



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:59 AM UTC

PDB ID : 4URS / pdb_00004urs
Title : Crystal Structure of GGDEF domain from T.maritima
Authors : Deepthi, A.; Liew, C.W.; Liang, Z.X.; Swaminathan, K.; Lescar, J.
Deposited on : 2014-07-02
Resolution : 2.27 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

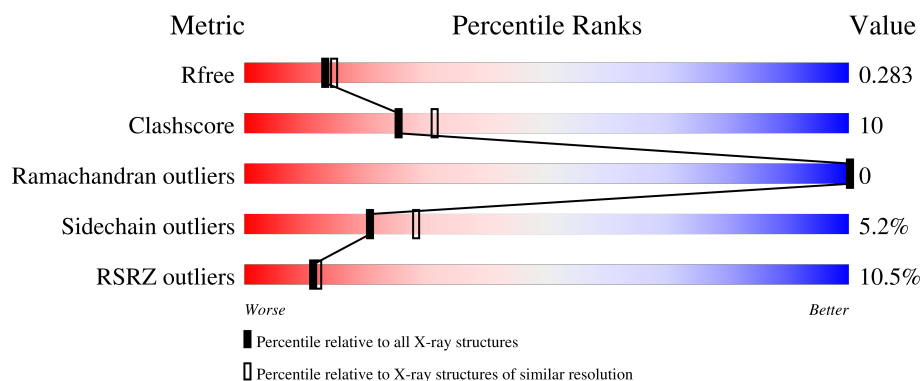
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	188	9% 63% 18% 5% 14%
1	B	188	10% 63% 20% • 14%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2980 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 DIGUANYLATE CYCLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	0	0	0
			1329	853	229	242	5			
1	B	162	Total	C	N	O	S	0	2	0
			1344	863	234	242	5			

There are 42 discrepancies between the modelled and reference sequences:

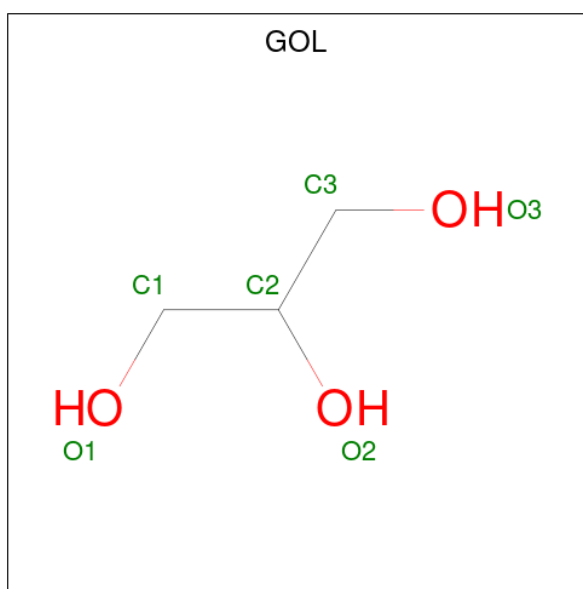
Chain	Residue	Modelled	Actual	Comment	Reference
A	61	MET	-	expression tag	UNP Q9X2A8
A	62	GLY	-	expression tag	UNP Q9X2A8
A	63	SER	-	expression tag	UNP Q9X2A8
A	64	SER	-	expression tag	UNP Q9X2A8
A	65	HIS	-	expression tag	UNP Q9X2A8
A	66	HIS	-	expression tag	UNP Q9X2A8
A	67	HIS	-	expression tag	UNP Q9X2A8
A	68	HIS	-	expression tag	UNP Q9X2A8
A	69	HIS	-	expression tag	UNP Q9X2A8
A	70	HIS	-	expression tag	UNP Q9X2A8
A	71	SER	-	expression tag	UNP Q9X2A8
A	72	SER	-	expression tag	UNP Q9X2A8
A	73	GLY	-	expression tag	UNP Q9X2A8
A	74	LEU	-	expression tag	UNP Q9X2A8
A	75	VAL	-	expression tag	UNP Q9X2A8
A	76	PRO	-	expression tag	UNP Q9X2A8
A	77	ARG	-	expression tag	UNP Q9X2A8
A	78	GLY	-	expression tag	UNP Q9X2A8
A	79	SER	-	expression tag	UNP Q9X2A8
A	80	HIS	-	expression tag	UNP Q9X2A8
A	81	MET	-	expression tag	UNP Q9X2A8
B	61	MET	-	expression tag	UNP Q9X2A8
B	62	GLY	-	expression tag	UNP Q9X2A8
B	63	SER	-	expression tag	UNP Q9X2A8
B	64	SER	-	expression tag	UNP Q9X2A8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	65	HIS	-	expression tag	UNP Q9X2A8
B	66	HIS	-	expression tag	UNP Q9X2A8
B	67	HIS	-	expression tag	UNP Q9X2A8
B	68	HIS	-	expression tag	UNP Q9X2A8
B	69	HIS	-	expression tag	UNP Q9X2A8
B	70	HIS	-	expression tag	UNP Q9X2A8
B	71	SER	-	expression tag	UNP Q9X2A8
B	72	SER	-	expression tag	UNP Q9X2A8
B	73	GLY	-	expression tag	UNP Q9X2A8
B	74	LEU	-	expression tag	UNP Q9X2A8
B	75	VAL	-	expression tag	UNP Q9X2A8
B	76	PRO	-	expression tag	UNP Q9X2A8
B	77	ARG	-	expression tag	UNP Q9X2A8
B	78	GLY	-	expression tag	UNP Q9X2A8
B	79	SER	-	expression tag	UNP Q9X2A8
B	80	HIS	-	expression tag	UNP Q9X2A8
B	81	MET	-	expression tag	UNP Q9X2A8

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



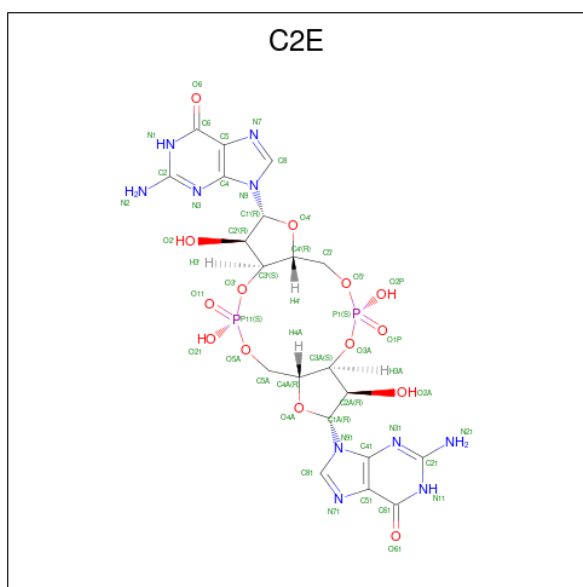
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	12	6	1	4	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-dioxidoctahydro-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) (CCD ID: C2E) (formula: $C_{20}H_{24}N_{10}O_{14}P_2$).



