



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 01:13 pm BST

PDB ID : 6PFV
Title : Structure of *S. venezuelae* RisG-WhiG-c-di-GMP complex: orthorhombic crystal form
Authors : Schumacher, M.A.
Deposited on : 2019-06-22
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

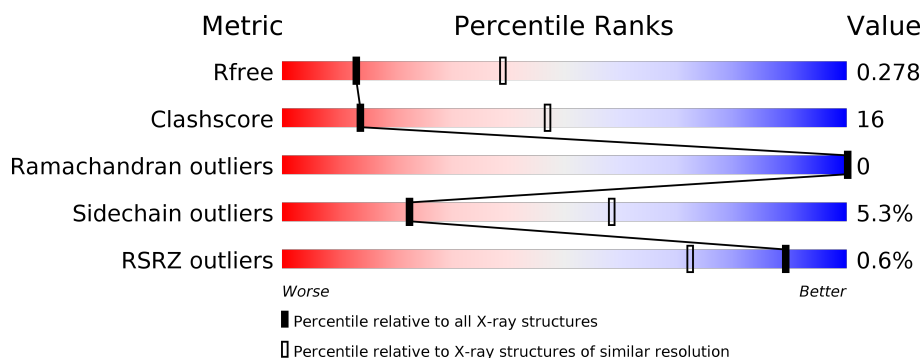
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	B	176	<div> <div>2%</div> <div> <div></div> <div>63%</div> <div>25%</div> <div>9%</div> </div> </div>
1	E	176	<div> <div>%</div> <div> <div></div> <div>55%</div> <div>34%</div> <div>10%</div> </div> </div>
1	T	176	<div> <div></div> <div> <div></div> <div>66%</div> <div>26%</div> <div>7%</div> </div> </div>
2	A	278	<div> <div></div> <div> <div></div> <div>51%</div> <div>26%</div> <div>21%</div> </div> </div>
2	D	278	<div> <div>%</div> <div> <div></div> <div>55%</div> <div>23%</div> <div>21%</div> </div> </div>
2	G	278	<div> <div></div> <div> <div></div> <div>56%</div> <div>22%</div> <div>20%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18372 atoms, of which 9070 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 AmfC protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	T	164	Total	C	H	N	O	S	0	0	0
			2614	788	1306	264	252	4			
1	B	160	Total	C	H	N	O	S	0	0	0
			2514	761	1252	251	246	4			
1	E	159	Total	C	H	N	O	S	0	0	0
			2535	764	1266	256	245	4			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	24	GLY	-	expression tag	UNP F2RFR7
T	25	SER	-	expression tag	UNP F2RFR7
T	91	GLY	PRO	engineered mutation	UNP F2RFR7
B	24	GLY	-	expression tag	UNP F2RFR7
B	25	SER	-	expression tag	UNP F2RFR7
B	91	GLY	PRO	engineered mutation	UNP F2RFR7
E	24	GLY	-	expression tag	UNP F2RFR7
E	25	SER	-	expression tag	UNP F2RFR7
E	91	GLY	PRO	engineered mutation	UNP F2RFR7

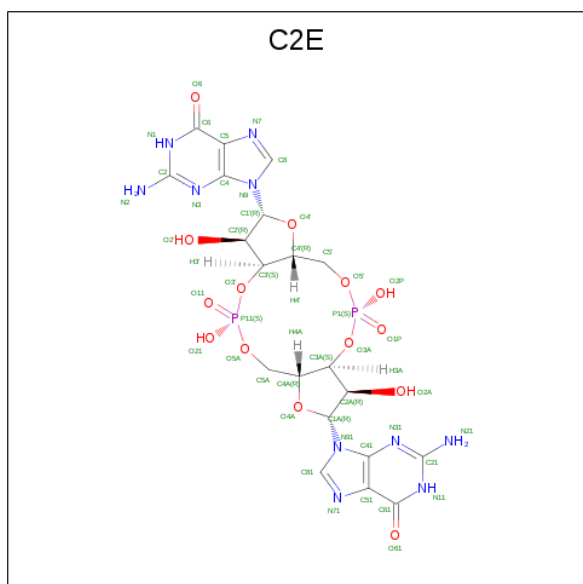
- Molecule 2 is a protein called RNA polymerase sigma factor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	A	220	Total	C	H	N	O	S	0	0	0
			3453	1089	1734	299	329	2			
2	D	220	Total	C	H	N	O	S	0	0	0
			3460	1091	1741	299	327	2			
2	G	223	Total	C	H	N	O	S	0	0	0
			3520	1110	1771	307	330	2			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	GLU	ASP	engineered mutation	UNP A0A3N1Q704
A	97	VAL	ILE	engineered mutation	UNP A0A3N1Q704
A	144	GLY	ARG	engineered mutation	UNP A0A3N1Q704
A	150	THR	SER	engineered mutation	UNP A0A3N1Q704
A	159	SER	THR	engineered mutation	UNP A0A3N1Q704
A	162	ASP	GLU	engineered mutation	UNP A0A3N1Q704
D	38	GLU	ASP	engineered mutation	UNP A0A3N1Q704
D	97	VAL	ILE	engineered mutation	UNP A0A3N1Q704
D	144	GLY	ARG	engineered mutation	UNP A0A3N1Q704
D	150	THR	SER	engineered mutation	UNP A0A3N1Q704
D	159	SER	THR	engineered mutation	UNP A0A3N1Q704
D	162	ASP	GLU	engineered mutation	UNP A0A3N1Q704
G	38	GLU	ASP	engineered mutation	UNP A0A3N1Q704
G	97	VAL	ILE	engineered mutation	UNP A0A3N1Q704
G	144	GLY	ARG	engineered mutation	UNP A0A3N1Q704
G	150	THR	SER	engineered mutation	UNP A0A3N1Q704
G	159	SER	THR	engineered mutation	UNP A0A3N1Q704
G	162	ASP	GLU	engineered mutation	UNP A0A3N1Q704

- Molecule 3 is 9,9'-[(2R,3R,3aS,5S,7aR,9R,10R,10aS,12S,14aR)-3,5,10,12-tetrahydro-5,12-dioxidooctahydro-2H,7H-difuro[3,2-d:3',2'-j][1,3,7,9,2,8]tetraoxadiphosphacyclodecine-2,9-diyl]bis(2-amino-1,9-dihydro-6H-purin-6-one) (three-letter code: C2E) (formula: C₂₀H₂₄N₁₀O₁₄P₂) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	T	1	Total	C	N	O	P	0	0
			46	20	10	14	2		

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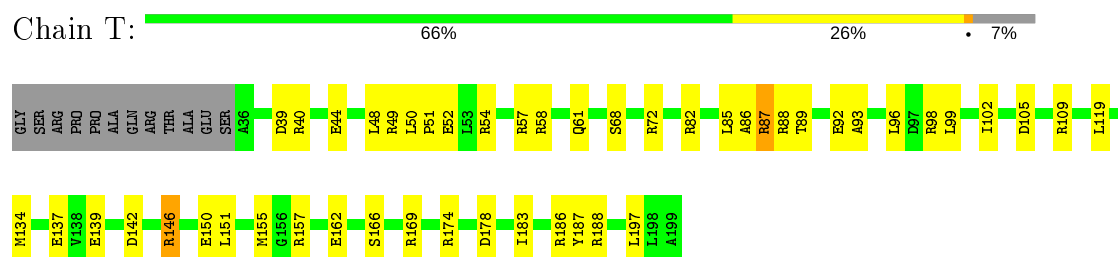
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	T	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
3	B	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
3	B	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
3	E	1	Total	C	N	O	P	0	0
			46	20	10	14	2		
3	E	1	Total	C	N	O	P	0	0
			46	20	10	14	2		

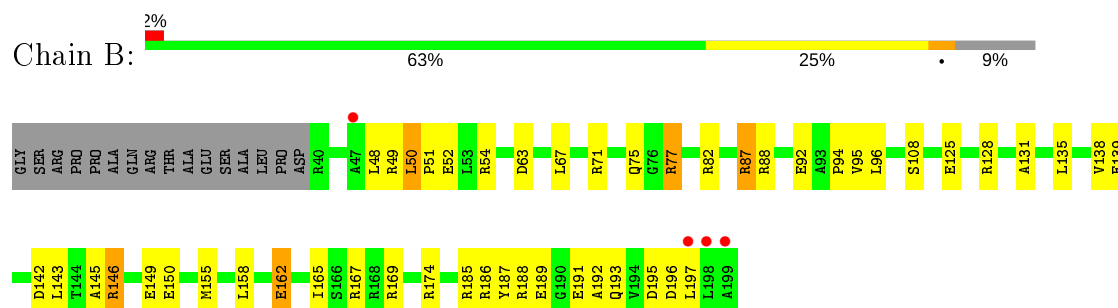
3 Residue-property plots [i](#)

