wwPDB X-ray Structure Validation Summary Report (i)

Sep 7, 2023 – 04:44 pm BST

PDB ID	:	6TD3
Title	:	Structure of DDB1 bound to CR8-engaged CDK12-cyclinK
Authors	:	Bunker, R.D.; Petzold, G.; Kozicka, Z.; Thoma, N.H.
Deposited on	:	2019-11-07
Resolution	:	3.46 Å(reported)

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	:	2.35
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)	:	2.35

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 3.46 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.
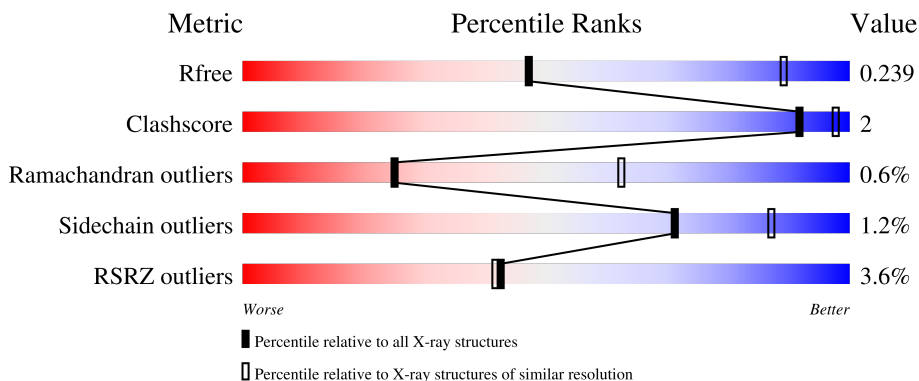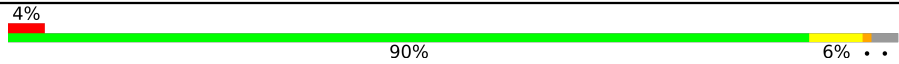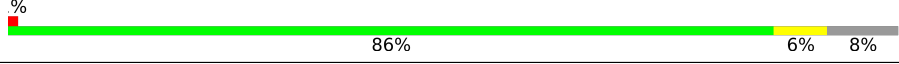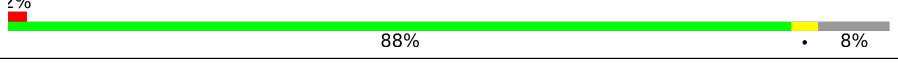

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)

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	840	3% / 93% / 5% ·
1	D	840	2% / 93% / 5% ·
1	G	840	6% / 94% / · ·
2	B	344	3% / 89% / 7% · ·
2	E	344	6% / 90% / 6% ·

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Mol	Chain	Length	Quality of chain
2	H	344	4% ... 90% ... 6%
3	C	271	3% ... 86% ... 6% 8%
3	F	271	.% ... 86% ... 6% 8%
3	I	271	2% ... 88% ... 8%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 67581 atoms, of which 33704 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 DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	826	Total 12937	C 4105	H 6450	N 1094	O 1252	S 36	6450	0	0
1	D	827	Total 12950	C 4111	H 6455	N 1095	O 1253	S 36	6455	0	0
1	G	826	Total 12936	C 4106	H 6450	N 1093	O 1251	S 36	6450	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q16531
A	-2	GLY	-	expression tag	UNP Q16531
A	-1	GLY	-	expression tag	UNP Q16531
A	0	ARG	-	expression tag	UNP Q16531
A	700	GLY	-	linker	UNP Q16531
A	701	ASN	-	linker	UNP Q16531
A	702	GLY	-	linker	UNP Q16531
A	703	ASN	-	linker	UNP Q16531
A	704	SER	-	linker	UNP Q16531
A	705	GLY	-	linker	UNP Q16531
A	706	GLU	-	linker	UNP Q16531
A	707	ILE	-	linker	UNP Q16531
D	-3	GLY	-	expression tag	UNP Q16531
D	-2	GLY	-	expression tag	UNP Q16531
D	-1	GLY	-	expression tag	UNP Q16531
D	0	ARG	-	expression tag	UNP Q16531
D	700	GLY	-	linker	UNP Q16531
D	701	ASN	-	linker	UNP Q16531
D	702	GLY	-	linker	UNP Q16531
D	703	ASN	-	linker	UNP Q16531
D	704	SER	-	linker	UNP Q16531
D	705	GLY	-	linker	UNP Q16531
D	706	GLU	-	linker	UNP Q16531

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W O R L D W I D E
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PROTEIN DATA BANK

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Chain	Residue	Modelled	Actual	Comment	Reference
D	707	ILE	-	linker	UNP Q16531
G	-3	GLY	-	expression tag	UNP Q16531
G	-2	GLY	-	expression tag	UNP Q16531
G	-1	GLY	-	expression tag	UNP Q16531
G	0	ARG	-	expression tag	UNP Q16531
G	700	GLY	-	linker	UNP Q16531
G	701	ASN	-	linker	UNP Q16531
G	702	GLY	-	linker	UNP Q16531
G	703	ASN	-	linker	UNP Q16531
G	704	SER	-	linker	UNP Q16531
G	705	GLY	-	linker	UNP Q16531
G	706	GLU	-	linker	UNP Q16531
G	707	ILE	-	linker	UNP Q16531

