



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 07:46 AM UTC

PDB ID : 2BW7 / pdb_00002bw7
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 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

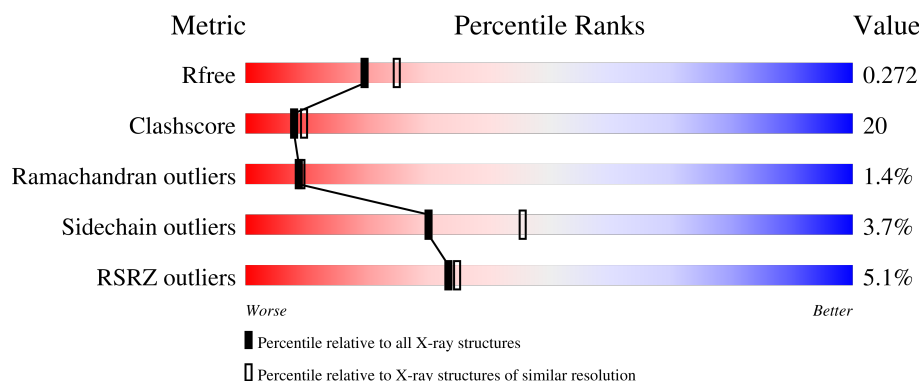
1 Overall quality at a glance

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	219	
1	B	219	
1	C	219	
1	D	219	

2 Entry composition [i](#)

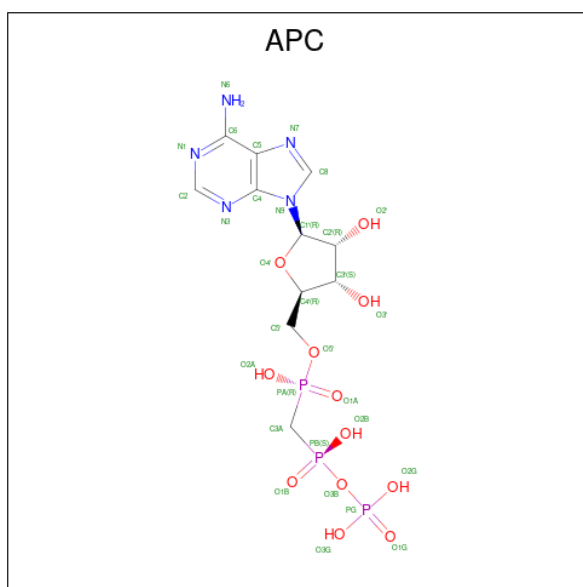
There are 6 unique types of molecules in this entry. The entry contains 6326 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: 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		

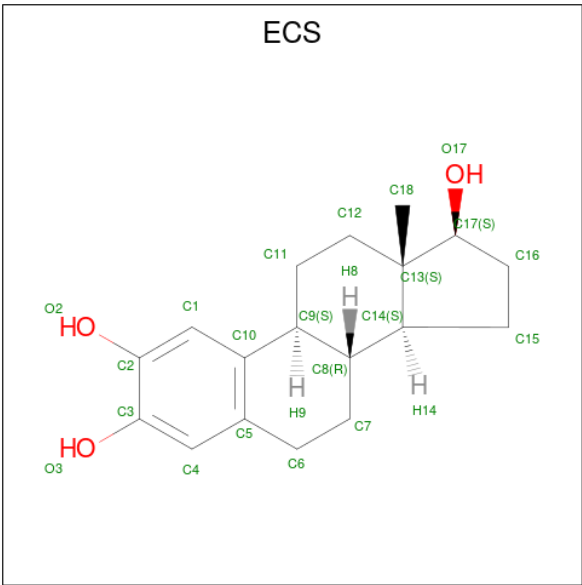
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 5 is 2,3,17BETA-TRIHYDROXY-1,3,5(10)-ESTRATRIENE (CCD ID: ECS) (formula: C₁₈H₂₄O₃).



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

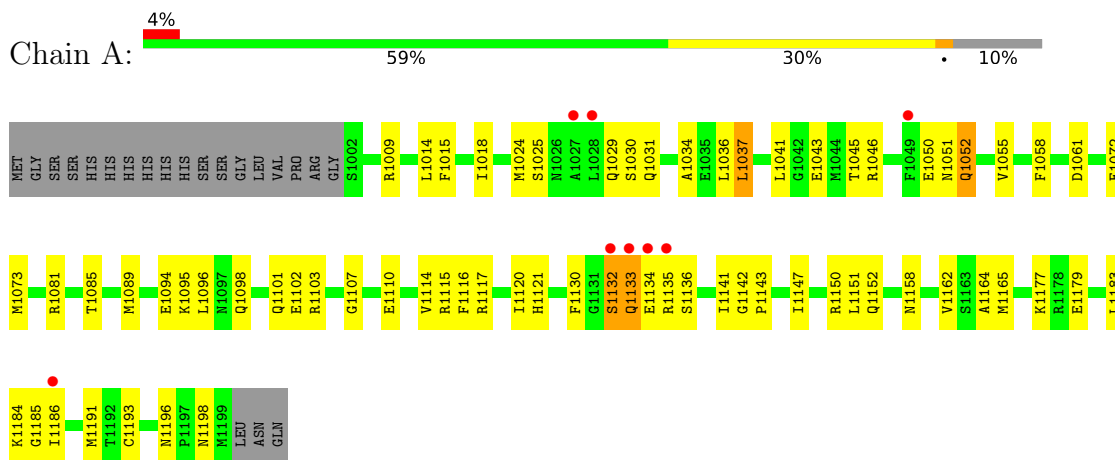
- Molecule 6 is water.

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

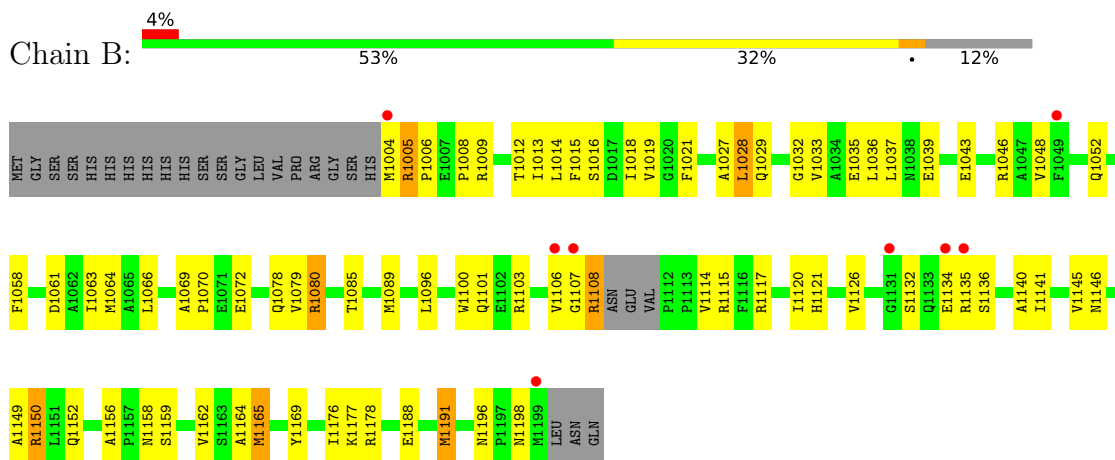
3 Residue-property plots

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.

