



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:23 AM UTC

PDB ID : 6Z2H / pdb_00006z2h
Title : Citryl-CoA lyase module of human ATP citrate lyase in complex with (3S)-citryl-CoA.
Authors : Verschueren, K.H.G.; Verstraete, K.
Deposited on : 2020-05-15
Resolution : 1.80 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

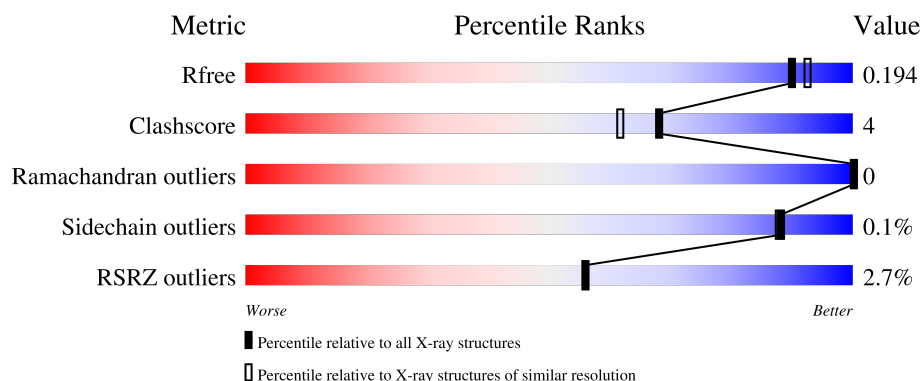
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	270	0% 92% 6% .
1	B	270	5% 90% 6% .
1	C	270	2% 92% 5% .
1	D	270	2% 87% 10% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17370 atoms, of which 8205 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.

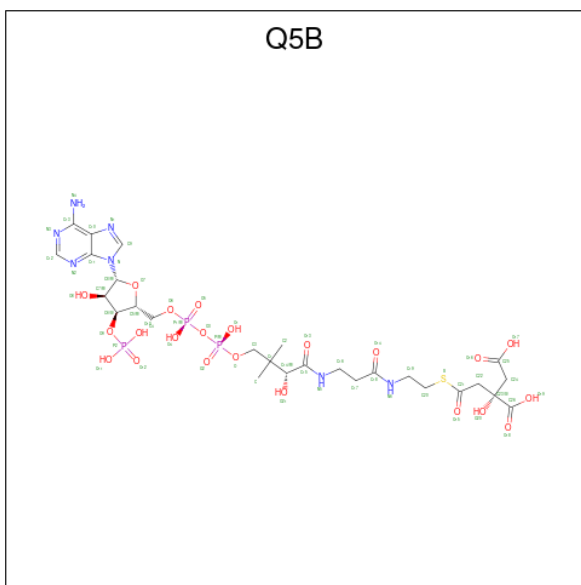
- Molecule 1 is a protein called ATP-citrate synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	264	Total	C	H	N	O	S	0	6	0
			4126	1321	2061	350	373	21			
1	B	261	Total	C	H	N	O	S	0	6	0
			4029	1298	2004	336	370	21			
1	C	263	Total	C	H	N	O	S	0	8	0
			4155	1333	2075	350	376	21			
1	D	261	Total	C	H	N	O	S	0	9	0
			4137	1327	2065	348	374	23			

There are 16 discrepancies between the modelled and reference sequences:

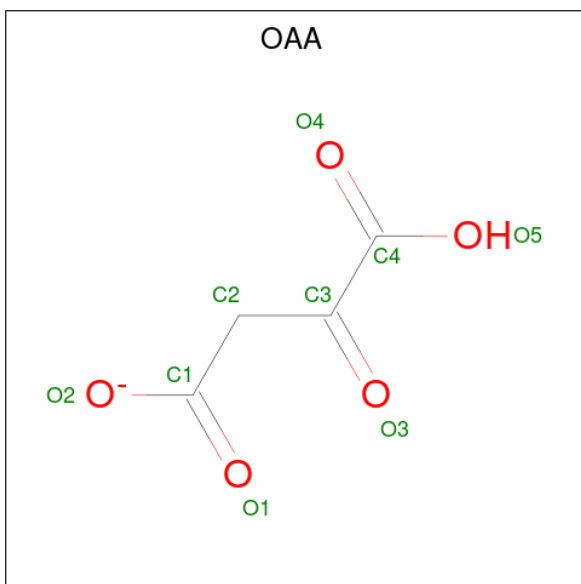
Chain	Residue	Modelled	Actual	Comment	Reference
A	832	GLY	-	expression tag	UNP P53396
A	833	SER	-	expression tag	UNP P53396
A	834	HIS	-	expression tag	UNP P53396
A	835	MET	-	expression tag	UNP P53396
B	832	GLY	-	expression tag	UNP P53396
B	833	SER	-	expression tag	UNP P53396
B	834	HIS	-	expression tag	UNP P53396
B	835	MET	-	expression tag	UNP P53396
C	832	GLY	-	expression tag	UNP P53396
C	833	SER	-	expression tag	UNP P53396
C	834	HIS	-	expression tag	UNP P53396
C	835	MET	-	expression tag	UNP P53396
D	832	GLY	-	expression tag	UNP P53396
D	833	SER	-	expression tag	UNP P53396
D	834	HIS	-	expression tag	UNP P53396
D	835	MET	-	expression tag	UNP P53396

- Molecule 2 is (3S)-citryl-Coenzyme A (CCD ID: Q5B) (formula: C₂₇H₄₂N₇O₂₂P₃S) (labeled as "Ligand of Interest" by depositor).



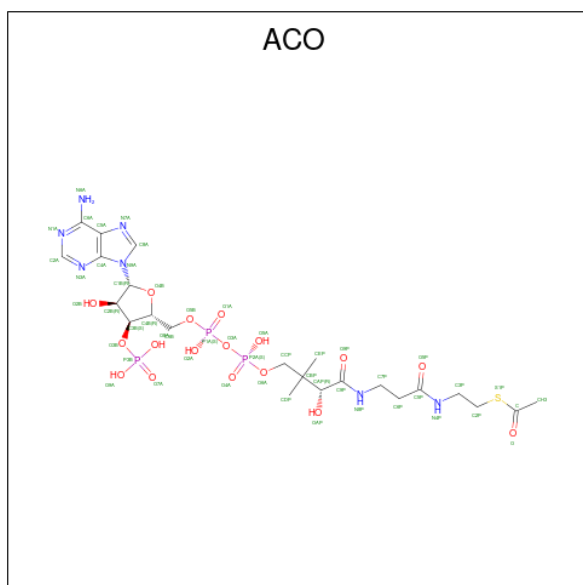
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	1
			60	27	7	22	3	1		
2	C	1	Total	C	N	O	P	S	0	1
			60	27	7	22	3	1		
2	D	1	Total	C	N	O	P	S	0	1
			60	27	7	22	3	1		

- Molecule 3 is OXALOACETATE ION (CCD ID: OAA) (formula: $C_4H_3O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 9 4 5	0	1
3	C	1	Total C O 9 4 5	0	1

- Molecule 4 is ACETYL COENZYME *A (CCD ID: ACO) (formula: $C_{23}H_{38}N_7O_{17}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P S 51 23 7 17 3 1	0	1
4	C	1	Total C N O P S 51 23 7 17 3 1	0	1

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	152	Total O 152 152	0	0
5	B	120	Total O 120 120	0	0
5	C	187	Total O 187 187	0	0
5	D	164	Total O 164 164	0	0