- Molecule 2 is a protein called Cyclin-dependent kinase 12.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
2	B	333	Total	C	H	N	O	P	S	2705	0	0
			5413	1735	2705	458	497	1	17			
2	E	333	Total	C	H	N	O	P	S	2707	0	0
			5415	1735	2707	458	497	1	17			
2	H	333	Total	C	H	N	O	P	S	2707	0	0
			5415	1735	2707	458	497	1	17			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	709	GLY	-	expression tag	UNP Q9NYV4
B	710	GLY	-	expression tag	UNP Q9NYV4
B	711	GLY	-	expression tag	UNP Q9NYV4
B	965	ARG	LYS	engineered mutation	UNP Q9NYV4
B	1052	GLN	-	expression tag	UNP Q9NYV4
E	709	GLY	-	expression tag	UNP Q9NYV4
E	710	GLY	-	expression tag	UNP Q9NYV4
E	711	GLY	-	expression tag	UNP Q9NYV4
E	965	ARG	LYS	engineered mutation	UNP Q9NYV4
E	1052	GLN	-	expression tag	UNP Q9NYV4
H	709	GLY	-	expression tag	UNP Q9NYV4
H	710	GLY	-	expression tag	UNP Q9NYV4
H	711	GLY	-	expression tag	UNP Q9NYV4
H	965	ARG	LYS	engineered mutation	UNP Q9NYV4
H	1052	GLN	-	expression tag	UNP Q9NYV4

WORLDWIDE
wwPDB
PROTEIN DATA BANK

- Molecule 3 is a protein called Cyclin-K.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	248	Total 4111	C 1341	H 2048	N 346	O 363	S 13	2048	0	0
3	F	248	Total 4111	C 1341	H 2048	N 346	O 363	S 13	2048	0	0
3	I	248	Total 4110	C 1341	H 2047	N 346	O 363	S 13	2047	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	expression tag	UNP O75909
C	-2	GLY	-	expression tag	UNP O75909
C	-1	GLY	-	expression tag	UNP O75909
C	0	ARG	-	expression tag	UNP O75909
F	-3	GLY	-	expression tag	UNP O75909
F	-2	GLY	-	expression tag	UNP O75909
F	-1	GLY	-	expression tag	UNP O75909
F	0	ARG	-	expression tag	UNP O75909
I	-3	GLY	-	expression tag	UNP O75909
I	-2	GLY	-	expression tag	UNP O75909
I	-1	GLY	-	expression tag	UNP O75909
I	0	ARG	-	expression tag	UNP O75909

- Molecule 4 is (2R)-2-({9-(1-methylethyl)-6-[(4-pyridin-2-ylbenzyl)amino]-9H-purin-2-yl }amino)butan-1-ol (three-letter code: RC8) (formula: $C_{24}H_{29}N_7O$) (labeled as "Ligand of Interest" by depositor).
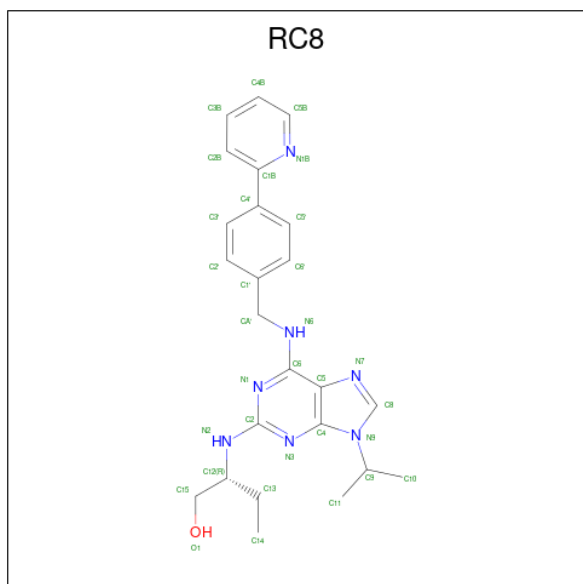
| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	H	N	O	29	0
			61	24	29	7	1		
4	E	1	Total	C	H	N	O	29	0
			61	24	29	7	1		
4	H	1	Total	C	H	N	O	29	0
			61	24	29	7	1		

