



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 7, 2022 – 09:49 AM EDT

PDB ID : 3N0S
Title : Crystal structure of BA2930 mutant (H183A) in complex with AcCoA
Authors : Klimecka, M.M.; Chruszcz, M.; Porebski, P.J.; Cymborowski, M.; Anderson, W.F.; Minor, W.; Center for Structural Genomics of Infectious Diseases (CS-GID)
Deposited on : 2010-05-14
Resolution : 2.15 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 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 : 2.27
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) : 2.27

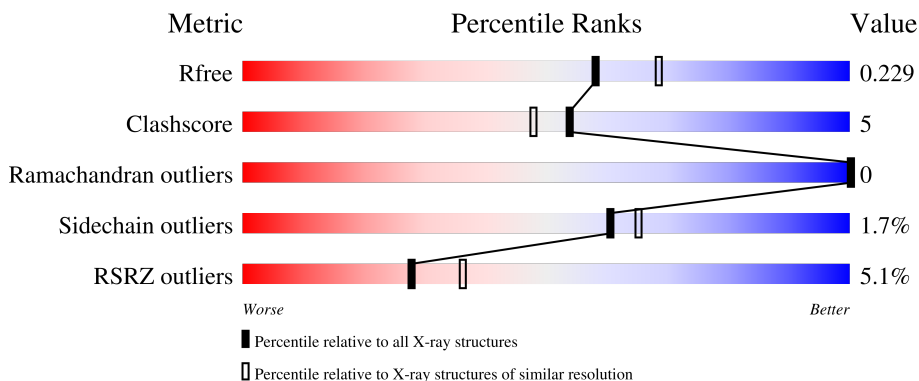
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	268	<div> <div>6%</div> <div> <div></div> <div>84%</div> <div>15%</div> <div>.</div> </div> </div>
1	B	268	<div> <div>4%</div> <div> <div></div> <div>86%</div> <div>13%</div> <div>.</div> </div> </div>
1	C	268	<div> <div>5%</div> <div> <div></div> <div>84%</div> <div>14%</div> <div>..</div> </div> </div>
1	D	268	<div> <div>5%</div> <div> <div></div> <div>91%</div> <div>7%</div> <div>..</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8881 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.

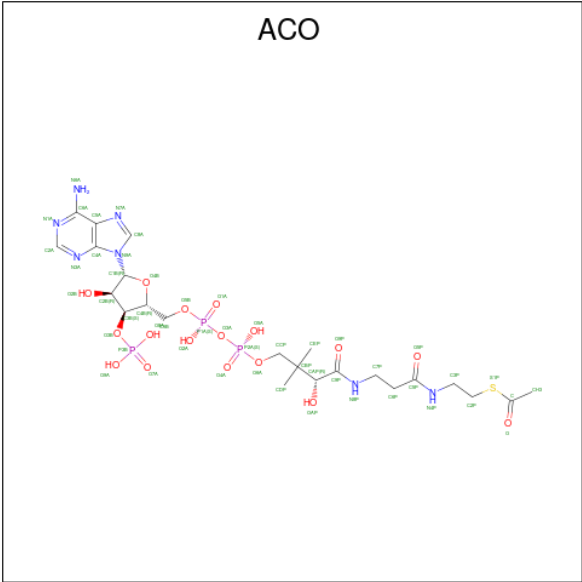
- Molecule 1 is a protein called Aminoglycoside N3-acetyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	Se	0	0	0
			2063	1306	351	394	3	9			
1	D	265	Total	C	N	O	S	Se	0	0	0
			2070	1311	353	394	3	9			
1	C	264	Total	C	N	O	S	Se	0	1	0
			2063	1307	352	392	3	9			
1	B	266	Total	C	N	O	S	Se	0	2	0
			2090	1326	356	396	3	9			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q81P86
A	-1	ASN	-	expression tag	UNP Q81P86
A	0	ALA	-	expression tag	UNP Q81P86
A	183	ALA	HIS	engineered mutation	UNP Q81P86
D	-2	SER	-	expression tag	UNP Q81P86
D	-1	ASN	-	expression tag	UNP Q81P86
D	0	ALA	-	expression tag	UNP Q81P86
D	183	ALA	HIS	engineered mutation	UNP Q81P86
C	-2	SER	-	expression tag	UNP Q81P86
C	-1	ASN	-	expression tag	UNP Q81P86
C	0	ALA	-	expression tag	UNP Q81P86
C	183	ALA	HIS	engineered mutation	UNP Q81P86
B	-2	SER	-	expression tag	UNP Q81P86
B	-1	ASN	-	expression tag	UNP Q81P86
B	0	ALA	-	expression tag	UNP Q81P86
B	183	ALA	HIS	engineered mutation	UNP Q81P86

- Molecule 2 is ACETYL COENZYME *A (three-letter code: ACO) (formula: C₂₃H₃₈N₇O₁₇P₃S).

