



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 26, 2026 – 11:51 AM EDT

PDB ID : 8BUQ / pdb_00008buq
Title : Structure of DDB1 bound to DS43-engaged CDK12-cyclin K
Authors : Kozicka, Z.; Kempf, G.; Focht, V.; Thoma, N.H.
Deposited on : 2022-11-30
Resolution : 3.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

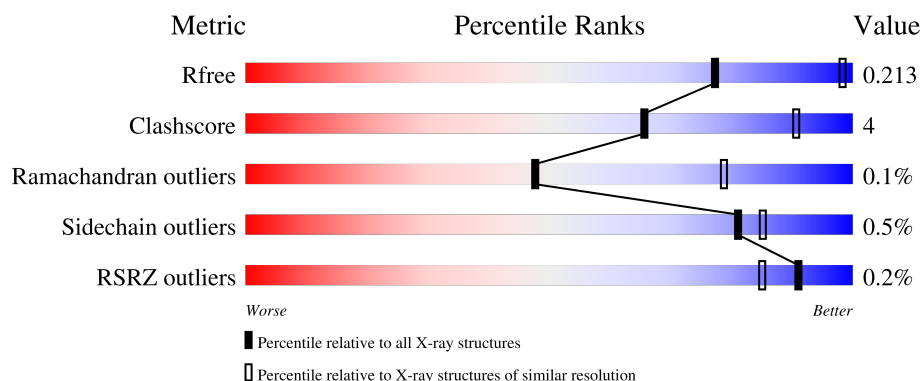
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	840	
1	D	840	
1	G	840	
2	B	344	
2	E	344	

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Mol	Chain	Length	Quality of chain
2	H	344	78% 14% • 7%
3	C	271	87% 5% 8%
3	F	271	90% • 8%
3	I	271	87% • 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 67017 atoms, of which 33441 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	822	Total	C	H	N	O	S	6423	0	0
			12881	4088	6423	1089	1245	36			
1	D	827	Total	C	H	N	O	S	6462	0	0
			12957	4111	6462	1095	1253	36			
1	G	826	Total	C	H	N	O	S	6452	0	0
			12938	4106	6452	1093	1251	36			

There are 39 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
A	708	GLN	-	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

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Chain	Residue	Modelled	Actual	Comment	Reference
D	706	GLU	-	linker	UNP Q16531
D	707	ILE	-	linker	UNP Q16531
D	708	GLN	-	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
G	708	GLN	-	linker	UNP Q16531

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

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
2	B	321	Total	C	H	N	O	P	S	2635	0	0
			5251	1677	2635	442	479	1	17			
2	E	313	Total	C	H	N	O	P	S	2579	0	0
			5128	1633	2579	431	469	1	15			
2	H	321	Total	C	H	N	O	P	S	2635	0	0
			5244	1672	2635	441	479	1	16			

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

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

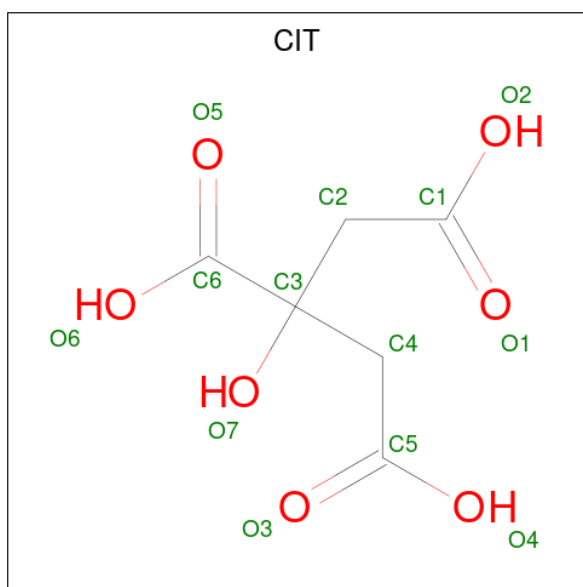
- Molecule 3 is a protein called Cyclin-K.

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 4111	C 1341	H 2048	N 346	O 363	S 13	2048	0	0

There are 12 discrepancies between the modelled and reference sequences:

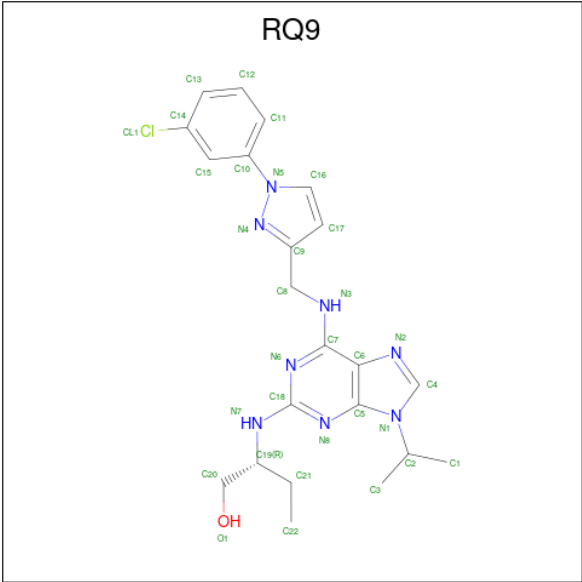
Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	expression tag	UNP O75909
C	-2	GLY	-	expression tag	UNP O75909
C	-1	GLY	-	expression tag	UNP O75909
C	0	ARG	-	expression tag	UNP O75909
F	-3	GLY	-	expression tag	UNP O75909
F	-2	GLY	-	expression tag	UNP O75909
F	-1	GLY	-	expression tag	UNP O75909
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 CITRIC ACID (CCD ID: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	5	0
			18	6	5	7		
4	C	1	Total	C	H	O	5	0
			18	6	5	7		
4	D	1	Total	C	H	O	5	0
			18	6	5	7		
4	F	1	Total	C	H	O	5	0
			18	6	5	7		
4	H	1	Total	C	H	O	5	0
			18	6	5	7		
4	I	1	Total	C	H	O	5	0
			18	6	5	7		

