



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 09:13 AM EDT

PDB ID : 1KRR  
Title : Galactoside Acetyltransferase in Complex with Acetyl-Coenzyme A  
Authors : Wang, X.-G.; Olsen, L.R.; Roderick, S.L.  
Deposited on : 2002-01-10  
Resolution : 2.50 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

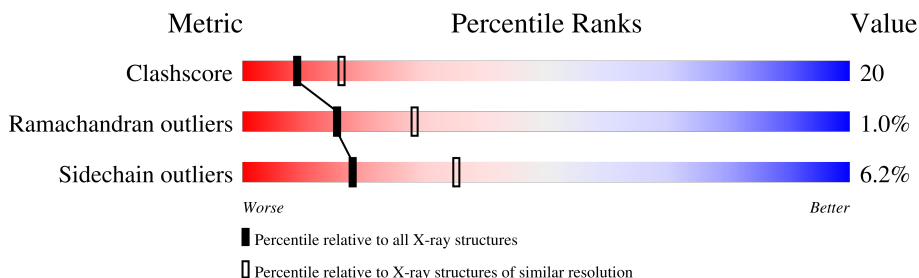
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	203	
1	B	203	
1	C	203	

## 2 Entry composition [i](#)

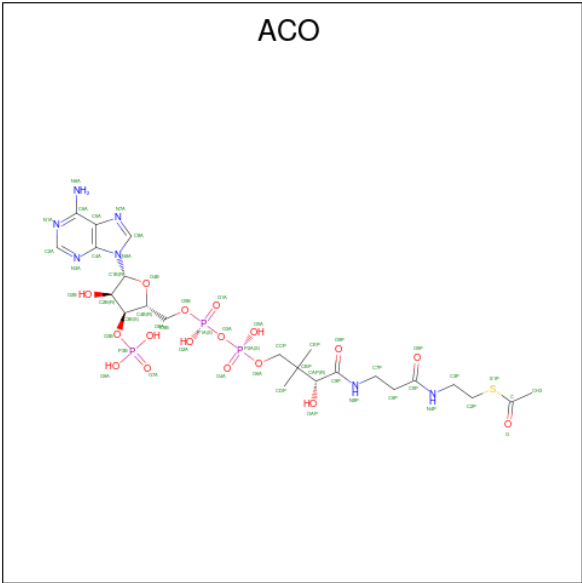
There are 3 unique types of molecules in this entry. The entry contains 4979 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GALACTOSIDE O-ACETYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	200	Total	C	N	O	S	0	0	0
			1569	998	269	294	8			
1	B	200	Total	C	N	O	S	0	0	0
			1565	996	269	292	8			
1	C	200	Total	C	N	O	S	0	0	0
			1579	1004	273	294	8			

- Molecule 2 is ACETYL COENZYME \*A (three-letter code: ACO) (formula: C<sub>23</sub>H<sub>38</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>S).



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		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	44	Total 44	O 44	0	0
3	B	34	Total 34	O 34	0	0
3	C	35	Total 35	O 35	0	0

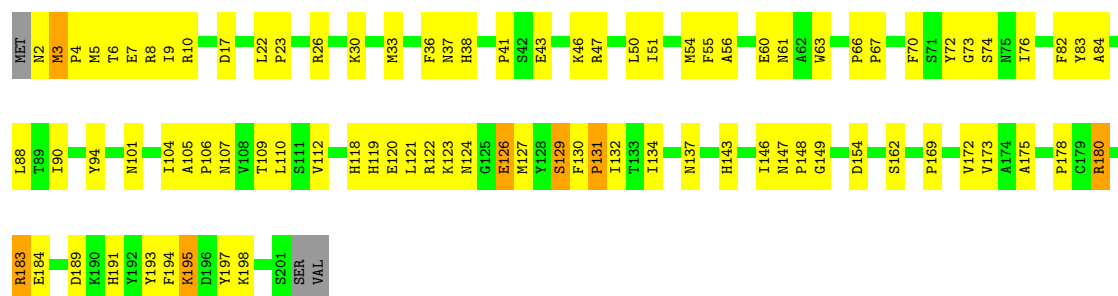
### 3 Residue-property plots [i](#)

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. 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. 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.

Note EDS was not executed.

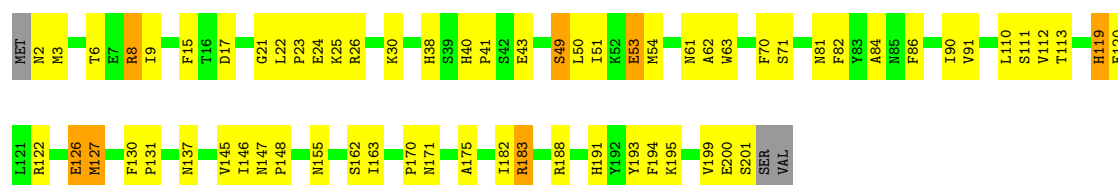
#### • Molecule 1: GALACTOSIDE O-ACETYLTRANSFERASE

