



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:03 PM UTC

PDB ID : 3H9J / pdb_00003h9j
Title : Crystal structure of E. coli MccB + AMPCPP + SeMeT MccA
Authors : Regni, C.A.; Roush, R.F.; Miller, D.; Nourse, A.; Walsh, C.T.; Schulman, B.A.
Deposited on : 2009-04-30
Resolution : 2.30 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

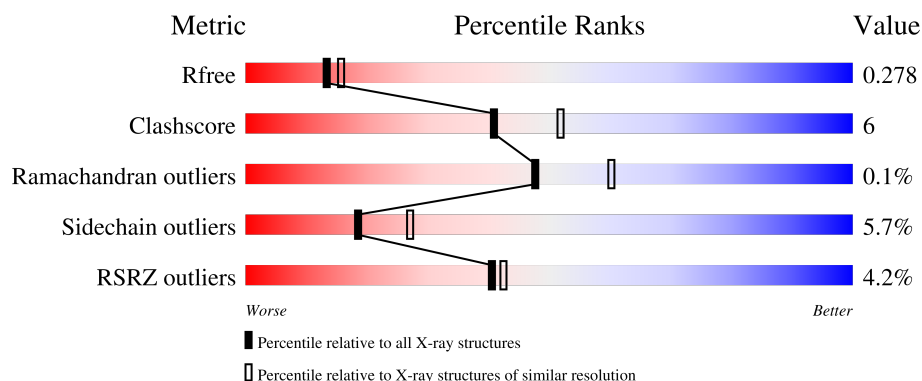
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	353	3% 82% 12% • •
1	B	353	6% 81% 13% • 5%
1	C	353	2% 84% 10% • •
1	D	353	5% 78% 13% • 5%
2	E	7	14% 86%

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Mol	Chain	Length	Quality of chain
2	F	7	14%86%
2	G	7	14%71%14%14%
2	H	7	14%86%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10848 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 MccB protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	0	0
			2616	1671	446	488	11			
1	B	336	Total	C	N	O	S	0	0	0
			2569	1646	432	480	11			
1	C	344	Total	C	N	O	S	0	0	0
			2658	1698	453	496	11			
1	D	334	Total	C	N	O	S	0	1	0
			2564	1638	439	476	11			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q47506
A	-1	SER	-	expression tag	UNP Q47506
A	0	HIS	-	expression tag	UNP Q47506
B	-2	GLY	-	expression tag	UNP Q47506
B	-1	SER	-	expression tag	UNP Q47506
B	0	HIS	-	expression tag	UNP Q47506
C	-2	GLY	-	expression tag	UNP Q47506
C	-1	SER	-	expression tag	UNP Q47506
C	0	HIS	-	expression tag	UNP Q47506
D	-2	GLY	-	expression tag	UNP Q47506
D	-1	SER	-	expression tag	UNP Q47506
D	0	HIS	-	expression tag	UNP Q47506

- Molecule 2 is a protein called Microcin C7 ANALOG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	1	Total	C	N	O	Se	0	0	0
			8	5	1	1	1			
2	F	1	Total	C	N	O	Se	0	0	0
			8	5	1	1	1			

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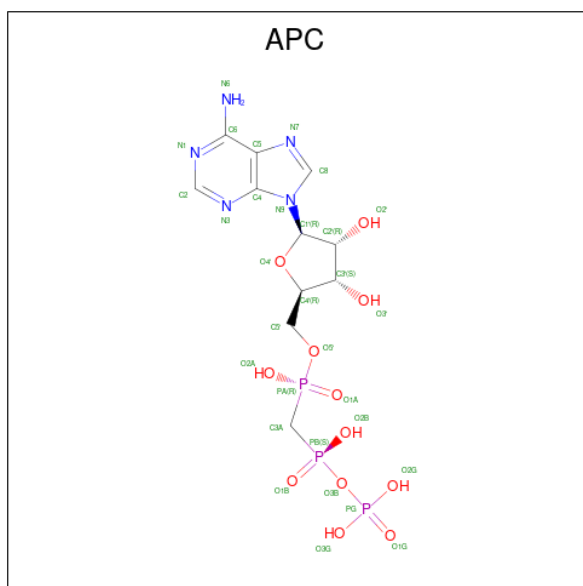
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	7	Total	C	N	O	Se	0	0	0
			52	28	12	11	1			
2	H	1	Total	C	N	O	Se	0	0	0
			8	5	1	1	1			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is DIPHOSPHOMETHYLPHOSPHONIC ACID ADENOSYL ESTER (CCD ID: APC) (formula: C₁₁H₁₈N₅O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
4	B	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
4	C	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
4	D	1	Total	C	O	P		0	0
			9	1	6	2			

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	S	0	0
			5	4	1		

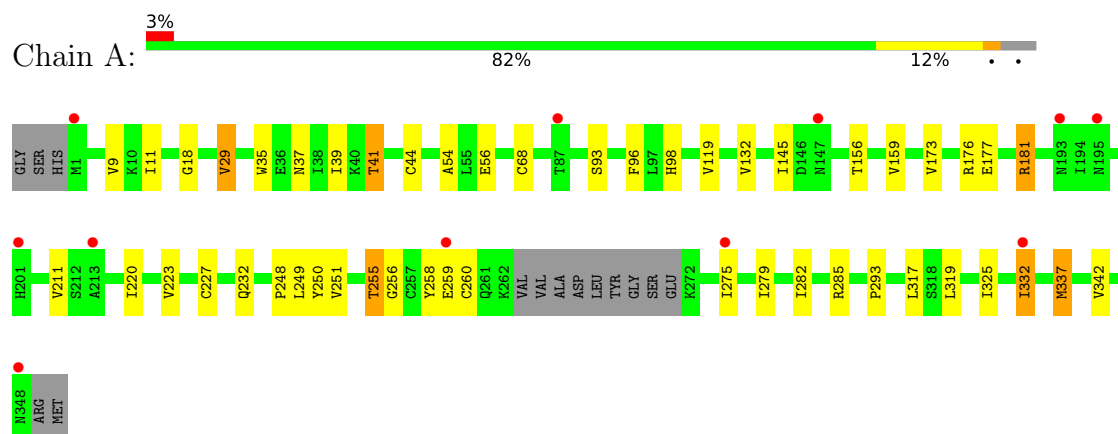
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	62	Total	O	0	0
			62	62		
6	B	44	Total	O	0	0
			44	44		
6	C	69	Total	O	0	0
			69	69		
6	D	47	Total	O	0	0
			47	47		
6	G	1	Total	O	0	0
			1	1		

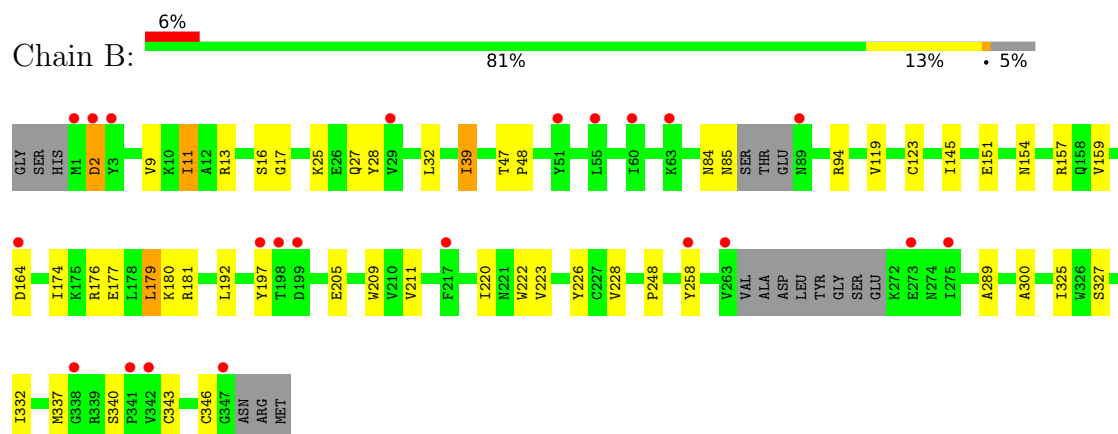
3 Residue-property plots [i](#)

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.

