Full wwPDB X-ray Structure Validation Report (i)

Oct 26, 2026 – 06:24 PM EDT

PDB ID	:	37TG / pdb_000037tg
Title	:	Minimal diadenylate cyclase from E. coli PanDA immune system - IEX
Authors	:	Nabhani, A.; Oh, N.; Otsuki, G.F.; Morehouse, B.R.
Deposited on	:	2026-08-04
Resolution	:	1.99 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 (i) 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 (i)) were used in the production of this report:

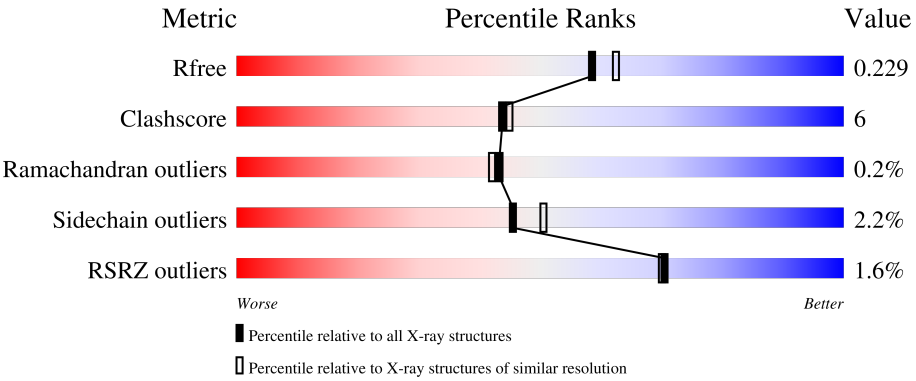
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 1.99 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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 <=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	146	2% 79% 18%
1	B	146	88% 10%
1	C	146	2% 88% 12%
1	D	146	2% 88% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	A1AEP	B	203	X	-	-	-
3	A1AEP	C	201	X	-	-	-

2 Entry composition

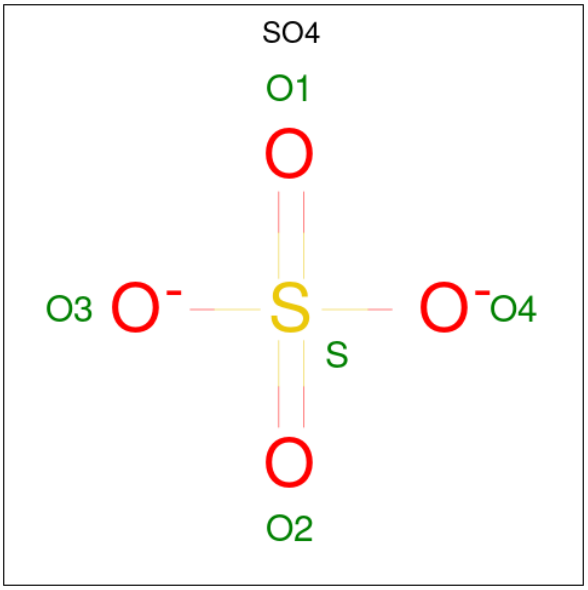
There are 4 unique types of molecules in this entry. The entry contains 4752 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Diadenylate cyclase PanS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	143	Total	C	N	O	S	0	0	0
			1136	727	186	220	3			
1	B	143	Total	C	N	O	S	0	0	0
			1136	725	186	222	3			
1	C	146	Total	C	N	O	S	0	0	0
			1161	740	191	227	3			
1	D	143	Total	C	N	O	S	0	0	0
			1136	725	186	222	3			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



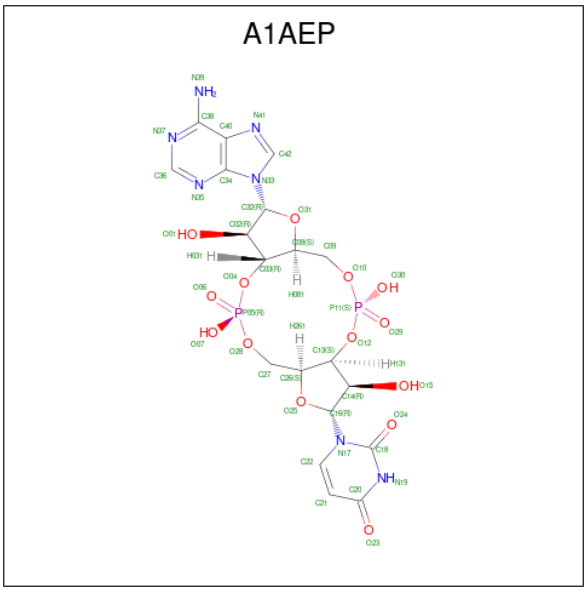
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 3 is 3'3'-cUMP-AMP (CCD ID: A1AEP) (formula: $C_{19}H_{23}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C N O P 42 19 7 14 2	0	0
3	C	1	Total C N O P 42 19 7 14 2	0	0

- Molecule 4 is water.

