



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:08 AM UTC

PDB ID : 2XTA / pdb_00002xta
Title : Crystal structure of the SucA domain of Mycobacterium smegmatis alpha-ketoglutarate decarboxylase in complex with acetyl-CoA (triclinic form)
Authors : Wagner, T.; Bellinzoni, M.; Wehenkel, A.M.; O'Hare, H.M.; Alzari, P.M.
Deposited on : 2010-10-05
Resolution : 2.20 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)
Xtrriage (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

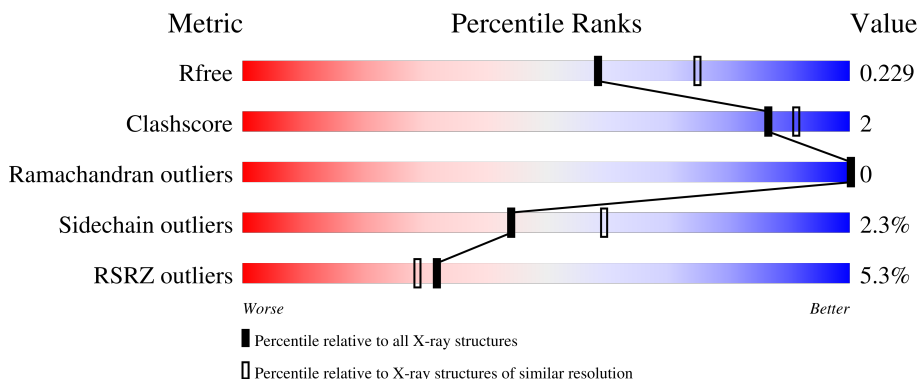
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	868	 5% 88% 7% • 5%
1	B	868	 6% 87% 6% 6%
1	C	868	 5% 87% 7% • 6%
1	D	868	 4% 87% 7% 6%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 26097 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.

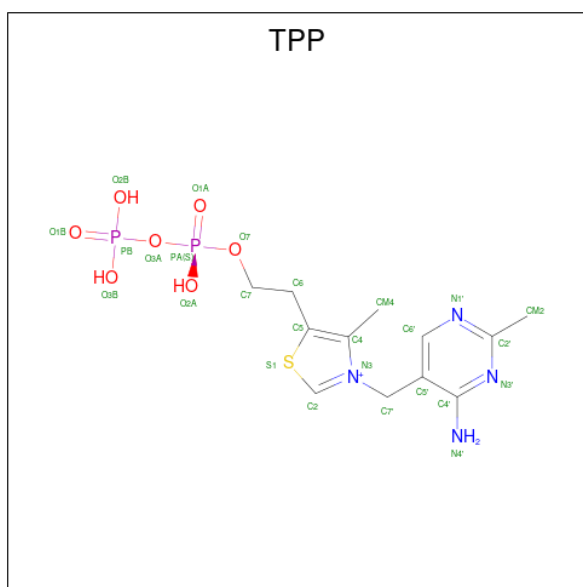
- Molecule 1 is a protein called 2-OXOGLUTARATE DECARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	826	Total 6360	C 4007	N 1128	O 1202	S 23	0	0	0
1	B	814	Total 6223	C 3925	N 1105	O 1169	S 24	0	0	0
1	C	817	Total 6309	C 3980	N 1112	O 1193	S 24	0	0	0
1	D	818	Total 6252	C 3939	N 1105	O 1184	S 24	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	360	GLY	-	expression tag	UNP A0R2B1
B	360	GLY	-	expression tag	UNP A0R2B1
C	360	GLY	-	expression tag	UNP A0R2B1
D	360	GLY	-	expression tag	UNP A0R2B1

- Molecule 2 is THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula: C₁₂H₁₉N₄O₇P₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
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		
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 (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

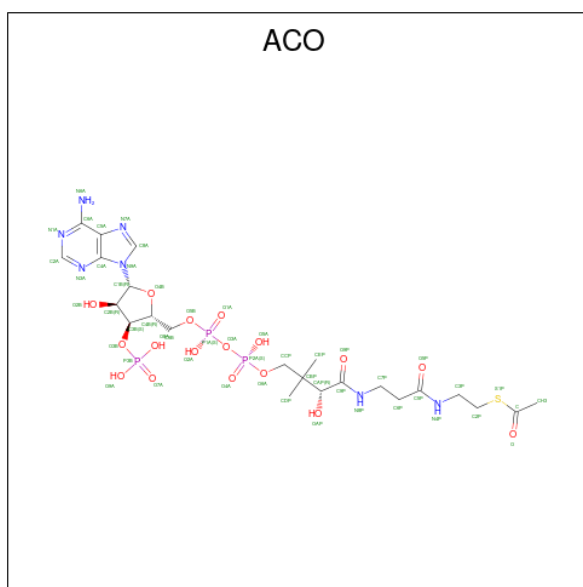
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
4	A	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Ca 1 1	0	0
4	C	1	Total Ca 1 1	0	0
4	D	1	Total Ca 1 1	0	0

- Molecule 5 is ACETYL COENZYME *A (CCD ID: ACO) (formula: $C_{23}H_{38}N_7O_{17}P_3S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O P 33 12 5 13 3	0	0
5	C	1	Total C N O P 33 12 5 13 3	0	0
5	D	1	Total C N O P 33 12 5 13 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	190	Total O 190 190	0	0
6	B	186	Total O 186 186	0	0
6	C	183	Total O 183 183	0	0

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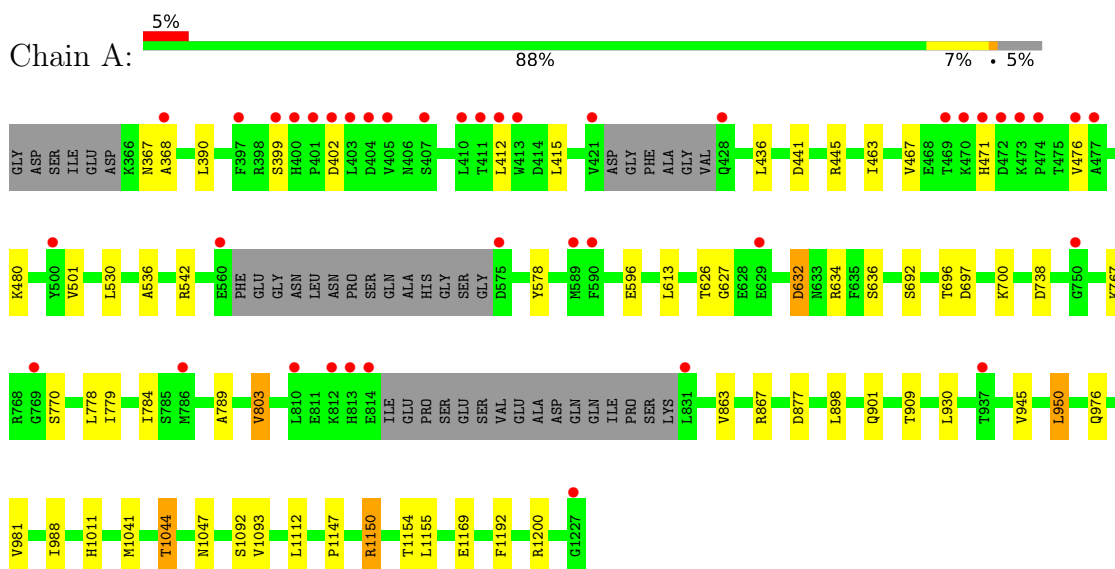
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	183	Total 183	O 183	0	0

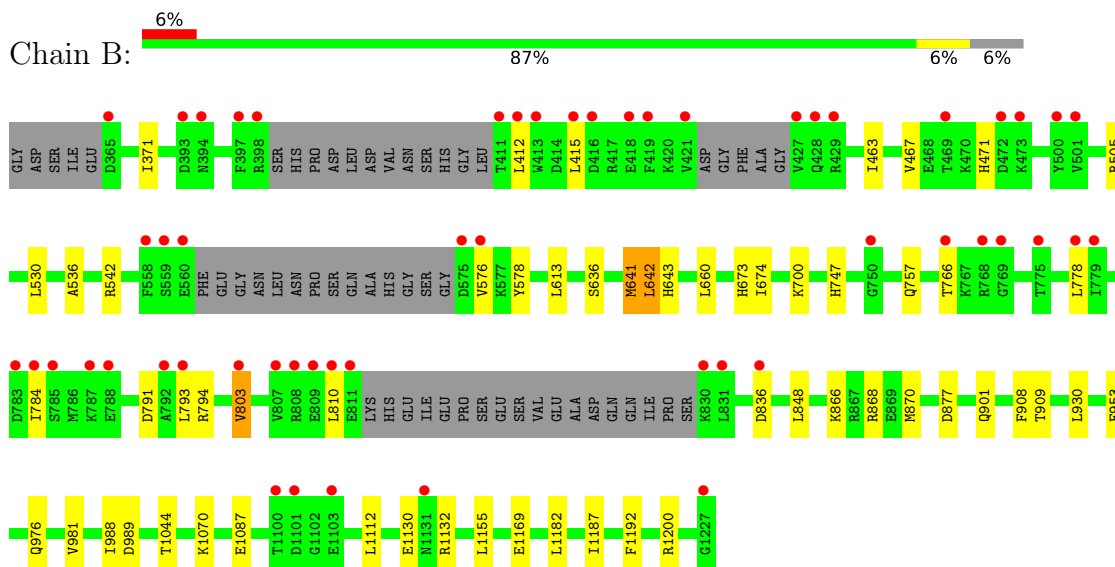
3 Residue-property plots [i](#)

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: 2-OXOGLUTARATE DECARBOXYLASE



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4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	80.55Å 83.58Å 160.07Å 99.59° 98.94° 100.68°	Depositor
Resolution (Å)	78.11 – 2.20 78.11 – 2.20	Depositor EDS
% Data completeness (in resolution range)	93.1 (78.11-2.20) 93.1 (78.11-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 2.20Å)	Xtrriage
Refinement program	BUSTER 2.9.3	Depositor
R, R_{free}	0.188 , 0.214 0.202 , 0.229	Depositor DCC
R_{free} test set	9391 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å ²)	31.4	Xtrriage
Anisotropy	0.617	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 58.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.022 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	26097	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: CA, ACO, 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	0.87	0/6492	1.24	11/8818 (0.1%)
1	B	0.86	1/6349 (0.0%)	1.24	11/8623 (0.1%)
1	C	0.88	1/6438 (0.0%)	1.24	10/8737 (0.1%)
1	D	0.87	1/6377 (0.0%)	1.24	19/8656 (0.2%)
All	All	0.87	3/25656 (0.0%)	1.24	51/34834 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	641	MET	SD-CE	-11.77	1.50	1.79
1	C	870	MET	SD-CE	-7.04	1.61	1.79
1	D	870	MET	SD-CE	-5.09	1.66	1.79

