Full wwPDB X-ray Structure Validation Report (i)

Apr 29, 2024 – 05:23 am BST

PDB ID	:	1W25
Title	:	Response regulator PleD in complex with c-diGMP
Authors	:	Chan, C.; Schirmer, T.; Jenal, U.
Deposited on	:	2004-06-28
Resolution	:	2.70 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:

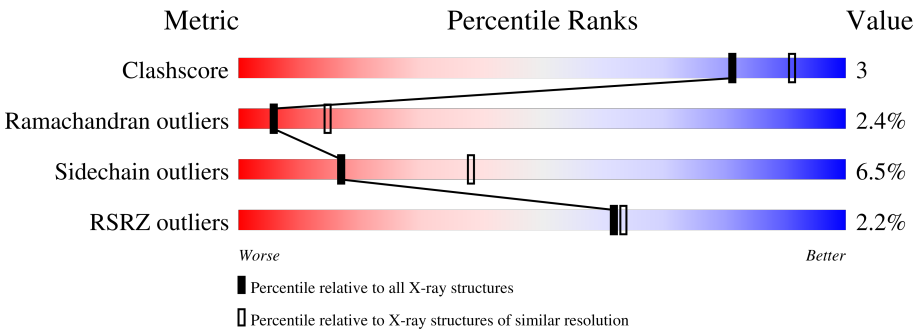
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.70 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))
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	459	2% 83% 12%
1	B	459	2% 84% 11%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7210 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 STALKED-CELL DIFFERENTIATION CONTROLLING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	454	3481	2166	639	661	15	164	0	0
1	B	454	3481	2166	639	661	15	164	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	455	HIS	-	expression tag	UNP Q9A5I5
A	456	HIS	-	expression tag	UNP Q9A5I5
A	457	HIS	-	expression tag	UNP Q9A5I5
A	458	HIS	-	expression tag	UNP Q9A5I5
A	459	HIS	-	expression tag	UNP Q9A5I5
A	460	HIS	-	expression tag	UNP Q9A5I5
B	455	HIS	-	expression tag	UNP Q9A5I5
B	456	HIS	-	expression tag	UNP Q9A5I5
B	457	HIS	-	expression tag	UNP Q9A5I5
B	458	HIS	-	expression tag	UNP Q9A5I5
B	459	HIS	-	expression tag	UNP Q9A5I5
B	460	HIS	-	expression tag	UNP Q9A5I5

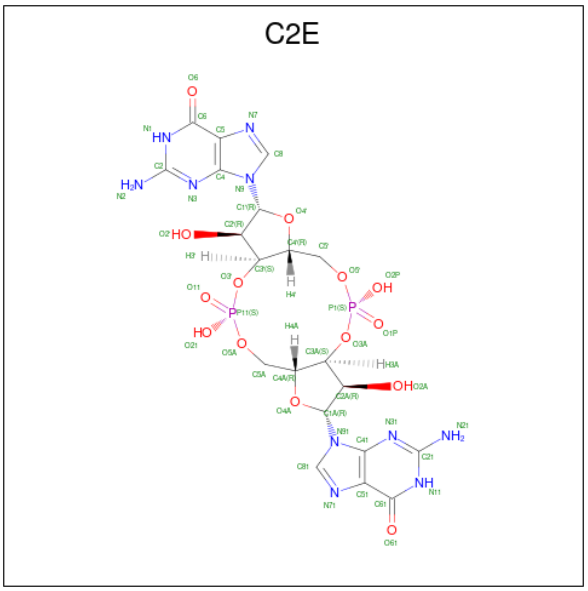
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	1	1	1	0	0

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

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

- Molecule 4 is 9,9'-[(2R,3R,3aS,5S,7aR,9R,10R,10aS,12S,14aR)-3,5,10,12-tetrahydroxy-5,12-dioxidooctahydro-2H,7H-difuro[3,2-d:3',2'-j][1,3,7,9,2,8]tetraoxadiphosphacyclododecine-2,9-diyl]bis(2-amino-1,9-dihydro-6H-purin-6-one) (three-letter code: C2E) (formula: $C_{20}H_{24}N_{10}O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	46	20	10	14	2	0	0
			Total	C	N	O	P		
4	A	1	46	20	10	14	2	0	0
			Total	C	N	O	P		
4	A	1	46	20	10	14	2	0	0
			Total	C	N	O	P		
4	B	1	46	20	10	14	2	0	0
			Total	C	N	O	P		
4	B	1	46	20	10	14	2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	7	7	7	0	0

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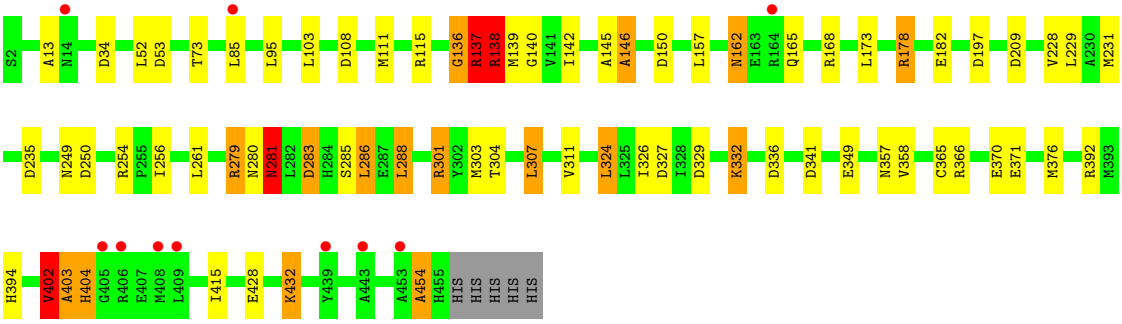
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	B	8	8	8	0	0

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.

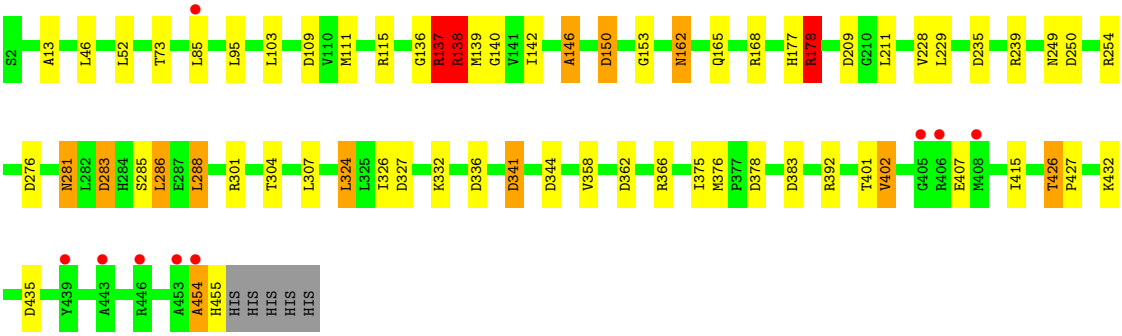
• Molecule 1: STALKED-CELL DIFFERENTIATION CONTROLLING PROTEIN

Chain A:



• Molecule 1: STALKED-CELL DIFFERENTIATION CONTROLLING PROTEIN

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	135.87Å 135.87Å 169.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 60.76 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.9 (50.00-2.70) 98.9 (60.76-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.03 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2.0001	Depositor
R, R_{free}	0.210 , 0.239 0.218 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	50.1	Xtriage
Anisotropy	0.371	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 29.1	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	7210	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, C2E, 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	0.91	9/3525 (0.3%)	1.43	32/4765 (0.7%)
1	B	0.92	6/3525 (0.2%)	1.33	27/4765 (0.6%)
All	All	0.91	15/7050 (0.2%)	1.38	59/9530 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
1	B	0	4
All	All	0	12

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	136	GLY	C-N	-29.09	0.67	1.34
1	B	301	ARG	CD-NE	-27.91	0.99	1.46
1	B	281	ASN	C-N	-27.30	0.71	1.34
1	A	281	ASN	C-N	-23.50	0.80	1.34
1	A	301	ARG	CD-NE	-18.24	1.15	1.46
1	B	281	ASN	CB-CG	-17.03	1.11	1.51
1	A	454	ALA	C-N	-15.58	0.98	1.34
1	B	332	LYS	CE-NZ	-13.69	1.14	1.49
1	B	136	GLY	C-N	-13.50	1.02	1.34
1	A	332	LYS	CE-NZ	-10.29	1.23	1.49
1	A	283	ASP	C-N	7.44	1.51	1.34
1	B	283	ASP	C-N	7.42	1.51	1.34
1	A	279	ARG	CG-CD	-6.76	1.35	1.51
1	A	402	VAL	CB-CG2	-5.96	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	402	VAL	CB-CG1	5.22	1.63	1.52

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	281	ASN	O-C-N	-53.76	36.68	122.70
1	B	281	ASN	O-C-N	-52.33	38.97	122.70
1	A	454	ALA	O-C-N	-47.08	47.37	122.70
1	B	454	ALA	O-C-N	-30.80	73.42	122.70
1	B	281	ASN	C-N-CA	-16.01	81.68	121.70
1	B	281	ASN	CA-C-N	-15.76	82.53	117.20
1	B	332	LYS	CD-CE-NZ	13.01	141.62	111.70
1	B	288	LEU	C-N-CA	12.57	153.13	121.70
1	A	332	LYS	CD-CE-NZ	11.77	138.76	111.70
1	A	281	ASN	CA-C-N	-10.25	94.65	117.20
1	A	281	ASN	CB-CG-ND2	-9.90	92.93	116.70
1	A	281	ASN	CA-CB-CG	-9.62	92.23	113.40
1	B	136	GLY	O-C-N	9.57	138.01	122.70
1	A	402	VAL	CA-CB-CG2	8.89	124.24	110.90
1	B	146	ALA	C-N-CA	-8.30	100.94	121.70
1	B	136	GLY	CA-C-N	-7.65	100.38	117.20
1	A	146	ALA	C-N-CA	-7.54	102.84	121.70
1	A	146	ALA	O-C-N	7.28	134.34	122.70
1	A	145	ALA	CA-C-N	-7.20	101.36	117.20
1	B	301	ARG	CG-CD-NE	6.37	125.17	111.80
1	A	150	ASP	CB-CG-OD2	6.32	123.99	118.30
1	B	138	ARG	C-N-CA	-6.30	105.95	121.70
1	A	402	VAL	CA-CB-CG1	6.29	120.34	110.90
1	B	150	ASP	CB-CG-OD2	6.19	123.87	118.30
1	A	138	ARG	C-N-CA	-5.97	106.78	121.70
1	A	108	ASP	CB-CG-OD2	5.94	123.65	118.30
1	A	288	LEU	CA-C-N	-5.94	104.14	117.20
1	A	301	ARG	CD-NE-CZ	-5.88	115.37	123.60
1	B	137	ARG	N-CA-C	-5.88	95.14	111.00
1	A	209	ASP	CB-CG-OD2	5.83	123.54	118.30
1	A	281	ASN	CB-CG-OD1	5.79	133.17	121.60
1	B	146	ALA	O-C-N	5.72	131.86	122.70
1	B	178	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	137	ARG	N-CA-CB	5.70	120.86	110.60
1	B	383	ASP	CB-CG-OD2	5.65	123.38	118.30
1	B	109	ASP	CB-CG-OD2	5.50	123.25	118.30
1	A	336	ASP	CB-CG-OD2	5.50	123.25	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	288	LEU	O-C-N	5.49	131.49	122.70
1	B	250	ASP	CB-CG-OD2	5.46	123.22	118.30
1	A	235	ASP	CB-CG-OD2	5.45	123.20	118.30
1	A	146	ALA	CA-C-N	-5.41	105.30	117.20
1	B	235	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	250	ASP	CB-CG-OD2	5.37	123.14	118.30
1	B	378	ASP	CB-CG-OD2	5.33	123.09	118.30
1	A	53	ASP	CB-CG-OD2	5.32	123.09	118.30
1	B	276	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	197	ASP	CB-CG-OD2	5.30	123.07	118.30
1	B	362	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	344	ASP	CB-CG-OD2	5.27	123.04	118.30
1	A	432	LYS	CB-CG-CD	5.25	125.24	111.60
1	B	341	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	435	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	329	ASP	CB-CG-OD2	5.21	122.99	118.30
1	B	336	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	34	ASP	CB-CG-OD2	5.17	122.95	118.30
1	B	209	ASP	CB-CG-OD2	5.15	122.94	118.30
1	A	327	ASP	CB-CG-OD2	5.14	122.93	118.30
1	A	145	ALA	O-C-N	5.09	130.85	122.70
1	A	136	GLY	C-N-CA	5.08	134.41	121.70

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	136	GLY	Mainchain
1	A	281	ASN	Peptide,Mainchain,Sidechain
1	A	288	LEU	Peptide
1	A	301	ARG	Sidechain
1	A	454	ALA	Peptide,Mainchain
1	B	281	ASN	Mainchain
1	B	288	LEU	Mainchain
1	B	454	ALA	Peptide,Mainchain

5.2 Too-close contacts (i)

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	3481	0	3548	21	3
1	B	3481	0	3548	15	6
2	A	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	138	0	66	1	0
4	B	92	0	44	1	0
5	A	7	0	0	1	0
5	B	8	0	0	1	0
All	All	7210	0	7206	36	9

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 3.