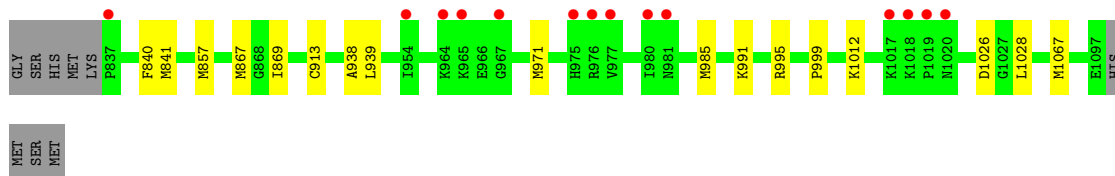
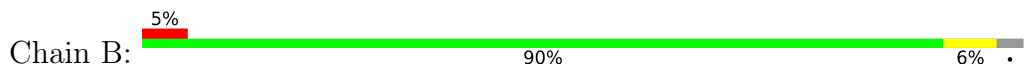
3 Residue-property plots

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

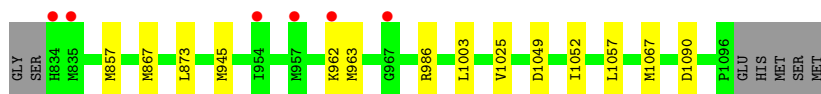
- Molecule 1: ATP-citrate synthase



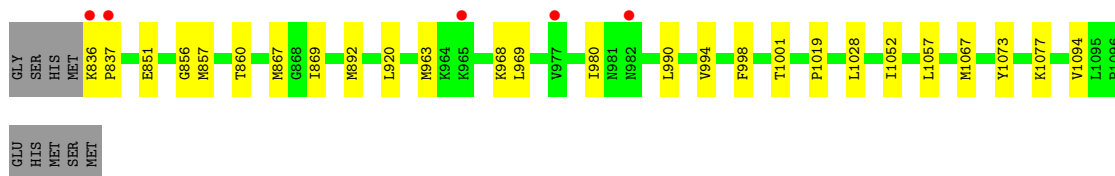
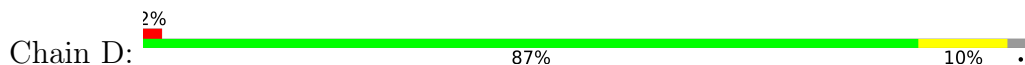
- Molecule 1: ATP-citrate synthase



- Molecule 1: ATP-citrate synthase



- Molecule 1: ATP-citrate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.44Å 114.27Å 144.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.28 – 1.80 44.28 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.28-1.80) 99.9 (44.28-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 1.79Å)	Xtriage
Refinement program	PHENIX 1.17_3644	Depositor
R, R_{free}	0.158 , 0.192 0.161 , 0.194	Depositor DCC
R_{free} test set	5263 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	20.9	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 36.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17370	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.76% 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: OAA, Q5B, ACO

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	0.48	0/2107	0.62	0/2843
1	B	0.48	0/2069	0.58	0/2796
1	C	0.52	0/2123	0.64	0/2865
1	D	0.49	0/2113	0.60	0/2850
All	All	0.49	0/8412	0.61	0/11354

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2065	2061	2056	12	0
1	B	2025	2004	1999	17	0
1	C	2080	2075	2063	14	0
1	D	2072	2065	2071	19	0
2	A	60	0	0	1	0
2	C	60	0	0	2	0
2	D	60	0	0	1	0
3	A	9	0	2	1	0
3	C	9	0	2	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	51	0	34	1	0
4	C	51	0	34	2	0
5	A	152	0	0	0	0
5	B	120	0	0	4	0
5	C	187	0	0	2	0
5	D	164	0	0	0	0
All	All	9165	8205	8261	60	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (60) 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:C:1049:ASP:OD1	5:C:1301:HOH:O	2.03	0.76
1:D:892[A]:MET:SD	1:D:990:LEU:HD23	2.31	0.70
1:D:994[A]:VAL:HG12	1:D:1001:THR:HG21	1.78	0.66
3:C:1202[B]:OAA:C3	4:C:1203[B]:ACO:HH32	2.26	0.65
1:D:1094:VAL:O	1:D:1094:VAL:HG23	1.97	0.63
1:A:1094:VAL:HG23	1:A:1094:VAL:O	2.00	0.62
2:C:1201[A]:Q5B:S	5:C:1410:HOH:O	2.57	0.60
1:C:962:LYS:HA	1:C:962:LYS:HE2	1.84	0.60
1:C:986:ARG:CZ	1:C:1025[A]:VAL:HG21	2.32	0.59
1:D:980:ILE:HD11	1:D:1019:PRO:HB3	1.84	0.58
1:B:857:MET:HE1	1:B:867[A]:MET:SD	2.44	0.58
1:C:857:MET:HE1	1:C:867[A]:MET:SD	2.48	0.54
3:A:1202[B]:OAA:C3	4:A:1203[B]:ACO:HH32	2.37	0.54
1:B:999:PRO:HD2	5:B:1266:HOH:O	2.10	0.52
5:B:1288:HOH:O	1:D:856:GLY:HA2	2.11	0.51
1:A:1067[A]:MET:HE1	1:B:869:ILE:HG23	1.94	0.50
1:B:1028:LEU:C	1:B:1028:LEU:HD13	2.36	0.49
1:B:991:LYS:NZ	5:B:1201:HOH:O	2.23	0.49
1:C:945:MET:SD	1:C:963:MET:HE2	2.52	0.49
1:A:994:VAL:HG12	1:A:1001:THR:HG21	1.93	0.49
1:A:1052:ILE:HD12	1:A:1057:LEU:HD11	1.95	0.49
2:C:1201[A]:Q5B:S	2:C:1201[A]:Q5B:C24	3.00	0.49
1:B:1012:LYS:HB3	1:B:1012:LYS:NZ	2.28	0.49
1:A:1079:LEU:HD22	1:B:841:MET:SD	2.53	0.48
1:D:851:GLU:OE2	1:D:860:THR:HG23	2.13	0.48
1:A:869:ILE:HG23	1:B:1067[A]:MET:HE1	1.96	0.48
1:C:1052:ILE:HD12	1:C:1057:LEU:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:959:PHE:O	1:A:963[A]:MET:HG2	2.13	0.48
1:D:994[A]:VAL:HG13	1:D:998:PHE:CD2	2.49	0.48
1:B:971:MET:HA	1:B:971:MET:HE2	1.96	0.48
1:C:1067[A]:MET:HE1	1:D:869:ILE:HG23	1.96	0.48
1:B:985:MET:HE3	1:B:985:MET:HA	1.96	0.47
1:D:994[A]:VAL:CG1	1:D:1001:THR:HG21	2.43	0.47
1:D:969:LEU:HD22	2:D:1201[A]:Q5B:C10	2.46	0.46
1:A:980:ILE:HG21	1:A:1015:THR:HB	1.96	0.46
1:B:991:LYS:HG2	1:B:995:ARG:HD3	1.97	0.46
1:B:867[B]:MET:HE1	5:B:1205:HOH:O	2.16	0.46
1:D:836:LYS:N	1:D:837:PRO:HD3	2.31	0.46
1:D:1052:ILE:HD13	1:D:1057[B]:LEU:HD13	1.97	0.46
1:C:1052:ILE:HD12	1:C:1057:LEU:CD1	2.46	0.46
3:C:1202[B]:OAA:C3	4:C:1203[B]:ACO:CH3	2.96	0.44
1:C:986:ARG:NE	1:C:1025[A]:VAL:HG21	2.32	0.43
1:D:1073:TYR:CZ	1:D:1077:LYS:HD2	2.53	0.43
1:A:839[A]:SER:OG	1:C:1090:ASP:OD2	2.37	0.43
1:C:1052:ILE:CD1	1:C:1057:LEU:HD11	2.49	0.43
1:C:986:ARG:CZ	1:C:1025[B]:VAL:HG11	2.49	0.43
1:A:912[A]:ILE:HD11	1:B:840:PHE:CZ	2.54	0.42
1:D:920:LEU:C	1:D:920:LEU:HD23	2.45	0.42
1:A:1028:LEU:C	1:A:1028:LEU:HD13	2.45	0.42
1:C:1003:LEU:HD12	1:C:1003:LEU:HA	1.90	0.41
1:B:939:LEU:H	1:B:939:LEU:HD12	1.86	0.41
1:D:857:MET:SD	1:D:867[A]:MET:SD	3.19	0.41
1:D:857:MET:HE1	1:D:867[A]:MET:SD	2.60	0.41
2:A:1201[A]:Q5B:S	2:A:1201[A]:Q5B:C24	3.09	0.41
1:B:938:ALA:HB3	1:B:1026:ASP:OD2	2.20	0.41
1:B:995:ARG:HE	1:B:995:ARG:HB2	1.77	0.41
1:D:963[A]:MET:HE3	1:D:968:LYS:CB	2.51	0.41
1:D:1028:LEU:HD13	1:D:1028:LEU:C	2.47	0.40
1:A:873:LEU:HD12	1:B:1067[B]:MET:SD	2.61	0.40
1:C:873:LEU:HD12	1:D:1067[A]:MET:SD	2.62	0.40

There are no symmetry-related clashes.