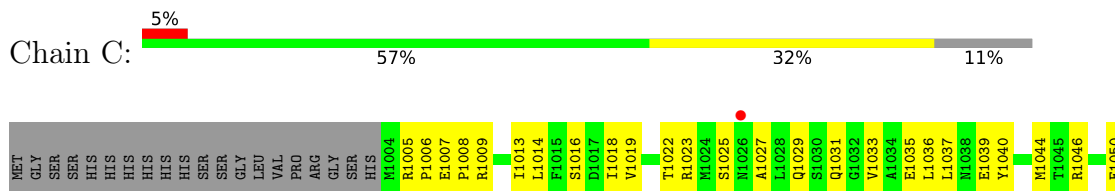
• Molecule 1: ADENYLATE CYCLASE

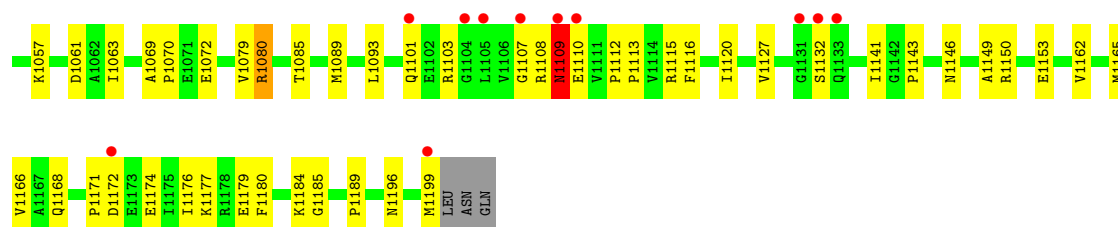


• Molecule 1: ADENYLATE CYCLASE

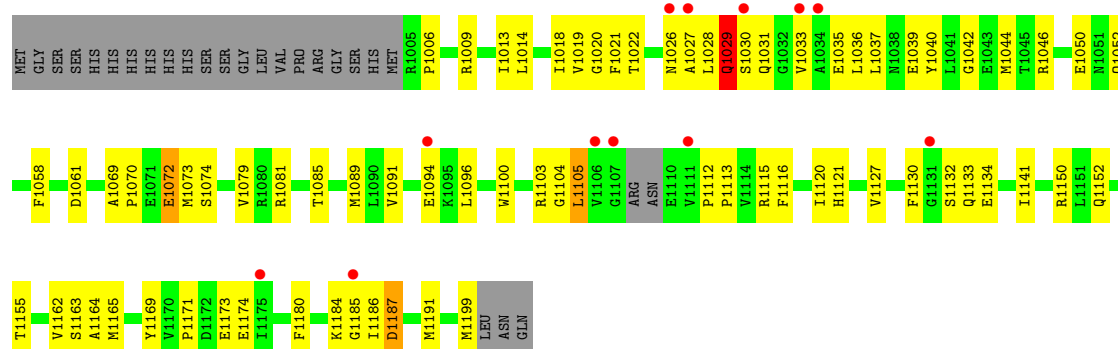


• Molecule 1: ADENYLATE CYCLASE





Molecule 1: ADENYLATE CYCLASE



4 Data and refinement statistics

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 15.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	0.9 (15.00-2.30) 93.0 (15.00-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.27Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.207 , 0.257 0.227 , 0.272	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)	0.36 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

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: ECS, CA, APC, 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	0.33	0/1553	0.90	4/2100 (0.2%)
1	B	0.31	0/1511	0.85	2/2040 (0.1%)
1	C	0.31	0/1536	0.82	0/2077
1	D	0.30	0/1508	0.84	2/2039 (0.1%)
All	All	0.31	0/6108	0.85	8/8256 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1028	LEU	N-CA-C	-5.95	106.16	113.41
1	B	1114	VAL	N-CA-C	5.76	117.02	109.58
1	A	1025	SER	N-CA-C	-5.32	106.63	113.01
1	D	1074	SER	CA-C-N	5.26	124.72	119.24
1	D	1074	SER	C-N-CA	5.26	124.72	119.24
1	A	1142	GLY	CA-C-N	5.26	125.32	119.32
1	A	1142	GLY	C-N-CA	5.26	125.32	119.32
1	A	1151	LEU	N-CA-C	-5.19	105.70	111.36