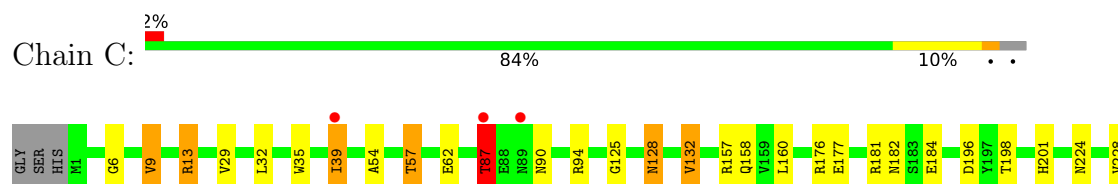
• Molecule 1: MccB protein



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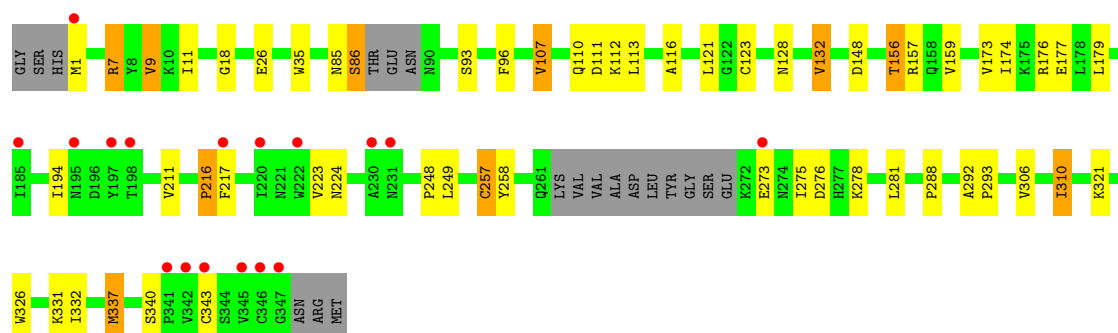
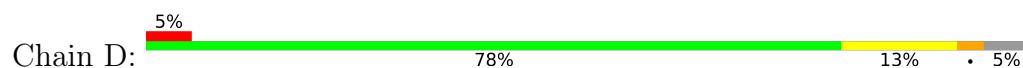


• Molecule 1: MccB protein

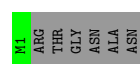




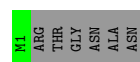
- Molecule 1: MccB protein



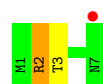
- Molecule 2: Microcin C7 ANALOG



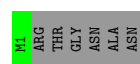
- Molecule 2: Microcin C7 ANALOG



- Molecule 2: Microcin C7 ANALOG



- Molecule 2: Microcin C7 ANALOG



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.84Å 138.00Å 80.82Å 90.00° 92.21° 90.00°	Depositor
Resolution (Å)	39.97 – 2.30 39.97 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.2 (39.97-2.30) 99.1 (39.97-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.95 (at 2.29Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.196 , 0.255 0.226 , 0.278	Depositor DCC
R_{free} test set	2715 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	37.9	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 28.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.035 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10848	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% 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: ZN, APC, SO4

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	0.62	0/2671	0.89	1/3630 (0.0%)
1	B	0.61	0/2622	0.87	0/3566
1	C	0.64	0/2713	0.86	0/3681
1	D	0.70	3/2623 (0.1%)	0.91	2/3563 (0.1%)
2	E	0.69	0/7	0.54	0/7
2	F	0.66	0/7	0.35	0/7
2	G	0.67	0/51	0.66	0/65
2	H	0.72	0/7	0.28	0/7
All	All	0.65	3/10701 (0.0%)	0.88	3/14526 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	273[A]	GLU	CG-CD	-10.36	1.26	1.52
1	D	273[B]	GLU	CG-CD	-10.36	1.26	1.52
1	D	86	SER	CB-OG	6.08	1.54	1.42

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	132	VAL	CB-CA-C	-6.82	103.25	111.97
1	D	9	VAL	N-CA-CB	5.89	116.95	110.53
1	A	260	CYS	N-CA-C	5.15	116.89	111.28

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	2616	0	2555	44	0
1	B	2569	0	2490	39	0
1	C	2658	0	2615	33	0
1	D	2564	0	2494	39	0
2	E	8	0	11	0	0
2	F	8	0	11	0	0
2	G	52	0	51	1	0
2	H	8	0	11	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	31	0	14	1	0
4	B	31	0	14	0	0
4	C	62	0	28	1	0
4	D	9	0	2	0	0
5	B	5	0	0	0	0
6	A	62	0	0	1	0
6	B	44	0	0	4	0
6	C	69	0	0	3	0
6	D	47	0	0	1	0
6	G	1	0	0	0	0
All	All	10848	0	10296	136	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 6.