- Molecule 5 is (2 {R})-2-[[6-[[1-(3-chlorophenyl)pyrazol-3-yl]methylamino]-9-propan-2-yl-purin-2-yl]amino]butan-1-ol (CCD ID: RQ9) (formula: C₂₂H₂₇ClN₈O) (labeled as "Ligand of Interest" by depositor).

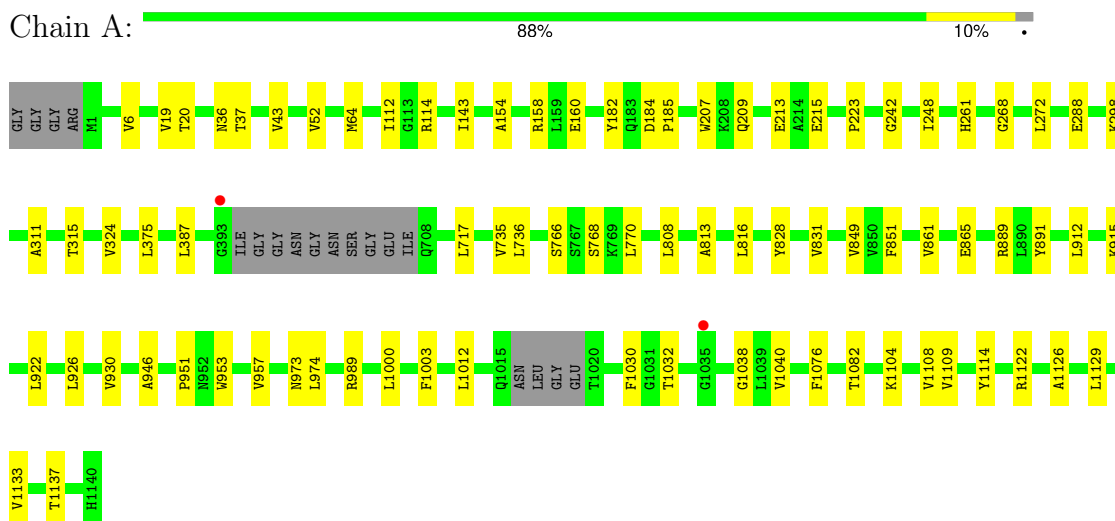


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	B	1	Total	C	Cl	H	N	O	27	0
			59	22	1	27	8	1		
5	E	1	Total	C	Cl	H	N	O	27	0
			59	22	1	27	8	1		
5	H	1	Total	C	Cl	H	N	O	27	0
			59	22	1	27	8	1		

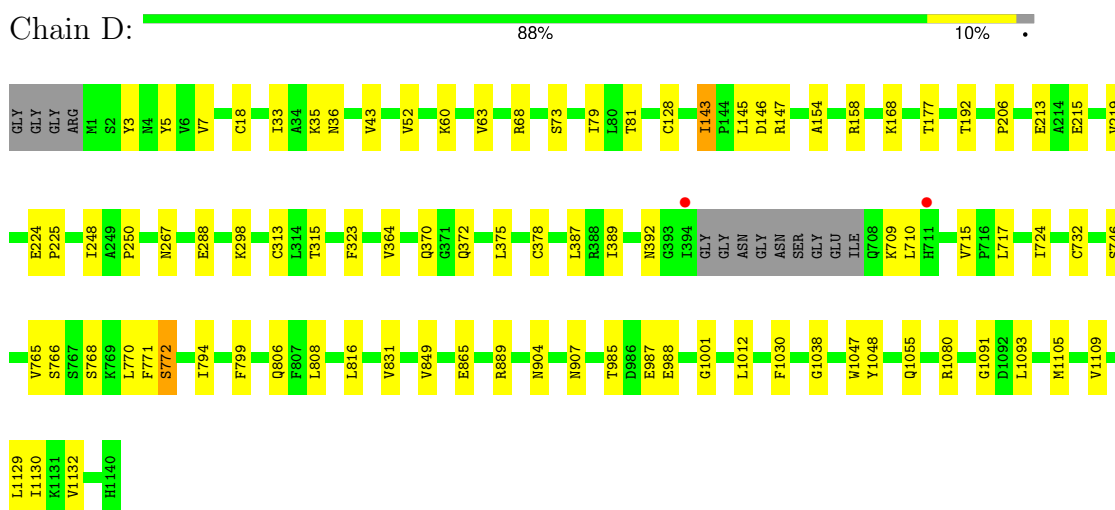
3 Residue-property plots [i](#)

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.

