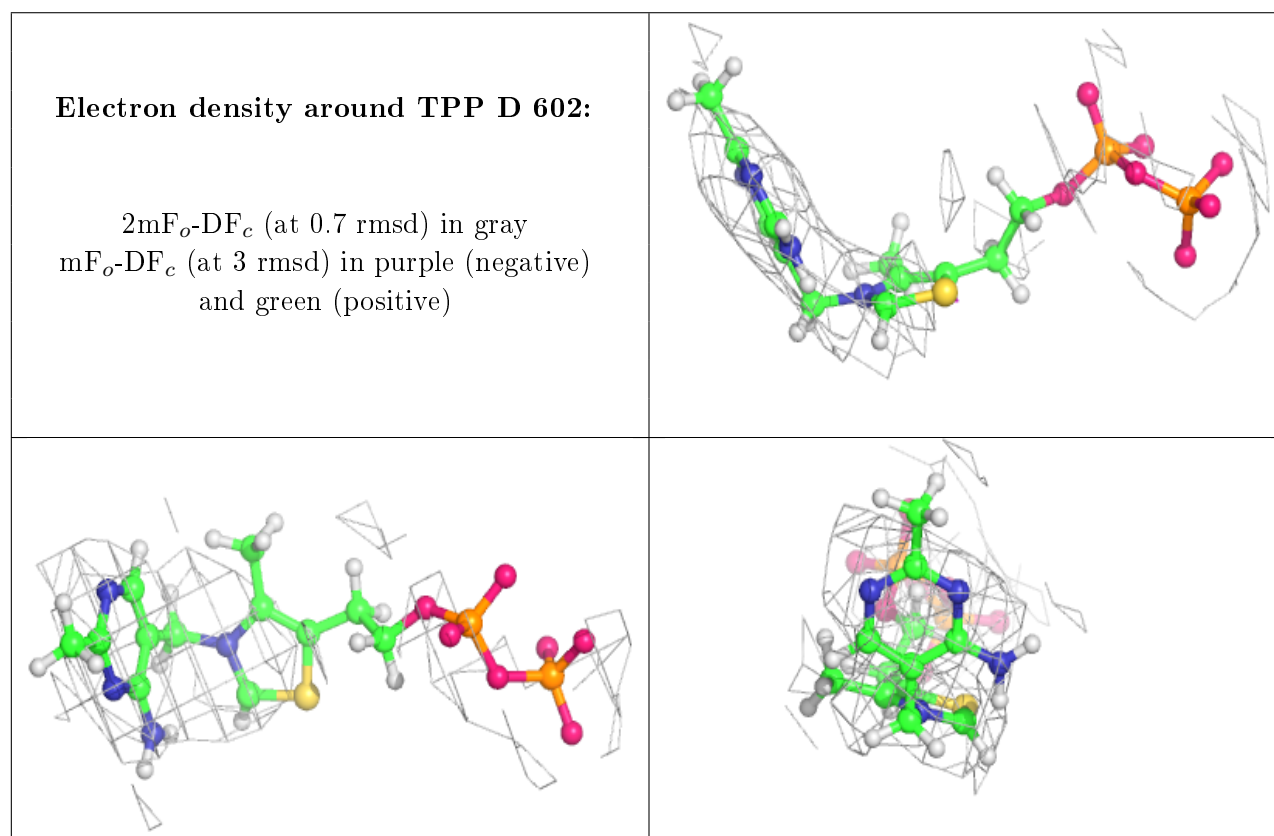
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	A	601	1/1	0.82	0.14	25,25,25,25	0
4	PEG	C	603	7/7	0.83	0.25	58,70,71,73	0
3	TPP	D	602	26/26	0.91	0.31	67,84,146,147	0
3	TPP	C	602	26/26	0.91	0.26	74,101,166,170	0
2	MG	C	601	1/1	0.94	0.10	162,162,162,162	0
3	TPP	B	602	26/26	0.94	0.31	60,75,147,155	0
3	TPP	A	602	26/26	0.95	0.23	27,83,122,142	0
2	MG	B	601	1/1	0.95	0.13	61,61,61,61	0