All (136) 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:181:ARG:NH1	1:B:159:VAL:O	1.95	0.98
1:C:285:ARG:HH11	1:C:285:ARG:HG2	1.37	0.89
1:B:248:PRO:HG3	1:B:337:MET:HE2	1.54	0.86
1:C:13:ARG:HH11	1:C:13:ARG:HG3	1.41	0.86
1:A:248:PRO:HG3	1:A:337:MET:CE	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:ARG:O	6:B:400:HOH:O	2.02	0.75
1:D:156:THR:HG22	1:D:157:ARG:HG3	1.67	0.75
1:C:128:ASN:O	1:C:132:VAL:HG23	1.87	0.74
1:D:121:LEU:HD11	1:D:194:ILE:HD11	1.70	0.74
1:C:157:ARG:HB2	6:C:421:HOH:O	1.90	0.72
1:A:279:ILE:HG13	1:B:39:ILE:HD12	1.72	0.71
1:A:29:VAL:HG22	1:A:35:TRP:HB2	1.71	0.71
1:B:258:TYR:HA	1:B:337:MET:HE1	1.74	0.70
1:A:159:VAL:O	1:B:181:ARG:NH1	2.25	0.70
1:D:248:PRO:HG3	1:D:337:MET:HE2	1.73	0.69
1:A:248:PRO:HG3	1:A:337:MET:HE1	1.74	0.69
1:C:296:ASN:ND2	6:C:421:HOH:O	2.22	0.68
1:C:87:THR:HG23	1:C:90:ASN:HB2	1.77	0.67
1:C:132:VAL:HG22	1:C:160:LEU:HD11	1.78	0.66
1:C:285:ARG:HG2	1:C:285:ARG:NH1	2.09	0.65
1:B:248:PRO:CG	1:B:337:MET:HE2	2.26	0.65
1:C:181:ARG:NH1	1:D:159:VAL:O	2.30	0.65
1:B:258:TYR:HA	1:B:337:MET:CE	2.27	0.64
4:A:359:APC:O3B	4:A:359:APC:H5'2	1.96	0.64
1:D:248:PRO:HG3	1:D:337:MET:CE	2.28	0.64
1:B:211:VAL:HG21	1:B:223:VAL:HG11	1.80	0.63
1:A:248:PRO:HG3	1:A:337:MET:HE2	1.79	0.63
1:A:317:LEU:HD11	1:B:327:SER:O	2.00	0.62
1:C:272:LYS:HB2	1:C:275:ILE:HD13	1.83	0.61
1:C:94:ARG:HH22	1:D:288:PRO:HD2	1.65	0.61
1:C:177:GLU:OE1	1:C:181:ARG:NH2	2.34	0.61
1:D:96:PHE:CE1	1:D:110:GLN:HG3	2.36	0.61
1:B:176:ARG:NH1	1:B:177:GLU:OE2	2.34	0.60
1:D:258:TYR:HA	1:D:337:MET:HE1	1.85	0.59
1:C:272:LYS:HB2	1:C:275:ILE:CD1	2.31	0.59
1:C:282:ILE:HG21	1:D:11:ILE:HD12	1.85	0.59
1:A:251:VAL:H	1:A:255:THR:CG2	2.16	0.59
1:C:35:TRP:O	1:C:39:ILE:HG23	2.03	0.58
1:D:123:CYS:HB3	1:D:174:ILE:HD12	1.86	0.58
1:C:325:ILE:HG12	1:C:332:ILE:HG12	1.86	0.57
1:C:13:ARG:HG3	1:C:13:ARG:NH1	2.15	0.57
1:D:123:CYS:HB3	1:D:174:ILE:CD1	2.35	0.57
1:D:110:GLN:NE2	6:D:376:HOH:O	2.37	0.56
1:A:258:TYR:HA	1:A:337:MET:HE1	1.88	0.56
1:A:41:THR:HG21	1:A:68:CYS:HB2	1.88	0.56
1:A:275:ILE:HD11	1:B:13:ARG:HH21	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:ILE:HG23	1:D:332:ILE:HG21	1.86	0.56
1:D:96:PHE:HE1	1:D:110:GLN:HG3	1.69	0.56
1:B:119:VAL:HG13	1:B:145:ILE:HD12	1.86	0.56
1:D:306:VAL:O	1:D:310:ILE:HG23	2.05	0.55
1:A:37:ASN:O	1:A:41:THR:HG23	2.06	0.55
1:A:176:ARG:NH1	1:A:177:GLU:OE2	2.40	0.54
1:B:157:ARG:NH1	6:B:397:HOH:O	2.40	0.54
1:A:332:ILE:HD11	1:B:332:ILE:HG22	1.89	0.54
1:B:154:ASN:HA	6:B:397:HOH:O	2.07	0.54
1:C:6:GLY:O	1:C:9:VAL:HG13	2.09	0.54
1:C:270:SER:OG	1:C:275:ILE:HD11	2.08	0.53
1:D:248:PRO:CG	1:D:337:MET:HE2	2.38	0.53
1:D:340:SER:HB3	1:D:343:CYS:HB2	1.90	0.53
1:A:332:ILE:HD11	1:B:332:ILE:N	2.23	0.53
1:B:248:PRO:HG3	1:B:337:MET:CE	2.34	0.52
1:A:211:VAL:HG21	1:A:223:VAL:HG11	1.92	0.52
1:C:39:ILE:HD11	1:D:278:LYS:HB2	1.91	0.51
4:C:359:APC:H3A2	6:C:414:HOH:O	2.10	0.51
1:A:250:TYR:HA	1:A:255:THR:HG21	1.93	0.51
1:D:113:LEU:HA	1:D:310:ILE:HD11	1.92	0.51
1:C:182:ASN:OD1	1:C:184:GLU:HB2	2.12	0.50
1:C:177:GLU:HB3	1:C:181:ARG:HH21	1.77	0.50
1:B:205:GLU:HA	6:B:371:HOH:O	2.12	0.49
1:A:35:TRP:CZ2	1:A:39:ILE:HD11	2.47	0.49
1:D:112:LYS:C	1:D:310:ILE:HD11	2.37	0.49
1:A:258:TYR:HA	1:A:337:MET:CE	2.43	0.49
1:B:228:VAL:HG11	1:B:346:CYS:HB3	1.94	0.49
1:B:340:SER:HB3	1:B:343:CYS:HB2	1.94	0.48
1:D:211:VAL:HG21	1:D:223:VAL:HG11	1.95	0.48
1:C:224:ASN:OD1	1:C:257:CYS:HB2	2.13	0.48
1:A:251:VAL:H	1:A:255:THR:HG21	1.78	0.48
1:D:116:ALA:HB2	1:D:310:ILE:HD13	1.94	0.48
1:A:293:PRO:HB3	1:B:300:ALA:O	2.13	0.48
1:D:326:TRP:CE2	1:D:331:LYS:HE3	2.49	0.47
1:A:342:VAL:HG12	1:A:342:VAL:O	2.16	0.46
1:D:113:LEU:HD23	1:D:310:ILE:CG1	2.45	0.46
1:B:179:LEU:HD12	1:B:179:LEU:HA	1.85	0.46
1:C:196:ASP:OD2	1:C:198:THR:OG1	2.32	0.45
1:C:198:THR:O	1:C:201:HIS:ND1	2.45	0.45
1:D:292:ALA:HB3	1:D:293:PRO:HD3	1.98	0.45
1:A:37:ASN:O	1:A:41:THR:CG2	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:VAL:HG13	1:A:145:ILE:HD12	1.98	0.45
1:B:325:ILE:HG12	1:B:332:ILE:HG13	1.99	0.45
1:C:224:ASN:O	1:C:228:VAL:HG23	2.16	0.45
1:B:84:ASN:O	1:B:85:ASN:C	2.59	0.45
1:D:224:ASN:HD21	1:D:257:CYS:HB2	1.83	0.44
1:D:337:MET:HE3	1:D:337:MET:HB3	1.79	0.44
1:A:227:CYS:HB3	1:A:232:GLN:O	2.18	0.44
1:A:282:ILE:HG21	1:B:11:ILE:HD12	1.99	0.44
1:B:17:GLY:HA2	1:B:32:LEU:HD13	2.01	0.43
1:A:220:ILE:HD12	1:A:258:TYR:CZ	2.53	0.43
1:A:337:MET:HE3	1:A:337:MET:HB3	1.84	0.43
1:A:173:VAL:HG13	1:A:176:ARG:HH21	1.83	0.43
1:A:332:ILE:CD1	1:B:332:ILE:HG22	2.48	0.43
1:B:2:ASP:OD1	1:B:48:PRO:HB2	2.18	0.43
1:A:248:PRO:CG	1:A:337:MET:HE2	2.46	0.43
1:D:248:PRO:HB3	1:D:337:MET:HE2	2.01	0.43
1:A:93:SER:O	1:A:96:PHE:HB2	2.18	0.43
1:B:123:CYS:HB3	1:B:174:ILE:HD12	2.00	0.43
1:C:228:VAL:HG11	1:C:346:CYS:HA	2.00	0.43
1:A:44:CYS:HB3	1:A:54:ALA:HB1	2.01	0.42
1:A:156:THR:HG21	6:A:421:HOH:O	2.18	0.42
1:A:255:THR:HG23	1:A:256:GLY:O	2.18	0.42
1:C:54:ALA:O	1:C:57:THR:HG22	2.20	0.42
1:D:93:SER:O	1:D:96:PHE:HB2	2.20	0.42
1:A:98:HIS:HA	1:B:289:ALA:HB1	2.01	0.42
1:A:332:ILE:HD11	1:B:332:ILE:H	1.84	0.41
1:C:125:GLY:HA2	1:C:158:GLN:HG2	2.02	0.41
1:D:176:ARG:NH1	1:D:177:GLU:OE2	2.51	0.41
1:D:216:PRO:HB2	1:D:217:PHE:H	1.64	0.41
1:D:86:SER:C	1:D:107:VAL:HG23	2.46	0.41
1:A:251:VAL:H	1:A:255:THR:HG22	1.85	0.41
1:A:279:ILE:CG1	1:B:39:ILE:HD12	2.47	0.41
1:A:275:ILE:CD1	1:B:13:ARG:HH21	2.32	0.41
1:B:197:TYR:HB2	1:B:222:TRP:CD1	2.55	0.41
1:B:209:TRP:CH2	1:B:226:TYR:CE2	3.08	0.41
1:B:16:SER:HB3	1:B:28:TYR:OH	2.20	0.41
1:A:18:GLY:HA3	1:A:35:TRP:CE2	2.55	0.41
1:C:285:ARG:O	1:D:7:ARG:HD2	2.21	0.41
1:A:220:ILE:HD12	1:A:258:TYR:OH	2.21	0.41
1:C:332:ILE:HG13	1:D:332:ILE:HG13	2.03	0.41
1:D:18:GLY:HA3	1:D:35:TRP:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:26:GLU:OE1	2:G:2:ARG:HD3	2.20	0.41
1:C:296:ASN:HD22	1:C:296:ASN:N	2.19	0.41
1:B:25:LYS:O	1:B:27:GLN:HG3	2.21	0.40
1:B:151:GLU:H	1:B:154:ASN:ND2	2.19	0.40
1:D:173:VAL:HG13	1:D:176:ARG:NH2	2.35	0.40
1:A:325:ILE:HG13	1:A:332:ILE:HG23	2.01	0.40
1:D:248:PRO:CB	1:D:337:MET:HE2	2.51	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	335/353 (95%)	327 (98%)	8 (2%)	0	100	100
1	B	330/353 (94%)	319 (97%)	11 (3%)	0	100	100
1	C	340/353 (96%)	330 (97%)	9 (3%)	1 (0%)	36	46
1	D	329/353 (93%)	319 (97%)	9 (3%)	1 (0%)	36	46
2	G	5/7 (71%)	5 (100%)	0	0	100	100
All	All	1339/1419 (94%)	1300 (97%)	37 (3%)	2 (0%)	48	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	216	PRO
1	C	87	THR