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	627	GLY	CA-C-N	7.14	129.73	120.44
1	A	627	GLY	C-N-CA	7.14	129.73	120.44
1	D	836	ASP	CA-CB-CG	6.42	119.02	112.60
1	A	399	SER	CA-C-N	6.25	127.78	122.28
1	A	399	SER	C-N-CA	6.25	127.78	122.28
1	C	1087	GLU	CB-CG-CD	5.96	122.72	112.60
1	B	836	ASP	CA-CB-CG	5.94	118.54	112.60
1	A	803	VAL	N-CA-CB	5.87	117.02	110.62
1	C	877	ASP	CA-CB-CG	5.78	118.38	112.60
1	D	576	VAL	CA-C-N	5.77	128.81	120.38
1	D	576	VAL	C-N-CA	5.77	128.81	120.38
1	D	700	LYS	CA-C-N	5.77	128.29	120.38
1	D	700	LYS	C-N-CA	5.77	128.29	120.38
1	C	627	GLY	CA-C-N	5.64	127.84	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	627	GLY	C-N-CA	5.64	127.84	120.28
1	C	463	ILE	CA-C-N	5.62	128.13	120.54
1	C	463	ILE	C-N-CA	5.62	128.13	120.54
1	D	877	ASP	CA-CB-CG	5.59	118.19	112.60
1	D	632	ASP	CA-CB-CG	5.58	118.18	112.60
1	D	791	ASP	CA-CB-CG	5.50	118.10	112.60
1	B	803	VAL	N-CA-CB	5.49	116.98	110.55
1	D	627	GLY	CA-C-N	5.49	127.95	120.54
1	D	627	GLY	C-N-CA	5.49	127.95	120.54
1	D	803	VAL	N-CA-CB	5.49	117.59	110.57
1	D	463	ILE	CA-C-N	5.46	127.92	120.54
1	D	463	ILE	C-N-CA	5.46	127.92	120.54
1	D	660	LEU	CA-C-N	5.33	127.68	120.38
1	D	660	LEU	C-N-CA	5.33	127.68	120.38
1	B	463	ILE	CA-C-N	5.33	127.73	120.54
1	B	463	ILE	C-N-CA	5.33	127.73	120.54
1	A	463	ILE	CA-C-N	5.32	127.72	120.54
1	A	463	ILE	C-N-CA	5.32	127.72	120.54
1	B	660	LEU	CA-C-N	5.31	128.13	120.38
1	B	660	LEU	C-N-CA	5.31	128.13	120.38
1	A	700	LYS	CA-C-N	5.30	127.65	120.38
1	A	700	LYS	C-N-CA	5.30	127.65	120.38
1	B	989	ASP	CA-CB-CG	5.27	117.87	112.60
1	B	700	LYS	CA-C-N	5.25	127.57	120.38
1	B	700	LYS	C-N-CA	5.25	127.57	120.38
1	C	700	LYS	CA-C-N	5.24	127.55	120.38
1	C	700	LYS	C-N-CA	5.24	127.55	120.38
1	D	830	LYS	CA-C-N	5.23	128.51	120.82
1	D	830	LYS	C-N-CA	5.23	128.51	120.82
1	A	632	ASP	CA-CB-CG	5.23	117.83	112.60
1	D	770	SER	CA-C-N	5.20	127.71	120.63
1	D	770	SER	C-N-CA	5.20	127.71	120.63
1	A	877	ASP	CA-CB-CG	5.17	117.77	112.60
1	B	877	ASP	CA-CB-CG	5.14	117.74	112.60
1	B	953	PHE	CA-CB-CG	5.14	118.94	113.80
1	C	660	LEU	CA-C-N	5.06	127.76	120.38
1	C	660	LEU	C-N-CA	5.06	127.76	120.38

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	6360	0	6105	28	0
1	B	6223	0	5967	25	0
1	C	6309	0	6084	26	0
1	D	6252	0	5998	28	0
2	A	26	0	16	1	0
2	B	26	0	16	2	0
2	C	26	0	16	1	0
2	D	26	0	16	1	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	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	33	0	13	0	0
5	C	33	0	13	0	0
5	D	33	0	13	0	0
6	A	190	0	0	0	0
6	B	186	0	0	0	0
6	C	183	0	0	0	0
6	D	183	0	0	1	0
All	All	26097	0	24257	103	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 2.

All (103) 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:641:MET:HE3	1:B:643:HIS:HE1	1.19	1.06
1:B:641:MET:HE3	1:B:643:HIS:CE1	2.01	0.94
1:B:641:MET:CE	1:B:643:HIS:HE1	1.94	0.80
1:B:641:MET:CE	1:B:643:HIS:CE1	2.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1044:THR:HG22	1:A:1047:ASN:H	1.54	0.70
1:D:1044:THR:HG22	1:D:1047:ASN:H	1.57	0.68
1:C:716:ALA:O	1:C:720:VAL:HG12	1.93	0.68
1:C:1044:THR:HG22	1:C:1047:ASN:H	1.57	0.67
1:D:1112:LEU:HD21	1:D:1155:LEU:HD22	1.76	0.67
1:B:1112:LEU:HD21	1:B:1155:LEU:HD22	1.78	0.66
1:B:848:LEU:HD12	1:B:868:ARG:HD2	1.76	0.65
1:C:1112:LEU:HD21	1:C:1155:LEU:HD22	1.78	0.64
1:D:494:THR:HG21	1:D:796:TYR:OH	1.96	0.64
1:A:1112:LEU:HD21	1:A:1155:LEU:HD22	1.78	0.64
1:A:368:ALA:HB1	1:B:371:ILE:HG13	1.78	0.64
1:C:912:HIS:HE1	1:D:755:MET:HE1	1.64	0.62
1:C:441:ASP:HA	1:C:445:ARG:HD3	1.81	0.61
1:C:912:HIS:HE1	1:D:755:MET:CE	2.13	0.61
1:A:441:ASP:HA	1:A:445:ARG:HD3	1.86	0.57
1:B:981:VAL:HG22	1:B:988:ILE:HD11	1.87	0.56
1:D:981:VAL:HG22	1:D:988:ILE:HD11	1.88	0.56
1:A:779:ILE:HD11	1:A:789:ALA:HB2	1.89	0.55
1:A:981:VAL:HG22	1:A:988:ILE:HD11	1.87	0.55
1:C:1011:HIS:HD2	1:C:1041:MET:HE1	1.72	0.55
1:A:1011:HIS:HD2	1:A:1041:MET:HE1	1.72	0.54
1:D:494:THR:HG23	1:D:800:LEU:HD13	1.91	0.53
1:D:876:ILE:HD11	1:D:1082:ILE:HD13	1.90	0.53
1:D:1169:GLU:O	1:D:1200:ARG:HD2	2.09	0.53
2:C:2001:TPP:H6'	1:D:901:GLN:OE1	2.10	0.51
1:B:866:LYS:HE3	1:B:870:MET:HE3	1.93	0.51
1:C:870:MET:HE1	1:C:877:ASP:CG	2.36	0.50
1:C:1218:GLN:O	1:C:1222:LEU:HD13	2.11	0.50
1:D:866:LYS:HE3	1:D:870:MET:HE3	1.93	0.50
1:D:447:VAL:HG22	1:D:709:VAL:HG12	1.94	0.49
1:D:709:VAL:HG11	1:D:720:VAL:HG21	1.94	0.49
1:A:901:GLN:OE1	2:B:2001:TPP:H6'	2.13	0.49
1:A:412:LEU:HA	1:A:415:LEU:HD12	1.95	0.49
2:A:2001:TPP:H6'	1:B:901:GLN:OE1	2.13	0.49
1:D:490:GLU:O	1:D:494:THR:HG22	2.13	0.49
1:B:505:ARG:HA	1:B:747:HIS:O	2.13	0.48
1:C:901:GLN:OE1	2:D:2001:TPP:H6'	2.13	0.48
1:C:1132:ARG:NH1	1:C:1226:PHE:O	2.46	0.48
1:B:641:MET:HE2	1:B:643:HIS:CE1	2.48	0.48
1:B:1130:GLU:HG3	1:B:1132:ARG:HG3	1.94	0.48
1:D:618:ARG:HH21	1:D:629:GLU:HG2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:510:GLY:O	1:C:741:CYS:HB2	2.15	0.47
1:D:776:GLU:HA	1:D:779:ILE:HD12	1.98	0.46
1:C:981:VAL:HG22	1:C:988:ILE:HD11	1.97	0.46
1:B:642:LEU:HD22	1:B:674:ILE:HB	1.98	0.46
1:B:1169:GLU:O	1:B:1200:ARG:HD2	2.16	0.46
1:D:1150:ARG:O	1:D:1154:THR:HG23	2.15	0.46
1:A:626:THR:HG21	1:A:636:SER:OG	2.17	0.45
1:C:412:LEU:HA	1:C:415:LEU:HD12	1.98	0.45
1:A:632:ASP:OD2	1:A:634:ARG:HB2	2.17	0.45
1:A:1150:ARG:O	1:A:1154:THR:HG23	2.16	0.44
1:D:510:GLY:O	1:D:741:CYS:HB2	2.16	0.44
1:B:412:LEU:HA	1:B:415:LEU:HD12	1.98	0.44
1:A:536:ALA:HB3	1:A:613:LEU:HD22	1.99	0.44
1:D:542:ARG:HD3	1:D:578:TYR:HA	2.00	0.43
1:D:751:ASP:HB2	6:D:3076:HOH:O	2.18	0.43
1:B:641:MET:HE2	1:B:673:HIS:CE1	2.52	0.43
1:A:1093:VAL:HB	1:A:1150:ARG:HD3	2.00	0.43
1:A:778:LEU:HB3	1:A:784:ILE:HG12	2.00	0.43
1:A:1092:SER:HB2	1:A:1147:PRO:HG3	2.01	0.43
1:C:831:LEU:HD23	1:C:1057:LYS:HE3	2.00	0.43
1:C:536:ALA:HB3	1:C:613:LEU:HD22	2.01	0.43
1:A:863:VAL:O	1:A:867:ARG:HG3	2.19	0.42
1:B:641:MET:HE2	1:B:673:HIS:ND1	2.34	0.42
1:A:476:VAL:HG12	1:A:480:LYS:HE3	2.01	0.42
1:D:476:VAL:HG12	1:D:480:LYS:HE2	2.00	0.42
1:B:778:LEU:HB3	1:B:784:ILE:HG12	2.01	0.42
1:B:1155:LEU:HD11	1:B:1192:PHE:CZ	2.55	0.42
1:D:760:MET:HG2	1:D:764:ILE:HD12	2.01	0.42
1:D:536:ALA:HB3	1:D:613:LEU:HD22	2.01	0.42
1:A:696:THR:HG21	1:A:738:ASP:HB2	2.01	0.42
1:A:1155:LEU:HD11	1:A:1192:PHE:CZ	2.55	0.42
1:D:415:LEU:HA	1:D:432:LEU:HB3	2.02	0.42
1:D:696:THR:HG21	1:D:738:ASP:HB2	2.02	0.42
1:A:950:LEU:HD11	2:B:2001:TPP:HM42	2.02	0.41
1:B:542:ARG:HD3	1:B:578:TYR:HA	2.02	0.41
1:C:626:THR:HG21	1:C:636:SER:OG	2.20	0.41
1:C:1155:LEU:HD11	1:C:1192:PHE:CZ	2.55	0.41
1:A:390:LEU:HD23	1:A:767:LYS:HD2	2.02	0.41
1:C:692:SER:HB2	1:C:697:ASP:OD2	2.19	0.41
1:A:898:LEU:O	1:A:945:VAL:HA	2.20	0.41
1:B:791:ASP:OD1	1:B:794:ARG:NH2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:ARG:HD3	1:A:578:TYR:HA	2.02	0.41
1:C:476:VAL:HG12	1:C:480:LYS:HE3	2.02	0.41
1:A:530:LEU:HD22	1:A:636:SER:HA	2.02	0.41
1:B:908:PHE:CZ	1:B:1070:LYS:HG2	2.55	0.41
1:C:632:ASP:OD2	1:C:634:ARG:HB2	2.20	0.41
1:C:753:PRO:HB2	1:C:761:TYR:CE2	2.56	0.41
1:A:692:SER:HB2	1:A:697:ASP:OD2	2.21	0.41
1:A:1112:LEU:CD2	1:A:1155:LEU:HD22	2.50	0.41
1:C:1109:VAL:HG21	1:C:1136:ALA:HB2	2.02	0.41
1:A:1169:GLU:O	1:A:1200:ARG:HD2	2.21	0.40
1:B:536:ALA:HB3	1:B:613:LEU:HD22	2.03	0.40
1:C:455:LEU:HD13	1:D:383:LEU:HD21	2.03	0.40
1:B:530:LEU:HD22	1:B:636:SER:HA	2.03	0.40
1:C:1093:VAL:HB	1:C:1150:ARG:HD3	2.03	0.40
1:C:898:LEU:O	1:C:945:VAL:HA	2.20	0.40
1:D:603:PRO:HD3	1:D:991:PHE:CZ	2.56	0.40
1:D:867:ARG:HG2	1:D:880:PHE:CD1	2.55	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	818/868 (94%)	800 (98%)	18 (2%)	0	100	100
1	B	804/868 (93%)	786 (98%)	18 (2%)	0	100	100
1	C	805/868 (93%)	789 (98%)	16 (2%)	0	100	100
1	D	808/868 (93%)	792 (98%)	16 (2%)	0	100	100
All	All	3235/3472 (93%)	3167 (98%)	68 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	649/726 (89%)	634 (98%)	15 (2%)	44	59
1	B	628/726 (86%)	612 (98%)	16 (2%)	42	56
1	C	648/726 (89%)	629 (97%)	19 (3%)	37	51
1	D	634/726 (87%)	624 (98%)	10 (2%)	55	71
All	All	2559/2904 (88%)	2499 (98%)	60 (2%)	44	59