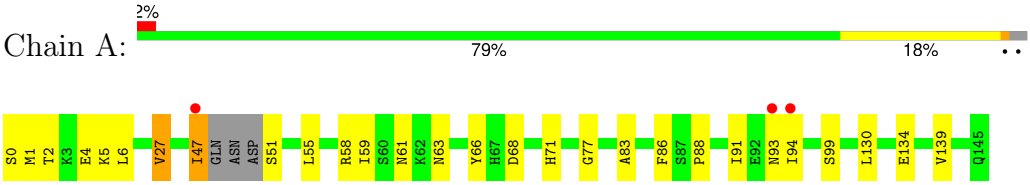
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	9	Total O 9 9	0	0
4	B	31	Total O 31 31	0	0
4	C	19	Total O 19 19	0	0
4	D	15	Total O 15 15	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

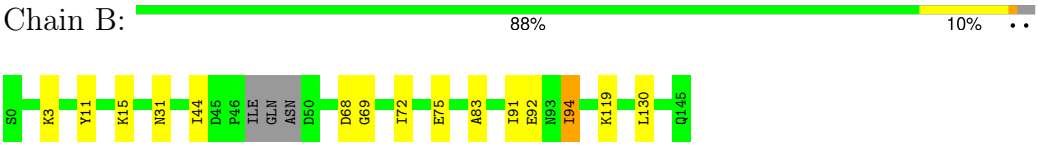
• Molecule 1: Diadenylate cyclase PanS

Chain A:



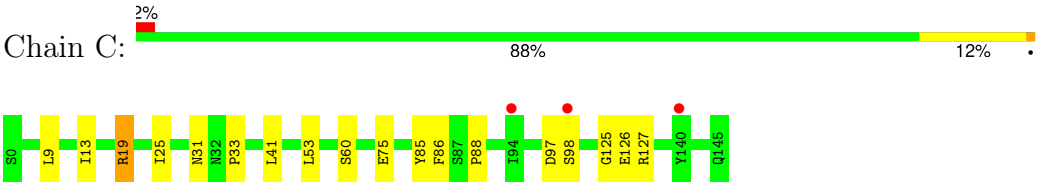
• Molecule 1: Diadenylate cyclase PanS

Chain B:



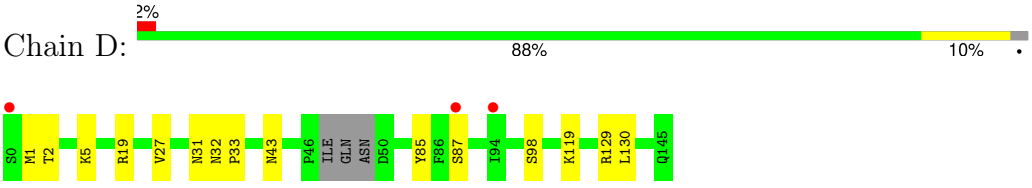
• Molecule 1: Diadenylate cyclase PanS

Chain C:



• Molecule 1: Diadenylate cyclase PanS

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	67.16Å 67.32Å 173.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.84 – 1.99 43.84 – 1.99	Depositor EDS
% Data completeness (in resolution range)	100.0 (43.84-1.99) 99.9 (43.84-1.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.35 (at 2.00Å)	Xtriage
Refinement program	PHENIX 2.1-6048	Depositor
R, R_{free}	0.191 , 0.230 0.193 , 0.229	Depositor DCC
R_{free} test set	1996 reflections (3.64%)	wwPDB-VP
Wilson B-factor (Å^2)	42.0	Xtriage
Anisotropy	0.556	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 47.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.066 for k,h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4752	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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: SO4, A1AEP

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	0.55	0/1158	0.73	0/1562
1	B	0.87	0/1158	0.93	0/1562
1	C	0.58	0/1184	0.79	0/1599
1	D	0.61	0/1158	0.81	0/1562
All	All	0.66	0/4658	0.82	0/6285