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	279/304 (92%)	265 (95%)	14 (5%)	22	33
1	B	270/304 (89%)	260 (96%)	10 (4%)	30	45
1	C	285/304 (94%)	266 (93%)	19 (7%)	15	21
1	D	271/304 (89%)	253 (93%)	18 (7%)	15	21
2	E	1/4 (25%)	1 (100%)	0	100	100
2	F	1/4 (25%)	1 (100%)	0	100	100
2	G	5/4 (125%)	3 (60%)	2 (40%)	0	0
2	H	1/4 (25%)	1 (100%)	0	100	100
All	All	1113/1232 (90%)	1050 (94%)	63 (6%)	18	27

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	VAL
1	A	11	ILE
1	A	29	VAL
1	A	41	THR
1	A	56	GLU
1	A	132	VAL
1	A	181	ARG
1	A	249	LEU
1	A	255	THR
1	A	259	GLU
1	A	285	ARG
1	A	319	LEU
1	A	332	ILE
1	A	337	MET
1	B	2	ASP
1	B	9	VAL
1	B	11	ILE
1	B	39	ILE
1	B	47	THR

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Mol	Chain	Res	Type
1	B	164	ASP
1	B	179	LEU
1	B	180	LYS
1	B	192	LEU
1	B	220	ILE
1	C	9	VAL
1	C	13	ARG
1	C	29	VAL
1	C	32	LEU
1	C	39	ILE
1	C	57	THR
1	C	62	GLU
1	C	87	THR
1	C	128	ASN
1	C	132	VAL
1	C	176	ARG
1	C	249	LEU
1	C	259	GLU
1	C	271	GLU
1	C	273	GLU
1	C	275	ILE
1	C	285	ARG
1	C	317	LEU
1	C	319	LEU
1	D	1	MET
1	D	7	ARG
1	D	9	VAL
1	D	85	ASN
1	D	107	VAL
1	D	111	ASP
1	D	128	ASN
1	D	132	VAL
1	D	148	ASP
1	D	156	THR
1	D	179	LEU
1	D	249	LEU
1	D	257	CYS
1	D	275	ILE
1	D	281	LEU
1	D	310	ILE
1	D	321	LYS
1	D	337	MET

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Mol	Chain	Res	Type
2	G	2	ARG
2	G	3	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	95	ASN
1	A	236	ASN
1	B	27	GLN
1	B	31	ASN
1	B	84	ASN
1	B	95	ASN
1	B	115	ASN
1	B	154	ASN
1	B	158	GLN
1	B	201	HIS
1	B	218	ASN
1	B	274	ASN
1	B	295	ASN
1	B	296	ASN
1	B	333	HIS
1	C	90	ASN
1	C	147	ASN
1	C	231	ASN
1	C	236	ASN
1	C	277	HIS
1	C	295	ASN
1	C	296	ASN
1	D	95	ASN
1	D	149	GLN
1	D	154	ASN
1	D	158	GLN
1	D	193	ASN
1	D	224	ASN
1	D	295	ASN
1	D	296	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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$
4	APC	C	359	-	29,33,33	1.35	3 (10%)	44,52,52	1.79	9 (20%)
4	APC	A	359	-	29,33,33	1.09	2 (6%)	44,52,52	1.90	11 (25%)
4	APC	B	359	-	29,33,33	1.19	4 (13%)	44,52,52	1.84	11 (25%)
4	APC	D	359	-	6,8,33	1.91	2 (33%)	12,13,52	1.64	4 (33%)
5	SO4	B	360	-	4,4,4	0.21	0	6,6,6	0.12	0
4	APC	C	360	-	29,33,33	1.14	1 (3%)	44,52,52	1.94	13 (29%)

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
4	APC	C	359	-	-	5/19/38/38	0/3/3/3
4	APC	A	359	-	-	4/19/38/38	0/3/3/3
4	APC	B	359	-	-	5/19/38/38	0/3/3/3
4	APC	D	359	-	-	3/6/6/38	-
4	APC	C	360	-	-	2/19/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	359	APC	PB-O3B	4.74	1.63	1.58
4	B	359	APC	PB-O3B	3.68	1.62	1.58
4	C	360	APC	PB-O3B	3.12	1.61	1.58
4	D	359	APC	PB-O3B	2.92	1.61	1.55
4	A	359	APC	PB-O3B	2.92	1.61	1.58
4	D	359	APC	PA-O5'	2.84	1.61	1.55
4	B	359	APC	C8-N7	2.07	1.35	1.31
4	B	359	APC	C4-N9	-2.05	1.33	1.37
4	C	359	APC	PB-O2B	-2.04	1.51	1.56
4	B	359	APC	C5-N7	-2.04	1.35	1.39
4	A	359	APC	C4-N9	-2.02	1.33	1.37
4	C	359	APC	C8-N7	2.01	1.35	1.31

