



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 11:49 pm BST

PDB ID : 3MK6  
Title : Substrate and Inhibitor Binding to Pank  
Authors : Yun, M.-K.; White, S.W.  
Deposited on : 2010-04-14  
Resolution : 1.98 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

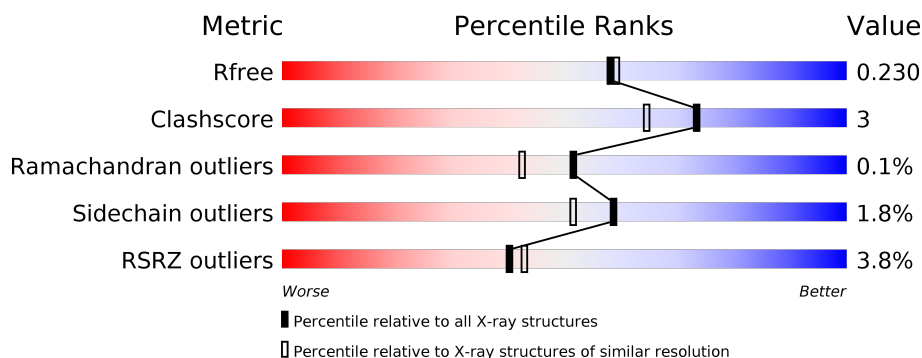
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.98 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	376	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>8%</div> <div>6%</div> </div> </div>
1	B	376	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>8%</div> <div>7%</div> </div> </div>
1	C	376	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>7%</div> <div>7%</div> </div> </div>
1	D	376	<div> <div>7%</div> <div> <div></div> <div>83%</div> <div>8%</div> <div>8%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11582 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 Pantothenate kinase 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	354	Total	C	N	O	S	0	1	0
			2725	1740	454	516	15			
1	B	351	Total	C	N	O	S	0	1	0
			2715	1733	457	510	15			
1	C	351	Total	C	N	O	S	0	2	0
			2708	1730	450	513	15			
1	D	345	Total	C	N	O	S	0	1	0
			2659	1699	444	502	14			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	EXPRESSION TAG	UNP Q9H999
A	-6	GLY	-	EXPRESSION TAG	UNP Q9H999
A	-5	SER	-	EXPRESSION TAG	UNP Q9H999
A	-4	SER	-	EXPRESSION TAG	UNP Q9H999
A	-3	HIS	-	EXPRESSION TAG	UNP Q9H999
A	-2	HIS	-	EXPRESSION TAG	UNP Q9H999
A	-1	HIS	-	EXPRESSION TAG	UNP Q9H999
A	0	HIS	-	EXPRESSION TAG	UNP Q9H999
A	1	HIS	-	EXPRESSION TAG	UNP Q9H999
A	2	HIS	-	EXPRESSION TAG	UNP Q9H999
A	3	SER	-	EXPRESSION TAG	UNP Q9H999
A	4	SER	-	EXPRESSION TAG	UNP Q9H999
A	5	GLY	-	EXPRESSION TAG	UNP Q9H999
A	6	LEU	-	EXPRESSION TAG	UNP Q9H999
A	7	VAL	-	EXPRESSION TAG	UNP Q9H999
A	8	PRO	-	EXPRESSION TAG	UNP Q9H999
A	9	ARG	-	EXPRESSION TAG	UNP Q9H999
A	10	GLY	-	EXPRESSION TAG	UNP Q9H999
A	11	SER	-	EXPRESSION TAG	UNP Q9H999
B	-7	MET	-	EXPRESSION TAG	UNP Q9H999
B	-6	GLY	-	EXPRESSION TAG	UNP Q9H999

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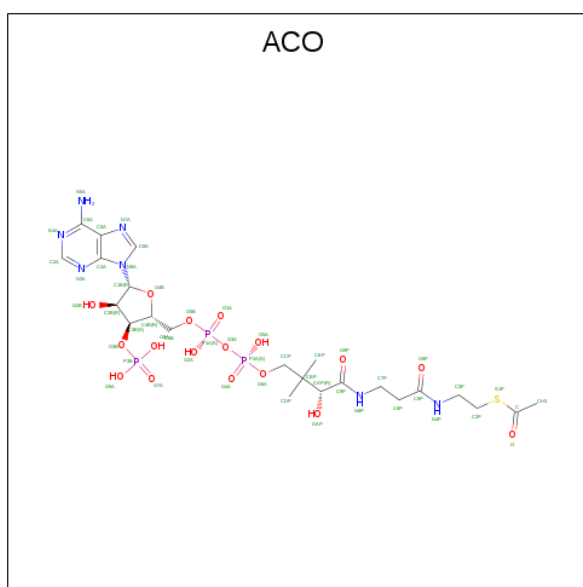
Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	SER	-	EXPRESSION TAG	UNP Q9H999
B	-4	SER	-	EXPRESSION TAG	UNP Q9H999
B	-3	HIS	-	EXPRESSION TAG	UNP Q9H999
B	-2	HIS	-	EXPRESSION TAG	UNP Q9H999
B	-1	HIS	-	EXPRESSION TAG	UNP Q9H999
B	0	HIS	-	EXPRESSION TAG	UNP Q9H999
B	1	HIS	-	EXPRESSION TAG	UNP Q9H999
B	2	HIS	-	EXPRESSION TAG	UNP Q9H999
B	3	SER	-	EXPRESSION TAG	UNP Q9H999
B	4	SER	-	EXPRESSION TAG	UNP Q9H999
B	5	GLY	-	EXPRESSION TAG	UNP Q9H999
B	6	LEU	-	EXPRESSION TAG	UNP Q9H999
B	7	VAL	-	EXPRESSION TAG	UNP Q9H999
B	8	PRO	-	EXPRESSION TAG	UNP Q9H999
B	9	ARG	-	EXPRESSION TAG	UNP Q9H999
B	10	GLY	-	EXPRESSION TAG	UNP Q9H999
B	11	SER	-	EXPRESSION TAG	UNP Q9H999
C	-7	MET	-	EXPRESSION TAG	UNP Q9H999
C	-6	GLY	-	EXPRESSION TAG	UNP Q9H999
C	-5	SER	-	EXPRESSION TAG	UNP Q9H999
C	-4	SER	-	EXPRESSION TAG	UNP Q9H999
C	-3	HIS	-	EXPRESSION TAG	UNP Q9H999
C	-2	HIS	-	EXPRESSION TAG	UNP Q9H999
C	-1	HIS	-	EXPRESSION TAG	UNP Q9H999
C	0	HIS	-	EXPRESSION TAG	UNP Q9H999
C	1	HIS	-	EXPRESSION TAG	UNP Q9H999
C	2	HIS	-	EXPRESSION TAG	UNP Q9H999
C	3	SER	-	EXPRESSION TAG	UNP Q9H999
C	4	SER	-	EXPRESSION TAG	UNP Q9H999
C	5	GLY	-	EXPRESSION TAG	UNP Q9H999
C	6	LEU	-	EXPRESSION TAG	UNP Q9H999
C	7	VAL	-	EXPRESSION TAG	UNP Q9H999
C	8	PRO	-	EXPRESSION TAG	UNP Q9H999
C	9	ARG	-	EXPRESSION TAG	UNP Q9H999
C	10	GLY	-	EXPRESSION TAG	UNP Q9H999
C	11	SER	-	EXPRESSION TAG	UNP Q9H999
D	-7	MET	-	EXPRESSION TAG	UNP Q9H999
D	-6	GLY	-	EXPRESSION TAG	UNP Q9H999
D	-5	SER	-	EXPRESSION TAG	UNP Q9H999
D	-4	SER	-	EXPRESSION TAG	UNP Q9H999
D	-3	HIS	-	EXPRESSION TAG	UNP Q9H999
D	-2	HIS	-	EXPRESSION TAG	UNP Q9H999