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

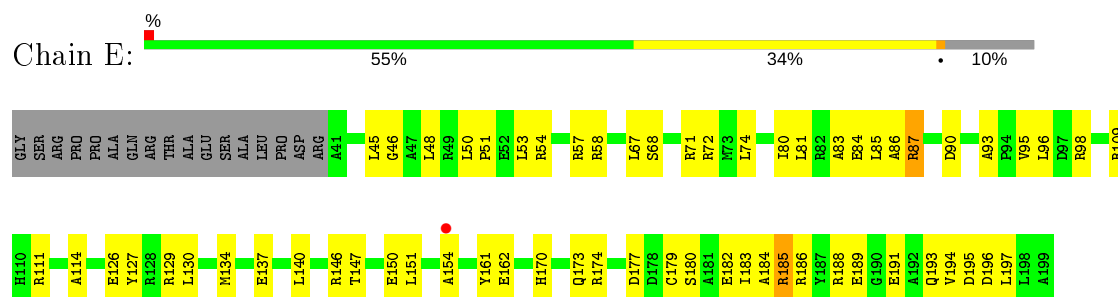
- Molecule 1: AmfC protein



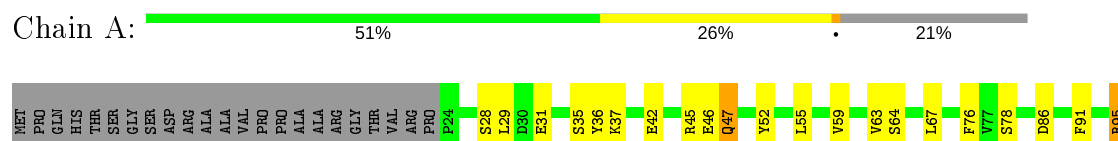
- Molecule 1: AmfC protein

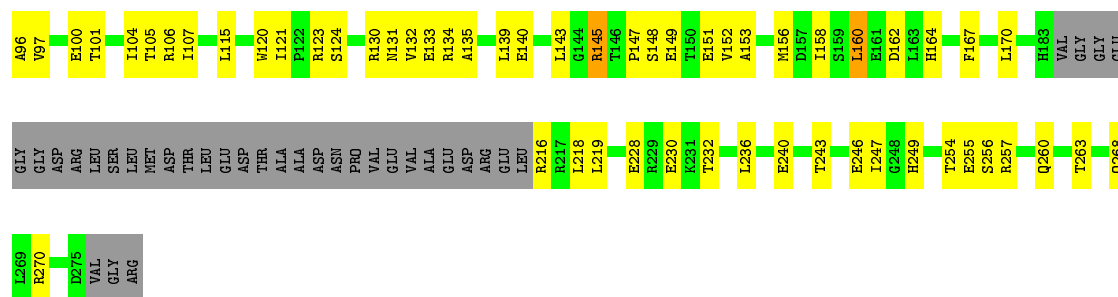


- Molecule 1: AmfC protein

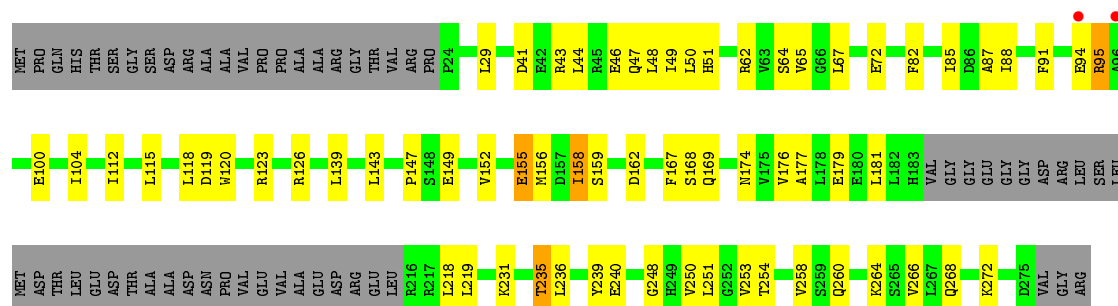


- Molecule 2: RNA polymerase sigma factor

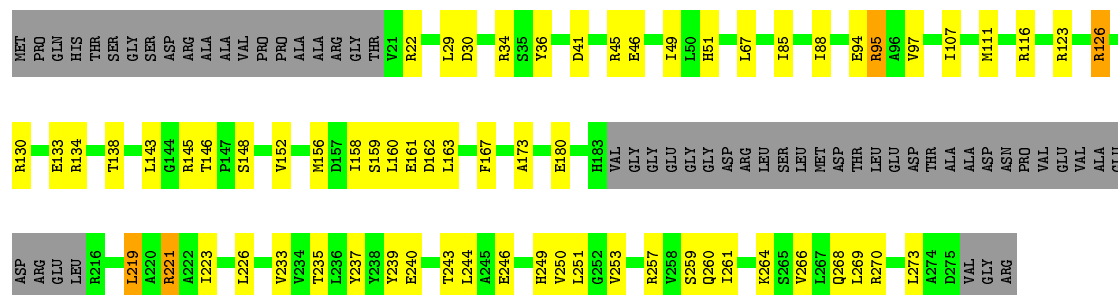




- Molecule 2: RNA polymerase sigma factor



- Molecule 2: RNA polymerase sigma factor



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.85Å 97.34Å 204.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.90 – 3.00 87.90 – 2.99	Depositor EDS
% Data completeness (in resolution range)	97.0 (87.90-3.00) 98.8 (87.90-2.99)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.214 , 0.278 0.214 , 0.278	Depositor DCC
R_{free} test set	1952 reflections (5.97%)	wwPDB-VP
Wilson B-factor (Å ²)	89.1	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 77.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18372	wwPDB-VP
Average B, all atoms (Å ²)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: C2E

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	B	0.30	0/1275	0.58	0/1718
1	E	0.29	0/1282	0.59	0/1725
1	T	0.30	0/1322	0.57	0/1780
2	A	0.31	0/1745	0.50	0/2368
2	D	0.30	0/1745	0.55	1/2368 (0.0%)
2	G	0.31	0/1777	0.53	1/2413 (0.0%)
All	All	0.30	0/9146	0.55	2/12372 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	219	LEU	CA-CB-CG	5.32	127.53	115.30
2	D	95	ARG	NE-CZ-NH1	5.12	122.86	120.30

There are no chirality outliers.

There are no planarity outliers.

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	B	1262	1252	1244	41	1
1	E	1269	1266	1264	47	2
1	T	1308	1306	1304	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1719	1734	1727	56	2
2	D	1719	1741	1734	43	0
2	G	1749	1771	1767	55	1
3	B	92	0	43	13	0
3	E	92	0	43	13	0
3	T	92	0	44	8	0
All	All	9302	9070	9170	292	3

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 16.