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.
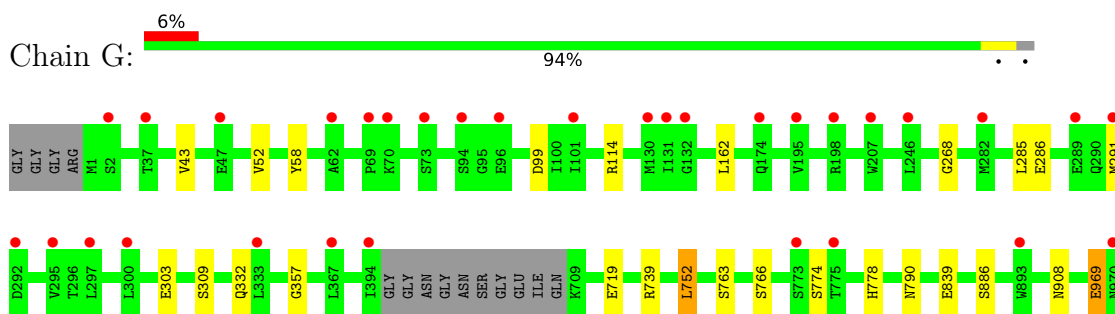
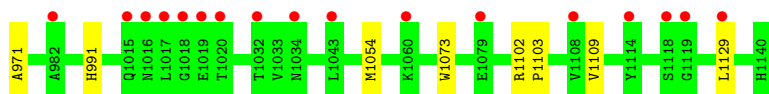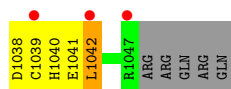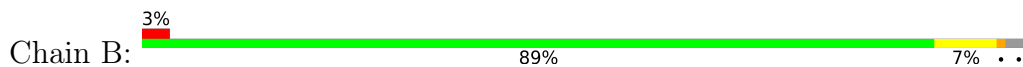- Molecule 1: DNA damage-binding protein 1
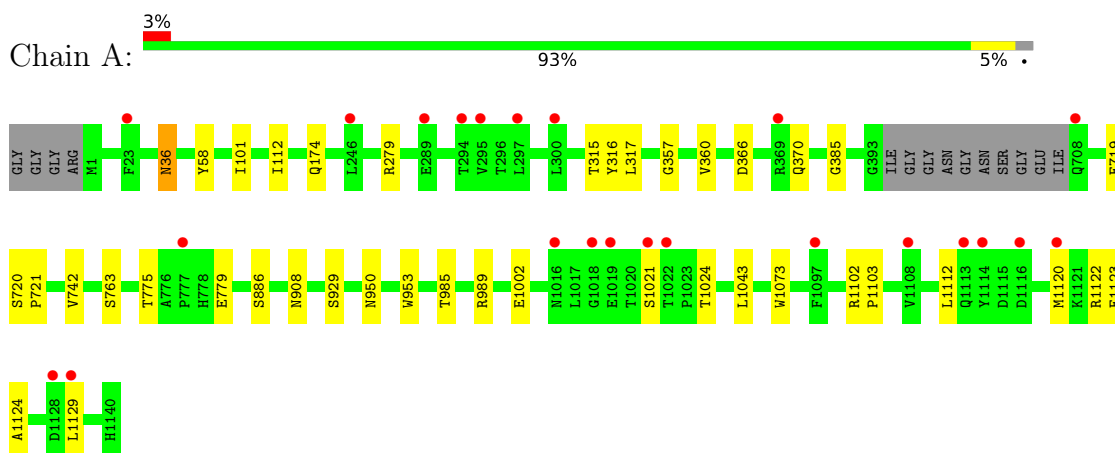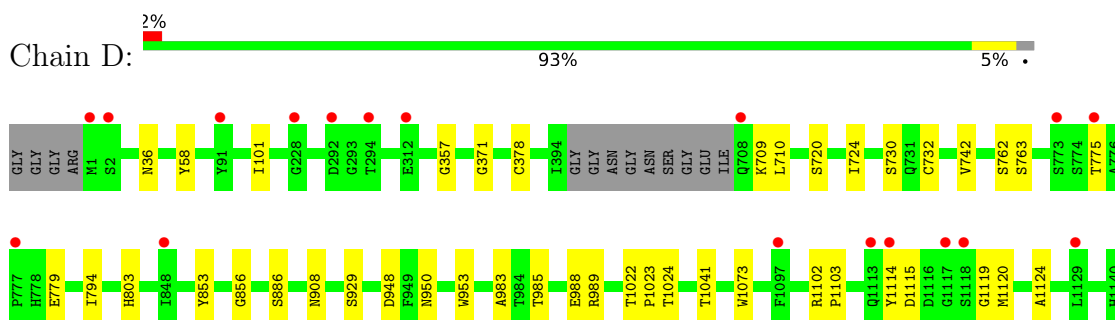
Chain A:

- Molecule 1: DNA damage-binding protein 1

Chain D:

- Molecule 1: DNA damage-binding protein 1

Chain G:

• Molecule 2: Cyclin-dependent kinase 12

Chain B:

• Molecule 2: Cyclin-dependent kinase 12

Chain E:

• Molecule 2: Cyclin-dependent kinase 12

Chain H:

• Molecule 3: Cyclin-K

Chain C:

• Molecule 3: Cyclin-K

Chain F:

GLY GLY GLY ARG MET LYS GLU ASN LYS GLU ASN SER SER PRO SER VAL THR SER ALA ASN LEU ASP HIS T20 W26 D27 K28 K29 L38 L64 M83 I146 S198 L199 Q200 Q223 S227 K228 P229 V239 Q263 Q264 M265 P266 H267

• Molecule 3: Cyclin-K

Chain I:

2%

88%

8%

GLY GLY GLY ARG MET LYS GLU ASN LYS GLU ASN SER SER PRO SER VAL THR SER ALA ASN LEU ASP HIS T20 K28 S36 Q37 L38 I146 Q200 R216 S227 V239 Q240 D241 K262 Q263 Q264 M265 P266 H267
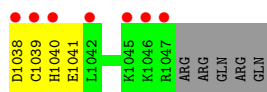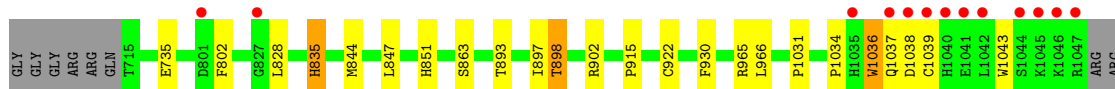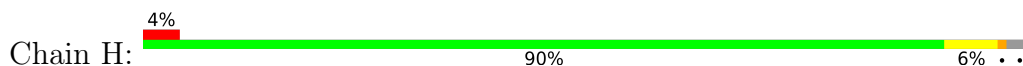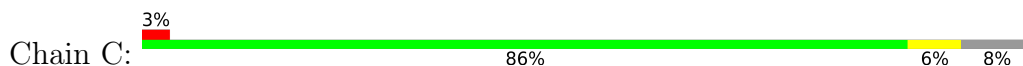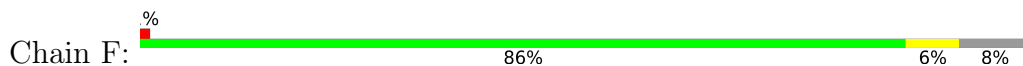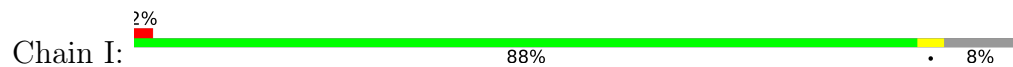
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	250.75Å 250.75Å 217.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	54.00 – 3.46 54.34 – 3.46	Depositor EDS
% Data completeness (in resolution range)	86.5 (54.00-3.46) 86.5 (54.34-3.46)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.28 (at 3.48Å)	Xtriage
Refinement program	BUSTER 2.11.7 (3-OCT-2019)	Depositor
R, R_{free}	0.194 , 0.220 0.214 , 0.239	Depositor DCC
R_{free} test set	4439 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å²)	118.9	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.31 , 48.0	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	67581	wwPDB-VP
Average B, all atoms (Å²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, RC8