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	367	ASN
1	A	402	ASP
1	A	436	LEU
1	A	467	VAL
1	A	471	HIS
1	A	501	VAL
1	A	596	GLU
1	A	770	SER
1	A	803	VAL
1	A	909	THR
1	A	930	LEU
1	A	950	LEU
1	A	976	GLN
1	A	1044	THR
1	A	1150	ARG
1	B	467	VAL
1	B	471	HIS
1	B	576	VAL
1	B	642	LEU
1	B	757	GLN
1	B	766	THR
1	B	793	LEU
1	B	803	VAL
1	B	810	LEU

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Mol	Chain	Res	Type
1	B	909	THR
1	B	930	LEU
1	B	976	GLN
1	B	1044	THR
1	B	1087	GLU
1	B	1182	LEU
1	B	1187	ILE
1	C	467	VAL
1	C	471	HIS
1	C	576	VAL
1	C	634	ARG
1	C	766	THR
1	C	767	LYS
1	C	779	ILE
1	C	793	LEU
1	C	803	VAL
1	C	831	LEU
1	C	909	THR
1	C	930	LEU
1	C	976	GLN
1	C	1044	THR
1	C	1146	LEU
1	C	1150	ARG
1	C	1182	LEU
1	C	1187	ILE
1	C	1222	LEU
1	D	467	VAL
1	D	471	HIS
1	D	803	VAL
1	D	909	THR
1	D	930	LEU
1	D	950	LEU
1	D	976	GLN
1	D	1044	THR
1	D	1087	GLU
1	D	1187	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	748	ASN
1	A	1016	GLN

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Mol	Chain	Res	Type
1	A	1219	GLN
1	B	524	GLN
1	B	748	ASN
1	B	757	GLN
1	B	933	ASN
1	B	1001	GLN
1	B	1016	GLN
1	B	1107	ASN
1	B	1219	GLN
1	C	503	GLN
1	C	748	ASN
1	C	912	HIS
1	C	1030	GLN
1	C	1219	GLN
1	D	503	GLN
1	D	524	GLN
1	D	748	ASN
1	D	797	GLN
1	D	985	GLN
1	D	1001	GLN
1	D	1107	ASN
1	D	1219	GLN

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 15 ligands modelled in this entry, 8 are monoatomic - leaving 7 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
5	ACO	D	2004	-	35,35,53	1.83	8 (22%)	51,54,79	2.07	13 (25%)
2	TPP	B	2001	3	26,27,27	1.32	2 (7%)	38,40,40	1.56	11 (28%)
5	ACO	C	2004	-	35,35,53	1.76	7 (20%)	51,54,79	2.19	13 (25%)
2	TPP	C	2001	3	26,27,27	1.45	3 (11%)	38,40,40	1.63	9 (23%)
2	TPP	D	2001	3	26,27,27	1.36	2 (7%)	38,40,40	1.58	8 (21%)
5	ACO	A	2004	-	35,35,53	1.94	8 (22%)	51,54,79	2.17	13 (25%)
2	TPP	A	2001	3	26,27,27	1.36	3 (11%)	38,40,40	1.62	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
5	ACO	D	2004	-	-	5/25/41/67	0/3/3/3
2	TPP	B	2001	3	-	3/17/17/17	0/2/2/2
5	ACO	C	2004	-	-	5/25/41/67	0/3/3/3
2	TPP	C	2001	3	-	3/17/17/17	0/2/2/2
2	TPP	D	2001	3	-	3/17/17/17	0/2/2/2
5	ACO	A	2004	-	-	5/25/41/67	0/3/3/3
2	TPP	A	2001	3	-	3/17/17/17	0/2/2/2

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	2004	ACO	P2A-O3A	5.74	1.65	1.59
5	A	2004	ACO	P2A-O3A	5.47	1.65	1.59
5	C	2004	ACO	P2A-O3A	4.66	1.64	1.59
5	C	2004	ACO	P1A-O3A	4.53	1.64	1.59
5	A	2004	ACO	P3B-O7A	4.18	1.63	1.50
5	A	2004	ACO	P1A-O3A	4.16	1.64	1.59
5	C	2004	ACO	P3B-O7A	4.01	1.63	1.50
2	D	2001	TPP	C4-N3	-3.93	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001	TPP	PB-O1B	3.89	1.62	1.50
2	C	2001	TPP	C4-N3	-3.72	1.32	1.39
5	D	2004	ACO	P3B-O7A	3.66	1.61	1.50
5	A	2004	ACO	P1A-O1A	3.53	1.63	1.50
5	D	2004	ACO	P1A-O3A	3.45	1.63	1.59
5	A	2004	ACO	P3B-O3B	3.43	1.65	1.59
2	C	2001	TPP	PA-O3A	3.40	1.63	1.59
2	D	2001	TPP	PB-O1B	3.37	1.60	1.50
5	C	2004	ACO	P1A-O1A	3.27	1.62	1.50
2	C	2001	TPP	PB-O1B	3.26	1.60	1.50
2	A	2001	TPP	C4-N3	-3.21	1.33	1.39
5	D	2004	ACO	P1A-O1A	3.15	1.61	1.50
2	A	2001	TPP	PB-O1B	3.10	1.60	1.50
2	B	2001	TPP	C4-N3	-3.03	1.33	1.39
5	A	2004	ACO	P2A-O4A	3.01	1.61	1.50
5	C	2004	ACO	P2A-O4A	2.81	1.60	1.50
5	D	2004	ACO	P3B-O8A	2.70	1.64	1.54
5	D	2004	ACO	P2A-O4A	2.56	1.59	1.50
5	C	2004	ACO	P3B-O8A	2.36	1.63	1.54
5	A	2004	ACO	P2A-O6A	2.31	1.68	1.59
5	D	2004	ACO	C5A-N7A	-2.19	1.35	1.39
2	A	2001	TPP	PA-O3A	2.16	1.61	1.59
5	C	2004	ACO	P3B-O3B	2.15	1.63	1.59
5	A	2004	ACO	O4B-C1B	2.05	1.46	1.42
5	D	2004	ACO	C5A-C4A	2.01	1.42	1.39