All (36) 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:165:GLN:HE22	1:B:254:ARG:HD2	1.56	0.71
1:B:73:THR:HG21	5:B:2004:HOH:O	1.92	0.69
1:B:228:VAL:H	1:B:249:ASN:HD22	1.41	0.68
1:B:162:ASN:C	1:B:162:ASN:HD22	2.01	0.61
1:A:231:MET:SD	1:A:256:ILE:HD11	2.41	0.60
1:A:111:MET:CE	1:A:115:ARG:HH22	2.16	0.58
1:B:111:MET:CE	1:B:115:ARG:HH22	2.17	0.56
1:B:426:THR:HG22	1:B:427:PRO:HD2	1.88	0.55
1:B:228:VAL:H	1:B:249:ASN:ND2	2.05	0.55
1:A:324:LEU:HD13	1:A:376:MET:CE	2.37	0.54
1:A:73:THR:HG21	5:A:2002:HOH:O	2.07	0.54
1:B:178:ARG:NH2	4:B:503:C2E:N7	2.60	0.50
1:A:157:LEU:HD11	1:A:182:GLU:HG3	1.95	0.48
1:A:178:ARG:NH2	4:A:503:C2E:N7	2.62	0.47
1:B:324:LEU:HD13	1:B:376:MET:CE	2.44	0.47
1:B:162:ASN:C	1:B:162:ASN:ND2	2.68	0.47
1:A:173:LEU:HD21	1:A:261:LEU:HG	1.96	0.47
1:A:162:ASN:C	1:A:162:ASN:HD22	2.18	0.46
1:B:326:ILE:HD13	1:B:415:ILE:HG23	1.97	0.46
1:A:307:LEU:HD22	1:A:311:VAL:HG23	1.97	0.46
1:A:324:LEU:HD13	1:A:376:MET:HE1	1.99	0.45
1:B:111:MET:HE2	1:B:115:ARG:HH22	1.82	0.45
1:A:326:ILE:HD13	1:A:415:ILE:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:ALA:O	1:A:404:HIS:C	2.56	0.44
1:A:428:GLU:OE1	1:A:428:GLU:N	2.50	0.44
1:A:324:LEU:HD13	1:A:376:MET:HE2	2.00	0.43
1:A:228:VAL:H	1:A:249:ASN:HD22	1.66	0.43
1:A:332:LYS:HE3	1:A:370:GLU:OE2	2.18	0.43
1:B:153:GLY:O	1:B:177:HIS:ND1	2.47	0.42
1:A:402:VAL:HB	1:A:403:ALA:H	1.58	0.42
1:A:303:MET:HB2	1:A:365:CYS:SG	2.60	0.42
1:B:46:LEU:HD21	1:B:73:THR:HG22	2.02	0.41
1:A:165:GLN:HE22	1:A:254:ARG:HD2	1.84	0.41
1:A:231:MET:SD	1:A:256:ILE:CD1	3.06	0.41
1:B:211:LEU:HD22	1:B:239:ARG:CZ	2.51	0.41
1:A:357:ASN:HD21	1:A:394:HIS:CE1	2.39	0.41

All (9) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:ARG:NH2	1:B:341:ASP:OD2[8_666]	0.63	1.57
1:A:138:ARG:NH2	1:A:341:ASP:OD2[8_666]	1.12	1.08
1:B:138:ARG:NH2	1:B:341:ASP:CG[8_666]	1.59	0.61
1:B:137:ARG:NH1	1:B:407:GLU:CG[8_666]	1.67	0.53
1:A:138:ARG:NH2	1:A:341:ASP:CG[8_666]	1.89	0.31
1:B:138:ARG:CZ	1:B:341:ASP:OD2[8_666]	1.95	0.25
1:A:138:ARG:CZ	1:A:341:ASP:OD2[8_666]	1.98	0.22
1:B:137:ARG:NH1	1:B:407:GLU:CD[8_666]	2.00	0.20
1:B:137:ARG:NH1	1:B:407:GLU:OE2[8_666]	2.18	0.02

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	452/459 (98%)	428 (95%)	11 (2%)	13 (3%)	4 10
1	B	452/459 (98%)	430 (95%)	13 (3%)	9 (2%)	7 19
All	All	904/918 (98%)	858 (95%)	24 (3%)	22 (2%)	6 15

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	ALA
1	A	281	ASN
1	A	286	LEU
1	A	403	ALA
1	B	146	ALA
1	B	286	LEU
1	A	13	ALA
1	A	137	ARG
1	A	140	GLY
1	A	142	ILE
1	A	402	VAL
1	B	13	ALA
1	B	140	GLY
1	B	142	ILE
1	A	280	ASN
1	A	283	ASP
1	A	404	HIS
1	B	137	ARG
1	B	283	ASP
1	A	285	SER
1	B	285	SER
1	B	402	VAL

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	369/374 (99%)	347 (94%)	22 (6%)	19 42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	369/374 (99%)	343 (93%)	26 (7%)	15	35
All	All	738/748 (99%)	690 (94%)	48 (6%)	17	38

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	LEU
1	A	85	LEU
1	A	95	LEU
1	A	103	LEU
1	A	137	ARG
1	A	138	ARG
1	A	139	MET
1	A	162	ASN
1	A	168	ARG
1	A	178	ARG
1	A	229	LEU
1	A	279	ARG
1	A	286	LEU
1	A	304	THR
1	A	307	LEU
1	A	324	LEU
1	A	349	GLU
1	A	358	VAL
1	A	366	ARG
1	A	371	GLU
1	A	392	ARG
1	A	432	LYS
1	B	52	LEU
1	B	85	LEU
1	B	95	LEU
1	B	103	LEU
1	B	137	ARG
1	B	138	ARG
1	B	139	MET
1	B	150	ASP
1	B	162	ASN
1	B	168	ARG
1	B	178	ARG
1	B	229	LEU
1	B	286	LEU
1	B	304	THR

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Mol	Chain	Res	Type
1	B	307	LEU
1	B	324	LEU
1	B	327	ASP
1	B	358	VAL
1	B	366	ARG
1	B	375	ILE
1	B	392	ARG
1	B	401	THR
1	B	402	VAL
1	B	426	THR
1	B	432	LYS
1	B	455	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	162	ASN
1	A	165	GLN
1	A	249	ASN
1	A	306	GLN
1	A	357	ASN
1	B	14	ASN
1	B	93	GLN
1	B	162	ASN
1	B	165	GLN
1	B	249	ASN
1	B	357	ASN
1	B	440	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	C2E	A	503	-	44,52,52	0.99	2 (4%)	52,82,82	1.16	7 (13%)
4	C2E	A	501	-	44,52,52	0.99	3 (6%)	52,82,82	1.18	8 (15%)
4	C2E	B	503	-	44,52,52	1.01	2 (4%)	52,82,82	1.15	6 (11%)
4	C2E	A	505	-	44,52,52	0.98	2 (4%)	52,82,82	1.21	8 (15%)
4	C2E	B	505	-	44,52,52	0.93	2 (4%)	52,82,82	1.23	8 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	C2E	A	503	-	-	0/22/62/62	0/6/7/7
4	C2E	A	501	-	-	1/22/62/62	0/6/7/7
4	C2E	B	503	-	-	0/22/62/62	0/6/7/7
4	C2E	A	505	-	-	0/22/62/62	0/6/7/7
4	C2E	B	505	-	-	0/22/62/62	0/6/7/7

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	C2E	C6-N1	-3.13	1.33	1.37
4	B	503	C2E	C6-N1	-2.99	1.33	1.37
4	A	501	C2E	C61-N11	-2.79	1.33	1.37
4	A	505	C2E	C6-N1	-2.77	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	505	C2E	C61-N11	-2.74	1.33	1.37
4	A	505	C2E	C61-N11	-2.73	1.33	1.37
4	B	503	C2E	C61-N11	-2.55	1.34	1.37
4	A	501	C2E	C6-N1	-2.45	1.34	1.37
4	A	503	C2E	C61-N11	-2.40	1.34	1.37
4	B	505	C2E	C6-N1	-2.04	1.34	1.37
4	A	501	C2E	O4A-C1A	2.01	1.43	1.41