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	0.42	0/6604	0.62	0/8931
1	D	0.42	0/6612	0.62	0/8942
1	G	0.42	0/6603	0.62	0/8930
2	B	0.47	0/2758	0.64	0/3720
2	E	0.47	0/2758	0.63	0/3720
2	H	0.49	0/2758	0.64	0/3720
3	C	0.40	0/2120	0.54	0/2868
3	F	0.44	0/2120	0.54	0/2868
3	I	0.43	0/2120	0.54	0/2868
All	All	0.44	0/34453	0.61	0/46567

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6487	6450	6453	22	0
1	D	6495	6455	6464	24	1
1	G	6486	6450	6456	16	0
2	B	2708	2705	2707	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	2708	2707	2707	15	0
2	H	2708	2707	2707	12	1
3	C	2063	2048	2048	9	0
3	F	2063	2048	2048	9	0
3	I	2063	2047	2048	6	0
4	B	32	29	29	0	0
4	E	32	29	29	0	0
4	H	32	29	29	0	0
All	All	33877	33704	33725	110	1

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 2.

The worst 5 of 110 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:F:239:VAL:HG23	3:F:239:VAL:O	1.86	0.76
1:G:1109:VAL:HG12	1:G:1129:LEU:HD12	1.72	0.72
2:E:828:LEU:O	2:E:1034:PRO:HD2	1.99	0.63
2:H:828:LEU:O	2:H:1034:PRO:HD2	1.98	0.62
2:B:828:LEU:O	2:B:1034:PRO:HD2	1.99	0.62

All (1) 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:D:730:SER:O	2:H:965:ARG:HH22[4_565]	1.47	0.13

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	A	822/840 (98%)	767 (93%)	49 (6%)	6 (1%)	22	60
1	D	823/840 (98%)	767 (93%)	51 (6%)	5 (1%)	25	62
1	G	822/840 (98%)	765 (93%)	55 (7%)	2 (0%)	47	80
2	B	330/344 (96%)	307 (93%)	20 (6%)	3 (1%)	17	54
2	E	330/344 (96%)	309 (94%)	19 (6%)	2 (1%)	25	62
2	H	330/344 (96%)	305 (92%)	23 (7%)	2 (1%)	25	62
3	C	246/271 (91%)	240 (98%)	4 (2%)	2 (1%)	19	57
3	F	246/271 (91%)	238 (97%)	7 (3%)	1 (0%)	34	70
3	I	246/271 (91%)	240 (98%)	5 (2%)	1 (0%)	34	70
All	All	4195/4365 (96%)	3938 (94%)	233 (6%)	24 (1%)	25	62

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1120	MET
1	A	1122	ARG
2	B	897	ILE
3	C	264	GLN
1	D	371	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	721/728 (99%)	714 (99%)	7 (1%)	76	89
1	D	722/728 (99%)	720 (100%)	2 (0%)	92	98
1	G	721/728 (99%)	711 (99%)	10 (1%)	67	85
2	B	297/308 (96%)	290 (98%)	7 (2%)	49	76
2	E	297/308 (96%)	294 (99%)	3 (1%)	76	89
2	H	297/308 (96%)	291 (98%)	6 (2%)	55	79
3	C	223/242 (92%)	220 (99%)	3 (1%)	69	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	223/242 (92%)	219 (98%)	4 (2%)	59	81
3	I	223/242 (92%)	220 (99%)	3 (1%)	69	86
All	All	3724/3834 (97%)	3679 (99%)	45 (1%)	71	87

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	291	MET
1	G	969	GLU
1	G	303	GLU
1	G	766	SER
2	H	863	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	778	HIS
1	G	790	ASN
1	D	970	ASN
1	D	990	GLN
2	E	740	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	TPO	B	893	2	8,10,11	1.24	1 (12%)	10,14,16	0.98	0
2	TPO	H	893	2	8,10,11	2.94	4 (50%)	10,14,16	2.21	4 (40%)
2	TPO	E	893	2	8,10,11	1.74	1 (12%)	10,14,16	1.26	1 (10%)

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
2	TPO	B	893	2	-	0/9/11/13	-
2	TPO	H	893	2	-	1/9/11/13	-
2	TPO	E	893	2	-	1/9/11/13	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	893	TPO	P-OG1	6.51	1.71	1.59
2	E	893	TPO	CB-CA	4.47	1.63	1.53
2	H	893	TPO	P-O1P	3.24	1.61	1.50
2	H	893	TPO	CB-CA	2.50	1.59	1.53
2	H	893	TPO	P-O2P	2.41	1.64	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	893	TPO	P-OG1-CB	4.88	137.95	123.21
2	H	893	TPO	O3P-P-OG1	2.91	119.01	105.99
2	E	893	TPO	O-C-CA	-2.48	118.28	124.78
2	H	893	TPO	CG2-CB-CA	-2.23	108.77	113.16
2	H	893	TPO	O-C-CA	-2.16	119.12	124.78

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	893	TPO	CG2-CB-OG1-P
2	E	893	TPO	CB-OG1-P-O2P

There are no ring outliers.

No monomer is involved in short contacts.

5.5   Carbohydrates (i)

There are no monosaccharides in this entry.