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2004	ACO	N3A-C2A-N1A	-5.87	119.69	128.58
5	C	2004	ACO	C5A-C4A-N3A	-5.60	119.01	126.72
5	D	2004	ACO	N3A-C2A-N1A	-5.57	120.15	128.58
5	C	2004	ACO	N3A-C2A-N1A	-5.53	120.21	128.58
5	D	2004	ACO	C5A-C4A-N3A	-5.19	119.58	126.72
5	C	2004	ACO	N3A-C4A-N9A	5.18	135.98	127.17
5	A	2004	ACO	P3B-O3B-C3B	-5.02	110.03	123.43
5	A	2004	ACO	C5A-C4A-N3A	-5.02	119.81	126.72
5	A	2004	ACO	N3A-C4A-N9A	4.81	135.35	127.17
5	C	2004	ACO	P3B-O3B-C3B	-4.68	110.94	123.43
5	D	2004	ACO	N3A-C4A-N9A	4.59	134.97	127.17
5	D	2004	ACO	P3B-O3B-C3B	-4.50	111.42	123.43
5	C	2004	ACO	C2A-N3A-C4A	4.30	122.32	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2004	ACO	C2A-N3A-C4A	4.11	121.87	111.83
5	C	2004	ACO	C5A-N7A-C8A	4.04	109.80	103.45
5	D	2004	ACO	C2A-N3A-C4A	4.03	121.66	111.83
2	C	2001	TPP	C6'-N1'-C2'	3.93	122.53	116.07
5	A	2004	ACO	C5A-N7A-C8A	3.90	109.58	103.45
5	C	2004	ACO	C2B-C1B-N9A	-3.84	103.76	113.30
5	D	2004	ACO	C5A-N7A-C8A	3.74	109.33	103.45
5	A	2004	ACO	O3A-P2A-O4A	-3.74	99.46	110.70
2	A	2001	TPP	C6'-N1'-C2'	3.72	122.18	116.07
5	A	2004	ACO	C2B-C1B-N9A	-3.70	104.12	113.30
5	D	2004	ACO	C2B-C1B-N9A	-3.69	104.13	113.30
2	B	2001	TPP	CM4-C4-C5	-3.68	118.33	127.75
2	D	2001	TPP	C6'-N1'-C2'	3.67	122.10	116.07
2	A	2001	TPP	CM4-C4-C5	-3.61	118.49	127.75
5	A	2004	ACO	N9A-C8A-N7A	-3.60	108.83	113.94
2	D	2001	TPP	C2-S1-C5	-3.58	88.84	91.22
2	C	2001	TPP	CM4-C4-C5	-3.52	118.72	127.75
5	C	2004	ACO	N9A-C8A-N7A	-3.50	108.97	113.94
5	C	2004	ACO	O3A-P2A-O4A	-3.41	100.43	110.70
2	A	2001	TPP	N1'-C2'-N3'	-3.38	119.91	125.53
5	D	2004	ACO	O3A-P2A-O4A	-3.29	100.82	110.70
2	B	2001	TPP	C6'-N1'-C2'	3.21	121.34	116.07
2	D	2001	TPP	CM4-C4-C5	-3.21	119.53	127.75
2	C	2001	TPP	N1'-C2'-N3'	-3.16	120.27	125.53
5	C	2004	ACO	C4A-N9A-C8A	3.05	108.94	105.74
2	D	2001	TPP	N1'-C2'-N3'	-3.03	120.49	125.53
2	B	2001	TPP	N1'-C2'-N3'	-2.99	120.55	125.53
5	A	2004	ACO	C4A-N9A-C8A	2.90	108.78	105.74
5	C	2004	ACO	C4A-C5A-N7A	-2.90	107.27	110.58
5	D	2004	ACO	C4A-C5A-N7A	-2.84	107.33	110.58
2	C	2001	TPP	C5'-C6'-N1'	-2.83	119.22	123.83
2	A	2001	TPP	CM2-C2'-N1'	2.81	120.19	117.20
5	D	2004	ACO	N9A-C8A-N7A	-2.77	110.00	113.94
2	B	2001	TPP	C5-C4-N3	2.60	116.40	111.67
2	C	2001	TPP	CM2-C2'-N1'	2.59	119.96	117.20
2	D	2001	TPP	C5-C4-N3	2.40	116.03	111.67
2	B	2001	TPP	CM2-C2'-N1'	2.40	119.75	117.20
2	A	2001	TPP	C5-C4-N3	2.34	115.93	111.67
2	B	2001	TPP	C4-C5-S1	-2.34	106.92	110.56
5	A	2004	ACO	O5A-P2A-O3A	2.32	113.55	107.27
5	C	2004	ACO	O5A-P2A-O3A	2.32	113.55	107.27
2	A	2001	TPP	N4'-C4'-N3'	2.30	120.14	117.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2001	TPP	C7-C6-C5	-2.29	105.55	112.73
5	A	2004	ACO	C4A-C5A-N7A	-2.28	107.97	110.58
2	C	2001	TPP	C5-C4-N3	2.28	115.82	111.67
2	D	2001	TPP	C5'-C6'-N1'	-2.28	120.12	123.83
2	B	2001	TPP	C2'-N3'-C4'	2.21	121.50	118.10
2	A	2001	TPP	C4-C5-S1	-2.19	107.15	110.56
2	A	2001	TPP	CM4-C4-N3	2.17	125.57	120.57
2	C	2001	TPP	C4-C5-S1	-2.16	107.19	110.56
5	C	2004	ACO	O4B-C1B-N9A	2.15	112.22	108.09
2	D	2001	TPP	CM2-C2'-N1'	2.14	119.48	117.20
2	A	2001	TPP	C5'-C6'-N1'	-2.14	120.35	123.83
2	B	2001	TPP	C5'-C6'-N1'	-2.12	120.38	123.83
5	A	2004	ACO	O8A-P3B-O3B	2.10	114.04	105.85
2	C	2001	TPP	CM4-C4-N3	2.10	125.41	120.57
2	B	2001	TPP	N4'-C4'-N3'	2.09	119.84	117.03
2	D	2001	TPP	C7-C6-C5	-2.07	106.25	112.73
5	D	2004	ACO	C2A-N1A-C6A	2.04	122.09	118.73
5	D	2004	ACO	O5A-P2A-O3A	2.04	112.79	107.27
5	D	2004	ACO	C4A-N9A-C8A	2.04	107.88	105.74
2	A	2001	TPP	C7-C6-C5	-2.03	106.38	112.73
2	B	2001	TPP	CM4-C4-N3	2.02	125.23	120.57
2	B	2001	TPP	C7-C6-C5	-2.00	106.44	112.73

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2001	TPP	PA-O3A-PB-O3B
2	C	2001	TPP	PA-O3A-PB-O3B
2	D	2001	TPP	PA-O3A-PB-O2B
2	D	2001	TPP	PA-O3A-PB-O3B
5	A	2004	ACO	C5B-O5B-P1A-O1A
5	A	2004	ACO	C5B-O5B-P1A-O3A
5	A	2004	ACO	CCP-O6A-P2A-O3A
5	C	2004	ACO	C5B-O5B-P1A-O1A
5	C	2004	ACO	C5B-O5B-P1A-O3A
5	C	2004	ACO	CCP-O6A-P2A-O3A
5	D	2004	ACO	C5B-O5B-P1A-O1A
5	D	2004	ACO	C5B-O5B-P1A-O3A
5	D	2004	ACO	CCP-O6A-P2A-O3A
5	A	2004	ACO	P2A-O3A-P1A-O5B
5	C	2004	ACO	P2A-O3A-P1A-O5B

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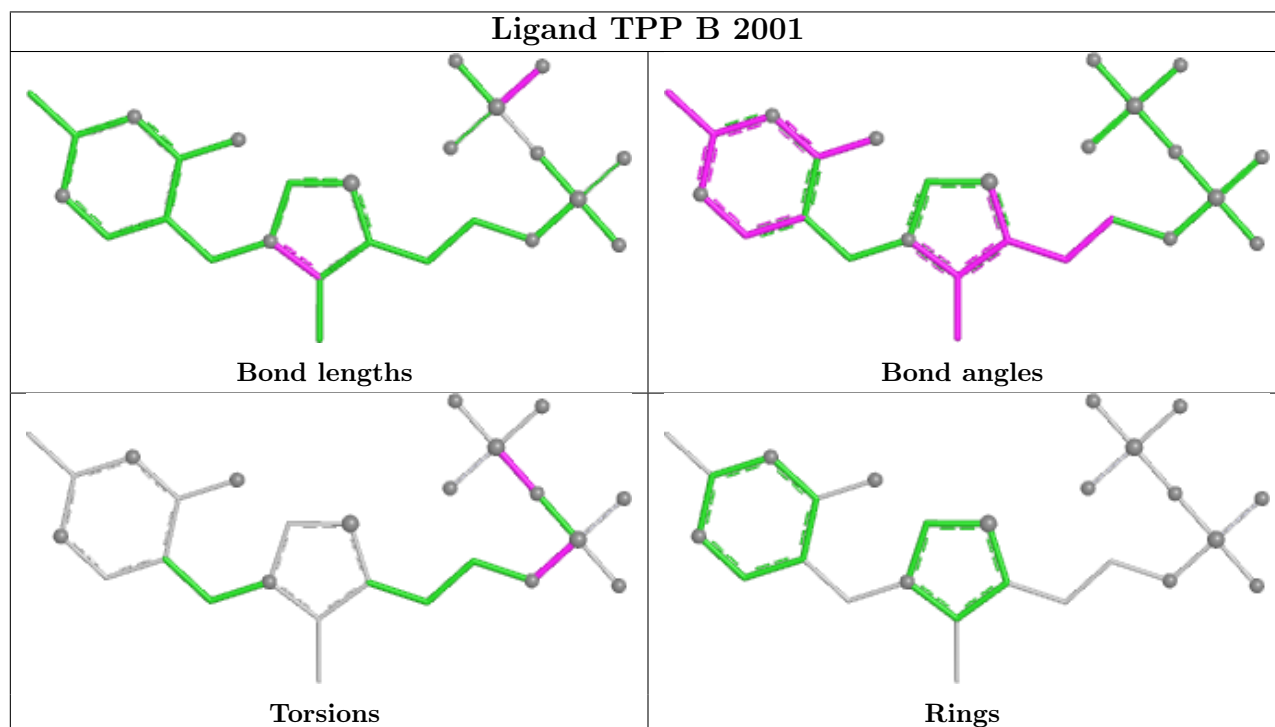
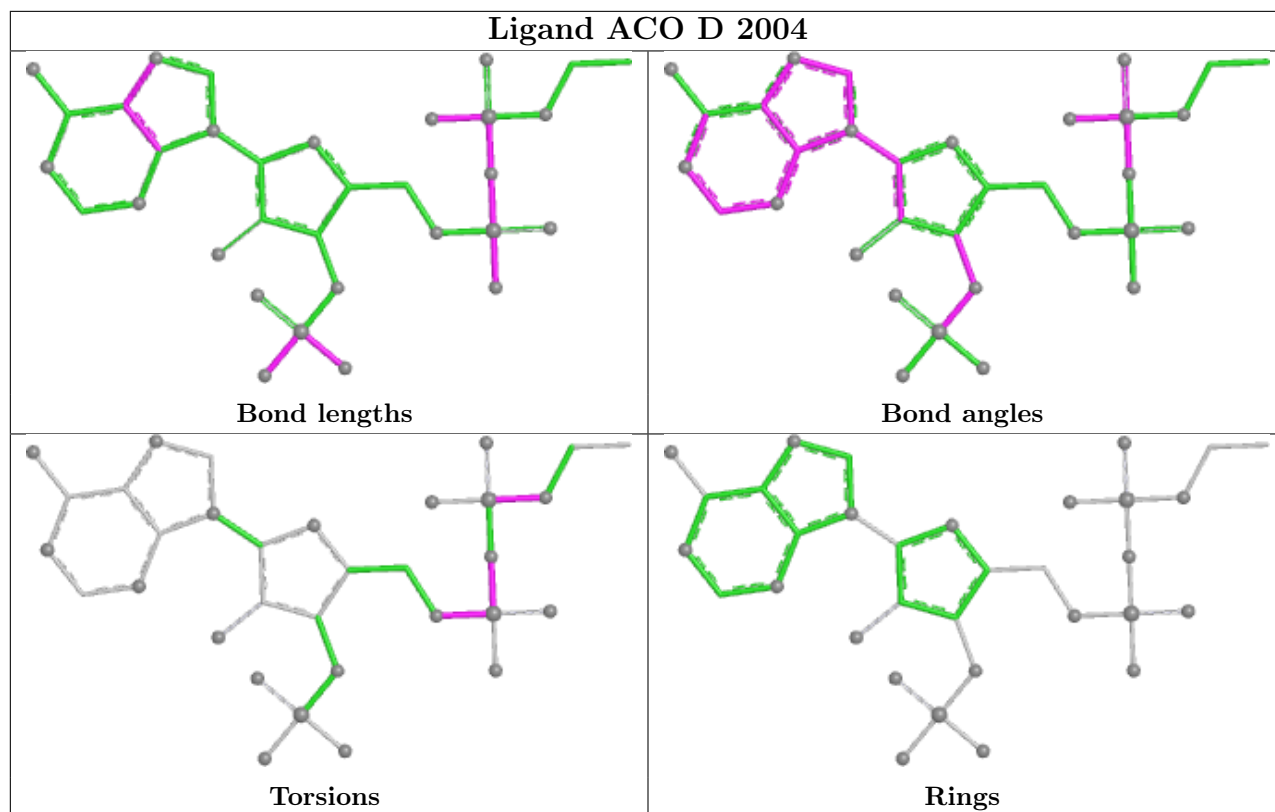
Mol	Chain	Res	Type	Atoms
5	D	2004	ACO	P2A-O3A-P1A-O5B
2	A	2001	TPP	PA-O3A-PB-O2B
2	B	2001	TPP	PA-O3A-PB-O2B
2	B	2001	TPP	PA-O3A-PB-O3B
2	C	2001	TPP	PA-O3A-PB-O2B
2	A	2001	TPP	C7-O7-PA-O1A
2	B	2001	TPP	C7-O7-PA-O1A
2	C	2001	TPP	C7-O7-PA-O1A
2	D	2001	TPP	C7-O7-PA-O1A
5	A	2004	ACO	C5B-O5B-P1A-O2A
5	C	2004	ACO	C5B-O5B-P1A-O2A
5	D	2004	ACO	C5B-O5B-P1A-O2A

