Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 04:04 am BST

PDB ID	:	2BW7
Title	:	A novel mechanism for adenylyl cyclase inhibition from the crystal structure of its complex with catechol estrogen
Authors	:	Steegborn, C.; Litvin, T.N.; Hess, K.C.; Capper, A.B.; Taussig, R.; Buck, J.; Levin, L.R.; Wu, H.
Deposited on	:	2005-07-12
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 following versions of software and data (see references ⓘ) were used in the production of this report:

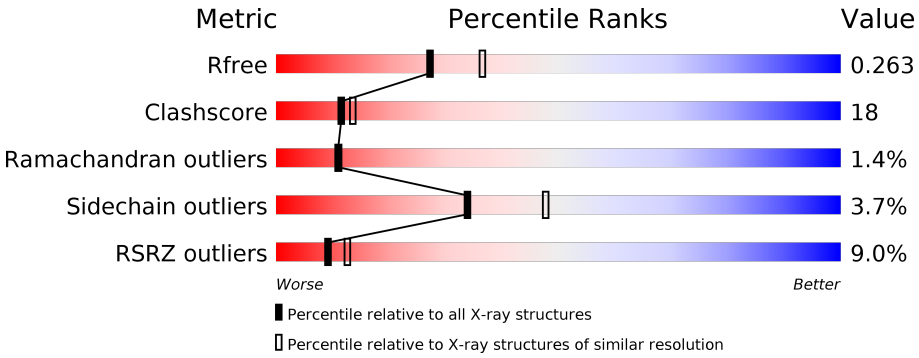
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 on 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 <=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	219	6% 62% 27% • 10%
1	B	219	9% 58% 28% • 12%
1	C	219	7% 58% 30% 11%
1	D	219	10% 58% 28% • 12%

2 Entry composition

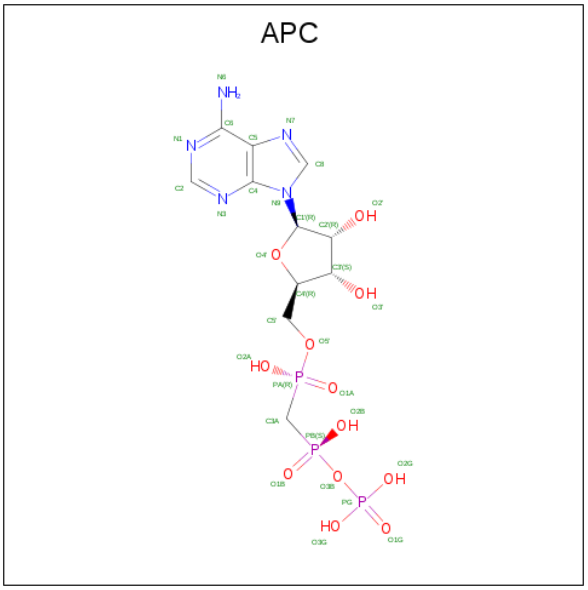
There are 6 unique types of molecules in this entry. The entry contains 6326 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ADENYLATE CYCLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	198	Total	C	N	O	S	3	0	0
			1528	958	269	288	13			
1	B	193	Total	C	N	O	S	4	0	0
			1488	935	261	279	13			
1	C	196	Total	C	N	O	S	7	0	0
			1512	949	265	285	13			
1	D	193	Total	C	N	O	S	14	0	0
			1485	934	258	281	12			

- Molecule 2 is DIPHOSPHOMETHYLPHOSPHONIC ACID ADENOSYL ESTER (three-letter code: APC) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



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

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

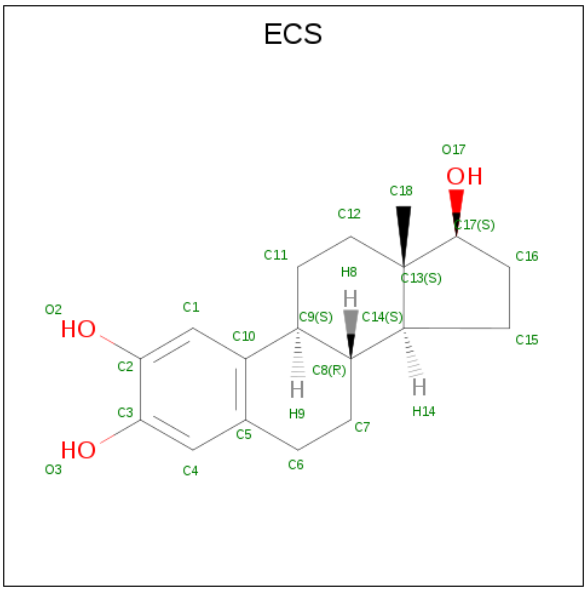
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	A	1	Total	Ca	0	0
			1	1		
4	D	1	Total	Ca	0	0
			1	1		
4	C	1	Total	Ca	0	0
			1	1		

- Molecule 5 is 2,3,17BETA-TRIHYDROXY-1,3,5(10)-ESTRATRIENE (three-letter code: ECS) (formula: $C_{18}H_{24}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 21 18 3	0	0
5	B	1	Total C O 21 18 3	0	0

- Molecule 6 is water.

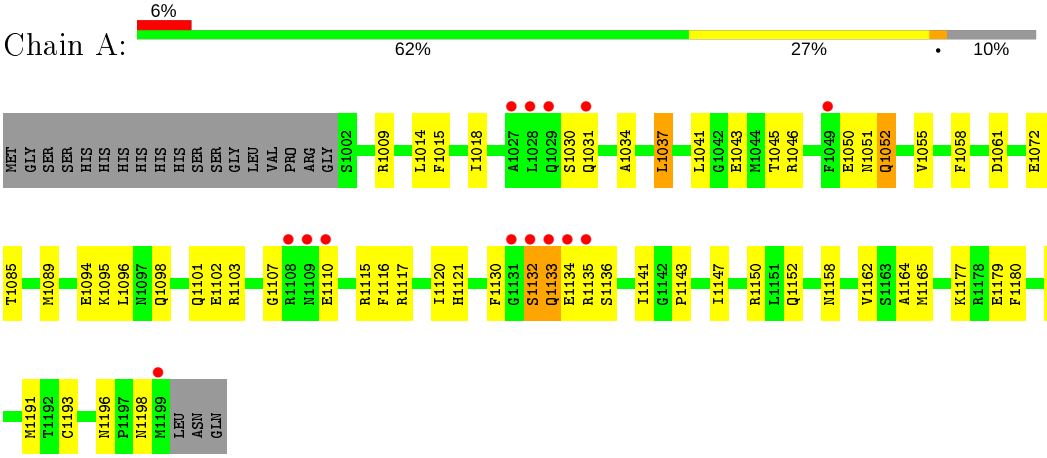
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	47	Total O 47 47	0	0
6	B	36	Total O 36 36	0	0
6	C	32	Total O 32 32	0	0
6	D	24	Total O 24 24	0	0

3 Residue-property plots (i)

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

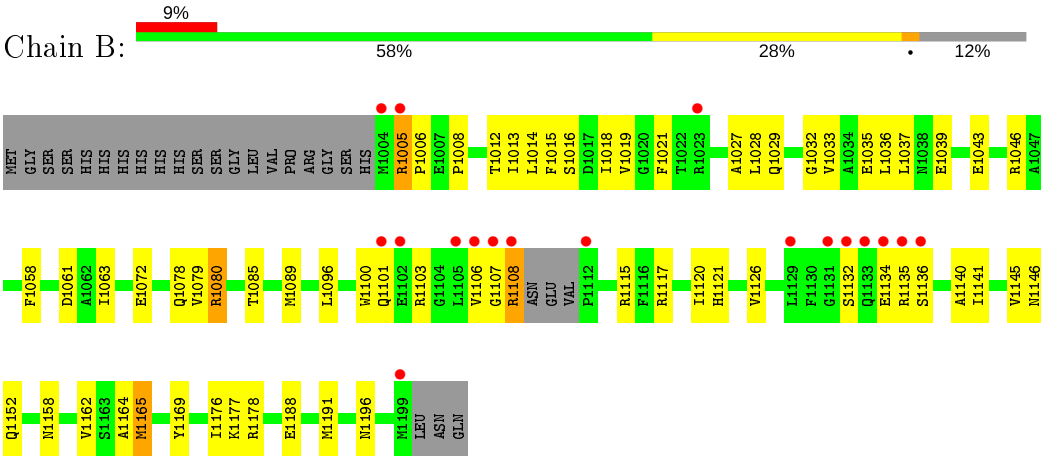
• Molecule 1: ADENYLATE CYCLASE

Chain A:



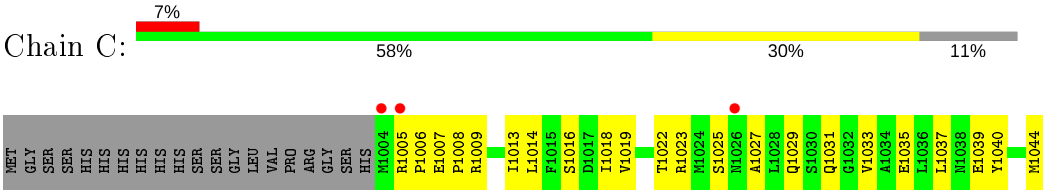
• Molecule 1: ADENYLATE CYCLASE

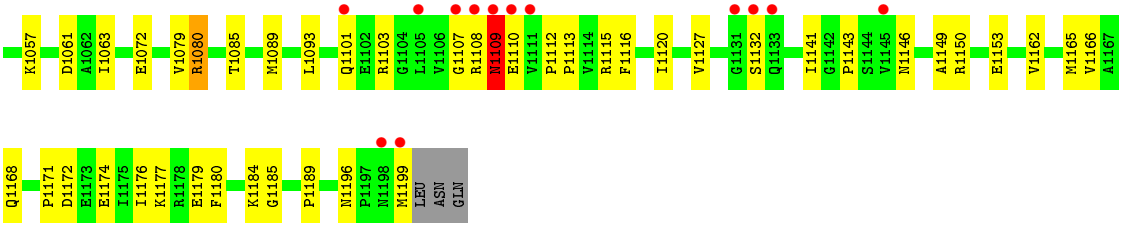
Chain B:



• Molecule 1: ADENYLATE CYCLASE

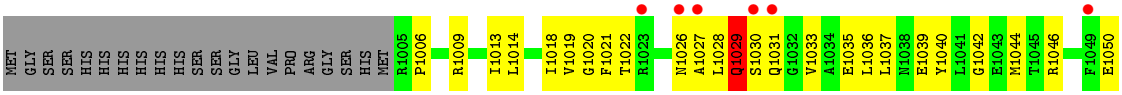
Chain C:

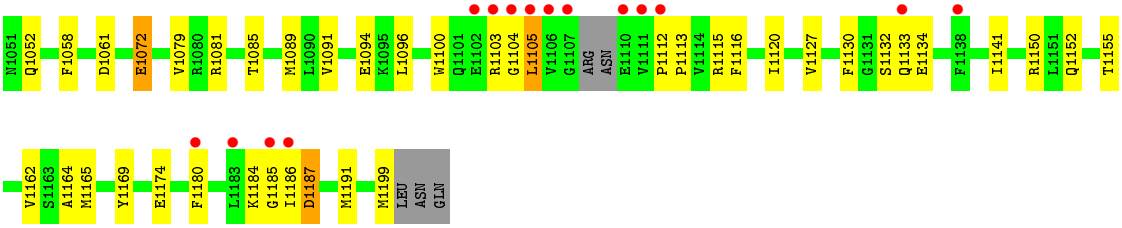




- Molecule 1: ADENYLATE CYCLASE

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	53.40Å 70.20Å 106.70Å 90.00° 96.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.30 38.25 – 2.27	Depositor EDS
% Data completeness (in resolution range)	0.9 (15.00-2.30) 91.9 (38.25-2.27)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 2.27Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.207 , 0.257 0.219 , 0.263	Depositor DCC
R_{free} test set	2451 reflections (6.98%)	wwPDB-VP
Wilson B-factor (Å^2)	28.0	Xtriage
Anisotropy	0.420	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 47.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6326	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.42% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: APC, CA, ECS, MG

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	0.29	0/1553	0.56	0/2100
1	B	0.27	0/1511	0.53	0/2040
1	C	0.26	0/1536	0.52	0/2077
1	D	0.26	0/1508	0.53	0/2039
All	All	0.27	0/6108	0.54	0/8256

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	1528	0	1532	50	0
1	B	1488	0	1499	67	0
1	C	1512	0	1520	61	0
1	D	1485	0	1491	54	0
2	A	31	0	14	6	0
2	B	31	0	14	6	0
2	C	31	0	14	0	0
2	D	31	0	14	3	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	21	0	23	2	0
5	B	21	0	23	3	0
6	A	47	0	0	5	0
6	B	36	0	0	1	0
6	C	32	0	0	2	0
6	D	24	0	0	1	0
All	All	6326	0	6144	216	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 18.