Chain A: 



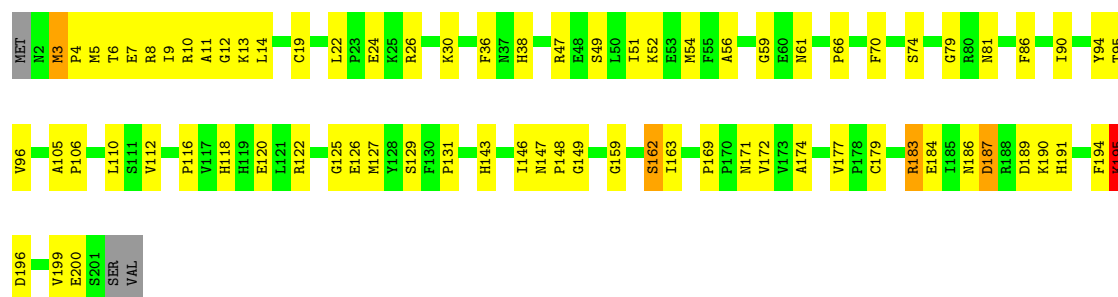
#### • Molecule 1: GALACTOSIDE O-ACETYLTRANSFERASE

Chain B: 



#### • Molecule 1: GALACTOSIDE O-ACETYLTRANSFERASE

Chain C: 



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.70Å 182.50Å 121.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.00 – 2.50	Depositor
% Data completeness (in resolution range)	90.1 (26.00-2.50)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.193 , 0.248	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4979	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.53	0/1609	0.72	0/2191
1	B	0.52	0/1605	0.73	0/2186
1	C	0.54	0/1619	0.73	0/2202
All	All	0.53	0/4833	0.73	0/6579

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

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	1569	0	1521	84	0
1	B	1565	0	1517	51	0
1	C	1579	0	1543	64	0
2	A	51	0	34	9	0
2	B	51	0	34	2	0
2	C	51	0	34	7	0
3	A	44	0	0	2	0
3	B	34	0	0	1	0
3	C	35	0	0	0	0
All	All	4979	0	4683	193	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 20.