All (292) 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:B:201:C2E:H5'2	3:B:201:C2E:H8	1.43	0.98
3:E:202:C2E:H5'2	3:E:202:C2E:H8	1.50	0.93
1:B:49:ARG:NH2	1:B:191:GLU:OE2	2.04	0.91
1:T:82:ARG:HB2	1:T:155:MET:HE1	1.62	0.82
3:B:202:C2E:H5'2	3:B:202:C2E:H8	1.64	0.79
2:G:22:ARG:NH2	2:G:41:ASP:OD2	2.17	0.78
3:E:202:C2E:C8	3:E:202:C2E:H5'2	2.14	0.77
2:D:231:LYS:O	2:D:235:THR:OG1	2.03	0.76
3:E:201:C2E:H8	3:E:201:C2E:H5'2	1.67	0.76
3:B:202:C2E:H5'2	3:B:202:C2E:C8	2.19	0.73
1:E:162:GLU:OE2	3:E:201:C2E:O2'	2.04	0.73
1:B:48:LEU:O	1:B:186:ARG:NH2	2.23	0.72
3:T:202:C2E:C8	3:T:202:C2E:H5'2	2.19	0.72
2:D:139:LEU:HD21	2:D:155:GLU:HG3	1.72	0.72
3:E:202:C2E:H5'1	3:E:202:C2E:H3A	1.71	0.71
1:B:87:ARG:NE	1:B:92:GLU:O	2.24	0.71
2:G:126:ARG:NH2	2:G:180:GLU:OE1	2.24	0.70
2:D:158:ILE:HG23	2:D:162:ASP:HB3	1.73	0.70
2:A:133:GLU:OE2	2:A:270:ARG:NH1	2.26	0.69
2:G:249:HIS:ND1	2:G:249:HIS:O	2.26	0.68
3:B:201:C2E:H5'1	3:B:201:C2E:C3A	2.24	0.68
3:B:201:C2E:H3A	3:B:201:C2E:H5'1	1.77	0.67
1:E:48:LEU:O	1:E:186:ARG:NH2	2.26	0.66
1:E:53:LEU:HD23	1:E:183:ILE:HG13	1.78	0.66
1:B:193:GLN:NE2	1:B:196:ASP:OD2	2.29	0.66
2:G:167:PHE:HB3	2:G:260:GLN:HB2	1.78	0.65
3:B:201:C2E:H5'2	3:B:201:C2E:C8	2.22	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:158:ILE:CG2	2:A:162:ASP:HB2	2.27	0.65
1:T:93:ALA:O	1:T:98:ARG:NH1	2.30	0.64
1:B:50:LEU:HD21	1:B:54:ARG:CZ	2.27	0.64
3:E:202:C2E:C5'	3:E:202:C2E:H8	2.27	0.64
2:A:42:GLU:OE2	2:A:45:ARG:NH1	2.31	0.64
2:A:64:SER:HA	2:A:67:LEU:HD12	1.78	0.64
2:D:181:LEU:HD22	2:D:266:VAL:HG23	1.80	0.63
1:B:145:ALA:HB3	1:B:146:ARG:NH1	2.13	0.63
1:T:174:ARG:CZ	2:D:72:GLU:HG3	2.28	0.62
1:B:149:GLU:OE1	1:B:149:GLU:N	2.28	0.62
3:B:202:C2E:H5'1	3:B:202:C2E:H3A	1.80	0.62
2:A:230:GLU:OE1	2:A:268:GLN:NE2	2.32	0.62
2:A:257:ARG:HH21	2:A:260:GLN:HG3	1.63	0.62
3:E:201:C2E:C3A	3:E:201:C2E:H5'1	2.29	0.62
2:D:236:LEU:HA	2:D:240:GLU:HB2	1.82	0.61
1:E:134:MET:HE1	1:E:161:TYR:HB3	1.82	0.61
1:B:88:ARG:NH2	1:B:143:LEU:O	2.33	0.61
1:E:191:GLU:N	1:E:191:GLU:OE2	2.33	0.61
2:G:49:ILE:HD12	2:G:85:ILE:HG12	1.82	0.61
3:T:202:C2E:H8	3:T:202:C2E:H5'2	1.82	0.61
1:B:142:ASP:O	1:B:146:ARG:NH1	2.34	0.60
1:E:197:LEU:HD11	2:G:240:GLU:HG2	1.84	0.60
1:T:169:ARG:NH2	3:T:201:C2E:O61	2.34	0.60
2:G:95:ARG:HB3	2:G:97:VAL:HG23	1.84	0.59
1:B:169:ARG:NH2	3:B:202:C2E:O11	2.34	0.59
2:G:226:LEU:HD11	2:G:269:LEU:HD21	1.83	0.59
1:E:53:LEU:HD21	1:E:182:GLU:HG3	1.84	0.59
1:B:49:ARG:NE	1:B:50:LEU:H	1.99	0.59
2:D:115:LEU:HA	2:D:118:LEU:HD12	1.85	0.59
2:D:64:SER:HA	2:D:67:LEU:HD12	1.85	0.59
2:A:130:ARG:HG2	2:A:130:ARG:HH11	1.68	0.58
1:T:57:ARG:NH2	2:A:240:GLU:O	2.36	0.58
2:G:49:ILE:HD13	2:G:88:ILE:HD12	1.84	0.58
2:A:228:GLU:O	2:A:232:THR:HG23	2.03	0.58
1:B:142:ASP:HB3	1:B:146:ARG:NH1	2.17	0.58
1:T:187:TYR:OH	1:T:197:LEU:HD11	2.01	0.58
2:G:133:GLU:OE1	2:G:270:ARG:HG2	2.04	0.58
2:G:158:ILE:HG22	2:G:159:SER:H	1.68	0.58
1:T:40:ARG:NH1	1:T:178:ASP:OD1	2.37	0.57
2:A:236:LEU:HA	2:A:240:GLU:HB2	1.86	0.57
1:B:125:GLU:HA	1:B:128:ARG:HD2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:143:LEU:HD22	2:G:145:ARG:HH21	1.69	0.57
3:E:201:C2E:H5'1	3:E:201:C2E:C5A	2.35	0.57
2:A:167:PHE:HB3	2:A:260:GLN:HB2	1.87	0.56
1:T:85:LEU:HD21	1:T:151:LEU:HB3	1.87	0.56
2:G:223:ILE:HA	2:G:226:LEU:CD1	2.35	0.56
2:G:158:ILE:HG22	2:G:162:ASP:HB2	1.87	0.56
2:G:163:LEU:HD21	2:G:167:PHE:CZ	2.41	0.56
1:E:126:GLU:O	1:E:129:ARG:HG2	2.06	0.56
2:D:158:ILE:HG23	2:D:162:ASP:CB	2.34	0.56
1:B:50:LEU:HD21	1:B:54:ARG:NE	2.21	0.55
1:B:67:LEU:HD22	1:B:165:ILE:HG23	1.88	0.55
1:E:86:ALA:O	1:E:90:ASP:HB2	2.06	0.55
2:A:158:ILE:HG22	2:A:162:ASP:HB2	1.86	0.55
2:A:59:VAL:O	2:A:63:VAL:HG12	2.07	0.55
2:A:86:ASP:OD2	2:A:106:ARG:NH2	2.34	0.55
1:T:98:ARG:O	1:T:102:ILE:HG13	2.07	0.55
2:A:131:ASN:HA	2:A:134:ARG:NH1	2.22	0.55
1:B:95:VAL:HG23	2:D:50:LEU:HD21	1.87	0.55
1:B:188:ARG:HH21	1:B:189:GLU:HG2	1.72	0.54
1:B:54:ARG:NH2	1:B:187:TYR:OH	2.40	0.54
2:A:145:ARG:H	2:A:145:ARG:HD3	1.73	0.54
2:D:167:PHE:HB3	2:D:260:GLN:HB2	1.89	0.54
2:G:243:THR:OG1	2:G:246:GLU:HG3	2.08	0.53
1:E:96:LEU:HD12	2:G:46:GLU:HG3	1.91	0.53
3:T:202:C2E:C5'	3:T:202:C2E:H8	2.38	0.53
2:A:140:GLU:HG2	2:A:147:PRO:HD3	1.90	0.53
2:G:134:ARG:O	2:G:138:THR:HG23	2.09	0.53
1:T:142:ASP:HB2	2:A:47:GLN:NE2	2.22	0.53
2:D:250:VAL:HG12	2:D:251:LEU:HD23	1.89	0.53
2:A:147:PRO:HB2	2:A:151:GLU:HB2	1.91	0.53
1:E:184:ALA:O	2:G:250:VAL:HG12	2.09	0.53
1:T:96:LEU:HD12	2:A:46:GLU:HG3	1.91	0.53
1:B:87:ARG:HG2	1:B:87:ARG:HH11	1.73	0.53
1:B:50:LEU:CD2	1:B:54:ARG:CZ	2.87	0.52
1:E:137:GLU:HB2	1:E:140:LEU:HD13	1.91	0.52
2:D:94:GLU:HB2	2:D:95:ARG:NH2	2.23	0.52
1:B:125:GLU:HG2	1:B:128:ARG:HD2	1.92	0.52
2:D:95:ARG:HH11	2:D:95:ARG:HG2	1.75	0.52
1:B:138:VAL:O	2:D:47:GLN:NE2	2.39	0.51
2:G:163:LEU:HD21	2:G:167:PHE:CE1	2.45	0.51
1:T:57:ARG:HD3	1:T:183:ILE:HD12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:ARG:HG3	1:B:51:PRO:HD2	1.92	0.51
2:D:248:GLY:HA2	2:D:258:VAL:HG21	1.92	0.51
1:E:93:ALA:HB3	1:E:98:ARG:HD3	1.93	0.51
1:T:119:LEU:HD23	2:A:59:VAL:HG22	1.93	0.51
2:A:95:ARG:HH21	2:A:97:VAL:HB	1.76	0.51
1:T:40:ARG:NH2	1:T:174:ARG:HG3	2.26	0.51
2:G:163:LEU:C	2:G:163:LEU:HD23	2.32	0.51
1:B:162:GLU:CD	3:B:201:C2E:HO2'	2.15	0.50
1:B:87:ARG:NH1	1:B:94:PRO:HA	2.27	0.50
2:D:82:PHE:HA	2:D:85:ILE:HG22	1.93	0.50
1:T:186:ARG:HH11	1:T:186:ARG:HG2	1.76	0.50
2:A:167:PHE:CB	2:A:260:GLN:HB2	2.42	0.50
2:G:233:VAL:HG21	2:G:261:ILE:HG21	1.93	0.50
2:G:36:TYR:CE1	2:G:45:ARG:HB2	2.46	0.50
2:A:153:ALA:HB1	2:A:158:ILE:O	2.12	0.50
2:G:156:MET:O	2:G:158:ILE:HG12	2.12	0.50
1:T:57:ARG:HH11	1:T:57:ARG:HB3	1.77	0.50
2:D:41:ASP:OD2	2:D:43:ARG:HB3	2.11	0.50
3:E:201:C2E:H5'1	3:E:201:C2E:H3A	1.92	0.50
1:E:83:ALA:O	1:E:87:ARG:HB3	2.11	0.50
3:T:202:C2E:H5'1	3:T:202:C2E:H3A	1.94	0.49
2:G:173:ALA:HB1	2:G:237:TYR:CZ	2.47	0.49
1:B:139:GLU:O	1:B:146:ARG:HD3	2.12	0.49
1:E:140:LEU:HD23	1:E:154:ALA:HB1	1.94	0.49
1:E:68:SER:O	1:E:72:ARG:HG2	2.12	0.49
2:D:139:LEU:O	2:D:143:LEU:HD12	2.12	0.49
2:G:219:LEU:HD13	2:G:223:ILE:HG13	1.93	0.49
3:E:201:C2E:H512	3:E:201:C2E:H5'1	1.95	0.48
1:T:68:SER:O	1:T:72:ARG:HG2	2.12	0.48
2:A:148:SER:O	2:A:152:VAL:HG23	2.12	0.48
1:E:170:HIS:HA	1:E:173:GLN:HG3	1.94	0.48
1:E:186:ARG:HG3	1:E:186:ARG:HH11	1.77	0.48
1:E:188:ARG:HG3	2:G:250:VAL:HA	1.96	0.48
2:A:52:TYR:O	2:A:55:LEU:HB2	2.14	0.48
1:B:188:ARG:NH2	1:B:189:GLU:HG2	2.29	0.48
2:D:158:ILE:HG22	2:D:159:SER:O	2.13	0.48
2:A:131:ASN:OD1	2:A:134:ARG:NH1	2.47	0.48
2:D:112:ILE:HD12	2:D:176:VAL:HG13	1.96	0.48
1:E:45:LEU:HA	1:E:48:LEU:HD12	1.95	0.48
2:G:30:ASP:O	2:G:34:ARG:HG3	2.13	0.48
2:G:94:GLU:OE2	2:G:94:GLU:N	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:95:ARG:HD2	2:A:96:ALA:H	1.78	0.48
1:B:49:ARG:HE	1:B:50:LEU:H	1.62	0.48
2:D:174:ASN:OD1	2:D:176:VAL:HB	2.14	0.48
1:E:54:ARG:HB3	1:E:58:ARG:NH2	2.28	0.48
1:B:77:ARG:HH22	2:D:51:HIS:HA	1.78	0.47
2:G:158:ILE:HG22	2:G:159:SER:N	2.27	0.47
2:A:254:THR:HG22	2:A:256:SER:H	1.79	0.47
1:E:147:THR:HG22	1:E:150:GLU:CG	2.44	0.47
1:E:182:GLU:OE1	1:E:185:ARG:HD3	2.14	0.47
2:D:120:TRP:HH2	2:D:177:ALA:HB2	1.79	0.47
1:E:193:GLN:HG3	1:E:194:VAL:N	2.29	0.47
2:G:148:SER:O	2:G:152:VAL:HG23	2.13	0.47
2:G:223:ILE:HA	2:G:226:LEU:HD12	1.97	0.47
2:D:119:ASP:OD1	2:D:126:ARG:NH1	2.48	0.47
1:T:68:SER:HG	3:T:202:C2E:HO2'	1.62	0.47
1:E:193:GLN:HG2	1:E:195:ASP:H	1.79	0.47
1:B:162:GLU:OE2	3:B:201:C2E:O2'	2.33	0.47
2:A:143:LEU:HD13	2:A:145:ARG:NH1	2.30	0.47
2:A:31:GLU:O	2:A:35:SER:OG	2.28	0.47
1:T:86:ALA:HA	1:T:89:THR:HG22	1.97	0.47
2:D:82:PHE:O	2:D:85:ILE:HG22	2.15	0.46
2:A:132:VAL:HG22	2:A:156:MET:SD	2.55	0.46
2:A:143:LEU:HD13	2:A:145:ARG:CZ	2.46	0.46
1:E:140:LEU:HD12	1:E:140:LEU:N	2.30	0.46
2:A:218:LEU:HD13	2:A:218:LEU:O	2.16	0.46
1:B:146:ARG:HG3	1:B:150:GLU:OE1	2.15	0.46
1:T:86:ALA:O	1:T:89:THR:HG22	2.16	0.46
2:A:101:THR:O	2:A:105:THR:HG23	2.15	0.46
1:T:139:GLU:O	1:T:146:ARG:NE	2.48	0.46
1:B:49:ARG:HG3	1:B:50:LEU:N	2.31	0.46
1:T:57:ARG:NH1	1:T:57:ARG:HB3	2.31	0.46
1:E:177:ASP:HA	1:E:180:SER:HB3	1.97	0.46
2:D:62:ARG:HA	2:D:65:VAL:HG23	1.98	0.45
1:B:82:ARG:HA	1:B:155:MET:HE1	1.98	0.45
2:G:235:THR:O	2:G:239:TYR:HB2	2.16	0.45
2:G:240:GLU:HA	2:G:240:GLU:OE1	2.15	0.45
2:G:250:VAL:HG23	2:G:251:LEU:HD12	1.98	0.45
2:A:59:VAL:HG11	2:A:107:ILE:HG22	1.98	0.45
1:E:147:THR:HG22	1:E:150:GLU:HG2	1.98	0.45
2:A:76:PHE:CD2	2:A:115:LEU:HD21	2.51	0.45
2:A:143:LEU:HD13	2:A:145:ARG:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:221:ARG:CZ	2:G:221:ARG:HB3	2.46	0.45
1:T:87:ARG:HD3	1:T:87:ARG:C	2.37	0.45
1:E:74:LEU:HD21	1:E:134:MET:HE2	1.99	0.45
1:E:85:LEU:HD21	1:E:151:LEU:HB2	1.99	0.45
1:T:49:ARG:HE	1:T:51:PRO:HG2	1.80	0.45
1:E:140:LEU:CD2	1:E:154:ALA:HB1	2.46	0.45
2:D:94:GLU:N	2:D:94:GLU:OE1	2.43	0.45
2:G:145:ARG:HG2	2:G:146:THR:N	2.32	0.45
2:G:158:ILE:HG22	2:G:162:ASP:CB	2.47	0.45
2:A:216:ARG:N	2:A:219:LEU:HD23	2.33	0.44
2:G:219:LEU:HA	2:G:273:LEU:HD21	1.99	0.44
2:D:268:GLN:O	2:D:272:LYS:HG3	2.17	0.44
2:A:170:LEU:HB2	2:A:263:THR:HG21	1.99	0.44
2:D:152:VAL:O	2:D:156:MET:HG3	2.18	0.44
2:A:145:ARG:HH12	2:A:147:PRO:HA	1.83	0.44
3:B:201:C2E:C5'	3:B:201:C2E:H8	2.32	0.44
1:E:57:ARG:HB2	1:E:179:CYS:HB3	1.99	0.44
1:B:77:ARG:HG2	1:B:158:LEU:HD13	1.99	0.44
1:B:167:ARG:HH22	1:B:174:ARG:HH22	1.66	0.44
1:E:54:ARG:HD3	1:E:58:ARG:HH12	1.82	0.44
2:G:107:ILE:O	2:G:111:MET:HG3	2.17	0.44
2:A:135:ALA:O	2:A:139:LEU:HB2	2.18	0.44
2:A:149:GLU:OE1	2:A:164:HIS:NE2	2.50	0.44
1:T:87:ARG:HD3	1:T:88:ARG:N	2.33	0.44
1:B:48:LEU:HG	1:B:49:ARG:N	2.33	0.43
1:E:67:LEU:HD23	1:E:67:LEU:HA	1.80	0.43
2:G:30:ASP:OD2	2:G:34:ARG:HD2	2.18	0.43
2:A:36:TYR:CE1	2:A:45:ARG:HB2	2.53	0.43
2:G:45:ARG:O	2:G:49:ILE:HG12	2.19	0.43
1:T:50:LEU:HD22	1:T:54:ARG:NH1	2.32	0.43
2:G:130:ARG:NH1	2:G:270:ARG:HH12	2.16	0.43
2:G:29:LEU:HD11	2:G:51:HIS:NE2	2.33	0.43
3:B:202:C2E:H8	3:B:202:C2E:C5'	2.43	0.43
1:E:57:ARG:HD3	1:E:183:ILE:HD12	2.00	0.43
2:G:257:ARG:HA	2:G:260:GLN:HG2	1.99	0.43
1:T:197:LEU:HD13	2:A:240:GLU:HG2	1.99	0.43
1:E:84:GLU:O	1:E:87:ARG:N	2.51	0.43
2:D:112:ILE:HD11	2:D:176:VAL:HG22	2.01	0.43
2:A:120:TRP:CH2	2:A:121:ILE:HD11	2.54	0.43
2:D:48:LEU:H	2:D:48:LEU:HD12	1.83	0.43
2:D:49:ILE:HG12	2:D:88:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:137:GLU:CD	1:T:157:ARG:HH22	2.19	0.43
1:E:50:LEU:N	1:E:51:PRO:HD2	2.33	0.43
2:A:130:ARG:HG2	2:A:130:ARG:NH1	2.33	0.43
1:B:187:TYR:HA	1:B:192:ALA:HB3	2.01	0.43
2:G:250:VAL:HG23	2:G:251:LEU:CD1	2.49	0.43
1:B:131:ALA:O	1:B:135:LEU:HG	2.19	0.43
2:D:44:LEU:O	2:D:47:GLN:N	2.50	0.43
2:A:37:LYS:NZ	2:A:91:PHE:O	2.35	0.42
3:E:201:C2E:H3A	3:E:201:C2E:C5'	2.48	0.42
1:T:146:ARG:HD3	1:T:150:GLU:OE1	2.20	0.42
1:B:48:LEU:HG	1:B:49:ARG:H	1.84	0.42
2:D:100:GLU:O	2:D:104:ILE:HG13	2.19	0.42
1:T:48:LEU:HG	2:D:169:GLN:NE2	2.35	0.42
1:T:99:LEU:HA	1:T:99:LEU:HD23	1.93	0.42
1:B:96:LEU:O	1:B:96:LEU:HD23	2.19	0.42
2:G:143:LEU:HD13	2:G:145:ARG:NH2	2.35	0.42
2:G:264:LYS:HG3	2:G:268:GLN:HE21	1.84	0.42
2:A:246:GLU:HA	2:A:249:HIS:ND1	2.34	0.42
1:E:114:ALA:HB3	2:G:244:LEU:HG	2.00	0.42
1:E:127:TYR:HA	1:E:130:LEU:HB3	2.01	0.42
1:T:49:ARG:HB2	1:T:52:GLU:OE2	2.20	0.42
2:D:139:LEU:HB2	2:D:147:PRO:HG3	2.01	0.42
1:E:134:MET:HE3	1:E:161:TYR:CD2	2.55	0.42
1:T:49:ARG:NH2	1:T:52:GLU:HG3	2.34	0.42
2:A:149:GLU:HB3	2:A:160:LEU:HD21	2.02	0.42
2:D:95:ARG:NH1	2:D:95:ARG:HG2	2.35	0.42
1:E:80:ILE:HG23	1:E:95:VAL:HG11	2.01	0.42
1:E:147:THR:HG22	1:E:150:GLU:CD	2.40	0.41
1:E:81:LEU:HD22	1:E:151:LEU:HD22	2.03	0.41
1:T:92:GLU:HG2	1:T:93:ALA:H	1.84	0.41
3:B:201:C2E:H3A	3:B:201:C2E:C5'	2.47	0.41
1:T:174:ARG:NH1	2:D:72:GLU:HG3	2.35	0.41
1:T:166:SER:HB3	3:T:201:C2E:O11	2.20	0.41
1:T:57:ARG:O	1:T:61:GLN:HG3	2.20	0.41
2:A:42:GLU:O	2:A:46:GLU:HB2	2.20	0.41
1:B:71:ARG:O	1:B:75:GLN:HG3	2.20	0.41
2:D:149:GLU:OE2	2:D:264:LYS:NZ	2.41	0.41
2:A:139:LEU:O	2:A:143:LEU:HG	2.21	0.41
2:D:235:THR:HG22	2:D:239:TYR:HD1	1.85	0.41
3:E:202:C2E:H512	3:E:202:C2E:C4'	2.51	0.41
1:T:146:ARG:HA	1:T:150:GLU:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:100:GLU:O	2:A:104:ILE:HG13	2.20	0.41
1:E:71:ARG:NH2	3:E:202:C2E:O61	2.53	0.41
2:G:160:LEU:HD23	2:G:160:LEU:HA	1.96	0.41
2:G:67:LEU:HD23	2:G:67:LEU:HA	1.96	0.41
1:T:162:GLU:OE2	3:T:201:C2E:O2'	2.39	0.41
1:T:58:ARG:NH1	1:T:58:ARG:HB2	2.36	0.41
1:E:147:THR:O	1:E:150:GLU:HG2	2.21	0.41
2:G:29:LEU:HD21	2:G:51:HIS:CD2	2.55	0.41
2:D:29:LEU:HD21	2:D:51:HIS:NE2	2.36	0.41
1:T:96:LEU:HD23	1:T:96:LEU:O	2.21	0.41
2:A:243:THR:O	2:A:247:ILE:HG13	2.21	0.40
2:G:266:VAL:HA	2:G:269:LEU:HB2	2.02	0.40
2:G:161:GLU:CD	2:G:161:GLU:H	2.24	0.40
2:A:254:THR:HG22	2:A:255:GLU:N	2.37	0.40
1:E:74:LEU:HD11	1:E:134:MET:CE	2.51	0.40
2:A:139:LEU:HD23	2:A:139:LEU:HA	1.89	0.40
2:D:87:ALA:O	2:D:91:PHE:HB2	2.21	0.40
1:E:96:LEU:HD23	1:E:96:LEU:O	2.21	0.40
2:G:269:LEU:HA	2:G:269:LEU:HD23	1.92	0.40