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	505	C2E	C3'-C2'-C1'	2.99	106.52	99.89
4	A	503	C2E	C8-N7-C5	2.77	108.26	102.99
4	B	503	C2E	C8-N7-C5	2.74	108.20	102.99
4	A	501	C2E	C3'-C2'-C1'	2.72	105.93	99.89
4	B	505	C2E	C3'-C2'-C1'	2.71	105.90	99.89
4	A	503	C2E	P11-O3'-C3'	-2.65	109.75	119.41
4	B	505	C2E	P1-O3A-C3A	-2.63	109.84	119.41
4	A	501	C2E	P1-O3A-C3A	-2.62	109.86	119.41
4	B	503	C2E	P1-O3A-C3A	-2.61	109.92	119.41
4	A	501	C2E	C3A-C2A-C1A	2.57	105.59	99.89
4	A	501	C2E	P11-O3'-C3'	-2.56	110.08	119.41
4	A	501	C2E	C8-N7-C5	2.54	107.82	102.99
4	B	503	C2E	P11-O3'-C3'	-2.52	110.23	119.41
4	A	503	C2E	P1-O3A-C3A	-2.50	110.31	119.41
4	A	503	C2E	C81-N71-C51	2.49	107.73	102.99
4	B	505	C2E	C5-C6-N1	2.46	118.29	113.95
4	B	503	C2E	C81-N71-C51	2.45	107.67	102.99
4	A	501	C2E	C81-N71-C51	2.45	107.66	102.99
4	A	505	C2E	C8-N7-C5	2.43	107.62	102.99
4	A	505	C2E	C81-N71-C51	2.43	107.61	102.99
4	A	503	C2E	C5-C6-N1	2.42	118.22	113.95
4	A	501	C2E	C5-C6-N1	2.40	118.19	113.95
4	A	505	C2E	P1-O3A-C3A	-2.40	110.69	119.41
4	B	505	C2E	C81-N71-C51	2.38	107.52	102.99
4	A	505	C2E	C3A-C2A-C1A	2.37	105.13	99.89
4	A	505	C2E	C5-C6-N1	2.37	118.13	113.95
4	B	505	C2E	O6-C6-C5	-2.36	119.76	124.37
4	B	505	C2E	C3A-C2A-C1A	2.36	105.12	99.89
4	A	505	C2E	P11-O3'-C3'	-2.36	110.83	119.41
4	B	505	C2E	P11-O3'-C3'	-2.33	110.92	119.41
4	A	503	C2E	C51-C61-N11	2.33	118.06	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	501	C2E	C51-C61-N11	2.24	117.91	113.95
4	B	503	C2E	C3A-C2A-C1A	2.24	104.85	99.89
4	B	503	C2E	C5-C6-N1	2.23	117.89	113.95
4	A	503	C2E	C3A-C2A-C1A	2.16	104.68	99.89
4	A	505	C2E	C2A-C3A-C4A	-2.10	99.50	103.22
4	B	505	C2E	C51-C61-N11	2.01	117.51	113.95

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	C2E	C5A-O5A-P11-O11

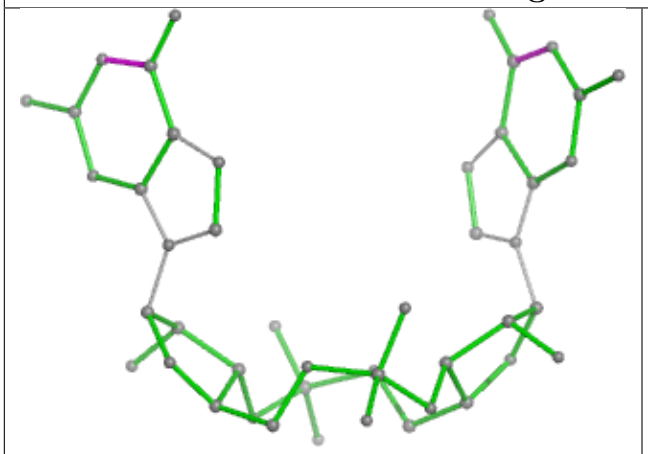
There are no ring outliers.

2 monomers are involved in 2 short contacts:

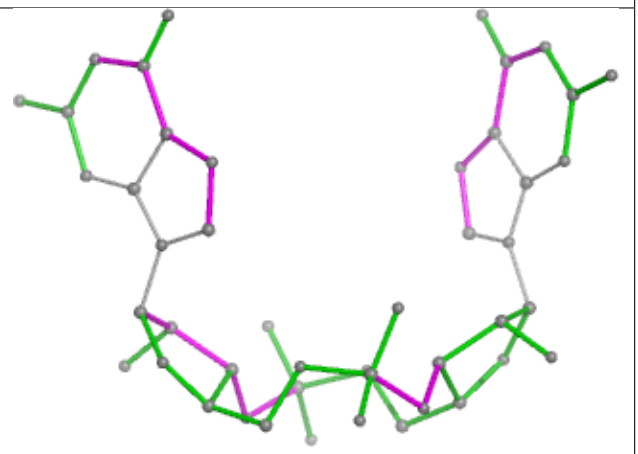
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	503	C2E	1	0
4	B	503	C2E	1	0

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.