All (193) 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:A:118:HIS:CD2	1:A:120:GLU:HB2	1.78	1.18
1:A:118:HIS:HD2	1:A:120:GLU:HB2	0.94	1.09
1:A:147:ASN:ND2	2:C:206:ACO:H61	1.81	0.95
1:A:180:ARG:CG	1:A:180:ARG:HH11	1.79	0.93
1:B:182:ILE:HG22	1:B:183:ARG:HG2	1.53	0.91
1:B:38:HIS:ND1	1:C:38:HIS:HE1	1.70	0.90
1:A:4:PRO:O	1:A:8:ARG:HG3	1.74	0.88
1:A:118:HIS:HD2	1:A:120:GLU:CB	1.86	0.86
1:A:180:ARG:HH11	1:A:180:ARG:HG3	1.42	0.84
1:A:124:ASN:HB2	1:A:126:GLU:OE2	1.80	0.82
1:B:111:SER:O	1:B:148:PRO:HD3	1.80	0.81
1:A:61:ASN:HB3	3:A:2056:HOH:O	1.80	0.80
1:A:118:HIS:CD2	1:A:120:GLU:CB	2.65	0.79
1:A:110:LEU:HD21	1:A:146:ILE:HD12	1.67	0.76
1:C:194:PHE:CZ	1:C:195:LYS:HD2	2.20	0.76
1:C:22:LEU:HB3	1:C:26:ARG:HH21	1.51	0.74
1:C:24:GLU:OE1	1:C:24:GLU:N	2.19	0.74
1:A:121:LEU:O	1:A:126:GLU:HG3	1.90	0.72
1:A:26:ARG:NH1	3:A:2010:HOH:O	2.22	0.72
1:A:147:ASN:HD21	2:C:206:ACO:H61	1.55	0.71
1:B:17:ASP:O	1:B:26:ARG:NH2	2.24	0.69
1:B:51:ILE:HA	1:B:54:MET:HE2	1.74	0.69
1:C:51:ILE:HA	1:C:54:MET:HE2	1.73	0.69
1:C:59:GLY:HA3	1:C:79:GLY:O	1.92	0.69
2:C:206:ACO:OAP	2:C:206:ACO:N7A	2.26	0.69
1:A:180:ARG:CG	1:A:180:ARG:NH1	2.48	0.69
1:A:6:THR:CG2	1:A:10:ARG:HH22	2.07	0.67
1:B:6:THR:HA	1:B:9:ILE:HD12	1.77	0.66
1:C:56:ALA:HB2	1:C:74:SER:O	1.95	0.66
1:A:51:ILE:HA	1:A:54:MET:HE2	1.77	0.65
1:C:14:LEU:HD21	1:C:116:PRO:HG3	1.78	0.65
1:A:107:ASN:HB2	1:A:143:HIS:HD2	1.62	0.64
1:A:94:TYR:CD2	1:A:131:PRO:HD3	2.33	0.64
1:C:3:MET:HE2	1:C:13:LYS:HE3	1.78	0.64
2:A:204:ACO:H61	1:B:147:ASN:HD21	1.62	0.64
1:A:105:ALA:HB2	2:A:204:ACO:H31	1.78	0.64
1:A:118:HIS:NE2	1:A:120:GLU:HG3	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:ASN:O	1:B:81:ASN:HA	1.99	0.63
1:A:110:LEU:CD2	1:A:146:ILE:HD12	2.28	0.63
1:A:6:THR:CG2	1:A:10:ARG:NH2	2.62	0.63
1:A:183:ARG:NH2	1:A:189:ASP:OD1	2.31	0.63
1:C:14:LEU:CD2	1:C:116:PRO:HG3	2.29	0.62
1:A:38:HIS:ND1	1:B:38:HIS:HE1	1.96	0.62
1:C:59:GLY:CA	1:C:79:GLY:O	2.47	0.62
1:A:180:ARG:HH11	1:A:180:ARG:HG2	1.62	0.62
1:C:105:ALA:HB2	2:C:206:ACO:H31	1.81	0.62
1:B:50:LEU:O	1:B:54:MET:HE2	2.00	0.62
2:B:205:ACO:H61	1:C:147:ASN:ND2	2.15	0.62
1:A:3:MET:SD	1:A:7:GLU:HB3	2.40	0.61
1:A:17:ASP:O	1:A:26:ARG:NH2	2.33	0.61
1:C:194:PHE:O	1:C:195:LYS:C	2.39	0.61
1:B:51:ILE:HA	1:B:54:MET:CE	2.29	0.61
1:A:180:ARG:NH1	1:A:180:ARG:HG2	2.16	0.61
1:B:110:LEU:CD2	1:B:146:ILE:HD12	2.31	0.61
1:A:3:MET:HE3	1:A:8:ARG:HG2	1.84	0.60
1:C:11:ALA:HB3	1:C:13:LYS:HD2	1.84	0.60
1:C:131:PRO:O	1:C:149:GLY:HA2	2.02	0.60
1:B:62:ALA:HB2	3:B:2099:HOH:O	2.01	0.60
1:B:191:HIS:O	1:B:199:VAL:HG23	2.02	0.59
1:A:105:ALA:HA	2:A:204:ACO:C	2.33	0.59
1:C:3:MET:HE2	1:C:13:LYS:CE	2.32	0.59
1:A:131:PRO:O	1:A:149:GLY:HA2	2.02	0.58
1:C:59:GLY:N	1:C:79:GLY:O	2.34	0.58
1:C:187:ASP:O	1:C:190:LYS:HB2	2.04	0.58
1:A:94:TYR:HD2	1:A:131:PRO:HD3	1.68	0.58
