



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 10:00 am BST

PDB ID : 2VJY
Title : Pyruvate decarboxylase from Kluyveromyces lactis in complex with the substrate analogue methyl acetylphosphonate
Authors : Kutter, S.; Wille, G.; Weiss, M.S.; Konig, S.
Deposited on : 2007-12-14
Resolution : 2.30 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 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

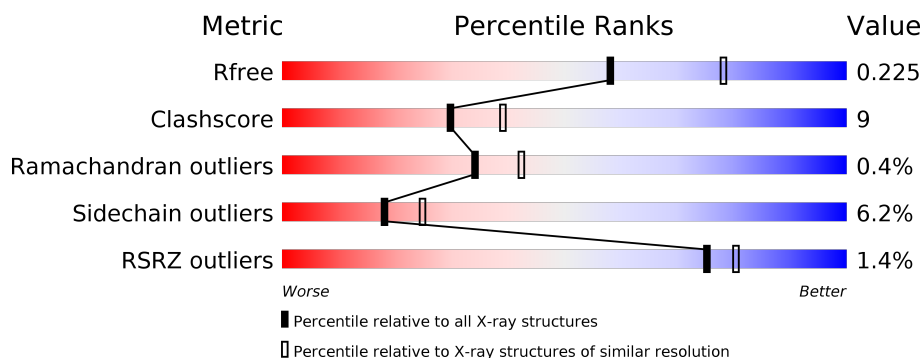
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 ≥ 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>%</div> <div> <div></div> <div>82%</div> <div>16%</div> <div>..</div> </div> </div>
1	B	563	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>13%</div> <div>.</div> </div> </div>
1	C	563	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>15%</div> <div>..</div> </div> </div>
1	D	563	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div>.</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	TPP	A	600	-	-	X	-
2	TPP	B	600	-	-	X	-
2	TPP	C	600	-	-	X	-
4	ALK	A	602	-	-	X	-
4	ALK	B	602	-	-	X	-
4	ALK	C	602	-	-	X	-
4	ALK	D	602	-	-	X	-

2 Entry composition [i](#)

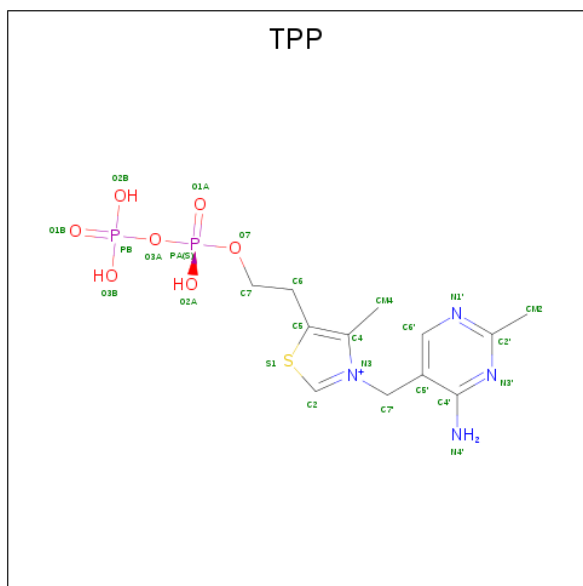
There are 6 unique types of molecules in this entry. The entry contains 18588 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PYRUVATE DECARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	562	Total	C	N	O	S	0	0	0
			4336	2760	725	837	14			
1	B	562	Total	C	N	O	S	0	0	0
			4336	2760	725	837	14			
1	C	562	Total	C	N	O	S	0	0	0
			4336	2760	725	837	14			
1	D	562	Total	C	N	O	S	0	0	0
			4336	2760	725	837	14			

- Molecule 2 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: C₁₂H₁₉N₄O₇P₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
2	B	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

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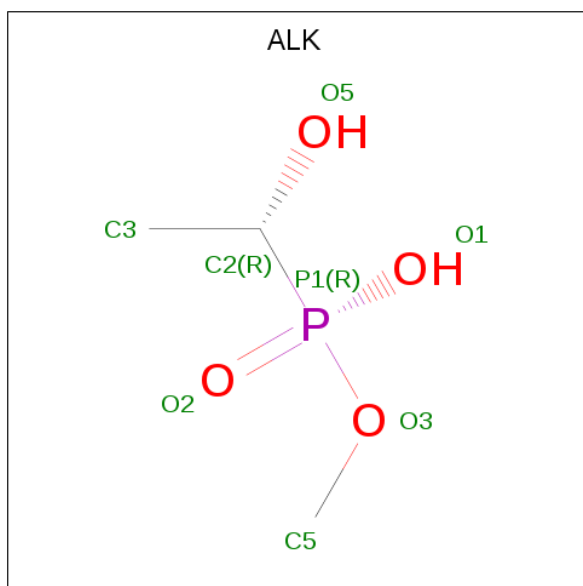
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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
2	D	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

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

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

- Molecule 4 is methoxy-[(1 {R})-1-oxidanylethyl]phosphinic acid (three-letter code: ALK) (formula: C₃H₉O₄P).



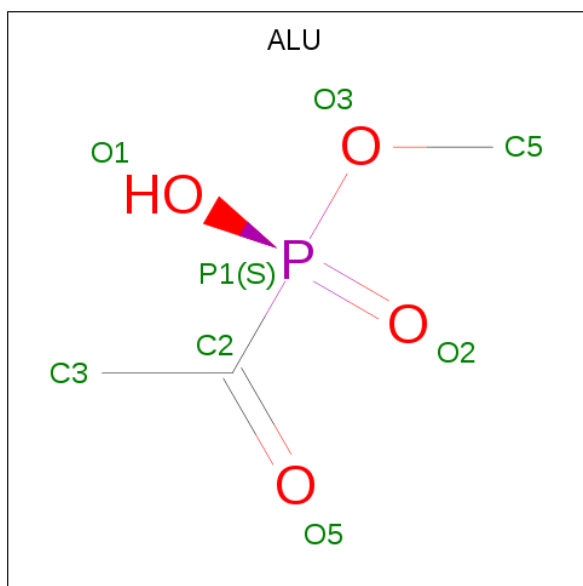
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			8	3	4	1		
4	A	1	Total	C	O	P	0	0
			8	3	4	1		
4	B	1	Total	C	O	P	0	0
			8	3	4	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	O	P	0	0
			8	3	4	1		
4	C	1	Total	C	O	P	0	0
			8	3	4	1		
4	C	1	Total	C	O	P	0	0
			8	3	4	1		
4	D	1	Total	C	O	P	0	0
			8	3	4	1		
4	D	1	Total	C	O	P	0	0
			8	3	4	1		

- Molecule 5 is METHYL HYDROGEN (S)-ACETYLPHOSPHONATE (three-letter code: ALU) (formula: C₃H₇O₄P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	P	0	0
			8	3	4	1		
5	B	1	Total	C	O	P	0	0
			8	3	4	1		
5	C	1	Total	C	O	P	0	0
			8	3	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	300	Total	O	0	0
			300	300		

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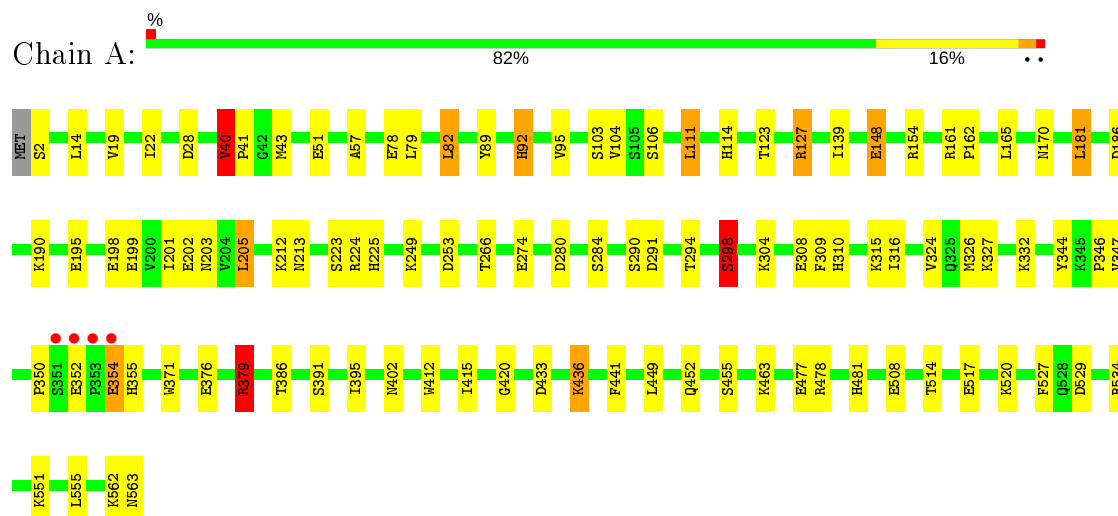
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	300	Total 300	O 300	0	0
6	C	220	Total 220	O 220	0	0
6	D	228	Total 228	O 228	0	0

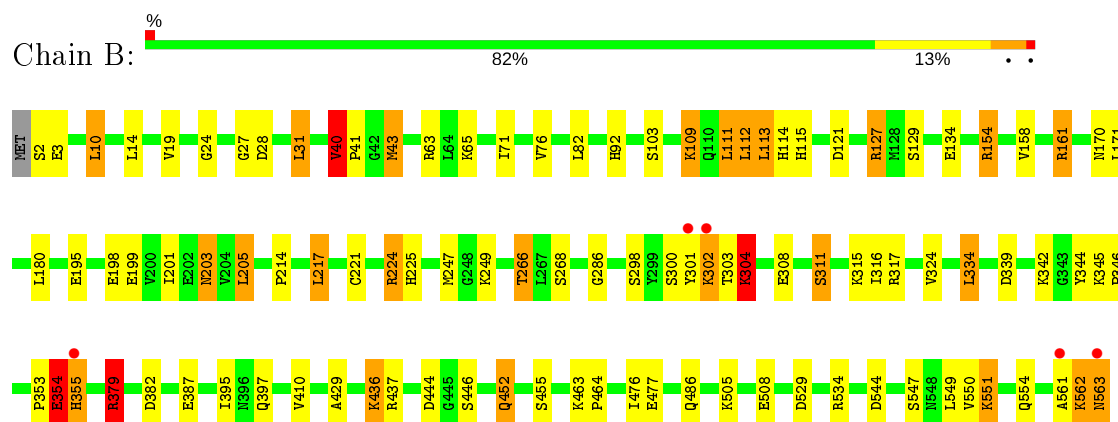
3 Residue-property plots

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.