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	268/270 (99%)	261 (97%)	7 (3%)	0	100	100
1	B	265/270 (98%)	257 (97%)	8 (3%)	0	100	100
1	C	269/270 (100%)	263 (98%)	6 (2%)	0	100	100
1	D	268/270 (99%)	262 (98%)	6 (2%)	0	100	100
All	All	1070/1080 (99%)	1043 (98%)	27 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	219/226 (97%)	219 (100%)	0	100	100
1	B	213/226 (94%)	211 (99%)	2 (1%)	70	67
1	C	220/226 (97%)	220 (100%)	0	100	100
1	D	221/226 (98%)	221 (100%)	0	100	100
All	All	873/904 (97%)	871 (100%)	2 (0%)	88	87

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	913[A]	CYS
1	B	913[B]	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	850	GLN
1	A	997	HIS
1	B	850	GLN
1	B	909	ASN
1	B	982	ASN
1	B	1039	ASN
1	C	879	GLN
1	D	981	ASN
1	D	1039	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](#)

7 ligands are modelled in this entry.

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	Q5B	A	1201[A]	-	60,62,62	0.51	0	87,93,93	0.95	2 (2%)
2	Q5B	D	1201[A]	-	60,62,62	0.47	0	87,93,93	0.64	0
3	OAA	C	1202[B]	-	8,8,8	2.36	3 (37%)	8,10,10	1.98	2 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ACO	C	1203[B]	-	51,53,53	1.18	5 (9%)	73,79,79	1.64	13 (17%)
3	OAA	A	1202[B]	-	8,8,8	2.20	4 (50%)	8,10,10	1.37	1 (12%)
2	Q5B	C	1201[A]	-	60,62,62	0.46	0	87,93,93	0.79	1 (1%)
4	ACO	A	1203[B]	-	51,53,53	1.17	5 (9%)	73,79,79	1.56	12 (16%)

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	Q5B	A	1201[A]	-	-	12/66/83/83	0/3/3/3
2	Q5B	D	1201[A]	-	-	9/66/83/83	0/3/3/3
3	OAA	C	1202[B]	-	-	2/8/8/8	-
4	ACO	C	1203[B]	-	-	9/51/67/67	0/3/3/3
3	OAA	A	1202[B]	-	-	1/8/8/8	-
2	Q5B	C	1201[A]	-	-	17/66/83/83	0/3/3/3
4	ACO	A	1203[B]	-	-	5/51/67/67	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1203[B]	ACO	C5A-C4A	4.93	1.47	1.39
3	C	1202[B]	OAA	O3-C3	4.72	1.32	1.23
4	A	1203[B]	ACO	C5A-C4A	4.71	1.47	1.39
3	A	1202[B]	OAA	O3-C3	4.09	1.31	1.23
3	C	1202[B]	OAA	O4-C4	3.74	1.31	1.22
3	A	1202[B]	OAA	O4-C4	3.06	1.30	1.22
3	A	1202[B]	OAA	O1-C1	2.92	1.31	1.22
4	A	1203[B]	ACO	C8A-N7A	2.68	1.36	1.31
4	C	1203[B]	ACO	C8A-N7A	2.67	1.36	1.31
4	A	1203[B]	ACO	C5A-C6A	2.56	1.48	1.41
3	C	1202[B]	OAA	O1-C1	2.51	1.30	1.22
4	A	1203[B]	ACO	C5A-N7A	-2.32	1.34	1.39
4	C	1203[B]	ACO	P1A-O3A	2.22	1.61	1.59
4	A	1203[B]	ACO	P1A-O3A	2.15	1.61	1.59
4	C	1203[B]	ACO	C5A-C6A	2.11	1.46	1.41
4	C	1203[B]	ACO	C4A-N9A	-2.05	1.33	1.37
3	A	1202[B]	OAA	C3-C4	-2.00	1.50	1.53

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1203[B]	ACO	C5A-C4A-N3A	-5.49	119.16	126.72
4	C	1203[B]	ACO	C5A-C4A-N3A	-5.47	119.18	126.72
2	A	1201[A]	Q5B	C23-C22-C21	5.18	128.07	114.70
4	C	1203[B]	ACO	N3A-C4A-N9A	5.04	135.75	127.17
4	A	1203[B]	ACO	N3A-C4A-N9A	4.41	134.66	127.17
2	C	1201[A]	Q5B	C23-C22-C21	4.29	125.77	114.70
4	C	1203[B]	ACO	N3A-C2A-N1A	-4.19	122.24	128.58
4	C	1203[B]	ACO	C2A-N3A-C4A	3.87	121.29	111.83
4	C	1203[B]	ACO	C4A-N9A-C8A	3.84	109.77	105.74
4	A	1203[B]	ACO	N3A-C2A-N1A	-3.67	123.03	128.58
4	A	1203[B]	ACO	C2A-N3A-C4A	3.66	120.78	111.83
3	C	1202[B]	OAA	O4-C4-C3	-3.66	117.26	121.81
4	A	1203[B]	ACO	C4A-C5A-N7A	-3.47	106.62	110.58
4	A	1203[B]	ACO	C4A-N9A-C8A	3.10	109.00	105.74
3	C	1202[B]	OAA	O5-C4-C3	2.89	121.60	113.59
4	C	1203[B]	ACO	O5P-C5P-C6P	-2.82	116.91	122.02
4	A	1203[B]	ACO	C5A-N7A-C8A	2.67	107.65	103.45
2	A	1201[A]	Q5B	P2-O9-C6	2.61	130.39	123.43
4	C	1203[B]	ACO	O4B-C1B-N9A	2.47	112.82	108.09
4	A	1203[B]	ACO	O6A-CCP-CBP	-2.44	106.62	110.55
4	C	1203[B]	ACO	N6A-C6A-N1A	2.43	123.80	118.38
3	A	1202[B]	OAA	O3-C3-C2	2.43	124.14	120.41
4	A	1203[B]	ACO	N9A-C8A-N7A	-2.37	110.57	113.94
4	C	1203[B]	ACO	C4A-C5A-N7A	-2.35	107.89	110.58
4	A	1203[B]	ACO	O5P-C5P-C6P	-2.30	117.86	122.02
4	A	1203[B]	ACO	C6A-C5A-N7A	2.25	136.43	132.09
4	C	1203[B]	ACO	C2B-C1B-N9A	-2.20	107.83	113.30
4	C	1203[B]	ACO	C2A-N1A-C6A	2.19	122.32	118.73
4	A	1203[B]	ACO	C2A-N1A-C6A	2.16	122.28	118.73
4	C	1203[B]	ACO	C5A-C6A-N6A	-2.11	118.05	123.29
4	C	1203[B]	ACO	O9A-P3B-O8A	2.04	115.44	107.80

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201[A]	Q5B	C3-O-P-O2
2	A	1201[A]	Q5B	N6-C19-C20-S
2	A	1201[A]	Q5B	C19-C20-S-C21
2	A	1201[A]	Q5B	C24-C23-C26-O18
2	A	1201[A]	Q5B	C24-C23-C26-O19