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	59	0
1	B	1488	0	1499	75	0
1	C	1512	0	1520	63	0
1	D	1485	0	1491	60	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
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	7	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	241	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (241) 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:1120:ILE:HB	1:B:1162:VAL:HG12	1.51	0.89
1:A:1121:HIS:HE1	1:A:1165:MET:HE2	1.37	0.88
1:B:1121:HIS:HE1	1:B:1165:MET:HE2	1.38	0.88
1:B:1134:GLU:HG3	1:B:1135:ARG:N	1.87	0.85
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:1004:MET:HE1	1:B:1009:ARG:HH22	1.56	0.70
1:D:1120:ILE:HB	1:D:1162:VAL:HG12	1.71	0.69
1:D:1132:SER:C	1:D:1134:GLU:H	1.99	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:D:1073:MET:HE2	1:D:1081:ARG:HH11	1.59	0.67
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: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:B:1121:HIS:CE1	1:B:1165:MET:HE2	2.29	0.63
1:D:1112:PRO:HB2	1:D:1113:PRO:HD2	1.80	0.63
1:A:1024:MET:HE1	1:A:1114:VAL:HG22	1.81	0.62
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:C:1014:LEU:C	1:C:1014:LEU:HD23	2.26	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:A:1179:GLU:O	1:A:1191:MET:HE3	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1115:ARG:HG3	1:C:1115:ARG:HH11	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:A:1073:MET:HE2	1:A:1081:ARG:HH11	1.70	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:N	1:C:1013:ILE:HD12	2.19	0.57
1:B:1018:ILE:HB	1:B:1061:ASP:OD2	2.05	0.57
1:D:1036:LEU:C	1:D:1036:LEU:HD23	2.29	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
1:D:1028:LEU:C	1:D:1029:GLN:HG2	2.29	0.56
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:B:1191:MET:HE3	1:B:1191:MET:HA	1.88	0.56
1:B:1080:ARG:HG2	1:B:1080:ARG:NH1	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:A:1132:SER:C	1:A:1134:GLU:H	2.10	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:B:1165:MET:HG3	1:C:1165:MET:HE1	1.88	0.54
1:C:1057:LYS:HE2	1:D:1058:PHE:O	2.07	0.54
1:D:1014:LEU:HD23	1:D:1014:LEU:C	2.33	0.54
1:B:1165:MET:SD	1:B:1165:MET:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1115:ARG:HG2	6:C:2013:HOH:O	2.08	0.53
1:A:1051:ASN:C	1:A:1052:GLN:HG2	2.34	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: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
1:A:1024:MET:HE2	6:A:2028:HOH:O	2.10	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:D:1021:PHE:CZ	1:D:1033:VAL:HG13	2.47	0.50
1:D:1073:MET:HE2	1:D:1081:ARG:NH1	2.26	0.50
1:A:1101:GLN:C	1:A:1103:ARG:H	2.20	0.50
1:B:1178:ARG:NH2	1:C:1168:GLN:NE2	2.60	0.50
1:A:1191:MET:HG3	6:A:2045:HOH:O	2.11	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:1073:MET:HE2	1:A:1081:ARG:NH1	2.27	0.49
1:B:1048:VAL:HG22	1:B:1085:THR:HG21	1.95	0.48
1:B:1064:MET:HE2	1:B:1066:LEU:HD21	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: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:A:1014:LEU:HD23	1:A:1014:LEU:C	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:1116:PHE:CD1	1:D:1116:PHE:C	2.92	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:B:1079:VAL:HG21	1:B:1169:TYR:CD1	2.50	0.47
1:C:1016:SER:HB3	1:C:1063:ILE:HB	1.97	0.47
1:C:1018:ILE:HB	1:C:1061:ASP:OD2	2.14	0.47
1:B:1014:LEU:C	1:B:1014:LEU:HD23	2.40	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:A:1196:ASN:C	1:A:1198:ASN:H	2.22	0.46
2:A:2200:APC:N3	5:B:2203:ECS:H161	2.30	0.46
1:C:1023:ARG:NH1	1:D:1187:ASP:OD2	2.48	0.46
1:D:1028:LEU:HD11	1:D:1105:LEU:HD22	1.97	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:D:1104:GLY:O	1:D:1105:LEU:C	2.58	0.45
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:1121:HIS:HD1	1:D:1163:SER:CB	2.28	0.45
1:D:1009:ARG:NH2	1:D:1072:GLU:OE1	2.50	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: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:HG3	1:D:1115:ARG:HH11	1.82	0.44
1:C:1036:LEU:C	1:C:1036:LEU:HD23	2.43	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:B:1069:ALA:HA	1:B:1070:PRO:C	2.42	0.44
1:C:1079:VAL:HG13	1:C:1166:VAL:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:1191:MET:HE2	6:A:2045:HOH:O	2.18	0.44
1:B:1196:ASN:C	1:B:1198:ASN:H	2.26	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:D:1069:ALA:HA	1:D:1070:PRO:C	2.42	0.43
1:A:1036:LEU:C	1:A:1036:LEU:HD23	2.43	0.43
1:B:1176:ILE:CD1	1:B:1196:ASN:HA	2.48	0.43
1:C:1069:ALA:HA	1:C:1070:PRO:C	2.42	0.43
1:C:1080:ARG:NH1	1:C:1080:ARG:HG3	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: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:B:1132:SER:C	1:B:1134:GLU:H	2.26	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:N7	1:B:1141:ILE:HD13	2.33	0.42
2:A:2200:APC:C8	1:B:1141:ILE:HA	2.49	0.42
1:B:1005:ARG:HH11	1:B:1005:ARG:CG	2.32	0.42
1:B:1108:ARG:NH1	1:B:1108:ARG:HG2	2.33	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:A:1029:GLN:O	1:A:1030:SER:C	2.62	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:A:1116:PHE:CD1	1:A:1116:PHE:C	2.97	0.42
1:D:1035:GLU:O	1:D:1039:GLU:HG3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:HA	1:C:1110:GLU:OE1	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: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:D:1171:PRO:C	1:D:1173:GLU:N	2.78	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:D:1165:MET:N	1:D:1165:MET:HE3	2.36	0.41
1:A:1121:HIS:CE1	1:A:1165:MET:HE2	2.30	0.41
1:B:1115:ARG:HA	1:B:1158:ASN:HD21	1.85	0.41
1:B:1005:ARG:HB3	1:B:1005:ARG:CZ	2.51	0.40
1:D:1132:SER:C	1:D:1134:GLU:N	2.67	0.40
1:A:1081:ARG:HG2	6:A:2013:HOH:O	2.20	0.40
1:B:1156:ALA:O	1:B:1159:SER:OG	2.35	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%)	12 15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	189/219 (86%)	173 (92%)	14 (7%)	2 (1%)	11	13
1	C	194/219 (89%)	181 (93%)	10 (5%)	3 (2%)	8	8
1	D	189/219 (86%)	178 (94%)	7 (4%)	4 (2%)	5	4
All	All	768/876 (88%)	719 (94%)	38 (5%)	11 (1%)	9	9

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 ⓘ

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%)	23	35
1	B	160/183 (87%)	150 (94%)	10 (6%)	16	23
1	C	163/183 (89%)	160 (98%)	3 (2%)	51	70
1	D	160/183 (87%)	157 (98%)	3 (2%)	50	69
All	All	648/732 (88%)	624 (96%)	24 (4%)	30	45

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	B	1191	MET
1	C	1072	GLU
1	C	1080	ARG
1	C	1109	ASN
1	D	1029	GLN
1	D	1072	GLU
1	D	1180	PHE

Sometimes 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	1152	GLN
1	A	1158	ASN
1	B	1026	ASN
1	B	1101	GLN
1	B	1146	ASN
1	B	1152	GLN
1	B	1158	ASN
1	B	1168	GLN
1	C	1026	ASN
1	C	1031	GLN
1	C	1101	GLN

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Mol	Chain	Res	Type
1	C	1122	GLN
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
1	D	1168	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
5	ECS	A	2203	3	24,24,24	3.11	14 (58%)	38,38,38	1.14	2 (5%)
2	APC	D	2200	3,4	29,33,33	1.41	4 (13%)	44,52,52	1.11	3 (6%)
5	ECS	B	2203	3	24,24,24	3.13	14 (58%)	38,38,38	1.15	4 (10%)
2	APC	C	2200	3,4	29,33,33	1.41	4 (13%)	44,52,52	1.31	8 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	APC	A	2200	3,4	29,33,33	1.89	6 (20%)	44,52,52	1.67	8 (18%)
2	APC	B	2200	3,4	29,33,33	2.10	9 (31%)	44,52,52	1.71	6 (13%)

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
5	ECS	A	2203	3	-	-	0/4/4/4
2	APC	D	2200	3,4	-	7/19/38/38	0/3/3/3
5	ECS	B	2203	3	-	-	0/4/4/4
2	APC	C	2200	3,4	-	9/19/38/38	0/3/3/3
2	APC	A	2200	3,4	-	7/19/38/38	0/3/3/3
2	APC	B	2200	3,4	-	9/19/38/38	0/3/3/3