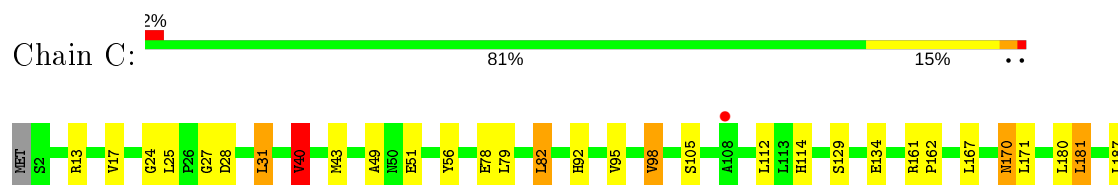
• Molecule 1: PYRUVATE DECARBOXYLASE



• Molecule 1: PYRUVATE DECARBOXYLASE



• Molecule 1: PYRUVATE DECARBOXYLASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.76Å 135.77Å 107.26Å 90.00° 103.88° 90.00°	Depositor
Resolution (Å)	20.19 – 2.30 20.19 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.19-2.30) 99.8 (20.19-2.30)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.154 , 0.225 0.153 , 0.225	Depositor DCC
R_{free} test set	1006 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å ²)	24.5	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18588	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ALU, ALK, 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	1.09	4/4428 (0.1%)	0.92	7/6028 (0.1%)
1	B	1.16	5/4428 (0.1%)	0.99	16/6028 (0.3%)
1	C	1.03	4/4428 (0.1%)	0.91	4/6028 (0.1%)
1	D	1.01	5/4428 (0.1%)	0.89	6/6028 (0.1%)
All	All	1.07	18/17712 (0.1%)	0.93	33/24112 (0.1%)

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	A	0	1
1	B	0	3
1	C	1	3
All	All	1	7

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	199	GLU	CD-OE1	7.69	1.34	1.25
1	D	198	GLU	CB-CG	-7.10	1.38	1.52
1	D	199	GLU	CD-OE2	6.94	1.33	1.25
1	C	202	GLU	CG-CD	6.30	1.61	1.51
1	B	40	VAL	CB-CG1	-6.12	1.40	1.52
1	C	98	VAL	CB-CG2	-5.92	1.40	1.52
1	A	195	GLU	CG-CD	5.66	1.60	1.51
1	A	441	PHE	CE2-CZ	5.62	1.48	1.37
1	B	198	GLU	CG-CD	5.49	1.60	1.51
1	B	354	GLU	CG-CD	5.34	1.59	1.51
1	D	315	LYS	CD-CE	5.34	1.64	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	357	GLU	CG-CD	5.32	1.59	1.51
1	A	127	ARG	CG-CD	5.28	1.65	1.51
1	C	199	GLU	CD-OE1	5.22	1.31	1.25
1	C	468	VAL	CB-CG2	-5.22	1.41	1.52
1	A	40	VAL	CB-CG1	-5.17	1.42	1.52
1	B	486	GLN	CG-CD	5.13	1.62	1.51
1	B	127	ARG	CG-CD	5.01	1.64	1.51

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	161	ARG	NE-CZ-NH2	-8.45	116.07	120.30
1	B	544	ASP	CB-CG-OD1	8.15	125.64	118.30
1	D	291	ASP	CB-CG-OD1	7.07	124.66	118.30
1	B	10	LEU	CB-CG-CD2	6.94	122.80	111.00
1	A	379	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	B	161	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	D	379	ARG	NE-CZ-NH2	-6.53	117.03	120.30
1	C	379	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	C	459	ARG	NE-CZ-NH1	-6.20	117.20	120.30
1	D	379	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	A	379	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	D	154	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	A	291	ASP	CB-CG-OD1	5.96	123.67	118.30
1	B	154	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	B	444	ASP	CB-CG-OD1	5.93	123.64	118.30
1	B	355	HIS	N-CA-C	-5.92	95.02	111.00
1	C	379	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	B	334	LEU	CA-CB-CG	5.75	128.52	115.30
1	A	478	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	B	379	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	D	199	GLU	OE1-CD-OE2	5.63	130.06	123.30
1	D	291	ASP	CB-CG-OD2	-5.62	113.24	118.30
1	B	379	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	A	181	LEU	CB-CG-CD1	5.60	120.52	111.00
1	A	529	ASP	CB-CG-OD1	5.56	123.31	118.30
1	C	40	VAL	CB-CA-C	5.56	121.96	111.40
1	B	217	LEU	CB-CG-CD2	5.39	120.16	111.00
1	A	298	SER	CB-CA-C	-5.36	99.92	110.10
1	B	334	LEU	CB-CG-CD1	5.33	120.05	111.00
1	B	301	TYR	N-CA-C	5.16	124.93	111.00
1	B	529	ASP	CB-CG-OD1	5.15	122.93	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	63	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	B	224	ARG	NE-CZ-NH2	-5.04	117.78	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	324	VAL	CA

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	350	PRO	Peptide
1	B	304	LYS	Peptide
1	B	561	ALA	Peptide
1	B	562	LYS	Peptide
1	C	353	PRO	Peptide
1	C	354	GLU	Peptide
1	C	561	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	4336	0	4310	73	0
1	B	4336	0	4310	83	0
1	C	4336	0	4310	72	0
1	D	4336	0	4310	63	0
2	A	26	0	16	9	0
2	B	26	0	16	10	0
2	C	26	0	16	10	0
2	D	26	0	16	7	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	16	0	15	23	0
4	B	16	0	16	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	16	0	15	20	0
4	D	16	0	15	19	0
5	A	8	0	7	0	0
5	B	8	0	7	0	0
5	C	8	0	7	1	0
6	A	300	0	0	6	0
6	B	300	0	0	5	0
6	C	220	0	0	1	0
6	D	228	0	0	3	0
All	All	18588	0	17386	327	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 9.