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Mol	Chain	Res	Type	Atoms
2	A	1201[A]	Q5B	O20-C23-C26-O18
2	A	1201[A]	Q5B	O20-C23-C26-O19
2	C	1201[A]	Q5B	C3-O-P-O2
2	C	1201[A]	Q5B	N6-C19-C20-S
2	C	1201[A]	Q5B	C19-C20-S-C21
2	C	1201[A]	Q5B	C24-C23-C26-O18
2	C	1201[A]	Q5B	C24-C23-C26-O19
2	C	1201[A]	Q5B	O20-C23-C26-O18
2	C	1201[A]	Q5B	O20-C23-C26-O19
2	D	1201[A]	Q5B	C3-O-P-O3
2	D	1201[A]	Q5B	C4-O6-P1-O3
2	D	1201[A]	Q5B	C4-O6-P1-O5
4	A	1203[B]	ACO	C5B-O5B-P1A-O2A
4	A	1203[B]	ACO	CCP-O6A-P2A-O3A
4	A	1203[B]	ACO	CCP-O6A-P2A-O5A
4	C	1203[B]	ACO	C5B-O5B-P1A-O2A
4	C	1203[B]	ACO	C5B-O5B-P1A-O3A
4	C	1203[B]	ACO	CCP-O6A-P2A-O3A
4	C	1203[B]	ACO	CCP-O6A-P2A-O5A
2	D	1201[A]	Q5B	C21-C22-C23-C24
2	D	1201[A]	Q5B	C21-C22-C23-C26
2	D	1201[A]	Q5B	O6-C4-C5-O7
2	D	1201[A]	Q5B	C21-C22-C23-O20
2	D	1201[A]	Q5B	O6-C4-C5-C6
4	A	1203[B]	ACO	P1A-O3A-P2A-O4A
4	C	1203[B]	ACO	P1A-O3A-P2A-O4A
2	A	1201[A]	Q5B	O15-C21-S-C20
2	C	1201[A]	Q5B	O15-C21-S-C20
2	C	1201[A]	Q5B	C22-C21-S-C20
2	C	1201[A]	Q5B	C2-C1-C3-O
4	C	1203[B]	ACO	CDP-CBP-CCP-O6A
2	C	1201[A]	Q5B	C14-C1-C3-O
2	D	1201[A]	Q5B	C3-O-P-O2
4	C	1203[B]	ACO	C5B-O5B-P1A-O1A
4	A	1203[B]	ACO	P1A-O3A-P2A-O5A
4	C	1203[B]	ACO	P1A-O3A-P2A-O5A
2	C	1201[A]	Q5B	C22-C23-C26-O18
2	C	1201[A]	Q5B	C22-C23-C26-O19
2	A	1201[A]	Q5B	C23-C24-C25-O17
2	C	1201[A]	Q5B	C23-C24-C25-O17
2	A	1201[A]	Q5B	C23-C24-C25-O16
2	C	1201[A]	Q5B	C23-C24-C25-O16

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Mol	Chain	Res	Type	Atoms
2	A	1201[A]	Q5B	C22-C21-S-C20
3	A	1202[B]	OAA	C1-C2-C3-O3
3	C	1202[B]	OAA	C1-C2-C3-O3
2	C	1201[A]	Q5B	C-C1-C3-O
4	C	1203[B]	ACO	CEP-CBP-CCP-O6A
3	C	1202[B]	OAA	C1-C2-C3-C4
2	A	1201[A]	Q5B	P1-O3-P-O1
2	C	1201[A]	Q5B	P1-O3-P-O1

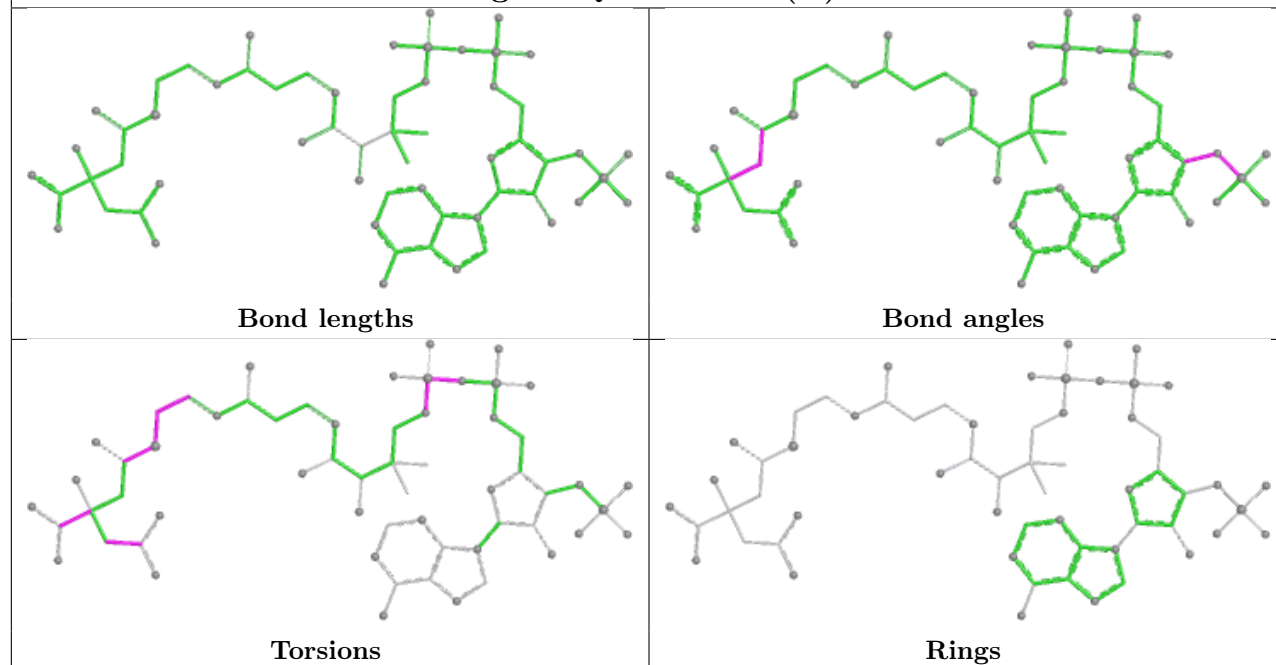
There are no ring outliers.

7 monomers are involved in 7 short contacts:

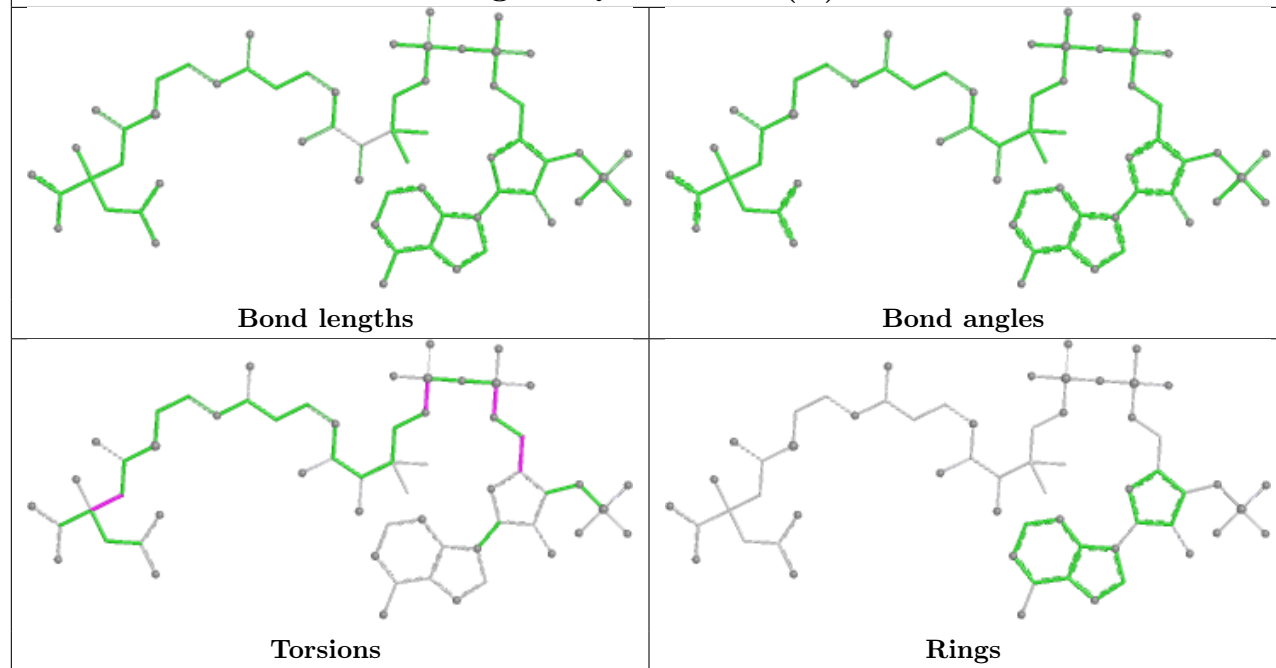
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201[A]	Q5B	1	0
2	D	1201[A]	Q5B	1	0
3	C	1202[B]	OAA	2	0
4	C	1203[B]	ACO	2	0
3	A	1202[B]	OAA	1	0
2	C	1201[A]	Q5B	2	0
4	A	1203[B]	ACO	1	0