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2200	APC	C4-N9	5.97	1.50	1.37
5	A	2203	ECS	C5-C10	5.96	1.49	1.40
5	A	2203	ECS	C9-C8	5.83	1.61	1.54
5	B	2203	ECS	C5-C10	5.78	1.49	1.40
2	B	2200	APC	C4-N9	5.74	1.49	1.37
5	B	2203	ECS	C9-C8	5.71	1.60	1.54
5	A	2203	ECS	C1-C10	4.63	1.47	1.39
5	B	2203	ECS	C1-C10	4.60	1.47	1.39
5	B	2203	ECS	C4-C5	4.22	1.46	1.39
5	B	2203	ECS	C4-C3	4.00	1.44	1.38
5	A	2203	ECS	C4-C3	3.95	1.44	1.38
5	A	2203	ECS	C4-C5	3.94	1.45	1.39
5	B	2203	ECS	C10-C9	3.86	1.57	1.52
5	A	2203	ECS	C10-C9	3.82	1.57	1.52
2	D	2200	APC	PA-O1A	3.81	1.60	1.51
2	D	2200	APC	C5'-C4'	3.77	1.62	1.51
2	A	2200	APC	C2-N3	3.77	1.40	1.33
5	B	2203	ECS	C1-C2	3.74	1.44	1.38
5	A	2203	ECS	C18-C13	3.62	1.60	1.54
5	B	2203	ECS	C18-C13	3.61	1.60	1.54
5	B	2203	ECS	C8-C14	3.59	1.60	1.53
2	B	2200	APC	C2-N3	3.59	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2203	ECS	C8-C14	3.56	1.60	1.53
5	B	2203	ECS	C13-C14	3.50	1.61	1.55
5	A	2203	ECS	C1-C2	3.47	1.43	1.38
2	B	2200	APC	O4'-C1'	3.38	1.49	1.42
5	A	2203	ECS	C13-C14	3.36	1.61	1.55
2	B	2200	APC	C1'-N9	3.33	1.55	1.46
2	B	2200	APC	C5'-C4'	3.33	1.61	1.51
5	B	2203	ECS	C11-C9	3.25	1.58	1.53
5	A	2203	ECS	C11-C9	3.21	1.58	1.53
2	C	2200	APC	PA-O1A	3.05	1.58	1.51
2	A	2200	APC	PB-O3B	3.02	1.61	1.58
2	B	2200	APC	PB-O3B	2.97	1.61	1.58
2	C	2200	APC	PB-O3B	2.93	1.61	1.58
2	A	2200	APC	C1'-N9	2.88	1.54	1.46
5	B	2203	ECS	C6-C5	2.83	1.55	1.51
5	A	2203	ECS	C6-C5	2.76	1.55	1.51
5	A	2203	ECS	C7-C6	2.71	1.57	1.52
2	A	2200	APC	O4'-C1'	2.70	1.48	1.42
2	D	2200	APC	C4-N9	2.59	1.43	1.37
5	B	2203	ECS	C7-C6	2.58	1.57	1.52
5	A	2203	ECS	C3-C2	2.54	1.44	1.40
5	B	2203	ECS	C3-C2	2.51	1.44	1.40
2	B	2200	APC	C2-N1	2.47	1.38	1.33
2	C	2200	APC	C4-N9	2.39	1.42	1.37
2	B	2200	APC	C5-C4	2.25	1.43	1.39
2	B	2200	APC	O3'-C3'	2.24	1.48	1.43
2	C	2200	APC	O4'-C1'	2.12	1.46	1.42
2	A	2200	APC	C2-N1	2.08	1.37	1.33
2	D	2200	APC	O4'-C1'	2.04	1.46	1.42

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2200	APC	C2'-C1'-N9	4.88	125.44	113.30
2	B	2200	APC	C4-N9-C1'	4.73	137.70	126.63
2	A	2200	APC	C4-N9-C1'	4.27	136.62	126.63
2	B	2200	APC	C1'-N9-C8	-3.98	118.25	127.09
2	B	2200	APC	C5-C4-N9	-3.92	101.54	105.81
2	A	2200	APC	C5-C4-N9	-3.77	101.70	105.81
2	B	2200	APC	N3-C4-N9	3.67	133.41	127.17
2	A	2200	APC	N3-C4-N9	3.60	133.29	127.17
2	A	2200	APC	C1'-N9-C8	-3.56	119.19	127.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2200	APC	O2B-PB-C3A	3.33	120.52	106.73
2	D	2200	APC	O3G-PG-O3B	3.30	115.70	104.64
2	C	2200	APC	O5'-C5'-C4'	3.29	120.19	108.99
2	C	2200	APC	O1A-PA-C3A	3.26	117.62	109.05
2	A	2200	APC	O4'-C1'-N9	3.23	114.30	108.09
2	A	2200	APC	C2'-C1'-N9	3.19	121.22	113.30
2	C	2200	APC	O2B-PB-C3A	3.09	119.51	106.73
2	C	2200	APC	PB-O3B-PG	-2.98	121.76	132.45
2	D	2200	APC	O1A-PA-C3A	2.82	116.48	109.05
5	B	2203	ECS	C15-C14-C13	-2.81	100.53	103.84
5	B	2203	ECS	C11-C9-C8	-2.73	107.88	111.45
5	A	2203	ECS	C15-C14-C13	-2.72	100.64	103.84
5	A	2203	ECS	C11-C9-C8	-2.63	108.01	111.45
2	A	2200	APC	C4'-O4'-C1'	-2.54	103.86	109.47
2	C	2200	APC	C5'-C4'-C3'	-2.48	106.29	115.21
2	C	2200	APC	O3G-PG-O3B	2.39	112.66	104.64
2	B	2200	APC	PB-O3B-PG	-2.35	124.03	132.45
2	C	2200	APC	O4'-C4'-C3'	2.18	109.48	105.15
2	A	2200	APC	O4'-C4'-C5'	2.11	116.10	109.33
2	C	2200	APC	C2'-C1'-N9	2.07	118.44	113.30
5	B	2203	ECS	C6-C7-C8	2.03	114.01	110.61
5	B	2203	ECS	C18-C13-C14	2.02	115.34	111.68

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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
2	B	2200	APC	PB-C3A-PA-O5'
2	B	2200	APC	C5'-O5'-PA-O1A
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	D	2200	APC	PA-C3A-PB-O1B

