



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:17 AM UTC

PDB ID : 2AG0 / pdb_00002ag0
Title : Crystal structure of Benzaldehyde lyase (BAL)- native
Authors : Mosbacher, T.G.; Mueller, M.; Schulz, G.E.
Deposited on : 2005-07-26
Resolution : 2.58 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

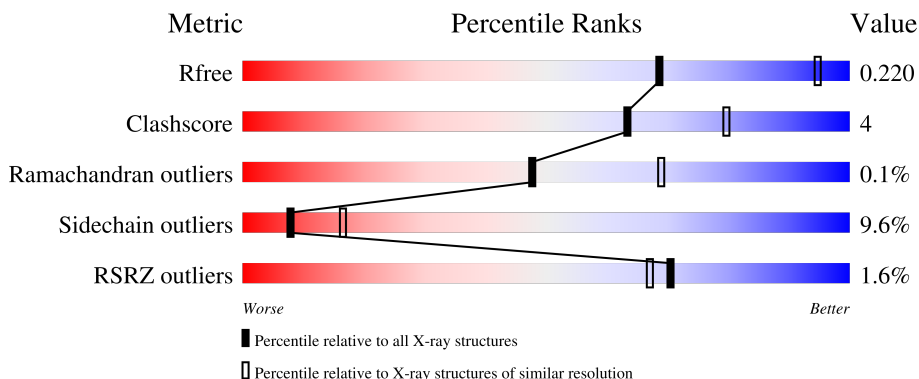
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.58 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	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (2.60-2.56)

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	563	2% 86% 11% ..
1	B	563	2% 85% 12% ..
1	C	563	2% 85% 12% ..
1	D	563	0% 85% 11% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16902 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.

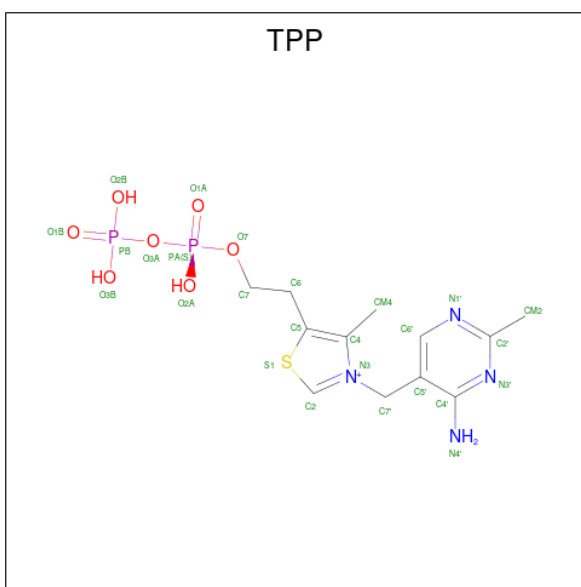
- Molecule 1 is a protein called benzaldehyde lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	554	Total	C	N	O	S	0	0	0
			4079	2576	723	764	16			
1	B	554	Total	C	N	O	S	0	0	0
			4079	2576	723	764	16			
1	C	554	Total	C	N	O	S	0	0	0
			4079	2576	723	764	16			
1	D	554	Total	C	N	O	S	0	0	0
			4079	2576	723	764	16			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula: C₁₂H₁₉N₄O₇P₂S).



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

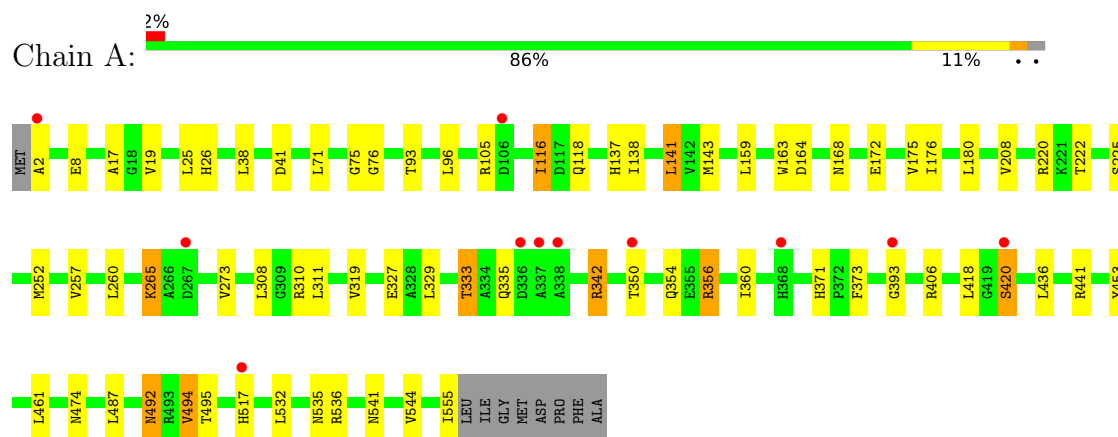
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	99	Total O 99 99	0	0
4	B	80	Total O 80 80	0	0
4	C	132	Total O 132 132	0	0
4	D	167	Total O 167 167	0	0

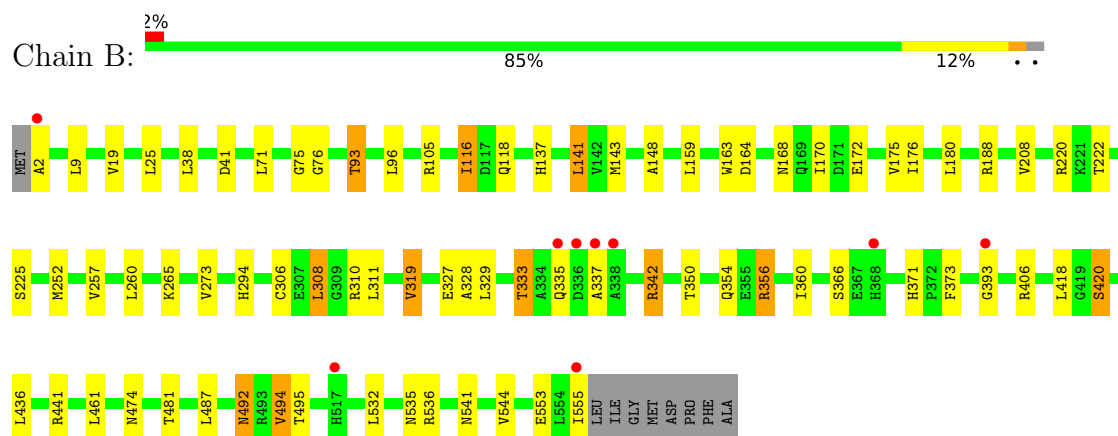
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