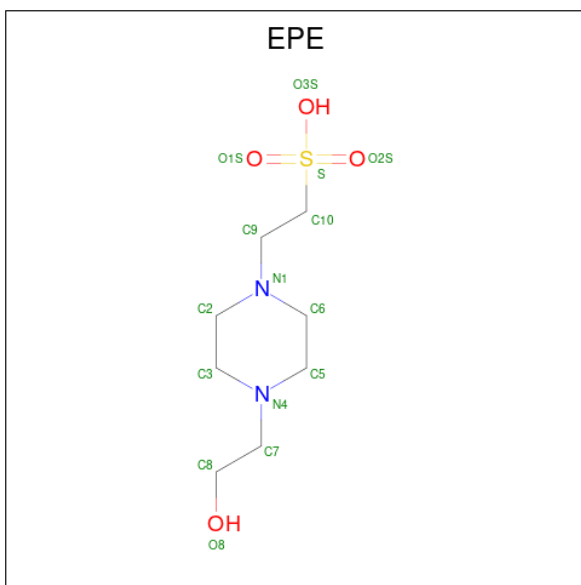


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

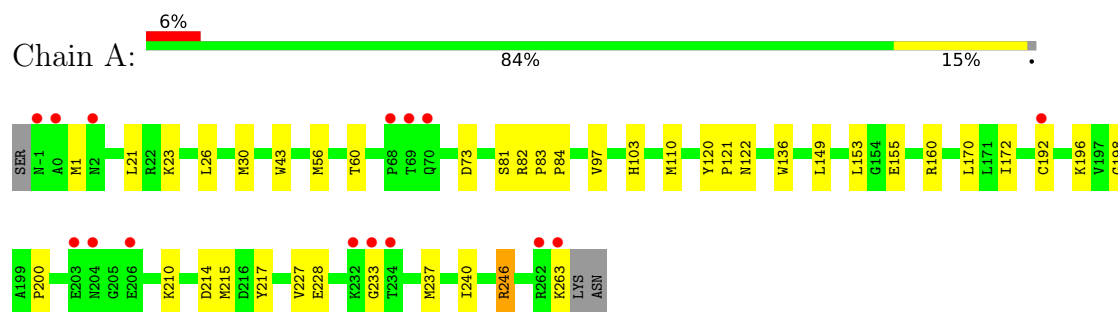
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	76	Total	O	0	0
			76	76		
5	D	100	Total	O	0	0
			100	100		
5	C	81	Total	O	0	0
			81	81		
5	B	117	Total	O	0	0
			117	117		

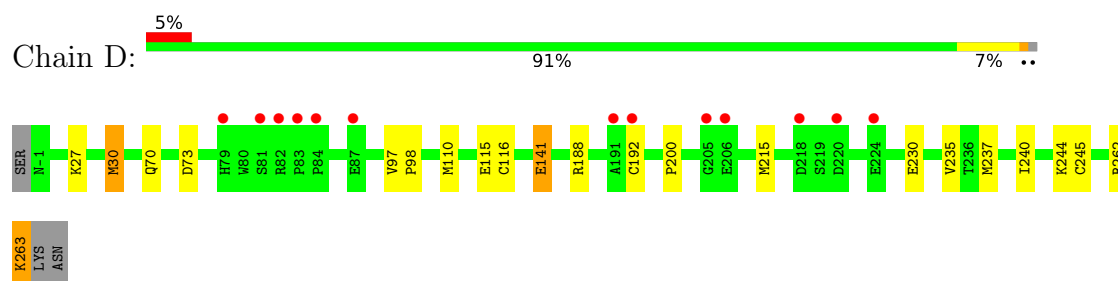
3 Residue-property plots [i](#)

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.

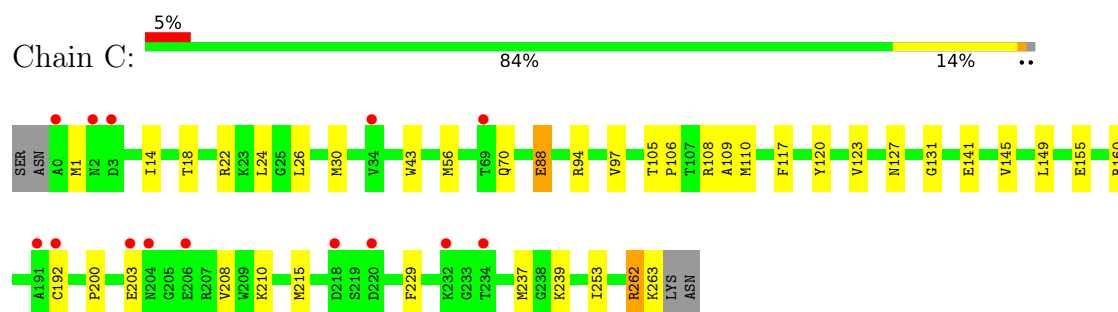
- Molecule 1: Aminoglycoside N3-acetyltransferase



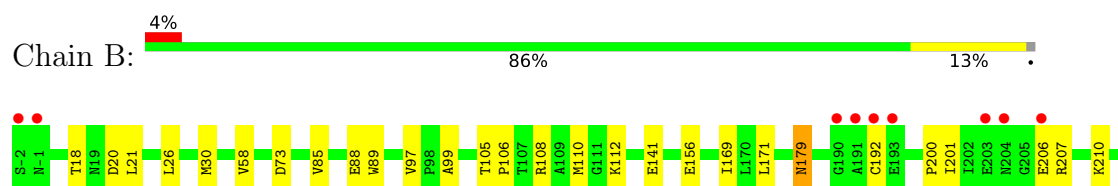
- Molecule 1: Aminoglycoside N3-acetyltransferase



- Molecule 1: Aminoglycoside N3-acetyltransferase



- Molecule 1: Aminoglycoside N3-acetyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.04Å 109.44Å 74.05Å 90.00° 111.86° 90.00°	Depositor
Resolution (Å)	50.00 – 2.15 30.24 – 2.14	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-2.15) 98.7 (30.24-2.14)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.173 , 0.228 0.177 , 0.229	Depositor DCC
R_{free} test set	2931 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	31.4	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8881	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.01 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.1708e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACO, MG, EPE

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	0/2098	0.80	1/2833 (0.0%)
1	B	0.94	1/2126 (0.0%)	0.86	1/2869 (0.0%)
1	C	0.91	0/2098	0.84	4/2832 (0.1%)
1	D	0.97	4/2105 (0.2%)	0.84	1/2840 (0.0%)
All	All	0.92	5/8427 (0.1%)	0.84	7/11374 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	192	CYS	CB-SG	8.53	1.96	1.82
1	D	116	CYS	CB-SG	-6.10	1.71	1.82
1	D	141	GLU	CG-CD	5.29	1.59	1.51
1	D	115	GLU	CG-CD	5.22	1.59	1.51
1	D	70	GLN	C-O	5.11	1.33	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	246	ARG	NE-CZ-NH1	-6.02	117.29	120.30
1	B	30	MSE	CG-SE-CE	-5.96	85.80	98.90
1	C	94	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	C	108	ARG	NE-CZ-NH2	5.33	122.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	30	MSE	CG-SE-CE	-5.17	87.53	98.90
1	C	24	LEU	CA-CB-CG	5.15	127.14	115.30
1	C	24	LEU	CB-CG-CD2	-5.06	102.39	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	233	GLY	Peptide