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	1136	0	1130	17	0
1	B	1136	0	1123	13	0
1	C	1161	0	1149	16	0
1	D	1136	0	1123	11	0
2	A	5	0	0	0	0
2	B	10	0	0	0	0
2	D	10	0	0	1	0
3	B	42	0	0	2	0
3	C	42	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	9	0	0	0	0
4	B	31	0	0	0	0
4	C	19	0	0	0	0
4	D	15	0	0	0	0
All	All	4752	0	4525	56	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 (56) 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)
3:C:201:A1AEP:C08	3:C:201:A1AEP:O31	1.65	1.25
1:B:31:ASN:H	1:B:119:LYS:HZ3	0.98	0.90
1:C:127:ARG:HD2	1:C:127:ARG:H	1.50	0.75
1:B:31:ASN:H	1:B:119:LYS:NZ	1.85	0.68
1:D:129:ARG:HH11	1:D:129:ARG:HG3	1.59	0.67
1:D:85:TYR:CE2	1:D:87:SER:HB2	2.36	0.60
1:D:2:THR:OG1	1:D:5:LYS:HG3	2.02	0.59
1:A:86:PHE:O	1:A:88:PRO:HD3	2.03	0.58
1:B:31:ASN:N	1:B:119:LYS:HZ3	1.84	0.55
1:A:61:ASN:HB3	1:A:63:ASN:OD1	2.07	0.55
1:C:13:ILE:HD13	1:C:53:LEU:HD12	1.90	0.53
1:A:86:PHE:CE2	1:A:88:PRO:HG3	2.44	0.53
1:C:9:LEU:O	1:C:13:ILE:HG12	2.09	0.53
1:A:47:ILE:HG13	1:A:58:ARG:HH22	1.75	0.52
1:A:130:LEU:C	1:A:130:LEU:HD23	2.36	0.51
1:C:25:ILE:HD12	1:C:60:SER:OG	2.11	0.51
1:B:75:GLU:OE2	1:B:119:LYS:HE2	2.13	0.48
1:D:31:ASN:C	1:D:33:PRO:HD3	2.38	0.48
1:B:119:LYS:N	1:B:119:LYS:HD2	2.30	0.47
1:B:69:GLY:HA2	3:B:203:A1AEP:C22	2.44	0.47
1:C:31:ASN:OD1	1:C:75:GLU:HG3	2.15	0.46
1:C:31:ASN:O	1:C:33:PRO:HD3	2.16	0.46
1:C:19:ARG:H	1:C:19:ARG:HG3	1.13	0.46
1:C:126:GLU:N	1:C:127:ARG:HH11	2.14	0.46
1:B:130:LEU:C	1:B:130:LEU:HD23	2.41	0.46
1:B:11:TYR:CZ	1:B:15:LYS:HE2	2.51	0.45
1:A:1:MET:HE2	1:A:77:GLY:HA2	1.99	0.45
1:C:41:LEU:HD21	1:C:85:TYR:HB2	1.98	0.45
1:B:68:ASP:O	1:B:83:ALA:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:GLU:H	1:C:127:ARG:HH11	1.62	0.45
1:A:55:LEU:O	1:A:59:ILE:HG12	2.17	0.45
1:A:134:GLU:HB3	1:A:139:VAL:HG11	1.99	0.44
1:A:91:ILE:HB	1:A:94:ILE:HG12	1.98	0.44
1:B:92:GLU:H	1:B:92:GLU:CD	2.26	0.43
1:A:2:THR:HG23	1:A:5:LYS:H	1.84	0.43
1:D:130:LEU:C	1:D:130:LEU:HD23	2.44	0.43
1:A:4:GLU:H	1:A:4:GLU:CD	2.27	0.43
1:A:86:PHE:O	3:B:203:A1AEP:N39	2.52	0.43
1:A:86:PHE:C	1:A:88:PRO:HD3	2.44	0.42
1:A:68:ASP:O	1:A:83:ALA:HA	2.20	0.42
1:B:91:ILE:HB	1:B:94:ILE:HG13	2.01	0.42
1:D:32:ASN:O	1:D:32:ASN:OD1	2.36	0.42
1:D:1:MET:O	1:D:119:LYS:HE2	2.19	0.42
1:D:129:ARG:HD2	2:D:202:SO4:O4	2.20	0.42
1:B:3:LYS:HB2	1:B:3:LYS:HE2	1.89	0.41
1:C:98:SER:HB3	1:D:43:ASN:ND2	2.34	0.41
1:C:86:PHE:O	1:C:88:PRO:HD3	2.20	0.41
1:C:98:SER:HB3	1:D:43:ASN:HD21	1.86	0.41
1:C:125:GLY:HA3	1:C:127:ARG:CD	2.49	0.41
1:A:66:TYR:O	1:A:71:HIS:HE1	2.03	0.41
1:A:6:LEU:HD11	1:A:27:VAL:HG21	2.02	0.41
1:B:44:ILE:HG21	1:B:44:ILE:HD13	1.66	0.41
1:C:125:GLY:HA3	1:C:127:ARG:HH11	1.86	0.41
1:C:125:GLY:CA	1:C:127:ARG:HH11	2.34	0.41
1:D:85:TYR:HE2	1:D:87:SER:HB2	1.85	0.41
1:A:0:SER:HB3	1:A:1:MET:H	1.60	0.41

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	139/146 (95%)	135 (97%)	4 (3%)	0	100 100
1	B	139/146 (95%)	137 (99%)	2 (1%)	0	100 100
1	C	144/146 (99%)	141 (98%)	2 (1%)	1 (1%)	18 14
1	D	139/146 (95%)	137 (99%)	2 (1%)	0	100 100
All	All	561/584 (96%)	550 (98%)	10 (2%)	1 (0%)	43 42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	97	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	126/129 (98%)	121 (96%)	5 (4%)	28 27
1	B	126/129 (98%)	124 (98%)	2 (2%)	55 62
1	C	129/129 (100%)	128 (99%)	1 (1%)	73 80
1	D	126/129 (98%)	123 (98%)	3 (2%)	43 47
All	All	507/516 (98%)	496 (98%)	11 (2%)	45 50