1:A:22:LEU:HB2	1:A:23:PRO:HD3	1.85	0.58
2:A:204:ACO:H61	1:B:147:ASN:ND2	2.19	0.58
1:A:147:ASN:HB3	1:A:148:PRO:HD2	1.85	0.57
1:A:38:HIS:ND1	1:B:38:HIS:CE1	2.73	0.57
1:A:193:TYR:CZ	1:A:197:TYR:HB3	2.40	0.57
1:B:21:GLY:HA2	1:B:24:GLU:OE1	2.05	0.57
1:B:22:LEU:HB2	1:B:23:PRO:HD3	1.86	0.57
1:C:174:ALA:HB1	1:C:179:CYS:SG	2.44	0.57
1:A:194:PHE:CE1	1:A:195:LYS:HE3	2.40	0.57
1:C:196:ASP:N	1:C:196:ASP:OD1	2.37	0.56
1:C:4:PRO:HB2	1:C:7:GLU:HG3	1.87	0.56
1:A:191:HIS:O	1:A:198:LYS:HA	2.06	0.56
1:B:201:SER:OG	1:C:13:LYS:HE2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ALA:HA	2:A:204:ACO:O	2.07	0.55
1:C:105:ALA:HB1	1:C:106:PRO:HD2	1.88	0.55
1:A:107:ASN:HB2	1:A:143:HIS:CD2	2.41	0.55
1:C:11:ALA:CB	1:C:13:LYS:HD2	2.36	0.55
1:B:38:HIS:ND1	1:C:38:HIS:CE1	2.62	0.55
1:C:163:ILE:HG12	1:C:177:VAL:HG22	1.87	0.55
1:B:145:VAL:HB	1:B:163:ILE:HD13	1.89	0.55
1:A:50:LEU:O	1:A:54:MET:HG3	2.07	0.55
1:C:22:LEU:HB3	1:C:26:ARG:NH2	2.21	0.54
1:C:118:HIS:CD2	1:C:120:GLU:HG3	2.42	0.54
1:A:5:MET:O	1:A:9:ILE:HG13	2.07	0.54
1:A:47:ARG:O	1:A:51:ILE:HG13	2.08	0.54
1:A:36:PHE:CE2	1:A:66:PRO:HG3	2.43	0.54
1:A:46:LYS:HE3	1:A:50:LEU:HG	1.90	0.54
2:A:204:ACO:OAP	2:A:204:ACO:N7A	2.39	0.54
1:B:70:PHE:HA	1:B:90:ILE:O	2.07	0.54
1:A:63:TRP:HD1	1:A:83:TYR:CE1	2.25	0.54
1:C:191:HIS:O	1:C:199:VAL:HG23	2.08	0.54
1:A:73:GLY:HA2	1:A:76:ILE:HD12	1.90	0.53
1:A:119:HIS:CE1	1:A:120:GLU:HG2	2.45	0.52
1:A:109:THR:OG1	1:C:143:HIS:NE2	2.30	0.52
1:A:43:GLU:O	1:A:47:ARG:HG3	2.10	0.51
1:C:171:ASN:O	1:C:184:GLU:HG3	2.10	0.51
1:B:63:TRP:HA	1:B:63:TRP:CE3	2.46	0.51
1:A:63:TRP:HD1	1:A:83:TYR:HE1	1.60	0.50
1:B:193:TYR:OH	1:C:12:GLY:O	2.24	0.50
1:B:15:PHE:CZ	1:B:127:MET:HG3	2.47	0.50
1:C:118:HIS:HD2	1:C:120:GLU:H	1.60	0.50
1:A:110:LEU:CD2	1:A:146:ILE:HB	2.42	0.49
1:A:88:LEU:HD21	1:A:90:ILE:HD11	1.94	0.49
1:A:82:PHE:CZ	1:A:84:ALA:HB2	2.47	0.49
1:B:110:LEU:HD23	1:B:146:ILE:HB	1.94	0.49
1:C:5:MET:O	1:C:9:ILE:HG13	2.12	0.49
1:B:26:ARG:HG2	1:B:71:SER:O	2.12	0.49
1:B:82:PHE:CZ	1:B:84:ALA:HB2	2.46	0.49
1:B:110:LEU:HD23	1:B:146:ILE:HD12	1.94	0.49
1:C:4:PRO:O	1:C:8:ARG:HG2	2.13	0.49
1:A:169:PRO:O	1:A:172:VAL:HG22	2.12	0.49
1:B:170:PRO:O	1:B:171:ASN:HB2	2.13	0.49
1:A:105:ALA:CB	2:A:204:ACO:H31	2.43	0.48
1:B:182:ILE:O	1:B:183:ARG:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:PRO:HG3	2:C:206:ACO:N3A	2.29	0.48
1:C:94:TYR:CD2	1:C:131:PRO:HD3	2.48	0.47
1:C:122:ARG:O	1:C:125:GLY:N	2.48	0.47
1:A:94:TYR:H	1:A:112:VAL:HG21	1.79	0.47
1:C:147:ASN:HB3	1:C:148:PRO:HD2	1.97	0.47
1:C:147:ASN:HB3	1:C:148:PRO:CD	2.44	0.47
1:B:111:SER:O	1:B:148:PRO:CD	2.57	0.47
1:A:30:LYS:HA	1:A:33:MET:HB3	1.98	0.47
1:B:3:MET:HB3	1:B:8:ARG:HD2	1.97	0.46
2:B:205:ACO:N7A	2:B:205:ACO:OAP	2.45	0.46
1:C:6:THR:HG22	1:C:10:ARG:NH2	2.30	0.46
1:A:137:ASN:HB3	1:B:119:HIS:HB2	1.96	0.46
1:A:162:SER:OG	1:A:175:ALA:HA	2.15	0.46