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	HIS	-	EXPRESSION TAG	UNP Q9H999
D	0	HIS	-	EXPRESSION TAG	UNP Q9H999
D	1	HIS	-	EXPRESSION TAG	UNP Q9H999
D	2	HIS	-	EXPRESSION TAG	UNP Q9H999
D	3	SER	-	EXPRESSION TAG	UNP Q9H999
D	4	SER	-	EXPRESSION TAG	UNP Q9H999
D	5	GLY	-	EXPRESSION TAG	UNP Q9H999
D	6	LEU	-	EXPRESSION TAG	UNP Q9H999
D	7	VAL	-	EXPRESSION TAG	UNP Q9H999
D	8	PRO	-	EXPRESSION TAG	UNP Q9H999
D	9	ARG	-	EXPRESSION TAG	UNP Q9H999
D	10	GLY	-	EXPRESSION TAG	UNP Q9H999
D	11	SER	-	EXPRESSION TAG	UNP Q9H999

- Molecule 2 is ACETYL COENZYME \*A (three-letter code: ACO) (formula:  $C_{23}H_{38}N_7O_{17}P_3S$ ).



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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

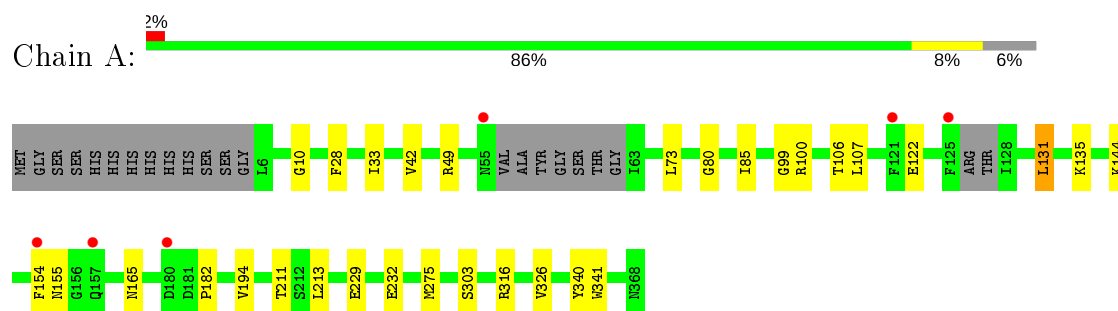
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	150	Total	O	0	0
			150	150		
4	B	105	Total	O	0	0
			105	105		
4	C	144	Total	O	0	0
			144	144		
4	D	124	Total	O	0	0
			124	124		

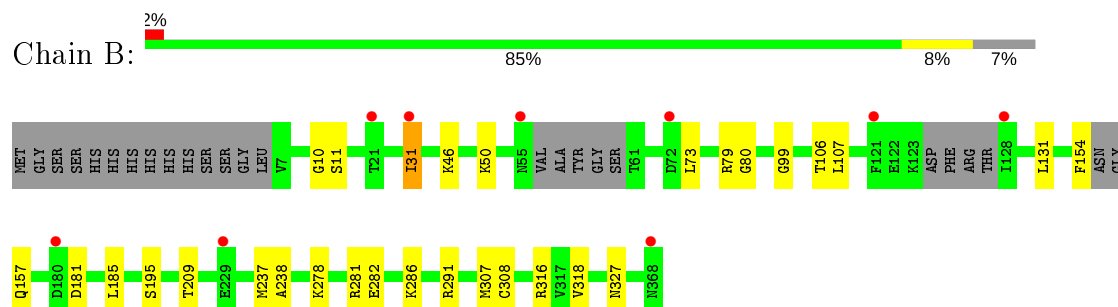
### 3 Residue-property plots [i](#)