All (327) 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:B:600:TPP:C2	4:B:602:ALK:H2	1.27	1.59
2:D:600:TPP:C2	4:D:602:ALK:H2	1.24	1.56
2:B:600:TPP:H2	4:B:602:ALK:C2	1.37	1.53
2:A:600:TPP:C2	4:A:602:ALK:H2	1.38	1.51
2:D:600:TPP:H2	4:D:602:ALK:C2	1.40	1.50
2:C:600:TPP:H2	4:C:602:ALK:C2	1.42	1.47
2:C:600:TPP:C2	4:C:602:ALK:H2	1.39	1.47
2:A:600:TPP:H2	4:A:602:ALK:C2	1.52	1.36
4:A:602:ALK:H3C2	4:A:602:ALK:C5	1.69	1.21
4:B:602:ALK:H5C3	4:B:602:ALK:H3C2	1.23	1.20
4:B:602:ALK:C5	4:B:602:ALK:H3C2	1.75	1.16
4:D:602:ALK:C3	4:D:602:ALK:H5C3	1.68	1.16
1:B:562:LYS:HG2	1:B:563:ASN:H	1.10	1.15
4:C:602:ALK:C5	4:C:602:ALK:H3C2	1.76	1.15
1:B:562:LYS:CG	1:B:563:ASN:H	1.62	1.11
4:D:602:ALK:C5	4:D:602:ALK:H3C2	1.79	1.10
4:A:602:ALK:H5C3	4:A:602:ALK:C3	1.69	1.10
1:A:92:HIS:CD2	1:A:225:HIS:HE1	1.70	1.10
1:A:92:HIS:HD2	1:A:225:HIS:CE1	1.69	1.09
2:B:600:TPP:H2	4:B:602:ALK:C3	1.83	1.08
1:C:114:HIS:CD2	4:D:602:ALK:H5C1	1.89	1.07
4:C:602:ALK:H5C3	4:C:602:ALK:H3C2	1.04	1.02
1:B:225:HIS:HD2	6:B:2090:HOH:O	1.43	1.01
4:C:602:ALK:H5C3	4:C:602:ALK:C3	1.89	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:HIS:HD2	1:B:225:HIS:HE1	1.01	0.99
2:C:600:TPP:H2	4:C:602:ALK:C3	1.93	0.98
1:D:317:ARG:HG2	1:D:317:ARG:HH11	1.29	0.97
1:B:92:HIS:CD2	1:B:225:HIS:HE1	1.83	0.97
1:A:103:SER:HB2	1:B:562:LYS:HD3	1.45	0.96
2:A:600:TPP:H2	4:A:602:ALK:C3	1.97	0.94
1:A:201:ILE:HG22	1:A:205:LEU:HD22	1.50	0.93
2:A:600:TPP:C2	4:A:602:ALK:C2	2.26	0.93
1:D:92:HIS:HD2	1:D:225:HIS:HE1	1.05	0.93
2:A:600:TPP:H2	4:A:602:ALK:H2	0.94	0.91
1:A:379:ARG:HD2	6:A:2205:HOH:O	1.69	0.91
1:B:562:LYS:CG	1:B:563:ASN:N	2.30	0.90
2:D:600:TPP:C2	4:D:602:ALK:C2	2.20	0.89
1:D:92:HIS:CD2	1:D:225:HIS:HE1	1.90	0.88
2:D:600:TPP:H2	4:D:602:ALK:C3	2.03	0.88
4:D:602:ALK:H5C3	4:D:602:ALK:H3C2	0.90	0.88
1:D:92:HIS:HD2	1:D:225:HIS:CE1	1.94	0.86
1:A:477:GLU:OE1	4:A:602:ALK:O1	1.93	0.86
1:C:92:HIS:CD2	1:C:225:HIS:HE1	1.93	0.86
2:B:600:TPP:C2	4:B:602:ALK:C2	2.19	0.85
4:A:602:ALK:O2	1:B:28:ASP:N	2.09	0.85
1:B:562:LYS:HG2	1:B:563:ASN:N	1.89	0.85
1:B:477:GLU:OE1	4:B:602:ALK:O1	1.93	0.85
1:C:92:HIS:HD2	1:C:225:HIS:HE1	1.24	0.84
1:B:3:GLU:OE1	6:B:2003:HOH:O	1.95	0.83
1:D:304:LYS:HE3	1:D:317:ARG:NH1	1.93	0.83
4:A:602:ALK:H5C1	1:B:114:HIS:NE2	1.93	0.83
1:C:558:ALA:HA	1:C:561:ALA:HB2	1.61	0.82
1:C:40:VAL:HG22	1:C:43:MET:HG3	1.59	0.82
1:C:477:GLU:OE1	4:C:602:ALK:O2	1.98	0.82
1:B:109:LYS:HG3	1:B:111:LEU:HD13	1.59	0.82
1:B:92:HIS:HD2	1:B:225:HIS:CE1	1.92	0.82
1:A:198:GLU:O	1:A:202:GLU:HG3	1.81	0.81
1:C:304:LYS:HE3	1:C:304:LYS:O	1.81	0.80
1:C:114:HIS:CD2	4:D:602:ALK:C5	2.63	0.80
1:D:477:GLU:OE1	4:D:602:ALK:O2	1.99	0.80
1:B:476:ILE:HG13	1:B:549:LEU:HD11	1.64	0.79
2:C:600:TPP:H2	4:C:602:ALK:H2	0.80	0.78
1:C:114:HIS:NE2	4:D:602:ALK:H5C1	1.98	0.78
4:A:602:ALK:C5	1:B:114:HIS:NE2	2.49	0.76
1:C:92:HIS:HD2	1:C:225:HIS:CE1	2.04	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:602:ALK:H5C2	4:D:602:ALK:O5	1.85	0.76
1:B:109:LYS:CG	1:B:111:LEU:HD13	2.15	0.76
2:C:600:TPP:N3	4:C:602:ALK:H2	2.00	0.75
1:A:114:HIS:CD2	4:B:602:ALK:H5C1	2.22	0.74
2:C:600:TPP:C2	4:C:602:ALK:C2	2.23	0.74
4:D:602:ALK:C5	4:D:602:ALK:O5	2.35	0.74
1:C:549:LEU:O	1:C:549:LEU:HD23	1.88	0.73
4:B:602:ALK:H5C2	4:B:602:ALK:H3C2	1.67	0.72
1:A:79:LEU:HA	1:A:82:LEU:HD22	1.71	0.72
4:B:602:ALK:H5C2	4:B:602:ALK:O5	1.89	0.72
1:D:304:LYS:HE3	1:D:317:ARG:HH11	1.53	0.71
1:A:201:ILE:HG22	1:A:205:LEU:CD2	2.19	0.70
1:C:563:ASN:O	1:C:563:ASN:CG	2.30	0.70
1:B:127:ARG:HB3	6:B:2068:HOH:O	1.91	0.70
1:B:40:VAL:HG22	1:B:43:MET:HG3	1.73	0.70
1:A:294:THR:O	1:A:298:SER:HB2	1.91	0.70
4:A:602:ALK:H3C2	4:A:602:ALK:H5C3	0.81	0.69
1:A:170:ASN:HB3	1:B:562:LYS:HB3	1.74	0.69
1:A:114:HIS:NE2	4:B:602:ALK:H5C1	2.08	0.69
2:B:600:TPP:N3	4:B:602:ALK:H2	2.03	0.69
1:C:549:LEU:CD2	1:C:549:LEU:O	2.40	0.69
1:D:317:ARG:HG2	1:D:317:ARG:NH1	1.97	0.69
4:C:602:ALK:H5C2	1:D:114:HIS:NE2	2.08	0.68
1:C:557:ALA:O	1:C:561:ALA:HB2	1.93	0.68
4:B:602:ALK:C3	4:B:602:ALK:H5C3	2.14	0.68
1:C:241:PRO:HB3	1:C:349:VAL:HG12	1.74	0.68
1:B:508:GLU:HB2	1:B:534:ARG:HG2	1.75	0.67
1:D:27:GLY:O	1:D:31:LEU:HD13	1.93	0.67
1:B:344:TYR:CE1	1:B:346:PRO:HA	2.29	0.67
1:C:31:LEU:HD23	1:D:481:HIS:HB3	1.76	0.67
1:A:92:HIS:CD2	1:A:225:HIS:CE1	2.58	0.67
1:B:27:GLY:O	1:B:31:LEU:HD13	1.95	0.66
4:A:602:ALK:C5	1:B:114:HIS:CD2	2.77	0.66
4:B:602:ALK:C5	4:B:602:ALK:C3	2.54	0.66
1:A:201:ILE:CG2	1:A:205:LEU:HD22	2.25	0.65
1:C:563:ASN:O	1:C:563:ASN:ND2	2.30	0.65
1:A:355:HIS:HD2	1:A:376:GLU:OE1	1.78	0.65
1:D:22:ILE:HD11	1:D:43:MET:HE2	1.78	0.65
2:A:600:TPP:N3	4:A:602:ALK:H2	2.07	0.64
2:D:600:TPP:H2	4:D:602:ALK:H2	0.65	0.63
4:A:602:ALK:H5C1	1:B:114:HIS:CD2	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:VAL:O	1:A:162:PRO:HA	1.99	0.63
1:D:123:THR:OG1	1:D:127:ARG:NH1	2.29	0.63
1:D:317:ARG:CG	1:D:317:ARG:HH11	2.06	0.63
1:D:369:TRP:CH2	1:D:373:GLN:HG2	2.34	0.62
1:A:114:HIS:CD2	4:B:602:ALK:C5	2.83	0.62
2:B:600:TPP:H2	4:B:602:ALK:H2	0.68	0.62
1:D:225:HIS:HD2	6:D:2060:HOH:O	1.82	0.62
4:A:602:ALK:H5C2	4:A:602:ALK:O5	1.99	0.62
4:A:602:ALK:C3	4:A:602:ALK:C5	2.44	0.62
1:B:92:HIS:CD2	1:B:225:HIS:CE1	2.75	0.61
1:C:370:VAL:O	1:C:374:VAL:HG23	2.03	0.59
1:D:508:GLU:HG3	1:D:532:ARG:HD2	1.85	0.59
1:C:92:HIS:CD2	1:C:225:HIS:CE1	2.82	0.59
4:B:602:ALK:C3	4:B:602:ALK:H5C2	2.25	0.59
1:C:199:GLU:O	1:C:203:ASN:HB2	2.03	0.58
1:C:28:ASP:N	4:D:602:ALK:O1	2.31	0.58
1:D:397:GLN:HG3	6:D:2153:HOH:O	2.03	0.58
1:B:303:THR:HG21	6:B:2144:HOH:O	2.03	0.58
1:B:547:SER:O	1:B:551:LYS:HD3	2.04	0.58
1:A:28:ASP:N	4:B:602:ALK:O2	2.22	0.58
4:C:602:ALK:C5	1:D:114:HIS:CD2	2.87	0.57
4:D:602:ALK:C3	4:D:602:ALK:C5	2.50	0.57
2:B:600:TPP:C2	4:B:602:ALK:C3	2.72	0.57
1:C:13:ARG:HD3	1:C:181:LEU:HD12	1.86	0.57
1:D:394:GLY:O	1:D:397:GLN:HG2	2.03	0.57
1:A:308:GLU:HB2	1:A:315:LYS:HB3	1.86	0.57
1:A:304:LYS:HE3	6:D:2074:HOH:O	2.04	0.57
1:D:92:HIS:CD2	1:D:225:HIS:CE1	2.81	0.57
1:A:103:SER:CB	1:B:562:LYS:HD3	2.28	0.57
1:C:249:LYS:HE2	1:C:395:ILE:O	2.04	0.57
1:C:170:ASN:HD22	1:C:170:ASN:H	1.52	0.57
1:B:550:VAL:O	1:B:554:GLN:HG3	2.05	0.56
1:C:304:LYS:HE2	1:C:317:ARG:HA	1.87	0.56
1:B:154:ARG:O	1:B:158:VAL:HG13	2.05	0.56
4:C:602:ALK:C5	4:C:602:ALK:C3	2.59	0.56
1:D:134:GLU:HG2	1:D:161:ARG:HB2	1.87	0.56
1:B:111:LEU:HB3	1:B:113:LEU:HD13	1.88	0.55
1:B:249:LYS:HE2	1:B:395:ILE:O	2.07	0.55
1:A:412:TRP:CE2	1:B:76:VAL:HG12	2.42	0.55
1:A:304:LYS:NZ	1:D:195:GLU:HG3	2.22	0.55
1:A:386:THR:HG21	1:A:395:ILE:HB	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:602:ALK:O1	1:D:28:ASP:N	2.27	0.55
1:A:170:ASN:ND2	1:B:562:LYS:HE3	2.22	0.54
1:D:353:PRO:C	1:D:354:GLU:HG2	2.27	0.54
1:A:78:GLU:O	1:A:82:LEU:HD13	2.08	0.54
1:B:304:LYS:HG2	1:B:317:ARG:HA	1.89	0.54
1:C:304:LYS:O	1:C:317:ARG:HG3	2.08	0.54
4:A:602:ALK:H5C2	1:B:114:HIS:CD2	2.41	0.54
1:B:308:GLU:HB2	1:B:315:LYS:HB2	1.89	0.54
1:A:104:VAL:HB	1:B:562:LYS:HE2	1.90	0.53
1:A:225:HIS:HD2	6:A:2082:HOH:O	1.89	0.53
1:C:17:VAL:HA	5:C:604:ALU:H3C1	1.90	0.53
2:D:600:TPP:H7'2	4:D:602:ALK:O5	2.08	0.53
1:D:427:PHE:O	1:D:431:GLU:HG3	2.07	0.53
1:C:24:GLY:C	1:C:25:LEU:HD12	2.29	0.53
1:C:476:ILE:O	1:C:480:ILE:HG13	2.09	0.53
1:C:386:THR:HG21	1:C:395:ILE:HB	1.91	0.52
1:C:508:GLU:HB2	1:C:534:ARG:HG2	1.92	0.52
4:A:602:ALK:H5C1	1:B:114:HIS:CE1	2.43	0.52
1:B:311:SER:HB2	4:B:603:ALK:O1	2.08	0.52