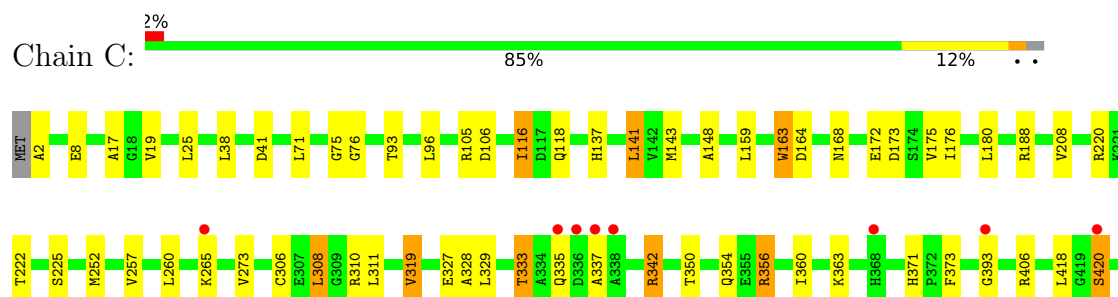
- Molecule 1: benzaldehyde lyase

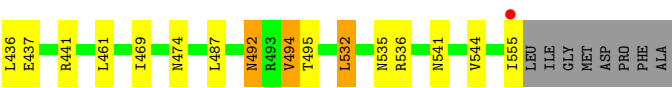


- Molecule 1: benzaldehyde lyase

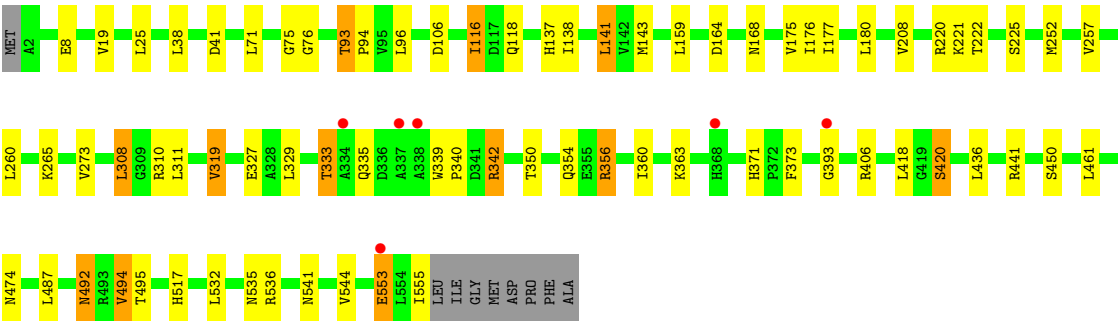
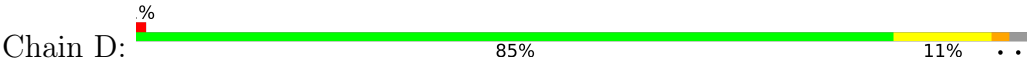


- Molecule 1: benzaldehyde lyase





● Molecule 1: benzaldehyde lyase



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	154.72Å 154.72Å 200.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.95 – 2.58 19.95 – 2.58	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.95-2.58) 97.9 (19.95-2.58)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.77 (at 2.59Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.200 , 0.220 0.200 , 0.220	Depositor DCC
R_{free} test set	4281 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	33.1	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.030 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16902	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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, 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	0.78	2/4162 (0.0%)	1.00	8/5677 (0.1%)
1	B	0.75	2/4162 (0.0%)	1.00	7/5677 (0.1%)
1	C	0.83	3/4162 (0.1%)	1.03	12/5677 (0.2%)
1	D	0.86	3/4162 (0.1%)	1.03	9/5677 (0.2%)
All	All	0.81	10/16648 (0.1%)	1.02	36/22708 (0.2%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	138	ILE	CA-CB	7.38	1.57	1.54
1	C	319	VAL	CA-CB	6.93	1.62	1.53
1	C	163	TRP	C-N	6.07	1.41	1.33
1	D	138	ILE	CA-CB	5.66	1.56	1.54
1	B	494	VAL	CA-CB	5.63	1.60	1.54
1	A	494	VAL	CA-CB	5.53	1.60	1.54
1	D	319	VAL	CA-CB	5.48	1.60	1.53
1	C	494	VAL	CA-CB	5.32	1.60	1.54
1	D	494	VAL	CA-CB	5.20	1.60	1.54
1	B	319	VAL	CA-CB	5.02	1.59	1.53

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	163	TRP	N-CA-C	9.63	122.78	111.71
1	B	164	ASP	N-CA-CB	-8.43	96.24	110.49
1	C	164	ASP	N-CA-CB	-8.31	97.18	109.82
1	A	164	ASP	N-CA-CB	-8.29	97.22	109.82
1	A	164	ASP	N-CA-C	7.39	120.04	111.02
1	C	164	ASP	N-CA-C	7.11	119.69	111.02
1	D	420	SER	N-CA-C	7.05	120.02	108.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	163	TRP	CB-CA-C	-6.75	98.14	110.63
1	D	553	GLU	CB-CA-C	-6.66	96.38	110.31
1	B	163	TRP	CB-CA-C	-6.64	96.44	110.31
1	B	420	SER	N-CA-C	6.63	119.33	108.52
1	C	420	SER	N-CA-C	6.47	119.06	108.52
1	D	164	ASP	N-CA-CB	-6.17	99.22	109.72
1	C	163	TRP	O-C-N	6.05	129.30	122.22
1	D	221	LYS	N-CA-C	5.94	117.42	111.07
1	B	393	GLY	N-CA-C	5.86	124.73	114.76
1	D	553	GLU	N-CA-C	5.71	119.51	112.54
1	A	105	ARG	N-CA-C	-5.66	103.02	110.43
1	A	163	TRP	CB-CA-C	-5.58	98.55	110.32
1	C	163	TRP	CA-C-N	5.55	128.51	120.79
1	C	163	TRP	C-N-CA	5.55	128.51	120.79
1	B	105	ARG	N-CA-C	-5.54	103.22	110.53
1	D	164	ASP	N-CA-C	5.45	120.31	111.37
1	D	393	GLY	N-CA-C	5.45	124.02	114.76
1	A	393	GLY	N-CA-C	5.33	123.83	114.76
1	B	553	GLU	CB-CA-C	-5.29	99.25	110.31
1	C	105	ARG	N-CA-C	-5.28	103.51	110.43
1	C	337	ALA	N-CA-C	5.28	119.56	113.38
1	C	393	GLY	N-CA-C	5.17	123.81	114.46
1	C	106	ASP	N-CA-C	5.16	118.87	112.47
1	A	420	SER	N-CA-C	5.15	116.91	108.52
1	A	163	TRP	CA-C-N	5.03	127.79	120.79
1	A	163	TRP	C-N-CA	5.03	127.79	120.79
1	D	106	ASP	N-CA-C	5.02	118.53	111.90
1	B	337	ALA	N-CA-C	5.01	119.25	113.38
1	D	450	SER	N-CA-C	5.00	116.73	111.28

There are no chirality outliers.

There are no planarity outliers.

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	4079	0	4069	30	2
1	B	4079	0	4069	33	0
1	C	4079	0	4069	33	1
1	D	4079	0	4069	40	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	0	16	0	0
3	B	26	0	16	0	0
3	C	26	0	16	0	0
3	D	26	0	16	1	0
4	A	99	0	0	4	0
4	B	80	0	0	4	0
4	C	132	0	0	1	0
4	D	167	0	0	13	0
All	All	16902	0	16340	130	2