All (216) 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:1178:ARG:HH12	1:C:1168:GLN:HE21	1.14	0.95
1:B:1134:GLU:HG3	1:B:1135:ARG:H	1.26	0.95
1:A:1101:GLN:HE22	1:A:1107:GLY:HA3	1.35	0.92
1:B:1101:GLN:HE22	1:B:1107:GLY:HA3	1.35	0.92
1:C:1143:PRO:HG3	1:D:1022:THR:HG23	1.52	0.89
1:B:1134:GLU:HG3	1:B:1135:ARG:N	1.87	0.89
1:B:1120:ILE:HB	1:B:1162:VAL:HG12	1.51	0.89
1:C:1120:ILE:HB	1:C:1162:VAL:HG12	1.58	0.84
1:A:1132:SER:O	1:A:1134:GLU:N	2.10	0.82
1:C:1132:SER:HB3	1:D:1042:GLY:HA2	1.64	0.80
1:B:1178:ARG:NH1	1:C:1168:GLN:HE21	1.79	0.80
1:A:1183:LEU:HB2	1:A:1186:ILE:HD12	1.67	0.76
1:A:1101:GLN:NE2	1:A:1107:GLY:HA3	2.00	0.76
1:B:1080:ARG:HG2	1:B:1080:ARG:HH11	1.49	0.75
1:C:1046:ARG:HD3	1:C:1050:GLU:OE2	1.88	0.74
1:A:1141:ILE:HG23	2:B:2200:APC:H8	1.69	0.73
1:B:1146:ASN:O	1:B:1150:ARG:HG2	1.89	0.73
1:A:1030:SER:CB	1:B:1008:PRO:HG3	2.19	0.72
1:A:1135:ARG:HG3	1:B:1058:PHE:CE1	2.24	0.72
1:B:1005:ARG:HD2	1:B:1006:PRO:HD2	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1085:THR:O	1:B:1089:MET:HG3	1.90	0.72
1:C:1107:GLY:O	1:C:1108:ARG:HG3	1.90	0.72
1:C:1150:ARG:HD2	1:C:1184:LYS:O	1.89	0.71
1:B:1117:ARG:HB2	1:B:1152:GLN:HE21	1.55	0.71
1:D:1120:ILE:HB	1:D:1162:VAL:HG12	1.71	0.69
1:A:1147:ILE:HG12	1:A:1186:ILE:HD13	1.74	0.69
1:C:1176:ILE:HD11	1:C:1196:ASN:HA	1.75	0.68
1:C:1101:GLN:OE1	1:C:1107:GLY:HA3	1.95	0.66
1:C:1019:VAL:HG12	1:C:1115:ARG:O	1.95	0.66
1:A:1018:ILE:HB	1:A:1061:ASP:OD2	1.95	0.66
1:B:1178:ARG:HH22	1:C:1168:GLN:NE2	1.93	0.66
1:D:1132:SER:C	1:D:1134:GLU:H	1.99	0.65
1:C:1146:ASN:HD21	2:D:2200:APC:H3A1	1.62	0.65
1:B:1019:VAL:HG12	1:B:1115:ARG:O	1.98	0.64
1:C:1184:LYS:HD3	1:C:1185:GLY:N	2.14	0.63
1:D:1112:PRO:HB2	1:D:1113:PRO:HD2	1.80	0.63
1:B:1101:GLN:NE2	1:B:1107:GLY:HA3	2.13	0.61
1:D:1022:THR:HG21	6:D:2004:HOH:O	2.00	0.61
1:D:1018:ILE:HB	1:D:1061:ASP:OD2	2.00	0.61
1:D:1013:ILE:HD12	1:D:1013:ILE:N	2.16	0.61
1:A:1115:ARG:HA	1:A:1158:ASN:HD21	1.66	0.60
1:B:1176:ILE:HD11	1:B:1196:ASN:HA	1.83	0.60
1:C:1085:THR:O	1:C:1089:MET:HG3	2.01	0.60
1:B:1146:ASN:HD21	1:B:1150:ARG:HD2	1.67	0.59
1:A:1134:GLU:HG3	1:A:1135:ARG:H	1.68	0.59
1:C:1115:ARG:HH11	1:C:1115:ARG:HG3	1.68	0.58
1:A:1046:ARG:O	1:A:1050:GLU:HG3	2.03	0.58
1:A:1043:GLU:HG3	1:A:1096:LEU:HD21	1.85	0.58
1:A:1164:ALA:HB2	1:A:1191:MET:HB3	1.86	0.58
1:C:1177:LYS:HE3	1:C:1179:GLU:OE2	2.03	0.58
1:A:1030:SER:OG	1:B:1008:PRO:HG3	2.04	0.57
1:C:1101:GLN:HE21	1:C:1108:ARG:CZ	2.17	0.57
1:D:1019:VAL:HG12	1:D:1115:ARG:O	2.03	0.57
1:D:1152:GLN:O	1:D:1155:THR:HG22	2.04	0.57
1:B:1013:ILE:HD13	1:B:1145:VAL:HG22	1.84	0.57
1:C:1007:GLU:OE2	1:C:1009:ARG:HD2	2.04	0.57
1:A:1117:ARG:HD2	1:A:1152:GLN:HE21	1.70	0.57
1:C:1013:ILE:HD12	1:C:1013:ILE:N	2.19	0.57
1:B:1018:ILE:HB	1:B:1061:ASP:OD2	2.05	0.57
1:A:1133:GLN:O	1:A:1133:GLN:HG3	2.05	0.57
1:A:1094:GLU:O	1:A:1098:GLN:HG3	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1021:PHE:HZ	1:D:1033:VAL:HG13	1.69	0.56
1:B:1005:ARG:HG3	1:B:1005:ARG:HH11	1.69	0.56
1:C:1014:LEU:C	1:C:1014:LEU:HD23	2.26	0.56
1:B:1080:ARG:NH1	1:B:1080:ARG:HG2	2.19	0.56
1:B:1149:ALA:O	1:B:1152:GLN:HB3	2.06	0.56
1:A:1120:ILE:HB	1:A:1162:VAL:HG12	1.88	0.56
1:C:1037:LEU:CD1	1:D:1141:ILE:HD13	2.35	0.56
1:A:1034:ALA:HB2	1:B:1126:VAL:HG11	1.89	0.55
1:B:1043:GLU:HG3	1:B:1096:LEU:HD21	1.88	0.55
1:D:1150:ARG:HD2	1:D:1184:LYS:O	2.06	0.55
1:A:1141:ILE:HD13	2:B:2200:APC:N7	2.22	0.55
1:B:1117:ARG:HH11	1:B:1152:GLN:NE2	2.05	0.55
1:C:1103:ARG:HD3	6:C:2012:HOH:O	2.06	0.54
1:A:1009:ARG:HD3	6:A:2004:HOH:O	2.06	0.54
1:C:1057:LYS:HE2	1:D:1058:PHE:O	2.07	0.54
1:B:1165:MET:N	1:B:1165:MET:SD	2.81	0.54
1:A:1018:ILE:HD12	1:A:1061:ASP:HB2	1.90	0.54
1:A:1095:LYS:HA	1:A:1098:GLN:NE2	2.23	0.54
1:C:1146:ASN:ND2	2:D:2200:APC:H3A1	2.22	0.54
1:C:1115:ARG:HG2	6:C:2013:HOH:O	2.08	0.53
1:C:1035:GLU:O	1:C:1039:GLU:HG3	2.08	0.53
1:D:1174:GLU:OE2	1:D:1199:MET:HA	2.08	0.53
1:C:1040:TYR:O	1:C:1044:MET:HG2	2.08	0.52
1:A:1130:PHE:O	1:A:1136:SER:HA	2.09	0.52
1:D:1036:LEU:HD23	1:D:1036:LEU:C	2.29	0.52
1:D:1028:LEU:C	1:D:1029:GLN:HG2	2.29	0.52
1:C:1177:LYS:HG2	1:C:1179:GLU:HG3	1.92	0.52
1:D:1006:PRO:HA	1:D:1127:VAL:O	2.09	0.52
2:A:2200:APC:C2	1:B:1145:VAL:HG11	2.40	0.52
1:C:1176:ILE:CD1	1:C:1196:ASN:HA	2.40	0.51
1:A:1037:LEU:HD22	1:A:1041:LEU:HG	1.92	0.51
1:C:1141:ILE:HD13	1:D:1037:LEU:CD1	2.40	0.51
1:C:1029:GLN:O	1:C:1033:VAL:HG23	2.11	0.51
1:A:1085:THR:O	1:A:1089:MET:HG3	2.11	0.51
1:B:1079:VAL:HG21	1:B:1169:TYR:HD1	1.75	0.51
1:B:1177:LYS:HE3	6:B:2022:HOH:O	2.10	0.51
1:C:1165:MET:O	1:C:1168:GLN:HB2	2.11	0.51
1:D:1046:ARG:HG2	1:D:1050:GLU:OE2	2.11	0.50
1:A:1180:PHE:HB2	1:A:1191:MET:HE1	1.94	0.50
1:D:1021:PHE:CZ	1:D:1033:VAL:HG13	2.47	0.50
1:B:1178:ARG:NH2	1:C:1168:GLN:NE2	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1191:MET:HG3	6:A:2045:HOH:O	2.11	0.49
1:D:1014:LEU:HD23	1:D:1014:LEU:C	2.33	0.49
1:B:1146:ASN:HD22	5:B:2203:ECS:H17	1.76	0.49
1:D:1052:GLN:HG3	1:D:1081:ARG:NH1	2.27	0.49
1:B:1100:TRP:HB3	1:B:1106:VAL:HG22	1.95	0.49
1:A:1177:LYS:O	1:A:1193:CYS:HA	2.13	0.49
5:A:2203:ECS:H161	2:B:2200:APC:H2'	1.94	0.49
1:B:1134:GLU:CG	1:B:1135:ARG:H	2.12	0.49
1:B:1164:ALA:HB2	1:B:1191:MET:HG2	1.94	0.49
1:A:1051:ASN:C	1:A:1052:GLN:HG2	2.34	0.49
1:B:1048:VAL:HG22	1:B:1085:THR:HG21	1.95	0.48
1:C:1184:LYS:HD3	1:C:1185:GLY:H	1.78	0.48
1:D:1164:ALA:HB2	1:D:1191:MET:HB3	1.95	0.48
1:B:1117:ARG:HH11	1:B:1152:GLN:HE22	1.60	0.48
1:B:1165:MET:HA	1:C:1165:MET:HE1	1.94	0.48
1:B:1146:ASN:ND2	1:B:1150:ARG:HD2	2.28	0.48
1:A:1143:PRO:HD2	6:A:2031:HOH:O	2.14	0.48
1:C:1149:ALA:O	1:C:1153:GLU:HG3	2.13	0.48
1:B:1117:ARG:HH22	2:B:2200:APC:PB	2.37	0.47
1:B:1035:GLU:O	1:B:1039:GLU:HG3	2.15	0.47
1:D:1079:VAL:HG21	1:D:1169:TYR:CD1	2.49	0.47
1:A:1116:PHE:H	1:A:1158:ASN:ND2	2.12	0.47
2:A:2200:APC:N7	1:B:1140:ALA:O	2.48	0.47
1:C:1018:ILE:HB	1:C:1061:ASP:OD2	2.14	0.47
1:C:1016:SER:HB3	1:C:1063:ILE:HB	1.97	0.47
1:B:1079:VAL:HG21	1:B:1169:TYR:CD1	2.50	0.47
1:D:1028:LEU:O	1:D:1029:GLN:HG2	2.15	0.47
1:C:1180:PHE:CZ	1:C:1189:PRO:HB2	2.50	0.46
1:A:1045:THR:HG21	1:A:1058:PHE:HZ	1.80	0.46
1:D:1132:SER:C	1:D:1134:GLU:N	2.67	0.46
2:A:2200:APC:N3	5:B:2203:ECS:H161	2.30	0.46
1:D:1028:LEU:HD11	1:D:1105:LEU:HD22	1.97	0.46
1:C:1023:ARG:NH1	1:D:1187:ASP:OD2	2.48	0.46
1:D:1052:GLN:HG3	1:D:1081:ARG:CZ	2.46	0.46
1:D:1091:VAL:O	1:D:1094:GLU:HG2	2.16	0.46
1:D:1031:GLN:HE22	1:D:1035:GLU:HG3	1.81	0.46
1:C:1171:PRO:HB2	1:C:1174:GLU:HG3	1.98	0.46
1:B:1021:PHE:HE1	1:B:1036:LEU:HD22	1.82	0.45
1:A:1045:THR:HG22	1:A:1055:VAL:HG21	1.98	0.45
1:D:1026:ASN:O	1:D:1027:ALA:HB3	2.16	0.45
1:D:1009:ARG:NH2	1:D:1072:GLU:OE1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1101:GLN:C	1:A:1103:ARG:H	2.20	0.45
1:B:1178:ARG:CZ	1:C:1168:GLN:HE21	2.29	0.45
1:C:1033:VAL:O	1:C:1037:LEU:HB2	2.17	0.45
1:A:1179:GLU:O	1:A:1191:MET:HE3	2.17	0.45
1:D:1130:PHE:CE2	1:D:1141:ILE:HD12	2.52	0.45
1:C:1112:PRO:HB2	1:C:1113:PRO:HD2	1.98	0.44
1:D:1046:ARG:HG3	1:D:1046:ARG:HH11	1.82	0.44
1:D:1096:LEU:HB3	1:D:1100:TRP:CH2	2.52	0.44
1:D:1115:ARG:HH11	1:D:1115:ARG:HG3	1.82	0.44
1:D:1185:GLY:O	1:D:1186:ILE:HD13	2.18	0.44
1:D:1019:VAL:CG1	1:D:1115:ARG:HB2	2.47	0.44
1:A:1183:LEU:CB	1:A:1186:ILE:HD12	2.43	0.44
2:A:2200:APC:H2'	5:B:2203:ECS:H161	1.99	0.44
1:C:1079:VAL:HG13	1:C:1166:VAL:HG13	1.99	0.44
1:A:1052:GLN:HG3	1:A:1081:ARG:CZ	2.48	0.44
1:B:1080:ARG:NH1	1:B:1080:ARG:CG	2.80	0.44
1:D:1079:VAL:HG21	1:D:1169:TYR:CE1	2.52	0.44
1:A:1095:LYS:HA	1:A:1098:GLN:HE21	1.83	0.44
1:C:1008:PRO:HD3	1:D:1030:SER:CB	2.48	0.43
1:D:1018:ILE:HD11	1:D:1040:TYR:CD2	2.53	0.43
1:B:1176:ILE:CD1	1:B:1196:ASN:HA	2.48	0.43
1:C:1080:ARG:HG3	1:C:1080:ARG:NH1	2.32	0.43
1:B:1117:ARG:NH1	1:B:1152:GLN:HE22	2.16	0.43
1:C:1006:PRO:HA	1:C:1127:VAL:O	2.18	0.43
1:C:1177:LYS:HG2	1:C:1179:GLU:CG	2.48	0.43
1:A:1014:LEU:C	1:A:1014:LEU:HD23	2.38	0.43
1:A:1121:HIS:HE1	1:A:1165:MET:CE	2.31	0.43
1:B:1132:SER:O	1:B:1136:SER:HB3	2.19	0.43
1:C:1109:ASN:O	1:C:1110:GLU:HB3	2.19	0.43
1:D:1033:VAL:O	1:D:1037:LEU:HB2	2.19	0.43
1:A:1141:ILE:HA	2:B:2200:APC:C8	2.49	0.43
1:C:1019:VAL:CG1	1:C:1115:ARG:HB2	2.49	0.43
1:C:1029:GLN:HB2	1:C:1031:GLN:HE21	1.84	0.43
1:D:1085:THR:O	1:D:1089:MET:HG3	2.19	0.43
1:B:1146:ASN:O	1:B:1150:ARG:CG	2.64	0.43
1:C:1008:PRO:HD3	1:D:1030:SER:OG	2.19	0.43
1:C:1005:ARG:HH11	1:C:1005:ARG:HG2	1.83	0.43
1:C:1022:THR:O	1:C:1025:SER:HB2	2.19	0.43
1:C:1101:GLN:NE2	1:C:1108:ARG:CZ	2.81	0.43
2:A:2200:APC:C8	1:B:1141:ILE:HA	2.49	0.42
2:A:2200:APC:N7	1:B:1141:ILE:HD13	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1005:ARG:CG	1:B:1005:ARG:HH11	2.32	0.42
1:B:1108:ARG:NH1	1:B:1108:ARG:HG2	2.33	0.42
1:D:1116:PHE:CD1	1:D:1116:PHE:C	2.92	0.42
1:A:1073:MET:CE	1:A:1081:ARG:HH11	2.32	0.42
1:D:1020:GLY:N	2:D:2200:APC:O1G	2.36	0.42
1:B:1028:LEU:O	1:B:1029:GLN:HB2	2.19	0.42
1:D:1052:GLN:HB2	1:D:1081:ARG:HD3	2.02	0.42
1:D:1112:PRO:CB	1:D:1113:PRO:HD2	2.47	0.42
1:D:1035:GLU:O	1:D:1039:GLU:HG3	2.18	0.42
1:A:1135:ARG:HG3	1:B:1058:PHE:CZ	2.54	0.42
5:A:2203:ECS:H161	2:B:2200:APC:N3	2.35	0.42
1:D:1040:TYR:O	1:D:1044:MET:HG2	2.20	0.42
1:A:1196:ASN:C	1:A:1198:ASN:H	2.22	0.42
1:B:1014:LEU:HD23	1:B:1014:LEU:C	2.40	0.42
1:C:1093:LEU:HD22	1:C:1116:PHE:CD2	2.54	0.42
1:B:1033:VAL:O	1:B:1037:LEU:HB2	2.20	0.42
1:C:1110:GLU:OE1	1:C:1110:GLU:HA	2.20	0.42
1:D:1100:TRP:HA	1:D:1103:ARG:HB2	2.01	0.42
1:B:1012:THR:OG1	1:B:1078:GLN:HB3	2.19	0.41
1:B:1121:HIS:HE1	1:B:1165:MET:CE	2.33	0.41
1:A:1009:ARG:HB2	6:A:2004:HOH:O	2.20	0.41
1:C:1019:VAL:HG11	1:C:1115:ARG:HB2	2.02	0.41
1:B:1016:SER:OG	1:B:1063:ILE:HB	2.20	0.41
1:A:1030:SER:HB3	1:B:1008:PRO:HG3	2.01	0.41
1:B:1046:ARG:HG3	1:B:1046:ARG:HH11	1.84	0.41
1:C:1174:GLU:OE2	1:C:1199:MET:HG3	2.21	0.41
1:A:1184:LYS:HG2	1:A:1185:GLY:N	2.36	0.41
1:B:1028:LEU:HB3	1:B:1032:GLY:HA3	2.03	0.41
1:B:1115:ARG:HA	1:B:1158:ASN:HD21	1.85	0.41
1:D:1104:GLY:O	1:D:1105:LEU:C	2.58	0.41
1:B:1005:ARG:CZ	1:B:1005:ARG:HB3	2.51	0.40
1:A:1081:ARG:HG2	6:A:2013:HOH:O	2.20	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	196/219 (90%)	187 (95%)	7 (4%)	2 (1%)	15 17
1	B	189/219 (86%)	173 (92%)	14 (7%)	2 (1%)	14 15
1	C	194/219 (89%)	181 (93%)	10 (5%)	3 (2%)	10 10
1	D	189/219 (86%)	178 (94%)	7 (4%)	4 (2%)	7 5
All	All	768/876 (88%)	719 (94%)	38 (5%)	11 (1%)	11 11