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	359	APC	N3-C2-N1	-5.48	120.29	128.58
4	C	360	APC	N3-C2-N1	-5.19	120.73	128.58
4	B	359	APC	N3-C2-N1	-5.16	120.76	128.58
4	C	360	APC	C5-C4-N3	-5.13	119.66	126.72
4	C	359	APC	N3-C2-N1	-4.82	121.29	128.58
4	B	359	APC	C5-C4-N3	-4.71	120.23	126.72
4	C	359	APC	C5-C4-N3	-4.51	120.50	126.72
4	A	359	APC	C5-C4-N3	-4.43	120.61	126.72
4	A	359	APC	N9-C8-N7	-3.97	108.30	113.94
4	C	359	APC	N9-C8-N7	-3.87	108.44	113.94
4	C	360	APC	C2-N3-C4	3.57	120.56	111.83
4	C	360	APC	N3-C4-N9	3.54	133.19	127.17
4	B	359	APC	N9-C8-N7	-3.53	108.93	113.94
4	A	359	APC	C2-N3-C4	3.51	120.41	111.83
4	A	359	APC	C4-N9-C8	3.45	109.36	105.74
4	C	360	APC	N9-C8-N7	-3.42	109.08	113.94
4	B	359	APC	C2-N3-C4	3.39	120.10	111.83
4	C	359	APC	C4-N9-C8	3.36	109.27	105.74
4	C	359	APC	N3-C4-N9	3.15	132.53	127.17
4	C	359	APC	C2-N3-C4	3.06	119.30	111.83
4	B	359	APC	N3-C4-N9	2.99	132.25	127.17
4	A	359	APC	N3-C4-N9	2.96	132.19	127.17
4	D	359	APC	O5'-PA-O1A	-2.80	105.14	112.39
4	A	359	APC	C4-C5-N7	-2.78	107.40	110.58
4	B	359	APC	C4-N9-C8	2.78	108.66	105.74
4	A	359	APC	C5-N7-C8	2.73	107.75	103.45
4	C	360	APC	C4-N9-C8	2.73	108.61	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	359	APC	O2B-PB-O1B	2.72	119.42	112.39
4	B	359	APC	C4-C5-N7	-2.70	107.49	110.58
4	C	359	APC	C5-N7-C8	2.70	107.69	103.45
4	C	360	APC	PB-O3B-PG	-2.69	122.81	132.45
4	A	359	APC	PB-O3B-PG	-2.64	122.98	132.45
4	C	360	APC	C3'-C2'-C1'	2.62	106.43	101.46
4	B	359	APC	O2B-PB-O1B	2.60	118.43	109.95
4	B	359	APC	O2A-PA-O1A	2.59	118.37	109.95
4	C	359	APC	C4-C5-N7	-2.58	107.63	110.58
4	C	360	APC	C5-N7-C8	2.57	107.48	103.45
4	C	360	APC	O2A-PA-O1A	2.57	118.30	109.95
4	C	360	APC	C4-C5-N7	-2.55	107.67	110.58
4	A	359	APC	O2B-PB-O1B	2.53	118.18	109.95
4	C	359	APC	O2B-PB-O1B	2.53	118.17	109.95
4	B	359	APC	C5-N7-C8	2.52	107.40	103.45
4	D	359	APC	O3B-PB-O1B	-2.44	106.08	112.39
4	C	360	APC	O2B-PB-O1B	2.42	117.82	109.95
4	D	359	APC	O2A-PA-O1A	2.36	118.49	112.39
4	B	359	APC	PB-O3B-PG	-2.25	124.38	132.45
4	A	359	APC	O3G-PG-O2G	2.09	115.63	107.80
4	C	360	APC	C2'-C1'-N9	-2.02	108.28	113.30

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	359	APC	PA-C3A-PB-O1B
4	A	359	APC	PA-C3A-PB-O2B
4	A	359	APC	PA-C3A-PB-O3B
4	A	359	APC	C5'-O5'-PA-O1A
4	B	359	APC	PA-C3A-PB-O1B
4	B	359	APC	PA-C3A-PB-O2B
4	B	359	APC	PA-C3A-PB-O3B
4	B	359	APC	C5'-O5'-PA-O1A
4	C	359	APC	PA-C3A-PB-O1B
4	C	359	APC	PA-C3A-PB-O2B
4	C	359	APC	PA-C3A-PB-O3B
4	C	359	APC	C5'-O5'-PA-C3A
4	C	360	APC	PB-C3A-PA-O1A
4	D	359	APC	PB-C3A-PA-O5'
4	C	360	APC	C5'-O5'-PA-O1A
4	D	359	APC	PB-C3A-PA-O2A

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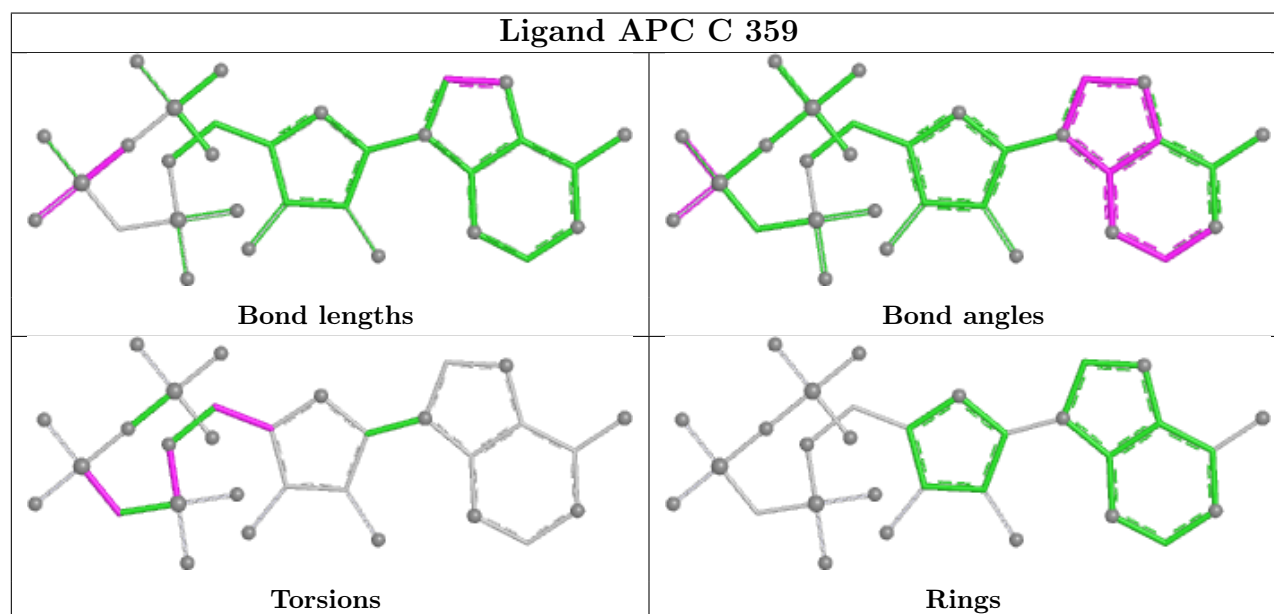
Mol	Chain	Res	Type	Atoms
4	C	359	APC	O4'-C4'-C5'-O5'
4	D	359	APC	PA-C3A-PB-O1B
4	B	359	APC	O4'-C4'-C5'-O5'

There are no ring outliers.