All (3) 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)
2:A:130:ARG:NH2	1:E:189:GLU:O[2_455]	2.10	0.10
2:A:123:ARG:NH2	1:E:46:GLY:O[2_455]	2.15	0.05
1:B:63:ASP:OD2	2:G:123:ARG:HH22[2_565]	1.59	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	B	158/176 (90%)	142 (90%)	16 (10%)	0	100	100
1	E	157/176 (89%)	144 (92%)	13 (8%)	0	100	100
1	T	162/176 (92%)	155 (96%)	7 (4%)	0	100	100
2	A	216/278 (78%)	196 (91%)	20 (9%)	0	100	100
2	D	216/278 (78%)	198 (92%)	18 (8%)	0	100	100
2	G	219/278 (79%)	200 (91%)	19 (9%)	0	100	100
All	All	1128/1362 (83%)	1035 (92%)	93 (8%)	0	100	100

There are no Ramachandran outliers to report.

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	B	129/145 (89%)	119 (92%)	10 (8%)	12	42
1	E	131/145 (90%)	124 (95%)	7 (5%)	22	58
1	T	135/145 (93%)	127 (94%)	8 (6%)	19	54
2	A	182/232 (78%)	174 (96%)	8 (4%)	28	65
2	D	182/232 (78%)	171 (94%)	11 (6%)	19	53
2	G	186/232 (80%)	180 (97%)	6 (3%)	39	74
All	All	945/1131 (84%)	895 (95%)	50 (5%)	22	58

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	T	39	ASP
1	T	44	GLU
1	T	87	ARG
1	T	105	ASP
1	T	109	ARG
1	T	134	MET
1	T	146	ARG

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Mol	Chain	Res	Type
1	T	188	ARG
2	A	28	SER
2	A	29	LEU
2	A	47	GLN
2	A	78	SER
2	A	95	ARG
2	A	124	SER
2	A	145	ARG
2	A	160	LEU
1	B	50	LEU
1	B	52	GLU
1	B	77	ARG
1	B	87	ARG
1	B	108	SER
1	B	146	ARG
1	B	162	GLU
1	B	185	ARG
1	B	195	ASP
1	B	197	LEU
2	D	46	GLU
2	D	123	ARG
2	D	155	GLU
2	D	158	ILE
2	D	168	SER
2	D	179	GLU
2	D	218	LEU
2	D	219	LEU
2	D	235	THR
2	D	253	VAL
2	D	254	THR
1	E	87	ARG
1	E	109	ARG
1	E	111	ARG
1	E	146	ARG
1	E	174	ARG
1	E	185	ARG
1	E	196	ASP
2	G	95	ARG
2	G	116	ARG
2	G	126	ARG
2	G	221	ARG
2	G	253	VAL

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Mol	Chain	Res	Type
2	G	259	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