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.

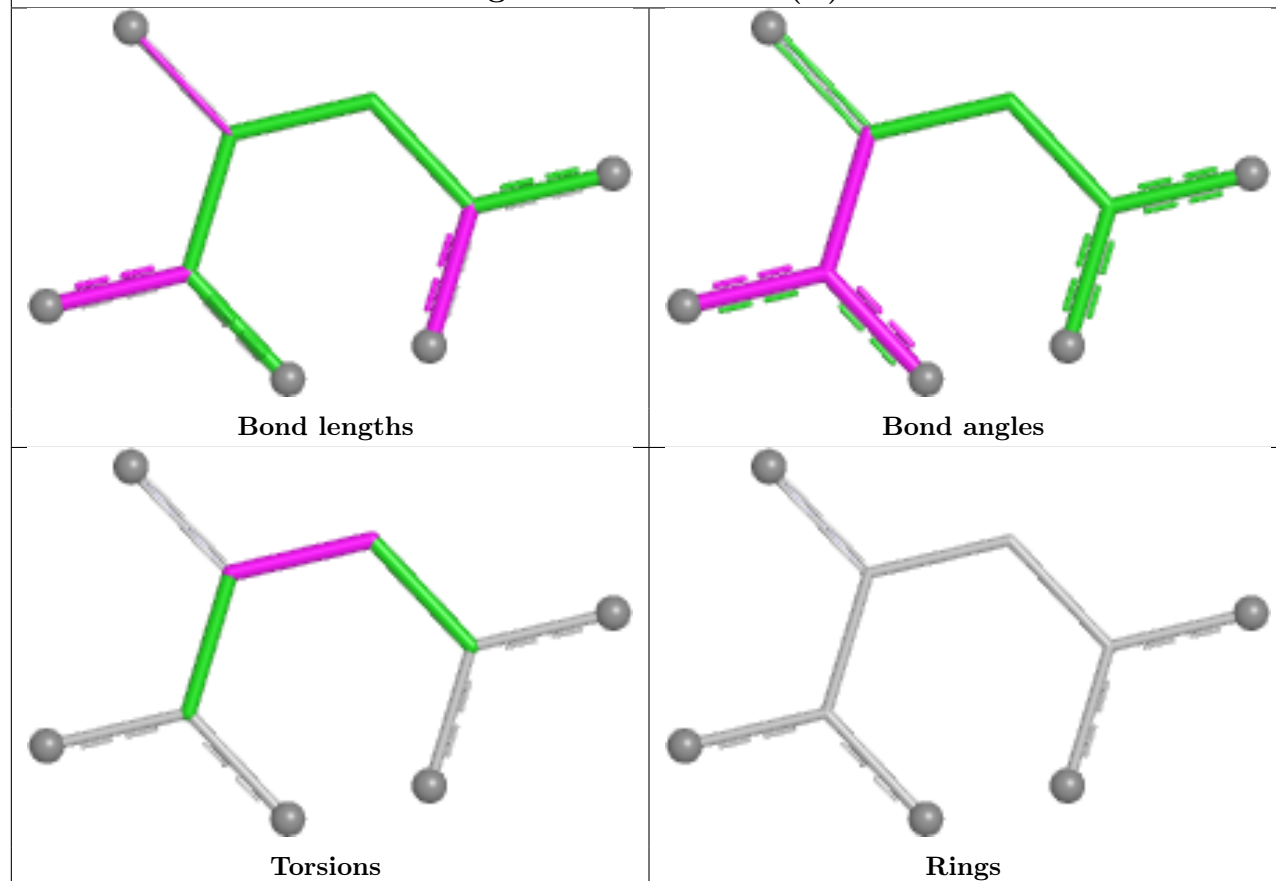
Ligand Q5B A 1201 (A)



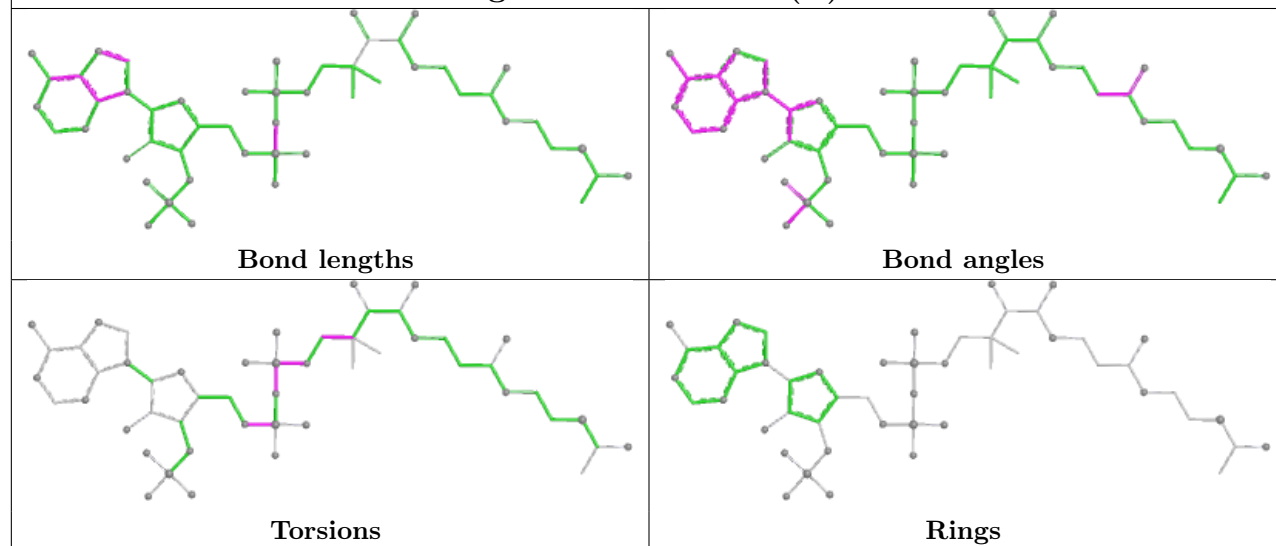
Ligand Q5B D 1201 (A)