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

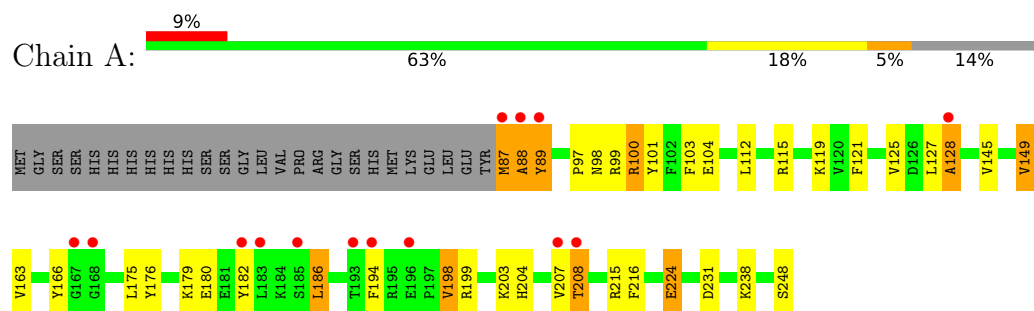
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	62	Total	O	0	0
			62	62		
5	B	31	Total	O	0	0
			31	31		

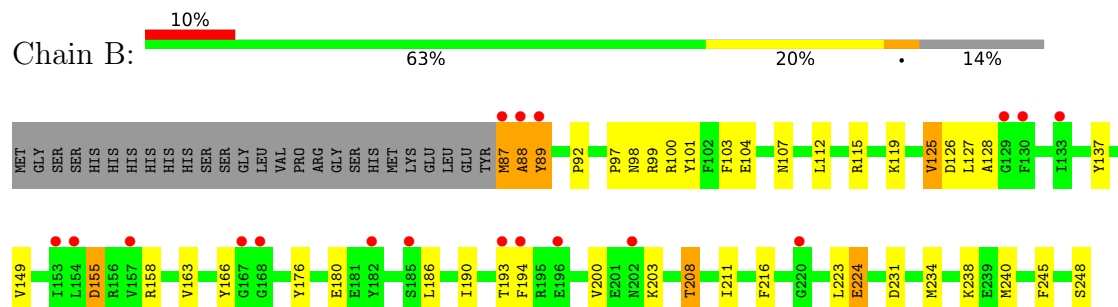
3 Residue-property plots

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

• Molecule 1: DIGUANYLATE CYCLASE



• Molecule 1: DIGUANYLATE CYCLASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	37.15Å 37.14Å 62.28Å 95.48° 100.23° 107.78°	Depositor
Resolution (Å)	32.58 – 2.27 32.58 – 2.27	Depositor EDS
% Data completeness (in resolution range)	95.6 (32.58-2.27) 95.7 (32.58-2.27)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.84 (at 2.26Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.218 , 0.268 0.224 , 0.283	Depositor DCC
R_{free} test set	682 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	33.1	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 65.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.036 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	2980	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.05% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MES, 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	A	0.83	0/1355	1.45	15/1820 (0.8%)
1	B	0.87	0/1377	1.41	10/1849 (0.5%)
All	All	0.85	0/2732	1.43	25/3669 (0.7%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	128	ALA	N-CA-C	9.50	121.23	111.07
1	A	231	ASP	CA-C-N	7.59	130.79	120.54
1	A	231	ASP	C-N-CA	7.59	130.79	120.54
1	B	231	ASP	CA-C-N	7.06	130.61	120.79
1	B	231	ASP	C-N-CA	7.06	130.61	120.79
1	A	208	THR	CB-CA-C	6.99	118.19	110.15
1	B	208	THR	CB-CA-C	6.91	118.10	110.15
1	A	238	LYS	CA-C-N	6.54	129.58	120.29
1	A	238	LYS	C-N-CA	6.54	129.58	120.29
1	A	88	ALA	CA-C-N	6.36	130.35	120.75
1	A	88	ALA	C-N-CA	6.36	130.35	120.75
1	B	88	ALA	CA-C-N	6.30	130.27	120.75
1	B	88	ALA	C-N-CA	6.30	130.27	120.75
1	B	238	LYS	CA-C-N	6.19	130.51	120.60
1	B	238	LYS	C-N-CA	6.19	130.51	120.60
1	B	155	ASP	CA-CB-CG	5.87	118.47	112.60
1	A	154	LEU	CA-C-N	5.56	128.49	120.38
1	A	154	LEU	C-N-CA	5.56	128.49	120.38
1	A	224	GLU	CB-CG-CD	5.49	121.93	112.60
1	B	224	GLU	CB-CG-CD	5.39	121.76	112.60
1	A	179	LYS	CA-C-N	5.31	127.66	120.38
1	A	179	LYS	C-N-CA	5.31	127.66	120.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	89	TYR	N-CA-C	5.25	117.49	110.35
1	A	89	TYR	N-CA-C	5.05	117.22	110.35
1	A	155	ASP	CA-CB-CG	5.03	117.63	112.60

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	1329	0	1348	35	0
1	B	1344	0	1368	32	0
2	A	6	0	8	0	0
2	B	12	0	16	1	0
3	A	12	0	13	0	0
4	A	92	0	44	2	0
4	B	92	0	44	4	0
5	A	62	0	0	2	0
5	B	31	0	0	0	0
All	All	2980	0	2841	55	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 10.