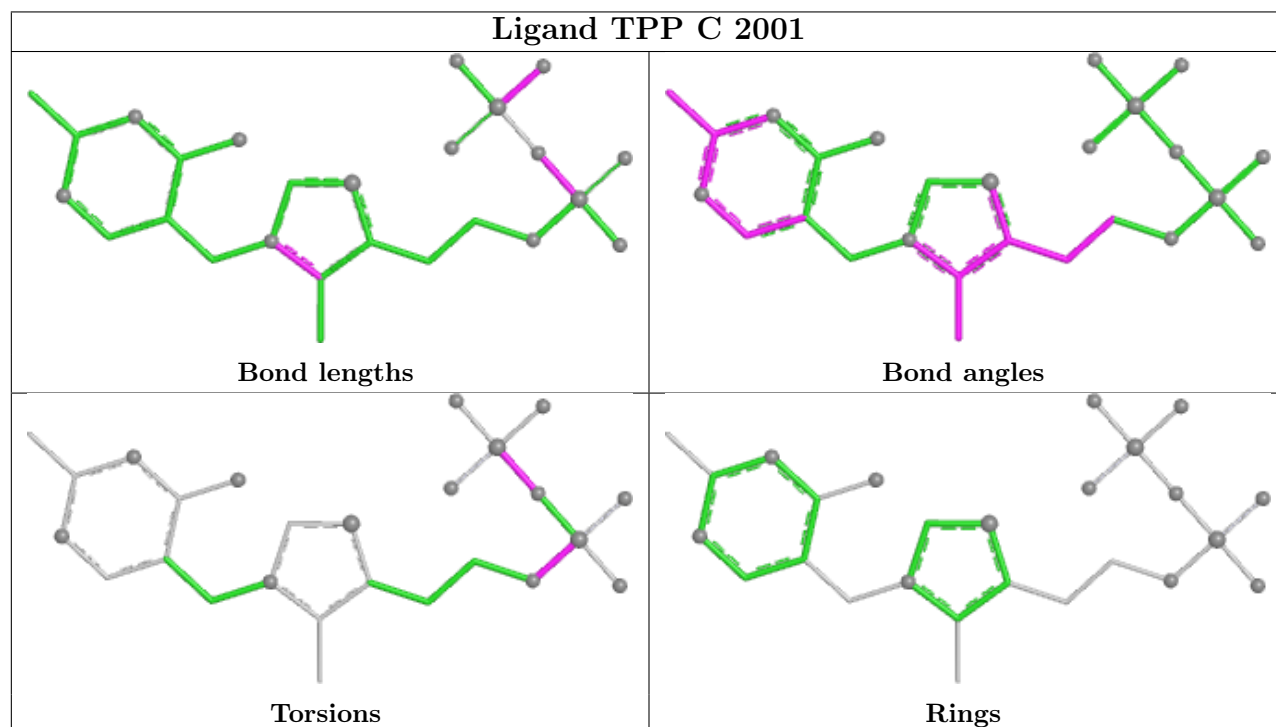
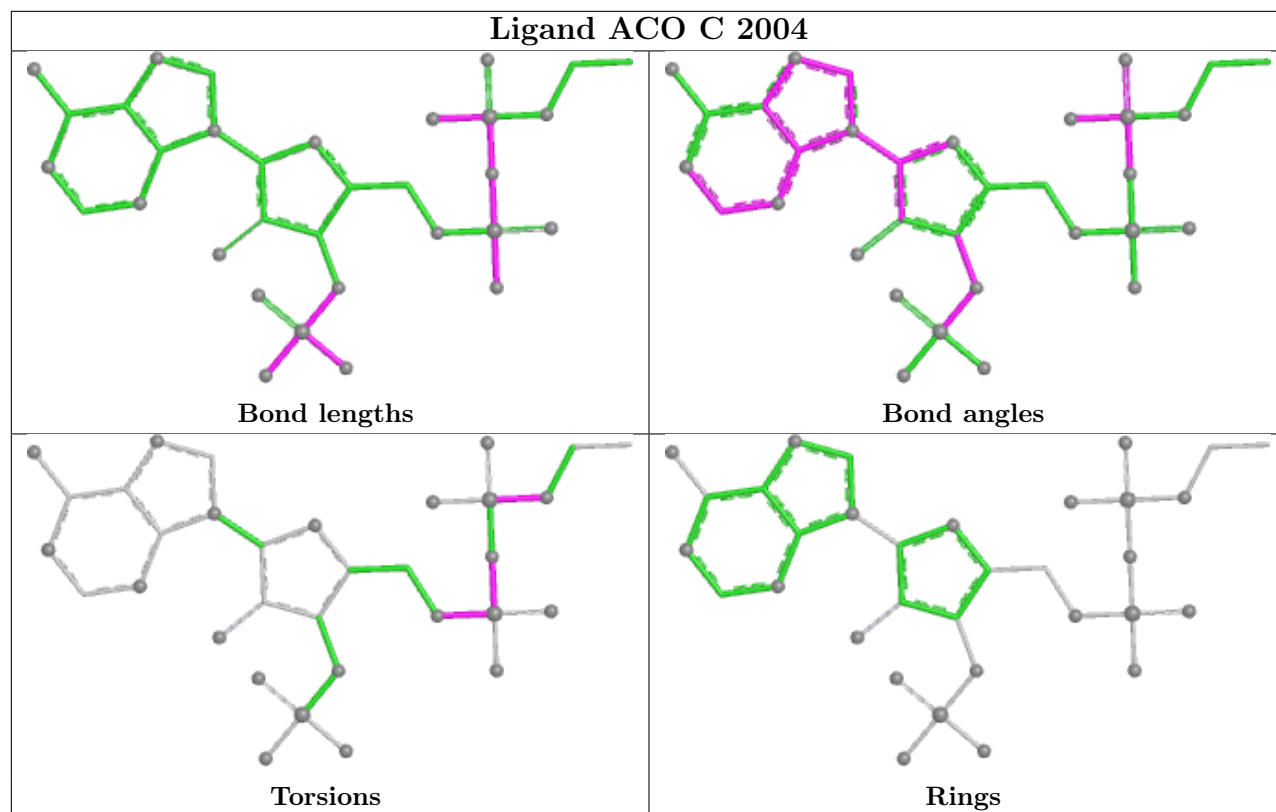
There are no ring outliers.