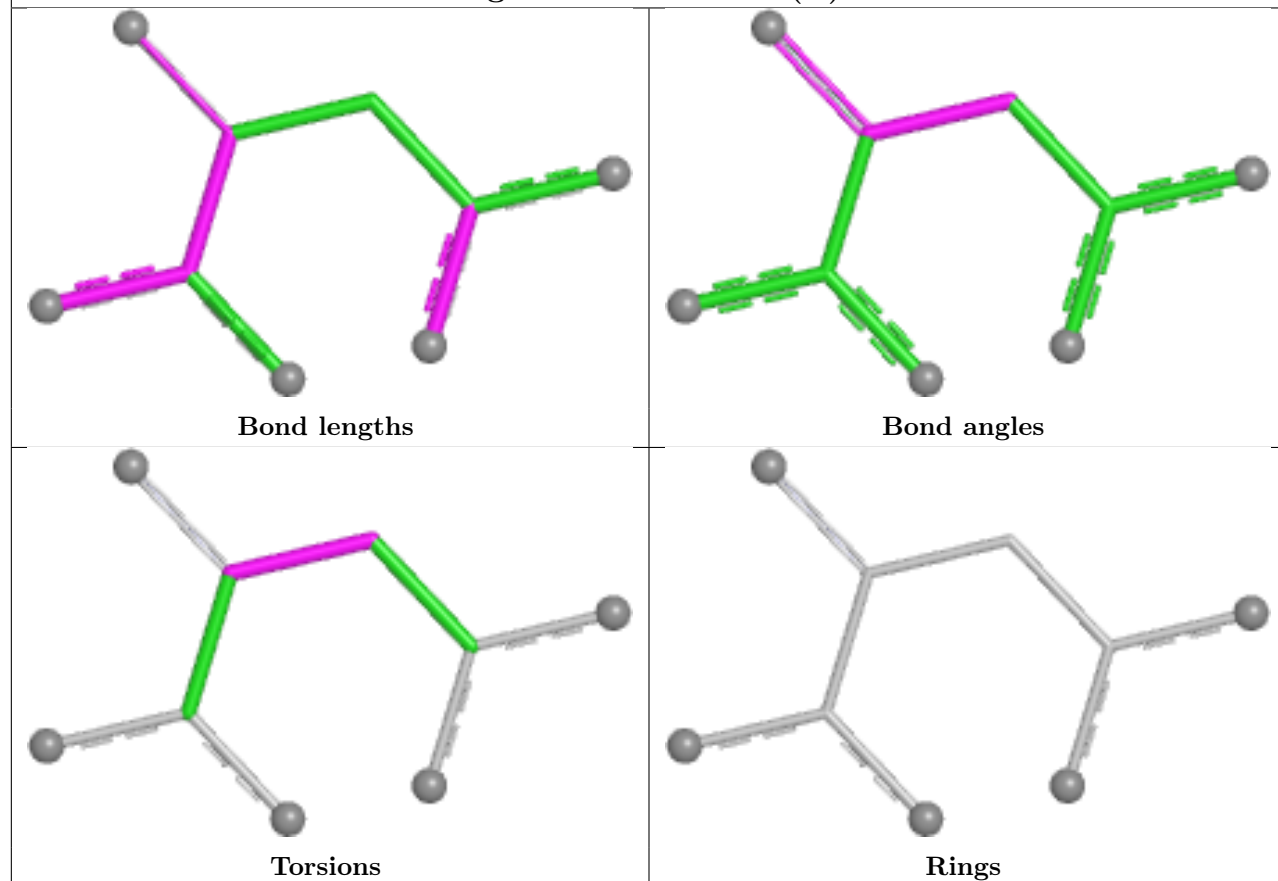
Ligand OAA C 1202 (B)



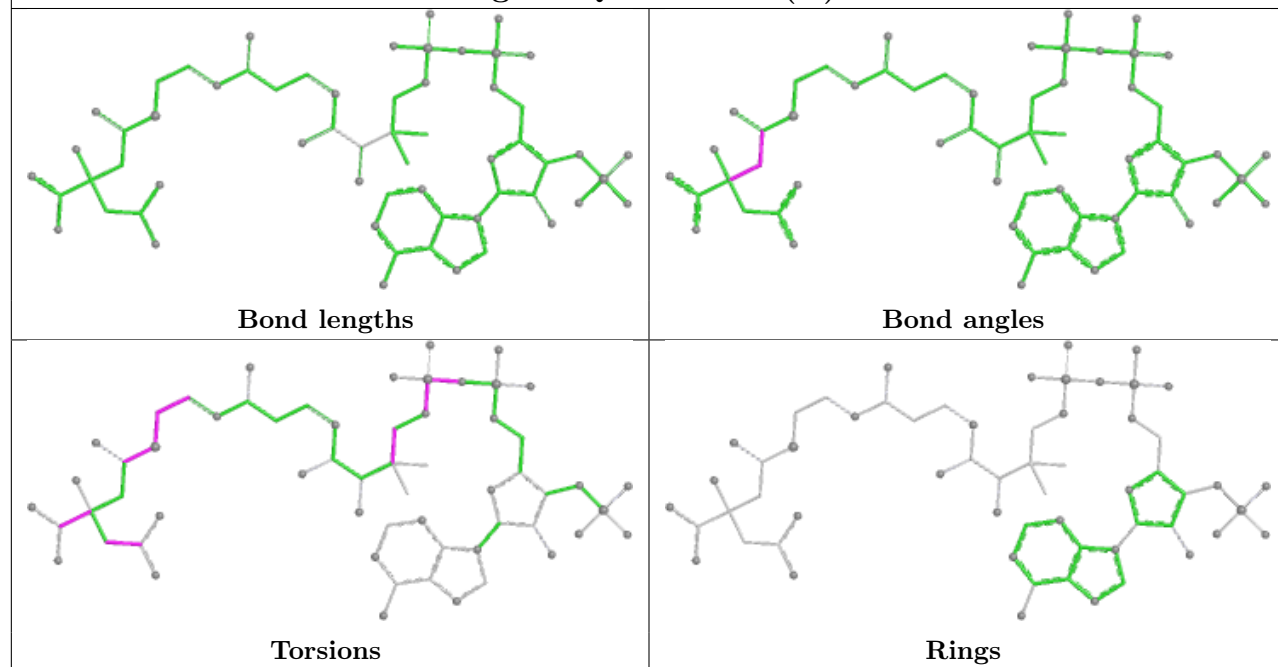
Ligand ACO C 1203 (B)

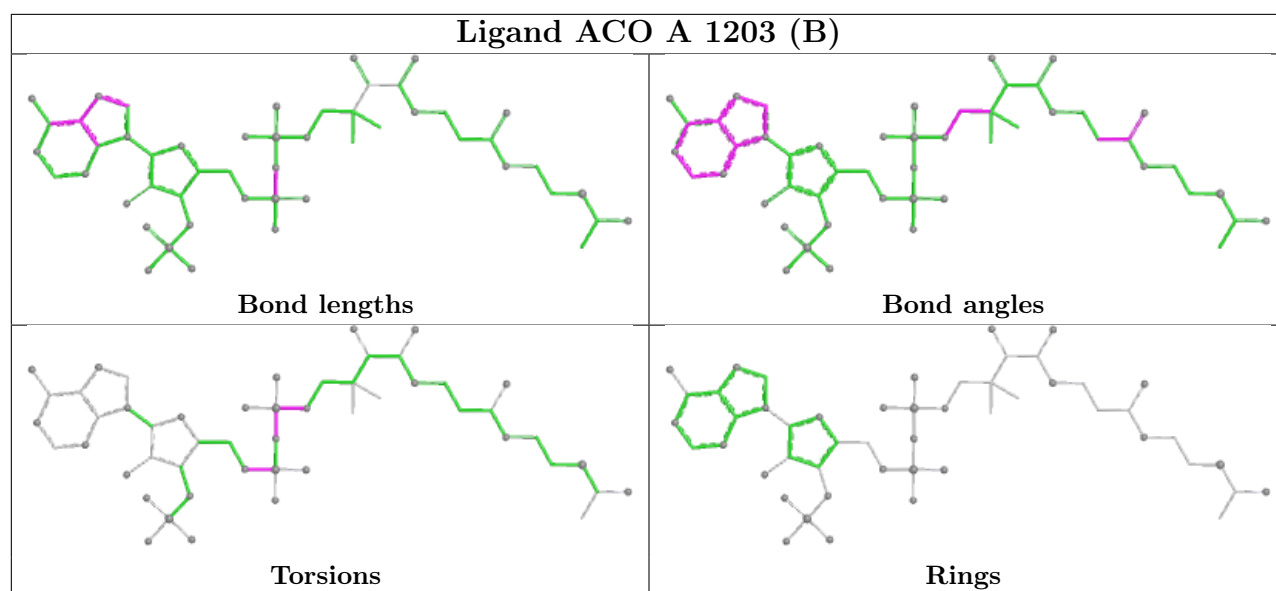


Ligand OAA A 1202 (B)