1:B:17:ASP:HB2	1:B:26:ARG:HH21	1.81	0.46
2:C:206:ACO:H4B	2:C:206:ACO:O8A	2.16	0.46
1:B:110:LEU:HD21	1:B:146:ILE:HD12	1.97	0.46
1:C:70:PHE:HA	1:C:90:ILE:O	2.16	0.46
1:B:49:SER:O	1:B:53:GLU:HB2	2.16	0.45
1:C:36:PHE:CE2	1:C:66:PRO:HG3	2.52	0.45
1:C:110:LEU:CD2	1:C:146:ILE:HD12	2.47	0.45
1:A:101:ASN:HB2	1:A:137:ASN:OD1	2.16	0.45
1:A:147:ASN:HB3	1:A:148:PRO:CD	2.47	0.45
1:A:55:PHE:HA	1:A:73:GLY:O	2.16	0.45
1:A:173:VAL:HG11	2:A:204:ACO:O5A	2.17	0.45
1:C:94:TYR:HD2	1:C:131:PRO:HD3	1.81	0.44
1:A:126:GLU:H	1:A:126:GLU:HG2	1.56	0.44
1:C:112:VAL:O	1:C:129:SER:HA	2.17	0.44
1:C:183:ARG:NH2	1:C:189:ASP:OD1	2.50	0.44
1:A:26:ARG:HG3	1:A:72:TYR:CE2	2.53	0.44
1:A:110:LEU:HD23	1:A:146:ILE:HB	1.99	0.44
1:A:122:ARG:HA	1:A:126:GLU:CG	2.48	0.44
1:C:51:ILE:HA	1:C:54:MET:CE	2.44	0.44
1:A:56:ALA:HB2	1:A:74:SER:O	2.17	0.44
1:B:40:HIS:HB3	1:B:43:GLU:HG3	2.00	0.44
1:C:61:ASN:HB3	1:C:81:ASN:HA	2.00	0.44
1:A:60:GLU:HG3	1:A:61:ASN:ND2	2.33	0.43
1:B:194:PHE:O	1:B:195:LYS:C	2.57	0.43
1:B:122:ARG:HA	1:B:126:GLU:HB2	2.00	0.43
1:C:24:GLU:H	1:C:24:GLU:CD	2.13	0.43
1:A:70:PHE:HA	1:A:90:ILE:O	2.18	0.43
1:B:137:ASN:O	1:B:155:ASN:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:ALA:CB	2:C:206:ACO:H31	2.48	0.43
1:C:147:ASN:HD22	1:C:147:ASN:HA	1.61	0.43
1:A:37:ASN:OD1	1:A:67:PRO:HA	2.19	0.43
1:B:91:VAL:O	1:B:112:VAL:HG22	2.19	0.43
1:B:63:TRP:HA	1:B:63:TRP:HE3	1.84	0.43
1:B:113:THR:CG2	1:B:127:MET:HB2	2.49	0.42
1:C:3:MET:CE	1:C:13:LYS:HE3	2.49	0.42
1:C:10:ARG:HG2	1:C:94:TYR:OH	2.19	0.42
1:A:130:PHE:HA	1:A:131:PRO:HD2	1.85	0.42
1:C:30:LYS:H	1:C:30:LYS:HG2	1.66	0.42
1:A:105:ALA:HA	2:A:204:ACO:CH3	2.49	0.42
1:A:132:ILE:HD13	1:A:146:ILE:HG22	2.02	0.42
1:C:169:PRO:O	1:C:172:VAL:HG22	2.19	0.42
1:C:47:ARG:NH2	1:C:66:PRO:HG2	2.35	0.41
1:C:26:ARG:O	1:C:30:LYS:HG2	2.19	0.41
1:B:90:ILE:HG12	1:B:110:LEU:HD12	2.02	0.41
1:C:116:PRO:HD2	1:C:126:GLU:O	2.20	0.41
1:A:41:PRO:HG3	1:B:30:LYS:O	2.21	0.41
1:C:95:THR:HG22	1:C:96:VAL:N	2.36	0.41
1:C:159:GLY:O	1:C:162:SER:OG	2.39	0.41
1:A:105:ALA:HB1	1:A:106:PRO:CD	2.51	0.41
1:C:24:GLU:N	1:C:24:GLU:CD	2.73	0.41
1:A:17:ASP:O	1:A:23:PRO:HD3	2.21	0.41
1:A:88:LEU:HD13	1:A:104:ILE:HG21	2.03	0.41
1:A:94:TYR:HB2	1:A:129:SER:HB3	2.03	0.40
1:A:118:HIS:CD2	1:A:120:GLU:H	2.39	0.40
1:B:41:PRO:HG3	1:C:30:LYS:O	2.21	0.40
1:B:130:PHE:HA	1:B:131:PRO:HD2	1.90	0.40
1:B:191:HIS:O	1:B:199:VAL:N	2.46	0.40
1:B:162:SER:OG	1:B:175:ALA:HA	2.21	0.40
1:A:46:LYS:HD2	1:A:46:LYS:HA	1.85	0.40
1:B:50:LEU:C	1:B:54:MET:HE2	2.41	0.40
1:C:186:ASN:HB2	1:C:187:ASP:H	1.75	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	198/203 (98%)	184 (93%)	12 (6%)	2 (1%)	15	28
1	B	198/203 (98%)	181 (91%)	15 (8%)	2 (1%)	15	28
1	C	198/203 (98%)	183 (92%)	13 (7%)	2 (1%)	15	28
All	All	594/609 (98%)	548 (92%)	40 (7%)	6 (1%)	15	28