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	VAL
1	A	47	ILE
1	A	51	SER
1	A	93	ASN
1	A	99	SER
1	B	72	ILE
1	B	94	ILE
1	C	19	ARG
1	D	19	ARG
1	D	27	VAL

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Mol	Chain	Res	Type
1	D	98	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	HIS
1	A	84	GLN
1	B	43	ASN
1	B	63	ASN
1	B	84	GLN
1	C	48	GLN
1	C	84	GLN
1	D	32	ASN
1	D	43	ASN
1	D	78	ASN
1	D	84	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry

7 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SO4	B	202	-	4,4,4	0.73	0	6,6,6	0.31	0
2	SO4	D	201	-	4,4,4	0.67	0	6,6,6	0.35	0
2	SO4	B	201	-	4,4,4	0.91	0	6,6,6	0.45	0
3	A1AEP	B	203	-	47,47,47	3.43	20 (42%)	69,73,73	3.38	39 (56%)
2	SO4	A	201	-	4,4,4	0.79	0	6,6,6	0.29	0
3	A1AEP	C	201	-	47,47,47	3.43	21 (44%)	69,73,73	3.17	28 (40%)
2	SO4	D	202	-	4,4,4	0.68	0	6,6,6	0.31	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A1AEP	B	203	-	4/4/10/10	7/30/62/62	0/5/6/6
3	A1AEP	C	201	-	2/2/10/10	3/30/62/62	0/5/6/6

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	201	A1AEP	O31-C08	9.25	1.65	1.45
3	C	201	A1AEP	C18-N19	8.58	1.52	1.38
3	B	203	A1AEP	O31-C08	8.15	1.63	1.45
3	C	201	A1AEP	C18-N17	8.11	1.51	1.38
3	B	203	A1AEP	C18-N17	7.84	1.50	1.38
3	B	203	A1AEP	C18-N19	7.54	1.51	1.38
3	B	203	A1AEP	C03-C08	-6.66	1.35	1.52
3	C	201	A1AEP	C13-C26	-6.56	1.35	1.52
3	B	203	A1AEP	C13-C26	-6.50	1.36	1.52
3	C	201	A1AEP	C03-C08	-5.59	1.38	1.52
3	B	203	A1AEP	C38-N39	5.52	1.48	1.34
3	C	201	A1AEP	O25-C26	5.47	1.57	1.45
3	B	203	A1AEP	O25-C26	5.36	1.56	1.45
3	C	201	A1AEP	C38-N39	5.34	1.47	1.34
3	B	203	A1AEP	O31-C32	-5.30	1.29	1.42
3	C	201	A1AEP	C20-N19	5.12	1.47	1.38
3	C	201	A1AEP	O25-C16	4.94	1.53	1.42
3	B	203	A1AEP	C22-N17	4.71	1.49	1.38
3	C	201	A1AEP	C22-C21	4.61	1.45	1.35
3	C	201	A1AEP	C14-C16	-4.59	1.39	1.53
3	B	203	A1AEP	C22-C21	4.47	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	203	A1AEP	C20-N19	4.46	1.46	1.38
3	B	203	A1AEP	O25-C16	4.30	1.51	1.42
3	B	203	A1AEP	C14-C16	-4.25	1.40	1.53
3	B	203	A1AEP	P05-O04	4.13	1.71	1.59
3	C	201	A1AEP	P05-O04	3.55	1.70	1.59
3	C	201	A1AEP	O31-C32	-3.49	1.33	1.42
3	B	203	A1AEP	C14-C13	3.44	1.60	1.53
3	B	203	A1AEP	P11-O12	3.39	1.69	1.59
3	C	201	A1AEP	C22-N17	3.30	1.46	1.38
3	C	201	A1AEP	O01-C02	-3.02	1.35	1.43
3	B	203	A1AEP	O01-C02	-3.01	1.35	1.43
3	B	203	A1AEP	C16-N17	2.78	1.55	1.47
3	C	201	A1AEP	P11-O12	2.68	1.67	1.59
3	C	201	A1AEP	C14-C13	2.50	1.58	1.53
3	C	201	A1AEP	C27-C26	2.34	1.58	1.51
3	C	201	A1AEP	P11-O10	2.30	1.68	1.59
3	C	201	A1AEP	O24-C18	-2.24	1.19	1.23
3	B	203	A1AEP	O23-C20	-2.10	1.20	1.24
3	C	201	A1AEP	O23-C20	-2.10	1.20	1.24
3	B	203	A1AEP	O24-C18	-2.06	1.19	1.23