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	2063	0	2046	28	0
1	B	2090	0	2083	23	0
1	C	2063	0	2052	26	0
1	D	2070	0	2066	12	0
2	A	51	0	34	1	0
2	B	51	0	34	1	0
2	C	51	0	34	1	0
2	D	51	0	34	1	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	B	15	0	17	1	0
5	A	76	0	0	0	0
5	B	117	0	0	1	0
5	C	81	0	0	1	0
5	D	100	0	0	1	0
All	All	8881	0	8400	89	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 5.

All (89) 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:248:MSE:HE3	1:B:253:ILE:HG21	1.35	1.07
1:A:110:MSE:HE1	2:A:266:ACO:H22	1.38	1.02
1:B:110:MSE:HE1	2:B:266:ACO:H22	1.45	0.99
1:D:110:MSE:HE1	2:D:266:ACO:H22	1.57	0.87
1:B:179:ASN:OD1	1:B:248:MSE:HE1	1.78	0.83
1:C:110:MSE:HE1	2:C:266:ACO:H22	1.60	0.83
1:A:56:MSE:HE3	1:A:136:TRP:CE2	2.18	0.78
1:C:97:VAL:HG13	1:C:200:PRO:HG3	1.66	0.78
1:A:192:CYS:HB2	1:A:215:MSE:SE	2.34	0.77
1:A:56:MSE:HE3	1:A:136:TRP:NE1	2.00	0.76
1:D:97:VAL:HG13	1:D:200:PRO:HG3	1.71	0.73
1:B:201:ILE:HD11	1:B:210:LYS:HD3	1.74	0.69
1:C:1:MSE:HE1	1:C:43:TRP:HD1	1.59	0.67
1:B:248:MSE:HE3	1:B:253:ILE:CG2	2.20	0.66
1:B:179:ASN:OD1	1:B:248:MSE:CE	2.44	0.65
1:C:155:GLU:OE1	1:C:160:ARG:NH1	2.28	0.65
1:C:26:LEU:HD12	1:C:30:MSE:SE	2.48	0.64
1:D:237:MSE:HE3	1:D:244:LYS:CE	2.30	0.62
1:A:56:MSE:CE	1:A:136:TRP:CE2	2.82	0.62
1:D:240:ILE:HG12	1:D:245:CYS:SG	2.40	0.61
1:D:262:ARG:HA	1:D:263:LYS:HB2	1.83	0.60
1:A:1:MSE:HE1	1:A:43:TRP:HD1	1.67	0.59
1:A:153:LEU:HD12	1:A:217:TYR:CD2	2.37	0.59
1:A:56:MSE:CE	1:A:136:TRP:NE1	2.66	0.57
1:C:192:CYS:O	1:C:215:MSE:HE2	2.07	0.55
1:A:97:VAL:HG13	1:A:200:PRO:HG3	1.89	0.55
1:C:117:PHE:O	1:C:123:VAL:HG21	2.07	0.55
1:C:239:LYS:NZ	5:C:370:HOH:O	2.40	0.54
1:B:21:LEU:HD22	1:B:26:LEU:HD22	1.90	0.54
1:A:26:LEU:HD12	1:A:30:MSE:HE1	1.90	0.53
1:A:215:MSE:HB3	1:A:217:TYR:CE1	2.43	0.53
1:B:88:GLU:O	1:B:88:GLU:HG2	2.09	0.53
1:A:149:LEU:HD21	1:A:210:LYS:HG2	1.91	0.53
1:A:21:LEU:HD23	1:A:240:ILE:HD11	1.91	0.52
1:C:127[B]:ASN:OD1	1:C:127[B]:ASN:C	2.49	0.51
1:B:73:ASP:OD1	1:B:108:ARG:HD2	2.10	0.51
4:B:268:EPE:O1S	4:B:268:EPE:N1	2.43	0.51
1:A:1:MSE:HE1	1:A:43:TRP:CD1	2.45	0.50
1:C:1:MSE:HE1	1:C:43:TRP:CD1	2.43	0.50
1:C:88:GLU:H	1:C:88:GLU:CD	2.14	0.50
1:C:141:GLU:O	1:C:145:VAL:HG13	2.11	0.50
1:B:248:MSE:CE	1:B:253:ILE:HG21	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:27:LYS:HB2	1:D:30:MSE:HE3	1.93	0.49
1:C:155:GLU:O	1:C:160:ARG:HG2	2.11	0.49
1:D:230:GLU:HG2	1:D:235:VAL:HG11	1.94	0.49
1:A:121:PRO:O	1:A:122:ASN:HB2	2.13	0.49
1:A:153:LEU:HD12	1:A:217:TYR:CE2	2.49	0.48
1:B:85:VAL:HB	1:B:89:TRP:CE3	2.50	0.47
1:B:88:GLU:O	1:B:88:GLU:CG	2.63	0.47
1:A:56:MSE:HE2	1:A:136:TRP:CZ2	2.50	0.46
1:B:156:GLU:OE1	1:B:156:GLU:HA	2.16	0.46
1:A:153:LEU:HB2	1:A:217:TYR:CZ	2.51	0.46
1:A:155:GLU:O	1:A:160:ARG:HG2	2.15	0.45
1:D:188:ARG:NH2	5:D:320:HOH:O	2.48	0.45
1:C:18:THR:HG22	1:C:22:ARG:NH1	2.30	0.45
1:C:192:CYS:HB2	1:C:215:MSE:CG	2.47	0.45
1:B:169:ILE:HD13	1:B:248:MSE:HE2	1.98	0.45
1:D:141:GLU:H	1:D:141:GLU:CD	2.20	0.45
1:C:56:MSE:HE1	1:C:120:TYR:CD2	2.52	0.45
1:D:192:CYS:HB2	1:D:215:MSE:SE	2.67	0.45
1:B:20:ASP:HB3	1:B:240:ILE:HD13	1.99	0.45
1:A:227:VAL:HG12	1:A:228:GLU:N	2.32	0.45
1:A:81:SER:O	1:A:84:PRO:HD3	2.16	0.45
1:B:222:PHE:CD1	1:B:222:PHE:N	2.85	0.44
1:D:98:PRO:HG3	1:C:14:ILE:HD11	2.00	0.44
1:B:18:THR:HG23	1:B:58:VAL:CG2	2.48	0.44
1:A:237:MSE:HE3	1:A:246:ARG:CG	2.47	0.44
1:A:82:ARG:HA	1:A:83:PRO:HA	1.81	0.43
1:B:105:THR:HA	1:B:106:PRO:HD3	1.90	0.43
1:A:170:LEU:HD21	1:A:172:ILE:HD11	2.01	0.43
1:B:223:VAL:O	1:B:227:VAL:HG23	2.18	0.43
1:C:109:ALA:O	1:C:110:MSE:HE2	2.18	0.43
1:B:97:VAL:HG13	1:B:200:PRO:HG3	2.00	0.43
1:B:112:LYS:HD2	5:B:314:HOH:O	2.18	0.42
1:A:56:MSE:HE1	1:A:120:TYR:CE2	2.54	0.42
1:C:18:THR:CG2	1:C:22:ARG:NH1	2.82	0.42
1:A:192:CYS:O	1:A:215:MSE:HE2	2.20	0.42
1:C:26:LEU:HD12	1:C:26:LEU:HA	1.95	0.42
1:B:171:LEU:O	1:B:245:CYS:HA	2.19	0.42
1:C:262:ARG:O	1:C:263:LYS:CB	2.67	0.42
1:D:262:ARG:O	1:D:262:ARG:HG3	2.19	0.42
1:C:149:LEU:HD21	1:C:210:LYS:HG2	2.02	0.41
1:A:56:MSE:HE3	1:A:136:TRP:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:GLY:HA2	1:A:210:LYS:O	2.21	0.41
1:C:237:MSE:HE3	1:C:237:MSE:HB3	1.98	0.41
1:C:70:GLN:HG2	1:C:131:GLY:HA2	2.02	0.41
1:C:229:PHE:CD2	1:C:253:ILE:HD13	2.56	0.41
1:B:99:ALA:HB2	1:B:207:ARG:HG3	2.02	0.41
1:C:105:THR:HA	1:C:106:PRO:HD3	1.91	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	263/268 (98%)	255 (97%)	8 (3%)	0	100	100
1	B	266/268 (99%)	258 (97%)	8 (3%)	0	100	100
1	C	263/268 (98%)	253 (96%)	10 (4%)	0	100	100
1	D	263/268 (98%)	255 (97%)	8 (3%)	0	100	100
All	All	1055/1072 (98%)	1021 (97%)	34 (3%)	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	228/224 (102%)	221 (97%)	7 (3%)	40	39
1	B	232/224 (104%)	229 (99%)	3 (1%)	69	74
1	C	228/224 (102%)	224 (98%)	4 (2%)	59	63
1	D	230/224 (103%)	228 (99%)	2 (1%)	78	83
All	All	918/896 (102%)	902 (98%)	16 (2%)	60	65