6 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	$\# Z > 2$
3	C2E	B	202	-	44,52,52	2.43	18 (40%)	54,82,82	2.42	10 (18%)
3	C2E	B	201	-	44,52,52	2.62	19 (43%)	54,82,82	2.45	12 (22%)
3	C2E	T	202	-	44,52,52	2.52	17 (38%)	54,82,82	2.38	10 (18%)
3	C2E	E	202	-	44,52,52	2.56	19 (43%)	54,82,82	2.32	9 (16%)
3	C2E	E	201	-	44,52,52	2.46	16 (36%)	54,82,82	2.45	10 (18%)
3	C2E	T	201	-	44,52,52	2.35	17 (38%)	54,82,82	2.30	10 (18%)

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	C2E	B	202	-	-	8/22/62/62	0/6/7/7
3	C2E	B	201	-	-	1/22/62/62	0/6/7/7
3	C2E	T	202	-	-	3/22/62/62	0/6/7/7
3	C2E	E	202	-	-	4/22/62/62	0/6/7/7
3	C2E	E	201	-	-	2/22/62/62	0/6/7/7
3	C2E	T	201	-	-	10/22/62/62	0/6/7/7

All (106) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	201	C2E	C2'-C1'	7.56	1.65	1.53
3	E	202	C2E	C2'-C1'	6.94	1.64	1.53
3	T	202	C2E	C2'-C1'	6.90	1.64	1.53
3	T	201	C2E	C6-N1	6.26	1.43	1.33
3	T	201	C2E	C2'-C1'	6.07	1.63	1.53
3	E	202	C2E	C61-N11	6.00	1.43	1.33
3	T	202	C2E	C6-N1	5.95	1.43	1.33
3	E	202	C2E	C6-N1	5.92	1.43	1.33
3	B	202	C2E	C6-N1	5.90	1.43	1.33
3	B	201	C2E	C61-N11	5.87	1.43	1.33
3	E	201	C2E	C6-N1	5.76	1.43	1.33
3	B	202	C2E	C61-N11	5.76	1.43	1.33
3	B	201	C2E	C6-N1	5.69	1.42	1.33
3	T	202	C2E	C61-N11	5.64	1.42	1.33
3	E	201	C2E	C2'-C1'	5.50	1.62	1.53
3	E	201	C2E	C61-N11	5.33	1.42	1.33
3	T	201	C2E	C61-N11	5.33	1.42	1.33
3	B	202	C2E	C2'-C1'	5.09	1.61	1.53
3	B	202	C2E	C2'-C3'	4.90	1.63	1.52
3	E	201	C2E	C2'-C3'	4.53	1.63	1.52
3	T	202	C2E	P11-O3'	4.46	1.72	1.60
3	E	202	C2E	C2'-C3'	4.43	1.62	1.52
3	T	202	C2E	C2'-C3'	4.40	1.62	1.52
3	E	202	C2E	P11-O3'	4.31	1.71	1.60
3	E	201	C2E	P11-O3'	4.31	1.71	1.60
3	B	201	C2E	O4'-C1'	4.28	1.47	1.41
3	B	201	C2E	C2'-C3'	4.16	1.62	1.52
3	E	201	C2E	P1-O3A	4.14	1.71	1.60
3	B	202	C2E	P11-O3'	3.99	1.71	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	201	C2E	O4'-C1'	3.97	1.46	1.41
3	B	201	C2E	P1-O3A	3.93	1.70	1.60
3	B	201	C2E	P11-O3'	3.89	1.70	1.60
3	B	201	C2E	O5'-C5'	-3.77	1.30	1.44
3	E	202	C2E	O4'-C1'	3.73	1.46	1.41
3	E	201	C2E	O5'-C5'	-3.69	1.30	1.44
3	T	201	C2E	P11-O3'	3.68	1.70	1.60
3	T	202	C2E	C2-N1	3.64	1.41	1.35
3	E	202	C2E	C2-N1	3.64	1.41	1.35
3	B	202	C2E	O5'-C5'	-3.59	1.31	1.44
3	E	201	C2E	C2-N1	3.58	1.41	1.35
3	B	202	C2E	O4'-C1'	3.53	1.46	1.41
3	T	202	C2E	O5'-C5'	-3.51	1.31	1.44
3	T	201	C2E	C2-N1	3.49	1.41	1.35
3	E	202	C2E	C21-N11	3.47	1.41	1.35
3	E	201	C2E	C21-N11	3.45	1.41	1.35
3	B	202	C2E	P1-O3A	3.31	1.69	1.60
3	T	202	C2E	O4'-C1'	3.31	1.45	1.41
3	B	202	C2E	C2-N1	3.29	1.41	1.35
3	B	201	C2E	C2-N1	3.24	1.41	1.35
3	B	201	C2E	C21-N11	3.21	1.41	1.35
3	E	202	C2E	P1-O3A	3.20	1.68	1.60
3	B	202	C2E	C21-N11	3.16	1.41	1.35
3	T	201	C2E	C2'-C3'	3.14	1.59	1.52
3	T	201	C2E	O4'-C1'	3.10	1.45	1.41
3	T	202	C2E	P1-O3A	3.05	1.68	1.60
3	T	201	C2E	P1-O3A	3.02	1.68	1.60
3	T	202	C2E	C21-N11	3.02	1.40	1.35
3	T	201	C2E	C4-N3	2.88	1.40	1.35
3	E	202	C2E	O5'-C5'	-2.88	1.33	1.44
3	T	201	C2E	C21-N11	2.85	1.40	1.35
3	T	202	C2E	C2A-C1A	2.80	1.58	1.53
3	B	201	C2E	C2A-C1A	2.79	1.58	1.53
3	T	201	C2E	O4A-C1A	-2.72	1.37	1.41
3	E	201	C2E	O2A-C2A	-2.69	1.36	1.43
3	B	202	C2E	O2A-C2A	-2.67	1.36	1.43
3	E	201	C2E	P11-O5A	2.60	1.69	1.59
3	E	202	C2E	C21-N21	2.57	1.39	1.33
3	B	201	C2E	P11-O5A	2.56	1.69	1.59
3	B	201	C2E	C21-N21	2.53	1.39	1.33
3	T	202	C2E	C21-N21	2.53	1.39	1.33
3	B	201	C2E	C5A-C4A	2.52	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	202	C2E	C2A-C1A	2.51	1.57	1.53
3	T	202	C2E	O2A-C2A	-2.50	1.37	1.43
3	B	201	C2E	O2A-C2A	-2.49	1.37	1.43
3	E	202	C2E	O2A-C2A	-2.48	1.37	1.43
3	E	202	C2E	C41-N31	2.47	1.39	1.35
3	B	202	C2E	P11-O5A	2.46	1.69	1.59
3	E	202	C2E	P1-O5'	2.44	1.69	1.59
3	T	201	C2E	O3'-C3'	-2.42	1.35	1.44
3	E	201	C2E	C4-N3	2.40	1.39	1.35
3	B	202	C2E	C41-N31	2.40	1.39	1.35
3	E	201	C2E	C2-N2	2.39	1.38	1.33
3	E	202	C2E	P11-O5A	2.39	1.69	1.59
3	B	201	C2E	C2-N2	2.37	1.38	1.33
3	B	202	C2E	C21-N21	2.34	1.38	1.33
3	T	202	C2E	C2-N2	2.34	1.38	1.33
3	T	201	C2E	C2-N2	2.34	1.38	1.33
3	T	201	C2E	O2A-C2A	-2.32	1.37	1.43
3	T	202	C2E	C4-N3	2.27	1.39	1.35
3	B	201	C2E	C41-N31	2.25	1.39	1.35
3	B	202	C2E	C5A-C4A	2.23	1.58	1.51
3	T	202	C2E	O3A-C3A	-2.22	1.36	1.44
3	E	201	C2E	C5A-C4A	2.18	1.58	1.51
3	T	202	C2E	P11-O5A	2.18	1.68	1.59
3	B	202	C2E	O3A-C3A	-2.17	1.36	1.44
3	T	201	C2E	P1-O5'	2.17	1.68	1.59
3	B	202	C2E	C2-N2	2.13	1.38	1.33
3	E	202	C2E	C4-N3	2.12	1.39	1.35
3	B	201	C2E	P1-O5'	2.11	1.67	1.59
3	T	201	C2E	C21-N21	2.10	1.38	1.33
3	E	202	C2E	C2A-C1A	2.09	1.56	1.53
3	E	202	C2E	C2-N2	2.09	1.38	1.33
3	B	201	C2E	C4-N3	2.07	1.38	1.35
3	E	202	C2E	C5A-C4A	2.04	1.58	1.51
3	T	201	C2E	O5'-C5'	-2.04	1.36	1.44
3	E	201	C2E	C2A-C1A	2.02	1.56	1.53