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 (130) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:420:SER:HB3	4:B:5023:HOH:O	1.39	1.18
1:D:420:SER:HB3	4:D:5045:HOH:O	1.01	1.17
1:D:517:HIS:HB3	4:D:5162:HOH:O	1.60	1.02
1:B:354:GLN:HE22	1:B:406:ARG:HH12	1.03	1.01
1:D:420:SER:CB	4:D:5045:HOH:O	1.69	0.98
1:C:354:GLN:HE22	1:C:406:ARG:HH12	1.15	0.94
1:D:354:GLN:HE22	1:D:406:ARG:HH12	1.13	0.94
1:A:354:GLN:HE22	1:A:406:ARG:HH12	1.15	0.93
1:B:354:GLN:NE2	1:B:406:ARG:HH12	1.66	0.92
1:D:342:ARG:HH11	1:D:342:ARG:HG3	1.34	0.92
1:C:342:ARG:HH11	1:C:342:ARG:HG3	1.36	0.91
1:B:342:ARG:HH11	1:B:342:ARG:HG3	1.35	0.91
1:A:342:ARG:HG3	1:A:342:ARG:HH11	1.36	0.90
1:D:354:GLN:NE2	1:D:406:ARG:HH12	1.71	0.88
1:C:354:GLN:NE2	1:C:406:ARG:HH12	1.74	0.85
1:A:354:GLN:NE2	1:A:406:ARG:HH12	1.73	0.85
1:B:143:MET:HE2	1:B:180:LEU:HD13	1.59	0.84
1:D:342:ARG:HH11	1:D:342:ARG:CG	1.90	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:ARG:HH11	1:B:342:ARG:CG	1.92	0.81
1:C:342:ARG:HH11	1:C:342:ARG:CG	1.94	0.81
1:D:143:MET:HE2	1:D:180:LEU:HD13	1.63	0.80
1:A:342:ARG:HH11	1:A:342:ARG:CG	1.95	0.78
1:A:371:HIS:HD2	1:A:373:PHE:H	1.29	0.78
1:D:371:HIS:HD2	1:D:373:PHE:H	1.29	0.78
1:A:143:MET:HE2	1:A:180:LEU:HD13	1.68	0.75
1:C:143:MET:HE2	1:C:180:LEU:HD13	1.69	0.75
1:B:371:HIS:HD2	1:B:373:PHE:H	1.33	0.74
1:C:371:HIS:HD2	1:C:373:PHE:H	1.34	0.74
1:D:517:HIS:HE1	4:D:5180:HOH:O	1.76	0.69
1:A:420:SER:OG	1:B:76:GLY:HA3	1.94	0.67
1:A:116:ILE:HD11	1:A:118:GLN:HE21	1.60	0.66
1:B:116:ILE:HD11	1:B:118:GLN:HE21	1.61	0.66
1:A:8:GLU:HG2	4:A:5026:HOH:O	1.95	0.66
1:C:310:ARG:HG3	1:C:311:LEU:HG	1.80	0.64
1:D:8:GLU:HG2	4:D:5126:HOH:O	1.97	0.63
1:D:220:ARG:HD3	1:D:327:GLU:OE1	1.99	0.63
1:C:220:ARG:HD3	1:C:327:GLU:OE1	1.99	0.63
1:B:93:THR:HG21	4:B:5033:HOH:O	1.97	0.62
1:A:2:ALA:HA	1:A:172:GLU:OE1	1.99	0.62
1:A:76:GLY:HA3	1:B:420:SER:OG	1.99	0.62
1:C:420:SER:OG	1:D:76:GLY:HA3	1.99	0.62
1:B:354:GLN:HE22	1:B:406:ARG:NH1	1.87	0.61
1:A:310:ARG:HG3	1:A:311:LEU:HG	1.82	0.61
1:A:220:ARG:HD3	1:A:327:GLU:OE1	2.01	0.61
1:D:342:ARG:HD3	4:D:5133:HOH:O	2.00	0.60
1:B:220:ARG:HD3	1:B:327:GLU:OE1	2.00	0.60
1:C:116:ILE:HD11	1:C:118:GLN:HE21	1.66	0.60
1:A:453:TYR:HB3	4:A:5025:HOH:O	2.00	0.60
1:B:310:ARG:HG3	1:B:311:LEU:HG	1.83	0.60
1:D:354:GLN:HE22	1:D:406:ARG:NH1	1.95	0.59
1:D:116:ILE:HD11	1:D:118:GLN:HE21	1.67	0.59
1:D:310:ARG:HG3	1:D:311:LEU:HG	1.86	0.58
1:B:2:ALA:HA	1:B:172:GLU:OE1	2.04	0.58
1:A:342:ARG:CG	1:A:342:ARG:NH1	2.64	0.56
1:D:177:ILE:HD11	4:D:5131:HOH:O	2.07	0.55
1:D:342:ARG:CD	4:D:5133:HOH:O	2.54	0.55
1:A:492:ASN:ND2	1:A:492:ASN:H	2.05	0.55
1:C:342:ARG:CG	1:C:342:ARG:NH1	2.62	0.54
1:B:420:SER:CB	4:B:5023:HOH:O	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:ASN:H	1:A:492:ASN:HD22	1.57	0.53
1:B:342:ARG:CG	1:B:342:ARG:NH1	2.61	0.53
1:C:8:GLU:HG2	4:C:5117:HOH:O	2.07	0.53
1:C:356:ARG:O	1:C:360:ILE:HG12	2.09	0.53
1:A:356:ARG:O	1:A:360:ILE:HG12	2.08	0.52
1:D:492:ASN:ND2	1:D:492:ASN:H	2.07	0.52
1:B:137:HIS:HB3	1:B:141:LEU:HD22	1.91	0.52
1:B:492:ASN:ND2	1:B:492:ASN:H	2.08	0.52
1:A:354:GLN:HE22	1:A:406:ARG:NH1	1.97	0.52
1:B:356:ARG:O	1:B:360:ILE:HG12	2.10	0.51
1:C:492:ASN:ND2	1:C:492:ASN:H	2.08	0.51
1:D:553:GLU:O	1:D:553:GLU:CG	2.59	0.51
1:A:329:LEU:O	1:A:333:THR:HB	2.10	0.50
1:C:2:ALA:HA	1:C:172:GLU:OE1	2.11	0.50
1:C:492:ASN:H	1:C:492:ASN:HD22	1.60	0.50
1:C:535:ASN:O	1:C:536:ARG:HG3	2.12	0.50
1:D:116:ILE:HD13	4:D:5149:HOH:O	2.10	0.50
1:A:342:ARG:HD3	4:A:5074:HOH:O	2.12	0.50
1:B:492:ASN:H	1:B:492:ASN:HD22	1.59	0.50
1:D:356:ARG:O	1:D:360:ILE:HG12	2.12	0.50
1:B:75:GLY:H	1:B:118:GLN:HE22	1.60	0.49
1:D:137:HIS:HB3	1:D:141:LEU:HD22	1.95	0.49
1:C:354:GLN:HE22	1:C:406:ARG:NH1	1.97	0.49
1:C:17:ALA:HB2	1:C:143:MET:HE1	1.95	0.49
1:D:474:ASN:HD22	1:D:541:ASN:HD21	1.60	0.49
1:D:517:HIS:CD2	4:D:5203:HOH:O	2.66	0.48
1:B:329:LEU:O	1:B:333:THR:HB	2.14	0.48
1:A:371:HIS:CD2	1:A:373:PHE:H	2.20	0.48
1:D:93:THR:HG21	4:D:5046:HOH:O	2.14	0.48
1:A:137:HIS:HB3	1:A:141:LEU:HD22	1.96	0.48
1:D:492:ASN:H	1:D:492:ASN:HD22	1.61	0.47
1:C:137:HIS:HB3	1:C:141:LEU:HD22	1.96	0.47
1:A:75:GLY:H	1:A:118:GLN:HE22	1.63	0.47
1:A:535:ASN:O	1:A:536:ARG:HG3	2.16	0.46
1:A:342:ARG:CD	4:A:5074:HOH:O	2.64	0.46
1:C:163:TRP:O	1:C:163:TRP:CD1	2.68	0.46
1:A:26:HIS:CD2	1:B:481:THR:HB	2.51	0.46
1:B:294:HIS:HD2	4:B:5053:HOH:O	1.99	0.45
1:C:75:GLY:H	1:C:118:GLN:HE22	1.63	0.45
1:A:17:ALA:HB2	1:A:143:MET:HE1	1.99	0.44
1:D:93:THR:HA	1:D:94:PRO:HD3	1.92	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:342:ARG:CG	1:D:342:ARG:NH1	2.60	0.44
1:D:75:GLY:H	1:D:118:GLN:HE22	1.65	0.44
1:C:76:GLY:HA3	1:D:420:SER:OG	2.17	0.44
1:C:329:LEU:O	1:C:333:THR:HB	2.17	0.43
1:D:339:TRP:HA	1:D:340:PRO:HD3	1.92	0.43
1:B:474:ASN:HD22	1:B:541:ASN:HD21	1.67	0.43
1:C:474:ASN:HD22	1:C:541:ASN:HD21	1.65	0.43
1:B:75:GLY:H	1:B:118:GLN:NE2	2.16	0.43
1:B:354:GLN:NE2	1:B:406:ARG:NH1	2.49	0.42
1:D:329:LEU:O	1:D:333:THR:HB	2.19	0.42
1:B:188:ARG:HD3	1:B:328:ALA:HB2	2.01	0.42
1:D:535:ASN:O	1:D:536:ARG:HG3	2.19	0.42
1:B:148:ALA:HB2	1:C:306:CYS:SG	2.59	0.42
1:A:474:ASN:HD22	1:A:541:ASN:HD21	1.68	0.42
1:A:143:MET:HE3	1:A:143:MET:HA	2.01	0.42
1:D:553:GLU:O	1:D:553:GLU:HG2	2.19	0.42
1:B:535:ASN:O	1:B:536:ARG:HG3	2.19	0.42
1:C:188:ARG:HD3	1:C:328:ALA:HB2	2.02	0.42
1:D:363:LYS:HE2	1:D:363:LYS:HB3	1.85	0.42
1:C:363:LYS:HE2	1:C:363:LYS:HB3	1.89	0.41
1:D:492:ASN:HD22	1:D:492:ASN:N	2.18	0.41
1:C:371:HIS:CD2	1:C:373:PHE:H	2.25	0.41
1:C:354:GLN:NE2	1:C:406:ARG:NH1	2.56	0.41
3:D:632:TPP:H62	3:D:632:TPP:HM41	1.89	0.41
1:B:9:LEU:HD11	1:B:170:ILE:HD11	2.02	0.41
1:D:177:ILE:CD1	4:D:5131:HOH:O	2.68	0.41
1:B:306:CYS:SG	1:C:148:ALA:HB2	2.62	0.40
1:C:75:GLY:H	1:C:118:GLN:NE2	2.19	0.40
1:D:517:HIS:HD2	4:D:5203:HOH:O	2.04	0.40
1:C:469:ILE:CD1	1:C:532:LEU:HD13	2.51	0.40