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LYS
1	A	60	THR
1	A	73	ASP
1	A	103	HIS
1	A	196	LYS
1	A	214	ASP
1	A	263	LYS
1	D	73	ASP
1	D	263	LYS
1	C	88	GLU
1	C	203	GLU
1	C	208	VAL
1	C	262	ARG
1	B	141	GLU
1	B	179	ASN
1	B	206	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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
2	ACO	D	266	-	45,53,53	1.30	5 (11%)	56,79,79	1.58	11 (19%)
2	ACO	C	266	-	45,53,53	1.23	3 (6%)	56,79,79	1.35	4 (7%)
2	ACO	A	266	-	45,53,53	1.03	2 (4%)	56,79,79	1.44	10 (17%)
2	ACO	B	266	-	45,53,53	1.23	2 (4%)	56,79,79	1.45	9 (16%)
4	EPE	B	268	-	15,15,15	1.45	1 (6%)	18,20,20	0.92	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	D	266	-	-	3/47/67/67	0/3/3/3
2	ACO	C	266	-	-	3/47/67/67	0/3/3/3
2	ACO	A	266	-	-	5/47/67/67	0/3/3/3
2	ACO	B	266	-	-	2/47/67/67	0/3/3/3
4	EPE	B	268	-	-	6/9/19/19	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	268	EPE	C10-S	4.60	1.84	1.77
2	C	266	ACO	O4B-C1B	4.43	1.47	1.41
2	C	266	ACO	P3B-O7A	3.74	1.62	1.50
2	D	266	ACO	C4A-N3A	-3.71	1.30	1.35
2	B	266	ACO	O4B-C1B	3.49	1.46	1.41
2	D	266	ACO	O4B-C1B	2.81	1.45	1.41
2	D	266	ACO	C5P-N4P	-2.40	1.27	1.33
2	A	266	ACO	C2B-C1B	-2.31	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	266	ACO	P3B-O7A	2.29	1.57	1.50
2	D	266	ACO	P3B-O3B	-2.23	1.55	1.59
2	A	266	ACO	C5A-N7A	-2.20	1.31	1.39
2	B	266	ACO	C5B-C4B	2.16	1.58	1.51
2	C	266	ACO	P2A-O5A	-2.02	1.45	1.55