2:C:600:TPP:C7'	4:C:602:ALK:H2	2.38	0.52
1:A:199:GLU:OE2	1:D:304:LYS:NZ	2.38	0.52
1:B:379:ARG:NH2	6:B:2204:HOH:O	2.43	0.51
4:C:602:ALK:C5	1:D:114:HIS:NE2	2.74	0.51
1:D:17:VAL:HG12	1:D:187:LEU:HD11	1.93	0.51
1:C:558:ALA:O	1:C:561:ALA:HB3	2.11	0.51
1:D:57:ALA:O	1:D:424:GLY:HA3	2.10	0.51
1:C:558:ALA:HA	1:C:561:ALA:CB	2.36	0.51
1:C:78:GLU:O	1:C:82:LEU:HD13	2.10	0.51
1:B:224:ARG:CZ	1:B:224:ARG:HA	2.41	0.51
1:C:360:ALA:O	1:C:363:THR:OG1	2.21	0.51
1:B:201:ILE:HG22	1:B:205:LEU:HD22	1.92	0.50
2:A:600:TPP:H2	4:A:602:ALK:H3C3	1.91	0.50
1:A:290:SER:HA	1:B:112:LEU:HG	1.92	0.50
1:A:123:THR:OG1	1:A:127:ARG:NH1	2.44	0.50
1:B:302:LYS:N	1:B:302:LYS:HD2	2.26	0.50
1:D:371:TRP:CZ2	1:D:391:SER:HA	2.46	0.50
1:D:117:LEU:HD22	1:D:124:VAL:HG11	1.94	0.50
4:B:602:ALK:C5	4:B:602:ALK:O5	2.58	0.49
1:A:253:ASP:HB3	1:A:402:ASN:OD1	2.12	0.49
1:A:92:HIS:HE1	6:A:2046:HOH:O	1.94	0.49
1:B:103:SER:HB2	1:B:170:ASN:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:THR:HB	1:B:298:SER:HB2	1.93	0.49
1:D:479:LEU:HD11	1:D:545:ALA:CB	2.42	0.49
1:A:57:ALA:HA	1:A:420:GLY:O	2.12	0.49
1:D:142:ILE:HD13	1:D:174:LEU:HB2	1.95	0.49
1:A:89:TYR:O	1:A:161:ARG:NH1	2.44	0.48
1:B:40:VAL:HA	1:B:41:PRO:HD3	1.81	0.48
1:D:476:ILE:HG13	1:D:549:LEU:HD11	1.95	0.48
1:A:563:ASN:ND2	6:A:2297:HOH:O	2.45	0.48
1:B:28:ASP:HA	1:B:31:LEU:HD22	1.94	0.48
1:B:339:ASP:O	1:B:342:LYS:HG2	2.12	0.48
1:B:382:ASP:OD1	1:B:437:ARG:HB2	2.13	0.48
4:C:602:ALK:H5C2	1:D:114:HIS:CD2	2.49	0.48
1:B:354:GLU:HB2	1:B:355:HIS:O	2.13	0.48
1:C:387:GLU:HG2	1:C:446:SER:CB	2.43	0.48
1:D:224:ARG:HA	1:D:224:ARG:CZ	2.44	0.48
1:A:266:THR:HG22	1:A:298:SER:OG	2.14	0.48
1:B:134:GLU:HB2	1:B:161:ARG:HB2	1.96	0.48
1:C:353:PRO:HB2	1:C:354:GLU:HB2	1.96	0.48
1:D:71:ILE:HG12	1:D:98:VAL:HB	1.94	0.48
1:B:109:LYS:HG3	1:B:111:LEU:CD1	2.37	0.48
1:A:190:LYS:HD3	6:A:2093:HOH:O	2.13	0.47
1:C:351:SER:O	1:C:352:GLU:HG2	2.13	0.47
1:A:154:ARG:HD2	1:A:186:ASP:O	2.14	0.47
1:D:154:ARG:HG3	1:D:186:ASP:O	2.15	0.47
1:A:266:THR:H	1:A:298:SER:HB3	1.79	0.47
2:C:600:TPP:H7'2	4:C:602:ALK:H2	1.97	0.47
1:C:28:ASP:HA	1:C:31:LEU:HD22	1.97	0.47
1:A:415:ILE:HG13	1:A:449:LEU:HD22	1.97	0.46
1:C:228:LYS:HE3	1:C:251:SER:HA	1.98	0.46
1:A:527:PHE:CE1	1:A:534:ARG:HD3	2.51	0.46
1:B:452:GLN:O	1:B:455:SER:HB3	2.15	0.46
1:C:224:ARG:HA	1:C:224:ARG:CZ	2.46	0.46
1:A:14:LEU:HB3	1:A:19:VAL:HB	1.96	0.46
1:B:429:ALA:HB1	1:B:436:LYS:HG3	1.97	0.46
1:D:13:ARG:HD3	1:D:181:LEU:HD12	1.98	0.46
1:D:37:ILE:HG23	1:D:43:MET:HG2	1.98	0.46
1:A:201:ILE:HG13	1:A:332:LYS:HG2	1.98	0.46
1:B:203:ASN:HB3	1:B:316:ILE:HD13	1.97	0.46
1:A:563:ASN:ND2	1:B:170:ASN:HD22	2.14	0.46
1:C:51:GLU:OE2	2:D:600:TPP:N1'	2.49	0.46
1:D:479:LEU:HD11	1:D:545:ALA:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:ASN:N	1:A:280:ASP:OD1	2.43	0.45
1:B:247:MET:HG3	1:B:410:VAL:HB	1.98	0.45
1:A:481:HIS:HB3	1:B:31:LEU:HD23	1.97	0.45
1:B:562:LYS:HG2	1:B:563:ASN:OD1	2.17	0.45
1:C:354:GLU:O	1:C:355:HIS:HB2	2.16	0.45
1:D:183:THR:HA	1:D:184:PRO:HD2	1.74	0.45
1:B:562:LYS:HG3	1:B:563:ASN:H	1.69	0.45
1:A:310:HIS:O	1:A:326:MET:HB3	2.17	0.45
1:C:105:SER:HB2	1:D:562:LYS:HZ1	1.82	0.45
1:A:40:VAL:HG22	1:A:43:MET:HG3	1.98	0.45
1:A:452:GLN:O	1:A:455:SER:HB3	2.16	0.45
1:C:362:SER:HB3	6:C:2151:HOH:O	2.17	0.45
4:A:602:ALK:H5C2	1:B:114:HIS:NE2	2.29	0.45
1:A:139:ILE:HD12	1:A:165:LEU:HD11	1.98	0.45
1:A:309:PHE:HB3	1:A:326:MET:HB2	1.99	0.44
1:A:249:LYS:HE2	1:A:395:ILE:O	2.18	0.44
1:B:221:CYS:HB2	1:B:286:GLY:CA	2.46	0.44
1:C:95:VAL:O	1:C:162:PRO:HA	2.18	0.44
1:A:203:ASN:HB3	1:A:316:ILE:HD13	2.00	0.44
1:A:40:VAL:HA	1:A:41:PRO:HD3	1.93	0.44
1:A:514:THR:OG1	1:A:517:GLU:HG3	2.16	0.44
2:A:600:TPP:H7'2	4:A:602:ALK:O5	2.18	0.44
2:B:600:TPP:C7'	4:B:602:ALK:H2	2.48	0.44
1:B:463:LYS:N	1:B:464:PRO:CD	2.80	0.44
1:C:56:TYR:CD2	1:C:417:PHE:HA	2.53	0.44
1:B:121:ASP:OD2	1:B:127:ARG:NH1	2.47	0.44
1:B:353:PRO:O	1:B:354:GLU:HB3	2.17	0.44
1:B:353:PRO:O	1:B:354:GLU:CB	2.66	0.44
1:B:550:VAL:CG2	1:B:551:LYS:N	2.81	0.44
1:B:563:ASN:N	1:B:563:ASN:OD1	2.50	0.44
1:C:223:SER:HB3	1:C:228:LYS:HD2	2.00	0.44
1:D:463:LYS:HG2	1:D:532:ARG:HA	2.00	0.44
1:C:105:SER:HB2	1:D:562:LYS:NZ	2.33	0.44
1:D:281:LEU:HD12	1:D:305:ASN:O	2.18	0.44
1:C:412:TRP:CE2	1:D:76:VAL:HG12	2.54	0.43
1:D:562:LYS:HE2	1:D:562:LYS:HB3	1.83	0.43
1:C:49:ALA:O	1:D:449:LEU:HG	2.17	0.43
1:C:27:GLY:O	1:C:31:LEU:HD13	2.18	0.43
1:C:476:ILE:HG21	2:C:600:TPP:S1	2.58	0.43
1:D:310:HIS:O	1:D:326:MET:HB3	2.19	0.43
1:D:177:PRO:O	1:D:180:LEU:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:291:ASP:HB3	1:D:297:PHE:CZ	2.53	0.43
1:B:436:LYS:HE2	1:B:436:LYS:HB3	1.82	0.43
1:C:473:GLY:HA2	1:C:490:ILE:HG12	2.01	0.43
1:C:170:ASN:CB	1:D:562:LYS:HB2	2.49	0.43
1:B:14:LEU:HB3	1:B:19:VAL:HB	2.01	0.43
1:B:315:LYS:HE2	1:B:315:LYS:HB3	1.87	0.43
1:A:354:GLU:HB3	1:A:355:HIS:CE1	2.54	0.42
1:D:11:PHE:CE1	1:D:33:LEU:HD22	2.54	0.42
1:A:139:ILE:CD1	1:A:165:LEU:HD11	2.49	0.42
1:B:303:THR:HG23	1:B:304:LYS:N	2.34	0.42
1:A:92:HIS:HA	1:A:161:ARG:HD3	2.00	0.42
1:A:344:TYR:CE1	1:A:346:PRO:HA	2.54	0.42
1:C:134:GLU:HB2	1:C:161:ARG:HB2	2.00	0.42
1:D:477:GLU:OE1	4:D:602:ALK:P1	2.77	0.42
1:C:221:CYS:HB2	1:C:286:GLY:CA	2.50	0.42
1:C:258:ARG:NH1	1:C:349:VAL:HG13	2.35	0.42
1:D:423:LEU:HD22	1:D:453:GLU:HG3	2.02	0.42
1:A:436:LYS:NZ	6:A:2227:HOH:O	2.45	0.42
1:A:148:GLU:HA	1:A:148:GLU:OE2	2.20	0.42
1:B:114:HIS:HD2	1:B:115:HIS:CE1	2.37	0.42
1:C:549:LEU:O	1:C:549:LEU:HD22	2.18	0.41
1:C:562:LYS:HD2	1:D:170:ASN:HB2	2.00	0.41
2:A:600:TPP:H7'2	4:A:602:ALK:C2	2.50	0.41
1:C:79:LEU:HA	1:C:79:LEU:HD23	1.84	0.41
1:A:371:TRP:CZ2	1:A:391:SER:HA	2.55	0.41
1:B:387:GLU:HG2	1:B:446:SER:CB	2.50	0.41
2:B:600:TPP:H7'2	4:B:602:ALK:C2	2.50	0.41
1:B:24:GLY:HA3	1:B:71:ILE:O	2.20	0.41
1:C:470:ASN:ND2	1:C:537:GLU:OE2	2.48	0.41
1:B:214:PRO:HD2	1:B:344:TYR:CE2	2.56	0.41
1:C:114:HIS:NE2	4:D:602:ALK:C5	2.77	0.41
1:A:22:ILE:HG12	1:A:43:MET:HE2	2.02	0.41
2:C:600:TPP:C2	4:C:602:ALK:C3	2.83	0.41
1:C:304:LYS:HE2	1:C:317:ARG:CA	2.50	0.41
1:A:274:GLU:HA	1:A:274:GLU:OE1	2.21	0.41
1:A:508:GLU:HB2	1:A:534:ARG:HG2	2.03	0.41
1:B:304:LYS:CG	1:B:317:ARG:HA	2.50	0.41
1:C:292:PHE:CZ	4:C:602:ALK:H5C1	2.56	0.41
1:D:320:THR:O	1:D:322:PRO:HD3	2.21	0.41
1:C:82:LEU:HD23	1:D:82:LEU:HD23	2.02	0.41
1:A:563:ASN:HD22	1:B:170:ASN:HD22	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:GLU:HB2	1:B:355:HIS:H	1.46	0.41
1:A:106:SER:HA	1:A:111:LEU:HD22	2.02	0.41
1:A:344:TYR:CZ	1:A:346:PRO:HA	2.56	0.41
1:C:330:LEU:O	1:C:334:LEU:HG	2.21	0.41
1:C:393:PHE:CG	1:C:549:LEU:HG	2.56	0.41
1:A:114:HIS:NE2	4:B:602:ALK:C5	2.79	0.40
1:A:433:ASP:HB3	1:A:436:LYS:HG3	2.03	0.40
1:A:51:GLU:OE2	2:B:600:TPP:N1'	2.55	0.40
1:D:75:GLY:O	1:D:79:LEU:HG	2.21	0.40
1:C:315:LYS:HB3	1:C:315:LYS:HE3	1.74	0.40
1:D:101:VAL:HB	1:D:102:PRO:HD2	2.03	0.40
1:B:199:GLU:O	1:B:203:ASN:HB2	2.22	0.40
1:C:317:ARG:HB3	1:C:318:SER:H	1.52	0.40
1:C:354:GLU:HB3	1:C:355:HIS:H	1.60	0.40
1:C:369:TRP:CH2	1:C:373:GLN:HG2	2.57	0.40
1:D:95:VAL:O	1:D:162:PRO:HA	2.21	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	560/563 (100%)	539 (96%)	21 (4%)	0	100	100
1	B	560/563 (100%)	536 (96%)	22 (4%)	2 (0%)	34	42
1	C	560/563 (100%)	533 (95%)	23 (4%)	4 (1%)	22	26
1	D	560/563 (100%)	536 (96%)	22 (4%)	2 (0%)	34	42
All	All	2240/2252 (100%)	2144 (96%)	88 (4%)	8 (0%)	34	42