All (55) 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)
5:A:2019:HOH:O	4:B:1249:C2E:H81	1.45	1.14
1:A:100:ARG:HG2	1:B:87:MET:HA	1.41	1.01
1:A:128:ALA:HB3	1:A:208:THR:HG23	1.69	0.74
1:A:89:TYR:HB3	1:A:98:ASN:HD21	1.52	0.73
1:B:89:TYR:HB3	1:B:98:ASN:HD21	1.51	0.73
1:B:92:PRO:HD3	2:B:1251:GOL:H12	1.69	0.71
1:A:88:ALA:HB3	1:B:104:GLU:HG3	1.74	0.68
1:A:104:GLU:HG3	1:B:88:ALA:HB3	1.76	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:MET:HE1	1:B:245:PHE:CD1	2.33	0.64
1:A:115:ARG:NH2	4:B:1249:C2E:N71	2.42	0.62
1:A:89:TYR:HB3	1:A:98:ASN:ND2	2.14	0.62
1:A:127:LEU:HD21	1:A:149:VAL:HG11	1.81	0.62
1:B:89:TYR:HB3	1:B:98:ASN:ND2	2.14	0.61
1:B:128:ALA:HB3	1:B:208:THR:HG23	1.85	0.59
1:A:176:TYR:CD2	1:B:112:LEU:HD11	2.38	0.58
4:A:1252:C2E:N7	1:B:115:ARG:NH2	2.50	0.57
1:B:127:LEU:HD21	1:B:194:PHE:CD1	2.41	0.56
1:A:182:TYR:CD2	4:A:1252:C2E:H511	2.42	0.55
1:A:127:LEU:HD23	1:A:207:VAL:HG21	1.88	0.55
1:A:87:MET:HB2	1:B:89:TYR:HB2	1.88	0.55
1:B:103:PHE:HE1	1:B:224:GLU:HG3	1.74	0.53
1:A:87:MET:O	1:B:88:ALA:HA	2.09	0.53
1:A:88:ALA:HA	1:B:87:MET:O	2.09	0.53
1:A:112:LEU:HD11	1:B:176:TYR:CD2	2.45	0.51
1:B:125:VAL:HG13	1:B:211:ILE:HG12	1.91	0.51
1:A:103:PHE:HE1	1:A:224:GLU:HG3	1.75	0.51
1:B:97:PRO:HD2	1:B:163:VAL:O	2.10	0.51
1:A:97:PRO:HD2	1:A:163:VAL:O	2.10	0.51
1:A:100:ARG:CG	1:B:87:MET:HA	2.28	0.50
1:A:87:MET:HA	1:B:100[B]:ARG:HD2	1.95	0.49
1:A:97:PRO:HB3	1:A:101:TYR:CD2	2.49	0.48
1:A:119:LYS:HE2	1:A:216:PHE:O	2.14	0.47
1:A:125:VAL:HG11	1:A:194:PHE:CE2	2.49	0.47
1:B:97:PRO:HB3	1:B:101:TYR:CD2	2.49	0.47
1:B:158:ARG:HG2	4:B:1252:C2E:H81	1.97	0.47
1:A:119:LYS:HG2	1:A:121:PHE:HE1	1.81	0.45
1:B:119:LYS:HD3	1:B:216:PHE:O	2.17	0.45
1:A:98:ASN:OD1	1:B:87:MET:N	2.49	0.45
1:A:119:LYS:NZ	1:A:215:ARG:HB3	2.32	0.45
1:A:145:VAL:HG13	1:A:198:VAL:HG11	1.99	0.44
1:A:153:ILE:HG12	1:A:194:PHE:CE2	2.53	0.44
1:A:87:MET:CB	1:B:89:TYR:HB2	2.47	0.44
1:A:104:GLU:CG	1:B:88:ALA:HB3	2.46	0.43
1:B:107:ASN:HD21	1:B:223:LEU:H	1.66	0.43
1:A:87:MET:N	1:B:98:ASN:OD1	2.51	0.43
1:B:126:ASP:HB2	1:B:234:MET:SD	2.59	0.43
1:B:99:ARG:HD3	1:B:166:TYR:O	2.18	0.42
1:A:99:ARG:HD3	1:A:166:TYR:O	2.18	0.42
1:A:175:LEU:CD1	1:A:186:LEU:HD21	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:LEU:HD13	1:A:186:LEU:HD21	2.01	0.42
1:B:190:ILE:HA	1:B:193:THR:HG22	2.01	0.41
1:A:121:PHE:HZ	1:A:180:GLU:HG3	1.86	0.41
1:B:137:TYR:CE1	1:B:203:LYS:HD3	2.55	0.41
1:A:199:ARG:HG2	1:A:204:HIS:CE1	2.56	0.41
5:A:2019:HOH:O	4:B:1249:C2E:C81	2.30	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	160/188 (85%)	157 (98%)	3 (2%)	0	100	100
1	B	162/188 (86%)	158 (98%)	4 (2%)	0	100	100
All	All	322/376 (86%)	315 (98%)	7 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	144/167 (86%)	137 (95%)	7 (5%)	22	31
1	B	146/167 (87%)	138 (94%)	8 (6%)	19	26

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	290/334 (87%)	275 (95%)	15 (5%)	21	28

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	MET
1	A	100	ARG
1	A	149	VAL
1	A	186	LEU
1	A	198	VAL
1	A	203	LYS
1	A	248	SER
1	B	87	MET
1	B	125	VAL
1	B	149	VAL
1	B	155	ASP
1	B	180	GLU
1	B	186	LEU
1	B	200	VAL
1	B	248	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	ASN
1	A	204	HIS
1	A	222	ASN
1	B	98	ASN
1	B	107	ASN
1	B	222	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	MES	A	1250	-	12,12,12	1.99	3 (25%)	15,16,16	1.48	2 (13%)
2	GOL	A	1249	-	5,5,5	0.50	0	5,5,5	0.15	0
2	GOL	B	1251	-	5,5,5	0.53	0	5,5,5	0.66	0
4	C2E	B	1249	-	52,52,52	2.00	11 (21%)	78,82,82	1.83	16 (20%)
4	C2E	A	1251	-	52,52,52	1.90	10 (19%)	78,82,82	1.87	17 (21%)
2	GOL	B	1250	-	5,5,5	0.45	0	5,5,5	0.15	0
4	C2E	B	1252	-	52,52,52	1.94	11 (21%)	78,82,82	1.86	16 (20%)
4	C2E	A	1252	-	52,52,52	2.00	7 (13%)	78,82,82	1.90	20 (25%)

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	MES	A	1250	-	-	3/6/14/14	0/1/1/1
2	GOL	A	1249	-	-	2/4/4/4	-
2	GOL	B	1251	-	-	2/4/4/4	-
4	C2E	B	1249	-	-	2/30/62/62	0/6/7/7
4	C2E	A	1251	-	-	1/30/62/62	0/6/7/7
2	GOL	B	1250	-	-	0/4/4/4	-
4	C2E	B	1252	-	-	0/30/62/62	0/6/7/7
4	C2E	A	1252	-	-	1/30/62/62	0/6/7/7