All (2) 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:A:265:LYS:O	1:A:265:LYS:O[6_555]	2.13	0.07
1:A:517:HIS:CD2	1:C:173:ASP:OD1[4_545]	2.14	0.06

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	552/563 (98%)	535 (97%)	17 (3%)	0	100	100
1	B	552/563 (98%)	532 (96%)	19 (3%)	1 (0%)	43	63
1	C	552/563 (98%)	534 (97%)	17 (3%)	1 (0%)	43	63
1	D	552/563 (98%)	534 (97%)	17 (3%)	1 (0%)	43	63
All	All	2208/2252 (98%)	2135 (97%)	70 (3%)	3 (0%)	48	69

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	308	LEU
1	C	308	LEU
1	D	308	LEU

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	412/419 (98%)	373 (90%)	39 (10%)	8	17
1	B	412/419 (98%)	372 (90%)	40 (10%)	8	16
1	C	412/419 (98%)	372 (90%)	40 (10%)	8	16
1	D	412/419 (98%)	373 (90%)	39 (10%)	8	17
All	All	1648/1676 (98%)	1490 (90%)	158 (10%)	8	16

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	VAL
1	A	25	LEU
1	A	38	LEU
1	A	41	ASP
1	A	71	LEU
1	A	93	THR
1	A	96	LEU
1	A	116	ILE
1	A	141	LEU
1	A	159	LEU
1	A	168	ASN
1	A	175	VAL
1	A	176	ILE
1	A	208	VAL
1	A	222	THR
1	A	225	SER
1	A	252	MET
1	A	257	VAL
1	A	260	LEU
1	A	265	LYS
1	A	273	VAL
1	A	308	LEU
1	A	319	VAL
1	A	333	THR
1	A	335	GLN
1	A	342	ARG
1	A	350	THR
1	A	356	ARG
1	A	418	LEU
1	A	436	LEU
1	A	441	ARG
1	A	461	LEU
1	A	487	LEU
1	A	492	ASN
1	A	494	VAL
1	A	495	THR
1	A	532	LEU
1	A	544	VAL
1	A	555	ILE
1	B	19	VAL
1	B	25	LEU
1	B	38	LEU
1	B	41	ASP

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Mol	Chain	Res	Type
1	B	71	LEU
1	B	93	THR
1	B	96	LEU
1	B	116	ILE
1	B	141	LEU
1	B	159	LEU
1	B	168	ASN
1	B	175	VAL
1	B	176	ILE
1	B	208	VAL
1	B	222	THR
1	B	225	SER
1	B	252	MET
1	B	257	VAL
1	B	260	LEU
1	B	265	LYS
1	B	273	VAL
1	B	308	LEU
1	B	319	VAL
1	B	333	THR
1	B	335	GLN
1	B	342	ARG
1	B	350	THR
1	B	356	ARG
1	B	366	SER
1	B	418	LEU
1	B	436	LEU
1	B	441	ARG
1	B	461	LEU
1	B	487	LEU
1	B	492	ASN
1	B	494	VAL
1	B	495	THR
1	B	532	LEU
1	B	544	VAL
1	B	555	ILE
1	C	19	VAL
1	C	25	LEU
1	C	38	LEU
1	C	41	ASP
1	C	71	LEU
1	C	93	THR

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Mol	Chain	Res	Type
1	C	96	LEU
1	C	116	ILE
1	C	141	LEU
1	C	159	LEU
1	C	168	ASN
1	C	175	VAL
1	C	176	ILE
1	C	208	VAL
1	C	222	THR
1	C	225	SER
1	C	252	MET
1	C	257	VAL
1	C	260	LEU
1	C	265	LYS
1	C	273	VAL
1	C	308	LEU
1	C	319	VAL
1	C	333	THR
1	C	335	GLN
1	C	342	ARG
1	C	350	THR
1	C	356	ARG
1	C	418	LEU
1	C	436	LEU
1	C	437	GLU
1	C	441	ARG
1	C	461	LEU
1	C	487	LEU
1	C	492	ASN
1	C	494	VAL
1	C	495	THR
1	C	532	LEU
1	C	544	VAL
1	C	555	ILE
1	D	19	VAL
1	D	25	LEU
1	D	38	LEU
1	D	41	ASP
1	D	71	LEU
1	D	93	THR
1	D	96	LEU
1	D	116	ILE

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Mol	Chain	Res	Type
1	D	141	LEU
1	D	159	LEU
1	D	168	ASN
1	D	175	VAL
1	D	176	ILE
1	D	208	VAL
1	D	222	THR
1	D	225	SER
1	D	252	MET
1	D	257	VAL
1	D	260	LEU
1	D	265	LYS
1	D	273	VAL
1	D	308	LEU
1	D	319	VAL
1	D	333	THR
1	D	335	GLN
1	D	342	ARG
1	D	350	THR
1	D	356	ARG
1	D	418	LEU
1	D	436	LEU
1	D	441	ARG
1	D	461	LEU
1	D	487	LEU
1	D	492	ASN
1	D	494	VAL
1	D	495	THR
1	D	532	LEU
1	D	544	VAL
1	D	555	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	HIS
1	A	113	GLN
1	A	118	GLN
1	A	258	GLN
1	A	259	ASN
1	A	294	HIS
1	A	297	GLN

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Mol	Chain	Res	Type
1	A	354	GLN
1	A	371	HIS
1	A	374	HIS
1	A	492	ASN
1	A	535	ASN
1	A	541	ASN
1	B	26	HIS
1	B	113	GLN
1	B	118	GLN
1	B	258	GLN
1	B	259	ASN
1	B	294	HIS
1	B	297	GLN
1	B	335	GLN
1	B	354	GLN
1	B	371	HIS
1	B	374	HIS
1	B	492	ASN
1	B	535	ASN
1	B	541	ASN
1	C	26	HIS
1	C	29	HIS
1	C	113	GLN
1	C	118	GLN
1	C	168	ASN
1	C	258	GLN
1	C	259	ASN
1	C	294	HIS
1	C	297	GLN
1	C	335	GLN
1	C	354	GLN
1	C	371	HIS
1	C	374	HIS
1	C	492	ASN
1	C	534	HIS
1	C	535	ASN
1	C	541	ASN
1	D	26	HIS
1	D	113	GLN
1	D	118	GLN
1	D	168	ASN
1	D	196	GLN