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

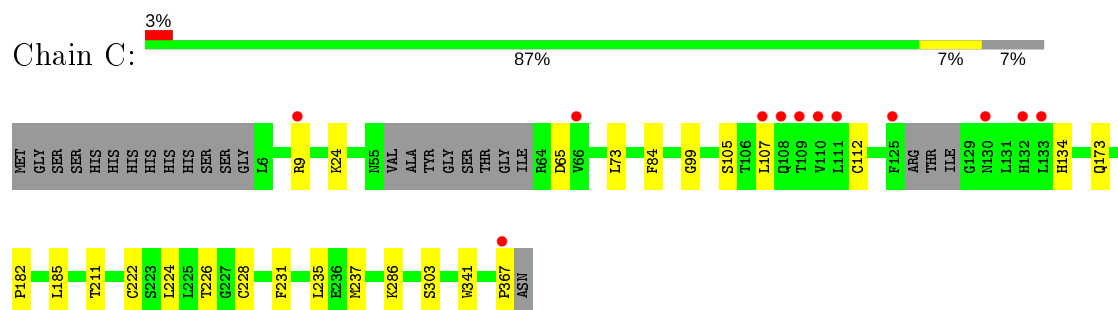
#### • Molecule 1: Pantothenate kinase 3



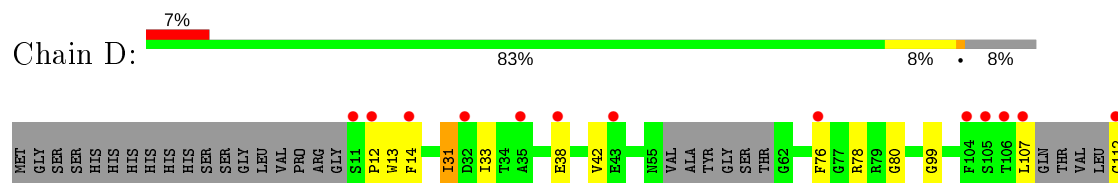
#### • Molecule 1: Pantothenate kinase 3

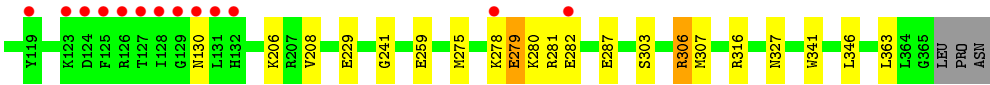


#### • Molecule 1: Pantothenate kinase 3



#### • Molecule 1: Pantothenate kinase 3







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.71 Å 180.38 Å 77.42 Å 90.00° 95.48° 90.00°	Depositor
Resolution (Å)	50.00 – 1.98 47.85 – 1.97	Depositor EDS
% Data completeness (in resolution range)	99.1 (50.00-1.98) 98.4 (47.85-1.97)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.26 (at 1.97 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.185 , 0.232 0.185 , 0.230	Depositor DCC
$R_{free}$ test set	5315 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.2	Xtriage
Anisotropy	0.450	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 51.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11582	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 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	0.72	0/2781	0.70	0/3758
1	B	0.63	0/2770	0.65	0/3738
1	C	0.68	1/2768 (0.0%)	0.67	0/3741
1	D	0.67	0/2714	0.68	0/3663
All	All	0.68	1/11033 (0.0%)	0.68	0/14900

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	222	CYS	CB-SG	-5.88	1.72	1.81

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	2725	0	2667	24	0
1	B	2715	0	2674	17	0
1	C	2708	0	2644	14	0
1	D	2659	0	2603	19	0
2	A	51	0	34	1	0
2	B	51	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	51	0	34	0	0
2	D	51	0	34	0	0
3	A	18	0	24	2	0
3	B	6	0	8	0	0
3	C	12	0	16	0	0
3	D	12	0	16	2	0
4	A	150	0	0	1	0
4	B	105	0	0	1	0
4	C	144	0	0	0	0
4	D	124	0	0	2	0
All	All	11582	0	10788	72	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 3.