5.6   Ligand geometry (i)

3 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	#$|Z| > 2$
4	RC8	H	1101	-	31,35,35	2.25	3 (9%)	33,48,48	5.74	13 (39%)
4	RC8	E	1101	-	31,35,35	2.26	3 (9%)	33,48,48	5.76	12 (36%)
4	RC8	B	1101	-	31,35,35	2.21	3 (9%)	33,48,48	5.75	12 (36%)

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	RC8	H	1101	-	-	6/17/21/21	0/4/4/4
4	RC8	E	1101	-	-	6/17/21/21	0/4/4/4
4	RC8	B	1101	-	-	6/17/21/21	0/4/4/4

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1101	RC8	C2-N2	9.79	1.47	1.34
4	E	1101	RC8	C2-N2	9.69	1.47	1.34
4	B	1101	RC8	C2-N2	9.43	1.46	1.34
4	E	1101	RC8	C6-N6	6.24	1.46	1.34
4	B	1101	RC8	C6-N6	6.07	1.45	1.34

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	1101	RC8	N2-C2-N1	23.43	152.36	117.18
4	B	1101	RC8	N2-C2-N1	23.29	152.15	117.18
4	H	1101	RC8	N2-C2-N1	23.24	152.08	117.18
4	E	1101	RC8	N2-C2-N3	-19.54	87.83	117.18
4	H	1101	RC8	N2-C2-N3	-19.52	87.86	117.18

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

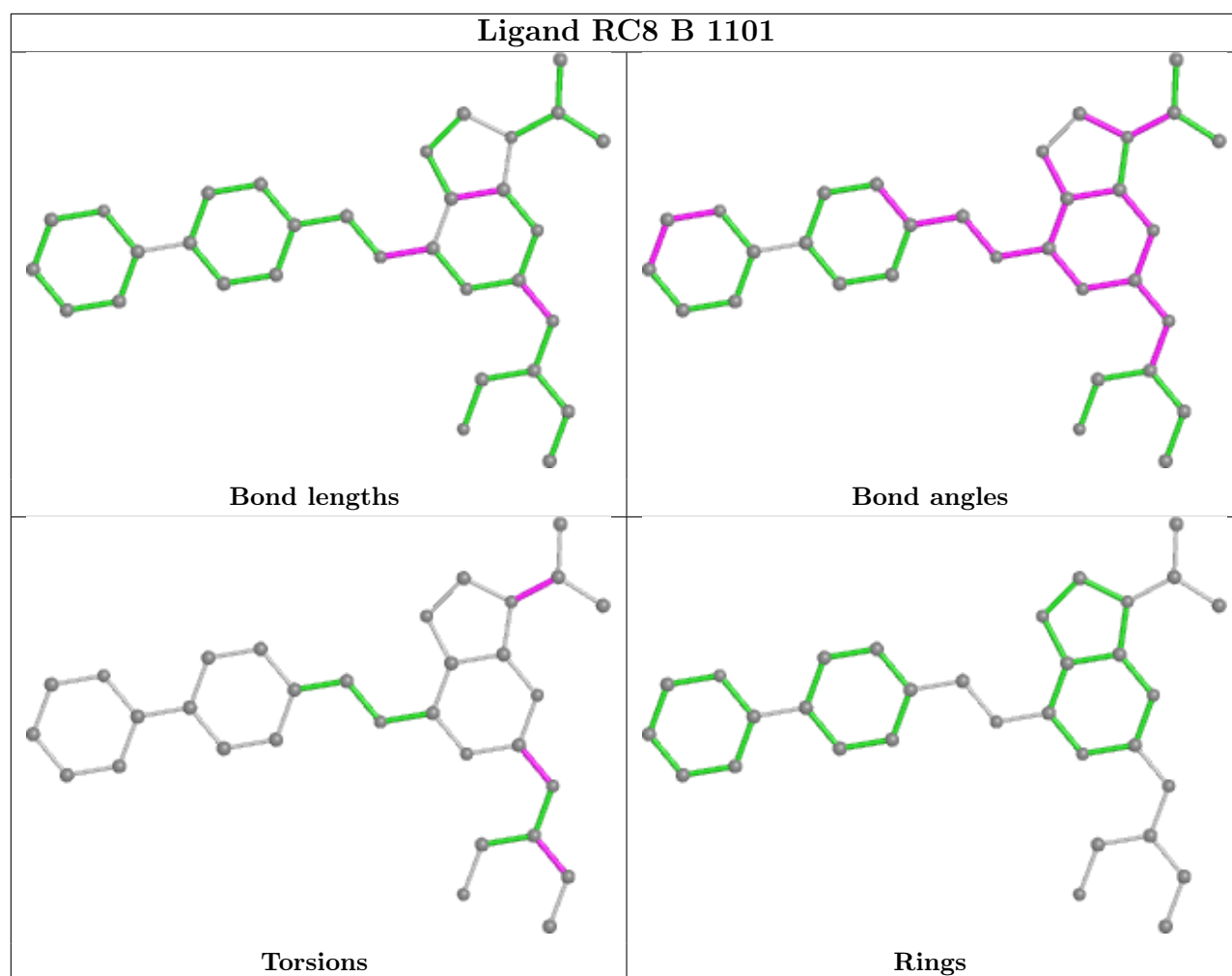| Mol	Chain	Res	Type	Atoms
4	B	1101	RC8	N1-C2-N2-C12
4	B	1101	RC8	N3-C2-N2-C12
4	B	1101	RC8	C10-C9-N9-C4
4	B	1101	RC8	C10-C9-N9-C8
4	B	1101	RC8	C15-C12-C13-C14

There are no ring outliers.

No monomer is involved in short contacts.