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1133	GLN
1	C	1027	ALA
1	D	1029	GLN
1	D	1105	LEU
1	A	1102	GLU
1	B	1027	ALA
1	B	1103	ARG
1	C	1109	ASN
1	D	1133	GLN
1	D	1187	ASP
1	C	1172	ASP

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	165/183 (90%)	157 (95%)	8 (5%)	25 36
1	B	160/183 (87%)	151 (94%)	9 (6%)	21 29
1	C	163/183 (89%)	160 (98%)	3 (2%)	59 75
1	D	160/183 (87%)	156 (98%)	4 (2%)	47 65
All	All	648/732 (88%)	624 (96%)	24 (4%)	34 48

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1015	PHE
1	A	1031	GLN
1	A	1037	LEU
1	A	1052	GLN
1	A	1072	GLU
1	A	1110	GLU
1	A	1132	SER
1	A	1150	ARG
1	B	1005	ARG
1	B	1015	PHE
1	B	1052	GLN
1	B	1072	GLU
1	B	1080	ARG
1	B	1108	ARG
1	B	1150	ARG
1	B	1165	MET
1	B	1188	GLU
1	C	1072	GLU
1	C	1080	ARG
1	C	1109	ASN
1	D	1029	GLN
1	D	1072	GLU
1	D	1165	MET
1	D	1180	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1026	ASN
1	A	1098	GLN
1	A	1101	GLN
1	A	1109	ASN
1	A	1122	GLN
1	A	1152	GLN
1	A	1158	ASN
1	B	1026	ASN
1	B	1101	GLN
1	B	1122	GLN
1	B	1146	ASN
1	B	1152	GLN
1	B	1158	ASN

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Mol	Chain	Res	Type
1	C	1026	ASN
1	C	1031	GLN
1	C	1101	GLN
1	C	1146	ASN
1	C	1152	GLN
1	C	1158	ASN
1	C	1168	GLN
1	D	1031	GLN
1	D	1088	GLN
1	D	1152	GLN
1	D	1158	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 14 ligands modelled in this entry, 8 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	$\#\|Z\| > 2$
2	APC	D	2200	3,4	27,33,33	1.62	5 (18%)	31,52,52	1.35	5 (16%)
2	APC	C	2200	3,4	27,33,33	1.54	4 (14%)	31,52,52	1.56	8 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	APC	A	2200	3,4	27,33,33	2.09	7 (25%)	31,52,52	1.49	3 (9%)
5	ECS	B	2203	3	24,24,24	3.08	14 (58%)	38,38,38	1.13	3 (7%)
5	ECS	A	2203	3	24,24,24	3.05	14 (58%)	38,38,38	1.12	2 (5%)
2	APC	B	2200	3,4	27,33,33	2.46	9 (33%)	31,52,52	1.55	3 (9%)

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	APC	D	2200	3,4	-	8/15/38/38	0/3/3/3
2	APC	C	2200	3,4	-	10/15/38/38	0/3/3/3
2	APC	A	2200	3,4	-	7/15/38/38	0/3/3/3
5	ECS	B	2203	3	-	-	0/4/4/4
5	ECS	A	2203	3	-	-	0/4/4/4
2	APC	B	2200	3,4	-	7/15/38/38	0/3/3/3

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2200	APC	O4'-C1'	6.26	1.49	1.41
2	B	2200	APC	PA-O5'	6.04	1.66	1.57
5	A	2203	ECS	C5-C10	6.03	1.49	1.40
5	B	2203	ECS	C5-C10	5.85	1.49	1.40
5	A	2203	ECS	C9-C8	5.77	1.61	1.54
5	B	2203	ECS	C9-C8	5.65	1.60	1.54
2	A	2200	APC	C2-N3	5.29	1.40	1.32
2	A	2200	APC	O4'-C1'	5.14	1.48	1.41
2	B	2200	APC	C2-N3	5.09	1.40	1.32
2	A	2200	APC	PA-O5'	4.70	1.64	1.57
5	A	2203	ECS	C1-C10	4.44	1.47	1.39
5	B	2203	ECS	C1-C10	4.41	1.47	1.39
2	C	2200	APC	O4'-C1'	4.17	1.46	1.41
2	D	2200	APC	O4'-C1'	4.04	1.46	1.41
5	B	2203	ECS	C4-C3	4.02	1.44	1.38
5	A	2203	ECS	C4-C3	3.97	1.44	1.38
5	B	2203	ECS	C4-C5	3.87	1.46	1.39
5	B	2203	ECS	C10-C9	3.79	1.57	1.52
5	B	2203	ECS	C1-C2	3.76	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2203	ECS	C10-C9	3.75	1.57	1.52
2	D	2200	APC	PA-O1A	3.73	1.60	1.51
2	D	2200	APC	C5'-C4'	3.62	1.62	1.51
5	A	2203	ECS	C4-C5	3.62	1.45	1.39
5	B	2203	ECS	C8-C14	3.53	1.60	1.53
5	A	2203	ECS	C8-C14	3.50	1.60	1.53
5	A	2203	ECS	C1-C2	3.49	1.43	1.38
5	A	2203	ECS	C18-C13	3.42	1.60	1.54
5	B	2203	ECS	C18-C13	3.41	1.60	1.54
5	B	2203	ECS	C13-C14	3.38	1.61	1.55
5	A	2203	ECS	C13-C14	3.24	1.61	1.55
2	B	2200	APC	C5'-C4'	3.20	1.61	1.51
2	D	2200	APC	C2-N3	3.15	1.37	1.32
5	B	2203	ECS	C11-C9	3.13	1.58	1.53
5	A	2203	ECS	C11-C9	3.08	1.58	1.53
2	A	2200	APC	PB-O3B	3.04	1.61	1.58
2	B	2200	APC	PB-O3B	3.00	1.61	1.58
2	C	2200	APC	PA-O1A	2.98	1.58	1.51
2	C	2200	APC	PB-O3B	2.96	1.61	1.58
2	B	2200	APC	C8-N7	-2.88	1.29	1.34
2	C	2200	APC	C2-N3	2.83	1.36	1.32
5	B	2203	ECS	C6-C5	2.75	1.55	1.51
5	A	2203	ECS	C6-C5	2.68	1.55	1.51
5	A	2203	ECS	C7-C6	2.66	1.57	1.52
2	A	2200	APC	C8-N7	-2.64	1.30	1.34
5	A	2203	ECS	C3-C2	2.64	1.44	1.40
5	B	2203	ECS	C3-C2	2.61	1.44	1.40
5	B	2203	ECS	C7-C6	2.53	1.57	1.52
2	B	2200	APC	C2'-C1'	-2.39	1.50	1.53
2	A	2200	APC	C2'-C1'	-2.38	1.50	1.53
2	B	2200	APC	C2-N1	2.38	1.38	1.33
2	B	2200	APC	O3'-C3'	2.35	1.48	1.43
2	D	2200	APC	C8-N7	-2.02	1.31	1.34
2	A	2200	APC	C2-N1	2.00	1.37	1.33