All (72) 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:228:CYS:HB3	1:C:237:MET:HE1	1.28	1.13
1:C:228:CYS:HB3	1:C:237:MET:CE	1.94	0.98
1:A:100:ARG:HH21	1:A:131:LEU:HD22	1.42	0.83
1:A:10:GLY:HA3	1:A:106:THR:HG23	1.61	0.82
1:A:10:GLY:HA3	1:A:106:THR:CG2	2.13	0.78
1:D:278:LYS:O	1:D:282:GLU:HG2	1.87	0.75
1:D:346:LEU:HA	3:D:370:GOL:H12	1.70	0.74
1:C:228:CYS:CB	1:C:237:MET:HE1	2.15	0.71
1:D:99:GLY:HA3	1:D:107:LEU:HD12	1.73	0.70
1:D:33:ILE:HD11	1:D:42:VAL:HG21	1.74	0.69
1:D:206:LYS:HE3	1:D:208:VAL:HG12	1.75	0.67
1:B:278:LYS:O	1:B:282:GLU:HG2	1.98	0.64
1:B:327:ASN:O	4:B:478:HOH:O	2.15	0.63
1:D:12:PRO:HG2	1:D:14:PHE:CZ	2.34	0.63
1:A:194:VAL:HB	1:A:211:THR:HG22	1.82	0.61
1:A:100:ARG:NH2	1:A:131:LEU:HB2	2.16	0.60
1:D:31:ILE:HG12	1:D:80:GLY:HA2	1.85	0.59
1:A:99:GLY:HA3	1:A:107:LEU:HD12	1.84	0.58
1:B:185:LEU:HD11	1:B:318:VAL:HG23	1.84	0.58
1:A:303:SER:HB2	1:A:341:TRP:CE2	2.39	0.57
1:C:112:CYS:SG	1:C:134:HIS:HB3	2.45	0.56
1:B:99:GLY:HA3	1:B:107:LEU:HD12	1.86	0.56
1:C:303:SER:HB2	1:C:341:TRP:CE2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:GLY:HA3	1:C:107:LEU:HD12	1.88	0.55
1:B:185:LEU:HD11	1:B:318:VAL:CG2	2.38	0.54
3:A:370:GOL:H32	4:A:386:HOH:O	2.10	0.51
1:A:100:ARG:HH21	1:A:131:LEU:CD2	2.21	0.51
1:A:49:ARG:HG3	1:A:85:ILE:HG21	1.92	0.51
1:A:33:ILE:HD11	1:A:42:VAL:HG21	1.93	0.51
1:A:340:TYR:HD1	3:A:370:GOL:H31	1.75	0.51
1:D:303:SER:HB2	1:D:341:TRP:CE2	2.45	0.50
1:B:278:LYS:HG3	1:B:281:ARG:NH2	2.27	0.49
1:C:226:THR:HA	1:C:286:LYS:HD2	1.94	0.49
1:A:10:GLY:HA3	1:A:106:THR:HG22	1.95	0.48
1:A:182:PRO:C	1:A:316:ARG:HH21	2.12	0.48
1:D:33:ILE:CD1	1:D:42:VAL:HG21	2.42	0.47
1:B:209:THR:HG21	1:B:308[B]:CYS:SG	2.55	0.46
1:A:194:VAL:HB	1:A:211:THR:CG2	2.44	0.46
1:C:9:ARG:HH12	1:C:367:PRO:HA	1.81	0.46
1:C:228:CYS:CB	1:C:237:MET:CE	2.80	0.46
1:A:229:GLU:HA	1:A:229:GLU:OE1	2.15	0.45
1:A:275:MET:HG3	1:C:224:LEU:HD11	1.99	0.44
1:B:131:LEU:HA	1:B:131:LEU:HD12	1.85	0.44
1:C:231:PHE:CZ	1:C:235:LEU:HD11	2.52	0.44
1:D:38:GLU:CD	1:D:78:ARG:HH12	2.20	0.44
1:A:232:GLU:HG3	1:A:326:VAL:CG1	2.47	0.44
1:A:213:LEU:N	1:A:213:LEU:HD12	2.33	0.44
1:A:135:LYS:NZ	2:A:1901:ACO:N1A	2.60	0.44
1:B:238:ALA:O	1:B:291:ARG:HD3	2.18	0.44
1:D:346:LEU:HA	3:D:370:GOL:C1	2.44	0.44
1:A:28:PHE:CE1	1:A:80:GLY:HA3	2.53	0.44
1:B:46:LYS:O	1:B:50:LYS:HG3	2.18	0.44
1:D:13:TRP:CH2	1:D:76:PHE:HB2	2.54	0.43
1:C:65:ASP:HB3	1:C:84:PHE:O	2.18	0.43
1:A:28:PHE:CZ	1:A:80:GLY:HA3	2.54	0.43
1:D:363:LEU:O	1:D:363:LEU:HD23	2.18	0.43
1:B:181:ASP:O	1:B:316:ARG:NH1	2.51	0.42
1:A:155:ASN:O	1:B:157:GLN:HA	2.18	0.42
1:D:306:ARG:HD3	4:D:468:HOH:O	2.18	0.42
1:D:316:ARG:NH1	4:D:499:HOH:O	2.52	0.42
1:B:10:GLY:HA3	1:B:106:THR:HG23	2.02	0.42
1:B:31:ILE:HB	1:B:80:GLY:HA2	2.02	0.42
1:C:182:PRO:O	1:C:185:LEU:HB2	2.20	0.42
1:B:307:MET:HE3	1:D:307:MET:HE1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ARG:HH21	1:A:131:LEU:HB2	1.85	0.41
1:D:279:GLU:HG2	1:D:280:LYS:N	2.36	0.41
1:B:237:MET:CE	1:B:286:LYS:HB3	2.51	0.41
1:A:144:LYS:HB2	1:A:144:LYS:HE2	1.70	0.41
1:D:275:MET:O	1:D:281:ARG:HD3	2.21	0.41
1:D:241:GLY:HA3	1:D:287:GLU:O	2.21	0.40
1:B:31:ILE:O	1:B:31:ILE:HG23	2.22	0.40
1:C:24:LYS:N	1:C:24:LYS:HD3	2.36	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	349/376 (93%)	341 (98%)	7 (2%)	1 (0%)	41	29
1	B	344/376 (92%)	338 (98%)	6 (2%)	0	100	100
1	C	347/376 (92%)	341 (98%)	6 (2%)	0	100	100
1	D	340/376 (90%)	336 (99%)	3 (1%)	1 (0%)	41	29
All	All	1380/1504 (92%)	1356 (98%)	22 (2%)	2 (0%)	51	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	GLU
1	D	327	ASN

### 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	289/316 (92%)	285 (99%)	4 (1%)	67	62
1	B	289/316 (92%)	283 (98%)	6 (2%)	53	47
1	C	288/316 (91%)	284 (99%)	4 (1%)	67	62
1	D	281/316 (89%)	274 (98%)	7 (2%)	47	39
All	All	1147/1264 (91%)	1126 (98%)	21 (2%)	59	51

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	LEU
1	A	131	LEU
1	A	154	PHE
1	A	165	ASN
1	B	11	SER
1	B	31	ILE
1	B	73	LEU
1	B	79	ARG
1	B	154	PHE
1	B	195	SER
1	C	73	LEU
1	C	105	SER
1	C	173	GLN
1	C	211	THR
1	D	31	ILE
1	D	112	CYS
1	D	130	ASN
1	D	229	GLU
1	D	259	GLU
1	D	279	GLU
1	D	306	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	ASN
1	B	67	HIS