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	202	C2E	C5-C6-N1	-9.13	110.95	123.43
3	B	202	C2E	C5-C6-N1	-9.00	111.12	123.43
3	B	201	C2E	C5-C6-N1	-8.96	111.18	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	202	C2E	C5-C6-N1	-8.91	111.25	123.43
3	E	201	C2E	C5-C6-N1	-8.87	111.30	123.43
3	T	201	C2E	C5-C6-N1	-8.83	111.35	123.43
3	E	201	C2E	C51-C61-N11	-8.76	111.44	123.43
3	E	202	C2E	C51-C61-N11	-8.37	111.98	123.43
3	B	201	C2E	C51-C61-N11	-8.36	112.00	123.43
3	T	202	C2E	C51-C61-N11	-8.35	112.02	123.43
3	B	202	C2E	C51-C61-N11	-8.33	112.03	123.43
3	T	201	C2E	C51-C61-N11	-8.29	112.09	123.43
3	T	202	C2E	C2-N3-C4	-5.32	109.29	115.36
3	B	201	C2E	C2-N3-C4	-5.28	109.33	115.36
3	T	201	C2E	C2-N3-C4	-5.20	109.42	115.36
3	B	202	C2E	C2-N3-C4	-5.08	109.56	115.36
3	E	202	C2E	C2-N3-C4	-5.02	109.62	115.36
3	E	201	C2E	C2-N3-C4	-4.95	109.71	115.36
3	B	202	C2E	C61-N11-C21	4.45	123.00	115.93
3	T	202	C2E	C6-N1-C2	4.41	122.94	115.93
3	B	201	C2E	C61-N11-C21	4.40	122.93	115.93
3	E	202	C2E	C6-N1-C2	4.37	122.88	115.93
3	B	202	C2E	C6-N1-C2	4.35	122.84	115.93
3	E	201	C2E	C6-N1-C2	4.35	122.84	115.93
3	T	202	C2E	C61-N11-C21	4.35	122.84	115.93
3	E	202	C2E	C61-N11-C21	4.33	122.81	115.93
3	B	201	C2E	C6-N1-C2	4.30	122.76	115.93
3	E	201	C2E	C61-N11-C21	4.27	122.71	115.93
3	E	201	C2E	C21-N31-C41	-4.22	110.53	115.36
3	B	202	C2E	C21-N31-C41	-4.12	110.66	115.36
3	T	201	C2E	C6-N1-C2	4.07	122.40	115.93
3	B	201	C2E	C21-N31-C41	-4.01	110.78	115.36
3	T	201	C2E	C61-N11-C21	3.96	122.22	115.93
3	E	202	C2E	C21-N31-C41	-3.90	110.90	115.36
3	T	202	C2E	C21-N31-C41	-3.83	110.98	115.36
3	B	202	C2E	O21-P11-O11	3.42	129.16	112.24
3	T	201	C2E	O21-P11-O11	3.41	129.11	112.24
3	B	201	C2E	O2P-P1-O1P	3.34	128.77	112.24
3	E	201	C2E	O2P-P1-O1P	3.32	128.68	112.24
3	B	201	C2E	C2'-C3'-C4'	3.31	109.09	103.22
3	E	201	C2E	C5'-C4'-C3'	-3.31	103.45	114.40
3	B	201	C2E	O21-P11-O11	3.26	128.34	112.24
3	T	202	C2E	O21-P11-O11	3.24	128.26	112.24
3	E	201	C2E	C2'-C3'-C4'	3.24	108.96	103.22
3	B	202	C2E	O2P-P1-O1P	3.20	128.08	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	202	C2E	O2P-P1-O1P	3.18	127.98	112.24
3	T	201	C2E	O2P-P1-O1P	3.16	127.85	112.24
3	E	202	C2E	O21-P11-O11	3.15	127.81	112.24
3	E	202	C2E	O2P-P1-O1P	3.15	127.81	112.24
3	E	201	C2E	O21-P11-O11	3.12	127.66	112.24
3	B	202	C2E	C5'-C4'-C3'	-3.09	104.15	114.40
3	B	201	C2E	C5'-C4'-C3'	-3.06	104.26	114.40
3	T	201	C2E	C21-N31-C41	-3.05	111.87	115.36
3	B	202	C2E	C2'-C3'-C4'	2.62	107.87	103.22
3	T	202	C2E	C5'-C4'-C3'	-2.30	106.78	114.40
3	T	201	C2E	O4A-C4A-C3A	2.23	109.64	104.87
3	B	201	C2E	C1'-N9-C4	2.19	130.48	126.64
3	E	202	C2E	C2'-C3'-C4'	2.16	107.06	103.22
3	T	201	C2E	O4'-C1'-C2'	2.16	110.08	106.93
3	T	202	C2E	C1'-N9-C4	2.15	130.42	126.64
3	B	201	C2E	O4A-C4A-C3A	2.05	109.25	104.87

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	202	C2E	C5A-O5A-P11-O21
3	E	201	C2E	C3'-O3'-P11-O5A
3	E	201	C2E	C5A-O5A-P11-O21
3	T	201	C2E	C3'-O3'-P11-O5A
3	T	201	C2E	O4A-C4A-C5A-O5A
3	T	202	C2E	C3'-C4'-C5'-O5'
3	T	201	C2E	O4'-C4'-C5'-O5'
3	T	201	C2E	C3'-C4'-C5'-O5'
3	T	201	C2E	C3A-C4A-C5A-O5A
3	B	202	C2E	C5A-O5A-P11-O3'
3	T	201	C2E	C5'-O5'-P1-O3A
3	T	201	C2E	C5A-O5A-P11-O3'
3	E	202	C2E	O4A-C4A-C5A-O5A
3	T	202	C2E	O4'-C4'-C5'-O5'
3	B	201	C2E	C3'-O3'-P11-O5A
3	T	202	C2E	C3'-O3'-P11-O5A
3	E	202	C2E	C3A-C4A-C5A-O5A
3	B	202	C2E	C3'-O3'-P11-O5A
3	E	202	C2E	C3'-O3'-P11-O5A
3	B	202	C2E	O4A-C4A-C5A-O5A
3	B	202	C2E	C5A-O5A-P11-O11

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Mol	Chain	Res	Type	Atoms
3	T	201	C2E	C5'-O5'-P1-O1P
3	T	201	C2E	C5A-O5A-P11-O11
3	B	202	C2E	C3'-C4'-C5'-O5'
3	E	202	C2E	C3'-C4'-C5'-O5'
3	B	202	C2E	C3A-O3A-P1-O5'
3	B	202	C2E	O4'-C4'-C5'-O5'
3	T	201	C2E	C4A-C3A-O3A-P1

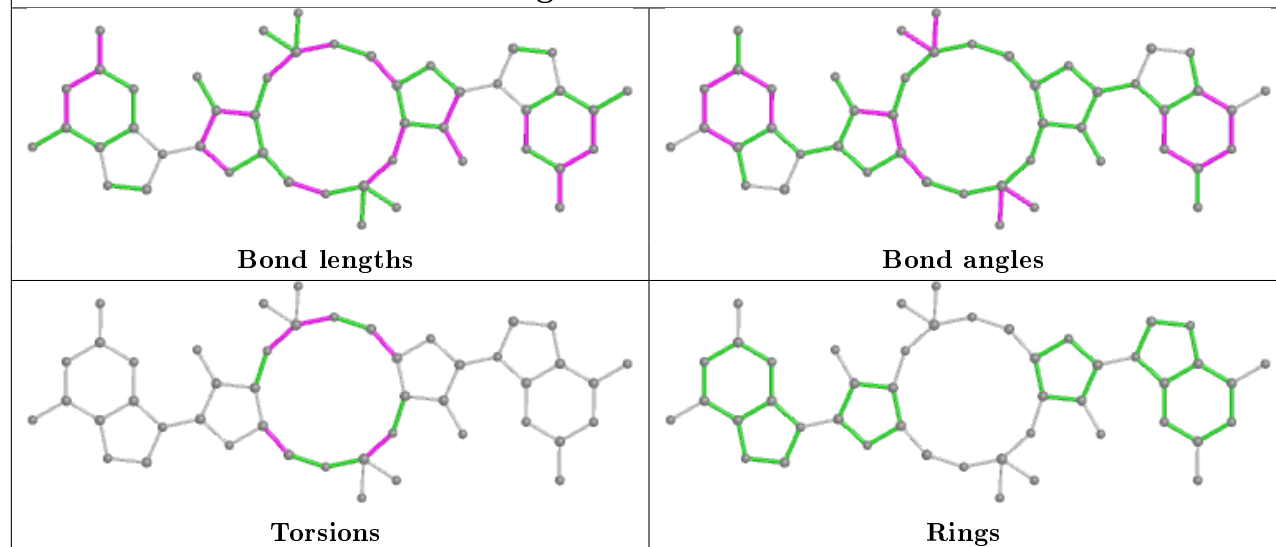
There are no ring outliers.

6 monomers are involved in 34 short contacts:

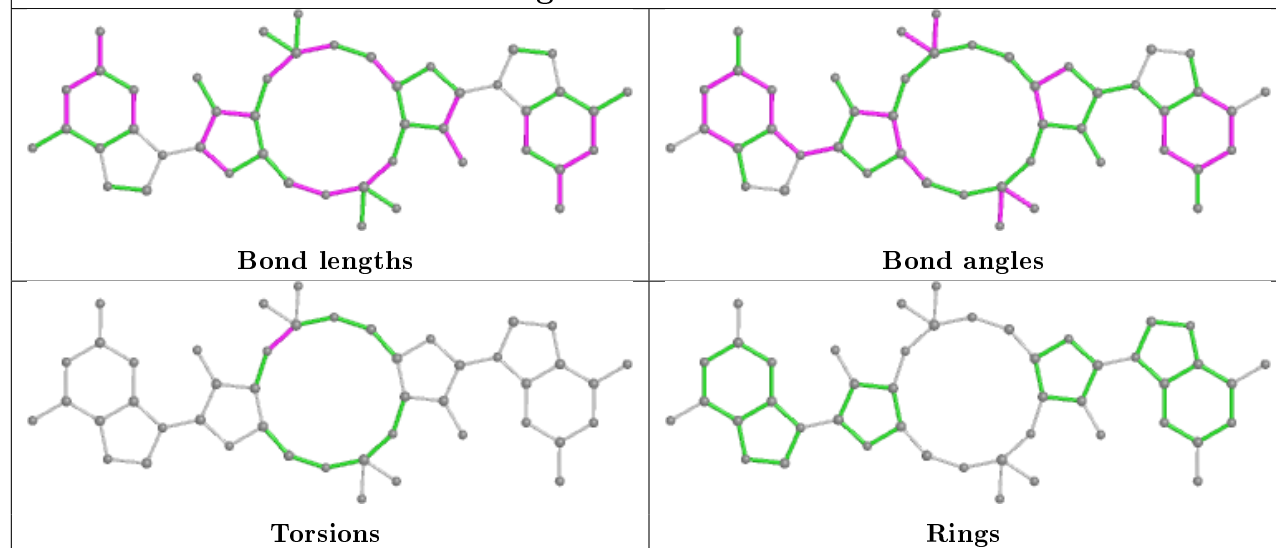
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	202	C2E	5	0
3	B	201	C2E	8	0
3	T	202	C2E	5	0
3	E	202	C2E	6	0
3	E	201	C2E	7	0
3	T	201	C2E	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