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2200	APC	C1'-N9-C4	6.29	137.70	126.64
2	A	2200	APC	C1'-N9-C4	5.68	136.62	126.64
2	D	2200	APC	O2B-PB-C3A	3.41	120.52	106.58
2	D	2200	APC	O3G-PG-O3B	3.30	115.70	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2200	APC	O5'-C5'-C4'	3.25	120.19	108.99
2	C	2200	APC	O1A-PA-C3A	3.23	117.62	109.07
2	C	2200	APC	O2B-PB-C3A	3.16	119.51	106.58
2	C	2200	APC	PG-O3B-PB	-3.08	121.76	132.62
2	A	2200	APC	C4-C5-N7	3.04	112.56	109.40
2	B	2200	APC	C4-C5-N7	3.03	112.56	109.40
2	D	2200	APC	O1A-PA-C3A	2.80	116.48	109.07
5	B	2203	ECS	C15-C14-C13	-2.75	100.53	103.84
5	A	2203	ECS	C15-C14-C13	-2.66	100.64	103.84
5	B	2203	ECS	C11-C9-C8	-2.61	107.88	111.39
5	A	2203	ECS	C11-C9-C8	-2.51	108.01	111.39
2	C	2200	APC	C4-C5-N7	2.45	111.95	109.40
2	B	2200	APC	PG-O3B-PB	-2.44	124.03	132.62
2	C	2200	APC	O3G-PG-O3B	2.39	112.66	104.64
2	D	2200	APC	C4-C5-N7	2.38	111.88	109.40
2	C	2200	APC	C5'-C4'-C3'	-2.37	106.29	115.18
2	C	2200	APC	O4'-C4'-C3'	2.21	109.48	105.11
2	D	2200	APC	O4'-C1'-C2'	-2.06	103.92	106.93
5	B	2203	ECS	C6-C7-C8	2.05	114.01	110.59
2	A	2200	APC	O4'-C4'-C5'	2.04	116.10	109.37

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	2200	APC	PA-C3A-PB-O1B
2	D	2200	APC	PA-C3A-PB-O2B
2	D	2200	APC	PA-C3A-PB-O3B
2	D	2200	APC	PB-C3A-PA-O1A
2	D	2200	APC	PB-C3A-PA-O5'
2	C	2200	APC	PA-C3A-PB-O1B
2	C	2200	APC	PA-C3A-PB-O3B
2	C	2200	APC	PB-C3A-PA-O1A
2	C	2200	APC	PB-C3A-PA-O2A
2	C	2200	APC	PB-C3A-PA-O5'
2	A	2200	APC	PB-O3B-PG-O2G
2	A	2200	APC	PB-C3A-PA-O1A
2	A	2200	APC	PB-C3A-PA-O2A
2	A	2200	APC	PB-C3A-PA-O5'
2	A	2200	APC	C5'-O5'-PA-O1A
2	B	2200	APC	PB-O3B-PG-O2G
2	B	2200	APC	PB-C3A-PA-O1A

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Mol	Chain	Res	Type	Atoms
2	B	2200	APC	PB-C3A-PA-O5'
2	B	2200	APC	C5'-O5'-PA-O1A
2	B	2200	APC	O4'-C4'-C5'-O5'
2	C	2200	APC	PB-O3B-PG-O2G
2	C	2200	APC	C3'-C4'-C5'-O5'
2	D	2200	APC	PB-C3A-PA-O2A
2	C	2200	APC	PA-C3A-PB-O2B
2	B	2200	APC	PB-C3A-PA-O2A
2	D	2200	APC	C5'-O5'-PA-O1A
2	A	2200	APC	C4'-C5'-O5'-PA
2	B	2200	APC	C5'-O5'-PA-O2A
2	C	2200	APC	O4'-C4'-C5'-O5'
2	D	2200	APC	C4'-C5'-O5'-PA
2	A	2200	APC	O4'-C4'-C5'-O5'
2	C	2200	APC	C5'-O5'-PA-O1A

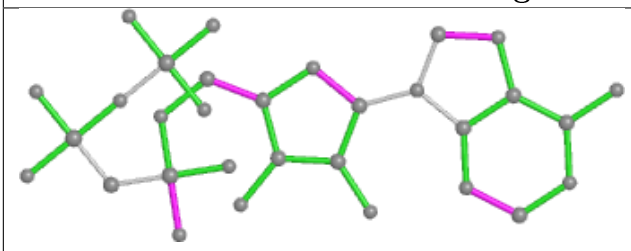
There are no ring outliers.

5 monomers are involved in 16 short contacts:

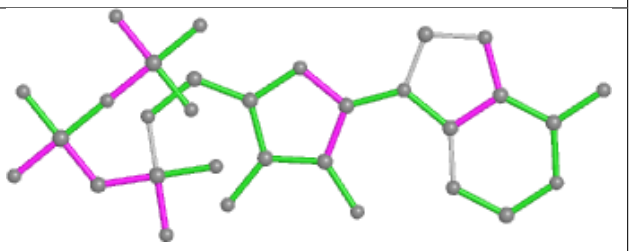
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2200	APC	3	0
2	A	2200	APC	6	0
5	B	2203	ECS	3	0
5	A	2203	ECS	2	0
2	B	2200	APC	6	0

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 then 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.