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1252	C2E	O61-C61	7.53	1.37	1.23
4	A	1252	C2E	O6-C6	7.09	1.37	1.23
4	B	1249	C2E	O6-C6	7.08	1.37	1.23
4	B	1252	C2E	O6-C6	6.91	1.36	1.23
4	A	1251	C2E	O6-C6	6.84	1.36	1.23
4	B	1252	C2E	O61-C61	6.68	1.36	1.23
4	B	1249	C2E	O61-C61	6.66	1.36	1.23
4	A	1251	C2E	O61-C61	6.55	1.36	1.23
4	A	1252	C2E	O4'-C1'	4.59	1.52	1.42
3	A	1250	MES	C8-S	4.22	1.83	1.77
4	B	1249	C2E	O4A-C1A	4.15	1.51	1.42
4	B	1252	C2E	O4'-C1'	3.47	1.50	1.42
4	B	1249	C2E	C51-N71	-3.31	1.32	1.39
3	A	1250	MES	O1S-S	3.20	1.54	1.45
3	A	1250	MES	O2S-S	3.15	1.54	1.45
4	A	1252	C2E	C5-N7	-3.10	1.32	1.39
4	A	1251	C2E	C51-N71	-3.10	1.32	1.39
4	A	1251	C2E	O4'-C1'	2.94	1.48	1.42
4	B	1249	C2E	C51-C61	-2.90	1.33	1.44
4	B	1252	C2E	C51-N71	-2.83	1.33	1.39
4	A	1251	C2E	C5-N7	-2.81	1.33	1.39
4	A	1251	C2E	C51-C61	-2.78	1.34	1.44
4	A	1251	C2E	C5-C6	-2.78	1.34	1.44
4	A	1252	C2E	C5-C6	-2.72	1.34	1.44
4	B	1252	C2E	O4A-C1A	2.67	1.48	1.42
4	B	1252	C2E	C5-C6	-2.66	1.34	1.44
4	B	1252	C2E	C5-N7	-2.66	1.33	1.39
4	B	1252	C2E	C51-C61	-2.65	1.34	1.44
4	B	1249	C2E	C61-N11	-2.61	1.34	1.38
4	B	1249	C2E	C5-N7	-2.59	1.33	1.39
4	B	1249	C2E	C6-N1	-2.57	1.34	1.38
4	A	1252	C2E	C51-N71	-2.56	1.33	1.39
4	A	1251	C2E	O4A-C1A	2.46	1.47	1.42
4	B	1249	C2E	C5-C6	-2.44	1.35	1.44
4	B	1249	C2E	C81-N91	-2.42	1.32	1.37
4	B	1252	C2E	C6-N1	-2.41	1.34	1.38
4	A	1252	C2E	C51-C61	-2.36	1.35	1.44
4	B	1249	C2E	O4'-C1'	2.24	1.47	1.42
4	A	1251	C2E	C6-N1	-2.15	1.34	1.38
4	B	1252	C2E	C61-N11	-2.13	1.34	1.38
4	A	1251	C2E	C81-N91	-2.09	1.32	1.37
4	B	1252	C2E	C81-N91	-2.04	1.33	1.37

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1252	C2E	C5-C4-N3	-5.88	119.04	128.39
4	B	1249	C2E	C51-C41-N31	-5.70	119.32	128.39
4	B	1252	C2E	C51-C41-N31	-5.70	119.32	128.39
4	B	1252	C2E	C5-C4-N3	-5.40	119.80	128.39
4	A	1251	C2E	C5-C4-N3	-5.35	119.88	128.39
4	A	1251	C2E	C51-C41-N31	-5.33	119.90	128.39
4	B	1249	C2E	C5-C4-N3	-5.14	120.21	128.39
4	A	1252	C2E	C51-C41-N31	-4.89	120.61	128.39
4	A	1251	C2E	C2-N3-C4	4.66	120.33	112.30
4	A	1252	C2E	C2-N3-C4	4.60	120.23	112.30
4	B	1249	C2E	C21-N31-C41	4.54	120.13	112.30
4	A	1252	C2E	C21-N31-C41	4.47	120.00	112.30
4	B	1252	C2E	C2-N3-C4	4.47	119.99	112.30
4	B	1252	C2E	C21-N31-C41	4.46	119.99	112.30
4	A	1251	C2E	C21-N31-C41	4.43	119.93	112.30
4	B	1249	C2E	C2-N3-C4	4.30	119.70	112.30
4	A	1252	C2E	O6-C6-C5	-3.97	116.04	126.53
4	B	1252	C2E	O4A-C1A-N91	3.92	117.25	108.36
4	A	1252	C2E	N9-C4-N3	3.80	133.56	125.95
4	A	1251	C2E	O61-C61-C51	-3.69	116.80	126.53
4	A	1252	C2E	C2-N1-C6	-3.61	118.56	125.11
4	B	1252	C2E	N91-C41-N31	3.60	133.15	125.95
4	B	1252	C2E	O61-C61-C51	-3.59	117.05	126.53
4	B	1249	C2E	O61-C61-C51	-3.58	117.09	126.53
4	A	1251	C2E	O6-C6-C5	-3.52	117.23	126.53
4	B	1249	C2E	N91-C41-N31	3.50	132.96	125.95
4	A	1251	C2E	O4'-C1'-N9	3.45	116.17	108.36
4	A	1251	C2E	N91-C41-N31	3.40	132.75	125.95
4	A	1251	C2E	C2-N1-C6	-3.32	119.08	125.11
4	B	1252	C2E	C21-N11-C61	-3.26	119.19	125.11
4	B	1252	C2E	C51-C61-N11	3.23	121.47	113.25
4	B	1252	C2E	O6-C6-C5	-3.20	118.08	126.53
4	A	1251	C2E	C5-C6-N1	3.10	121.15	113.25
4	A	1251	C2E	N9-C4-N3	3.07	132.10	125.95
4	B	1252	C2E	C5-C6-N1	3.06	121.04	113.25
4	B	1249	C2E	C21-N11-C61	-3.06	119.56	125.11
4	B	1252	C2E	C2-N1-C6	-3.05	119.57	125.11
4	A	1251	C2E	C21-N11-C61	-3.04	119.59	125.11
4	A	1252	C2E	C5-C6-N1	3.04	120.98	113.25
4	B	1252	C2E	N9-C4-N3	3.04	132.03	125.95
4	A	1251	C2E	C51-C61-N11	3.03	120.97	113.25
4	A	1252	C2E	O61-C61-C51	-2.99	118.63	126.53
4	A	1252	C2E	C21-N11-C61	-2.94	119.78	125.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1249	C2E	C51-C61-N11	2.90	120.62	113.25
3	A	1250	MES	O1S-S-C8	2.82	110.99	106.73
4	A	1251	C2E	O4A-C1A-N91	2.81	114.72	108.36
4	B	1249	C2E	N9-C4-N3	2.80	131.55	125.95
4	A	1251	C2E	N9-C8-N7	-2.76	108.29	113.40
4	A	1252	C2E	N91-C81-N71	-2.69	108.41	113.40
4	A	1252	C2E	C51-C61-N11	2.67	120.06	113.25
4	B	1249	C2E	O6-C6-C5	-2.65	119.54	126.53
4	B	1249	C2E	C5-C6-N1	2.63	119.95	113.25
4	A	1252	C2E	C1'-N9-C8	-2.62	119.28	126.73
4	A	1252	C2E	N91-C41-N31	2.57	131.09	125.95
4	A	1252	C2E	N9-C8-N7	-2.54	108.69	113.40
4	B	1249	C2E	C2-N1-C6	-2.52	120.53	125.11
4	A	1252	C2E	C81-N71-C51	2.35	108.45	104.26
4	B	1249	C2E	C1A-N91-C81	-2.33	120.10	126.73
4	B	1252	C2E	N9-C8-N7	-2.33	109.08	113.40
4	A	1251	C2E	N91-C81-N71	-2.28	109.17	113.40
4	B	1249	C2E	O4A-C1A-N91	2.26	113.48	108.36
4	A	1252	C2E	C1'-N9-C4	2.25	133.14	126.49
4	A	1252	C2E	C41-C51-N71	-2.23	107.13	110.67
4	B	1249	C2E	N9-C8-N7	-2.17	109.39	113.40
4	A	1252	C2E	O5'-C5'-C4'	2.16	116.35	108.99
4	A	1252	C2E	C8-N7-C5	2.15	108.09	104.26
4	B	1249	C2E	C1A-N91-C41	2.14	132.81	126.49
3	A	1250	MES	C6-C5-N4	2.14	113.36	110.12
4	B	1252	C2E	O4'-C1'-N9	2.13	113.19	108.36
4	B	1252	C2E	N91-C81-N71	-2.04	109.62	113.40
4	A	1251	C2E	C8-N7-C5	2.02	107.86	104.26