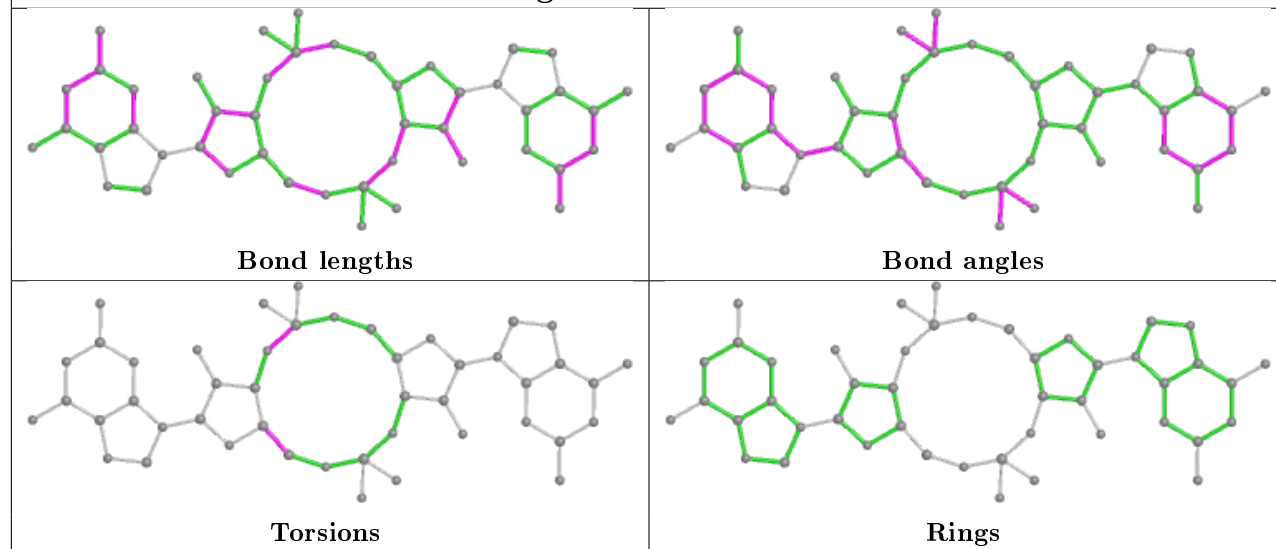
Ligand C2E B 202



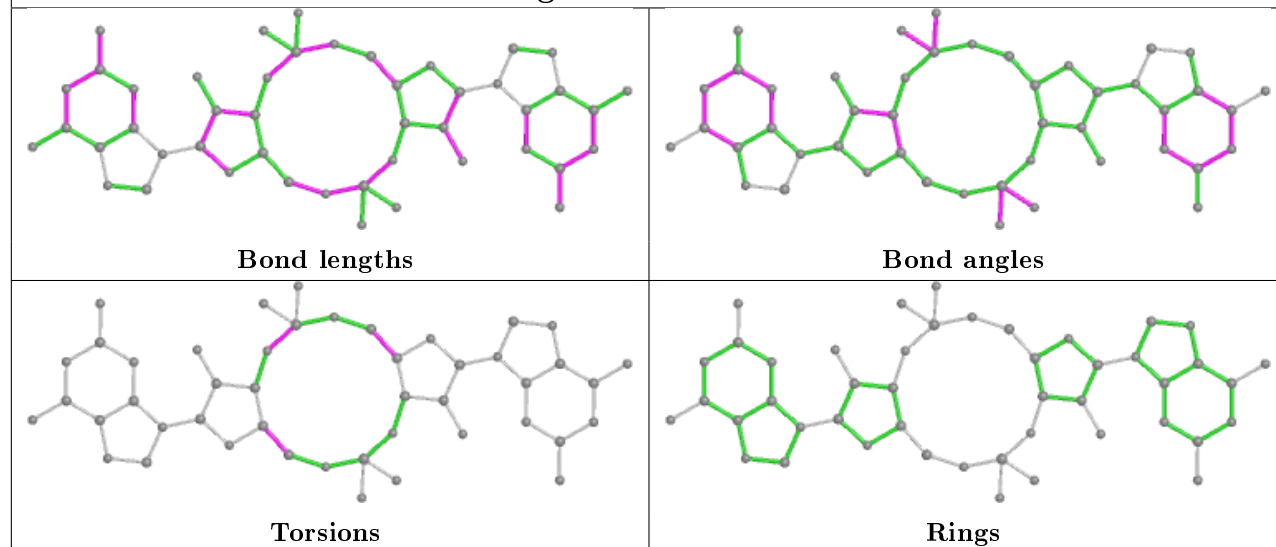
Ligand C2E B 201



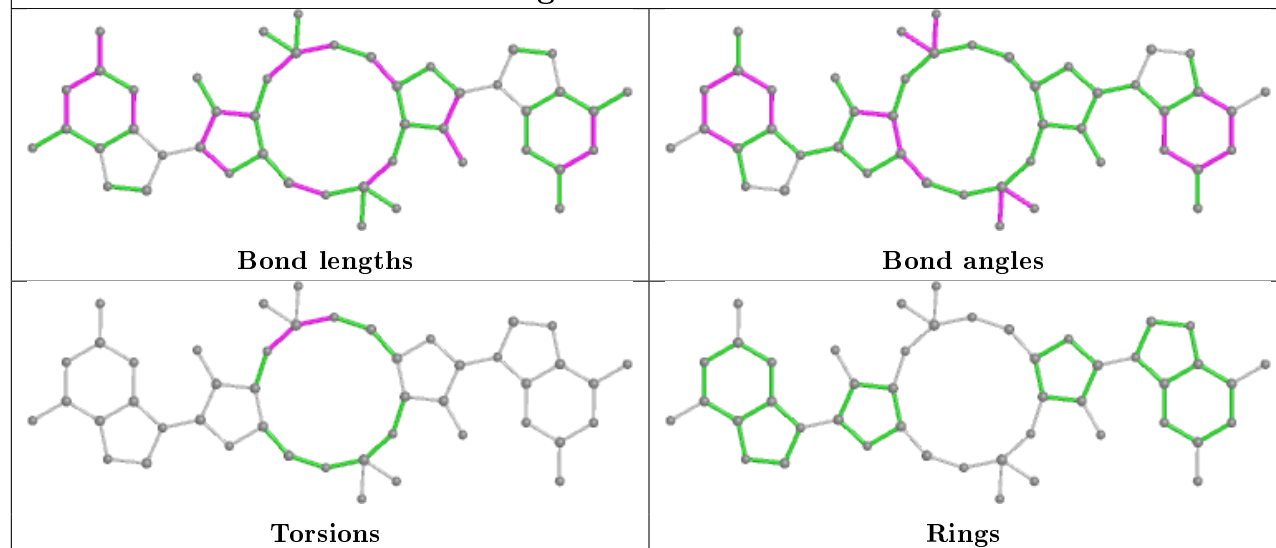
Ligand C2E T 202



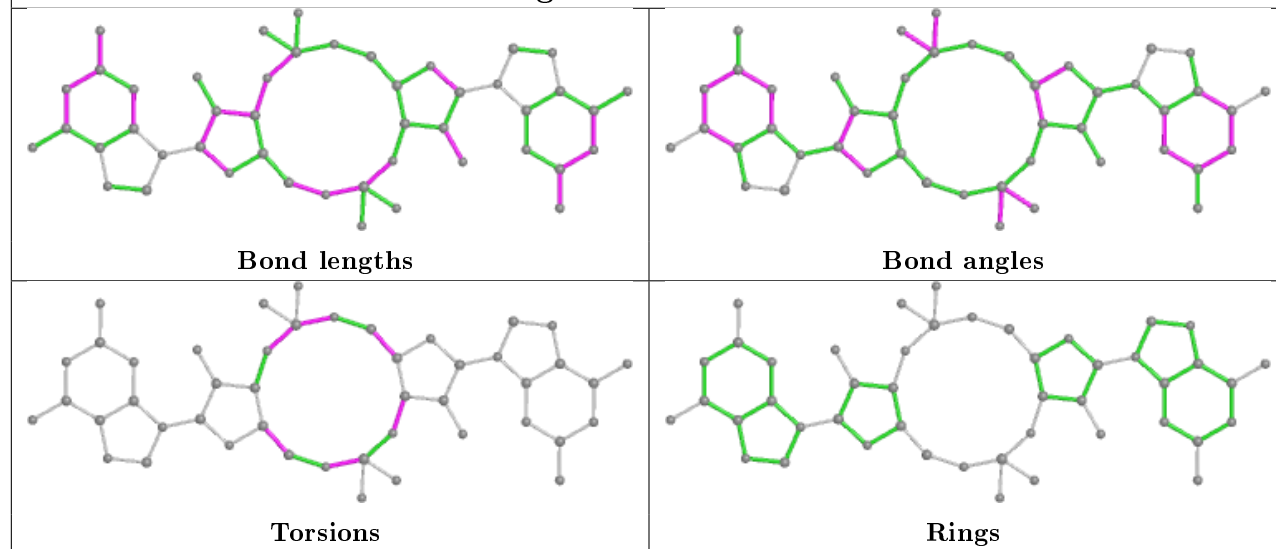
Ligand C2E E 202



Ligand C2E E 201



Ligand C2E T 201



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	B	160/176 (90%)	0.02	4 (2%) 57 29	74, 109, 169, 192	0
1	E	159/176 (90%)	-0.02	1 (0%) 89 72	72, 106, 146, 172	0
1	T	164/176 (93%)	-0.29	0 100 100	59, 93, 137, 169	0
2	A	220/278 (79%)	-0.12	0 100 100	48, 90, 156, 188	0
2	D	220/278 (79%)	-0.15	2 (0%) 84 63	60, 98, 151, 194	0
2	G	223/278 (80%)	-0.17	0 100 100	64, 96, 139, 176	0
All	All	1146/1362 (84%)	-0.13	7 (0%) 89 72	48, 99, 153, 194	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	199	ALA	3.3
1	B	197	LEU	3.0
2	D	96	ALA	2.8
1	E	154	ALA	2.4
2	D	94	GLU	2.1
1	B	47	ALA	2.0
1	B	198	LEU	2.0

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 carbohydrates in this entry.

6.4 Ligands [i](#)

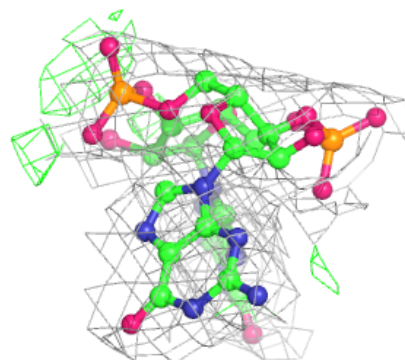
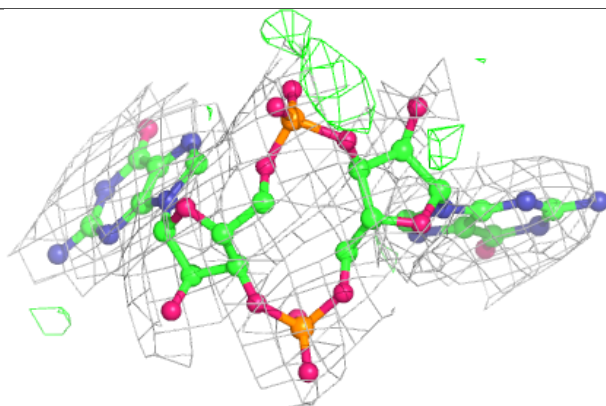
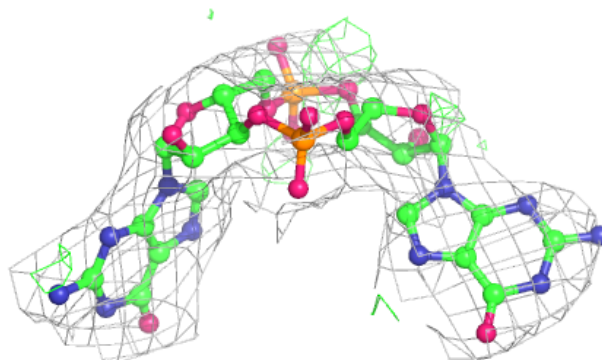
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	C2E	E	202	46/46	0.93	0.22	47,75,111,137	0
3	C2E	E	201	46/46	0.93	0.23	61,100,134,164	0
3	C2E	B	201	46/46	0.95	0.20	55,76,92,103	0
3	C2E	B	202	46/46	0.96	0.22	55,74,96,112	0
3	C2E	T	202	46/46	0.97	0.22	42,62,95,108	0
3	C2E	T	201	46/46	0.97	0.20	32,57,78,91	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.