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	266	ACO	N3A-C2A-N1A	-5.57	119.97	128.68
2	C	266	ACO	N3A-C2A-N1A	-5.12	120.68	128.68
2	B	266	ACO	N3A-C2A-N1A	-4.79	121.20	128.68
2	A	266	ACO	N3A-C2A-N1A	-4.32	121.93	128.68
2	D	266	ACO	C7P-C6P-C5P	-3.45	106.61	112.36
2	D	266	ACO	C3P-N4P-C5P	-3.41	116.51	122.84
2	C	266	ACO	C2P-C3P-N4P	-3.24	105.60	112.42
2	A	266	ACO	C7P-C6P-C5P	-3.24	106.96	112.36
2	D	266	ACO	O6A-P2A-O4A	-3.23	96.47	109.07
2	B	266	ACO	C1B-N9A-C4A	-3.02	121.33	126.64
2	D	266	ACO	C1B-N9A-C4A	-2.99	121.39	126.64
2	C	266	ACO	P2A-O3A-P1A	-2.94	122.74	132.83
2	A	266	ACO	C2P-C3P-N4P	-2.81	106.52	112.42
2	B	266	ACO	C2P-C3P-N4P	-2.76	106.62	112.42
2	B	266	ACO	C4A-C5A-N7A	-2.73	106.56	109.40
2	A	266	ACO	C2A-N1A-C6A	2.61	123.22	118.75
2	A	266	ACO	C5A-C6A-N6A	2.53	124.20	120.35
2	A	266	ACO	P2A-O3A-P1A	-2.51	124.20	132.83
2	B	266	ACO	C7P-N8P-C9P	-2.50	118.13	122.59
2	A	266	ACO	C4A-C5A-N7A	-2.45	106.85	109.40
2	B	266	ACO	O2B-C2B-C1B	-2.44	101.86	110.85
2	D	266	ACO	C4A-C5A-N7A	-2.42	106.87	109.40
2	D	266	ACO	C2P-C3P-N4P	-2.42	107.33	112.42
2	D	266	ACO	O2B-C2B-C1B	-2.31	102.34	110.85
2	A	266	ACO	O3B-C3B-C2B	-2.21	103.66	111.68
2	B	266	ACO	O9A-P3B-O3B	2.21	115.91	105.99
2	D	266	ACO	P2A-O3A-P1A	-2.20	125.29	132.83
2	D	266	ACO	O9A-P3B-O3B	2.17	115.74	105.99
2	B	266	ACO	C2A-N1A-C6A	2.16	122.44	118.75
2	C	266	ACO	C1B-N9A-C4A	-2.13	122.90	126.64
2	D	266	ACO	C2A-N1A-C6A	2.11	122.36	118.75
2	A	266	ACO	O9A-P3B-O8A	2.07	115.56	107.64
2	A	266	ACO	O3B-P3B-O7A	-2.05	101.49	109.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	266	ACO	C6P-C7P-N8P	-2.01	107.83	111.90

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	266	ACO	C3B-O3B-P3B-O7A
2	C	266	ACO	C3B-O3B-P3B-O9A
4	B	268	EPE	C9-C10-S-O2S
4	B	268	EPE	C9-C10-S-O3S
2	A	266	ACO	S1P-C2P-C3P-N4P
2	A	266	ACO	O-C-S1P-C2P
2	C	266	ACO	O-C-S1P-C2P
4	B	268	EPE	N4-C7-C8-O8
2	A	266	ACO	C3B-C4B-C5B-O5B
4	B	268	EPE	C10-C9-N1-C2
4	B	268	EPE	C10-C9-N1-C6
2	C	266	ACO	CH3-C-S1P-C2P
2	B	266	ACO	P1A-O3A-P2A-O4A
4	B	268	EPE	C9-C10-S-O1S
2	A	266	ACO	CH3-C-S1P-C2P
2	D	266	ACO	O-C-S1P-C2P
2	D	266	ACO	C4B-C5B-O5B-P1A
2	B	266	ACO	P1A-O3A-P2A-O5A
2	D	266	ACO	CH3-C-S1P-C2P

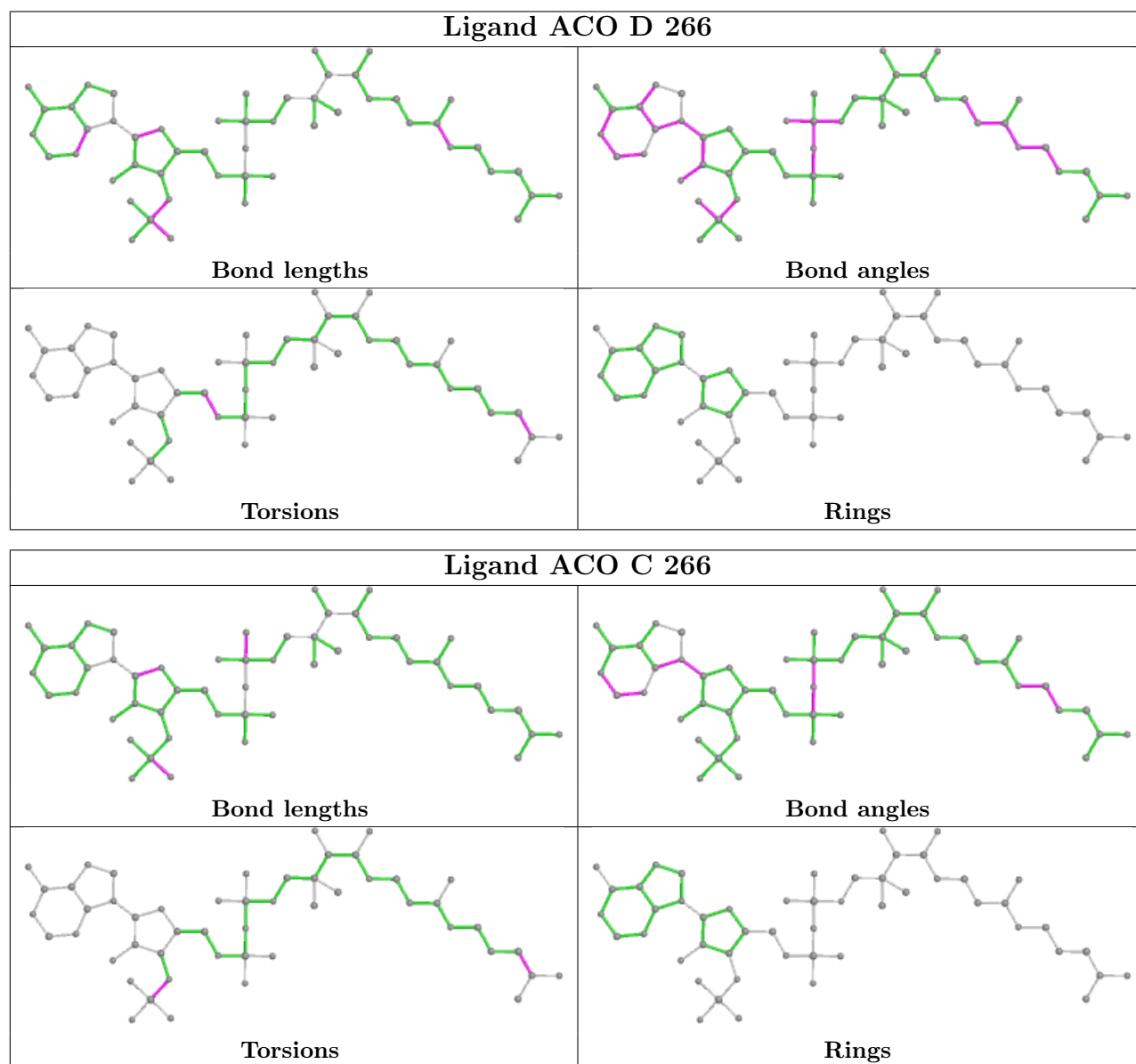
There are no ring outliers.