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1249	GOL	C1-C2-C3-O3
4	B	1249	C2E	C5A-O5A-P11-O11
3	A	1250	MES	C7-C8-S-O3S
2	A	1249	GOL	O2-C2-C3-O3
2	B	1251	GOL	O1-C1-C2-O2
3	A	1250	MES	C7-C8-S-O1S
3	A	1250	MES	C7-C8-S-O2S
4	A	1251	C2E	C5'-O5'-P1-O2P
4	A	1252	C2E	O4A-C4A-C5A-O5A

Continued on next page...

Continued from previous page...

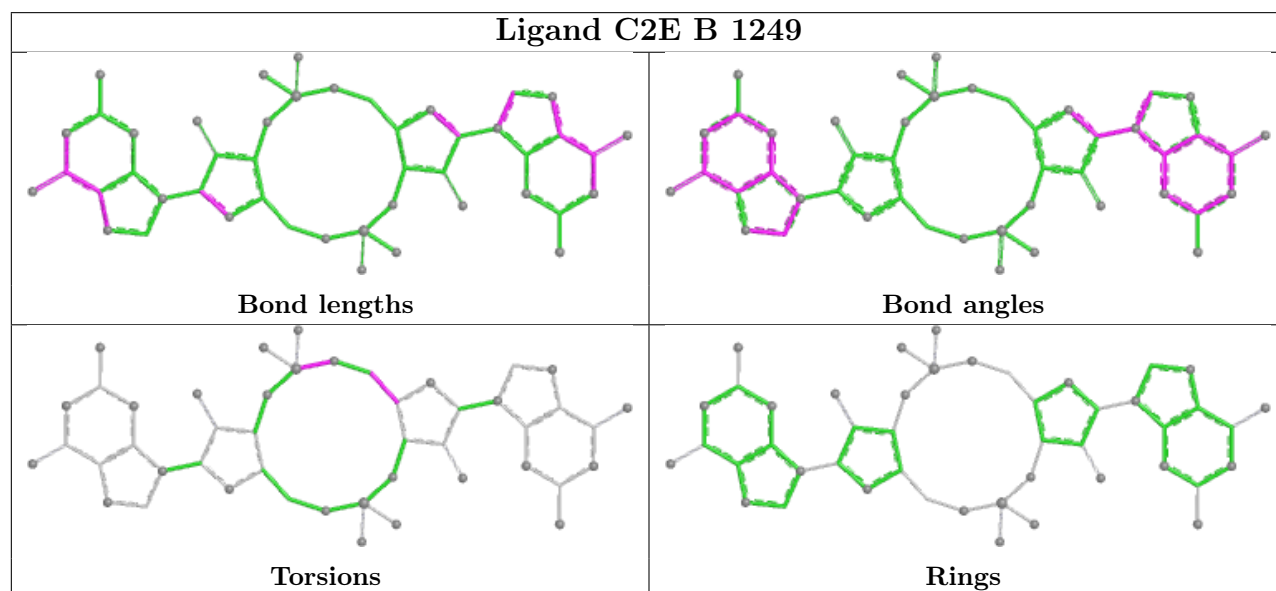
Mol	Chain	Res	Type	Atoms
4	B	1249	C2E	O4A-C4A-C5A-O5A
2	B	1251	GOL	O2-C2-C3-O3