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 RC8 H 1101

Bond lengths

Bond angles

Torsions

Rings

Ligand RC8 E 1101

Bond lengths

Bond angles

Torsions

Rings

Ligand RC8 B 1101

Bond lengths

Bond angles

Torsions

Rings
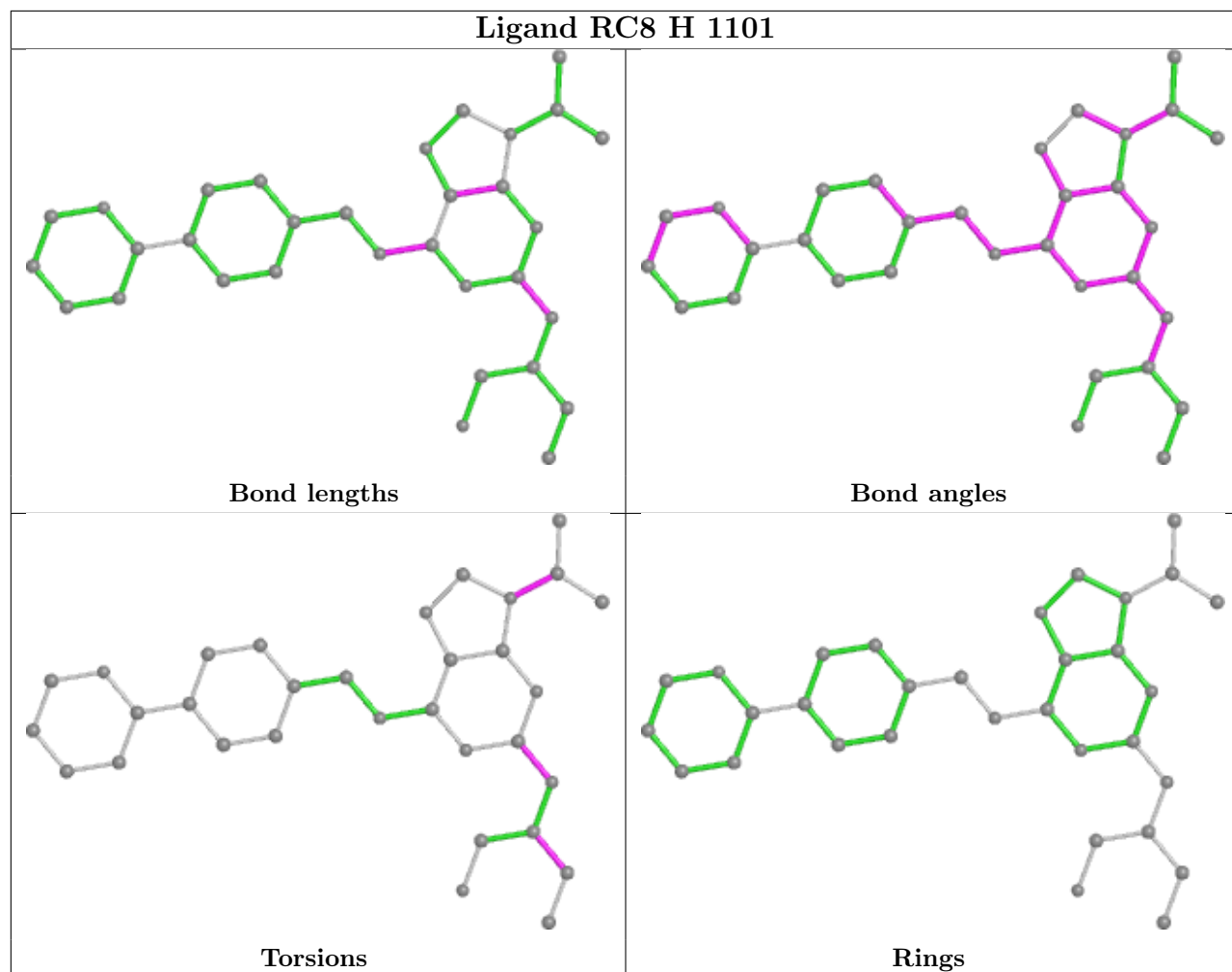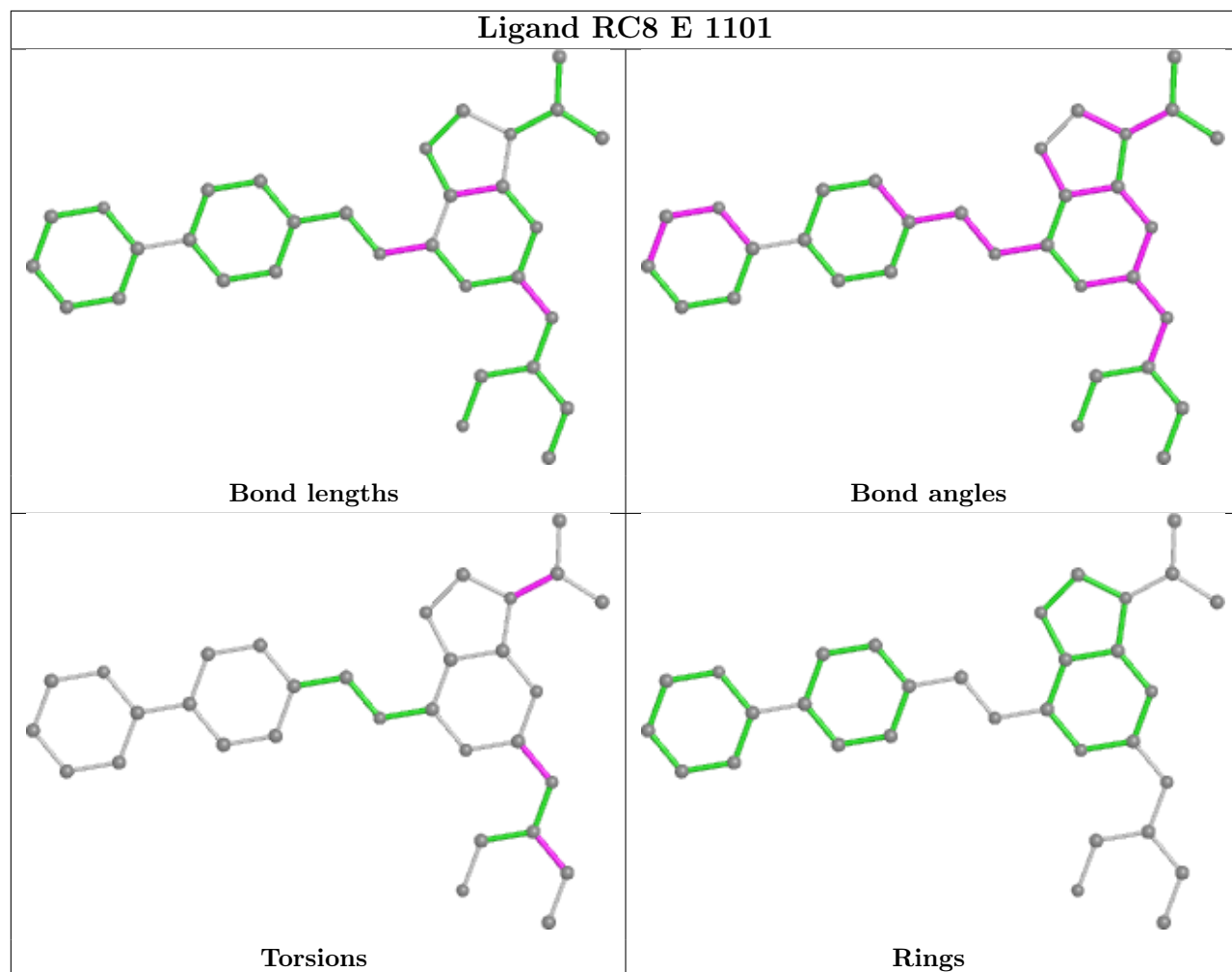
5.7 Other polymers ⓘ