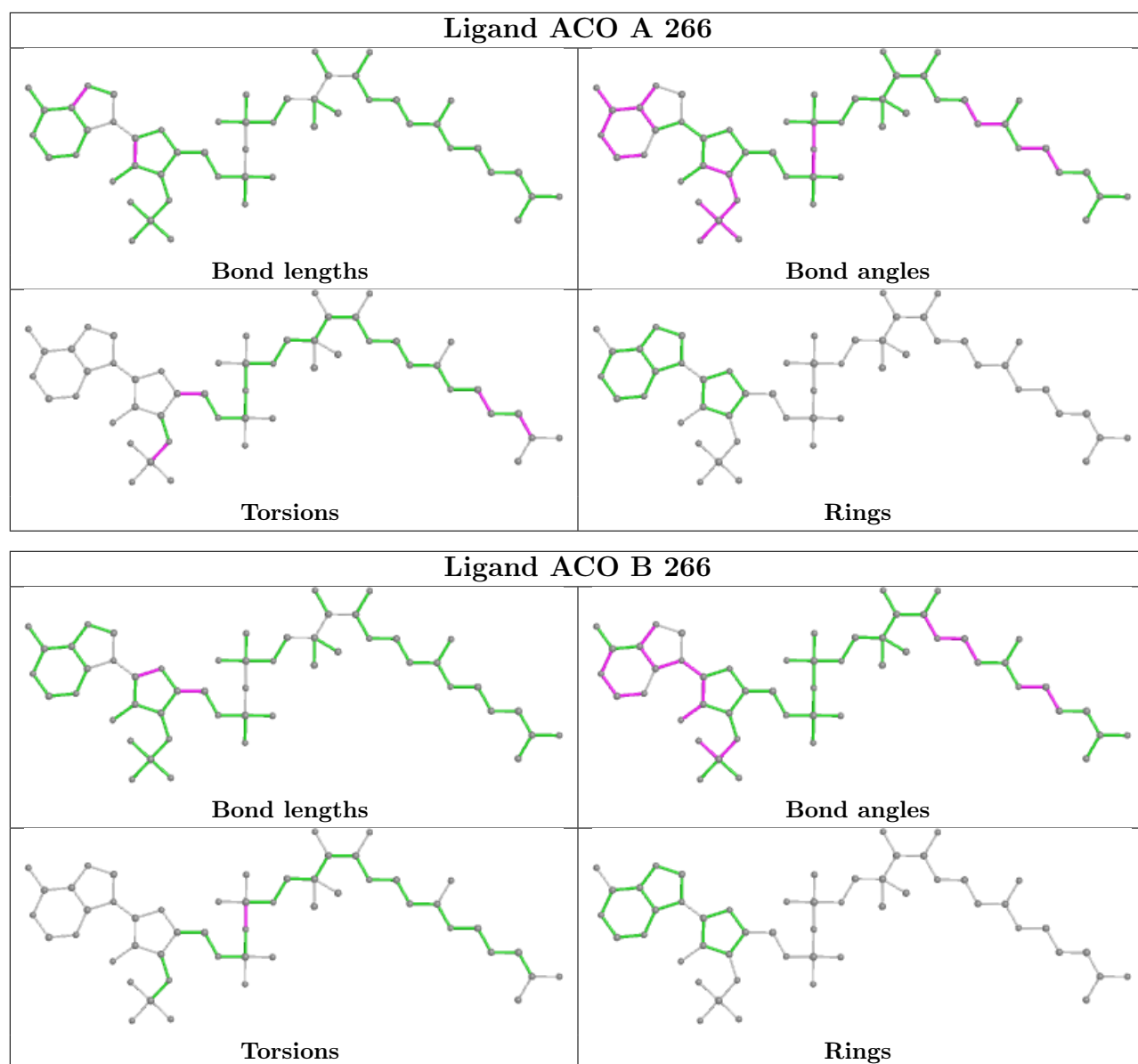
5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	266	ACO	1	0
2	C	266	ACO	1	0
2	A	266	ACO	1	0
2	B	266	ACO	1	0
4	B	268	EPE	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	256/268 (95%)	0.22	15 (5%)	22 30	4, 12, 30, 47	7 (2%)
1	B	257/268 (95%)	0.02	10 (3%)	39 48	4, 12, 30, 46	8 (3%)
1	C	255/268 (95%)	0.20	14 (5%)	25 34	3, 11, 30, 35	4 (1%)
1	D	256/268 (95%)	0.06	13 (5%)	28 36	4, 12, 29, 37	4 (1%)
All	All	1024/1072 (95%)	0.12	52 (5%)	28 36	3, 12, 30, 47	23 (2%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	233	GLY	4.8
1	D	82	ARG	4.7
1	B	-2	SER	4.5
1	A	0	ALA	4.4
1	D	192	CYS	4.3
1	A	-1	ASN	4.3
1	B	191	ALA	4.1
1	D	191	ALA	3.7
1	B	192	CYS	3.7
1	C	204	ASN	3.6
1	B	-1	ASN	3.6
1	D	83	PRO	3.5
1	C	191	ALA	3.4
1	D	220	ASP	3.1
1	C	2	ASN	3.1
1	A	232	LYS	3.1
1	B	204	ASN	3.0
1	C	0	ALA	3.0
1	A	204	ASN	3.0
1	C	234	THR	3.0
1	A	262	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	203	GLU	2.9
1	C	203	GLU	2.8
1	A	192	CYS	2.8
1	D	205	GLY	2.8
1	C	220	ASP	2.7
1	A	234	THR	2.7
1	B	193	GLU	2.6
1	C	192	CYS	2.6
1	B	203	GLU	2.5
1	A	70	GLN	2.5
1	C	3	ASP	2.5
1	C	34	VAL	2.5
1	D	79	HIS	2.5
1	D	81	SER	2.5
1	A	206	GLU	2.5
1	C	232	LYS	2.5
1	B	220	ASP	2.4
1	B	206	GLU	2.4
1	B	190	GLY	2.4
1	C	218	ASP	2.3
1	C	69	THR	2.3
1	A	263	LYS	2.3
1	A	2	ASN	2.2
1	D	206	GLU	2.2
1	D	84	PRO	2.1
1	D	224	GLU	2.1
1	A	69	THR	2.1
1	C	206	GLU	2.1
1	D	87	GLU	2.1
1	D	218	ASP	2.0
1	A	68	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](#)