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Mol	Chain	Res	Type
1	D	259	ASN
1	D	294	HIS
1	D	297	GLN
1	D	335	GLN
1	D	354	GLN
1	D	371	HIS
1	D	374	HIS
1	D	415	HIS
1	D	492	ASN
1	D	535	ASN
1	D	541	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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	TPP	B	612	2	26,27,27	2.60	7 (26%)	38,40,40	3.14	14 (36%)
3	TPP	C	622	2	26,27,27	2.78	6 (23%)	38,40,40	2.59	9 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	TPP	D	632	2	26,27,27	2.86	8 (30%)	38,40,40	2.32	10 (26%)
3	TPP	A	602	2	26,27,27	2.72	6 (23%)	38,40,40	2.60	10 (26%)

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	B	612	2	-	8/17/17/17	0/2/2/2
3	TPP	C	622	2	-	5/17/17/17	0/2/2/2
3	TPP	D	632	2	-	7/17/17/17	0/2/2/2
3	TPP	A	602	2	-	4/17/17/17	0/2/2/2

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	632	TPP	CM4-C4	-8.35	1.32	1.49
3	C	622	TPP	CM4-C4	-8.26	1.33	1.49
3	A	602	TPP	CM4-C4	-8.04	1.33	1.49
3	B	612	TPP	CM4-C4	-8.00	1.33	1.49
3	D	632	TPP	C6-C5	-6.66	1.36	1.50
3	A	602	TPP	C6-C5	-6.58	1.36	1.50
3	C	622	TPP	C6-C5	-6.58	1.36	1.50
3	D	632	TPP	C2-N3	6.41	1.48	1.32
3	C	622	TPP	C2-N3	6.14	1.47	1.32
3	A	602	TPP	C2-N3	5.99	1.47	1.32
3	B	612	TPP	C2-N3	5.86	1.46	1.32
3	B	612	TPP	C6-C5	-5.53	1.38	1.50
3	A	602	TPP	C5'-C4'	4.59	1.50	1.42
3	C	622	TPP	C5'-C4'	4.22	1.49	1.42
3	D	632	TPP	C5'-C4'	4.03	1.49	1.42
3	B	612	TPP	C5'-C4'	3.87	1.49	1.42
3	D	632	TPP	C2-S1	2.85	1.77	1.69
3	C	622	TPP	PA-O3A	2.74	1.62	1.59
3	D	632	TPP	PA-O3A	2.68	1.62	1.59
3	C	622	TPP	C2-S1	2.63	1.77	1.69
3	B	612	TPP	C2'-N1'	2.61	1.38	1.34
3	A	602	TPP	C2-S1	2.52	1.76	1.69
3	B	612	TPP	PA-O3A	2.51	1.62	1.59
3	A	602	TPP	C5-S1	-2.48	1.66	1.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	632	TPP	C4-N3	-2.29	1.35	1.39
3	B	612	TPP	C2-S1	2.24	1.76	1.69
3	D	632	TPP	C2'-N1'	2.21	1.37	1.34

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	612	TPP	C2-S1-C5	9.73	97.66	91.22
3	A	602	TPP	C2-S1-C5	8.89	97.10	91.22
3	B	612	TPP	S1-C2-N3	-8.84	101.10	112.30
3	A	602	TPP	S1-C2-N3	-8.69	101.29	112.30
3	C	622	TPP	S1-C2-N3	-8.19	101.92	112.30
3	C	622	TPP	C2-S1-C5	7.64	96.28	91.22
3	D	632	TPP	S1-C2-N3	-6.80	103.68	112.30
3	D	632	TPP	C7-C6-C5	5.74	130.74	112.73
3	C	622	TPP	C7-C6-C5	5.58	130.25	112.73
3	B	612	TPP	C7-C6-C5	5.54	130.11	112.73
3	B	612	TPP	CM2-C2'-N1'	5.28	122.82	117.20
3	B	612	TPP	C6'-N1'-C2'	5.08	124.42	116.07
3	B	612	TPP	C7'-N3-C2	-4.85	113.37	123.48
3	D	632	TPP	CM2-C2'-N1'	4.56	122.06	117.20
3	A	602	TPP	C7-C6-C5	4.50	126.85	112.73
3	D	632	TPP	C2-S1-C5	4.27	94.04	91.22
3	B	612	TPP	C5'-C6'-N1'	-4.03	117.28	123.83
3	D	632	TPP	C6-C5-C4	-3.73	118.80	128.17
3	C	622	TPP	C6'-N1'-C2'	3.67	122.11	116.07
3	A	602	TPP	C6'-N1'-C2'	3.66	122.09	116.07
3	A	602	TPP	C7'-N3-C2	-3.57	116.04	123.48
3	C	622	TPP	C7'-N3-C2	-3.53	116.12	123.48
3	D	632	TPP	C6'-N1'-C2'	3.51	121.84	116.07
3	D	632	TPP	C6-C5-S1	3.44	128.94	120.90
3	C	622	TPP	C6-C5-S1	3.18	128.35	120.90
3	B	612	TPP	C6-C5-S1	3.09	128.14	120.90
3	A	602	TPP	CM2-C2'-N1'	2.87	120.26	117.20
3	C	622	TPP	C6-C5-C4	-2.81	121.12	128.17
3	D	632	TPP	N1'-C2'-N3'	-2.80	120.86	125.53
3	B	612	TPP	C7'-N3-C4	2.77	129.70	122.36
3	B	612	TPP	N1'-C2'-N3'	-2.75	120.95	125.53
3	A	602	TPP	N1'-C2'-N3'	-2.65	121.11	125.53
3	C	622	TPP	N1'-C2'-N3'	-2.62	121.17	125.53
3	D	632	TPP	C7'-N3-C2	-2.60	118.06	123.48
3	C	622	TPP	N4'-C4'-N3'	2.57	120.50	117.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	612	TPP	C6-C5-C4	-2.34	122.31	128.17
3	A	602	TPP	C5'-C6'-N1'	-2.16	120.32	123.83
3	B	612	TPP	C2-N3-C4	2.12	116.92	114.06
3	B	612	TPP	C5'-C4'-N4'	-2.11	119.30	122.14
3	B	612	TPP	CM4-C4-C5	-2.10	122.36	127.75
3	A	602	TPP	C7'-N3-C4	2.10	127.93	122.36
3	D	632	TPP	O3A-PB-O1B	-2.05	100.24	111.04
3	A	602	TPP	O3B-PB-O2B	2.01	115.34	107.80

There are no chirality outliers.

All (24) torsion outliers are listed below:

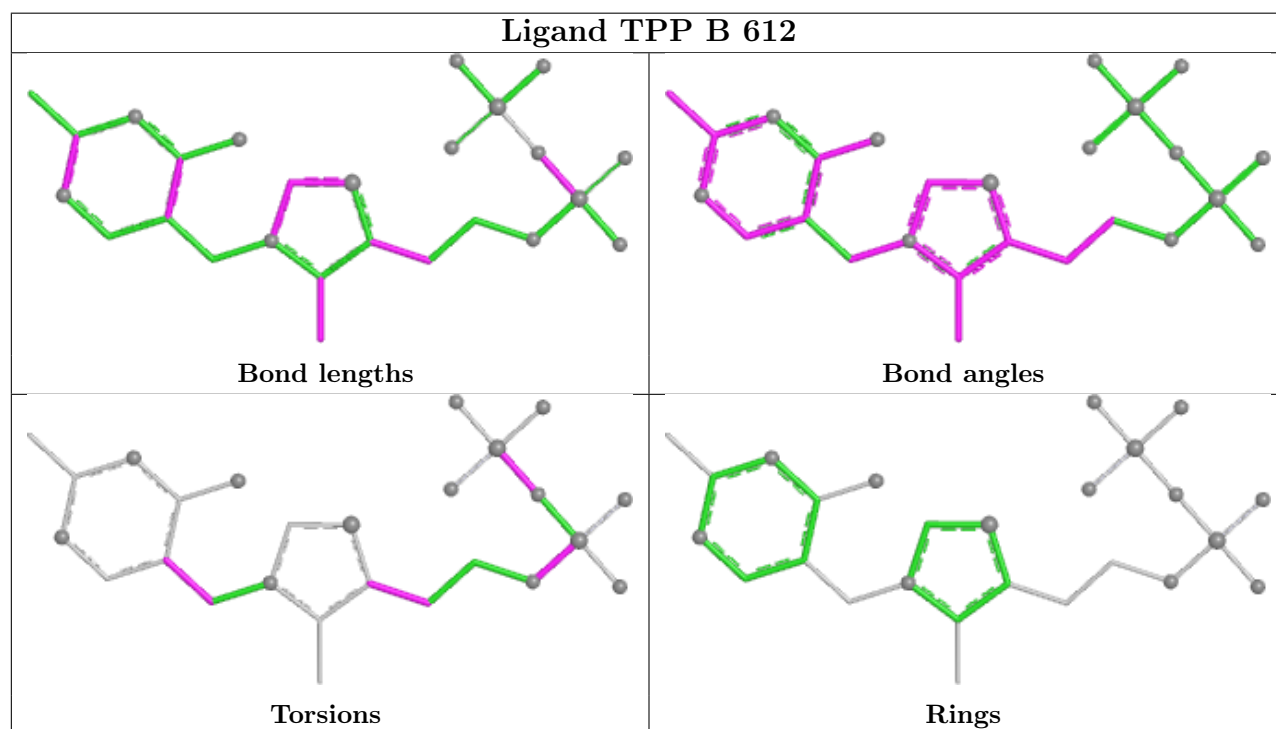
Mol	Chain	Res	Type	Atoms
3	B	612	TPP	C7-O7-PA-O2A
3	B	612	TPP	C7-O7-PA-O3A
3	C	622	TPP	C7-O7-PA-O2A
3	C	622	TPP	C7-O7-PA-O3A
3	D	632	TPP	C7-O7-PA-O2A
3	D	632	TPP	PA-O3A-PB-O3B
3	A	602	TPP	PA-O3A-PB-O1B
3	B	612	TPP	PA-O3A-PB-O1B
3	D	632	TPP	PA-O3A-PB-O1B
3	B	612	TPP	C6'-C5'-C7'-N3
3	A	602	TPP	S1-C5-C6-C7
3	B	612	TPP	S1-C5-C6-C7
3	C	622	TPP	S1-C5-C6-C7
3	D	632	TPP	S1-C5-C6-C7
3	A	602	TPP	PA-O3A-PB-O3B
3	B	612	TPP	PA-O3A-PB-O3B
3	A	602	TPP	C4-C5-C6-C7
3	B	612	TPP	C4-C5-C6-C7
3	C	622	TPP	C4-C5-C6-C7
3	D	632	TPP	C4-C5-C6-C7
3	B	612	TPP	C4'-C5'-C7'-N3
3	D	632	TPP	C7-O7-PA-O1A
3	D	632	TPP	C7-O7-PA-O3A
3	C	622	TPP	PA-O3A-PB-O1B

There are no ring outliers.

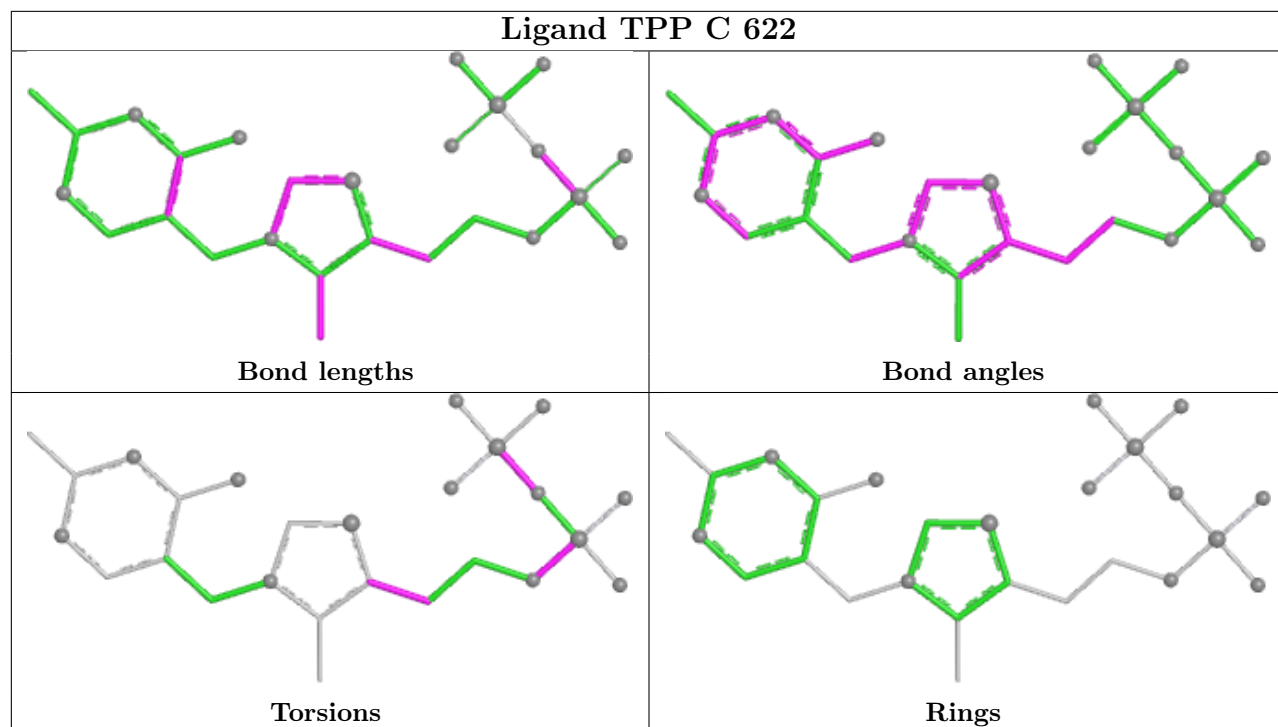
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	632	TPP	1	0

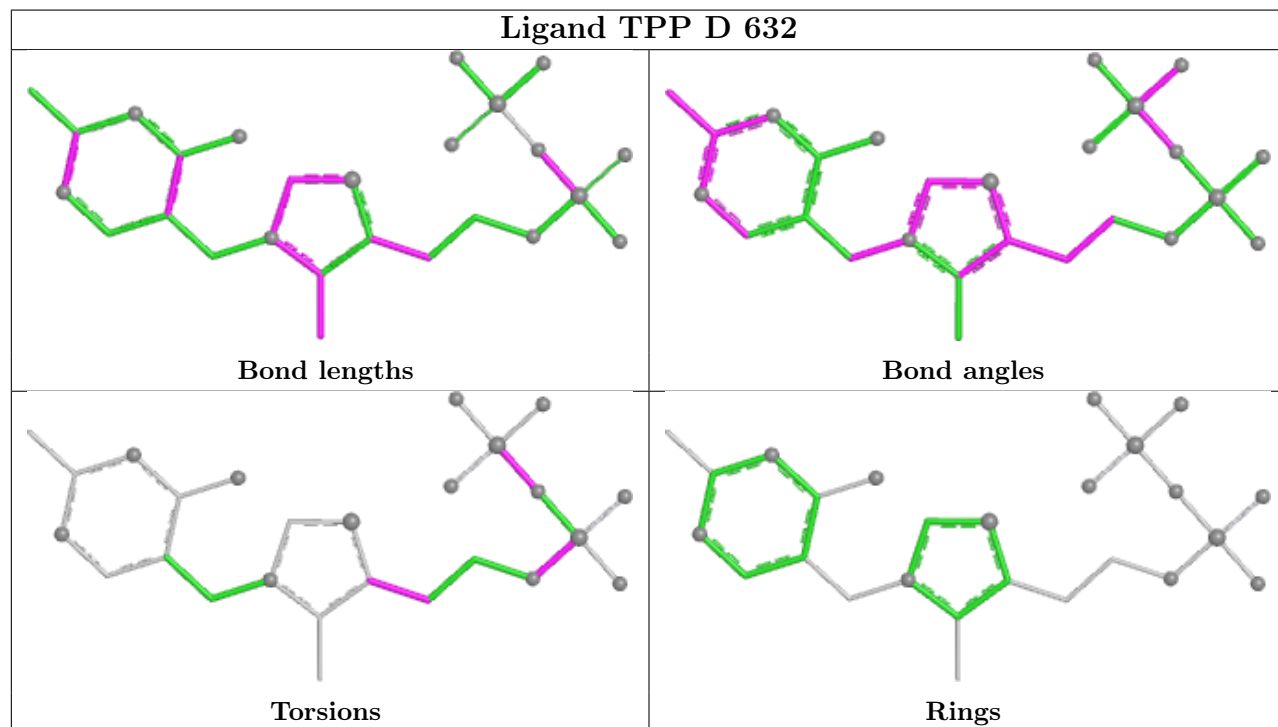
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