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	354	GLU
1	B	304	LYS
1	C	354	GLU
1	C	355	HIS
1	D	112	LEU
1	D	352	GLU
1	C	561	ALA
1	C	352	GLU

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	473/474 (100%)	448 (95%)	25 (5%)	22	31
1	B	473/474 (100%)	439 (93%)	34 (7%)	14	18
1	C	473/474 (100%)	437 (92%)	36 (8%)	13	16
1	D	473/474 (100%)	450 (95%)	23 (5%)	25	35
All	All	1892/1896 (100%)	1774 (94%)	118 (6%)	18	25

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	40	VAL
1	A	82	LEU
1	A	92	HIS
1	A	111	LEU
1	A	148	GLU
1	A	181	LEU
1	A	205	LEU
1	A	212	LYS
1	A	223	SER
1	A	224	ARG
1	A	284	SER
1	A	298	SER
1	A	324	VAL

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Mol	Chain	Res	Type
1	A	327	LYS
1	A	347	VAL
1	A	352	GLU
1	A	354	GLU
1	A	379	ARG
1	A	436	LYS
1	A	463	LYS
1	A	520	LYS
1	A	551	LYS
1	A	555	LEU
1	A	562	LYS
1	B	2	SER
1	B	10	LEU
1	B	31	LEU
1	B	40	VAL
1	B	43	MET
1	B	65	LYS
1	B	82	LEU
1	B	109	LYS
1	B	111	LEU
1	B	112	LEU
1	B	113	LEU
1	B	129	SER
1	B	171	LEU
1	B	180	LEU
1	B	195	GLU
1	B	203	ASN
1	B	205	LEU
1	B	217	LEU
1	B	266	THR
1	B	268	SER
1	B	300	SER
1	B	302	LYS
1	B	304	LYS
1	B	311	SER
1	B	324	VAL
1	B	334	LEU
1	B	345	LYS
1	B	379	ARG
1	B	397	GLN
1	B	436	LYS
1	B	452	GLN

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Mol	Chain	Res	Type
1	B	505	LYS
1	B	551	LYS
1	B	563	ASN
1	C	31	LEU
1	C	40	VAL
1	C	82	LEU
1	C	98	VAL
1	C	112	LEU
1	C	129	SER
1	C	167	LEU
1	C	170	ASN
1	C	171	LEU
1	C	180	LEU
1	C	181	LEU
1	C	187	LEU
1	C	190	LYS
1	C	203	ASN
1	C	212	LYS
1	C	267	LEU
1	C	296	SER
1	C	300	SER
1	C	302	LYS
1	C	304	LYS
1	C	317	ARG
1	C	324	VAL
1	C	332	LYS
1	C	337	VAL
1	C	352	GLU
1	C	355	HIS
1	C	379	ARG
1	C	397	GLN
1	C	463	LYS
1	C	483	GLU
1	C	510	VAL
1	C	525	GLU
1	C	549	LEU
1	C	551	LYS
1	C	555	LEU
1	C	563	ASN
1	D	14	LEU
1	D	33	LEU
1	D	43	MET

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Mol	Chain	Res	Type
1	D	82	LEU
1	D	112	LEU
1	D	117	LEU
1	D	134	GLU
1	D	167	LEU
1	D	180	LEU
1	D	181	LEU
1	D	198	GLU
1	D	232	LYS
1	D	296	SER
1	D	300	SER
1	D	304	LYS
1	D	311	SER
1	D	317	ARG
1	D	342	LYS
1	D	355	HIS
1	D	379	ARG
1	D	452	GLN
1	D	505	LYS
1	D	520	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	HIS
1	A	225	HIS
1	A	355	HIS
1	A	563	ASN
1	B	92	HIS
1	B	225	HIS
1	C	92	HIS
1	C	170	ASN
1	C	203	ASN
1	C	225	HIS
1	C	563	ASN
1	D	92	HIS
1	D	225	HIS
1	D	397	GLN
1	D	563	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 19 ligands modelled in this entry, 4 are monoatomic - leaving 15 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	TPP	A	600	3	22,27,27	1.59	3 (13%)	29,40,40	2.12	8 (27%)
2	TPP	C	600	3	22,27,27	2.20	7 (31%)	29,40,40	1.72	5 (17%)
4	ALK	B	602	-	5,7,7	2.08	2 (40%)	6,10,10	4.13	4 (66%)
4	ALK	B	603	1	5,7,7	4.20	3 (60%)	6,10,10	2.98	4 (66%)
4	ALK	D	603	1	5,7,7	4.14	3 (60%)	6,10,10	1.39	1 (16%)
4	ALK	A	603	1	5,7,7	3.59	2 (40%)	6,10,10	2.56	4 (66%)
4	ALK	C	603	1	5,7,7	4.47	3 (60%)	6,10,10	2.50	3 (50%)
2	TPP	D	600	3	22,27,27	1.70	5 (22%)	29,40,40	1.79	8 (27%)
4	ALK	C	602	-	5,7,7	2.20	1 (20%)	6,10,10	2.77	3 (50%)
5	ALU	A	604	-	4,7,7	1.57	1 (25%)	3,10,10	3.12	2 (66%)
2	TPP	B	600	3	22,27,27	1.90	6 (27%)	29,40,40	1.96	7 (24%)
4	ALK	A	602	-	5,7,7	2.76	3 (60%)	6,10,10	4.09	4 (66%)
5	ALU	C	604	-	4,7,7	1.78	2 (50%)	3,10,10	3.28	1 (33%)
5	ALU	B	604	-	4,7,7	1.71	2 (50%)	3,10,10	1.39	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ALK	D	602	-	5,7,7	2.53	1 (20%)	6,10,10	2.50	2 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TPP	A	600	3	-	5/16/17/17	0/2/2/2
2	TPP	C	600	3	-	4/16/17/17	0/2/2/2
4	ALK	B	602	-	-	2/7/9/9	-
4	ALK	B	603	1	-	0/7/9/9	-
4	ALK	D	603	1	-	1/7/9/9	-
4	ALK	A	603	1	-	1/7/9/9	-
4	ALK	C	603	1	-	1/7/9/9	-
2	TPP	D	600	3	-	3/16/17/17	0/2/2/2
4	ALK	C	602	-	-	6/7/9/9	-
5	ALU	A	604	-	-	0/2/9/9	-
2	TPP	B	600	3	-	5/16/17/17	0/2/2/2
4	ALK	A	602	-	-	2/7/9/9	-
5	ALU	C	604	-	-	1/2/9/9	-
5	ALU	B	604	-	-	1/2/9/9	-
4	ALK	D	602	-	-	2/7/9/9	-