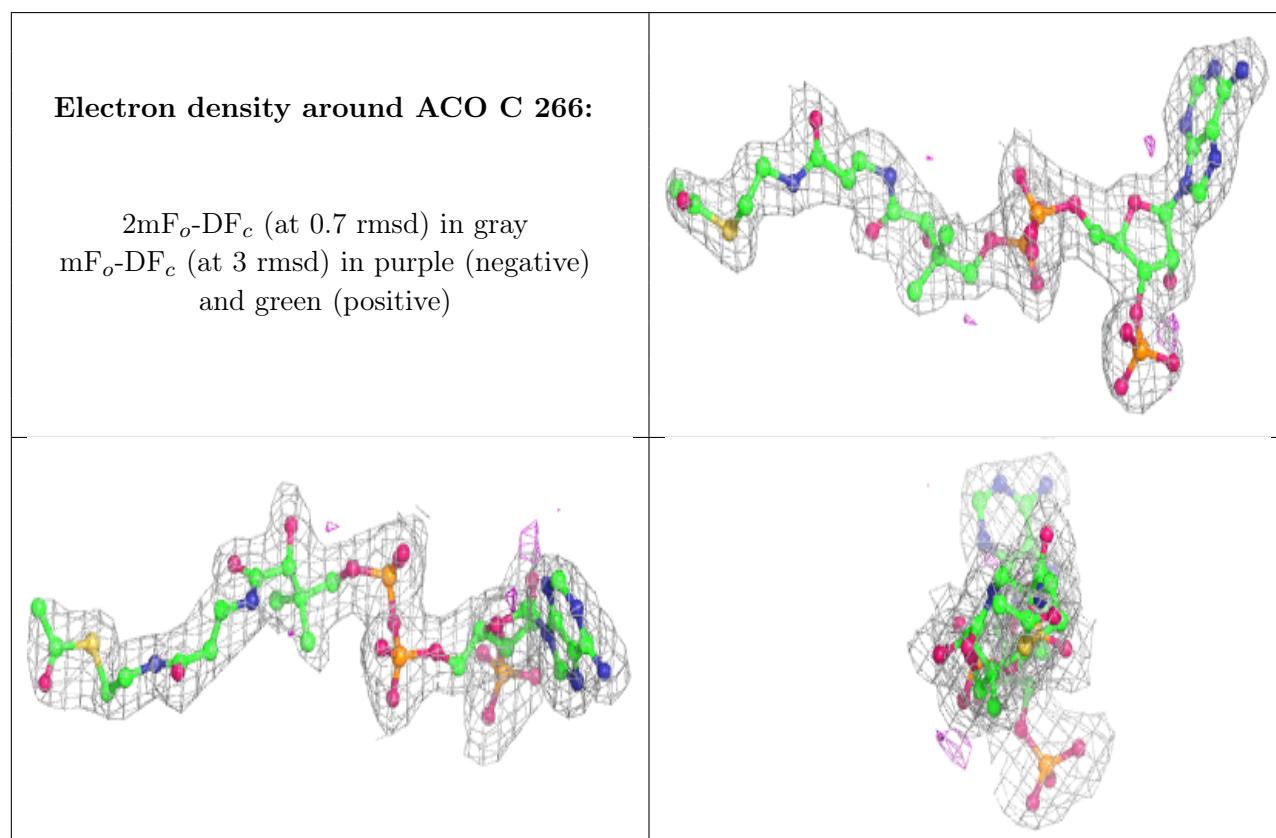
There are no monosaccharides in this entry.