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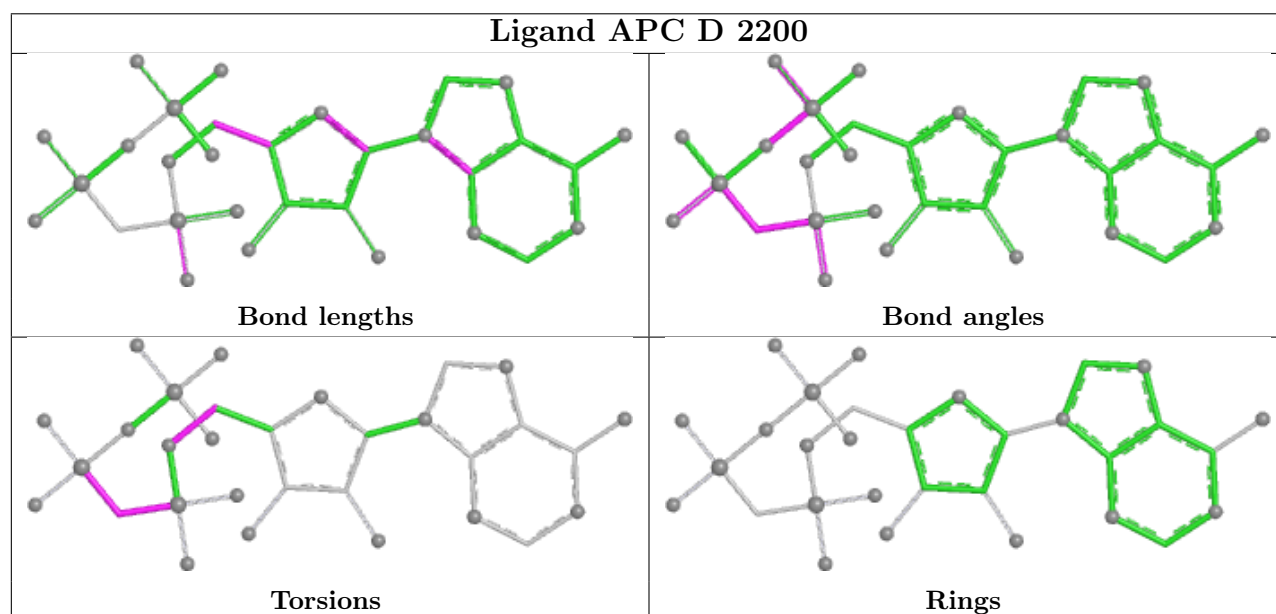
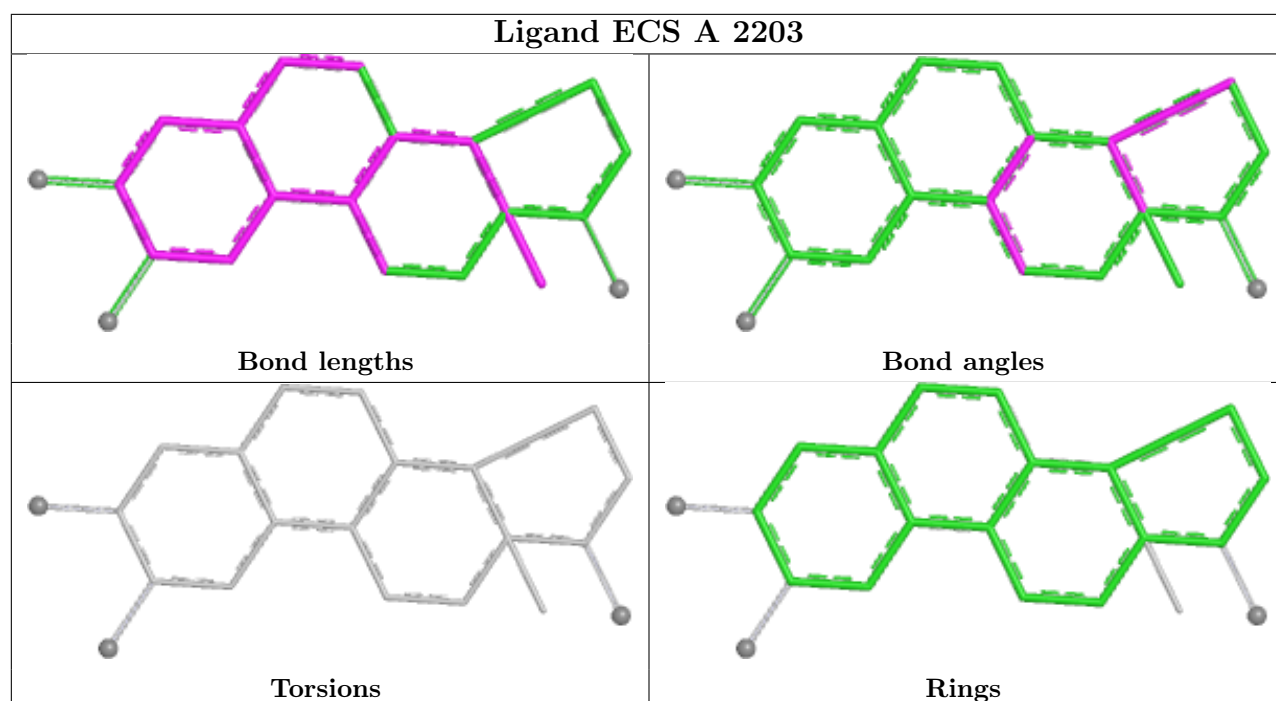
Mol	Chain	Res	Type	Atoms
2	D	2200	APC	PA-C3A-PB-O2B
2	D	2200	APC	PA-C3A-PB-O3B
2	D	2200	APC	PB-C3A-PA-O1A
2	D	2200	APC	PB-C3A-PA-O5'
2	B	2200	APC	C2'-C1'-N9-C4
2	B	2200	APC	C2'-C1'-N9-C8
2	B	2200	APC	O4'-C4'-C5'-O5'
2	C	2200	APC	PB-O3B-PG-O2G
2	C	2200	APC	C3'-C4'-C5'-O5'
2	B	2200	APC	PB-C3A-PA-O2A
2	C	2200	APC	PA-C3A-PB-O2B
2	D	2200	APC	PB-C3A-PA-O2A
2	B	2200	APC	C5'-O5'-PA-O2A
2	A	2200	APC	C4'-C5'-O5'-PA
2	A	2200	APC	O4'-C1'-N9-C8
2	D	2200	APC	C4'-C5'-O5'-PA
2	C	2200	APC	O4'-C4'-C5'-O5'