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	603	ALK	P1-O1	-7.55	1.39	1.56
4	D	603	ALK	P1-O1	-7.51	1.39	1.56
4	A	603	ALK	P1-O1	-7.22	1.40	1.56
4	C	603	ALK	P1-O1	-6.98	1.40	1.56
2	B	600	TPP	C6-C5	6.33	1.53	1.50
4	C	603	ALK	P1-O2	-5.39	1.38	1.50
4	D	602	ALK	P1-O1	-5.31	1.44	1.56
2	C	600	TPP	C6-C5	5.22	1.53	1.50
4	B	603	ALK	P1-O2	-5.05	1.39	1.50
2	C	600	TPP	C4-N3	-4.80	1.35	1.39
4	A	602	ALK	P1-O1	-4.62	1.45	1.56
4	C	603	ALK	P1-O3	-4.61	1.50	1.57
4	D	603	ALK	P1-O2	-4.53	1.40	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	602	ALK	P1-O1	-4.33	1.46	1.56
2	D	600	TPP	C6-C5	4.28	1.52	1.50
2	A	600	TPP	C6-C5	4.23	1.52	1.50
2	C	600	TPP	C6'-N1'	3.74	1.42	1.34
2	C	600	TPP	C4'-N3'	3.70	1.40	1.35
2	A	600	TPP	C2'-N1'	3.48	1.40	1.34
4	B	602	ALK	P1-O1	-3.45	1.48	1.56
4	A	603	ALK	P1-O2	-3.24	1.43	1.50
2	D	600	TPP	C2'-N1'	3.12	1.39	1.34
2	D	600	TPP	C2'-N3'	3.05	1.39	1.34
2	D	600	TPP	C4'-N3'	3.02	1.39	1.35
4	A	602	ALK	P1-O3	-3.01	1.52	1.57
2	C	600	TPP	C2'-N1'	3.00	1.39	1.34
4	B	602	ALK	P1-O2	-2.95	1.43	1.50
2	B	600	TPP	C2'-N1'	2.78	1.38	1.34
4	D	603	ALK	P1-O3	-2.73	1.53	1.57
2	A	600	TPP	C6'-N1'	2.62	1.40	1.34
2	B	600	TPP	C4-N3	-2.48	1.37	1.39
5	B	604	ALU	P1-C2	-2.45	1.71	1.79
5	C	604	ALU	P1-C2	-2.45	1.71	1.79
5	C	604	ALU	P1-O3	2.42	1.61	1.57
2	B	600	TPP	C4'-N3'	2.38	1.38	1.35
4	A	602	ALK	P1-O2	-2.37	1.45	1.50
5	B	604	ALU	P1-O3	2.36	1.61	1.57
2	D	600	TPP	C2-N3	2.35	1.40	1.36
2	C	600	TPP	C2'-N3'	2.34	1.38	1.34
4	B	603	ALK	P1-O3	-2.27	1.54	1.57
2	B	600	TPP	C5'-C4'	-2.22	1.39	1.42
2	C	600	TPP	C2-N3	2.11	1.40	1.36
5	A	604	ALU	P1-O3	2.11	1.60	1.57
2	B	600	TPP	C6'-N1'	2.05	1.38	1.34

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	602	ALK	O1-P1-O2	6.36	127.09	111.58
2	B	600	TPP	CM2-C2'-N1'	6.25	124.02	117.14
4	A	602	ALK	O2-P1-C2	-6.19	102.42	113.69
4	B	602	ALK	O3-P1-O2	-6.09	101.92	114.92
4	B	602	ALK	P1-C2-O5	-5.87	93.35	108.05
5	C	604	ALU	O3-P1-O2	-5.34	94.29	114.51
4	C	603	ALK	O3-P1-O2	-5.08	104.07	114.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	603	ALK	O3-P1-O2	-4.99	104.26	114.92
5	A	604	ALU	O3-P1-O2	-4.79	96.38	114.51
2	C	600	TPP	N1'-C2'-N3'	-4.75	117.36	125.54
2	A	600	TPP	CM2-C2'-N1'	4.75	122.37	117.14
4	C	602	ALK	O1-P1-O2	4.61	122.82	111.58
4	D	602	ALK	P1-C2-O5	-4.58	96.58	108.05
4	B	602	ALK	O2-P1-C2	-4.53	105.44	113.69
2	C	600	TPP	CM2-C2'-N1'	4.51	122.10	117.14
2	A	600	TPP	C5'-C6'-N1'	-4.20	116.82	123.82
4	C	602	ALK	O3-P1-O2	-4.20	105.95	114.92
2	D	600	TPP	C6'-C5'-C4'	4.01	121.17	115.72
2	A	600	TPP	C6'-N1'-C2'	3.97	122.72	115.96
4	A	603	ALK	O1-P1-O2	3.95	121.19	111.58
2	A	600	TPP	CM4-C4-N3	3.81	127.39	122.53
2	A	600	TPP	N1'-C2'-N3'	-3.74	119.10	125.54
4	B	603	ALK	P1-O3-C5	3.58	132.16	122.32
2	A	600	TPP	C6'-C5'-C4'	3.52	120.51	115.72
4	A	602	ALK	O3-P1-O2	-3.48	107.49	114.92
2	B	600	TPP	C6'-C5'-C4'	3.44	120.40	115.72
2	B	600	TPP	N1'-C2'-N3'	-3.37	119.73	125.54
2	D	600	TPP	CM4-C4-N3	3.34	126.79	122.53
2	B	600	TPP	C5'-C6'-N1'	-3.24	118.43	123.82
2	C	600	TPP	C2'-N3'-C4'	3.06	122.86	118.08
4	D	602	ALK	P1-O3-C5	-3.03	114.01	122.32
2	B	600	TPP	C6'-N1'-C2'	2.86	120.84	115.96
4	A	603	ALK	O3-P1-O2	-2.76	109.03	114.92
4	B	603	ALK	O1-P1-O2	2.75	118.27	111.58
2	D	600	TPP	N1'-C2'-N3'	-2.71	120.88	125.54
4	B	602	ALK	P1-O3-C5	-2.70	114.91	122.32
2	B	600	TPP	CM4-C4-N3	2.69	125.96	122.53
2	C	600	TPP	C6'-N1'-C2'	2.63	120.44	115.96
4	A	603	ALK	O2-P1-C2	-2.61	108.94	113.69
2	D	600	TPP	C5'-C6'-N1'	-2.56	119.56	123.82
2	D	600	TPP	C7'-C5'-C6'	-2.54	115.83	120.69
4	C	602	ALK	O5-C2-C3	-2.47	104.53	109.17
2	D	600	TPP	C5'-C4'-N3'	-2.47	117.37	121.24
2	D	600	TPP	C6'-N1'-C2'	2.44	120.12	115.96
4	B	603	ALK	O5-C2-C3	-2.42	104.62	109.17
4	D	603	ALK	O2-P1-C2	-2.36	109.39	113.69
2	D	600	TPP	CM2-C2'-N1'	2.33	119.70	117.14
4	A	603	ALK	O5-C2-C3	-2.32	104.80	109.17
4	A	602	ALK	P1-O3-C5	-2.30	116.00	122.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	603	ALK	O5-C2-C3	-2.23	104.97	109.17
2	B	600	TPP	C2'-N3'-C4'	2.21	121.53	118.08
2	A	600	TPP	CM4-C4-C5	-2.19	122.81	127.60
2	C	600	TPP	CM2-C2'-N3'	2.17	120.54	117.15
5	B	604	ALU	O1-P1-O2	2.16	118.63	110.62
5	A	604	ALU	O1-P1-O2	2.12	118.47	110.62
2	A	600	TPP	C5'-C7'-N3	-2.07	109.82	113.28
4	C	603	ALK	P1-C2-O5	2.00	113.07	108.05

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	TPP	PA-O3A-PB-O3B
2	C	600	TPP	PA-O3A-PB-O3B
4	B	602	ALK	C5-O3-P1-C2
4	A	603	ALK	O5-C2-P1-O1
4	D	602	ALK	C5-O3-P1-C2
2	D	600	TPP	C4-C5-C6-C7
2	B	600	TPP	C4-C5-C6-C7
2	B	600	TPP	PA-O3A-PB-O3B
4	A	602	ALK	C5-O3-P1-C2
5	C	604	ALU	C5-O3-P1-C2
4	C	602	ALK	C5-O3-P1-C2
4	C	602	ALK	C3-C2-P1-O3
4	C	602	ALK	O5-C2-P1-O1
4	B	602	ALK	C5-O3-P1-O2
4	D	602	ALK	C5-O3-P1-O2
4	A	602	ALK	C5-O3-P1-O2
2	D	600	TPP	PA-O3A-PB-O1B
4	C	603	ALK	C5-O3-P1-O2
2	C	600	TPP	C7-O7-PA-O1A
5	B	604	ALU	C5-O3-P1-O2
2	A	600	TPP	C4-C5-C6-C7
4	C	602	ALK	C3-C2-P1-O2
2	A	600	TPP	PB-O3A-PA-O1A
2	B	600	TPP	PB-O3A-PA-O1A
2	A	600	TPP	PA-O3A-PB-O1B
2	C	600	TPP	PA-O3A-PB-O1B
2	B	600	TPP	PA-O3A-PB-O1B
4	D	603	ALK	C5-O3-P1-O2
2	A	600	TPP	PA-O3A-PB-O2B

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Mol	Chain	Res	Type	Atoms
2	D	600	TPP	PA-O3A-PB-O2B
2	C	600	TPP	C7-O7-PA-O3A
2	B	600	TPP	PB-O3A-PA-O2A
4	C	602	ALK	O5-C2-P1-O3
4	C	602	ALK	C5-O3-P1-O2

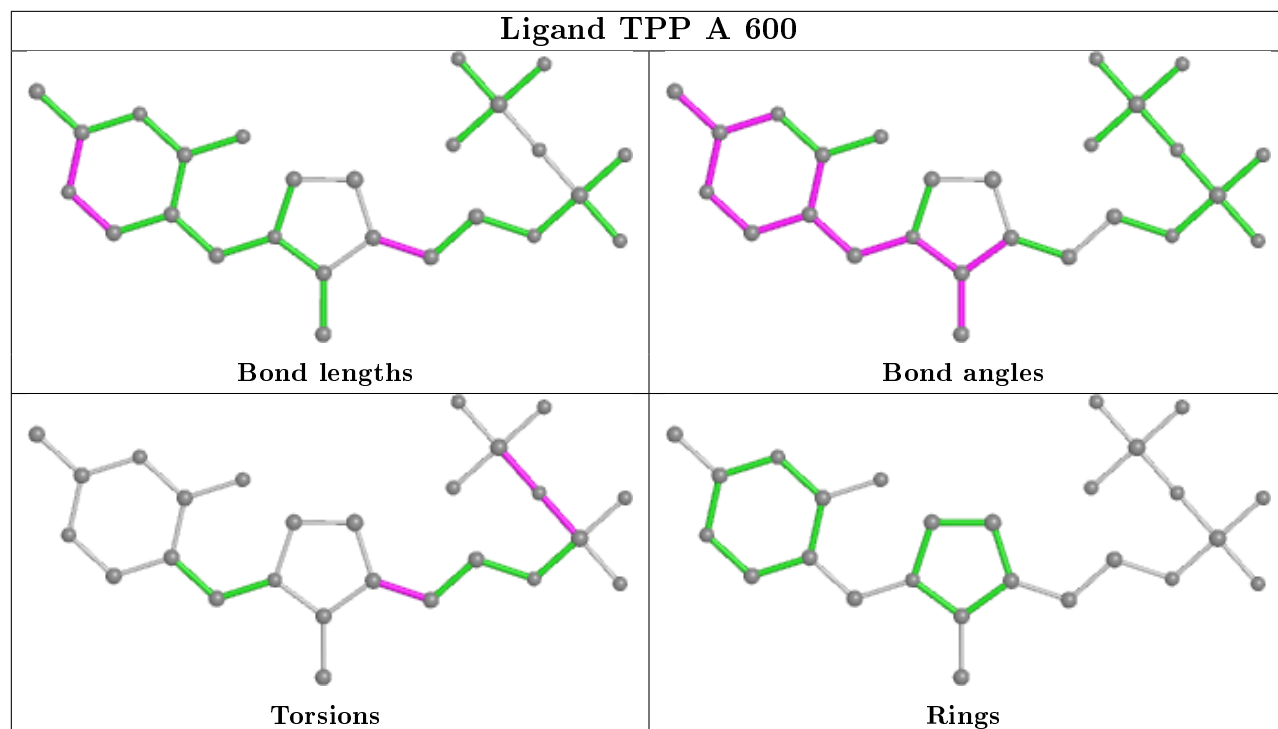
There are no ring outliers.