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Mol	Chain	Res	Type
1	B	130	ASN
1	B	157	GLN
1	B	165	ASN
1	D	130	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

12 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	ACO	A	1901	-	45,53,53	1.08	3 (6%)	56,79,79	1.31	6 (10%)
3	GOL	C	370	-	5,5,5	0.47	0	5,5,5	1.17	0
3	GOL	A	370	-	5,5,5	0.36	0	5,5,5	0.39	0
3	GOL	D	370	-	5,5,5	0.39	0	5,5,5	0.66	0
2	ACO	B	1902	-	45,53,53	1.11	3 (6%)	56,79,79	1.58	10 (17%)
3	GOL	A	369	-	5,5,5	0.49	0	5,5,5	0.67	0
3	GOL	C	369	-	5,5,5	0.50	0	5,5,5	0.43	0
2	ACO	C	1903	-	45,53,53	1.07	3 (6%)	56,79,79	1.31	6 (10%)
3	GOL	A	371	-	5,5,5	0.25	0	5,5,5	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	D	369	-	5,5,5	0.37	0	5,5,5	0.58	0
2	ACO	D	1904	-	45,53,53	1.09	2 (4%)	56,79,79	1.33	5 (8%)
3	GOL	B	369	-	5,5,5	0.45	0	5,5,5	0.63	0

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	ACO	A	1901	-	-	2/47/67/67	0/3/3/3
3	GOL	C	370	-	-	4/4/4/4	-
3	GOL	A	370	-	-	2/4/4/4	-
3	GOL	D	370	-	-	3/4/4/4	-
2	ACO	B	1902	-	-	1/47/67/67	0/3/3/3
3	GOL	A	369	-	-	0/4/4/4	-
3	GOL	C	369	-	-	0/4/4/4	-
2	ACO	C	1903	-	-	2/47/67/67	0/3/3/3
3	GOL	A	371	-	-	2/4/4/4	-
3	GOL	D	369	-	-	2/4/4/4	-
2	ACO	D	1904	-	-	2/47/67/67	0/3/3/3
3	GOL	B	369	-	-	0/4/4/4	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1904	ACO	O-C	4.51	1.42	1.20
2	B	1902	ACO	O-C	4.34	1.41	1.20
2	C	1903	ACO	O-C	4.32	1.41	1.20
2	A	1901	ACO	O-C	4.32	1.41	1.20
2	B	1902	ACO	O4B-C1B	2.64	1.44	1.41
2	C	1903	ACO	O4B-C1B	2.52	1.44	1.41
2	B	1902	ACO	P3B-O3B	2.35	1.63	1.59
2	A	1901	ACO	O4B-C1B	2.23	1.44	1.41
2	C	1903	ACO	C2A-N3A	2.17	1.35	1.32
2	D	1904	ACO	O4B-C1B	2.06	1.44	1.41
2	A	1901	ACO	P3B-O3B	2.01	1.63	1.59

All (27) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1902	ACO	N3A-C2A-N1A	-5.44	120.17	128.68
2	D	1904	ACO	N3A-C2A-N1A	-5.21	120.54	128.68
2	C	1903	ACO	N3A-C2A-N1A	-4.96	120.93	128.68
2	A	1901	ACO	N3A-C2A-N1A	-4.92	120.98	128.68
2	B	1902	ACO	C7P-N8P-C9P	3.95	129.63	122.59
2	D	1904	ACO	C7P-N8P-C9P	3.82	129.40	122.59
2	B	1902	ACO	C7P-C6P-C5P	-3.40	106.69	112.36
2	B	1902	ACO	C2P-C3P-N4P	-3.25	105.59	112.42
2	C	1903	ACO	C2P-C3P-N4P	-3.09	105.92	112.42
2	D	1904	ACO	O9A-P3B-O8A	2.88	118.65	107.64
2	B	1902	ACO	C1B-N9A-C4A	-2.79	121.74	126.64
2	B	1902	ACO	C6P-C7P-N8P	-2.69	106.47	111.90
2	C	1903	ACO	C6P-C7P-N8P	-2.68	106.50	111.90
2	A	1901	ACO	P2A-O3A-P1A	-2.65	123.72	132.83
2	A	1901	ACO	O2A-P1A-O1A	2.33	123.77	112.24
2	B	1902	ACO	P2A-O3A-P1A	-2.29	124.97	132.83
2	D	1904	ACO	C2P-C3P-N4P	-2.27	107.64	112.42
2	A	1901	ACO	C2A-N1A-C6A	2.18	122.48	118.75
2	C	1903	ACO	O9A-P3B-O8A	2.17	115.94	107.64
2	A	1901	ACO	C6P-C7P-N8P	-2.17	107.52	111.90
2	D	1904	ACO	P2A-O3A-P1A	-2.15	125.44	132.83
2	C	1903	ACO	C3P-N4P-C5P	2.15	126.83	122.84
2	B	1902	ACO	C3P-N4P-C5P	2.13	126.79	122.84
2	C	1903	ACO	C7P-N8P-C9P	2.11	126.36	122.59
2	A	1901	ACO	C7P-N8P-C9P	2.08	126.29	122.59
2	B	1902	ACO	OAP-CAP-CBP	-2.03	105.47	110.25
2	B	1902	ACO	C2A-N1A-C6A	2.03	122.23	118.75

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	370	GOL	O1-C1-C2-C3
3	D	370	GOL	C1-C2-C3-O3
3	A	371	GOL	C1-C2-C3-O3
3	C	370	GOL	O1-C1-C2-O2
3	A	371	GOL	O2-C2-C3-O3
3	C	370	GOL	C1-C2-C3-O3
3	A	370	GOL	O1-C1-C2-C3
3	C	370	GOL	O2-C2-C3-O3
3	A	370	GOL	O1-C1-C2-O2
3	D	370	GOL	O2-C2-C3-O3
2	B	1902	ACO	P2A-O3A-P1A-O1A