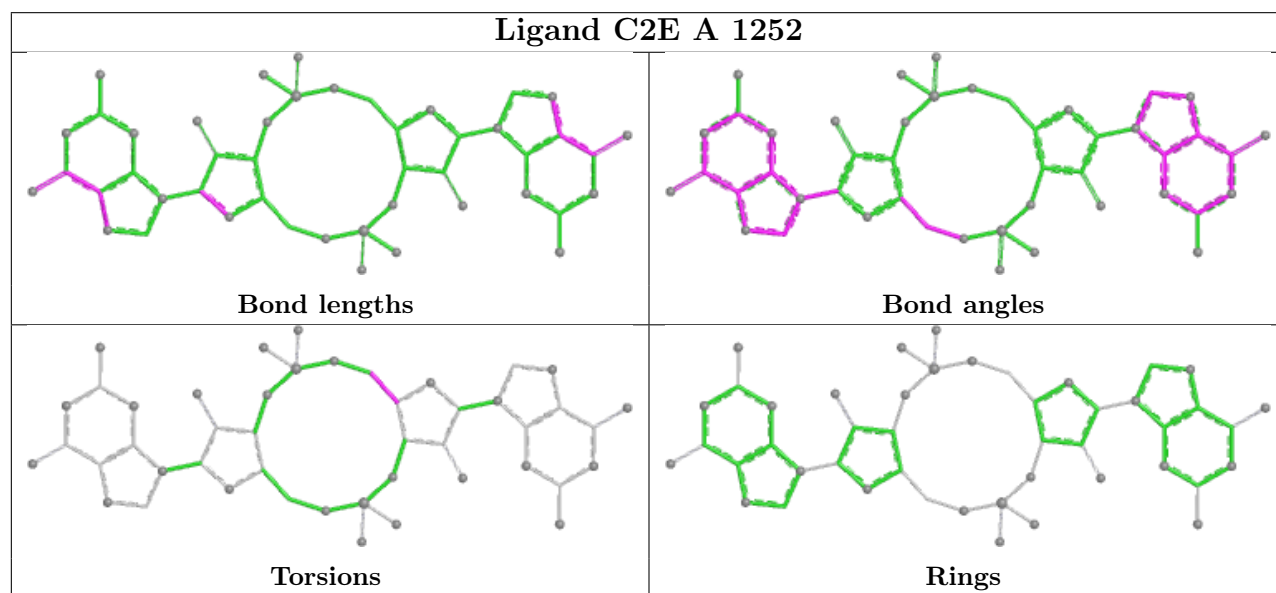
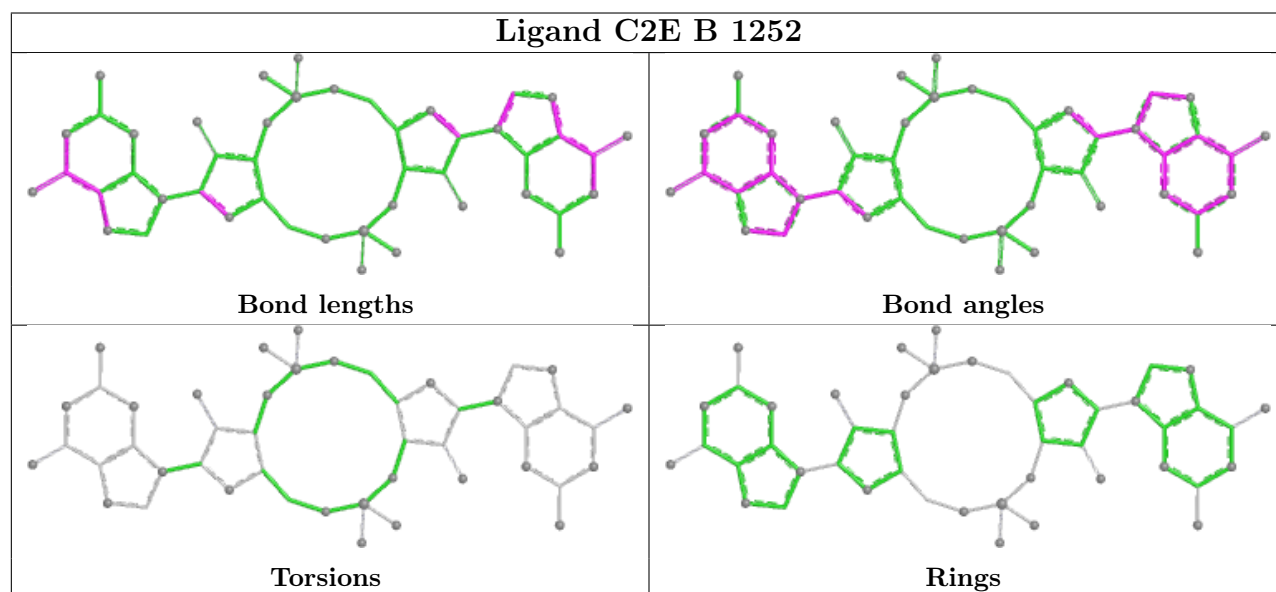
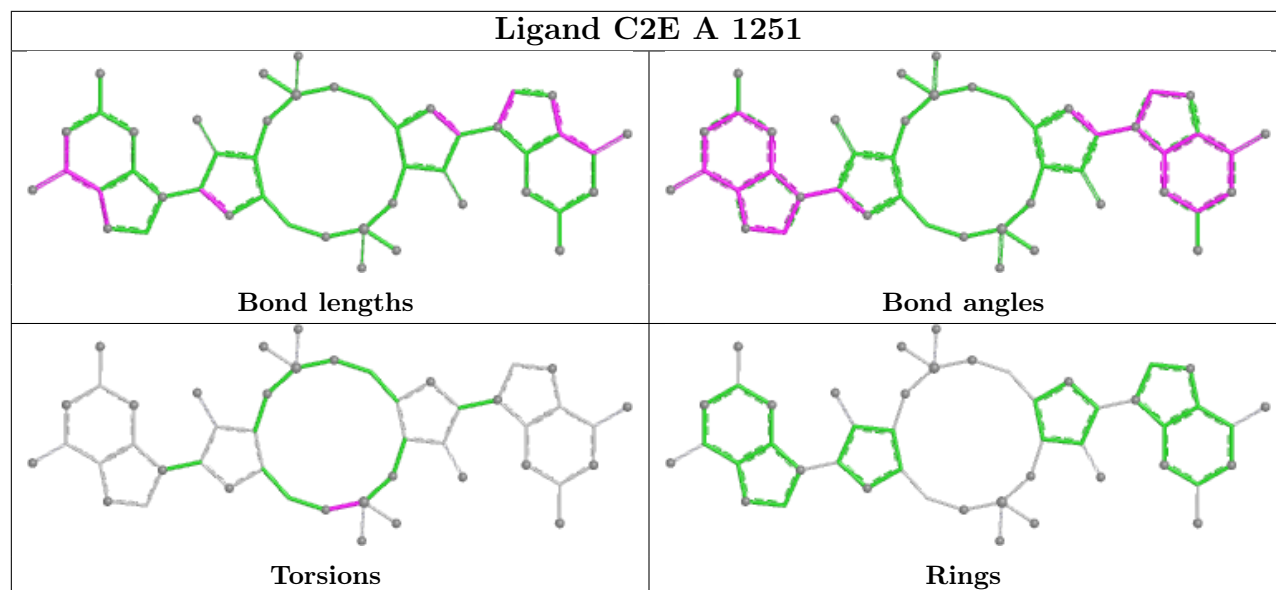
There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1251	GOL	1	0
4	B	1249	C2E	3	0
4	B	1252	C2E	1	0
4	A	1252	C2E	2	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	162/188 (86%)	0.79	16 (9%) 13 14	16, 38, 59, 67	0
1	B	162/188 (86%)	0.84	18 (11%) 10 11	17, 37, 58, 69	2 (1%)
All	All	324/376 (86%)	0.81	34 (10%) 11 12	16, 37, 58, 69	2 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	194	PHE	5.4
1	B	182	TYR	5.0
1	A	182	TYR	4.6
1	A	87	MET	4.5
1	B	194	PHE	4.1
1	B	88	ALA	3.9
1	B	87	MET	3.7
1	A	88	ALA	3.3
1	B	168	GLY	3.3
1	B	130	PHE	3.1
1	B	202	ASN	3.1
1	B	193	THR	3.1
1	A	89	TYR	3.0
1	A	193	THR	2.9
1	B	129	GLY	2.8
1	A	128	ALA	2.8
1	A	168	GLY	2.7
1	B	133	ILE	2.6
1	B	167	GLY	2.6
1	B	157	VAL	2.5
1	B	220	GLY	2.5
1	A	207	VAL	2.4
1	B	185	SER	2.4
1	B	89	TYR	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	185	SER	2.4
1	A	155	ASP	2.3
1	A	208	THR	2.2
1	B	153	ILE	2.1
1	B	154	LEU	2.1
1	A	196	GLU	2.1
1	A	154	LEU	2.1
1	B	196	GLU	2.1
1	A	183	LEU	2.1
1	A	167	GLY	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