10 monomers are involved in 90 short contacts:

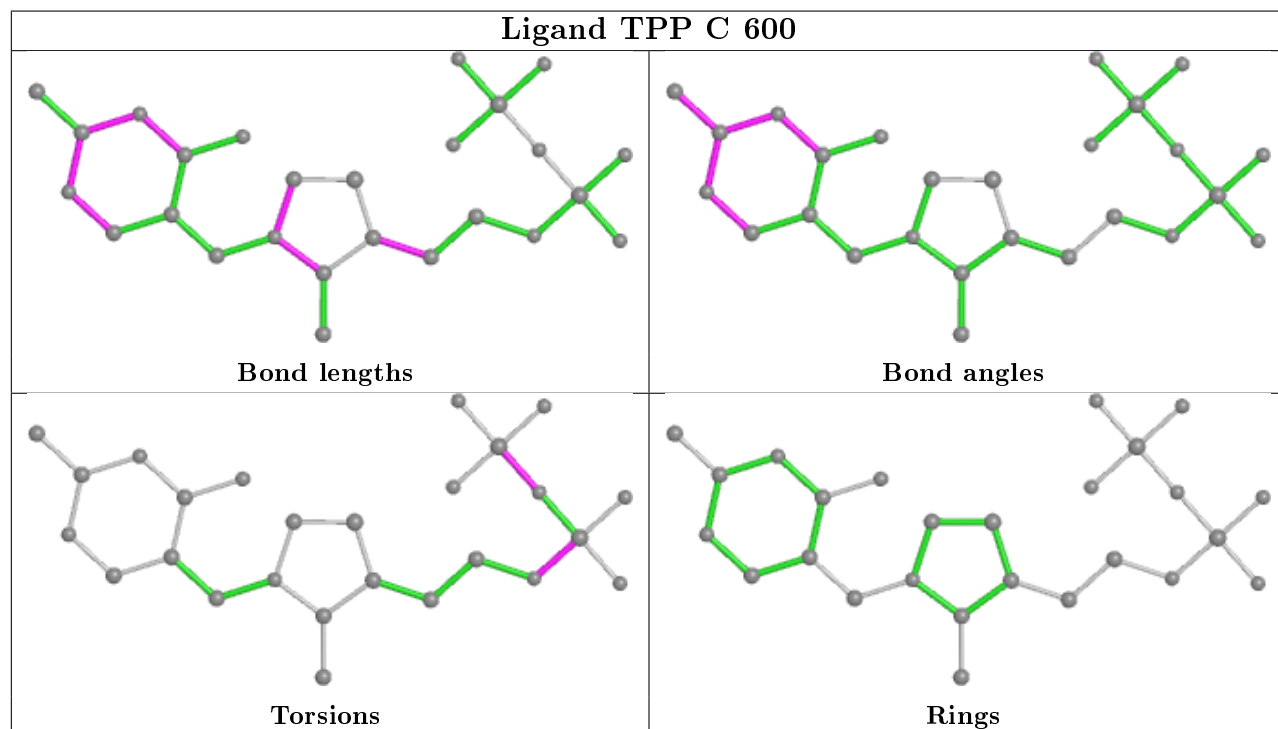
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	TPP	9	0
2	C	600	TPP	10	0
4	B	602	ALK	23	0
4	B	603	ALK	1	0
2	D	600	TPP	7	0
4	C	602	ALK	20	0
2	B	600	TPP	10	0
4	A	602	ALK	23	0
5	C	604	ALU	1	0
4	D	602	ALK	19	0

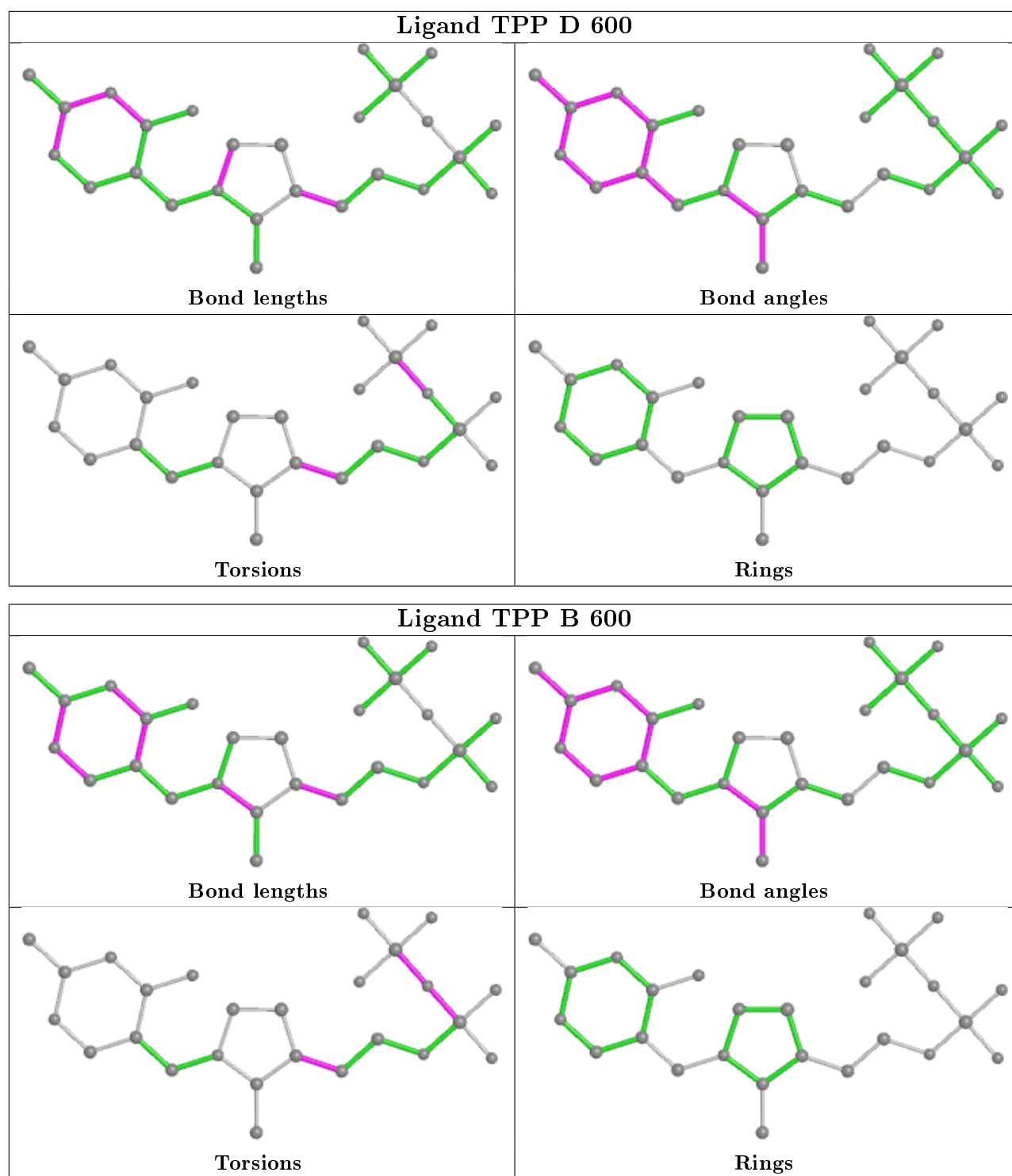
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 TPP A 600



Ligand TPP C 600





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, 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	562/563 (99%)	-0.61	4 (0%) 87 91	12, 22, 35, 61	0
1	B	562/563 (99%)	-0.64	5 (0%) 84 88	11, 20, 35, 61	0
1	C	562/563 (99%)	-0.31	14 (2%) 57 64	18, 29, 44, 87	0
1	D	562/563 (99%)	-0.41	8 (1%) 75 80	17, 27, 42, 63	0
All	All	2248/2252 (99%)	-0.49	31 (1%) 75 80	11, 24, 40, 87	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	563	ASN	7.2
1	C	558	ALA	6.3
1	C	557	ALA	5.4
1	C	562	LYS	4.8
1	B	563	ASN	4.6
1	C	354	GLU	4.3
1	C	559	THR	4.2
1	D	563	ASN	4.0
1	D	353	PRO	4.0
1	C	561	ALA	3.9
1	A	353	PRO	3.9
1	C	351	SER	3.8
1	C	553	ALA	3.5
1	D	357	GLU	3.5
1	C	556	THR	3.2
1	C	353	PRO	2.8
1	B	301	TYR	2.8
1	D	561	ALA	2.7
1	A	354	GLU	2.7
1	D	354	GLU	2.6
1	A	352	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	352	GLU	2.5
1	B	302	LYS	2.4
1	B	355	HIS	2.4
1	D	355	HIS	2.3
1	C	108	ALA	2.2
1	C	357	GLU	2.1
1	C	216	ILE	2.1
1	B	561	ALA	2.0
1	D	505	LYS	2.0
1	A	351	SER	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	ALU	B	604	8/8	0.75	0.28	15,21,24,24	8
5	ALU	C	604	8/8	0.81	0.26	13,20,23,24	8
4	ALK	A	602	8/8	0.83	0.35	20,27,29,29	8
4	ALK	C	602	8/8	0.85	0.31	33,37,39,40	8
4	ALK	D	602	8/8	0.86	0.36	29,33,34,36	8
5	ALU	A	604	8/8	0.88	0.20	18,24,28,29	8
4	ALK	B	602	8/8	0.93	0.34	33,35,37,39	8
3	MG	C	601	1/1	0.96	0.09	30,30,30,30	0
3	MG	D	601	1/1	0.97	0.08	20,20,20,20	0
2	TPP	C	600	26/26	0.98	0.09	17,22,26,27	0
4	ALK	A	603	8/8	0.98	0.09	20,25,26,27	0
4	ALK	B	603	8/8	0.98	0.07	15,19,22,22	0
3	MG	B	601	1/1	0.98	0.06	15,15,15,15	0