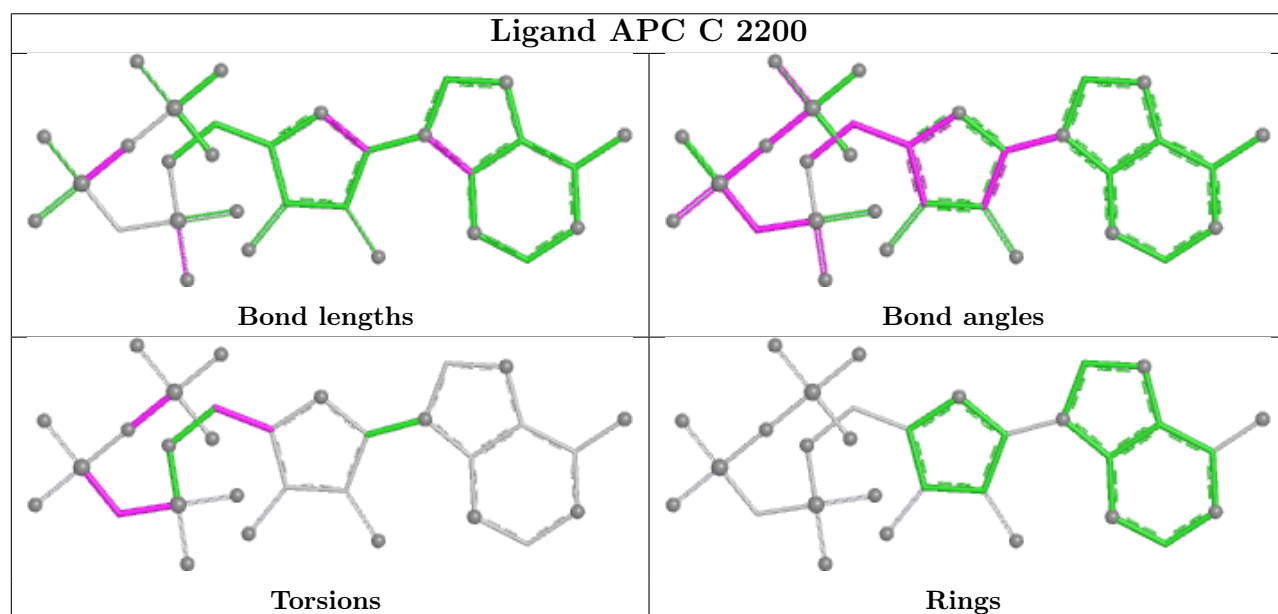
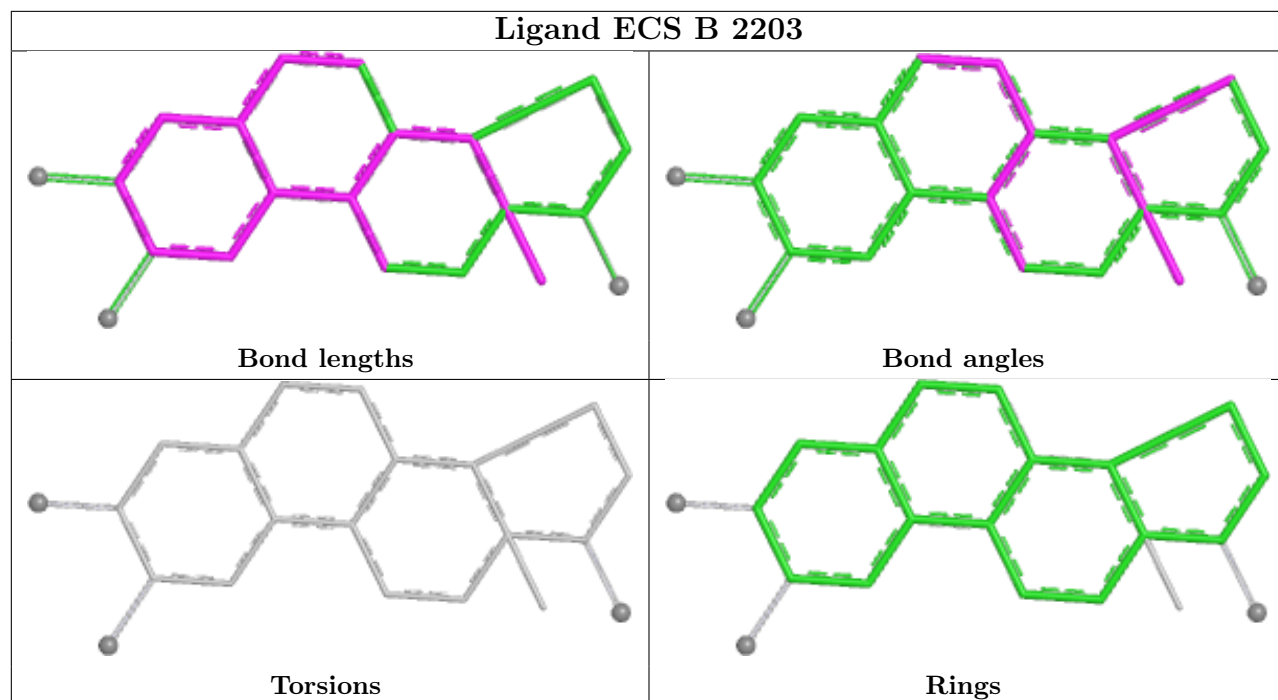
There are no ring outliers.

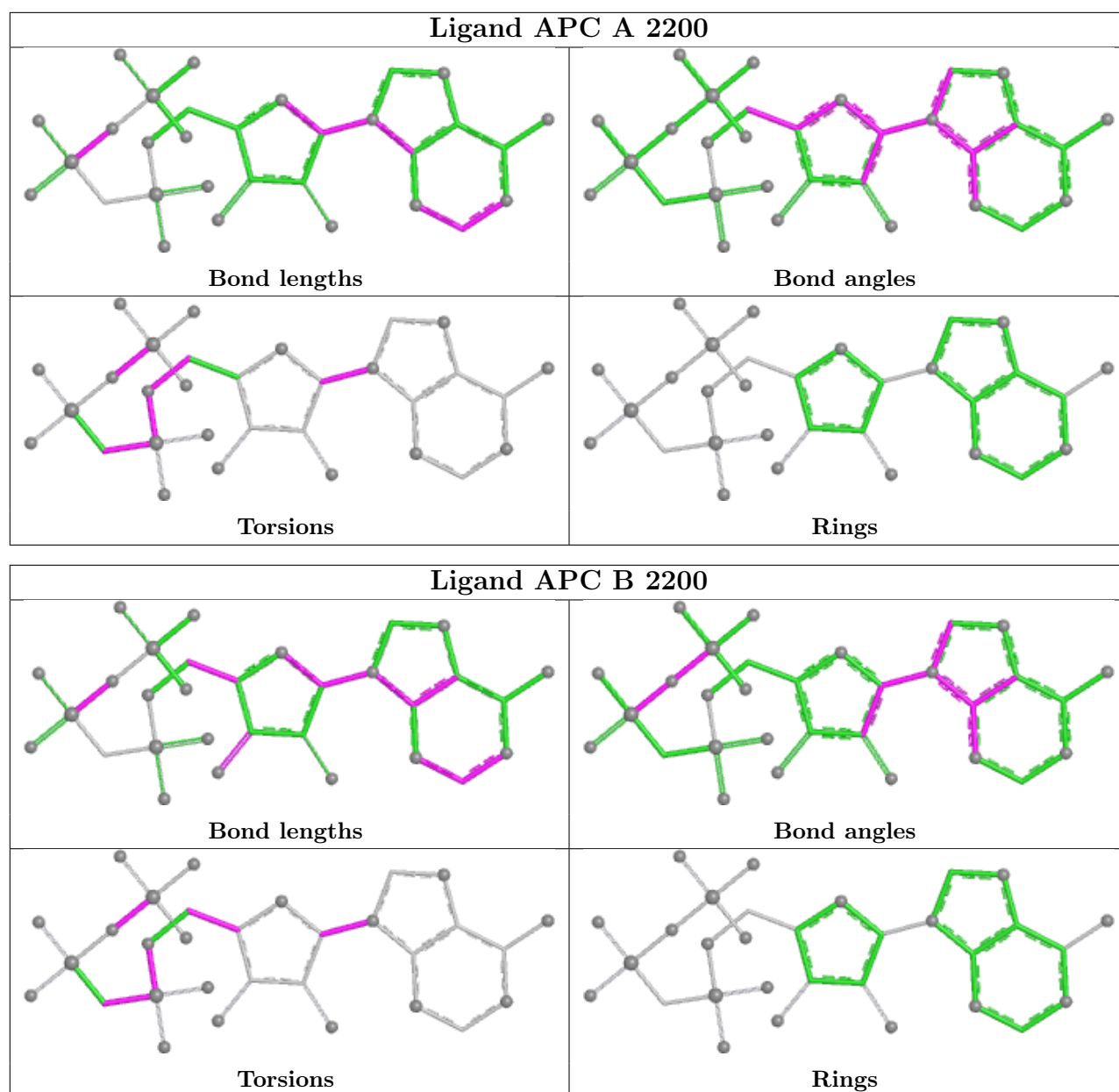
5 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2203	ECS	2	0
2	D	2200	APC	3	0
5	B	2203	ECS	3	0
2	A	2200	APC	6	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 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	198/219 (90%)	0.10	8 (4%)	42	44	12, 25, 59, 77	1 (0%)
1	B	193/219 (88%)	0.25	8 (4%)	41	43	15, 28, 70, 83	1 (0%)
1	C	196/219 (89%)	0.36	12 (6%)	27	29	17, 32, 63, 81	2 (1%)
1	D	193/219 (88%)	0.49	12 (6%)	26	28	13, 35, 74, 90	4 (2%)
All	All	780/876 (89%)	0.30	40 (5%)	33	35	12, 30, 68, 90	8 (1%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1131	GLY	6.1
1	A	1132	SER	4.7
1	C	1109	ASN	4.4
1	D	1107	GLY	3.0
1	B	1107	GLY	3.0
1	D	1034	ALA	2.9
1	A	1134	GLU	2.9
1	B	1131	GLY	2.8
1	B	1135	ARG	2.8
1	A	1135	ARG	2.8
1	D	1030	SER	2.8
1	D	1106	VAL	2.6
1	C	1104	GLY	2.6
1	B	1004	MET	2.6
1	C	1105	LEU	2.5
1	D	1027	ALA	2.4
1	C	1107	GLY	2.3
1	B	1199	MET	2.3
1	B	1049	PHE	2.3
1	D	1111	VAL	2.3
1	A	1133	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	1026	ASN	2.3
1	A	1028	LEU	2.2
1	C	1199	MET	2.2
1	D	1094	GLU	2.2
1	C	1172	ASP	2.1
1	B	1134	GLU	2.1
1	C	1110	GLU	2.1
1	D	1026	ASN	2.1
1	D	1033	VAL	2.1
1	A	1049	PHE	2.1
1	D	1185	GLY	2.1
1	D	1175	ILE	2.1
1	C	1132	SER	2.1
1	A	1027	ALA	2.1
1	B	1106	VAL	2.1
1	D	1131	GLY	2.1
1	C	1101	GLN	2.0
1	C	1133	GLN	2.0
1	A	1186	ILE	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
2	APC	A	2200	31/31	0.88	0.17	22,59,69,69	0
2	APC	C	2200	31/31	0.88	0.12	30,39,45,47	0
5	ECS	A	2203	21/21	0.88	0.10	27,30,31,32	0
2	APC	B	2200	31/31	0.89	0.16	29,64,71,72	0