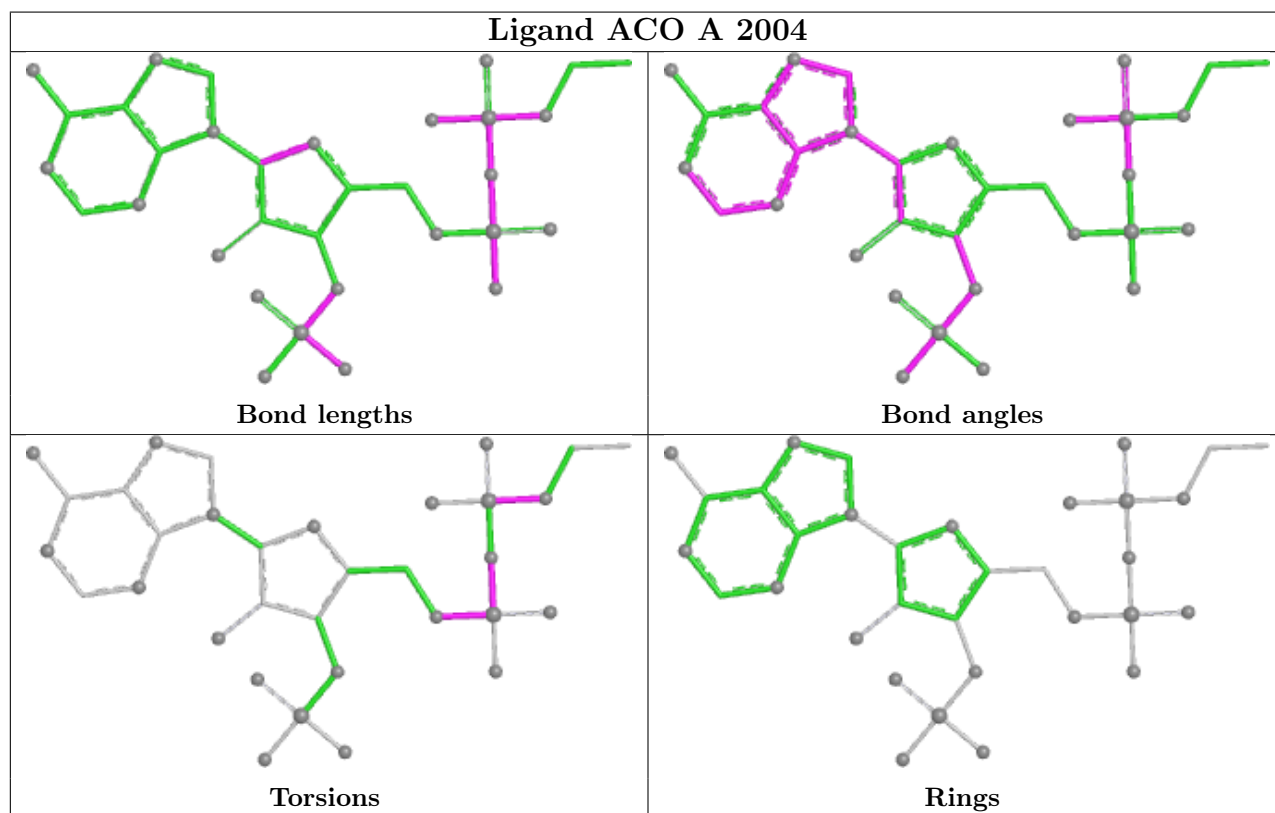
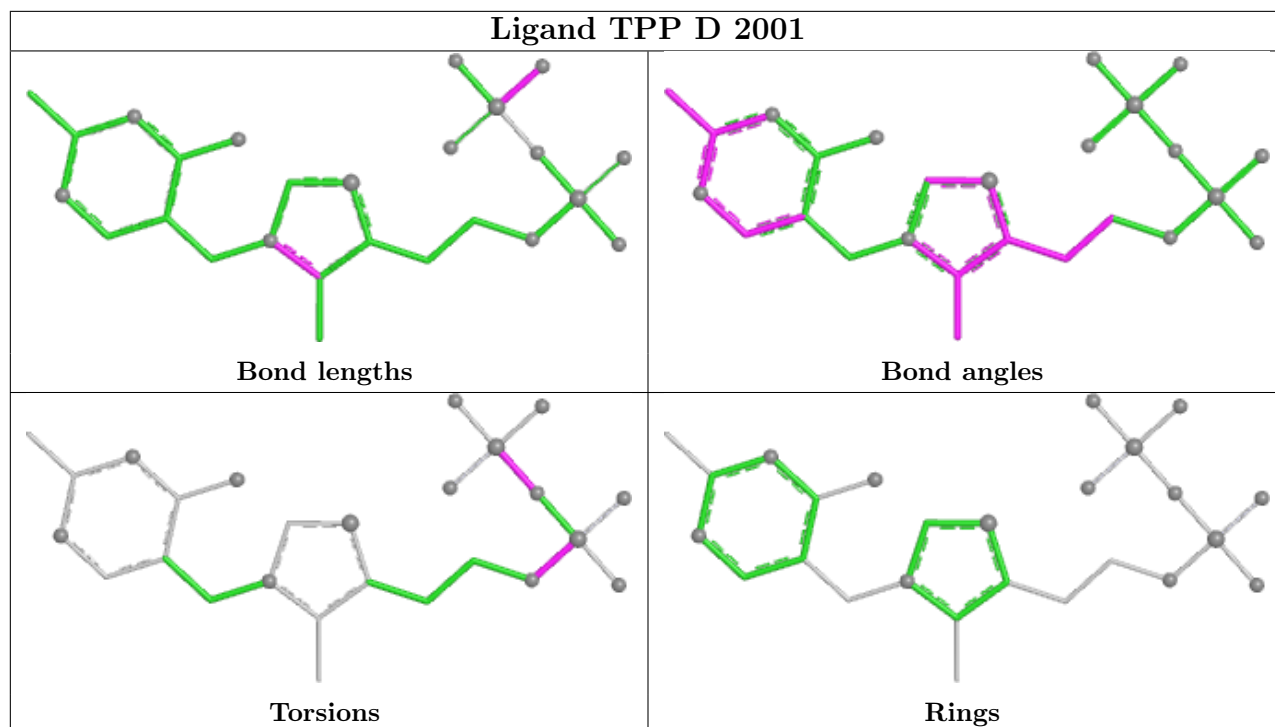
4 monomers are involved in 5 short contacts:

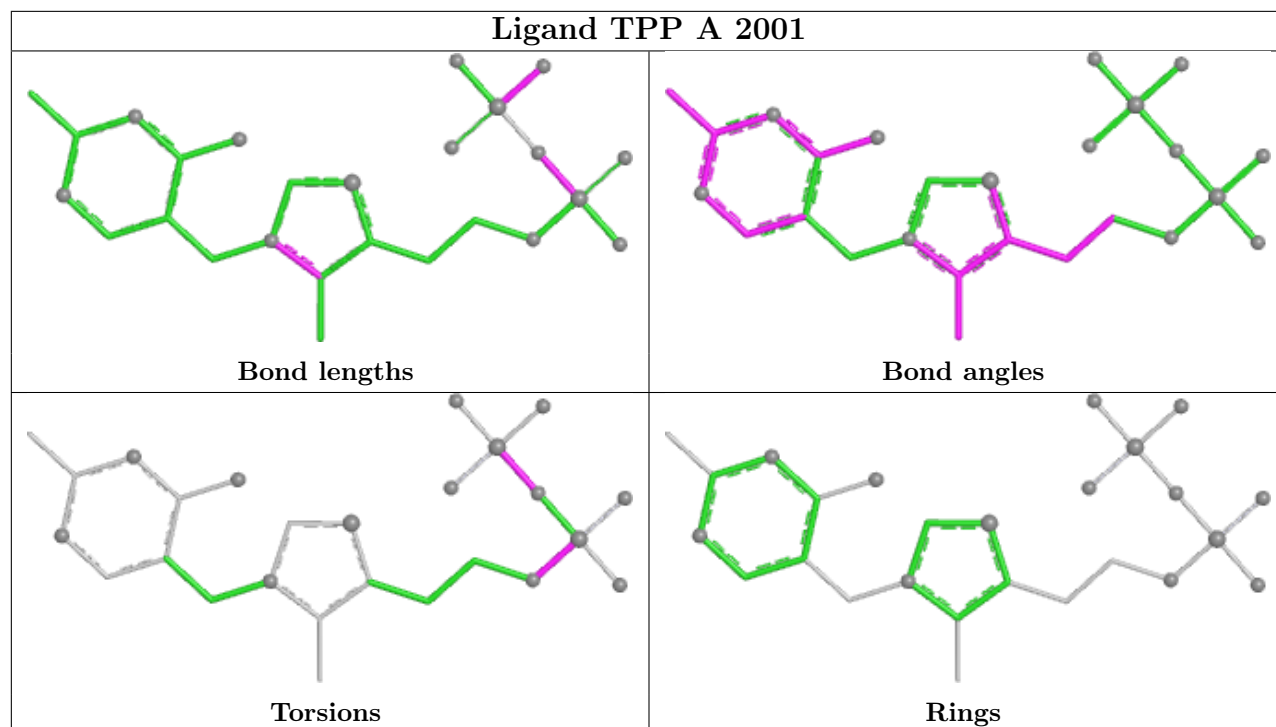
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2001	TPP	2	0
2	C	2001	TPP	1	0
2	D	2001	TPP	1	0
2	A	2001	TPP	1	0

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.









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	826/868 (95%)	0.35	40 (4%) 35 32	23, 40, 81, 111	0
1	B	814/868 (93%)	0.41	54 (6%) 24 21	21, 41, 80, 108	0
1	C	817/868 (94%)	0.30	42 (5%) 33 30	20, 39, 78, 105	0
1	D	818/868 (94%)	0.32	39 (4%) 35 32	18, 39, 78, 107	0
All	All	3275/3472 (94%)	0.35	175 (5%) 32 29	18, 40, 79, 111	0

All (175) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	413	TRP	6.1
1	D	397	PHE	5.4
1	D	472	ASP	5.2
1	A	412	LEU	5.1
1	B	560	GLU	4.6
1	B	421	VAL	4.5
1	A	400	HIS	4.3
1	D	814	GLU	4.2
1	D	632	ASP	4.2
1	D	471	HIS	4.1
1	A	750	GLY	4.1
1	B	398	ARG	4.1
1	D	574	GLY	4.0
1	A	831	LEU	3.9
1	B	810	LEU	3.9
1	A	813	HIS	3.8
1	D	422	ASP	3.8
1	B	394	ASN	3.7
1	C	365	ASP	3.7
1	B	411	THR	3.7
1	A	413	TRP	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	421	VAL	3.7
1	A	560	GLU	3.6
1	A	814	GLU	3.6
1	C	575	ASP	3.5
1	D	427	VAL	3.5
1	C	769	GLY	3.5
1	A	476	VAL	3.4
1	B	365	ASP	3.4
1	C	366	LYS	3.4
1	C	813	HIS	3.3
1	A	399	SER	3.3
1	C	750	GLY	3.3
1	C	779	ILE	3.3
1	B	750	GLY	3.3
1	B	472	ASP	3.3
1	D	560	GLU	3.2
1	B	779	ILE	3.2
1	C	830	LYS	3.2
1	D	575	ASP	3.2
1	C	395	THR	3.2
1	C	560	GLU	3.2
1	D	836	ASP	3.2
1	D	590	PHE	3.1
1	D	364	GLU	3.1
1	C	633	ASN	3.1
1	A	402	ASP	3.1
1	C	404	ASP	3.1
1	A	590	PHE	3.1
1	D	365	ASP	3.1
1	B	501	VAL	3.1
1	C	831	LEU	3.1
1	D	473	LYS	3.0
1	B	473	LYS	3.0
1	A	397	PHE	3.0
1	C	397	PHE	3.0
1	D	829	SER	3.0
1	B	1101	ASP	3.0
1	C	401	PRO	3.0
1	B	793	LEU	2.9
1	C	400	HIS	2.9
1	C	471	HIS	2.9
1	A	470	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	429	ARG	2.9
1	C	402	ASP	2.9
1	D	769	GLY	2.9
1	C	629	GLU	2.8
1	B	418	GLU	2.8
1	B	775	THR	2.8
1	B	428	GLN	2.8
1	A	410	LEU	2.8
1	B	427	VAL	2.8
1	A	575	ASP	2.8
1	A	401	PRO	2.8
1	B	558	PHE	2.8
1	D	628	GLU	2.7
1	C	403	LEU	2.7
1	B	429	ARG	2.7
1	C	632	ASP	2.7
1	D	416	ASP	2.7
1	B	412	LEU	2.7
1	D	419	PHE	2.7
1	A	405	VAL	2.6
1	A	1227	GLY	2.6
1	B	784	ILE	2.6
1	B	413	TRP	2.6
1	B	778	LEU	2.6
1	B	803	VAL	2.6
1	C	474	PRO	2.6
1	C	630	GLY	2.6
1	D	421	VAL	2.6
1	D	469	THR	2.6
1	C	470	LYS	2.6
1	B	769	GLY	2.6
1	D	501	VAL	2.6
1	D	428	GLN	2.5
1	D	808	ARG	2.5
1	A	471	HIS	2.5
1	C	428	GLN	2.5
1	A	589	MET	2.5
1	A	477	ALA	2.5
1	A	469	THR	2.5
1	D	626	THR	2.5
1	A	407	SER	2.5
1	C	501	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	412	LEU	2.5
1	A	786	MET	2.5
1	A	769	GLY	2.5
1	C	808	ARG	2.5
1	B	576	VAL	2.4
1	B	500	TYR	2.4
1	B	831	LEU	2.4
1	B	575	ASP	2.4
1	D	770	SER	2.4
1	B	830	LYS	2.4
1	D	831	LEU	2.4
1	A	629	GLU	2.4
1	B	766	THR	2.4
1	D	804	PHE	2.4
1	A	403	LEU	2.4
1	C	784	ILE	2.4
1	D	779	ILE	2.4
1	C	810	LEU	2.4
1	C	789	ALA	2.3
1	C	469	THR	2.3
1	B	785	SER	2.3
1	A	428	GLN	2.3
1	D	809	GLU	2.3
1	B	393	ASP	2.3
1	A	473	LYS	2.3
1	B	809	GLU	2.3
1	B	787	LYS	2.3
1	A	368	ALA	2.3
1	B	469	THR	2.3
1	A	474	PRO	2.3
1	C	768	ARG	2.3
1	B	397	PHE	2.2
1	B	1131	ASN	2.2
1	B	792	ALA	2.2
1	B	811	GLU	2.2
1	B	1103	GLU	2.2
1	B	559	SER	2.2
1	D	558	PHE	2.2
1	C	394	ASN	2.2
1	A	937	THR	2.2
1	B	808	ARG	2.2
1	C	778	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	782	GLY	2.2
1	B	768	ARG	2.1
1	B	415	LEU	2.1
1	C	413	TRP	2.1
1	B	783	ASP	2.1
1	B	419	PHE	2.1
1	C	539	HIS	2.1
1	A	812	LYS	2.1
1	D	1187	ILE	2.1
1	D	394	ASN	2.1
1	B	1100	THR	2.1
1	C	786	MET	2.1
1	D	589	MET	2.1
1	C	415	LEU	2.1
1	A	500	TYR	2.1
1	B	807	VAL	2.1
1	C	1227	GLY	2.1
1	B	788	GLU	2.1
1	A	810	LEU	2.1
1	D	797	GLN	2.1
1	B	1227	GLY	2.1
1	D	470	LYS	2.0
1	A	411	THR	2.0
1	A	404	ASP	2.0
1	A	472	ASP	2.0
1	B	836	ASP	2.0
1	D	1060	ILE	2.0
1	B	416	ASP	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,