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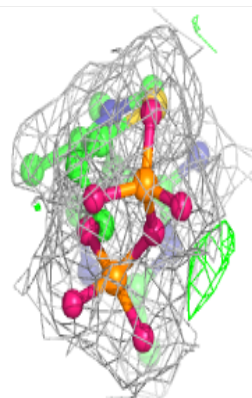
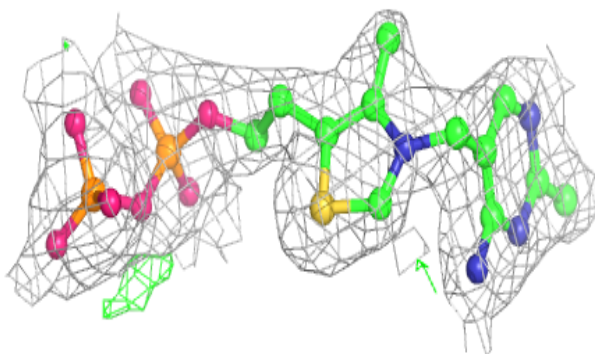
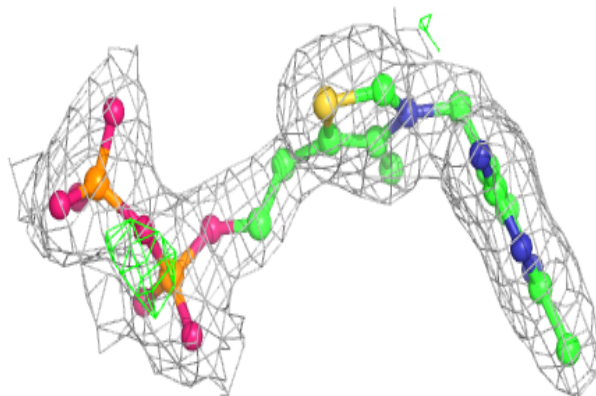
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	TPP	B	600	26/26	0.99	0.09	11,15,19,19	0
4	ALK	C	603	8/8	0.99	0.07	21,22,27,29	0
2	TPP	D	600	26/26	0.99	0.07	11,21,25,26	0
3	MG	A	601	1/1	0.99	0.05	20,20,20,20	0
2	TPP	A	600	26/26	0.99	0.09	11,16,20,22	0
4	ALK	D	603	8/8	0.99	0.07	20,25,27,28	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.

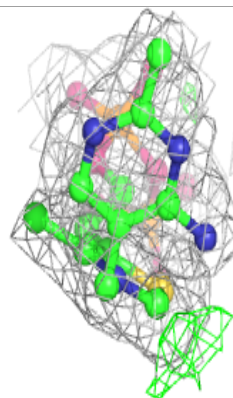
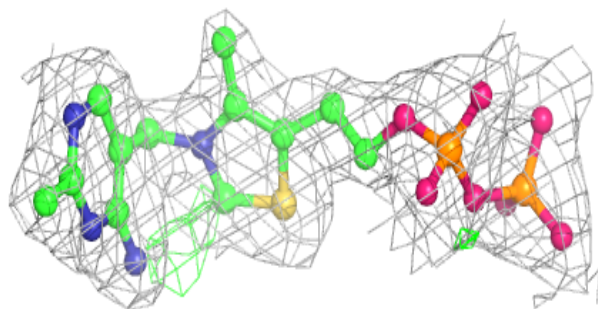
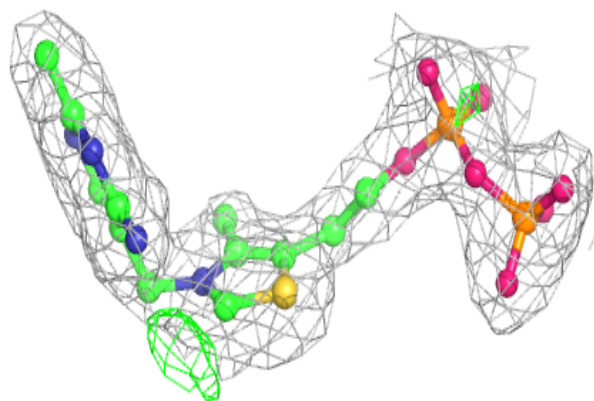
Electron density around TPP C 600:

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

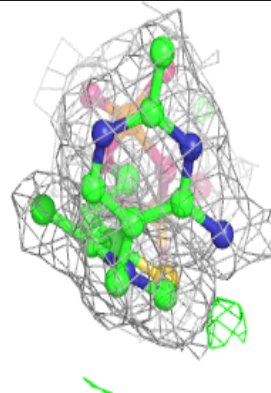
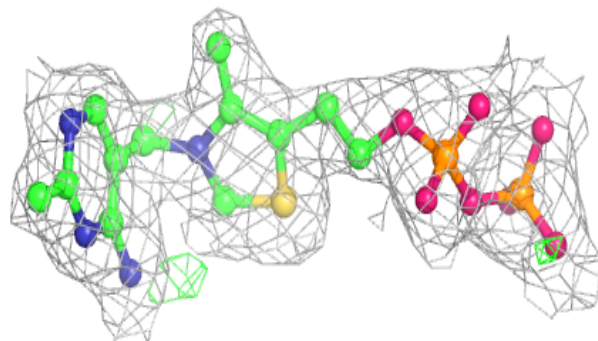
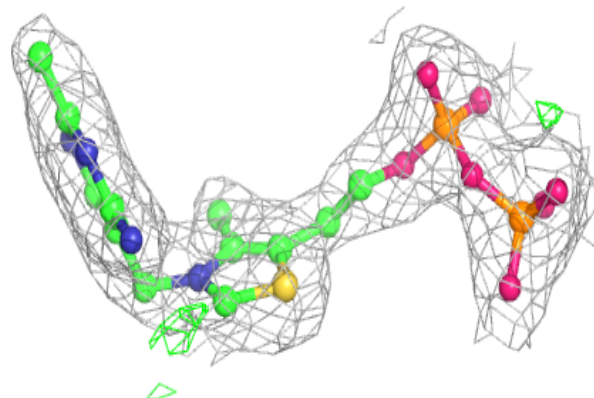


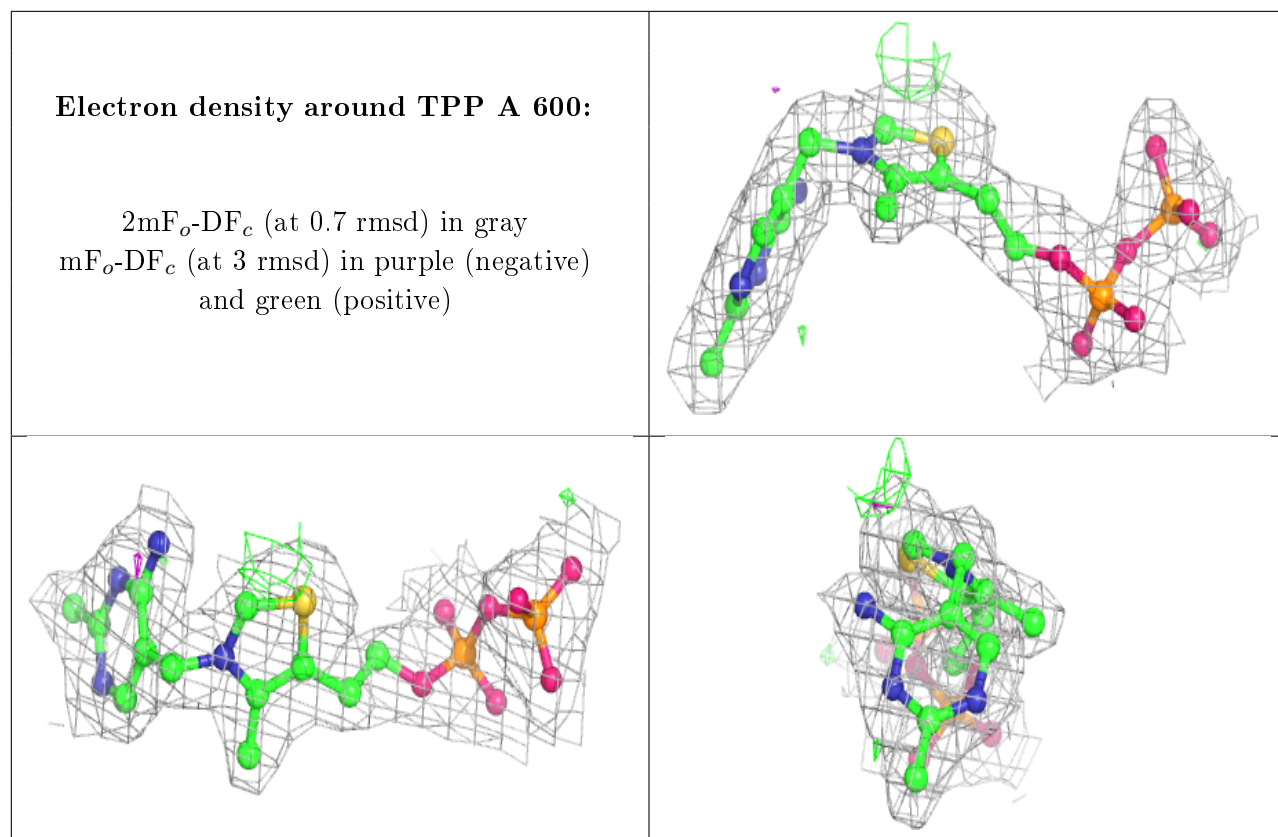
Electron density around TPP B 600:

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

**Electron density around TPP D 600:**

$2mF_o-DF_c$ (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.