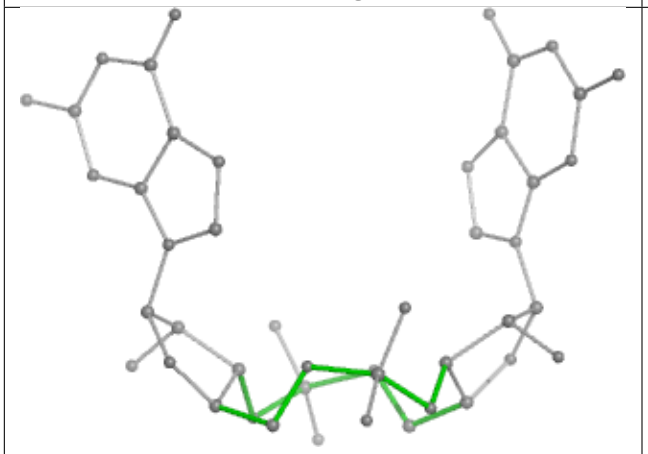
Ligand C2E A 503



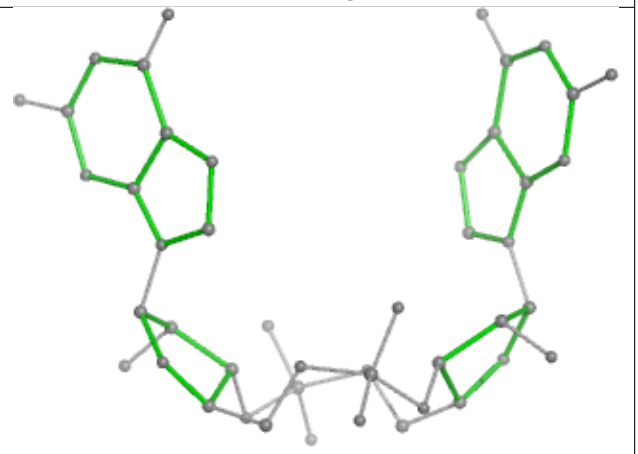
Bond lengths



Bond angles

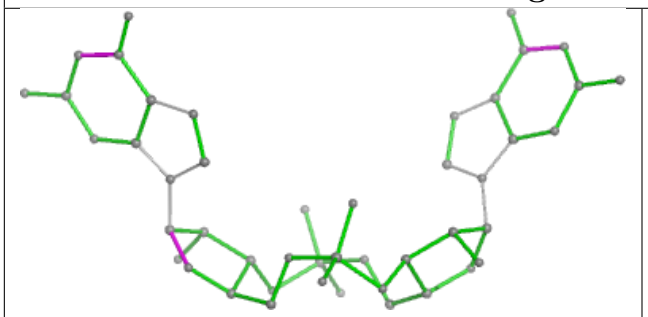


Torsions

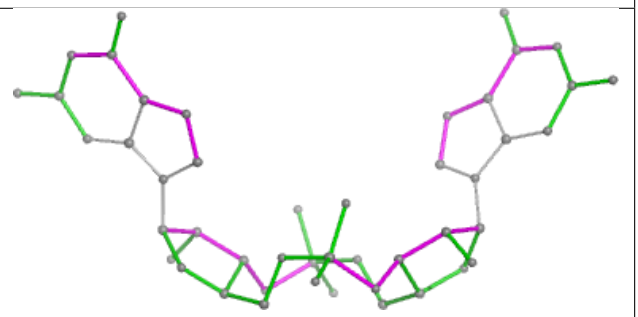


Rings

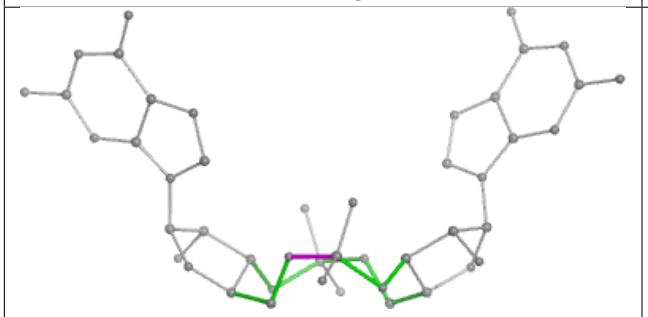
Ligand C2E A 501



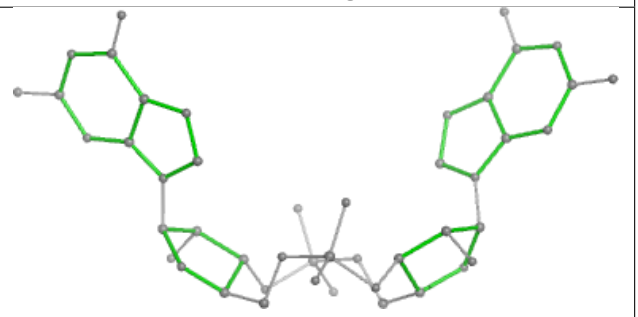
Bond lengths



Bond angles

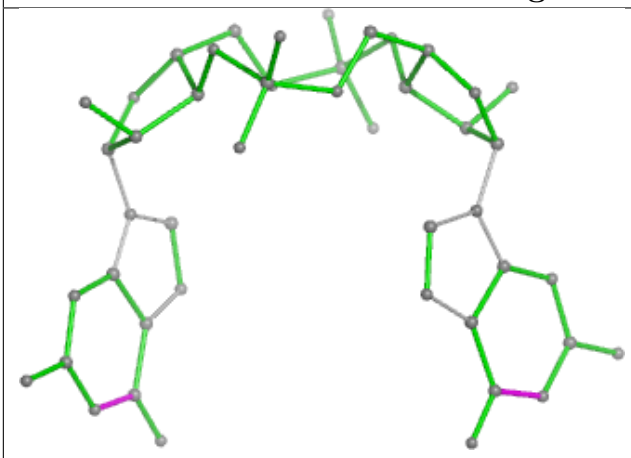


Torsions

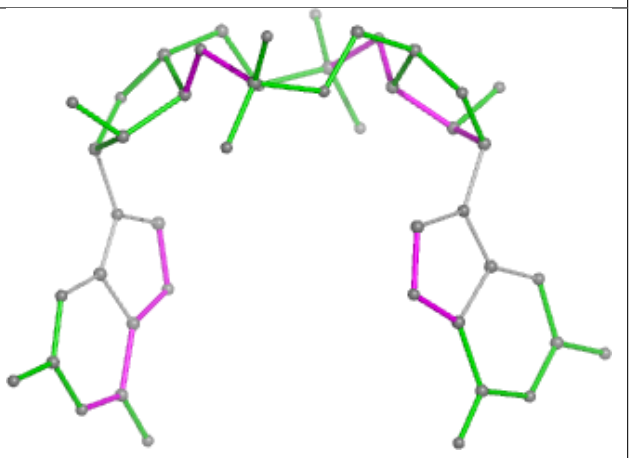


Rings

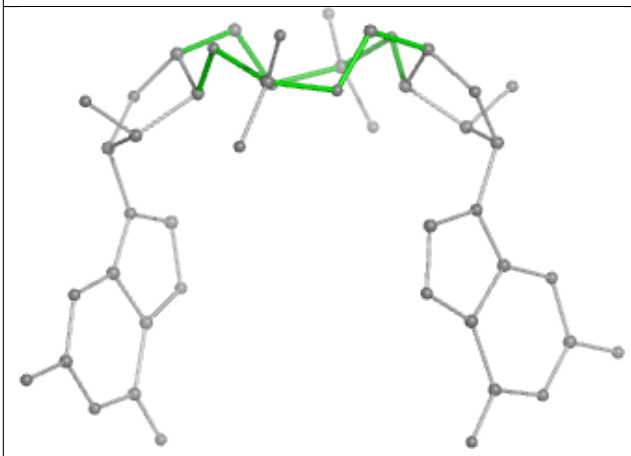