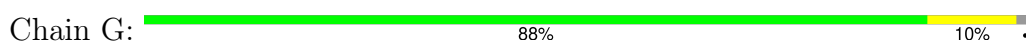
- Molecule 1: DNA damage-binding protein 1

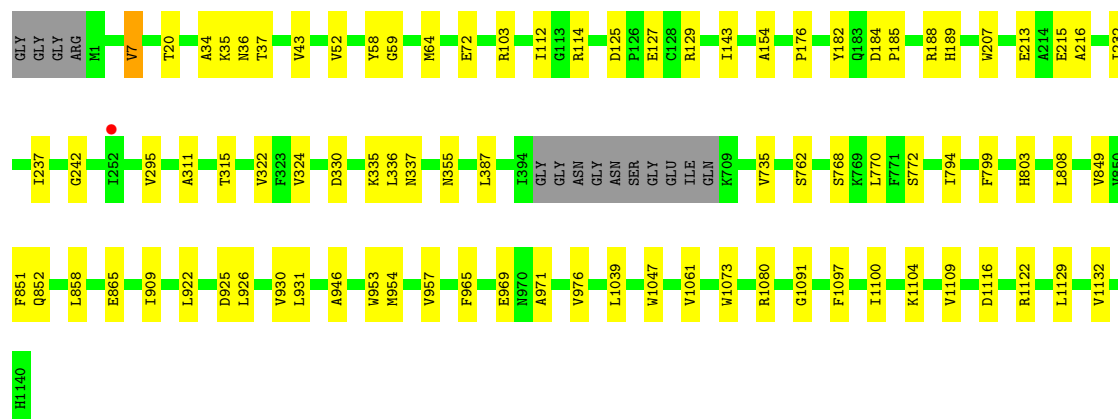


- Molecule 1: DNA damage-binding protein 1



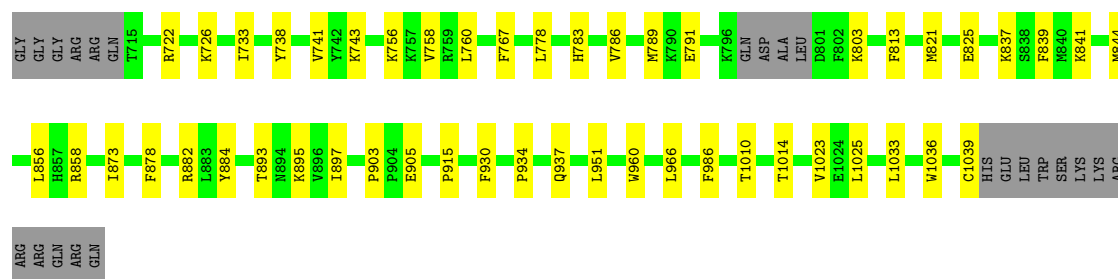
- Molecule 1: DNA damage-binding protein 1





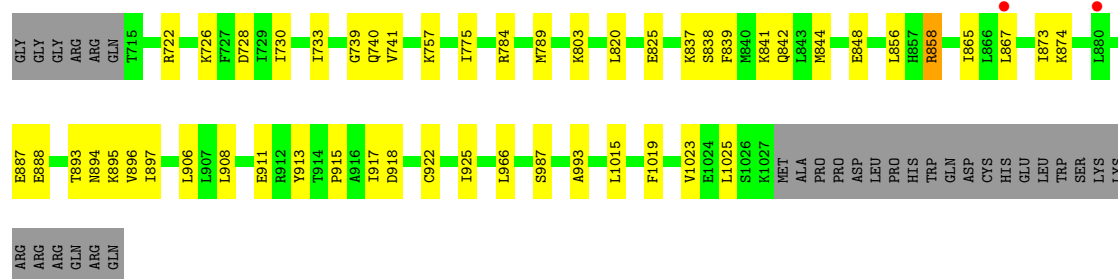
• Molecule 2: Cyclin-dependent kinase 12

Chain B: 79% 14% 7%

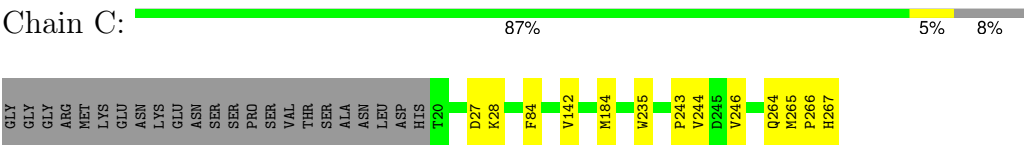


• Molecule 2: Cyclin-dependent kinase 12

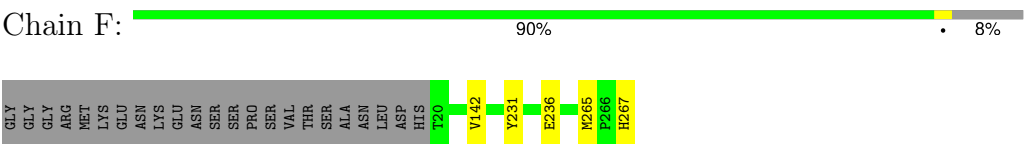
Chain E: 76% 15% 9%



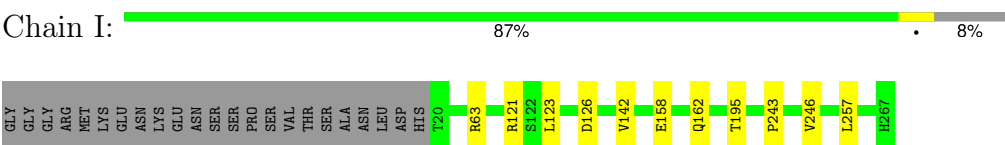
● Molecule 3: Cyclin-K



● Molecule 3: Cyclin-K



● Molecule 3: Cyclin-K



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	250.16Å 250.16Å 218.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	54.30 – 3.20 54.30 – 3.20	Depositor EDS
% Data completeness (in resolution range)	80.7 (54.30-3.20) 80.8 (54.30-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.195 , 0.216 0.194 , 0.213	Depositor DCC
R_{free} test set	5174 reflections (3.98%)	wwPDB-VP
Wilson B-factor (Å ²)	121.3	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 84.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	67017	wwPDB-VP
Average B, all atoms (Å ²)	144.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% 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: RQ9, CIT, TPO