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, 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.

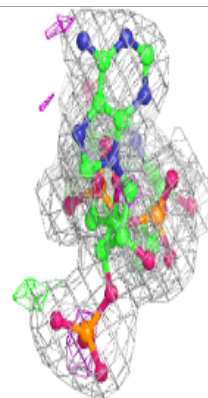
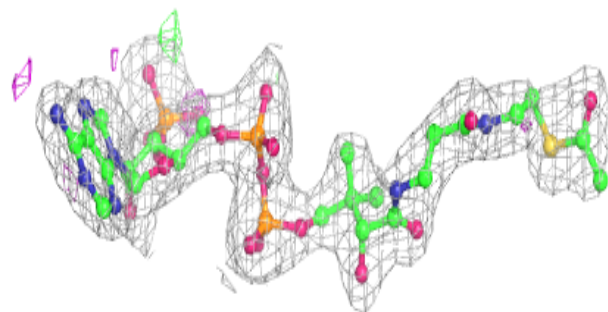
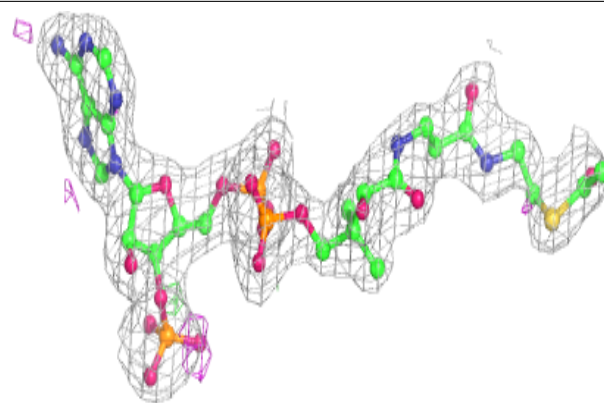
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	EPE	B	268	15/15	0.58	0.24	64,68,82,82	0
3	MG	D	267	1/1	0.83	0.23	45,45,45,45	0
3	MG	B	267	1/1	0.87	0.19	37,37,37,37	0
2	ACO	C	266	51/51	0.95	0.10	17,28,48,49	0
2	ACO	A	266	51/51	0.95	0.10	20,31,51,52	0
2	ACO	B	266	51/51	0.96	0.10	15,27,44,47	0
2	ACO	D	266	51/51	0.96	0.10	14,27,48,50	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.

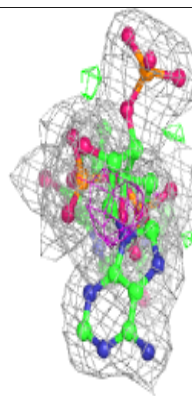
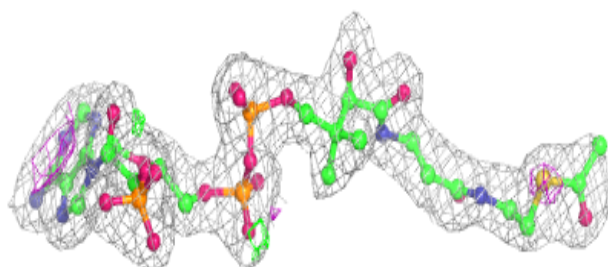
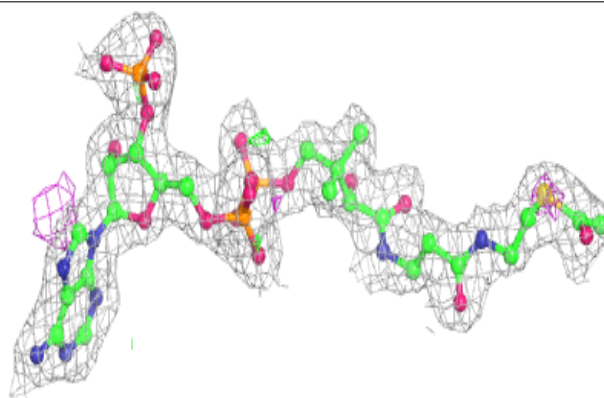


Electron density around ACO A 266:

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

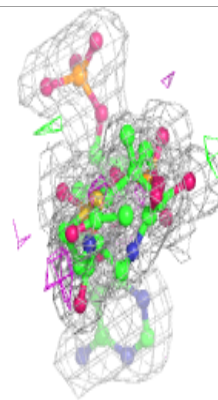
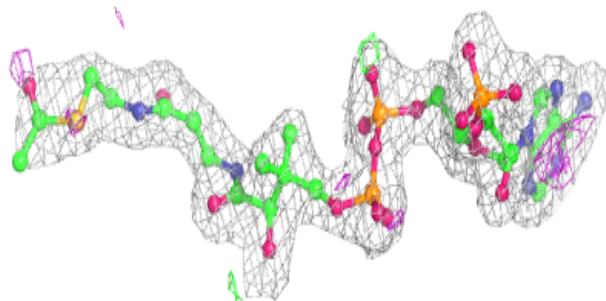
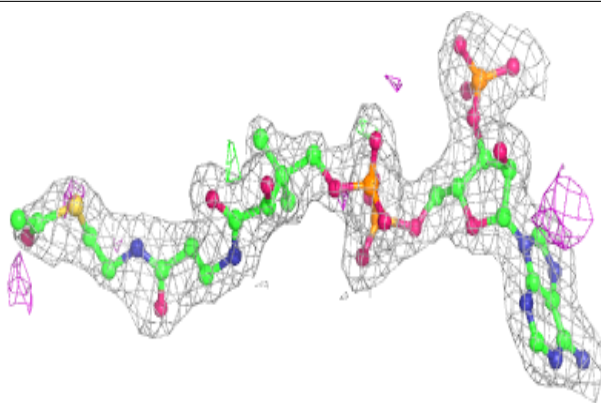
**Electron density around ACO B 266:**

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



Electron density around ACO D 266:

$2mF_o-DF_c$ (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.