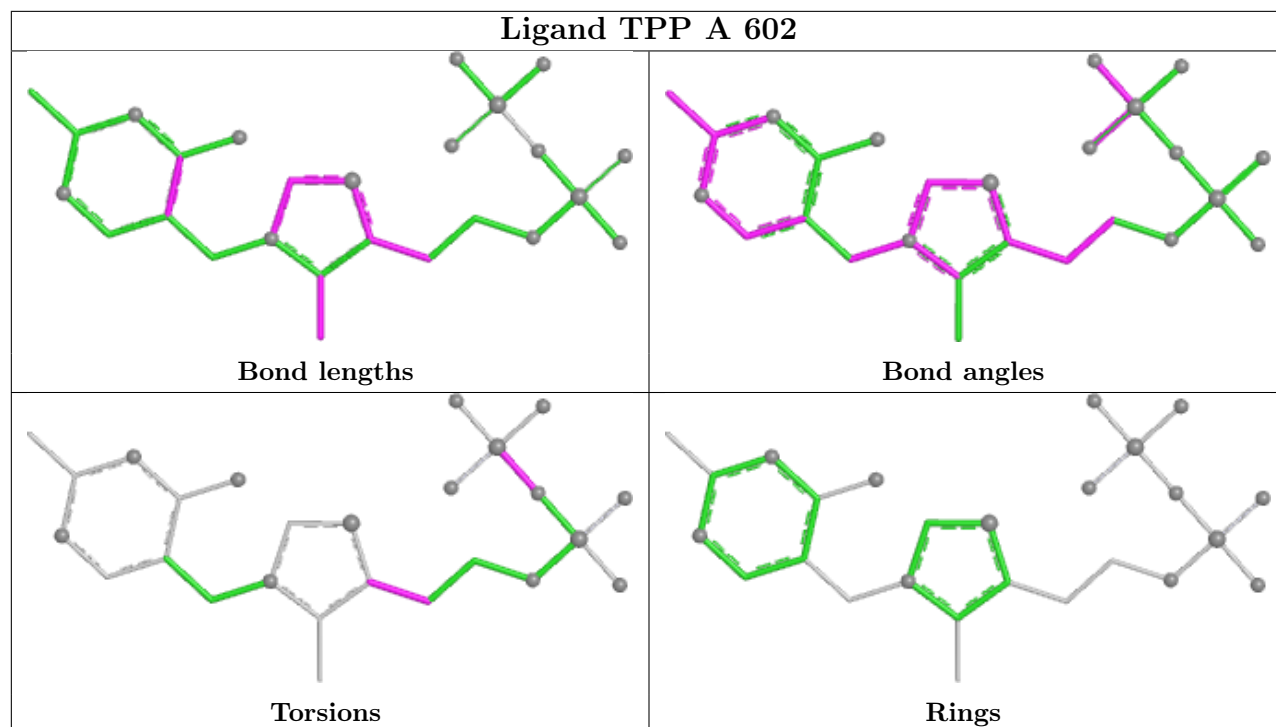


Ligand TPP C 622



Ligand TPP D 632





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	554/563 (98%)	-0.07	11 (1%) 65 61	18, 38, 68, 94	0
1	B	554/563 (98%)	-0.09	9 (1%) 70 67	22, 41, 66, 84	0
1	C	554/563 (98%)	-0.34	9 (1%) 70 67	15, 28, 49, 62	0
1	D	554/563 (98%)	-0.41	6 (1%) 78 75	14, 25, 38, 55	0
All	All	2216/2252 (98%)	-0.23	35 (1%) 70 67	14, 32, 62, 94	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	337	ALA	5.3
1	C	337	ALA	5.2
1	B	335	GLN	5.0
1	B	338	ALA	4.6
1	B	2	ALA	4.4
1	C	338	ALA	4.1
1	B	336	ASP	3.9
1	A	338	ALA	3.9
1	A	336	ASP	3.7
1	A	368	HIS	3.7
1	C	393	GLY	3.3
1	B	337	ALA	3.2
1	A	517	HIS	3.1
1	D	368	HIS	3.1
1	C	368	HIS	3.0
1	B	393	GLY	2.9
1	C	336	ASP	2.9
1	A	267	ASP	2.8
1	C	335	GLN	2.8
1	B	517	HIS	2.7
1	A	2	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	334	ALA	2.6
1	A	350	THR	2.5
1	A	393	GLY	2.4
1	C	555	ILE	2.4
1	B	368	HIS	2.4
1	D	393	GLY	2.3
1	C	420	SER	2.2
1	D	337	ALA	2.2
1	D	553	GLU	2.2
1	D	338	ALA	2.1
1	B	555	ILE	2.1
1	A	106	ASP	2.1
1	A	420	SER	2.1
1	C	265	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

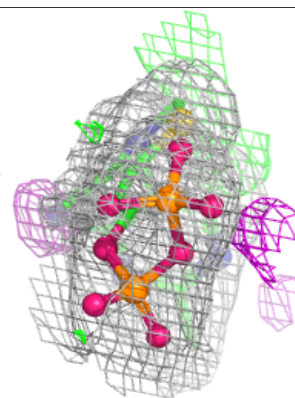
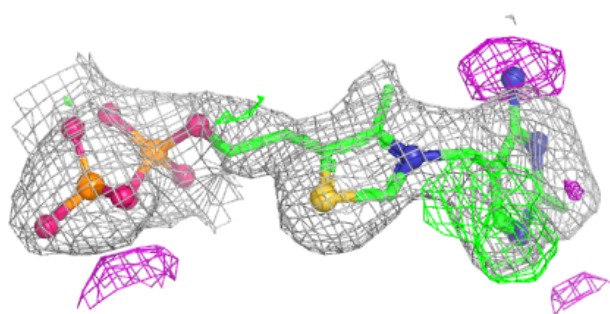
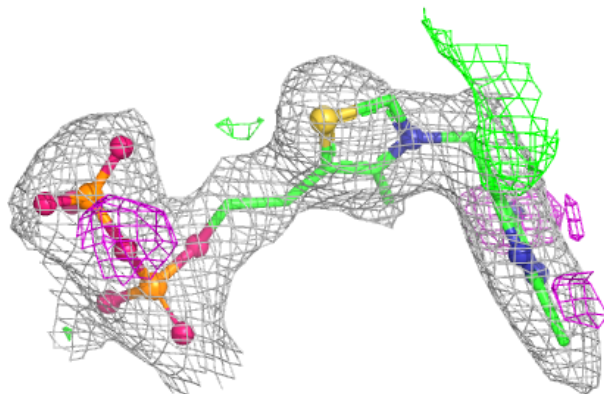
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	TPP	B	612	26/26	0.92	0.10	32,37,38,39	0
3	TPP	A	602	26/26	0.94	0.09	39,42,44,44	0
2	MG	A	601	1/1	0.96	0.05	47,47,47,47	0
3	TPP	C	622	26/26	0.97	0.06	22,27,28,29	0
3	TPP	D	632	26/26	0.98	0.05	16,18,20,21	0
2	MG	C	621	1/1	0.99	0.03	22,22,22,22	0
2	MG	D	631	1/1	0.99	0.03	18,18,18,18	0
2	MG	B	611	1/1	0.99	0.04	31,31,31,31	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.