Ligand Q5B C 1201 (A)





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	264/270 (97%)	-0.42	3 (1%) 78 78	8, 24, 45, 61	6 (2%)
1	B	261/270 (96%)	-0.10	14 (5%) 31 30	8, 27, 59, 70	6 (2%)
1	C	263/270 (97%)	-0.41	6 (2%) 61 61	7, 21, 44, 68	8 (3%)
1	D	261/270 (96%)	-0.40	5 (1%) 66 66	7, 23, 47, 71	9 (3%)
All	All	1049/1080 (97%)	-0.33	28 (2%) 56 56	7, 24, 50, 71	29 (2%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	967	GLY	6.0
1	D	836	LYS	4.1
1	C	834	HIS	3.7
1	B	837	PRO	3.6
1	B	976	ARG	3.3
1	B	980	ILE	3.2
1	B	967	GLY	3.1
1	A	967	GLY	3.1
1	B	975	HIS	3.0
1	B	965	LYS	3.0
1	B	1020	ASN	2.9
1	B	954	ILE	2.8
1	B	1019	PRO	2.7
1	B	981	ASN	2.7
1	D	837	PRO	2.6
1	B	1018	LYS	2.5
1	B	977	VAL	2.5
1	C	835	MET	2.5
1	D	982	ASN	2.4
1	C	954	ILE	2.3
1	C	957[A]	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1089	ASP	2.2
1	C	962	LYS	2.2
1	D	977	VAL	2.2
1	B	964	LYS	2.1
1	B	1017	LYS	2.1
1	D	965	LYS	2.0
1	A	1096	PRO	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](#)

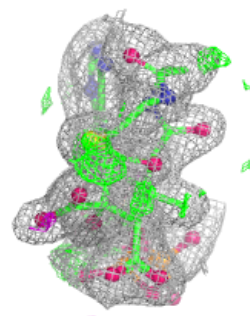
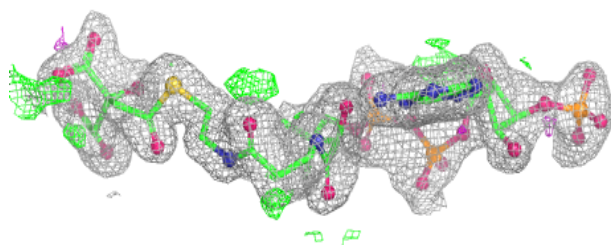
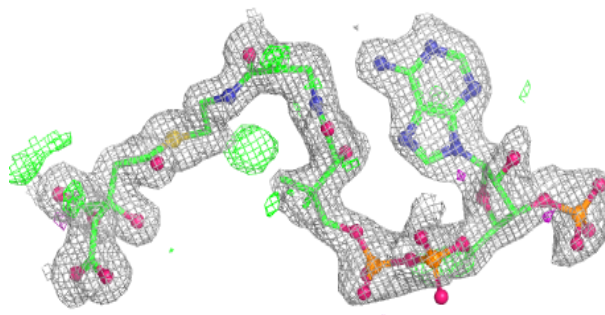
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	Q5B	D	1201[A]	60/60	0.89	0.11	25,42,73,89	0
2	Q5B	C	1201[A]	60/60	0.92	0.10	11,24,55,67	60
4	ACO	A	1203[B]	51/51	0.92	0.10	15,26,56,72	51
4	ACO	C	1203[B]	51/51	0.93	0.09	16,27,56,67	51
2	Q5B	A	1201[A]	60/60	0.94	0.09	13,24,57,74	60
3	OAA	A	1202[B]	9/9	0.97	0.05	13,17,23,24	9
3	OAA	C	1202[B]	9/9	0.97	0.06	15,18,21,24	9

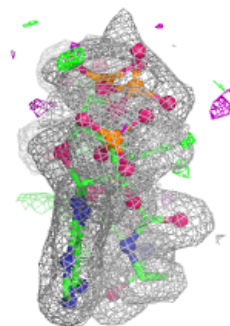
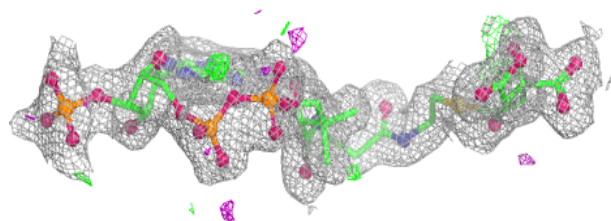
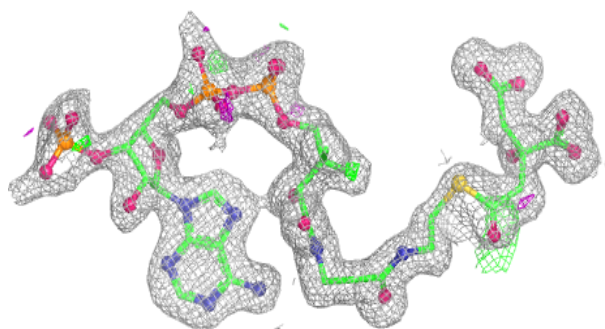
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Q5B D 1201 (A):

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

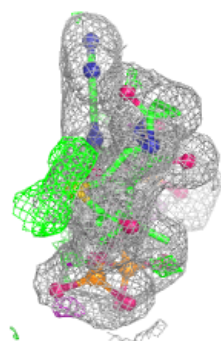
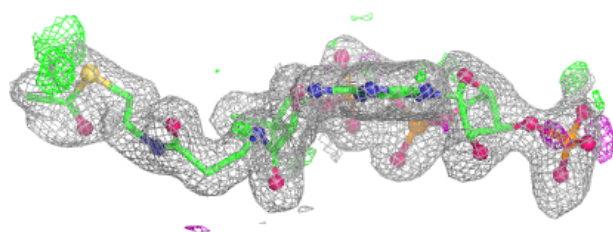
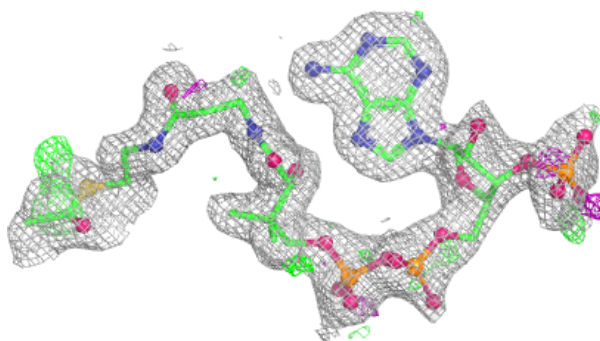
**Electron density around Q5B C 1201 (A):**

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

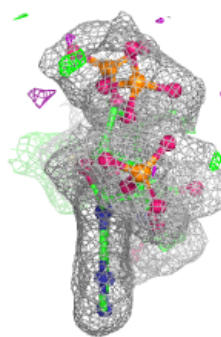
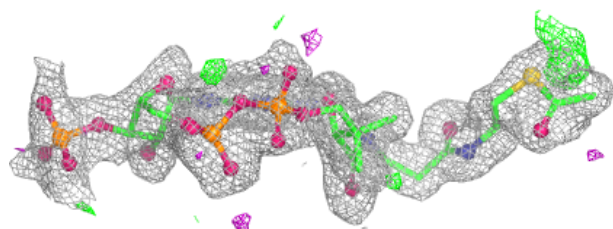
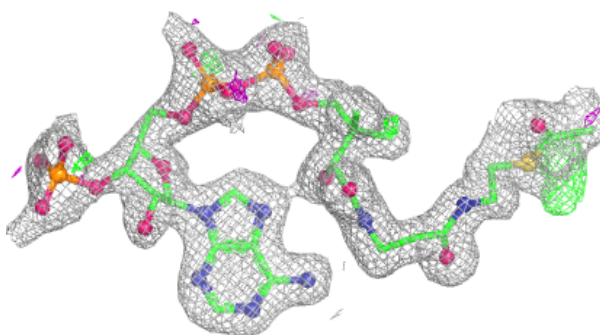