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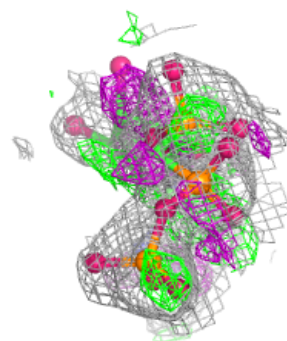
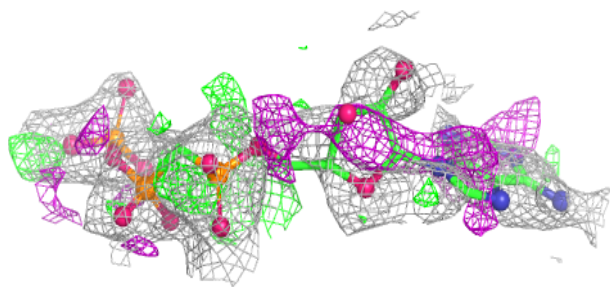
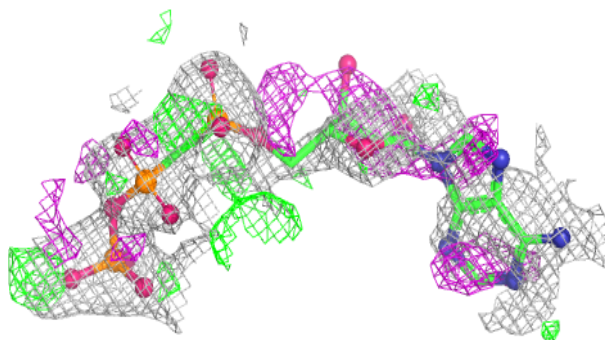
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	APC	D	2200	31/31	0.90	0.10	38,42,46,46	0
3	MG	D	2201	1/1	0.91	0.07	22,22,22,22	0
5	ECS	B	2203	21/21	0.91	0.09	22,26,33,36	0
4	CA	A	2202	1/1	0.95	0.04	31,31,31,31	0
4	CA	B	2202	1/1	0.95	0.05	36,36,36,36	0
3	MG	B	2201	1/1	0.96	0.06	13,13,13,13	0
3	MG	A	2201	1/1	0.96	0.03	6,6,6,6	0
4	CA	D	2202	1/1	0.97	0.04	32,32,32,32	0
3	MG	C	2201	1/1	0.97	0.10	14,14,14,14	0
4	CA	C	2202	1/1	0.97	0.03	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.

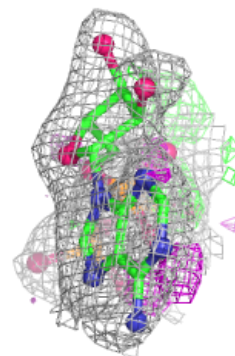
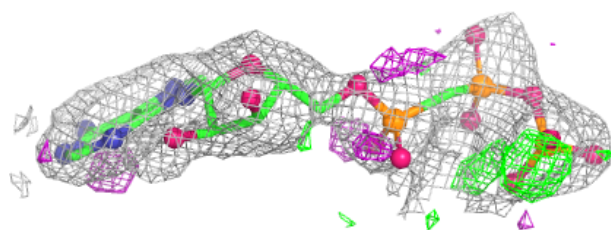
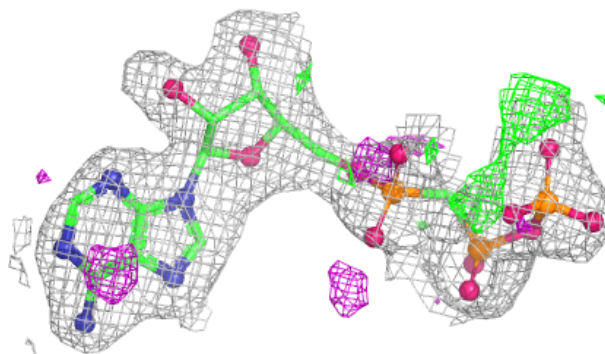
Electron density around APC A 2200:

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

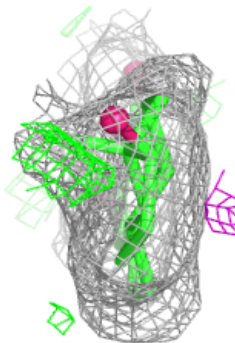
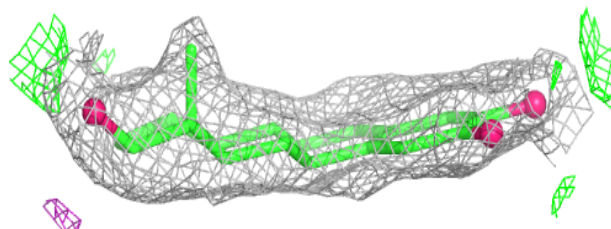
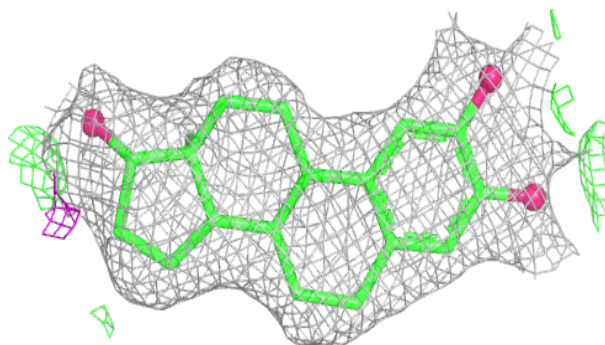