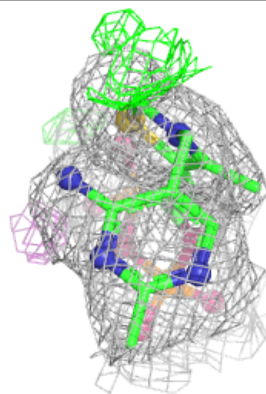
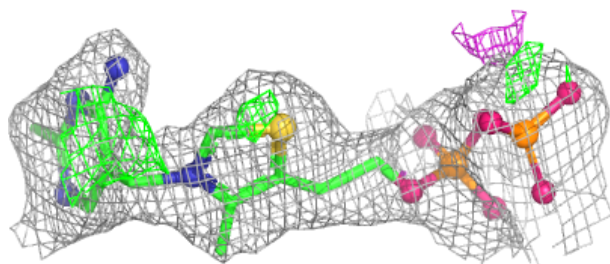
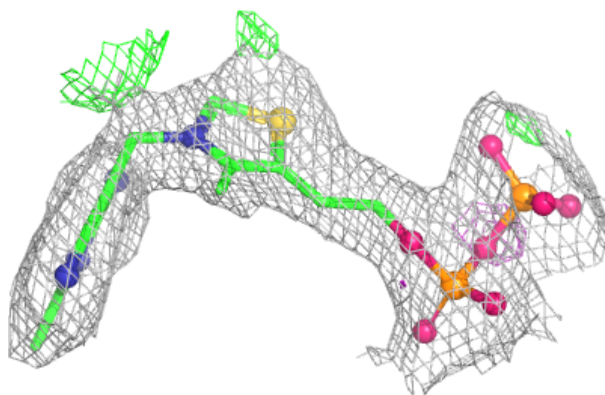
Electron density around TPP B 612:

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

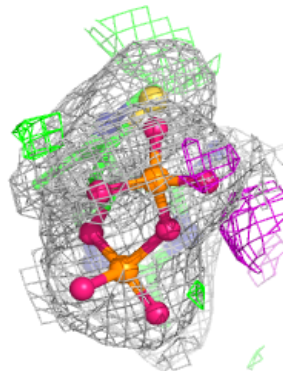
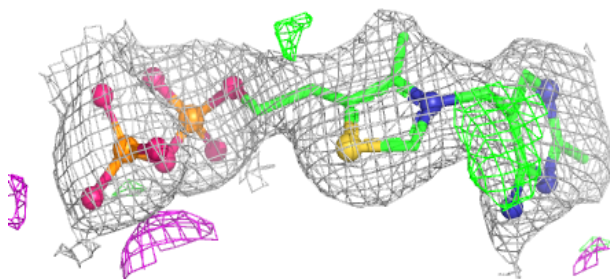
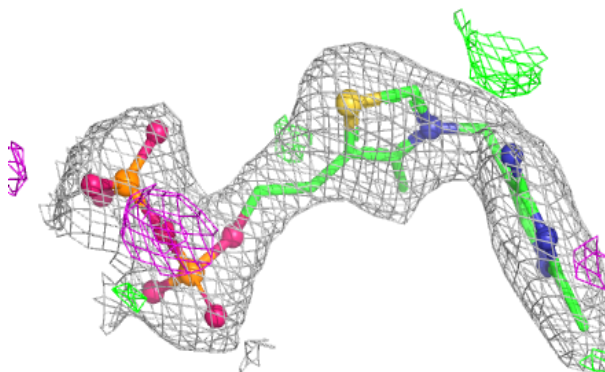


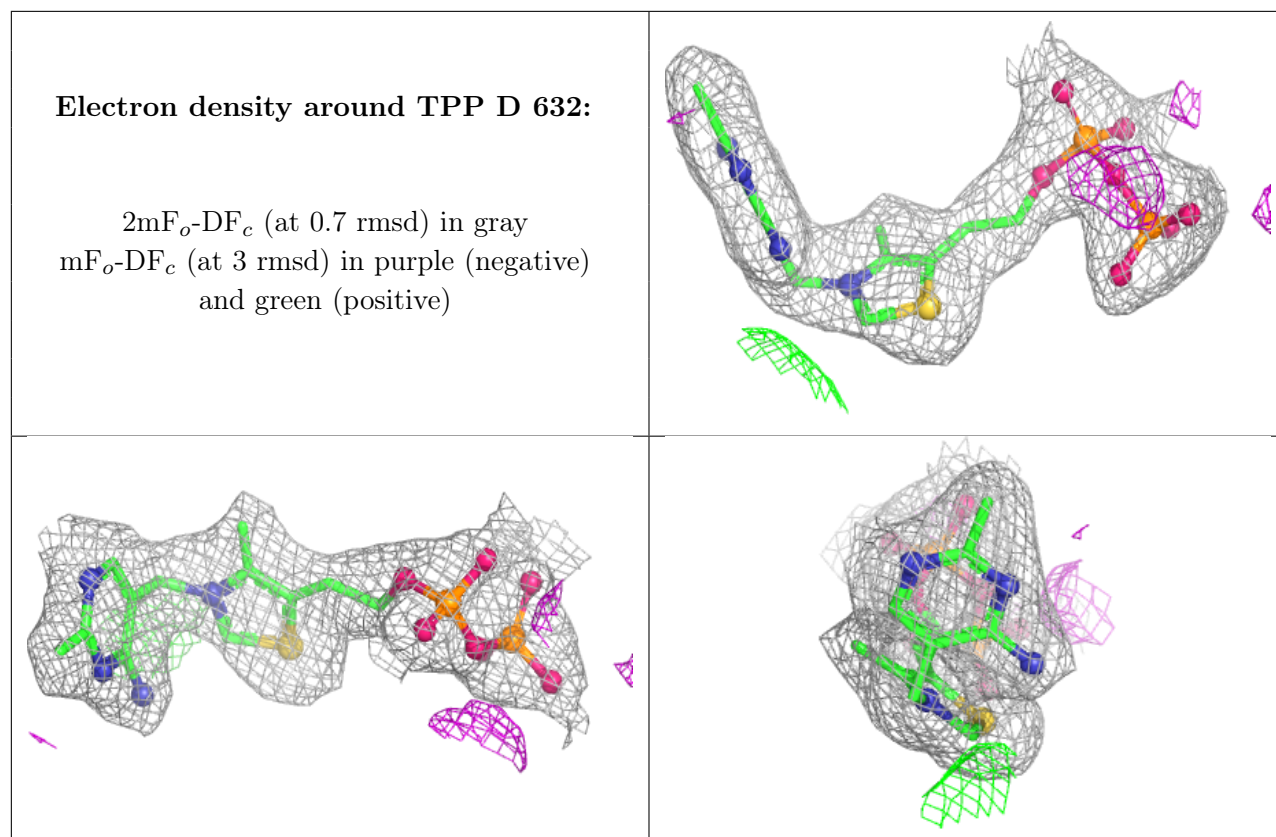
Electron density around TPP A 602:

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

**Electron density around TPP C 622:**

$2mF_o-DF_c$ (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.