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	201	A1AEP	C02-C03-C08	-13.19	80.14	103.24
3	B	203	A1AEP	C02-C32-N33	9.39	136.63	113.30
3	C	201	A1AEP	C02-C32-N33	8.48	134.37	113.30
3	C	201	A1AEP	O31-C32-N33	-7.28	94.10	108.09
3	B	203	A1AEP	O31-C32-N33	-7.25	94.16	108.09
3	B	203	A1AEP	C40-C34-N35	-7.21	116.78	126.72
3	B	203	A1AEP	O28-C27-C26	-7.19	84.51	108.99
3	C	201	A1AEP	O15-C14-C13	-7.04	91.49	111.19
3	B	203	A1AEP	O10-C09-C08	-6.94	85.35	108.99
3	B	203	A1AEP	N35-C34-N33	6.64	138.45	127.17
3	B	203	A1AEP	O25-C16-C14	-6.24	93.26	106.62
3	B	203	A1AEP	C21-C20-N19	6.19	123.48	114.80
3	C	201	A1AEP	C40-C34-N35	-5.05	119.76	126.72
3	B	203	A1AEP	C16-N17-C18	5.00	126.57	117.59
3	C	201	A1AEP	O31-C32-C02	-4.97	95.98	106.62
3	B	203	A1AEP	C14-C16-N17	4.92	126.94	113.25
3	C	201	A1AEP	O23-C20-C21	-4.91	116.70	125.16
3	C	201	A1AEP	C14-C13-C26	4.61	111.30	103.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	203	A1AEP	C22-C21-C20	-4.53	113.74	119.53
3	C	201	A1AEP	C21-C20-N19	4.47	121.06	114.80
3	B	203	A1AEP	C16-N17-C22	-4.30	111.59	120.78
3	B	203	A1AEP	C32-N33-C42	-4.29	117.58	127.09
3	B	203	A1AEP	C38-C40-C34	4.24	122.97	117.18
3	B	203	A1AEP	C13-C14-C16	4.15	109.02	99.89
3	C	201	A1AEP	C13-C14-C16	4.07	108.85	99.89
3	C	201	A1AEP	N37-C36-N35	-4.01	122.51	128.58
3	C	201	A1AEP	N35-C34-N33	3.94	133.87	127.17
3	B	203	A1AEP	C08-O31-C32	-3.85	100.97	109.47
3	B	203	A1AEP	C14-C13-C26	-3.80	96.59	103.24
3	B	203	A1AEP	N39-C38-N37	3.73	126.69	118.38
3	B	203	A1AEP	C40-C38-N39	-3.72	114.08	123.29
3	C	201	A1AEP	C08-O31-C32	-3.63	101.45	109.47
3	C	201	A1AEP	O12-C13-C14	3.60	124.57	111.68
3	C	201	A1AEP	C34-N33-C42	3.52	109.43	105.74
3	C	201	A1AEP	N33-C42-N41	-3.49	108.98	113.94
3	B	203	A1AEP	O24-C18-N17	3.39	127.21	122.80
3	C	201	A1AEP	C36-N35-C34	3.35	120.00	111.83
3	B	203	A1AEP	O23-C20-C21	-3.32	119.44	125.16
3	C	201	A1AEP	C20-N19-C18	-3.30	122.52	126.61
3	B	203	A1AEP	O15-C14-C16	3.24	121.28	110.10
3	B	203	A1AEP	C34-N33-C32	3.23	134.19	126.63
3	C	201	A1AEP	O12-C13-C26	3.20	121.31	110.03
3	B	203	A1AEP	C38-C40-N41	-3.06	126.19	132.09
3	B	203	A1AEP	C36-N35-C34	2.98	119.11	111.83
3	B	203	A1AEP	C26-O25-C16	-2.95	102.96	109.47
3	C	201	A1AEP	C34-N33-C32	-2.89	119.88	126.63
3	B	203	A1AEP	C02-C03-C08	-2.85	98.25	103.24
3	B	203	A1AEP	O25-C26-C13	2.83	110.89	104.92
3	C	201	A1AEP	O12-P11-O29	-2.78	100.91	109.81
3	C	201	A1AEP	O01-C02-C03	2.57	118.38	111.19
3	B	203	A1AEP	C27-C26-C13	2.57	122.94	114.38
3	B	203	A1AEP	O25-C16-N17	2.53	114.10	108.36
3	C	201	A1AEP	O10-C09-C08	-2.46	100.63	108.99
3	B	203	A1AEP	O12-C13-C26	2.40	118.49	110.03
3	B	203	A1AEP	O01-C02-C32	-2.36	101.97	110.10
3	B	203	A1AEP	O07-P05-O06	2.35	123.39	112.44
3	C	201	A1AEP	C40-N41-C42	2.30	107.07	103.45
3	C	201	A1AEP	O24-C18-N19	2.30	125.72	121.49
3	B	203	A1AEP	O30-P11-O12	2.24	115.81	106.70
3	B	203	A1AEP	C34-N33-C42	2.23	108.08	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	201	A1AEP	C34-C40-N41	-2.15	108.13	110.58
3	B	203	A1AEP	C20-N19-C18	-2.13	123.97	126.61
3	B	203	A1AEP	O31-C08-C03	2.12	109.39	104.92
3	B	203	A1AEP	N19-C18-N17	-2.11	112.15	114.89
3	C	201	A1AEP	O30-P11-O12	2.07	115.11	106.70
3	C	201	A1AEP	O04-P05-O06	-2.06	103.23	109.81
3	B	203	A1AEP	O12-P11-O29	-2.05	103.24	109.81

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	203	A1AEP	C14
3	B	203	A1AEP	C08
3	B	203	A1AEP	C26
3	B	203	A1AEP	C02
3	C	201	A1AEP	C13
3	C	201	A1AEP	C02

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	203	A1AEP	O25-C16-N17-C22
3	B	203	A1AEP	O25-C16-N17-C18
3	C	201	A1AEP	C14-C13-O12-P11
3	B	203	A1AEP	C13-C26-C27-O28
3	C	201	A1AEP	O25-C26-C27-O28
3	B	203	A1AEP	O31-C32-N33-C34
3	C	201	A1AEP	C13-C26-C27-O28
3	B	203	A1AEP	O31-C32-N33-C42
3	B	203	A1AEP	C03-C08-C09-O10
3	B	203	A1AEP	C27-O28-P05-O06

There are no ring outliers.