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	195	LYS
1	B	86	PHE
1	C	86	PHE
1	A	195	LYS
1	A	154	ASP
1	B	119	HIS

### 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	173/179 (97%)	162 (94%)	11 (6%)	17	33
1	B	172/179 (96%)	161 (94%)	11 (6%)	17	33
1	C	175/179 (98%)	165 (94%)	10 (6%)	20	39
All	All	520/537 (97%)	488 (94%)	32 (6%)	18	35

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	3	MET
1	A	123	LYS
1	A	126	GLU
1	A	127	MET
1	A	129	SER
1	A	131	PRO
1	A	134	ILE
1	A	180	ARG
1	A	183	ARG
1	A	184	GLU
1	B	2	ASN
1	B	8	ARG
1	B	25	LYS
1	B	49	SER
1	B	53	GLU
1	B	120	GLU
1	B	126	GLU
1	B	127	MET
1	B	183	ARG
1	B	188	ARG
1	B	200	GLU
1	C	3	MET
1	C	19	CYS
1	C	49	SER
1	C	52	LYS
1	C	127	MET
1	C	162	SER
1	C	183	ARG
1	C	187	ASP
1	C	195	LYS
1	C	200	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	118	HIS
1	A	147	ASN
1	B	118	HIS
1	B	147	ASN

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Mol	Chain	Res	Type
1	C	38	HIS
1	C	118	HIS
1	C	147	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

3 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	C	206	-	47,53,53	1.47	5 (10%)	60,79,79	1.25	7 (11%)
2	ACO	A	204	-	47,53,53	1.29	3 (6%)	60,79,79	1.36	11 (18%)
2	ACO	B	205	-	47,53,53	1.46	3 (6%)	60,79,79	1.26	6 (10%)

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	C	206	-	-	19/47/67/67	0/3/3/3
2	ACO	A	204	-	-	15/47/67/67	0/3/3/3
2	ACO	B	205	-	-	15/47/67/67	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	205	ACO	P2A-O3A	7.38	1.67	1.59
2	C	206	ACO	P2A-O3A	6.93	1.67	1.59
2	A	204	ACO	P2A-O3A	4.94	1.64	1.59
2	B	205	ACO	C2A-N1A	2.68	1.38	1.33
2	A	204	ACO	C6P-C5P	2.48	1.56	1.51
2	C	206	ACO	C2A-N1A	2.36	1.38	1.33
2	C	206	ACO	C1B-N9A	-2.33	1.44	1.49
2	C	206	ACO	O-C	2.04	1.31	1.21
2	A	204	ACO	O6A-CCP	2.02	1.50	1.43
2	B	205	ACO	O-C	2.01	1.31	1.21
2	C	206	ACO	P1A-O3A	-2.01	1.57	1.59

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	205	ACO	O3B-C3B-C4B	4.11	124.51	110.03
2	A	204	ACO	C6P-C5P-N4P	-3.83	109.36	116.34
2	C	206	ACO	O3B-C3B-C4B	3.65	122.91	110.03
2	A	204	ACO	O5P-C5P-N4P	3.22	129.34	123.03
2	A	204	ACO	C5A-C6A-N6A	3.14	125.09	120.31
2	A	204	ACO	O3B-C3B-C4B	2.94	120.41	110.03
2	B	205	ACO	O2A-P1A-O3A	2.71	114.59	107.27
2	C	206	ACO	CEP-CBP-CCP	2.68	112.65	108.22
2	C	206	ACO	C4A-C5A-N7A	2.68	112.17	109.34
2	B	205	ACO	CEP-CBP-CCP	2.57	112.47	108.22
2	B	205	ACO	C5A-C6A-N6A	2.55	124.20	120.31
2	C	206	ACO	O6A-CCP-CBP	2.47	114.52	110.55
2	A	204	ACO	CEP-CBP-CCP	2.46	112.28	108.22
2	C	206	ACO	C5A-C6A-N6A	2.43	124.01	120.31
2	A	204	ACO	O6A-CCP-CBP	2.38	114.38	110.55
2	A	204	ACO	O4B-C1B-N9A	2.30	111.80	108.75
2	A	204	ACO	O3A-P1A-O1A	2.26	117.51	110.70
2	A	204	ACO	P3B-O3B-C3B	-2.20	117.56	123.43
2	A	204	ACO	C2B-C3B-C4B	-2.15	99.47	103.24
2	A	204	ACO	C1B-N9A-C4A	-2.12	122.91	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	205	ACO	C2P-C3P-N4P	-2.08	108.08	112.41
2	C	206	ACO	C2B-C3B-C4B	-2.02	99.71	103.24
2	B	205	ACO	C1B-N9A-C4A	-2.01	123.11	126.64
2	C	206	ACO	O4B-C1B-N9A	2.01	111.41	108.75