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	0.15	0/6574	0.35	0/8889
1	D	0.15	1/6612 (0.0%)	0.35	0/8942
1	G	0.14	0/6603	0.35	0/8930
2	B	0.14	0/2662	0.35	0/3586
2	E	0.14	0/2590	0.35	0/3486
2	H	0.16	0/2654	0.39	0/3576
3	C	0.12	0/2120	0.31	0/2868
3	F	0.13	0/2120	0.32	0/2868
3	I	0.12	0/2120	0.31	0/2868
All	All	0.14	1/34055 (0.0%)	0.35	0/46013

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	143	ILE	CA-C	-5.15	1.49	1.53

There are no bond angle outliers.

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	A	6458	6423	6424	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	6495	6462	6464	51	0
1	G	6486	6452	6454	52	0
2	B	2616	2635	2634	32	0
2	E	2549	2579	2579	30	0
2	H	2609	2635	2635	38	0
3	C	2063	2048	2048	9	0
3	F	2063	2048	2048	4	0
3	I	2063	2048	2048	8	0
4	A	13	5	5	0	0
4	C	13	5	5	0	0
4	D	13	5	5	0	0
4	F	13	5	5	0	0
4	H	13	5	5	0	0
4	I	13	5	5	0	0
5	B	32	27	0	1	0
5	E	32	27	0	0	0
5	H	32	27	0	0	0
All	All	33576	33441	33364	253	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 4.

The worst 5 of 253 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)
2:H:867:LEU:HD21	2:H:1031:PRO:HG2	1.75	0.68
1:G:770:LEU:HD21	1:G:865:GLU:HB2	1.76	0.67
2:E:856:LEU:HD11	2:E:915:PRO:HG3	1.77	0.65
2:H:733:ILE:HD11	2:H:741:VAL:HG12	1.78	0.64
1:D:375:LEU:HB2	1:D:1012:LEU:HD21	1.84	0.60

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	816/840 (97%)	794 (97%)	22 (3%)	0	100	100
1	D	823/840 (98%)	803 (98%)	19 (2%)	1 (0%)	48	79
1	G	822/840 (98%)	803 (98%)	18 (2%)	1 (0%)	48	79
2	B	316/344 (92%)	309 (98%)	7 (2%)	0	100	100
2	E	310/344 (90%)	303 (98%)	6 (2%)	1 (0%)	36	68
2	H	318/344 (92%)	309 (97%)	9 (3%)	0	100	100
3	C	246/271 (91%)	244 (99%)	2 (1%)	0	100	100
3	F	246/271 (91%)	243 (99%)	3 (1%)	0	100	100
3	I	246/271 (91%)	244 (99%)	2 (1%)	0	100	100
All	All	4143/4365 (95%)	4052 (98%)	88 (2%)	3 (0%)	48	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	772	SER
2	E	895	LYS
1	G	772	SER

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	718/728 (99%)	716 (100%)	2 (0%)	86	88
1	D	722/728 (99%)	720 (100%)	2 (0%)	86	88
1	G	721/728 (99%)	719 (100%)	2 (0%)	86	88
2	B	289/308 (94%)	284 (98%)	5 (2%)	53	75
2	E	281/308 (91%)	278 (99%)	3 (1%)	65	79
2	H	288/308 (94%)	285 (99%)	3 (1%)	68	80
3	C	223/242 (92%)	223 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	223/242 (92%)	223 (100%)	0	100	100
3	I	223/242 (92%)	223 (100%)	0	100	100
All	All	3688/3834 (96%)	3671 (100%)	17 (0%)	81	85

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	770	THR
2	H	1025	LEU
1	D	766	SER
1	D	849	VAL
2	E	728	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	796	GLN
1	G	991	HIS
1	G	797	HIS
1	G	877	ASN
1	G	1034	ASN

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	H	893	2	8,10,11	1.65	1 (12%)	10,14,16	1.15	1 (10%)
2	TPO	E	893	2	8,10,11	1.67	1 (12%)	10,14,16	1.29	1 (10%)
2	TPO	B	893	2	8,10,11	1.61	1 (12%)	10,14,16	1.42	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	H	893	2	-	5/9/11/13	-
2	TPO	E	893	2	-	4/9/11/13	-
2	TPO	B	893	2	-	2/9/11/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	893	TPO	P-O1P	3.56	1.61	1.50
2	B	893	TPO	P-O1P	3.56	1.61	1.50
2	H	893	TPO	P-O1P	3.53	1.61	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	893	TPO	P-OG1-CB	-3.85	112.88	123.33
2	H	893	TPO	P-OG1-CB	-2.91	115.43	123.33
2	E	893	TPO	P-OG1-CB	-2.84	115.60	123.33