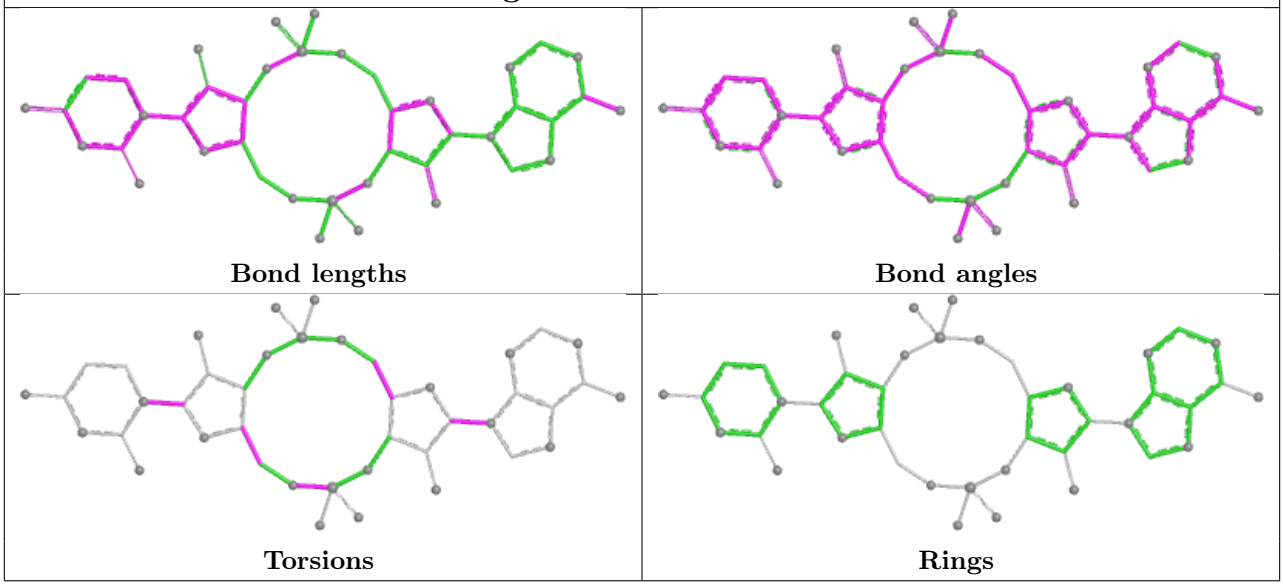
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	203	A1AEP	2	0
3	C	201	A1AEP	1	0
2	D	202	SO4	1	0

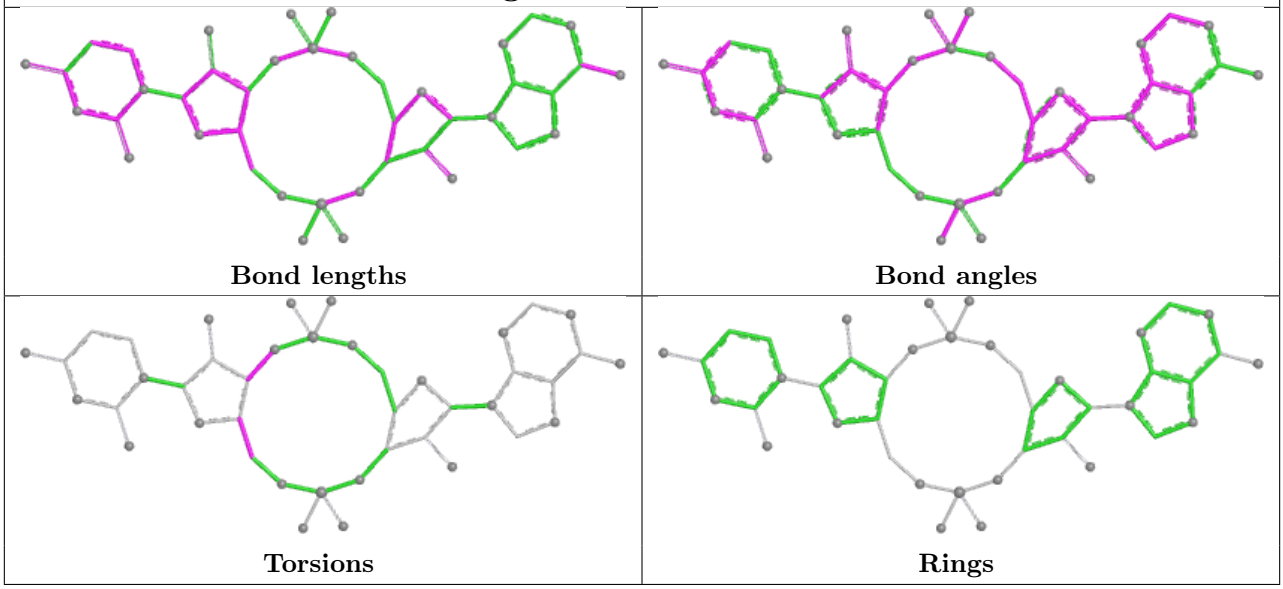
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 A1AEP B 203