Ligand C2E B 503



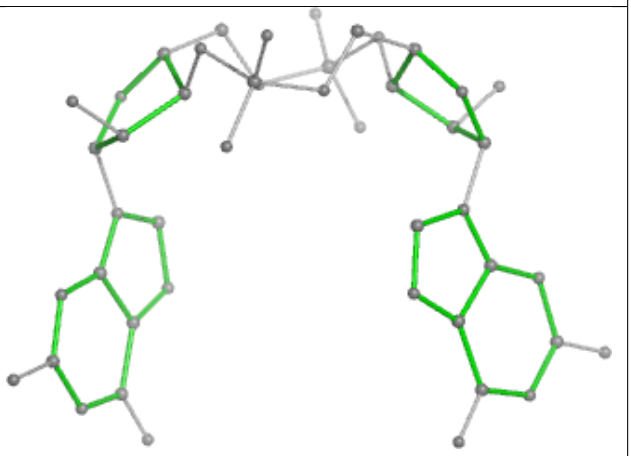
Bond lengths



Bond angles

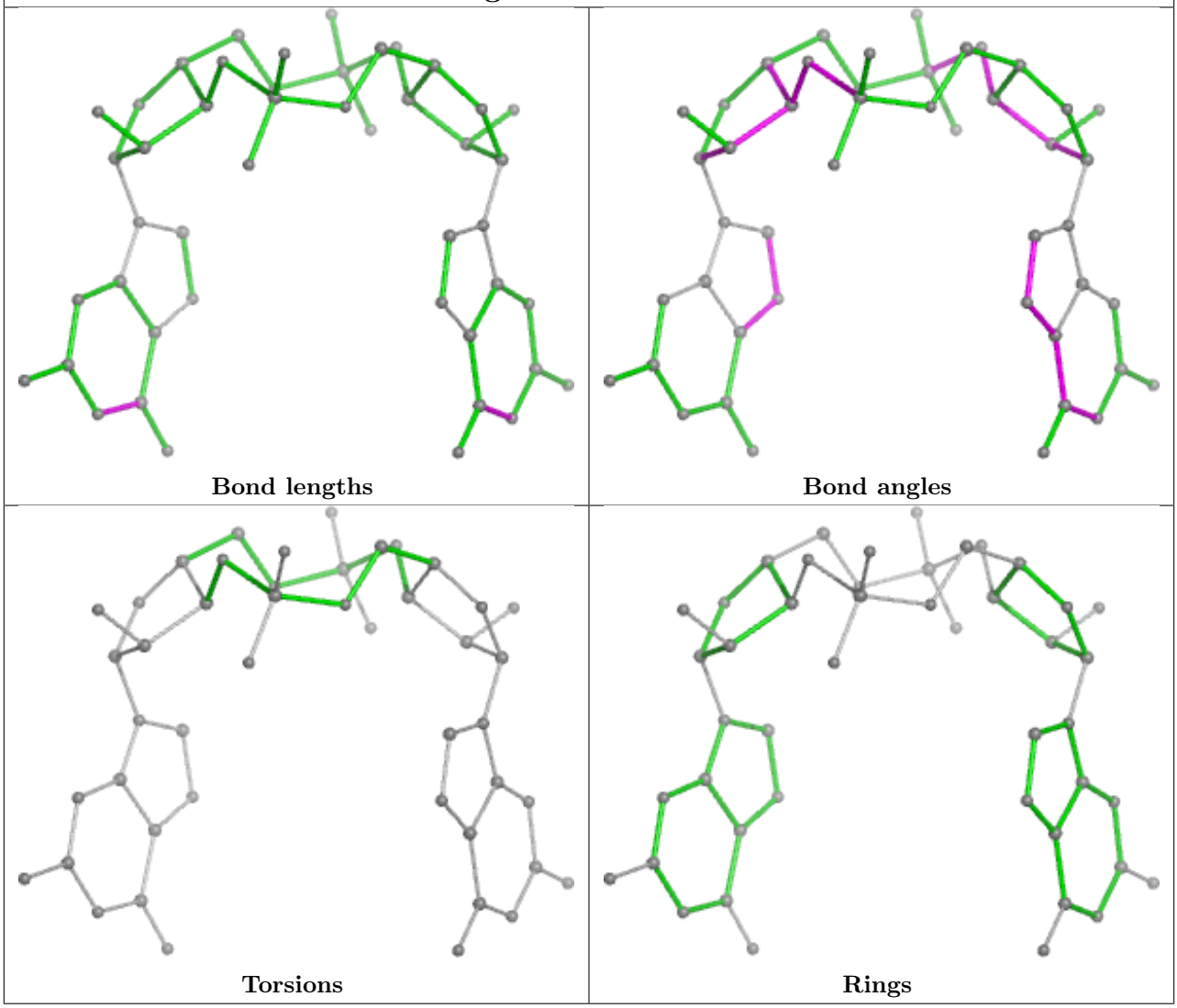


Torsions

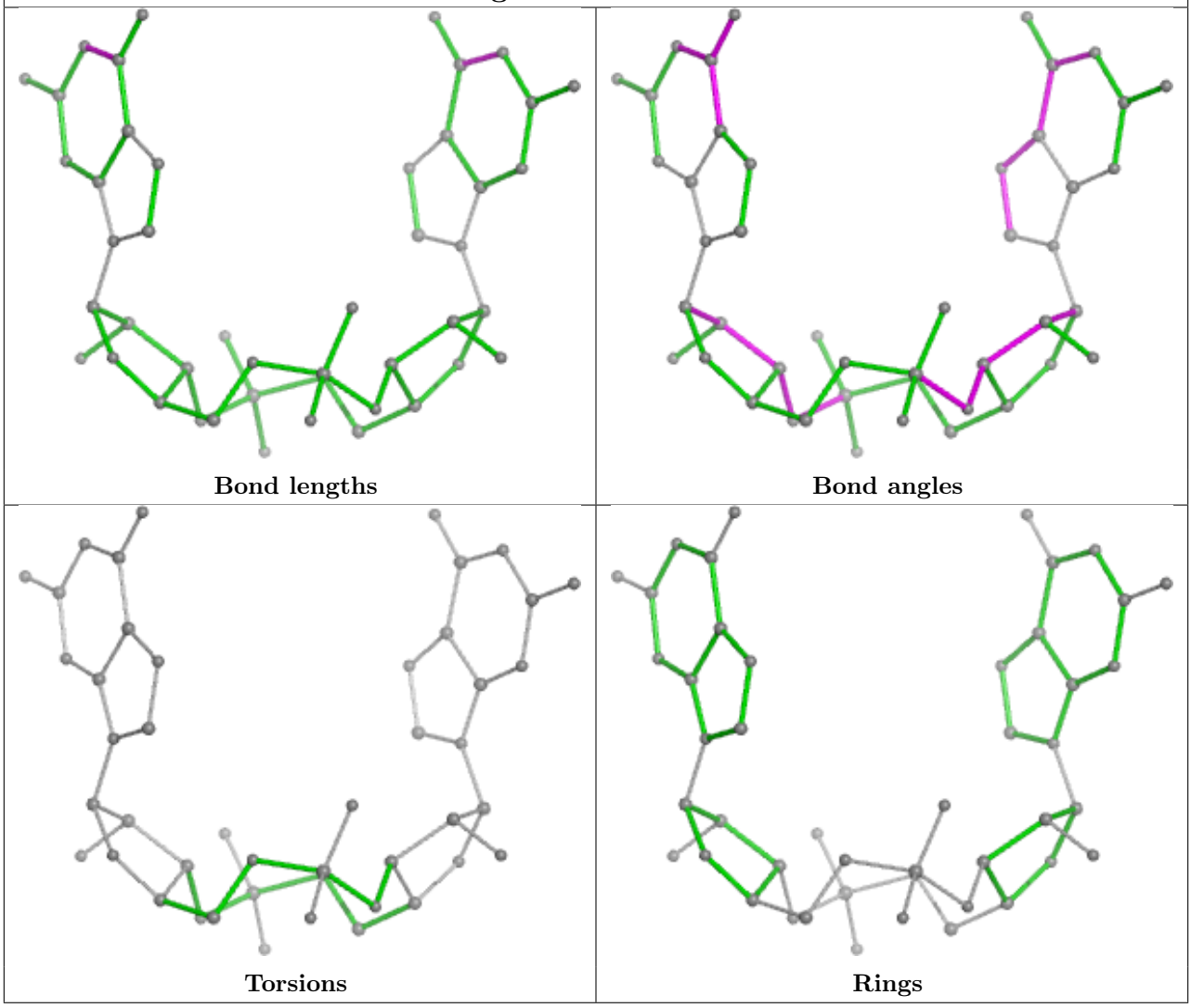


Rings

Ligand C2E A 505



Ligand C2E B 505



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3
1	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	136:GLY	C	137:ARG	N	1.03
1	A	454:ALA	C	455:HIS	N	0.98
1	A	281:ASN	C	282:LEU	N	0.80
1	B	281:ASN	C	282:LEU	N	0.71
1	A	136:GLY	C	137:ARG	N	0.67