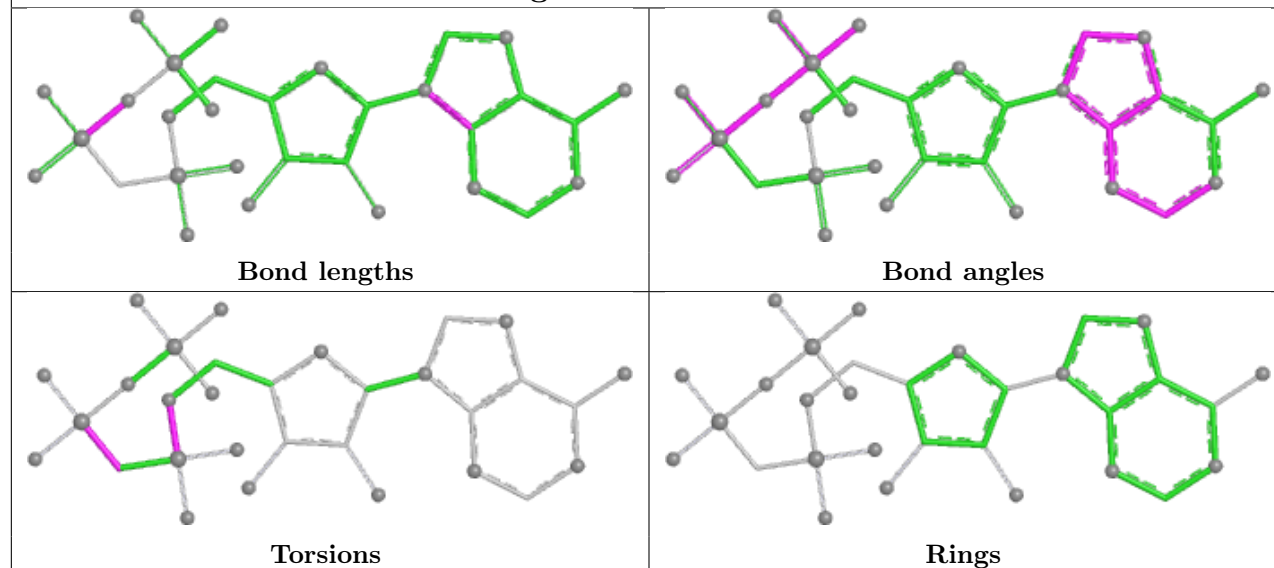
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	359	APC	1	0
4	A	359	APC	1	0

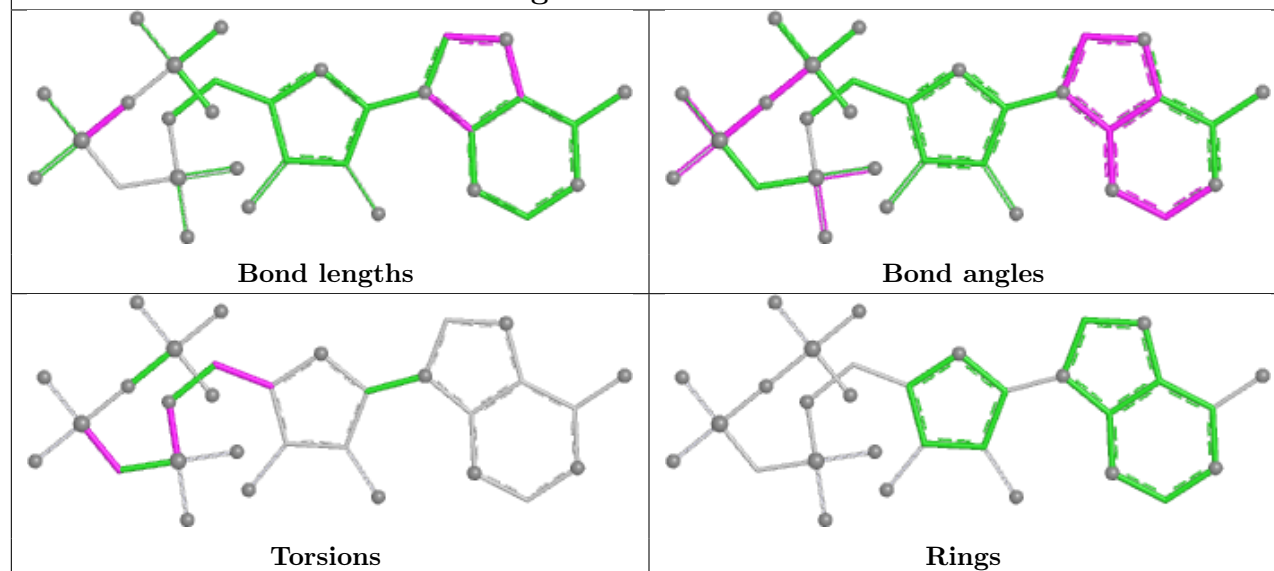
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