Ligand A1AEP C 201



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, 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	143/146 (97%)	0.55	3 (2%) 63 63	40, 70, 97, 110	0
1	B	143/146 (97%)	0.17	0 100 100	34, 46, 79, 110	0
1	C	146/146 (100%)	0.41	3 (2%) 63 63	41, 61, 95, 120	0
1	D	143/146 (97%)	0.26	3 (2%) 63 63	40, 57, 90, 115	0
All	All	575/584 (98%)	0.35	9 (1%) 70 70	34, 58, 96, 120	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	47	ILE	5.0
1	C	98	SER	4.2
1	D	87	SER	3.9
1	C	94	ILE	2.7
1	C	140	TYR	2.3
1	A	94	ILE	2.2
1	A	93	ASN	2.2
1	D	94	ILE	2.1
1	D	0	SER	2.1

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands (i)

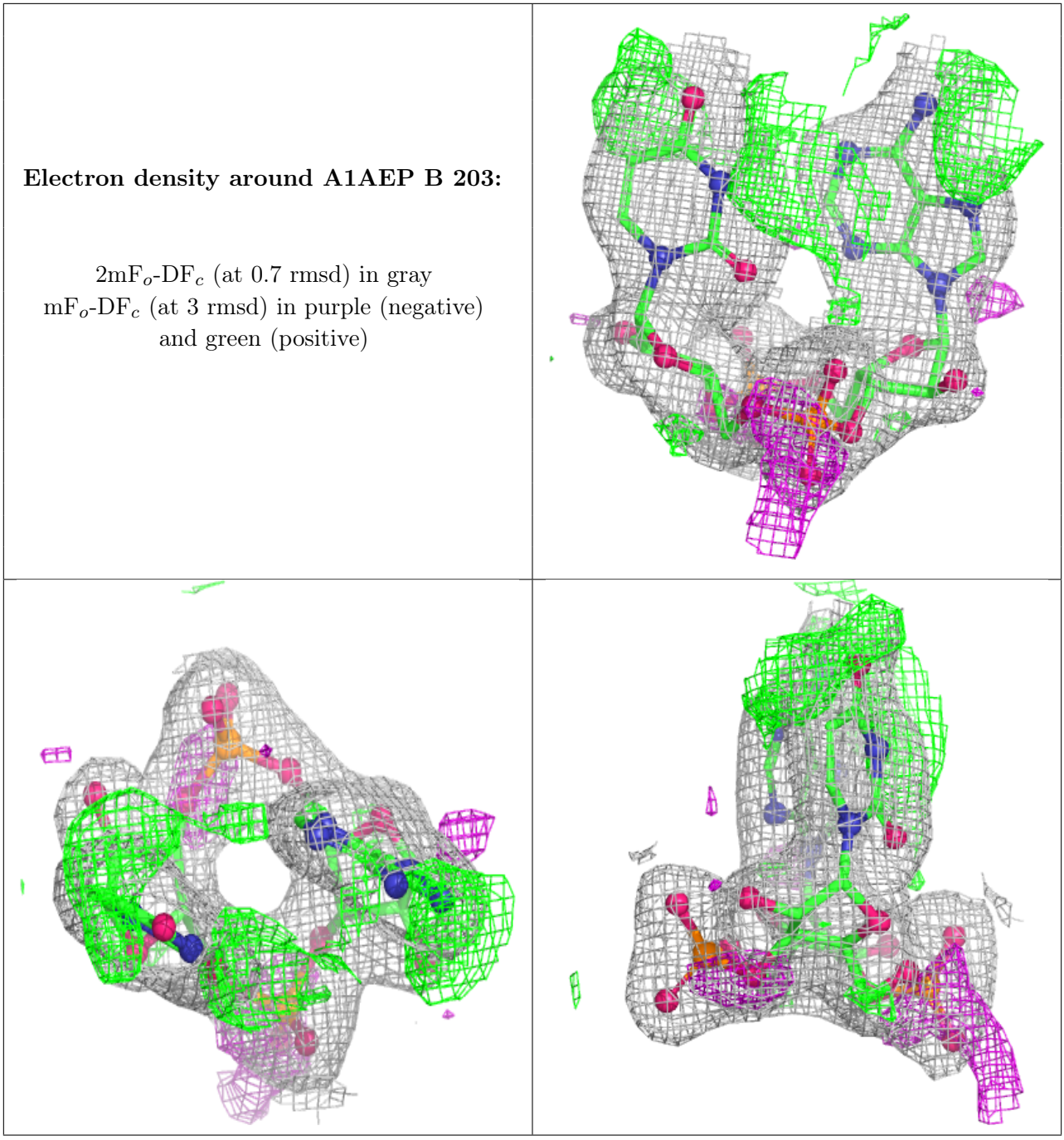
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	A1AEP	B	203	42/42	0.92	0.11	36,49,58,65	0
2	SO4	A	201	5/5	0.94	0.07	68,71,83,86	0
3	A1AEP	C	201	42/42	0.95	0.08	40,49,59,73	0
2	SO4	B	202	5/5	0.96	0.07	44,54,68,72	0
2	SO4	B	201	5/5	0.97	0.09	38,43,50,52	0
2	SO4	D	201	5/5	0.97	0.05	44,55,60,65	0
2	SO4	D	202	5/5	0.98	0.04	50,53,64,68	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.