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	A	826/840 (98%)	0.36	23 (2%)	53	51	17, 61, 110, 160	0
1	D	827/840 (98%)	0.36	18 (2%)	62	59	15, 55, 104, 152	0
1	G	826/840 (98%)	0.55	49 (5%)	22	23	27, 69, 122, 206	0
2	B	332/344 (96%)	0.36	11 (3%)	46	44	39, 63, 121, 159	0
2	E	332/344 (96%)	0.46	19 (5%)	23	23	26, 55, 114, 183	0
2	H	332/344 (96%)	0.36	13 (3%)	39	38	4, 42, 101, 164	0
3	C	248/271 (91%)	0.25	7 (2%)	53	51	19, 51, 80, 121	0
3	F	248/271 (91%)	0.22	4 (1%)	72	69	3, 31, 66, 111	0
3	I	248/271 (91%)	0.23	6 (2%)	59	56	10, 35, 73, 114	0
All	All	4219/4365 (96%)	0.38	150 (3%)	42	41	3, 55, 111, 206	0

The worst 5 of 150 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	1039	CYS	6.5
2	H	1047	ARG	6.1
1	G	291	MET	5.8
2	E	1045	LYS	5.6
2	E	1042	LEU	5.4

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

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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
2	TPO	E	893	11/12	0.69	0.24	83,103,187,190	6
2	TPO	B	893	11/12	0.74	0.30	87,100,188,190	5
2	TPO	H	893	11/12	0.83	0.25	41,52,86,88	5

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
4	RC8	E	1101	32/32	0.91	0.37	20,35,53,75	29
4	RC8	B	1101	32/32	0.92	0.30	36,56,88,125	29
4	RC8	H	1101	32/32	0.93	0.27	32,41,72,75	29