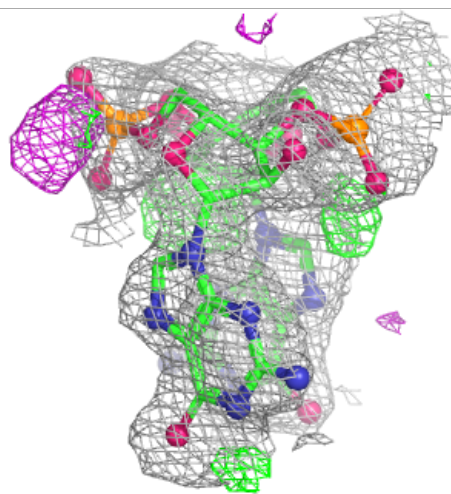
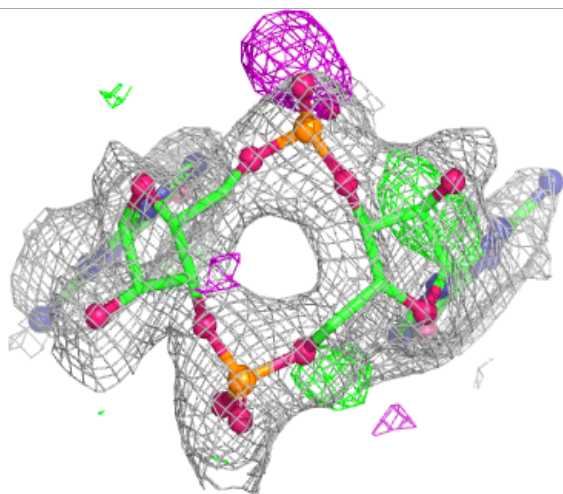
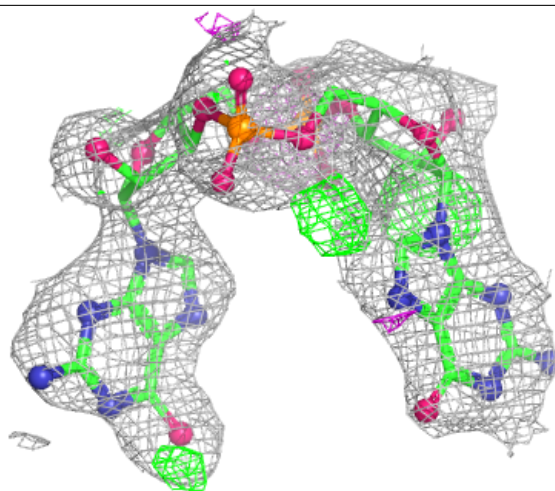
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MES	A	1250	12/12	0.69	0.19	63,66,72,75	0
2	GOL	B	1250	6/6	0.76	0.11	58,61,63,66	0
4	C2E	A	1252	46/46	0.76	0.13	34,44,49,53	0
4	C2E	B	1249	46/46	0.79	0.12	33,47,53,55	0
2	GOL	B	1251	6/6	0.83	0.14	27,32,38,40	0
2	GOL	A	1249	6/6	0.84	0.12	49,51,56,57	0
4	C2E	B	1252	46/46	0.86	0.10	38,43,52,56	0
4	C2E	A	1251	46/46	0.87	0.10	31,45,53,57	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.

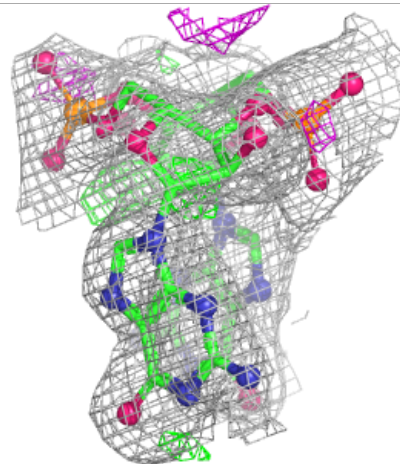
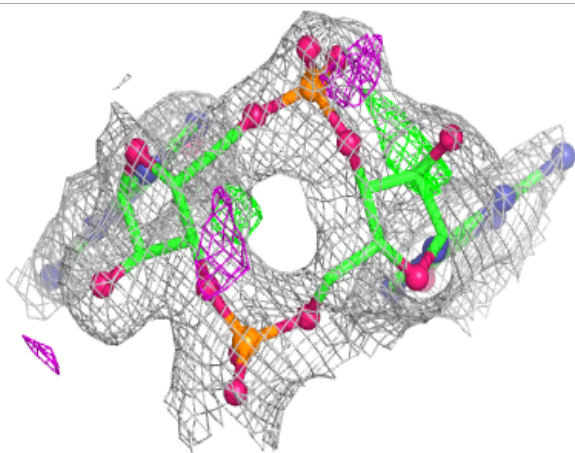
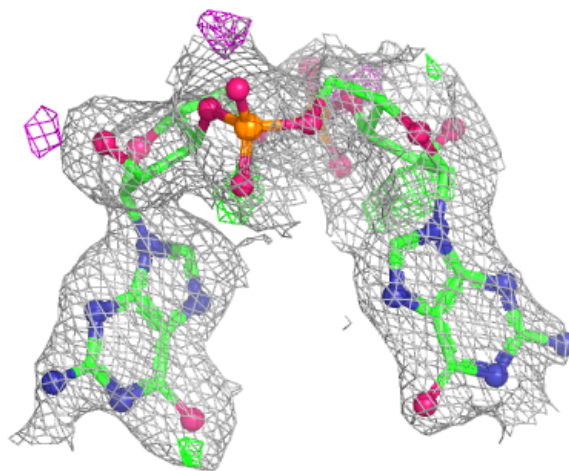
Electron density around C2E A 1252:

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



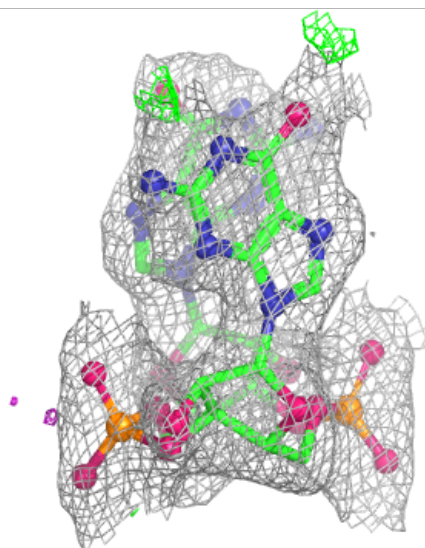
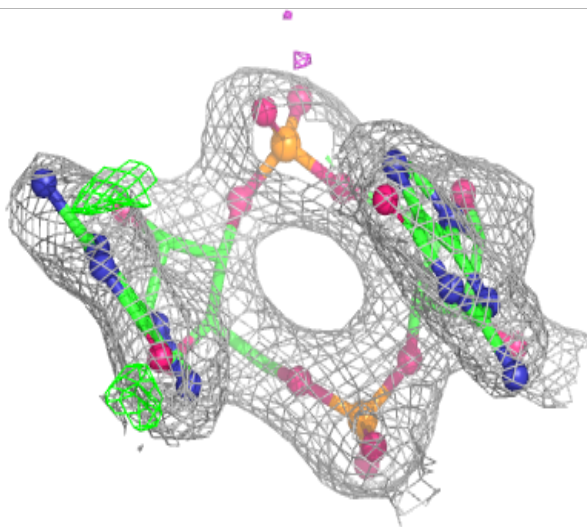
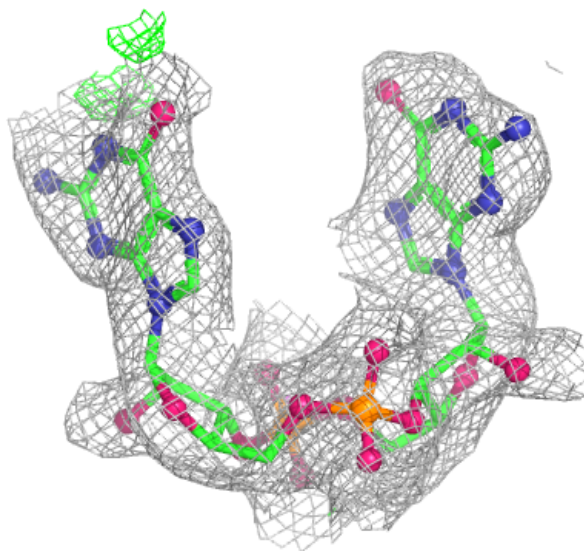
Electron density around C2E B 1249:

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



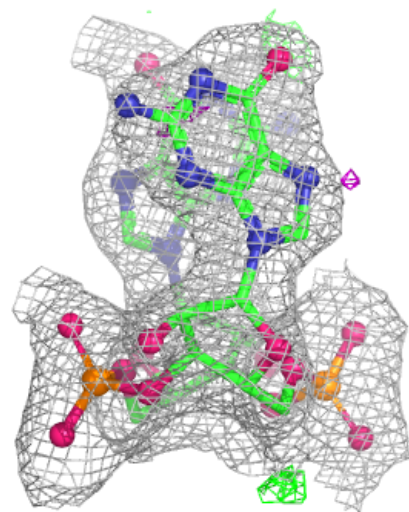
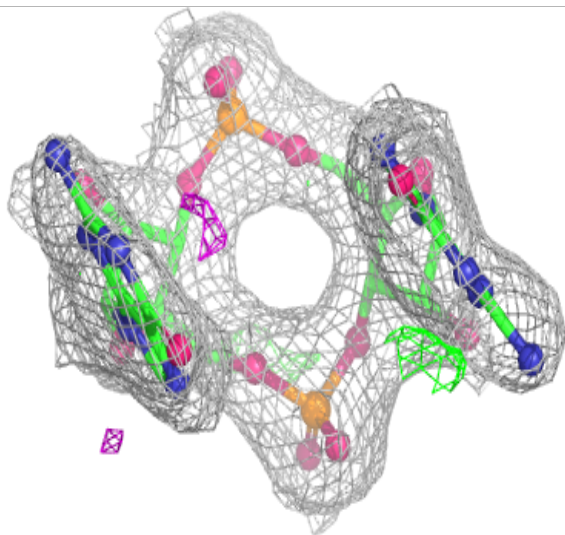
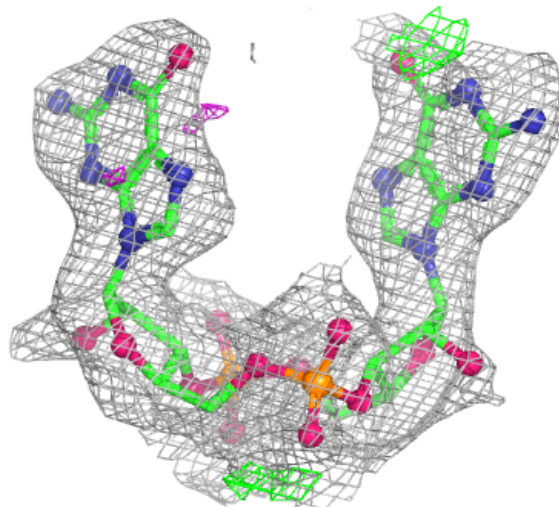
Electron density around C2E B 1252:

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



Electron density around C2E A 1251:

$2mF_o-DF_c$ (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.