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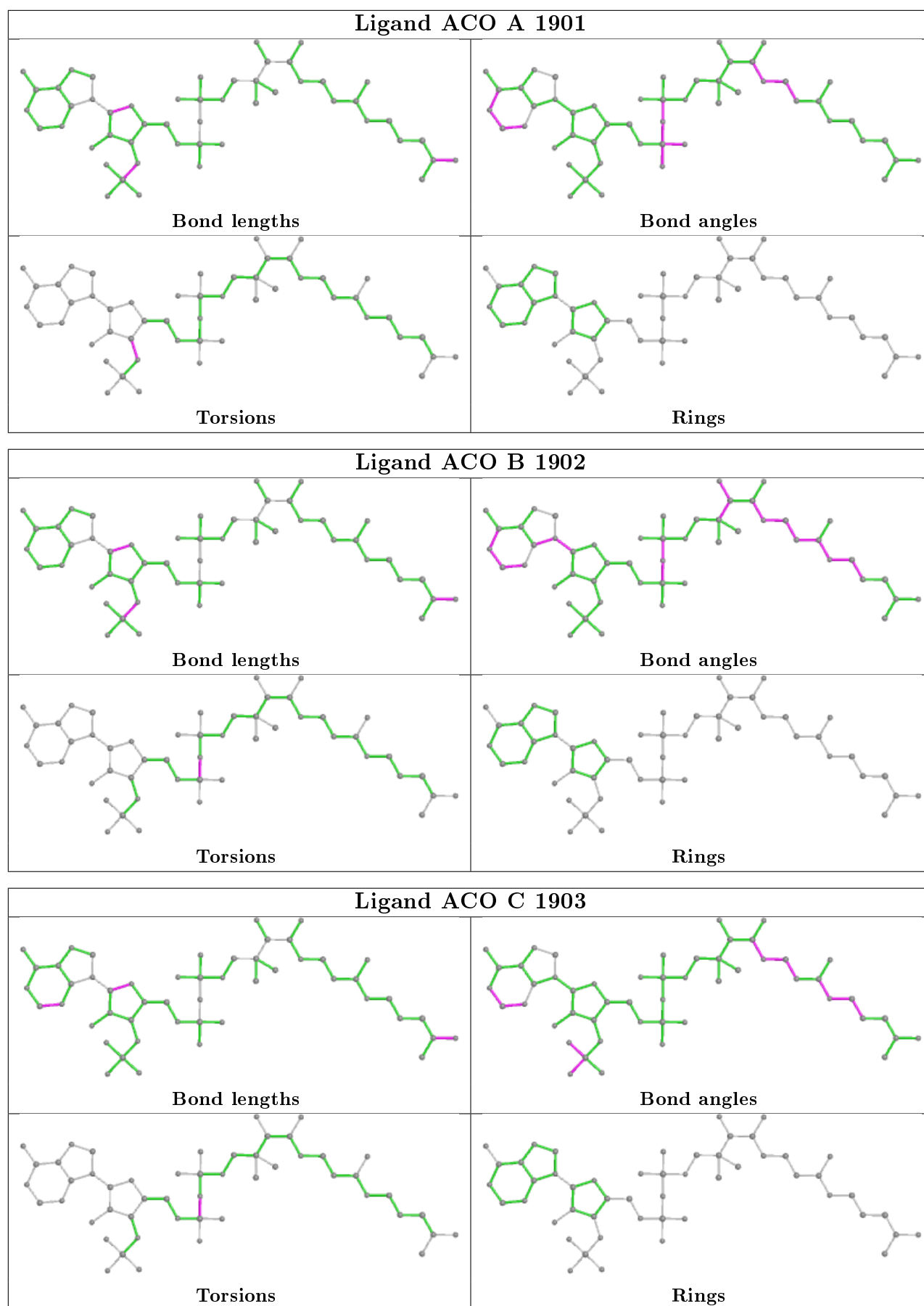
Mol	Chain	Res	Type	Atoms
2	C	1903	ACO	P2A-O3A-P1A-O1A
3	D	369	GOL	O2-C2-C3-O3
2	D	1904	ACO	P2A-O3A-P1A-O1A
2	C	1903	ACO	P2A-O3A-P1A-O2A
3	D	370	GOL	O1-C1-C2-C3
3	D	369	GOL	C1-C2-C3-O3
2	A	1901	ACO	C2B-C3B-O3B-P3B
2	D	1904	ACO	C5B-O5B-P1A-O1A
2	A	1901	ACO	C4B-C3B-O3B-P3B