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.
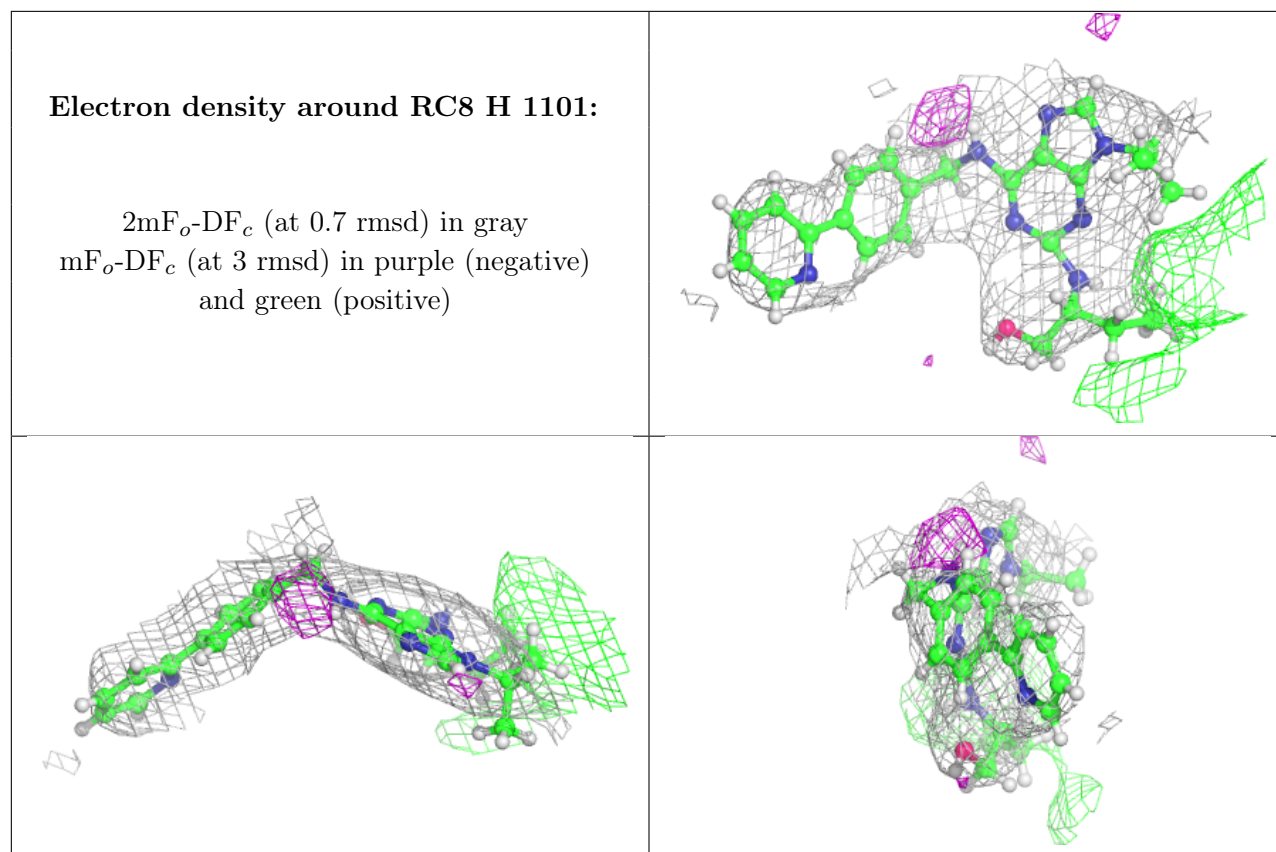
Electron density around RC8 E 1101:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
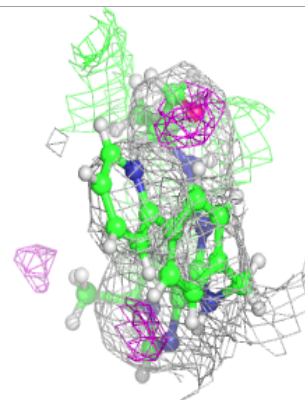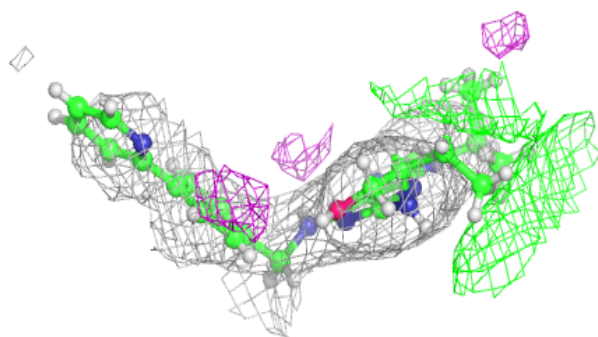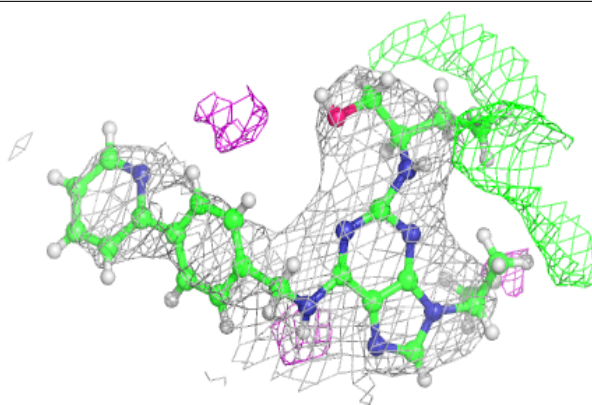
Electron density around RC8 B 1101:

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

Electron density around RC8 H 1101:

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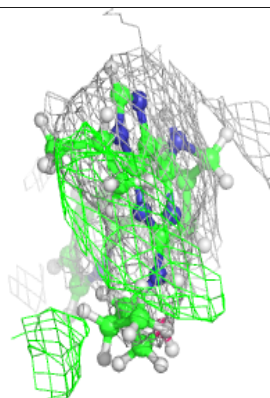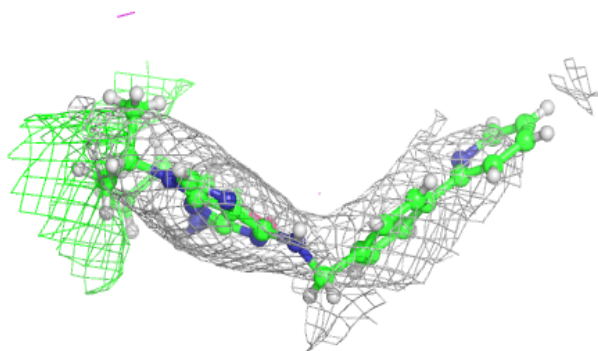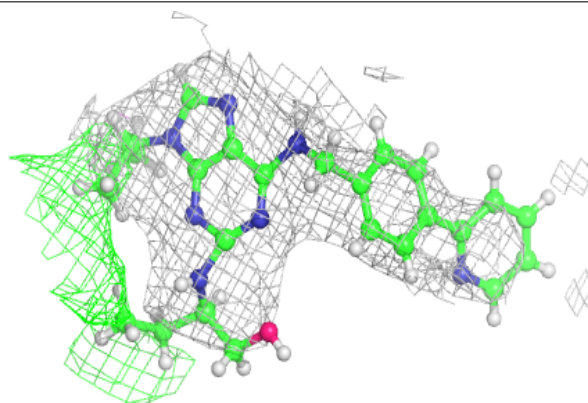
6.5   Other polymers (i)

There are no such residues in this entry.