Electron density around ACO A 1203 (B):

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

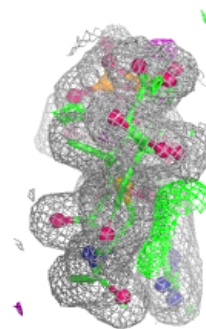
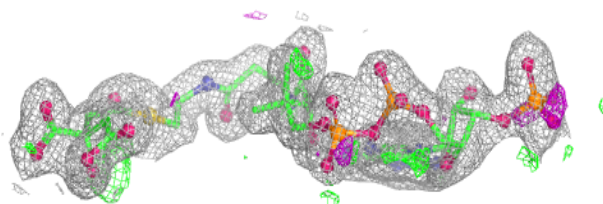
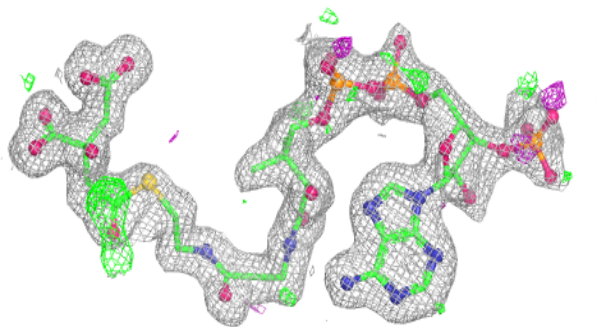
**Electron density around ACO C 1203 (B):**

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



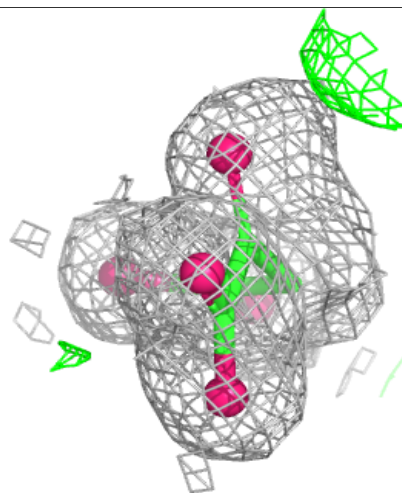
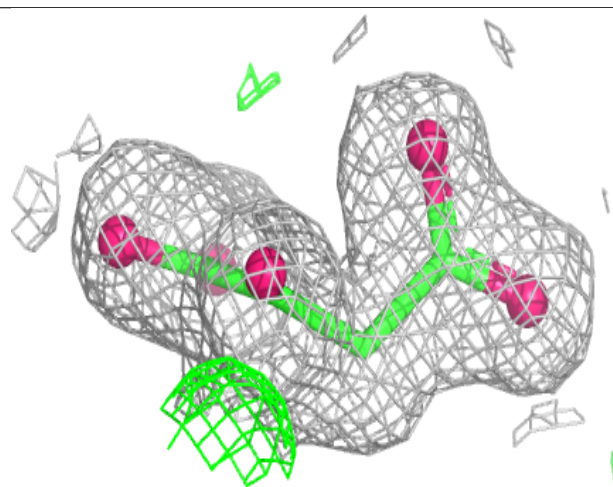
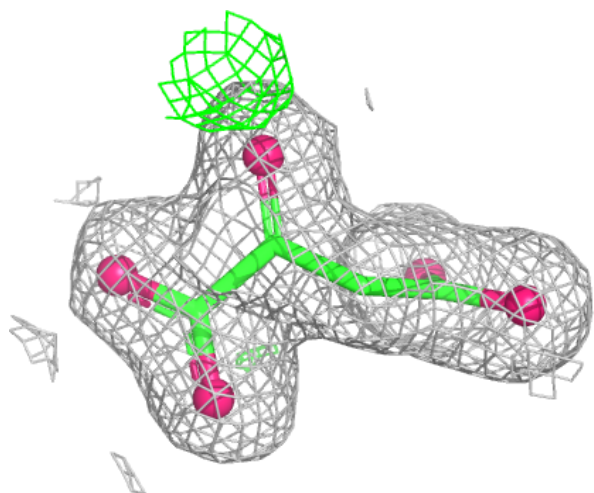
Electron density around Q5B A 1201 (A):

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



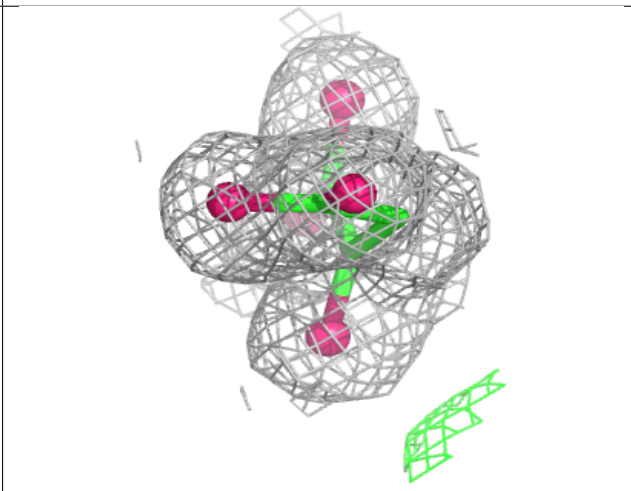
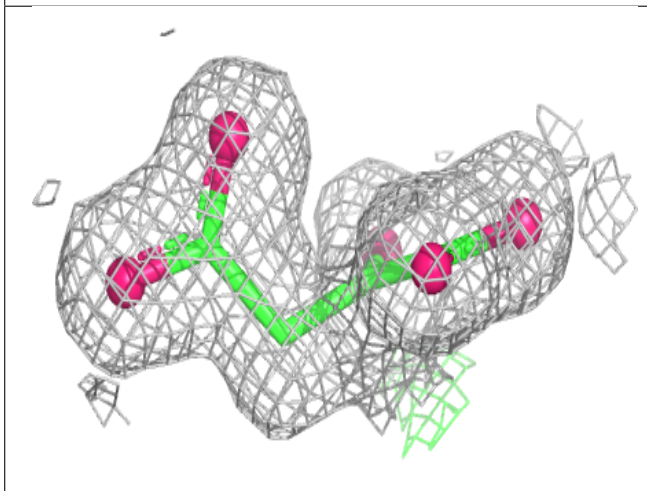
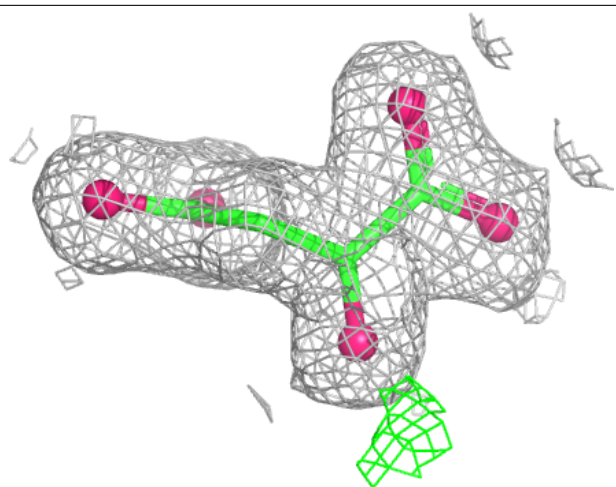
Electron density around OAA A 1202 (B):

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



Electron density around OAA C 1202 (B):

$2mF_o-DF_c$ (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.