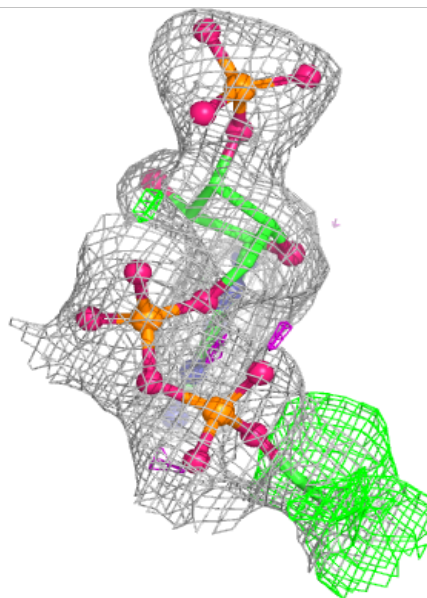
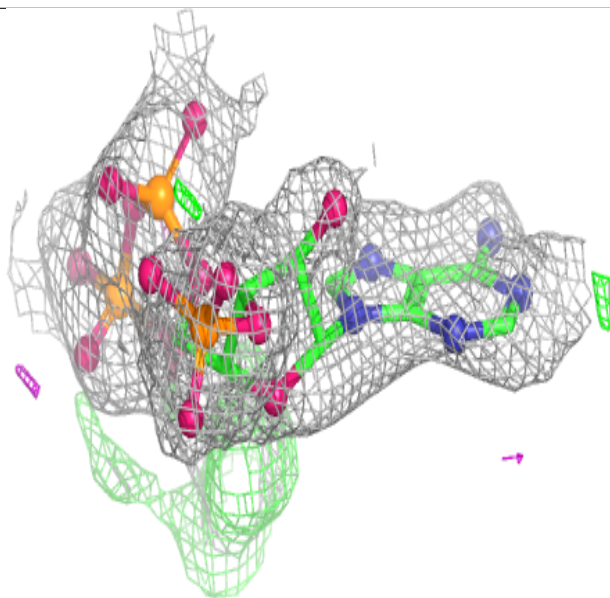
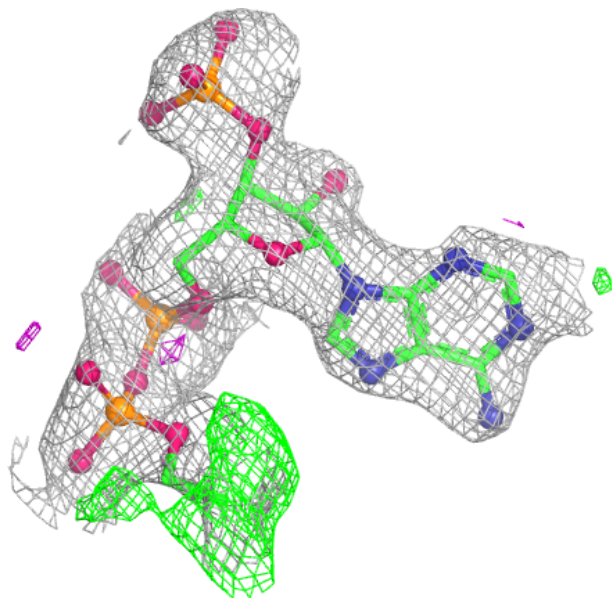
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	ACO	D	2004	33/51	0.72	0.15	53,75,91,92	0
5	ACO	A	2004	33/51	0.86	0.12	47,60,77,77	0
5	ACO	C	2004	33/51	0.87	0.11	43,54,78,82	0
4	CA	A	2003	1/1	0.94	0.09	75,75,75,75	0
4	CA	B	2003	1/1	0.95	0.15	74,74,74,74	0
4	CA	C	2003	1/1	0.95	0.14	55,55,55,55	0
4	CA	D	2003	1/1	0.95	0.16	57,57,57,57	0
2	TPP	D	2001	26/26	0.97	0.08	18,27,40,55	0
2	TPP	B	2001	26/26	0.97	0.08	18,30,44,50	0
2	TPP	A	2001	26/26	0.98	0.06	19,28,38,50	0
3	MG	C	2002	1/1	0.98	0.04	18,18,18,18	0
2	TPP	C	2001	26/26	0.98	0.07	18,30,43,49	0
3	MG	A	2002	1/1	0.99	0.05	18,18,18,18	0
3	MG	D	2002	1/1	0.99	0.03	23,23,23,23	0
3	MG	B	2002	1/1	0.99	0.04	23,23,23,23	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.

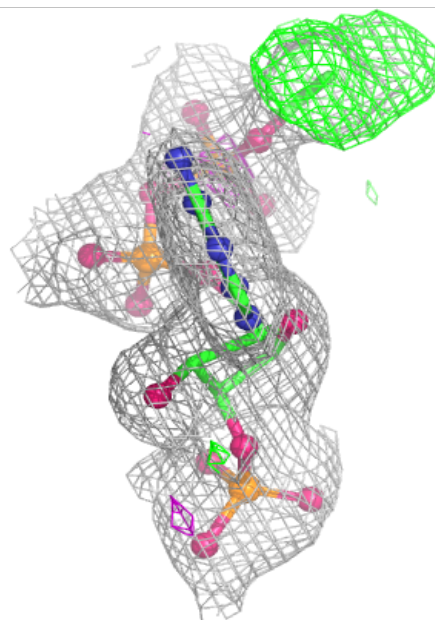
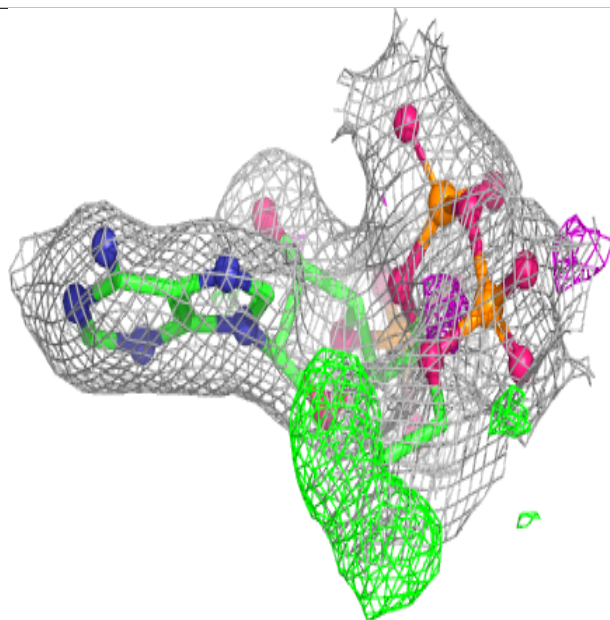
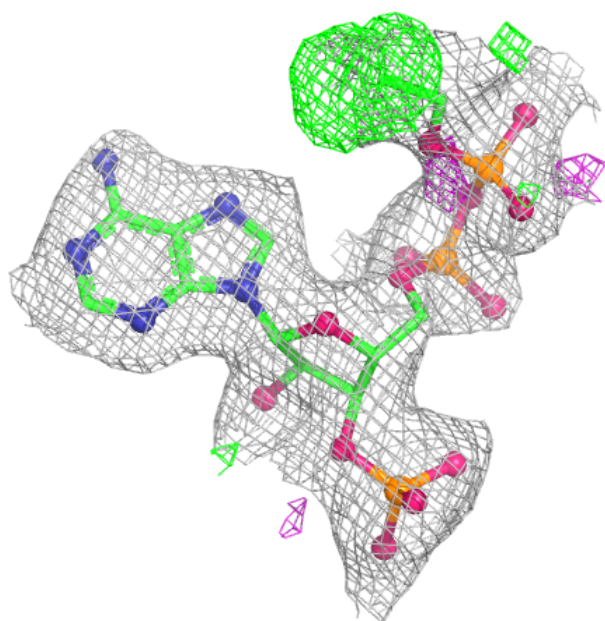
Electron density around ACO D 2004:

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



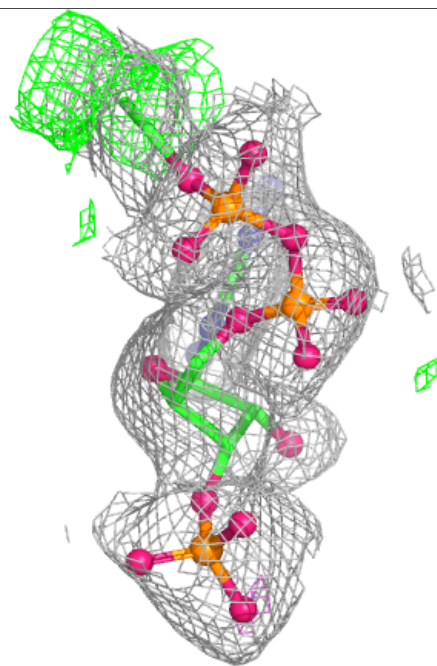
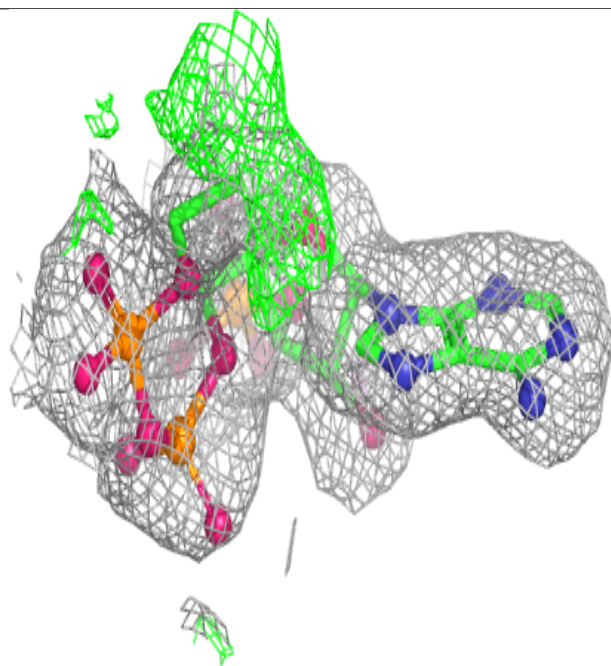
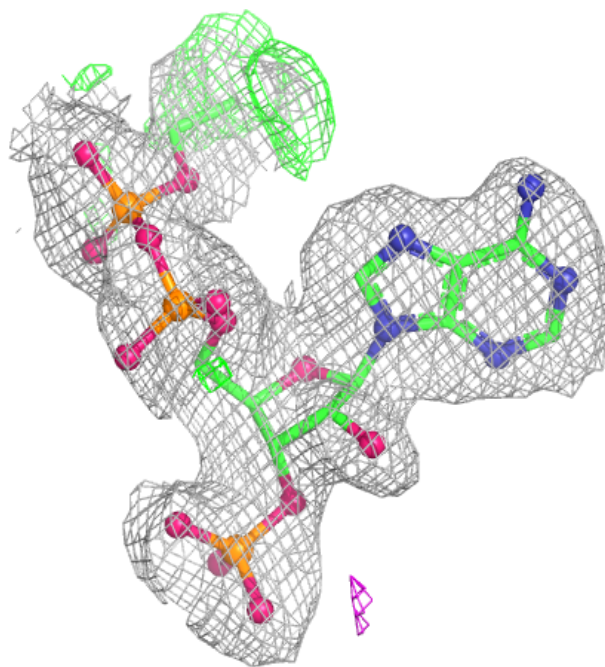
Electron density around ACO A 2004:

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



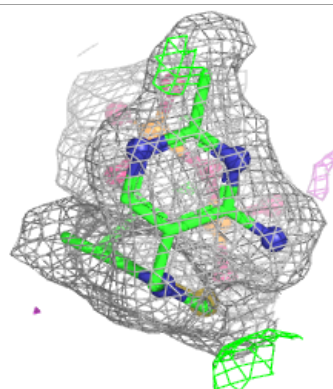
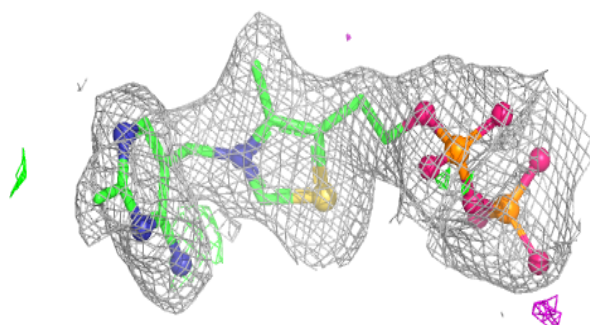
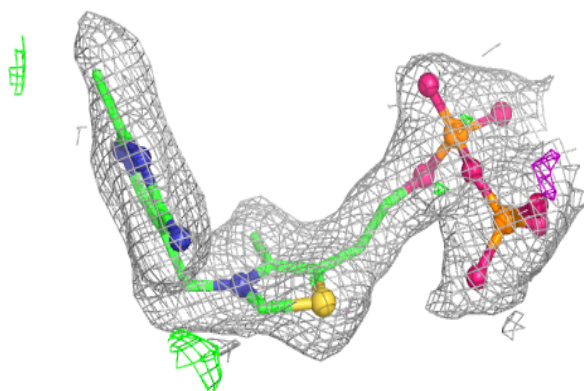
Electron density around ACO C 2004:

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

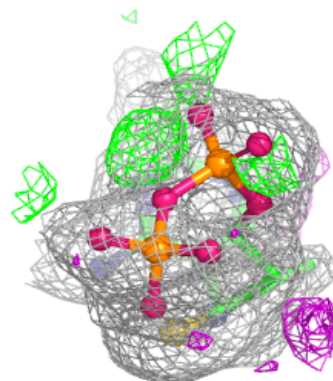
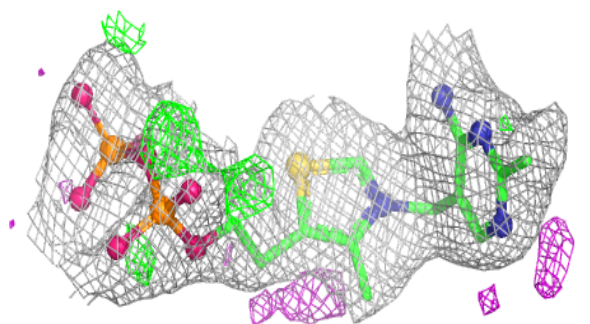
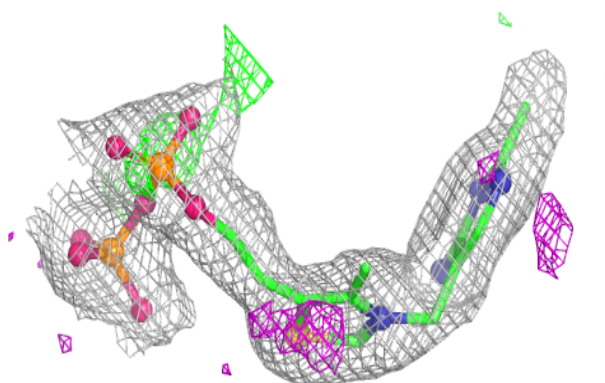


Electron density around TPP D 2001:

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

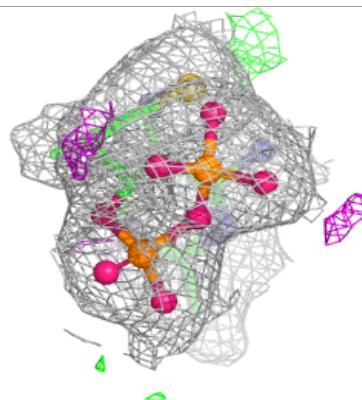
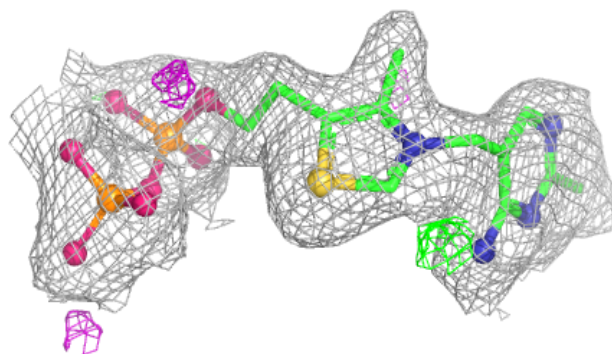
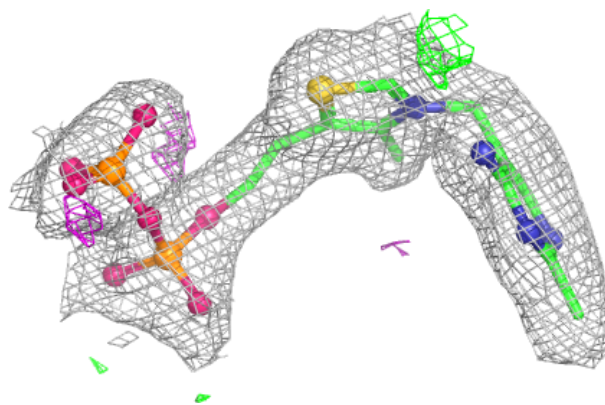
**Electron density around TPP B 2001:**

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

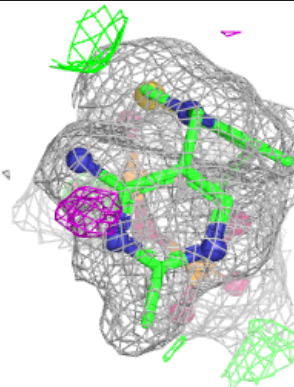
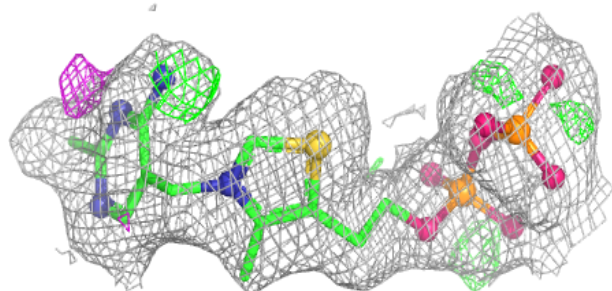
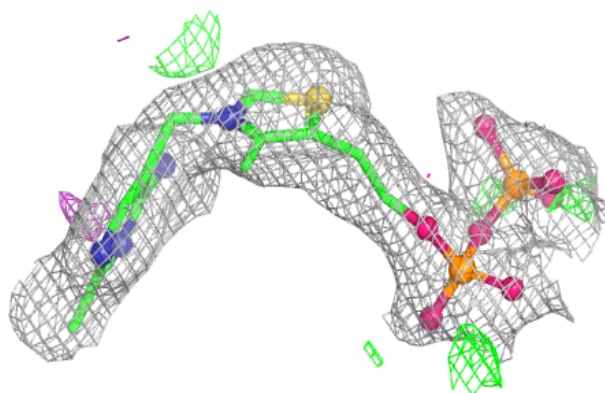


Electron density around TPP A 2001:

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

**Electron density around TPP C 2001:**

$2mF_o-DF_c$ (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.