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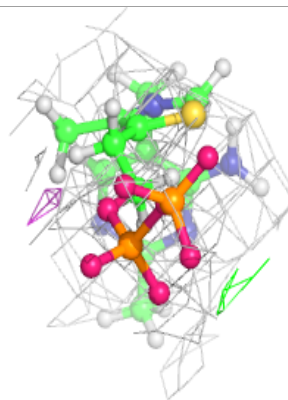
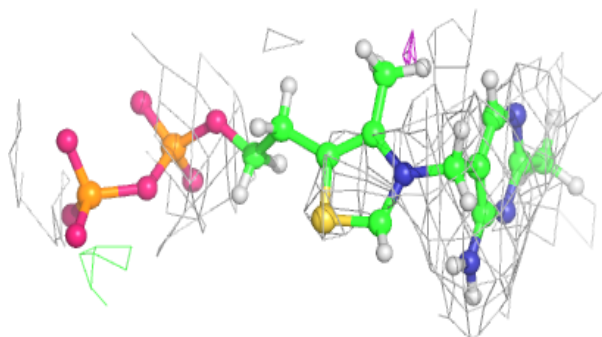
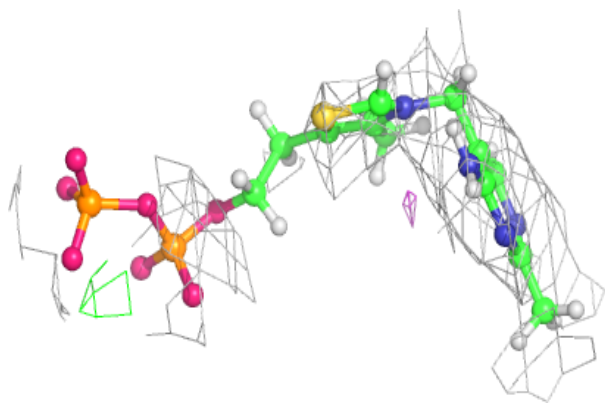
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	D	601	1/1	0.95	0.13	75,75,75,75	0

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.

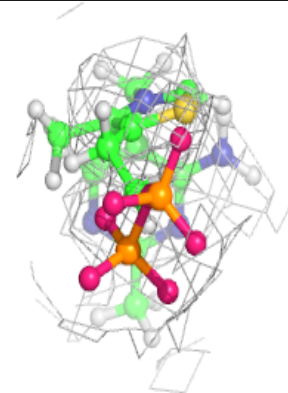
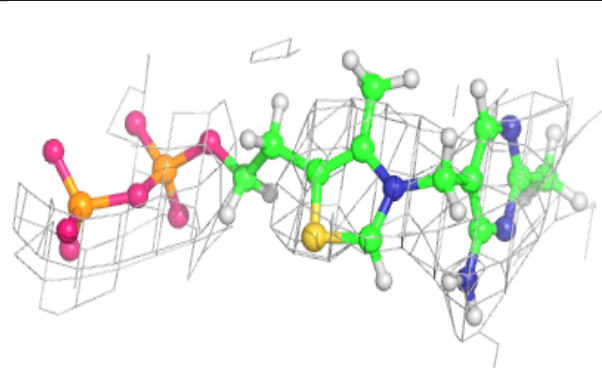
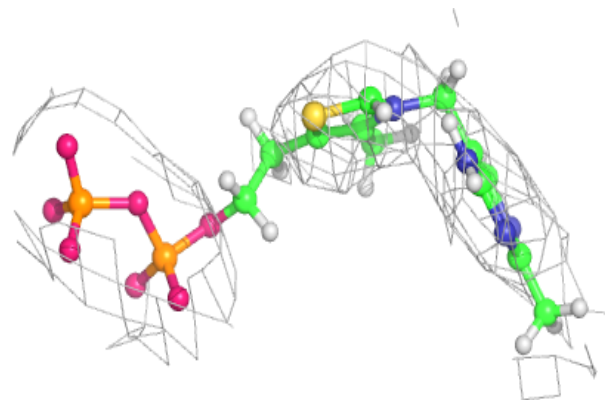