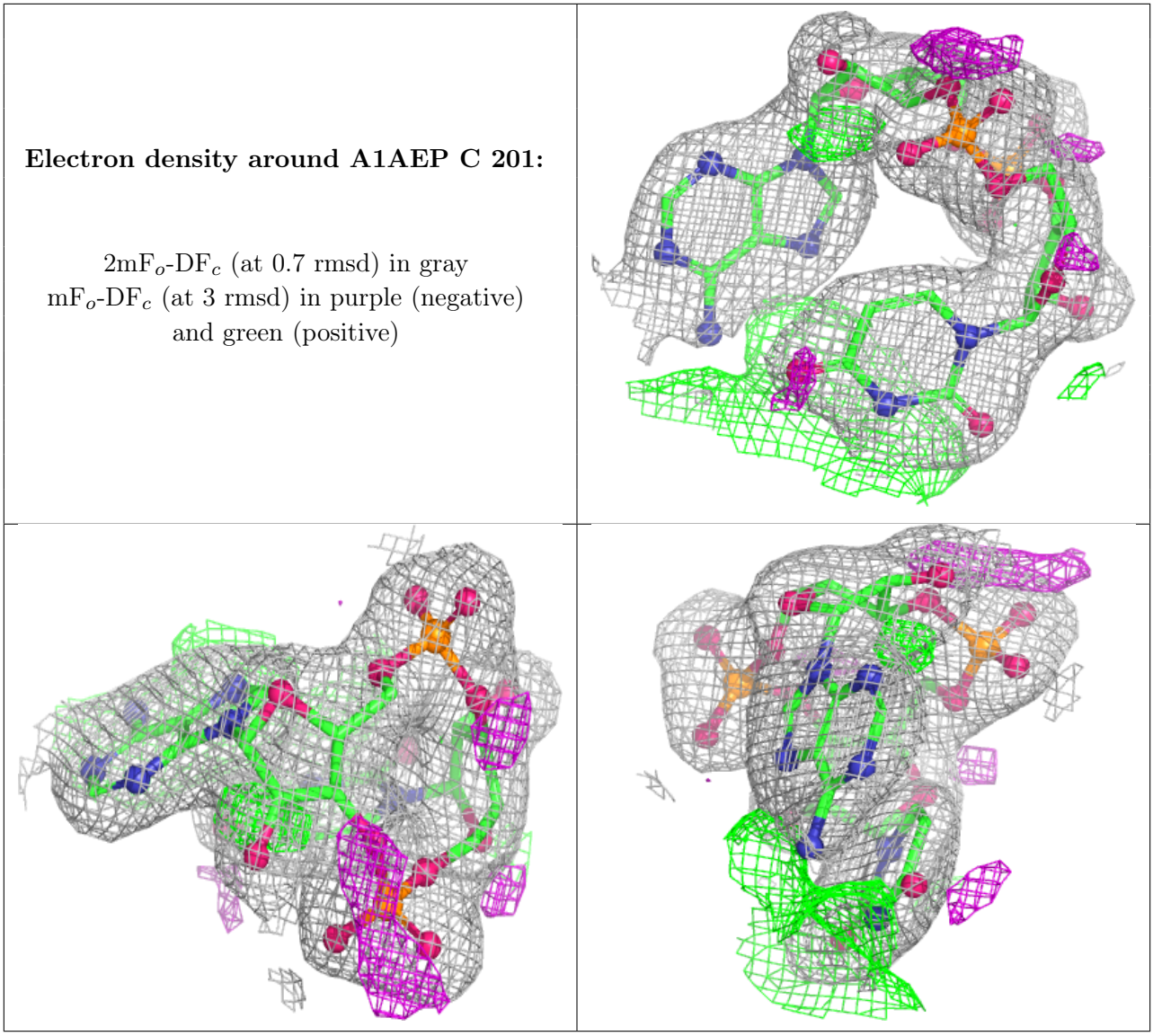
Electron density around A1AEP B 203:

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



Electron density around A1AEP C 201:

$2mF_o$-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.