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	436/459 (94%)	0.13	10 (2%)	60	62	17, 27, 37, 44	9 (2%)
1	B	436/459 (94%)	0.14	9 (2%)	63	65	17, 27, 37, 44	9 (2%)
All	All	872/918 (94%)	0.14	19 (2%)	62	63	17, 27, 37, 44	18 (2%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	446	ARG	4.3
1	B	454	ALA	4.2
1	B	405	GLY	3.3
1	A	443	ALA	3.1
1	A	408	MET	3.1
1	B	408	MET	2.7
1	B	453	ALA	2.6
1	A	409	LEU	2.5
1	B	406	ARG	2.4
1	B	85	LEU	2.4
1	A	405	GLY	2.4
1	B	439	TYR	2.3
1	A	14	ASN	2.2
1	A	85	LEU	2.2
1	B	443	ALA	2.2
1	A	406	ARG	2.2
1	A	164	ARG	2.1
1	A	453	ALA	2.1
1	A	439	TYR	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 monosaccharides in this entry.

6.4 Ligands (i)

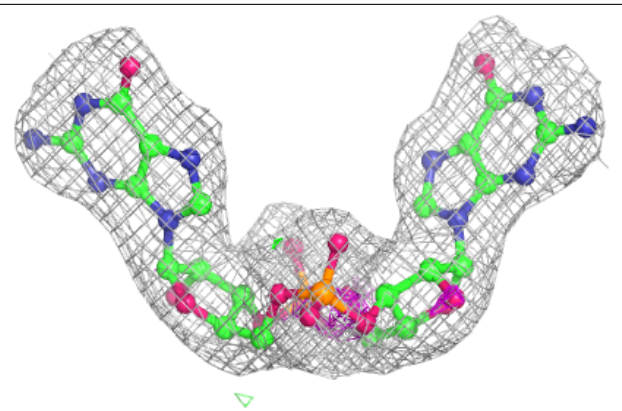
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

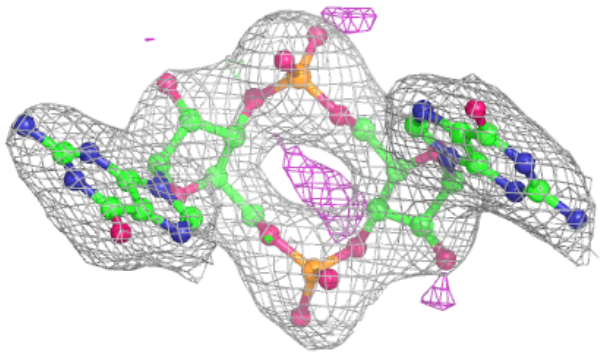
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	B	500	1/1	0.73	0.10	39,39,39,39	0
3	MG	A	500	1/1	0.83	0.09	43,43,43,43	0
4	C2E	A	501	46/46	0.95	0.16	58,61,66,68	0
2	ZN	A	499	1/1	0.96	0.14	86,86,86,86	0
4	C2E	A	503	46/46	0.97	0.14	20,24,26,27	0
4	C2E	B	503	46/46	0.97	0.14	20,24,25,27	0
4	C2E	B	505	46/46	0.97	0.15	13,21,23,24	0
4	C2E	A	505	46/46	0.98	0.15	13,21,23,24	0

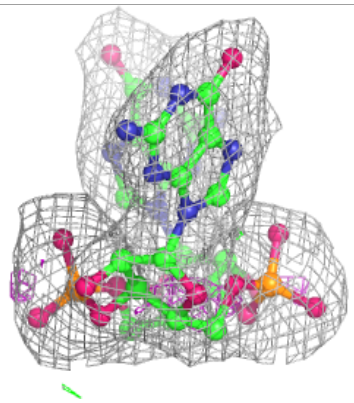
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around C2E A 501:

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

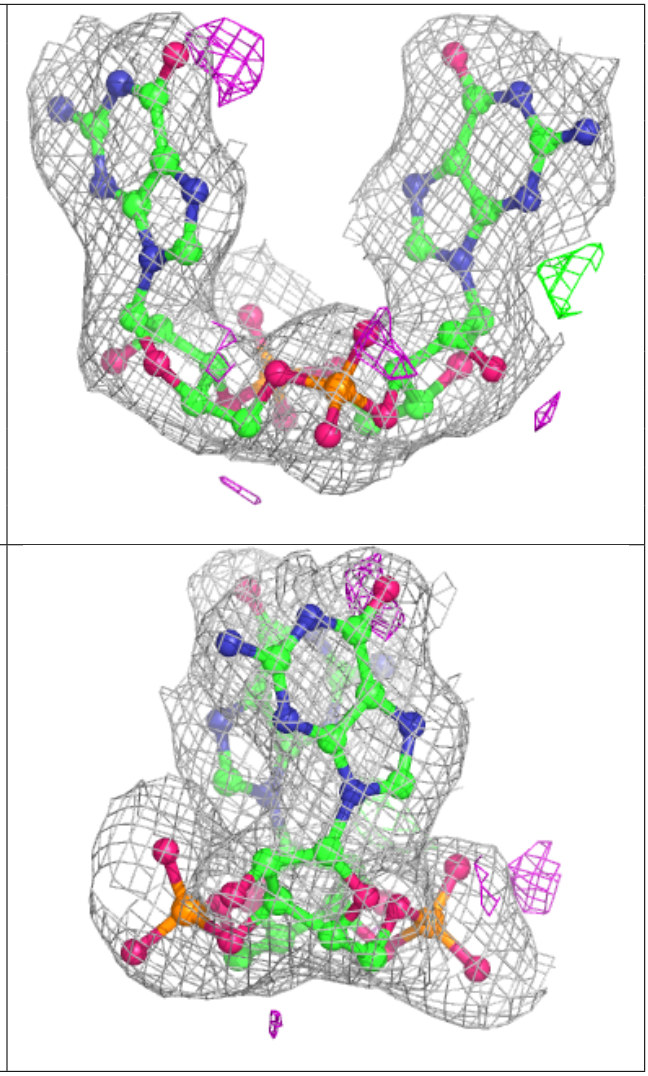






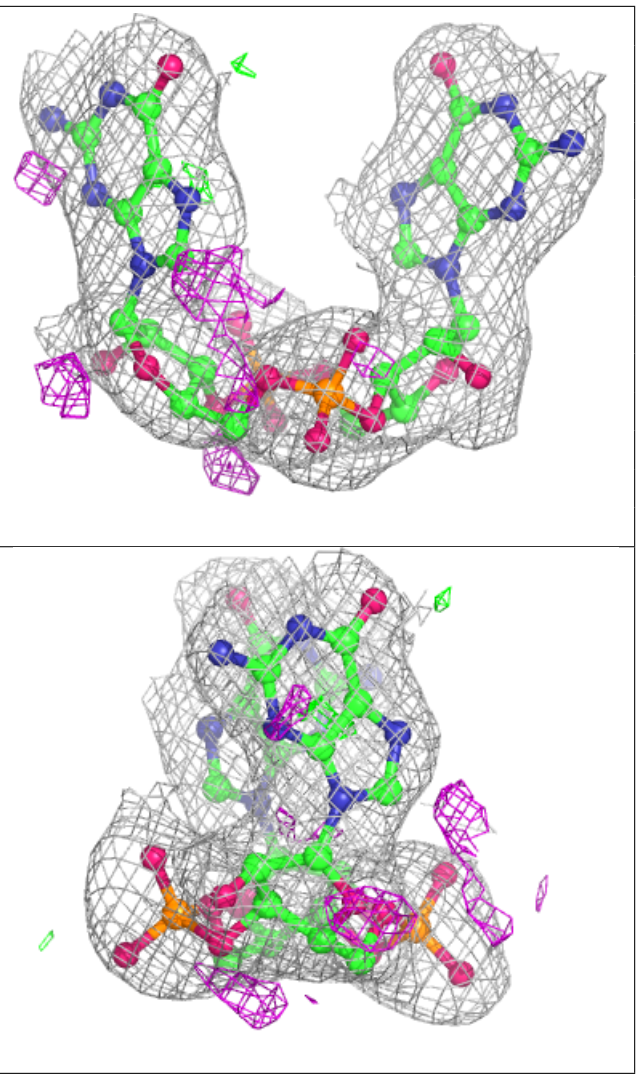
Electron density around C2E A 503:

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



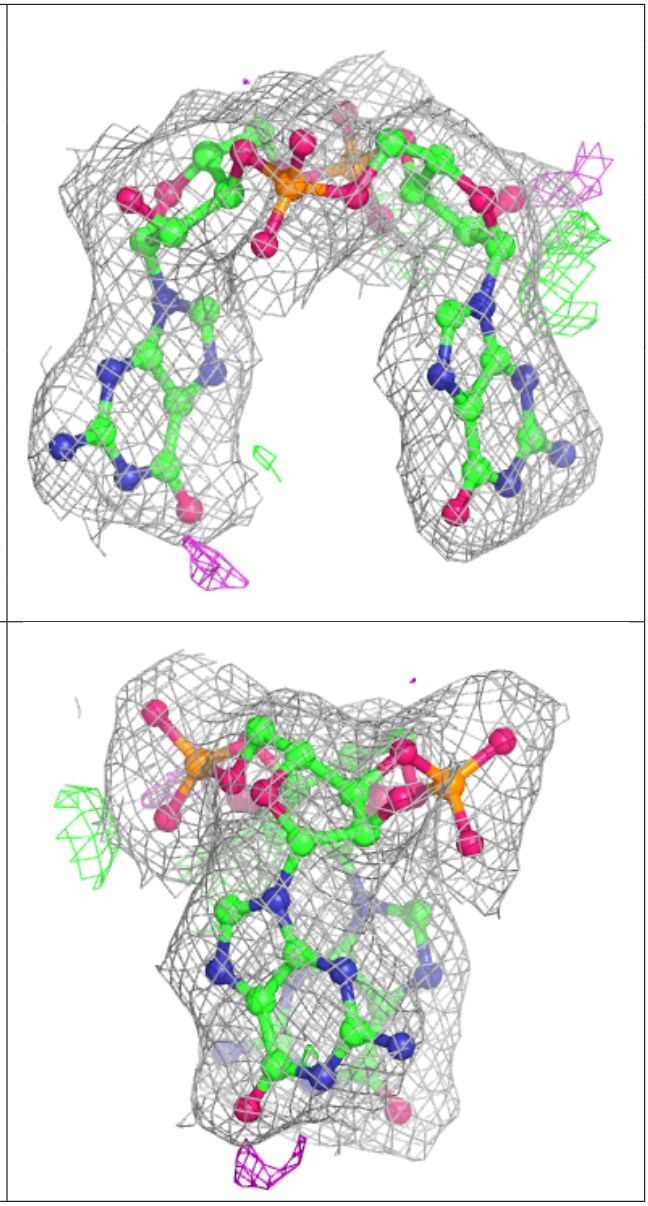
Electron density around C2E B 503:

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



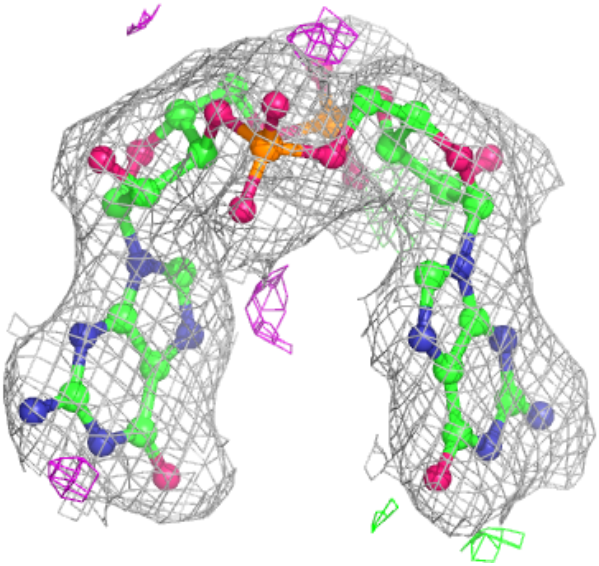
Electron density around C2E B 505:

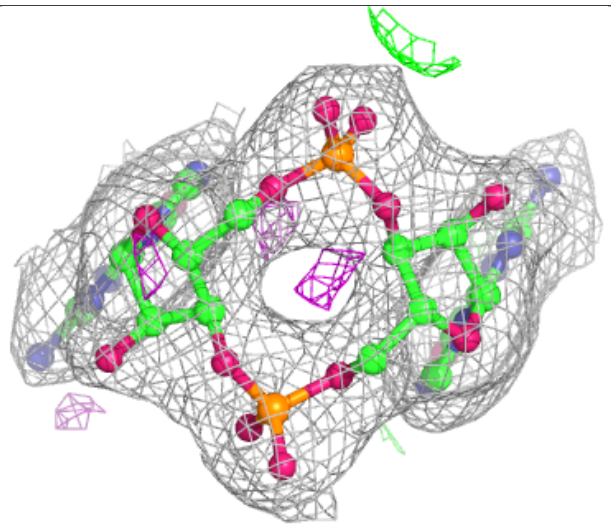
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

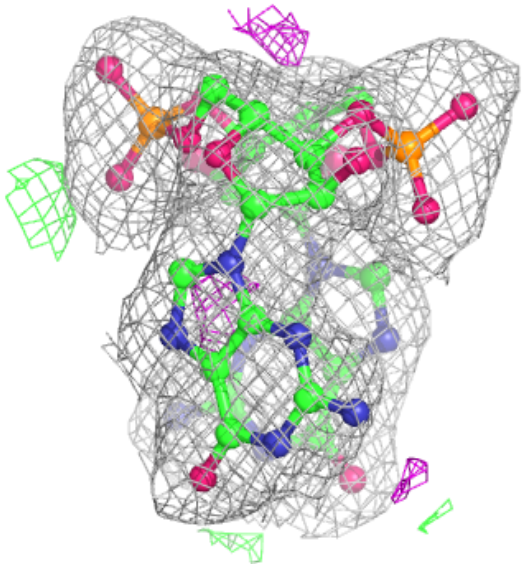


Electron density around C2E A 505:

$2mF_o$-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.