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	893	TPO	O-C-CA-CB
2	E	893	TPO	N-CA-CB-CG2
2	E	893	TPO	N-CA-CB-OG1
2	E	893	TPO	C-CA-CB-CG2
2	E	893	TPO	CG2-CB-OG1-P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	893	TPO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 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	CIT	F	301	-	12,12,12	1.09	0	17,17,17	1.44	1 (5%)
4	CIT	A	1201	-	12,12,12	1.10	0	17,17,17	1.45	1 (5%)
5	RQ9	E	1101	-	35,35,35	0.26	0	47,49,49	0.62	0
4	CIT	I	301	-	12,12,12	1.09	0	17,17,17	1.49	1 (5%)
4	CIT	C	301	-	12,12,12	1.06	0	17,17,17	1.48	2 (11%)
4	CIT	H	1102	-	12,12,12	1.13	0	17,17,17	1.45	1 (5%)
4	CIT	D	1201	-	12,12,12	1.11	0	17,17,17	1.35	2 (11%)
5	RQ9	H	1101	-	35,35,35	0.25	0	47,49,49	0.56	0
5	RQ9	B	1101	-	35,35,35	0.26	0	47,49,49	0.65	1 (2%)

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	CIT	F	301	-	-	0/16/16/16	-
4	CIT	A	1201	-	-	9/16/16/16	-
5	RQ9	E	1101	-	-	5/21/21/21	0/4/4/4
4	CIT	I	301	-	-	1/16/16/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CIT	C	301	-	-	2/16/16/16	-
4	CIT	H	1102	-	-	2/16/16/16	-
4	CIT	D	1201	-	-	2/16/16/16	-
5	RQ9	H	1101	-	-	4/21/21/21	0/4/4/4
5	RQ9	B	1101	-	-	3/21/21/21	0/4/4/4

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	301	CIT	O6-C6-C3	4.03	120.86	113.14
4	A	1201	CIT	O6-C6-C3	3.99	120.80	113.14
4	H	1102	CIT	O6-C6-C3	3.96	120.74	113.14
4	C	301	CIT	O6-C6-C3	3.87	120.56	113.14
4	F	301	CIT	O6-C6-C3	3.79	120.41	113.14

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1201	CIT	C1-C2-C3-O7
4	A	1201	CIT	C1-C2-C3-C4
4	A	1201	CIT	O7-C3-C6-O5
4	A	1201	CIT	O7-C3-C6-O6
4	A	1201	CIT	C4-C3-C6-O5

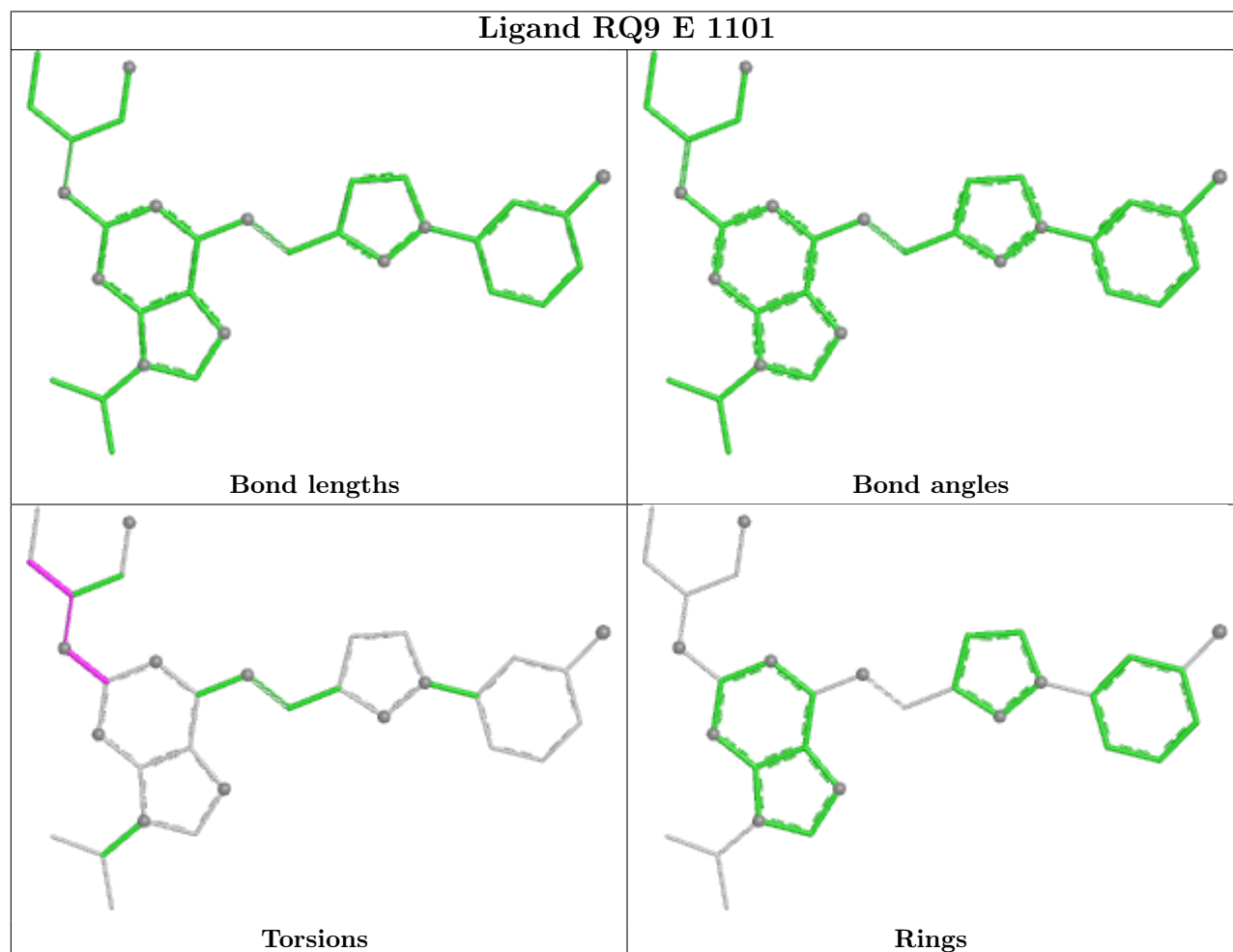
There are no ring outliers.