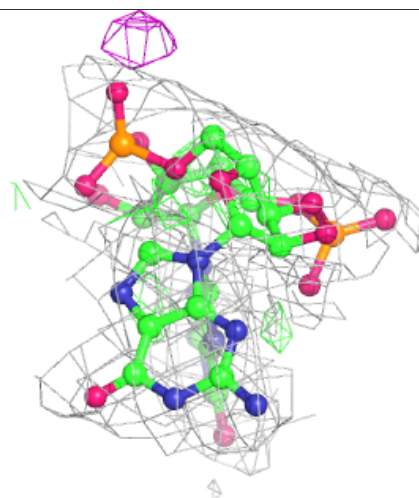
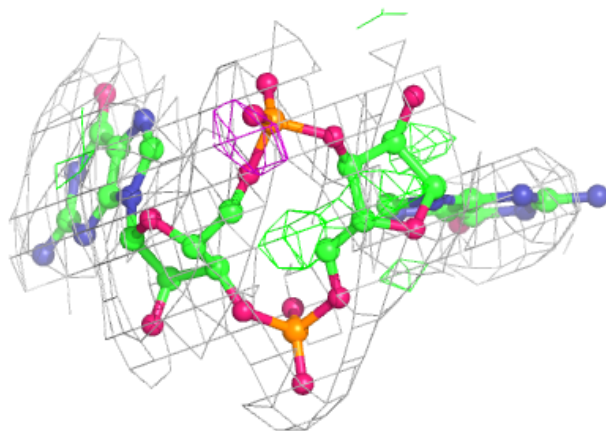
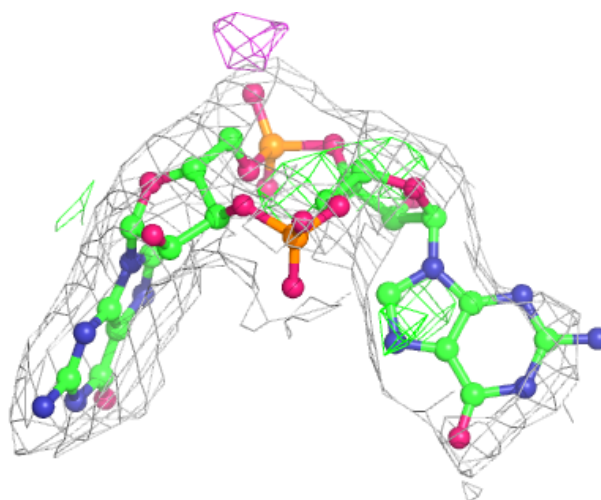
Electron density around C2E E 202:

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



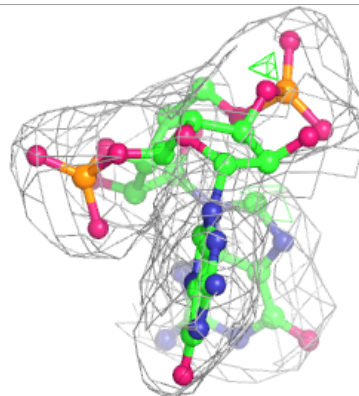
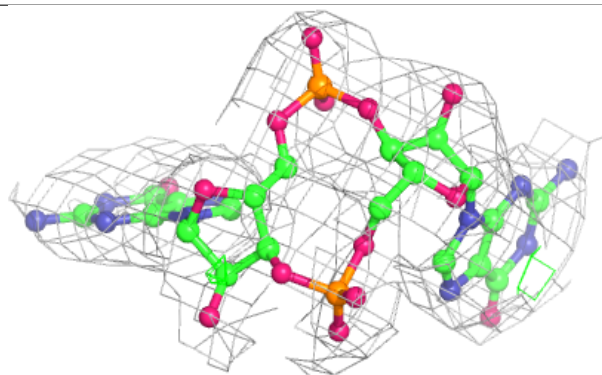
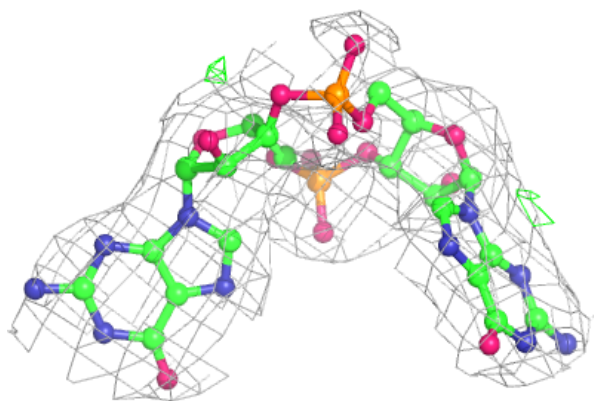
Electron density around C2E E 201:

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

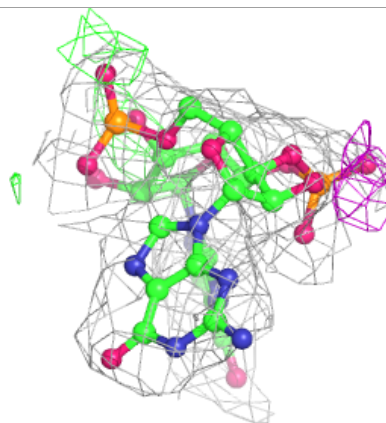
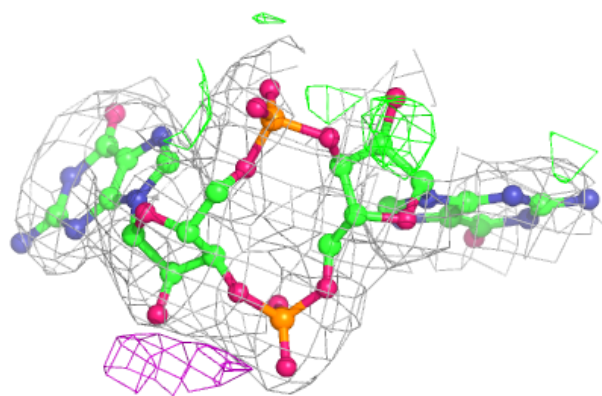
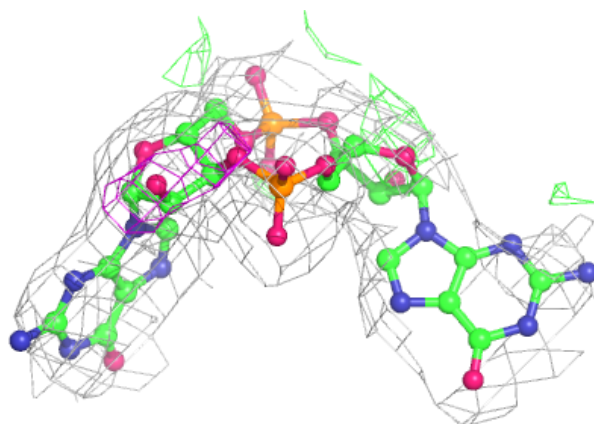


Electron density around C2E B 201:

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

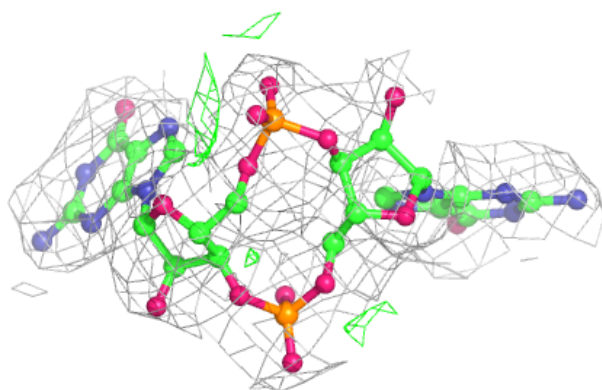
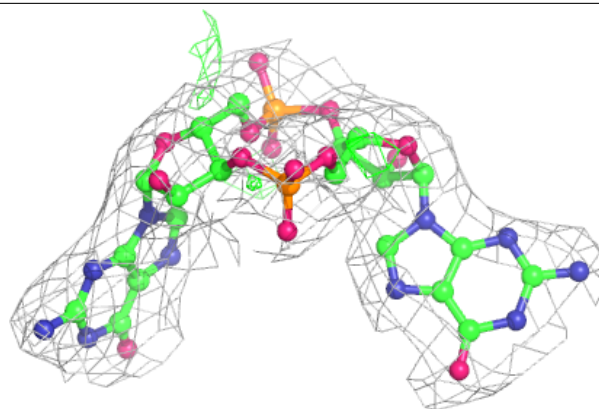
**Electron density around C2E B 202:**

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

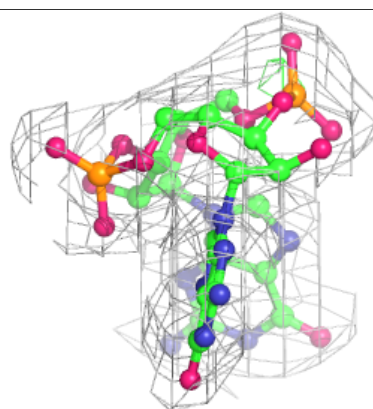
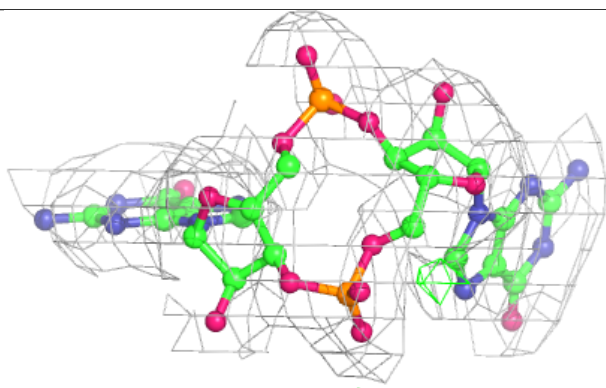
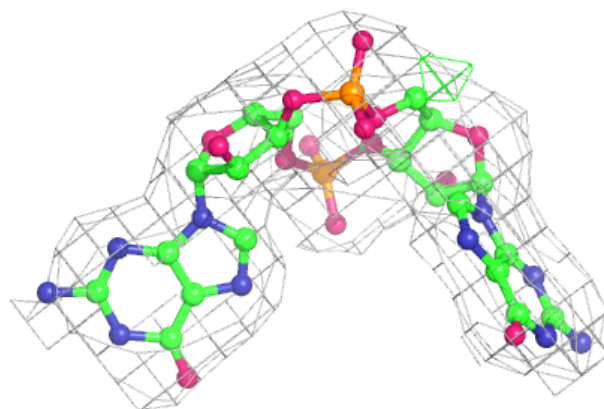


Electron density around C2E T 202:

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

**Electron density around C2E T 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

There are no such residues in this entry.