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	204	ACO	CCP-O6A-P2A-O3A
2	A	204	ACO	CCP-O6A-P2A-O4A
2	A	204	ACO	CCP-O6A-P2A-O5A
2	A	204	ACO	CDP-CBP-CCP-O6A
2	A	204	ACO	CEP-CBP-CCP-O6A
2	A	204	ACO	CAP-CBP-CCP-O6A
2	A	204	ACO	O-C-S1P-C2P
2	A	204	ACO	CH3-C-S1P-C2P
2	B	205	ACO	C5B-O5B-P1A-O2A
2	B	205	ACO	C5B-O5B-P1A-O3A
2	B	205	ACO	O-C-S1P-C2P
2	B	205	ACO	CH3-C-S1P-C2P
2	C	206	ACO	C5B-O5B-P1A-O1A
2	C	206	ACO	C5B-O5B-P1A-O2A
2	C	206	ACO	C5B-O5B-P1A-O3A
2	C	206	ACO	P1A-O3A-P2A-O6A
2	C	206	ACO	CCP-O6A-P2A-O3A
2	C	206	ACO	CCP-O6A-P2A-O4A
2	C	206	ACO	CCP-O6A-P2A-O5A
2	C	206	ACO	CDP-CBP-CCP-O6A
2	C	206	ACO	CEP-CBP-CCP-O6A
2	C	206	ACO	CAP-CBP-CCP-O6A
2	C	206	ACO	O-C-S1P-C2P
2	B	205	ACO	C4B-C3B-O3B-P3B
2	A	204	ACO	C2B-C3B-O3B-P3B
2	A	204	ACO	C4B-C3B-O3B-P3B
2	B	205	ACO	C2B-C3B-O3B-P3B
2	C	206	ACO	C2B-C3B-O3B-P3B
2	C	206	ACO	C4B-C3B-O3B-P3B
2	C	206	ACO	CH3-C-S1P-C2P
2	B	205	ACO	S1P-C2P-C3P-N4P
2	A	204	ACO	P1A-O3A-P2A-O6A
2	B	205	ACO	CDP-CBP-CCP-O6A