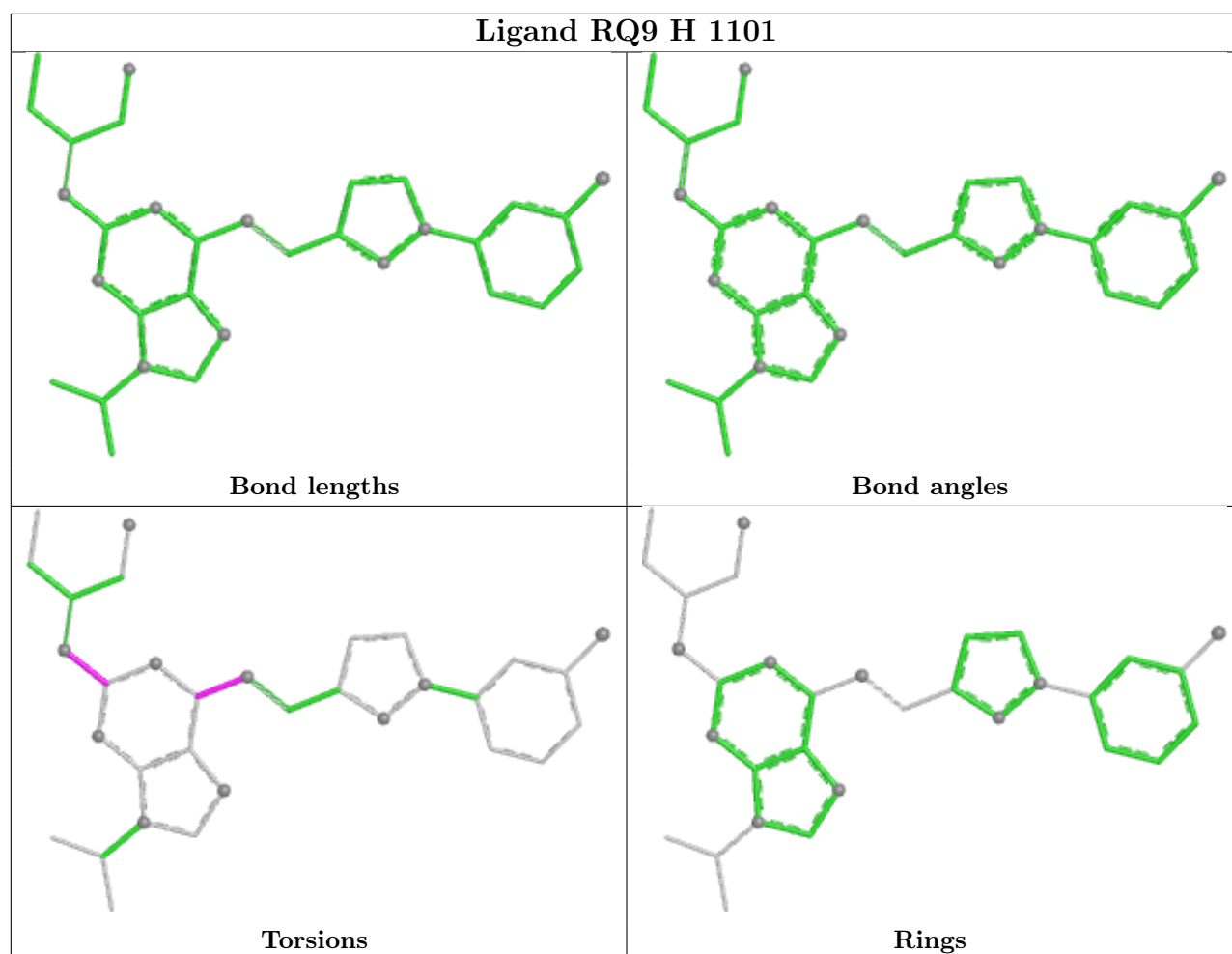
1 monomer is involved in 1 short contact:

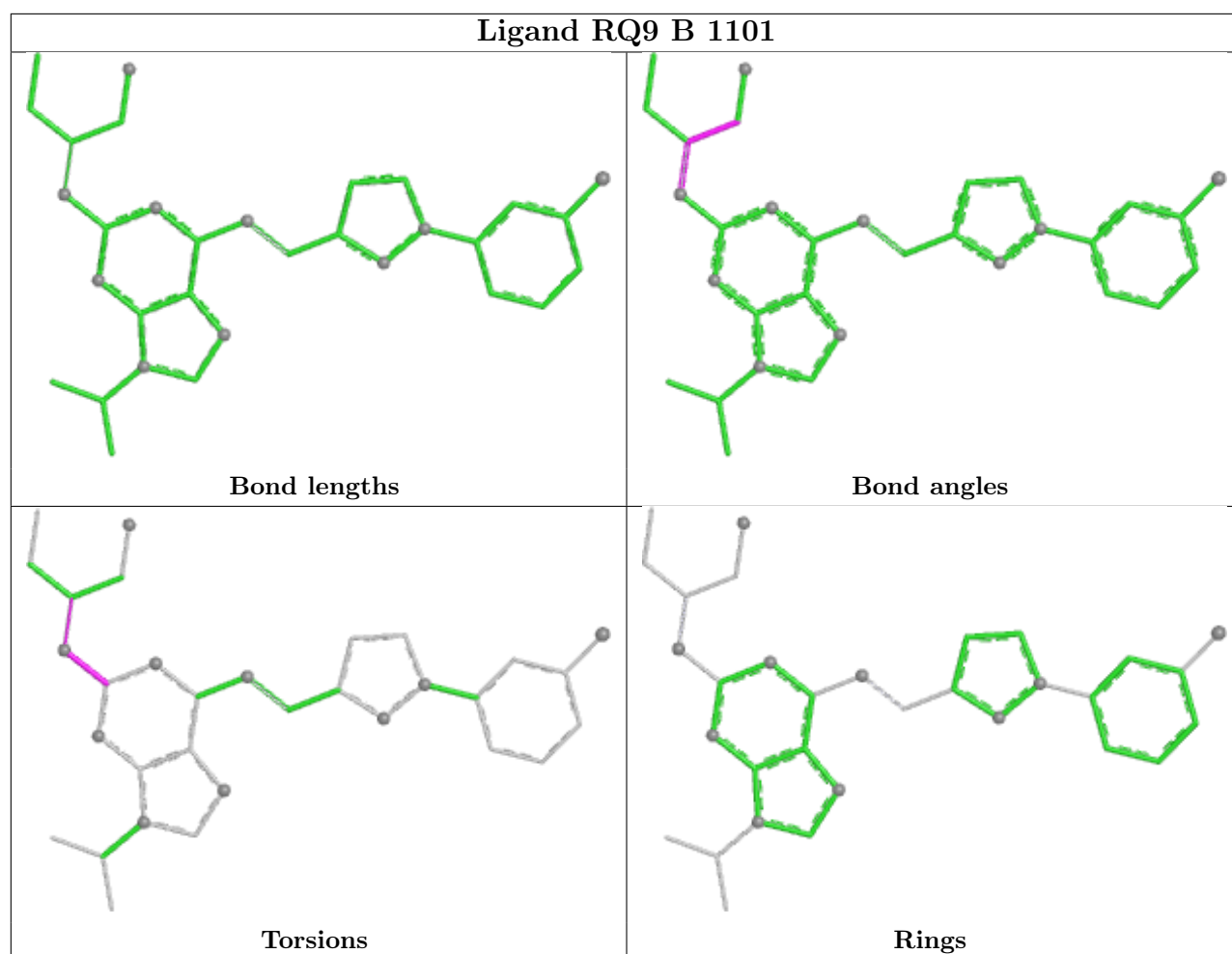
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1101	RQ9	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	822/840 (97%)	-0.51	2 (0%) 91 85	38, 64, 111, 185	0
1	D	827/840 (98%)	-0.53	2 (0%) 91 85	37, 63, 107, 194	0
1	G	826/840 (98%)	-0.46	1 (0%) 92 89	42, 68, 118, 189	0
2	B	320/344 (93%)	-0.35	0 100 100	45, 71, 121, 176	0
2	E	312/344 (90%)	-0.35	2 (0%) 85 73	40, 67, 107, 155	0
2	H	320/344 (93%)	-0.33	1 (0%) 90 81	35, 56, 105, 165	0
3	C	248/271 (91%)	-0.62	0 100 100	41, 62, 99, 120	0
3	F	248/271 (91%)	-0.64	0 100 100	34, 52, 87, 121	0
3	I	248/271 (91%)	-0.65	0 100 100	37, 54, 93, 132	0
All	All	4171/4365 (95%)	-0.49	8 (0%) 91 85	34, 63, 110, 194	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	394	ILE	3.2
2	E	880	LEU	2.7
2	H	1031	PRO	2.3
1	A	1035	GLY	2.2
1	G	252	ILE	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	TPO	B	893	11/12	0.75	0.13	202,225,270,277	6
2	TPO	E	893	11/12	0.76	0.11	204,229,281,287	6
2	TPO	H	893	11/12	0.77	0.16	133,154,180,180	5