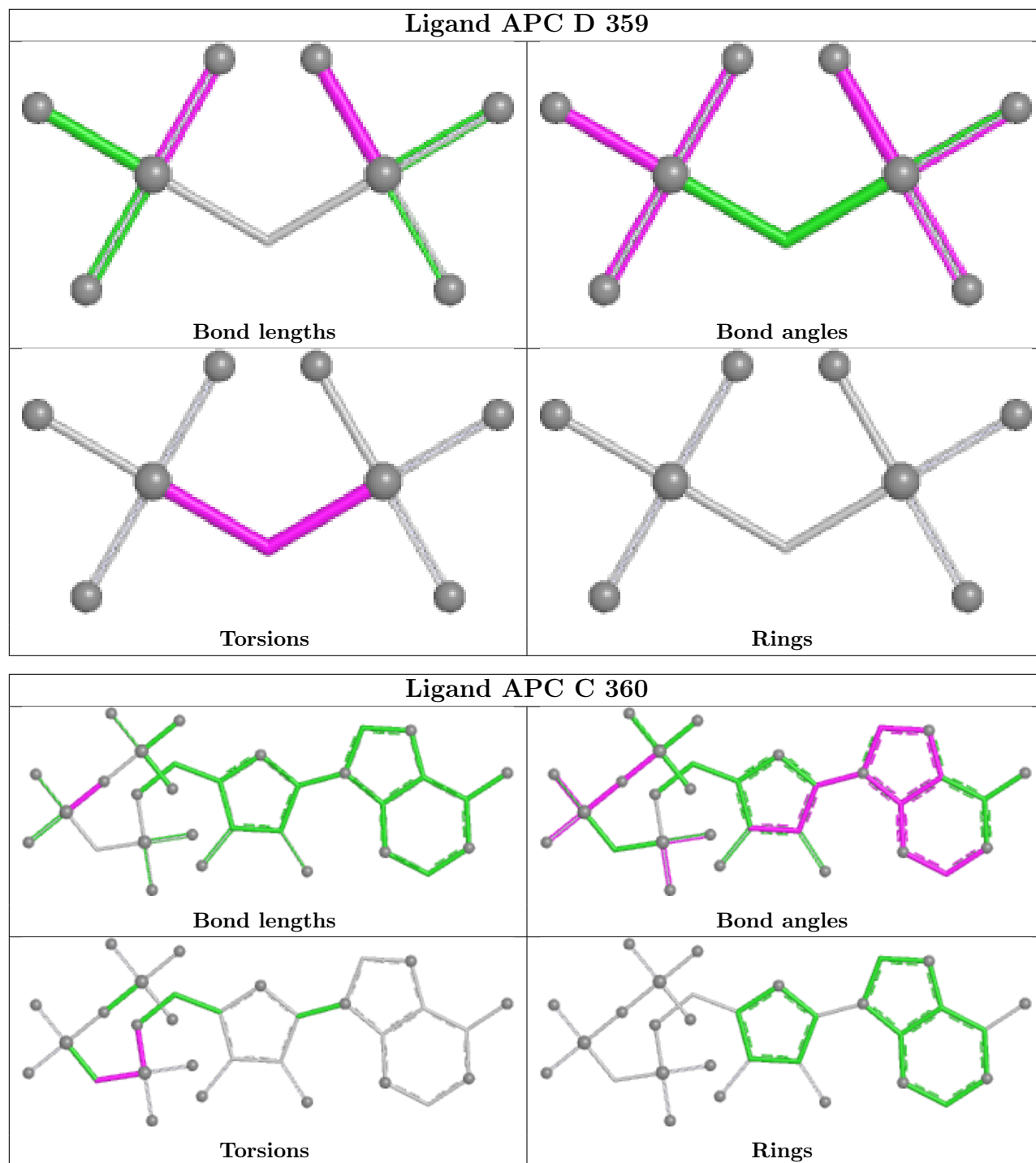


Ligand APC A 359



Ligand APC B 359





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	339/353 (96%)	0.57	11 (3%) 50 52	33, 43, 55, 62	0
1	B	336/353 (95%)	0.76	22 (6%) 25 27	31, 42, 55, 66	0
1	C	344/353 (97%)	0.48	6 (1%) 69 70	31, 42, 56, 67	0
1	D	334/353 (94%)	0.63	17 (5%) 33 35	28, 42, 56, 66	1 (0%)
2	E	0/7	-	-	-	-
2	F	0/7	-	-	-	-
2	G	6/7 (85%)	1.60	1 (16%) 4 5	64, 65, 67, 67	0
2	H	0/7	-	-	-	-
All	All	1359/1440 (94%)	0.61	57 (4%) 40 42	28, 42, 56, 67	1 (0%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	347	GLY	3.9
1	D	273[A]	GLU	3.6
1	D	342	VAL	3.6
1	C	89	ASN	3.3
1	B	1	MET	3.2
1	D	1	MET	3.2
1	D	222	TRP	3.2
1	D	197	TYR	3.1
1	D	341	PRO	3.0
1	C	87	THR	3.0
1	D	198	THR	3.0
1	B	198	THR	3.0
1	B	197	TYR	2.9
1	D	217	PHE	2.8
1	A	259	GLU	2.8
1	D	220	ILE	2.7
1	C	348	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	348	ASN	2.6
1	D	347	GLY	2.6
1	B	275	ILE	2.6
1	A	147	ASN	2.5
1	B	342	VAL	2.5
1	C	264	VAL	2.5
1	B	89	ASN	2.5
1	B	29	VAL	2.4
1	D	346	CYS	2.4
1	A	1	MET	2.4
1	A	213	ALA	2.4
1	B	263	VAL	2.4
1	D	343	CYS	2.4
1	C	341	PRO	2.3
1	D	230	ALA	2.3
1	A	332	ILE	2.3
1	D	195	ASN	2.3
1	B	217	PHE	2.2
1	A	193	ASN	2.2
1	B	199	ASP	2.2
1	B	60	ILE	2.2
1	A	195	ASN	2.2
1	B	2	ASP	2.2
1	B	273	GLU	2.2
1	A	201	HIS	2.2
1	B	338	GLY	2.1
1	B	341	PRO	2.1
1	D	345	VAL	2.1
1	B	63	LYS	2.1
1	A	275	ILE	2.1
1	B	51	TYR	2.1
1	C	39	ILE	2.1
1	D	185	ILE	2.1
2	G	7	ASN	2.1
1	B	3	TYR	2.1
1	B	258	TYR	2.1
1	B	55	LEU	2.0
1	B	164	ASP	2.0
1	D	231	ASN	2.0
1	A	87	THR	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](#)

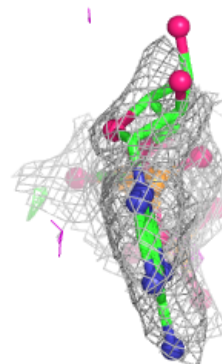
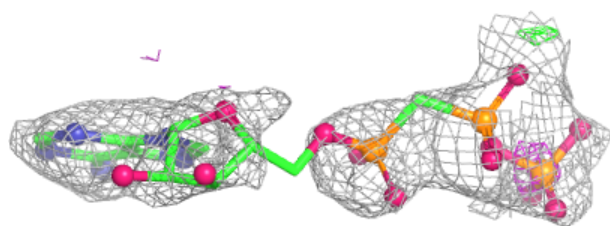
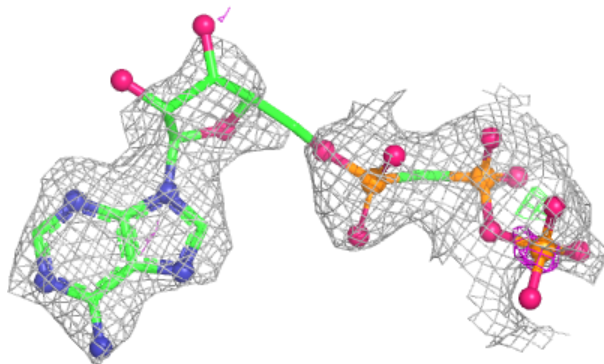
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SO4	B	360	5/5	0.66	0.15	95,95,96,96	0
4	APC	C	360	31/31	0.68	0.16	85,89,105,106	0
4	APC	B	359	31/31	0.69	0.15	81,82,94,94	0
4	APC	D	359	9/31	0.70	0.13	89,90,90,90	0
4	APC	A	359	31/31	0.81	0.11	53,55,74,74	0
4	APC	C	359	31/31	0.83	0.11	37,42,70,71	0
3	ZN	D	500	1/1	0.90	0.09	86,86,86,86	0
3	ZN	B	500	1/1	0.99	0.03	58,58,58,58	0
3	ZN	C	500	1/1	0.99	0.04	34,34,34,34	0
3	ZN	A	500	1/1	0.99	0.03	46,46,46,46	0

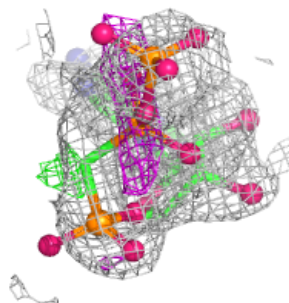
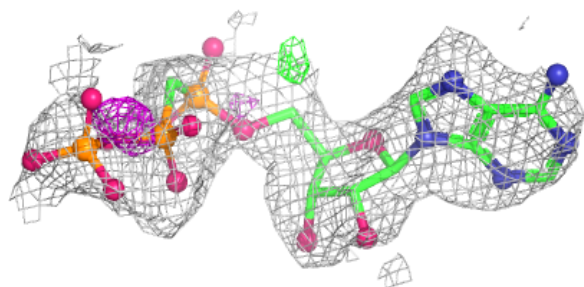
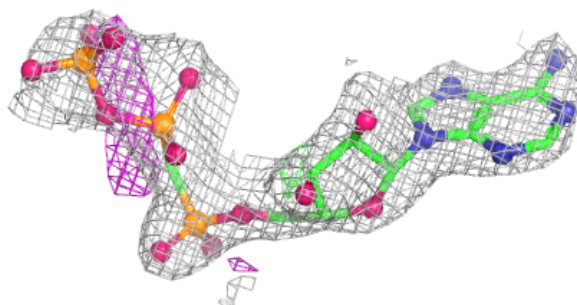
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around APC C 360:

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

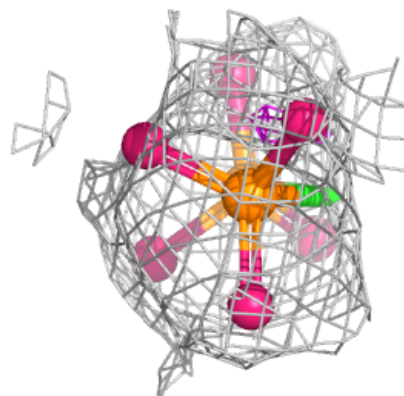
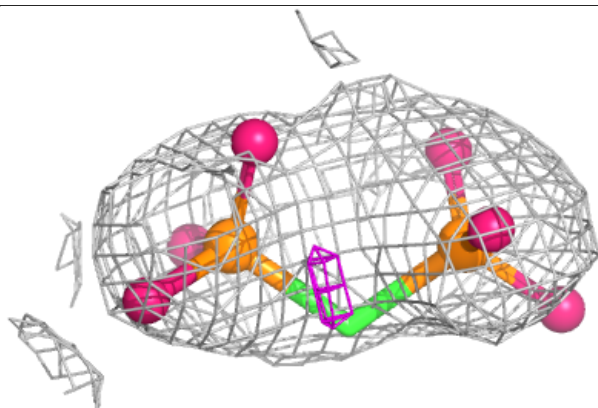
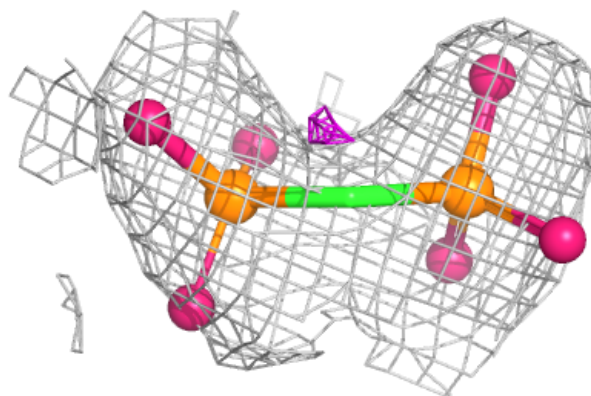
**Electron density around APC B 359:**

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

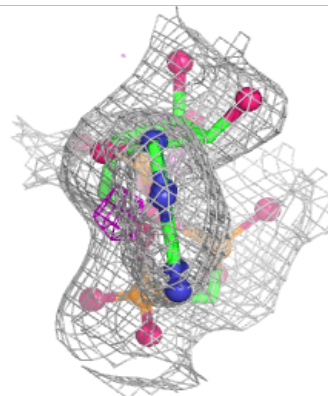
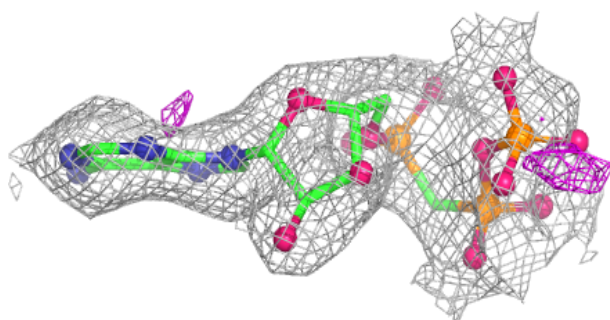
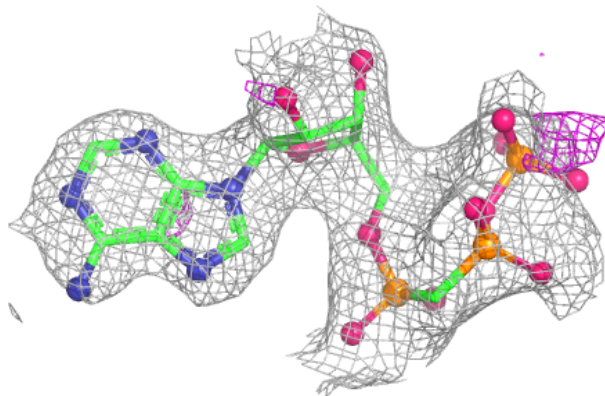


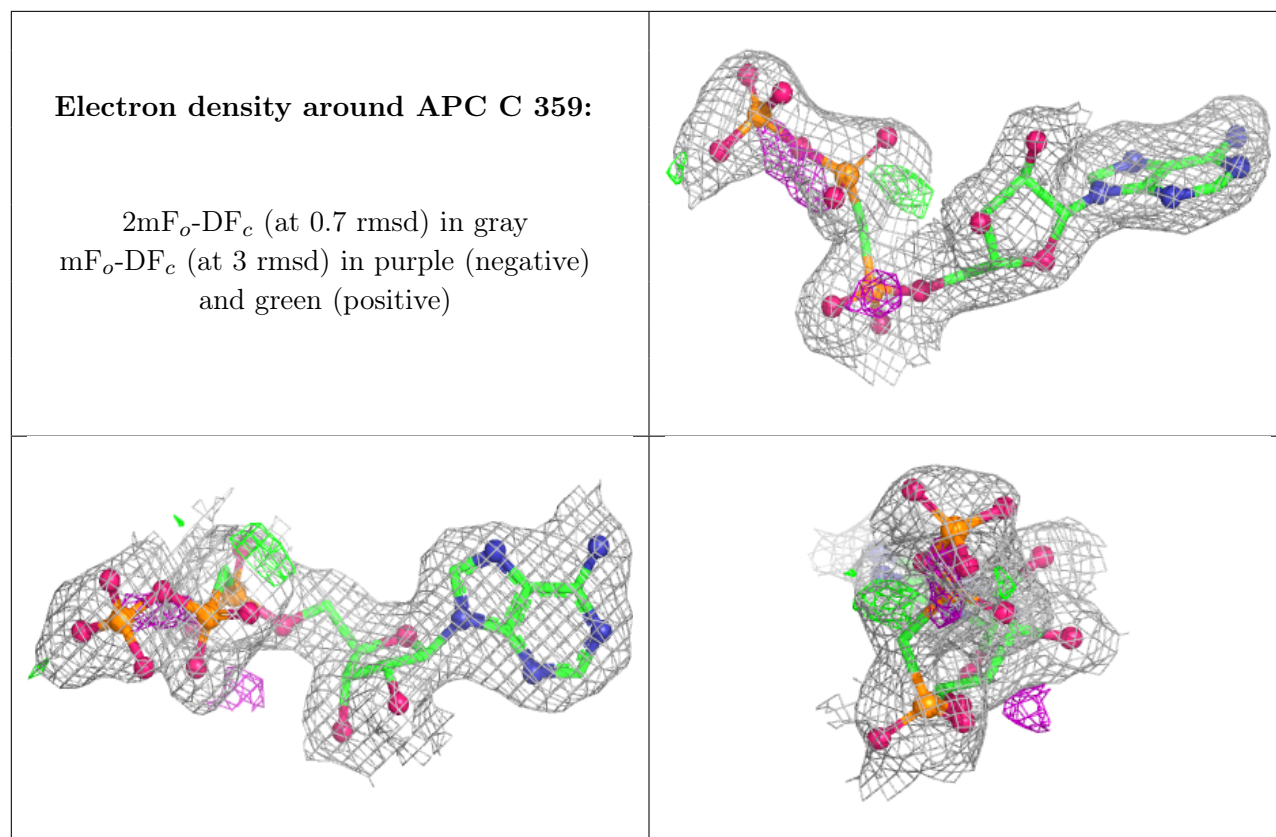
Electron density around APC D 359:

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

**Electron density around APC A 359:**

$2mF_o-DF_c$ (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.