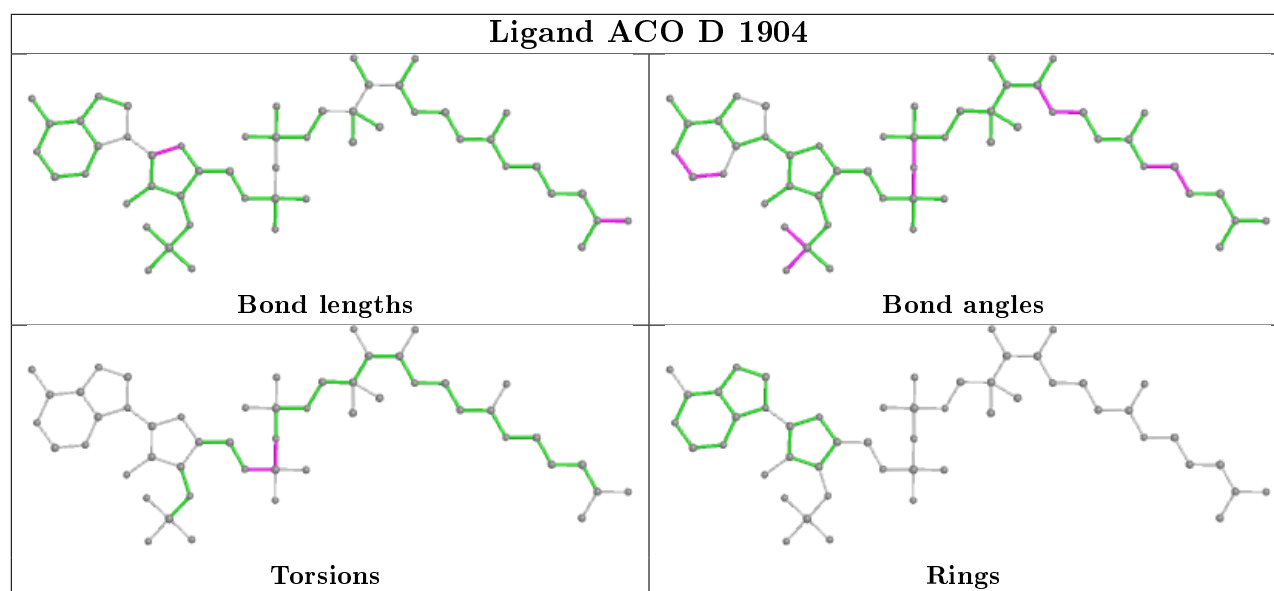
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1901	ACO	1	0
3	A	370	GOL	2	0
3	D	370	GOL	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	354/376 (94%)	0.32	6 (1%) 70 71	19, 29, 44, 52	0
1	B	351/376 (93%)	0.31	9 (2%) 56 58	23, 33, 48, 59	0
1	C	351/376 (93%)	0.20	12 (3%) 45 48	20, 31, 49, 59	0
1	D	345/376 (91%)	0.35	26 (7%) 14 16	21, 32, 55, 65	0
All	All	1401/1504 (93%)	0.29	53 (3%) 40 43	19, 31, 48, 65	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	128	ILE	15.0
1	C	109	THR	7.9
1	C	110	VAL	5.9
1	D	132	HIS	5.2
1	D	107	LEU	4.9
1	D	105	SER	4.7
1	D	126	ARG	4.7
1	A	55	ASN	4.2
1	D	112	CYS	3.9
1	C	107	LEU	3.7
1	C	367	PRO	3.6
1	A	121	PHE	3.5
1	C	108	GLN	3.5
1	D	106	THR	3.5
1	C	132	HIS	3.5
1	D	127	THR	3.4
1	D	129	GLY	3.3
1	B	368	ASN	3.1
1	A	125	PHE	3.0
1	D	76	PHE	3.0
1	D	282	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	35	ALA	2.9
1	A	180	ASP	2.8
1	D	130	ASN	2.8
1	D	32	ASP	2.8
1	C	130	ASN	2.8
1	D	104	PHE	2.7
1	D	131	LEU	2.7
1	D	119	TYR	2.7
1	A	154	PHE	2.5
1	D	123	LYS	2.5
1	B	21	THR	2.5
1	D	125	PHE	2.4
1	B	72	ASP	2.4
1	D	11	SER	2.4
1	C	133	LEU	2.4
1	C	9	ARG	2.4
1	B	55	ASN	2.4
1	D	278	LYS	2.3
1	B	128	ILE	2.3
1	C	125	PHE	2.3
1	B	31	ILE	2.3
1	B	121	PHE	2.2
1	D	124	ASP	2.2
1	D	43	GLU	2.2
1	C	111	LEU	2.2
1	B	180	ASP	2.2
1	B	229	GLU	2.1
1	D	12	PRO	2.1
1	D	14	PHE	2.1
1	A	157	GLN	2.1
1	D	38	GLU	2.0
1	C	66	VAL	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

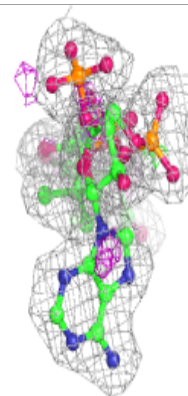
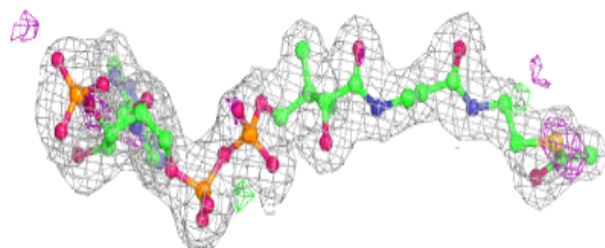
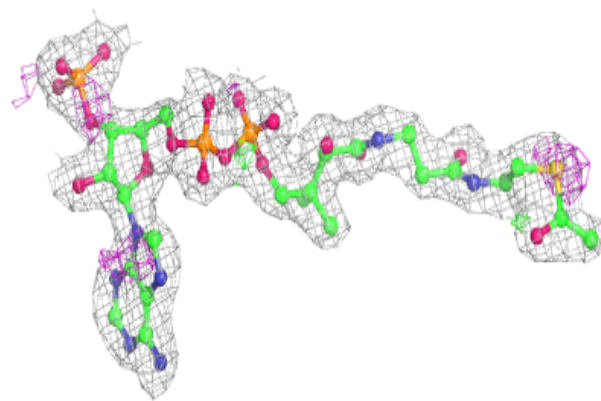
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	GOL	C	370	6/6	0.84	0.23	37,45,47,49	0
3	GOL	D	370	6/6	0.84	0.19	38,47,50,53	0
3	GOL	A	370	6/6	0.89	0.29	54,57,58,59	0
3	GOL	D	369	6/6	0.91	0.12	35,39,40,42	0
3	GOL	B	369	6/6	0.91	0.19	33,38,42,45	0
3	GOL	A	371	6/6	0.92	0.08	35,41,42,44	0
3	GOL	A	369	6/6	0.95	0.11	35,38,39,40	0
2	ACO	C	1903	51/51	0.96	0.10	20,32,44,47	0
2	ACO	B	1902	51/51	0.96	0.10	17,29,46,49	0
2	ACO	A	1901	51/51	0.96	0.09	17,26,52,54	0
2	ACO	D	1904	51/51	0.96	0.10	23,31,39,42	0
3	GOL	C	369	6/6	0.96	0.10	37,39,40,40	0