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

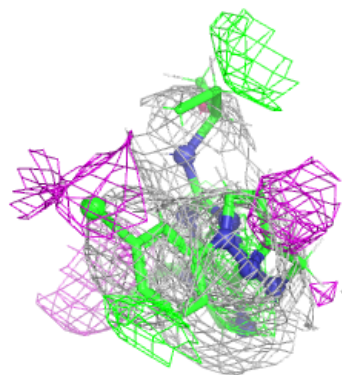
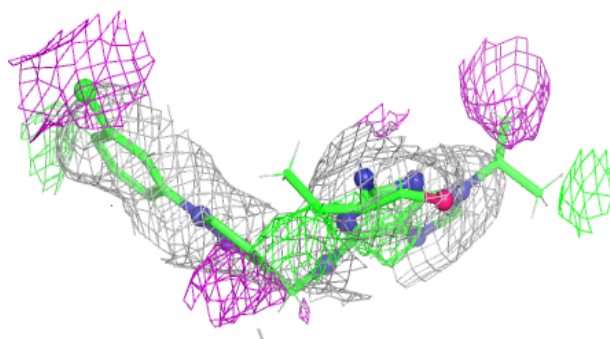
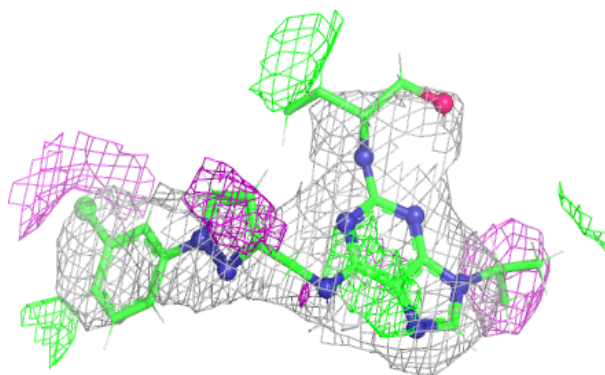
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	CIT	I	301	13/13	0.60	0.09	141,155,187,187	5
4	CIT	H	1102	13/13	0.61	0.11	141,165,186,189	5
4	CIT	C	301	13/13	0.69	0.09	154,169,203,203	5
4	CIT	A	1201	13/13	0.70	0.12	146,169,209,209	5
4	CIT	F	301	13/13	0.76	0.10	134,158,175,193	5
4	CIT	D	1201	13/13	0.77	0.10	147,168,202,202	5
5	RQ9	E	1101	32/32	0.88	0.19	114,143,175,183	27
5	RQ9	H	1101	32/32	0.90	0.17	104,127,165,179	27
5	RQ9	B	1101	32/32	0.91	0.14	115,133,161,180	27

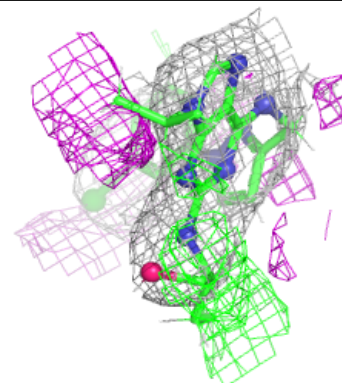
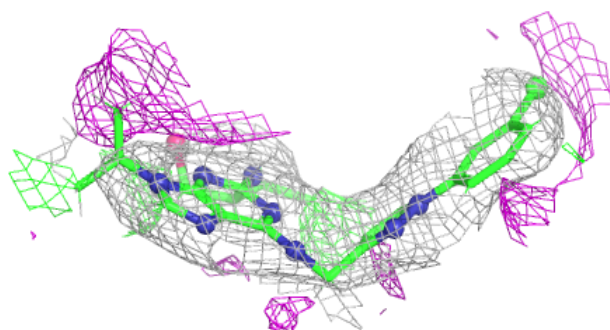
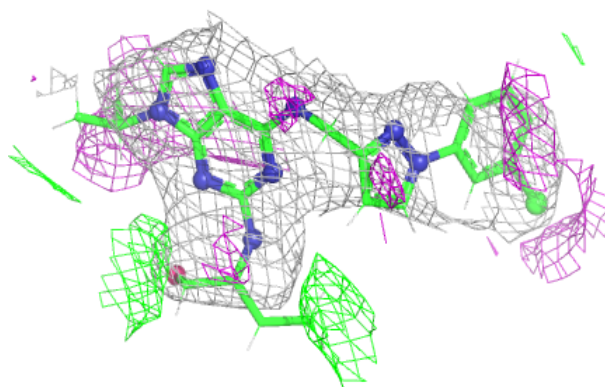
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around RQ9 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)

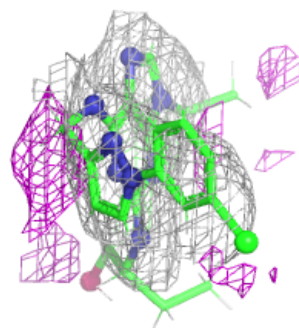
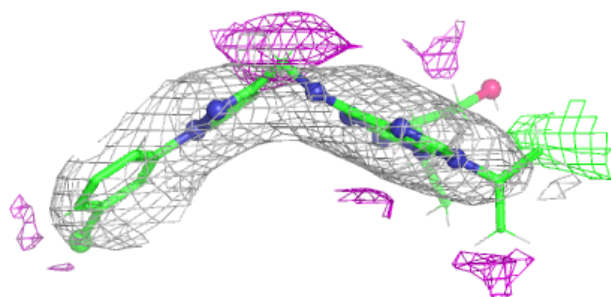
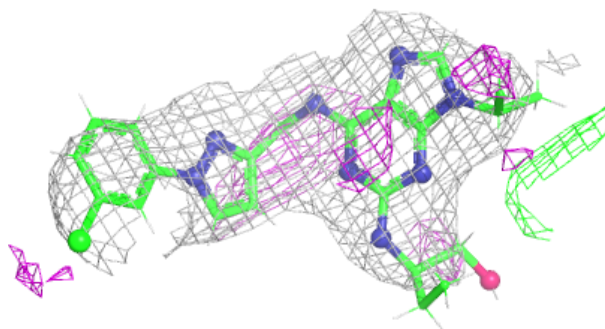
**Electron density around RQ9 H 1101:**

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



Electron density around RQ9 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.