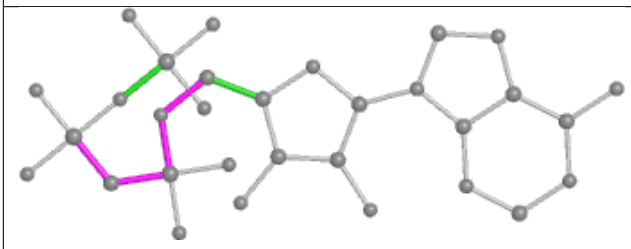
Ligand APC D 2200



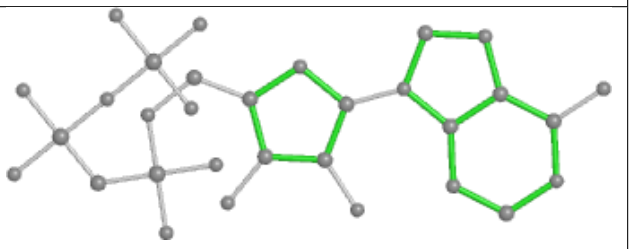
Bond lengths



Bond angles

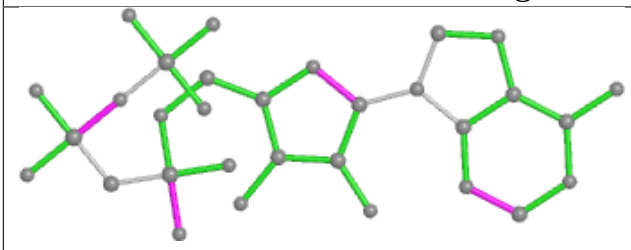


Torsions

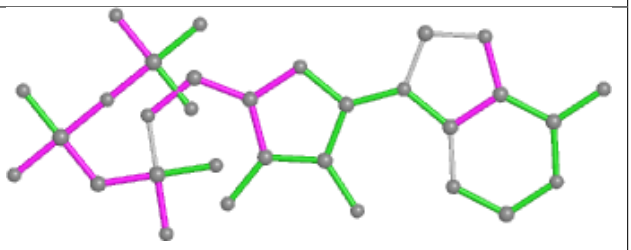


Rings

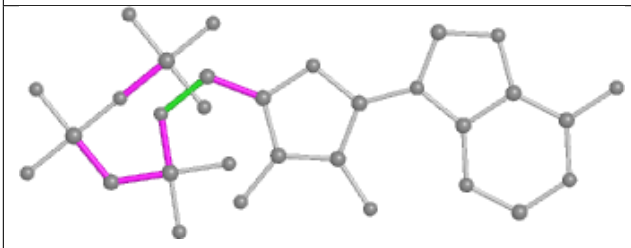
Ligand APC C 2200



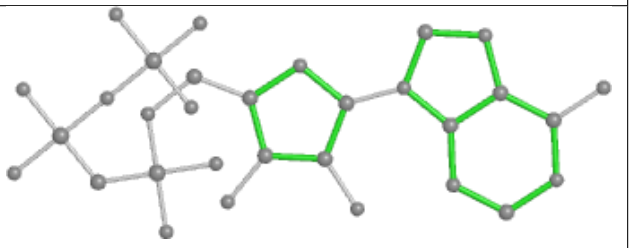
Bond lengths



Bond angles

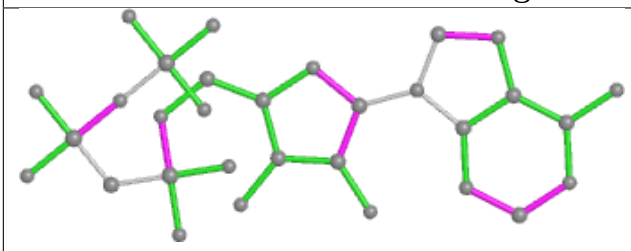


Torsions

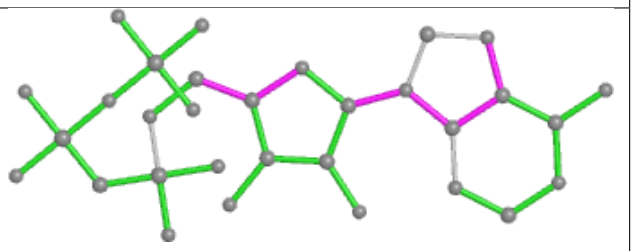


Rings

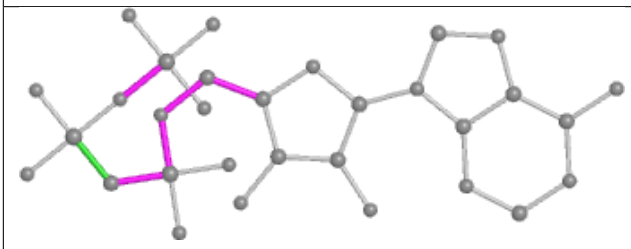
Ligand APC A 2200



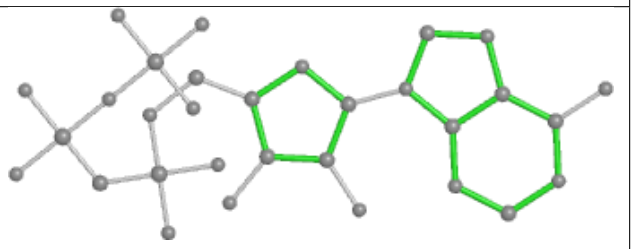
Bond lengths



Bond angles

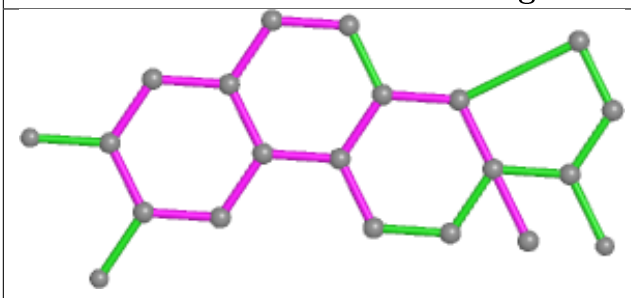


Torsions

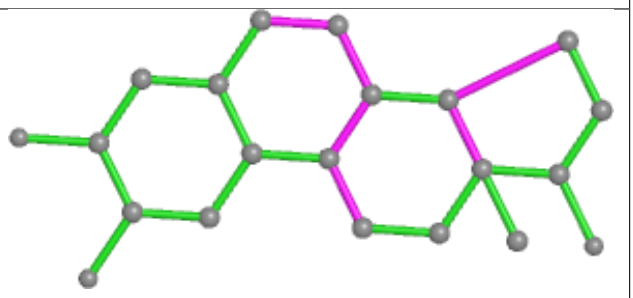


Rings

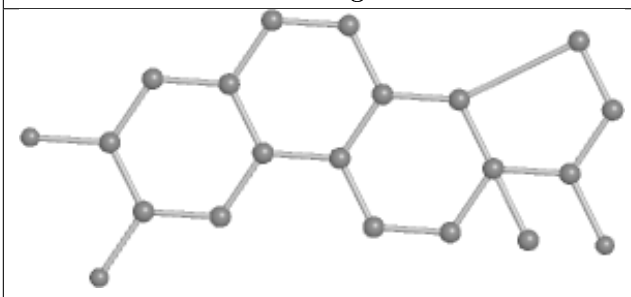
Ligand ECS B 2203



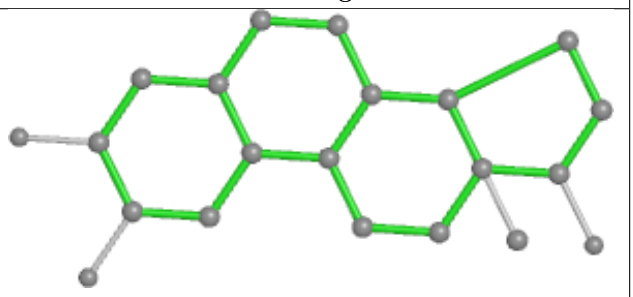
Bond lengths



Bond angles

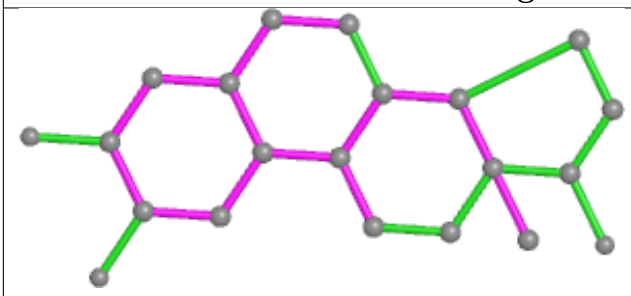


Torsions

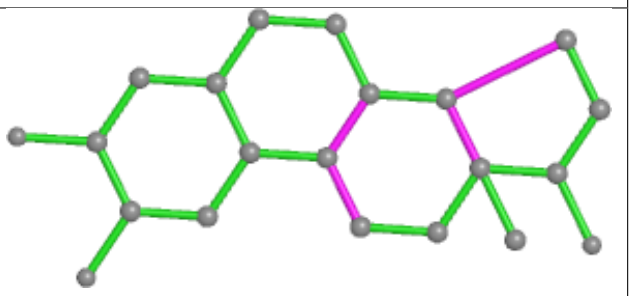


Rings

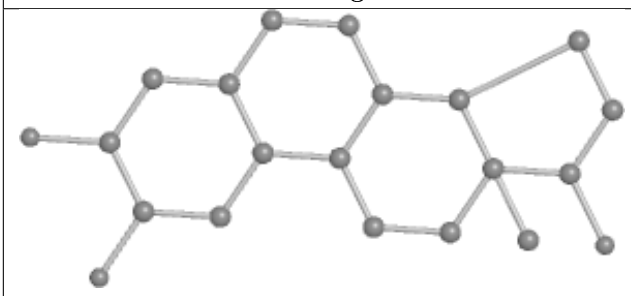
Ligand ECS A 2203



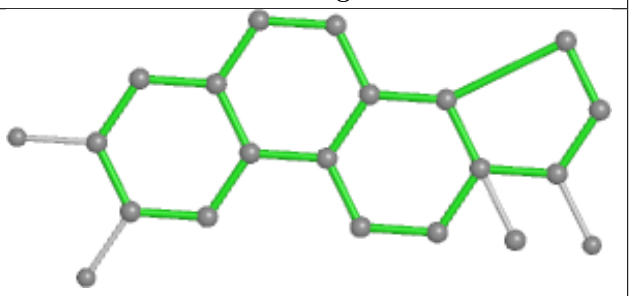
Bond lengths



Bond angles

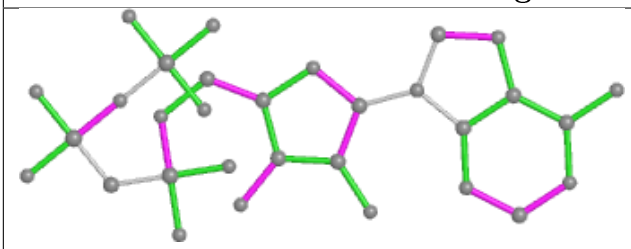


Torsions

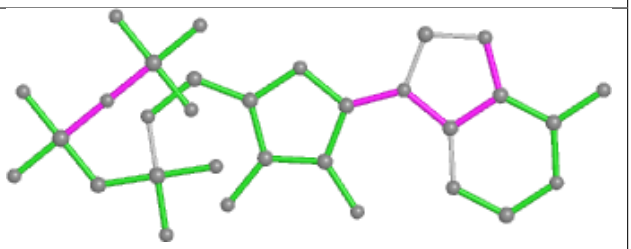


Rings

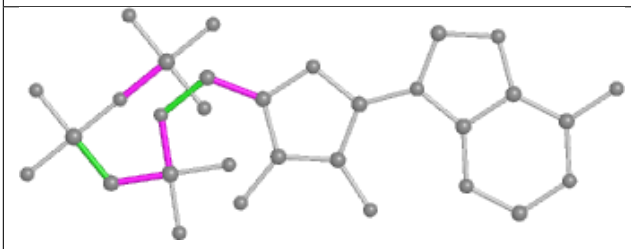
Ligand APC B 2200



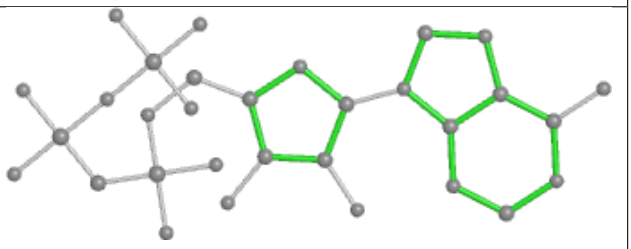
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	198/219 (90%)	0.30	14 (7%) 16 21	12, 25, 59, 77	1 (0%)
1	B	193/219 (88%)	0.38	19 (9%) 7 10	15, 29, 72, 83	1 (0%)
1	C	196/219 (89%)	0.52	16 (8%) 11 15	17, 32, 65, 81	2 (1%)
1	D	193/219 (88%)	0.66	21 (10%) 5 8	13, 35, 76, 91	4 (2%)
All	All	780/876 (89%)	0.47	70 (8%) 9 12	12, 30, 70, 91	8 (1%)