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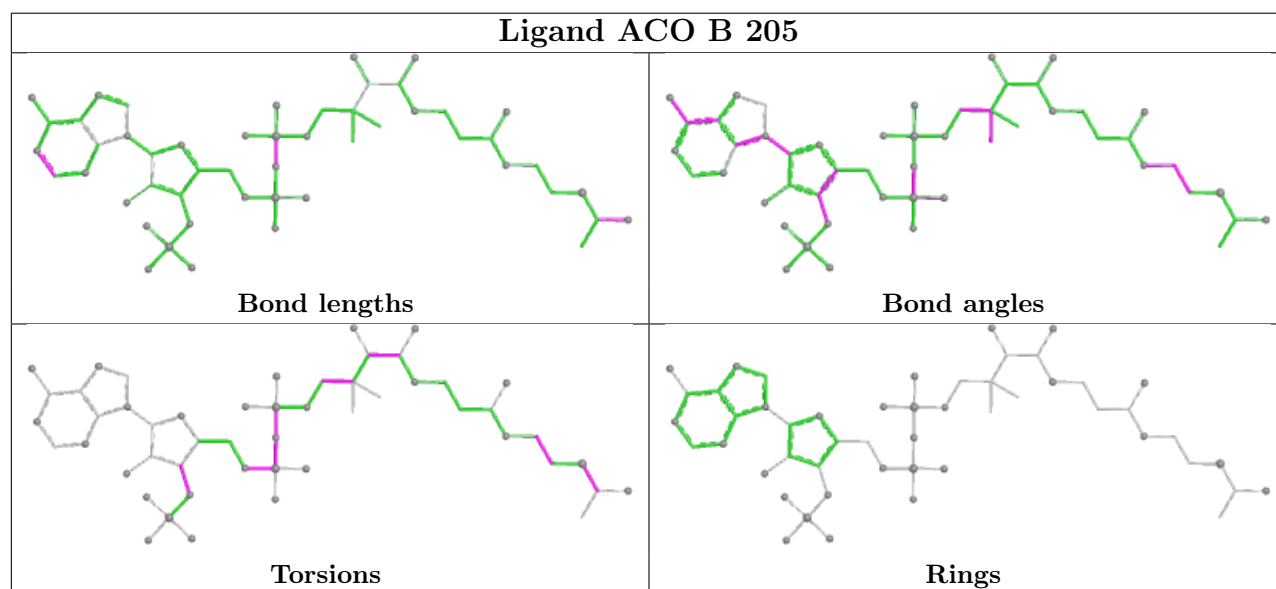
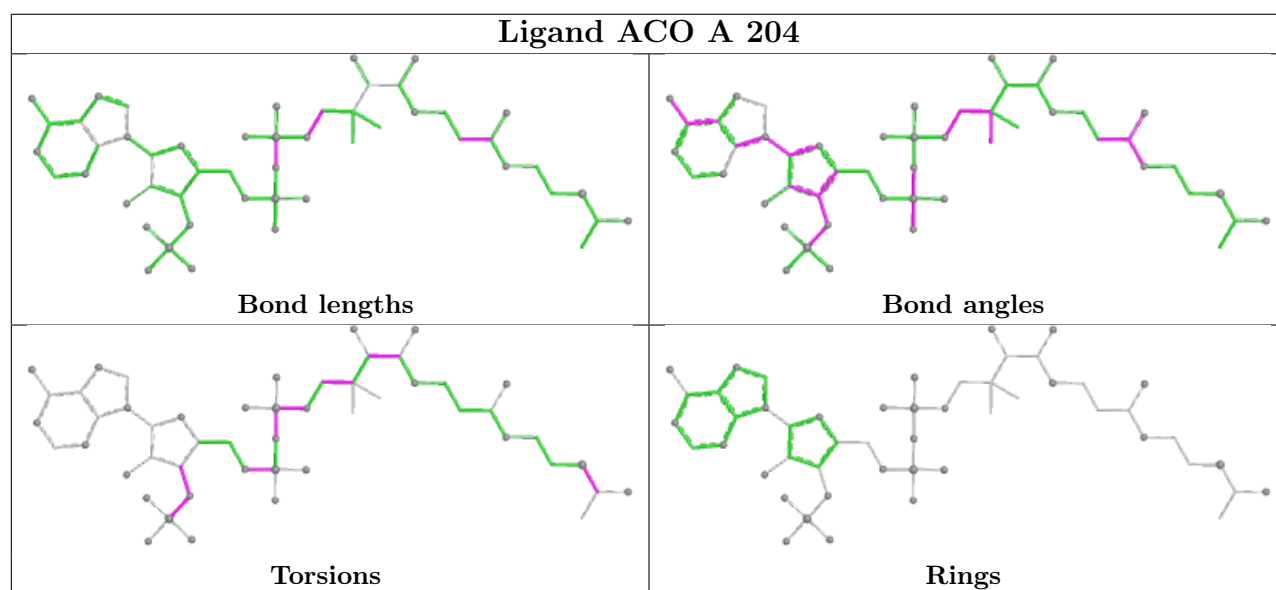
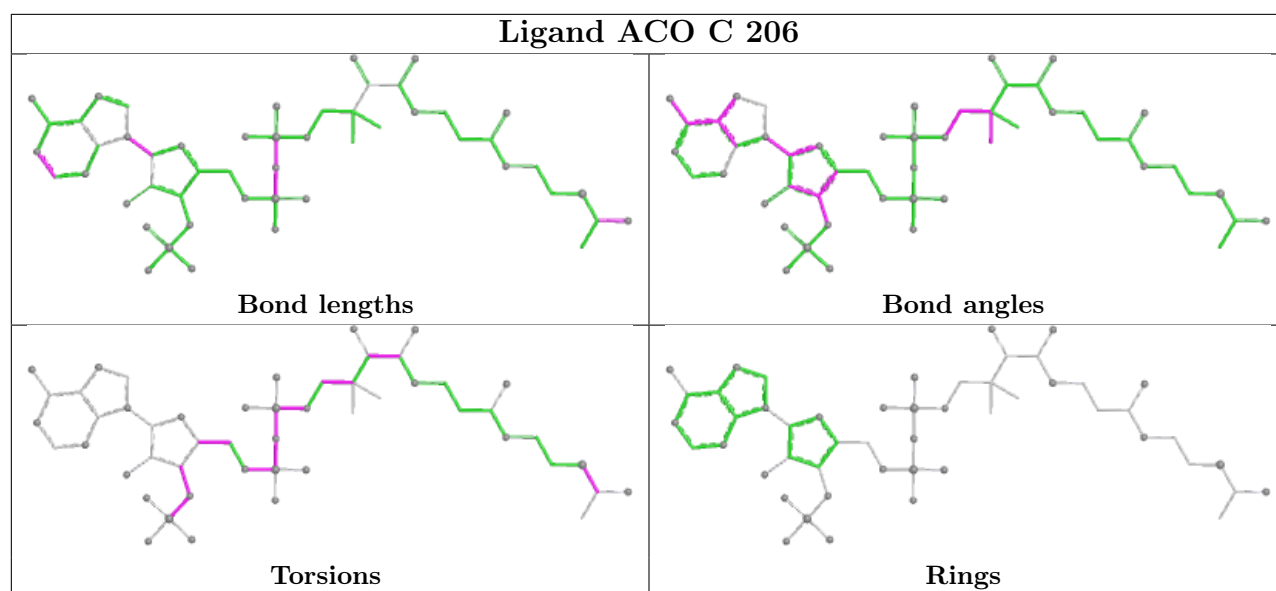
Mol	Chain	Res	Type	Atoms
2	B	205	ACO	CEP-CBP-CCP-O6A
2	A	204	ACO	C5B-O5B-P1A-O1A
2	B	205	ACO	C5B-O5B-P1A-O1A
2	B	205	ACO	P1A-O3A-P2A-O5A
2	C	206	ACO	C3B-O3B-P3B-O9A
2	B	205	ACO	P2A-O3A-P1A-O1A
2	C	206	ACO	O4B-C4B-C5B-O5B
2	B	205	ACO	P2A-O3A-P1A-O2A
2	C	206	ACO	C3B-O3B-P3B-O8A
2	A	204	ACO	O9P-C9P-CAP-OAP
2	A	204	ACO	C3B-O3B-P3B-O7A
2	A	204	ACO	N8P-C9P-CAP-OAP
2	B	205	ACO	N8P-C9P-CAP-OAP
2	C	206	ACO	N8P-C9P-CAP-OAP
2	B	205	ACO	CAP-CBP-CCP-O6A
2	C	206	ACO	P2A-O3A-P1A-O2A

There are no ring outliers.

3 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	206	ACO	7	0
2	A	204	ACO	9	0
2	B	205	ACO	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.