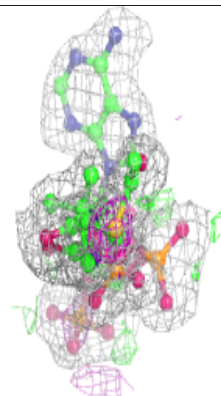
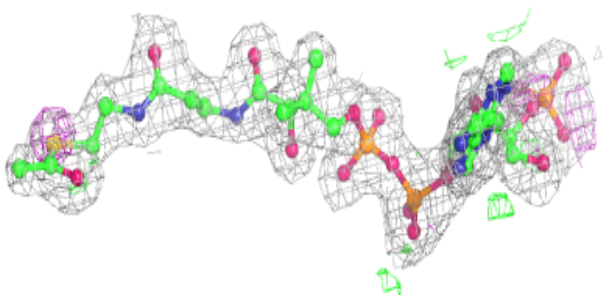
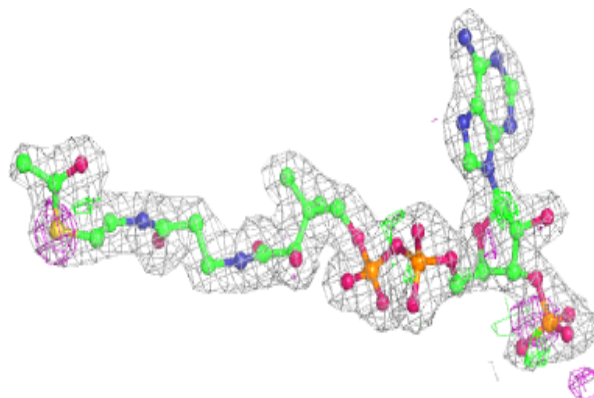
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ACO C 1903:**

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

**Electron density around ACO B 1902:**

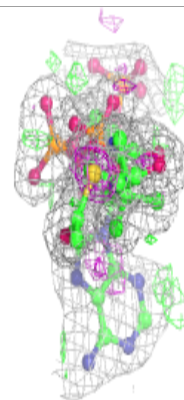
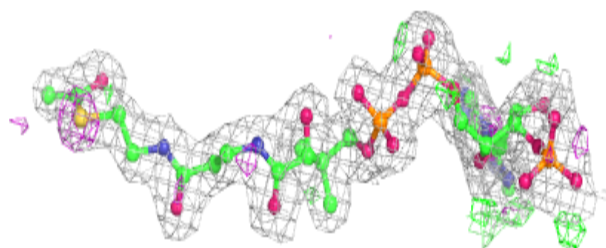
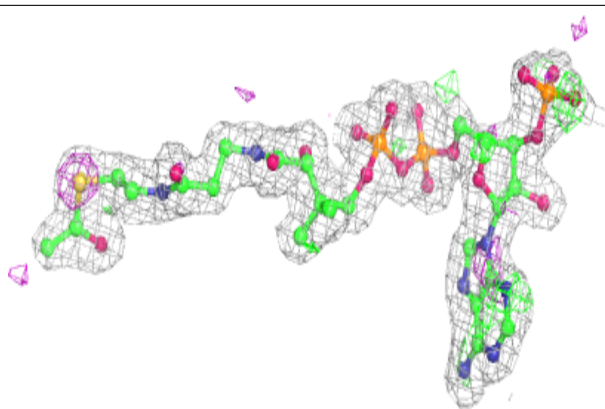
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



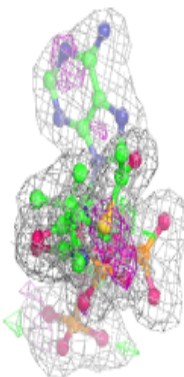
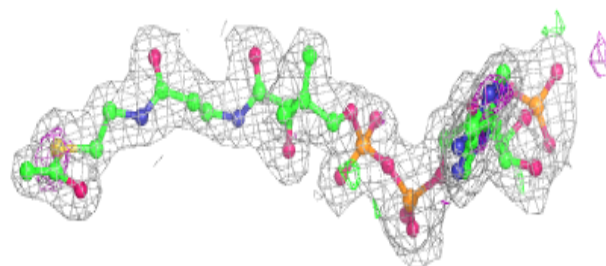
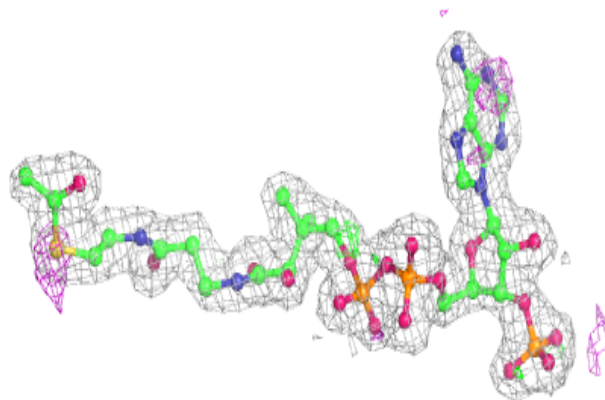


**Electron density around ACO A 1901:**

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

**Electron density around ACO D 1904:**

$2mF_o-DF_c$  (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.