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1110	GLU	7.4
1	B	1004	MET	6.8
1	B	1107	GLY	6.5
1	C	1004	MET	5.7
1	C	1131	GLY	5.6
1	D	1111	VAL	5.5
1	C	1133	GLN	5.5
1	D	1104	GLY	5.3
1	D	1026	ASN	5.3
1	C	1109	ASN	5.2
1	B	1105	LEU	5.1
1	A	1134	GLU	5.0
1	D	1105	LEU	4.9
1	C	1110	GLU	4.9
1	A	1135	ARG	4.3
1	A	1108	ARG	4.3
1	C	1199	MET	4.2
1	B	1131	GLY	4.1
1	A	1133	GLN	4.0
1	B	1134	GLU	4.0
1	D	1027	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	1109	ASN	3.9
1	C	1005	ARG	3.9
1	A	1132	SER	3.9
1	D	1023	ARG	3.8
1	D	1107	GLY	3.7
1	A	1028	LEU	3.7
1	B	1023	ARG	3.6
1	B	1108	ARG	3.6
1	D	1112	PRO	3.6
1	D	1180	PHE	3.5
1	B	1135	ARG	3.5
1	D	1103	ARG	3.3
1	D	1138	PHE	3.3
1	B	1199	MET	3.3
1	B	1112	PRO	3.2
1	C	1026	ASN	3.2
1	A	1199	MET	3.1
1	B	1136	SER	3.0
1	C	1107	GLY	2.9
1	B	1106	VAL	2.9
1	C	1132	SER	2.9
1	D	1183	LEU	2.9
1	B	1005	ARG	2.9
1	D	1185	GLY	2.8
1	C	1105	LEU	2.8
1	D	1102	GLU	2.8
1	A	1031	GLN	2.8
1	A	1029	GLN	2.8
1	D	1133	GLN	2.7
1	A	1049	PHE	2.7
1	A	1110	GLU	2.7
1	B	1049	PHE	2.6
1	C	1145	VAL	2.6
1	C	1198	ASN	2.6
1	B	1102	GLU	2.5
1	D	1031	GLN	2.5
1	C	1101	GLN	2.4
1	C	1108	ARG	2.4
1	D	1106	VAL	2.4
1	B	1132	SER	2.4
1	A	1131	GLY	2.3
1	B	1101	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	1049	PHE	2.2
1	A	1027	ALA	2.2
1	D	1186	ILE	2.2
1	B	1129	LEU	2.2
1	B	1133	GLN	2.2
1	D	1030	SER	2.1
1	C	1111	VAL	2.1

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 carbohydrates 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

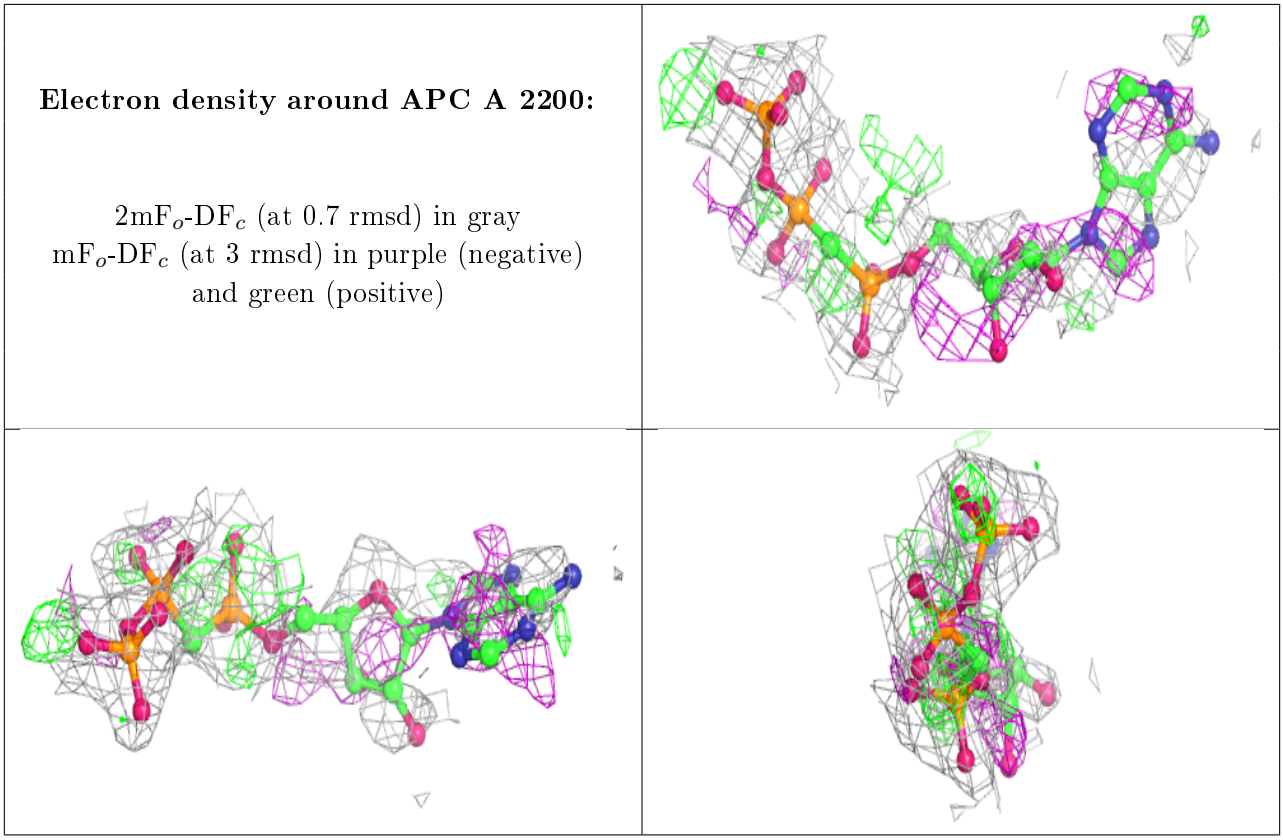
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	APC	A	2200	31/31	0.89	0.28	22,59,69,69	0
5	ECS	A	2203	21/21	0.92	0.18	27,30,31,32	0
2	APC	B	2200	31/31	0.92	0.25	29,64,71,72	0
2	APC	C	2200	31/31	0.93	0.16	30,39,45,47	0
3	MG	D	2201	1/1	0.93	0.25	22,22,22,22	0
5	ECS	B	2203	21/21	0.94	0.15	22,26,33,36	0
2	APC	D	2200	31/31	0.94	0.18	38,42,46,46	0
4	CA	B	2202	1/1	0.95	0.09	36,36,36,36	0
3	MG	A	2201	1/1	0.95	0.13	6,6,6,6	0
4	CA	D	2202	1/1	0.95	0.10	32,32,32,32	0
4	CA	A	2202	1/1	0.95	0.14	31,31,31,31	0
3	MG	B	2201	1/1	0.96	0.12	13,13,13,13	0
3	MG	C	2201	1/1	0.98	0.22	14,14,14,14	0
4	CA	C	2202	1/1	0.99	0.07	23,23,23,23	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.