Electron density around APC C 2200:

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

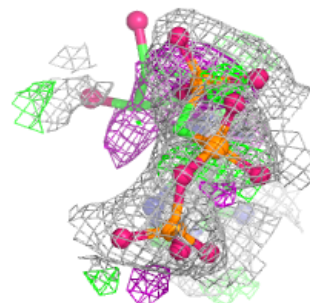
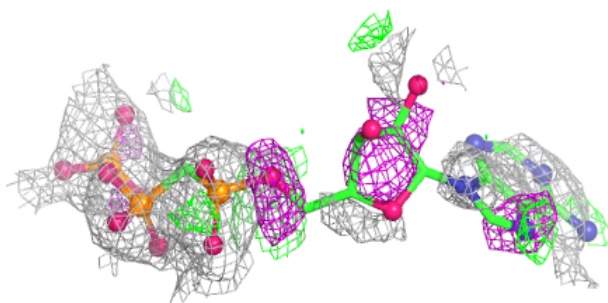
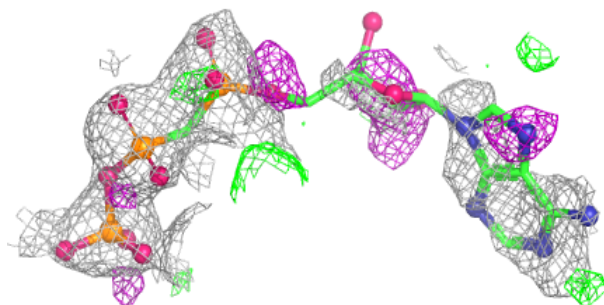
**Electron density around ECS A 2203:**

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

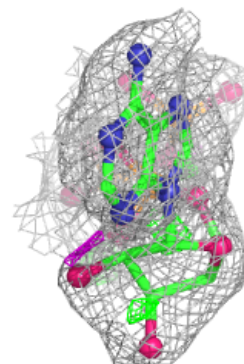
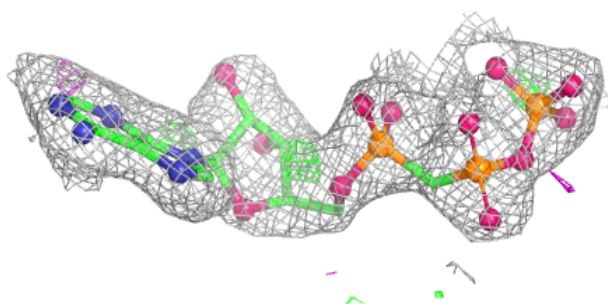
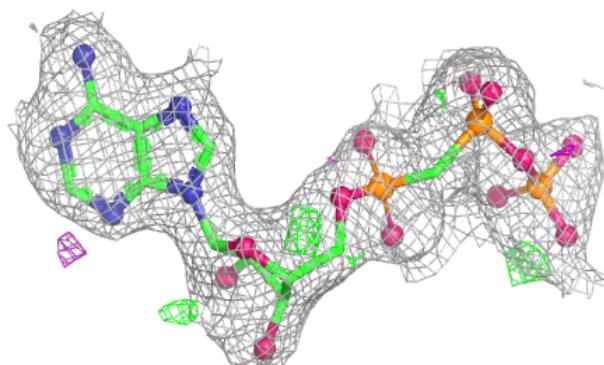


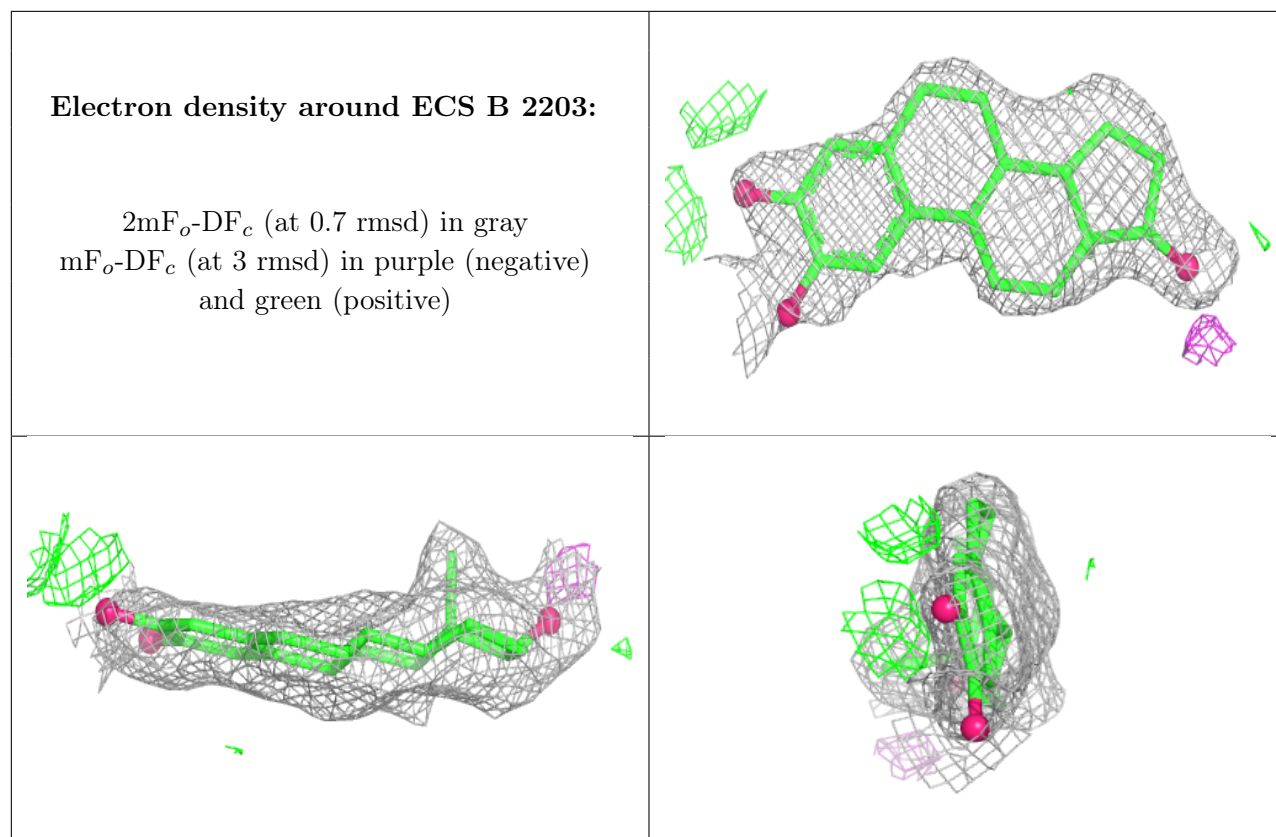
Electron density around APC B 2200:

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

**Electron density around APC 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.