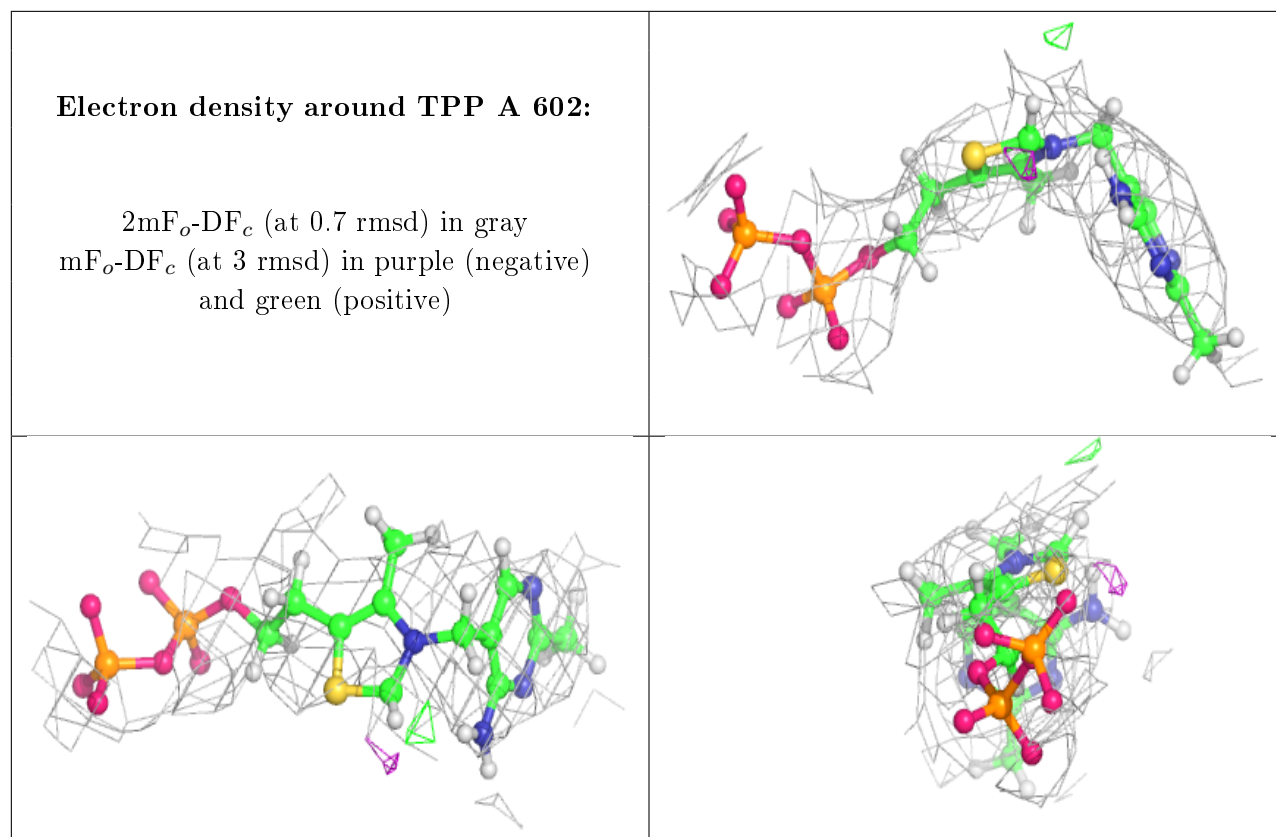
**Electron density around TPP C 602:**

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

**Electron density around TPP B 602:**

$2mF_o-DF_c$  (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.