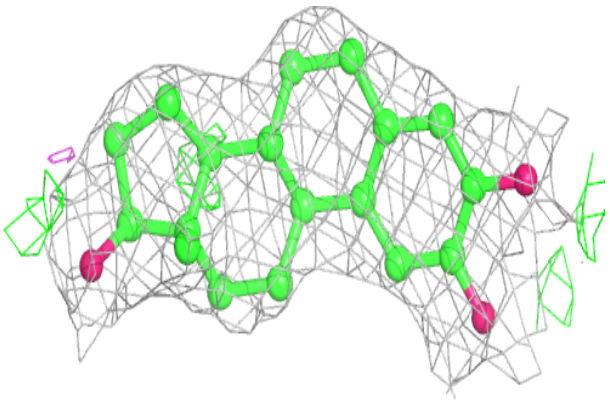
Electron density around APC A 2200:

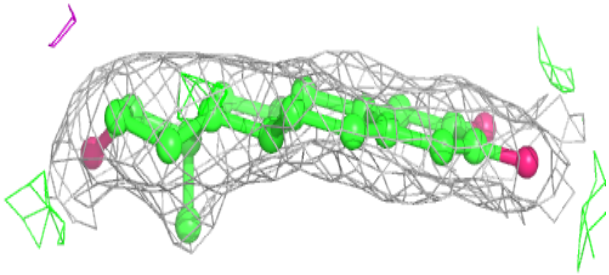
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

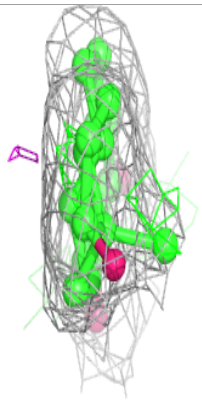


Electron density around ECS A 2203:

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

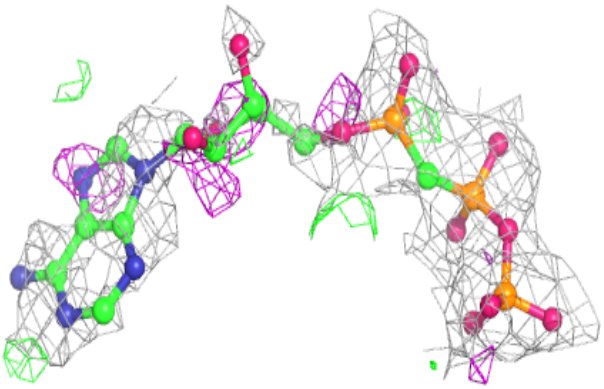


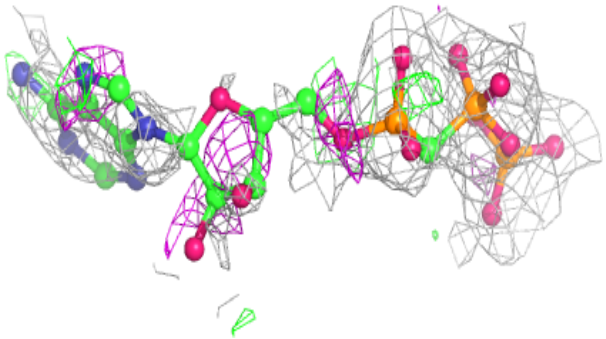


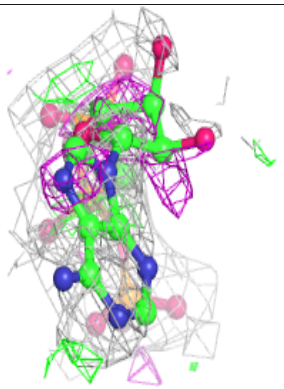


Electron density around APC B 2200:

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

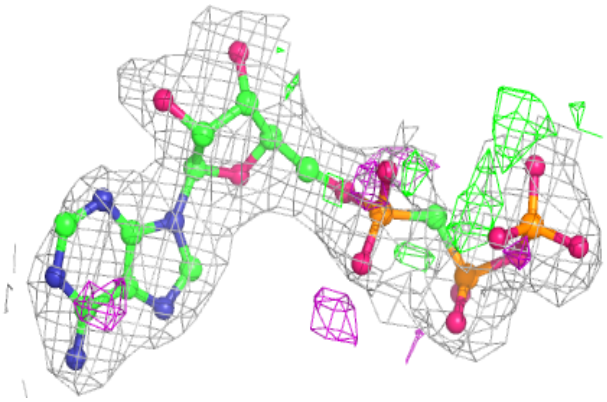


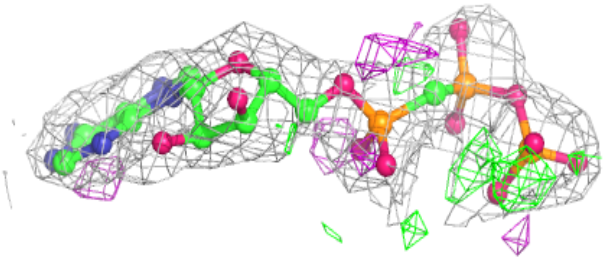


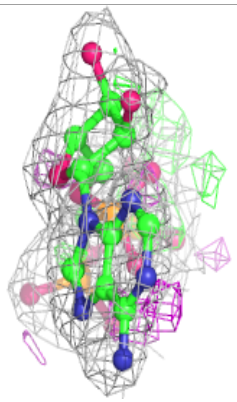


Electron density around APC C 2200:

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

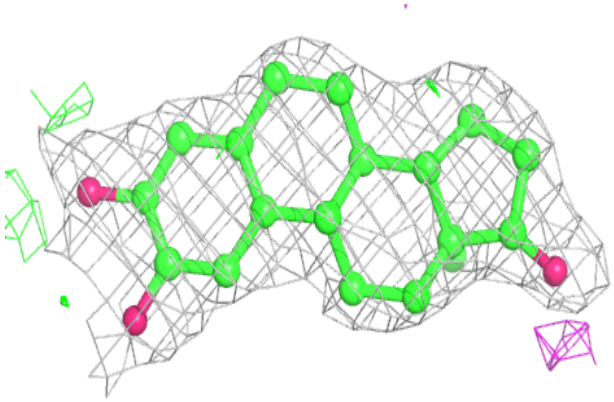


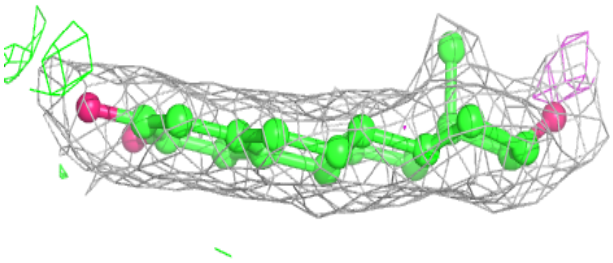


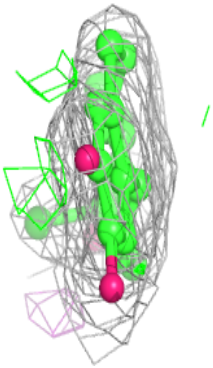


Electron density around ECS B 2203:

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

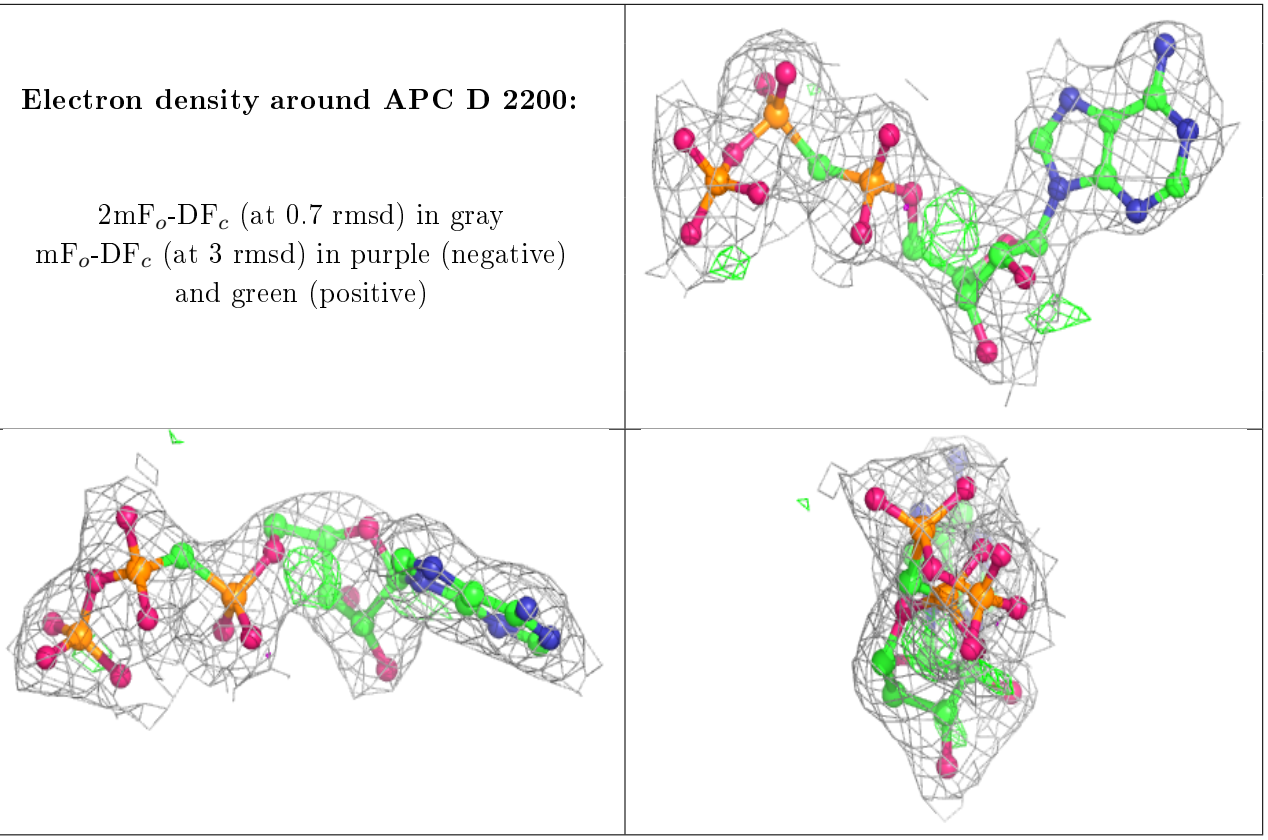






Electron density around APC D 2200:

$2mF_o$-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.