

wwPDB X-ray Structure Validation Summary Report (i)

Sep 7, 2023 – 01:33 pm BST

PDB ID : 8BU5

Title: Structure of DDB1 bound to SR-4835-engaged CDK12-cyclin K

Authors: Kozicka, Z.; Kempf, G.; Petzold, G.; Thoma, N.H.

Deposited on : 2022-11-30

Resolution : 3.13 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 (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) 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)

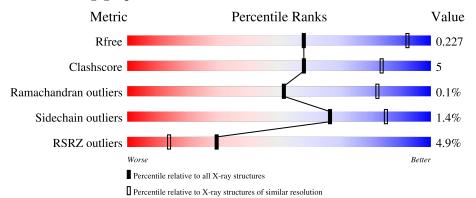
Validation Pipeline (wwPDB-VP) : 2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$

The reported resolution of this entry is 3.13 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	1626 (3.18-3.10)
Clashscore	141614	1735 (3.18-3.10)
Ramachandran outliers	138981	1677 (3.18-3.10)
Sidechain outliers	138945	1677 (3.18-3.10)
RSRZ outliers	127900	1588 (3.18-3.10)

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	Λ	840	5%	
1	A	040	4%	15% •
1	D	840	89%	10% •
1	G	840	8%	17% •
_			8%	27,70
2	В	344	79%	15% • •
9	E	344		17% • •
	B E	344		15% 17%



Continued from previous page...

Mol	Chain	Length	Quality of chain	
2	Н	344	5% 85%	10% • •
3	С	271	86%	6% 8%
3	F	271	85%	6% 8%
3	I	271	87%	• 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	CIT	I	301	-	X	_	-



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 67681 atoms, of which 33741 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						AltConf	Trace
1	Λ	826	Total	С	Н	N	О	S	6485	0	0
1	Λ	020	12936	4105	6449	1094	1252	36	0400	0	
1	D	827	Total	С	Н	N	О	S	6462	0	0
1	D	021	12957	4111	6462	1095	1253	36	0402	0	0
1	С	826	Total	С	Н	N	О	S	6452	0	0
1	G	020	12938	4106	6452	1093	1251	36	0452	U	0

There are 30 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
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
G	-3	GLY	-	expression tag	UNP Q16531
G	-2	GLY	-	expression tag	UNP Q16531
G	-1	GLY	-	expression tag	UNP Q16531



Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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

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

Mol	Chain	Residues		Atoms						ZeroOcc	AltConf	Trace
2	R	332	Total	С	Н	N	О	Р	S	2723	0	0
	D	332	5436	1737	2723	461	497	1	17	2120	U	U
9	E	331	Total	С	Η	N	O	Р	S	2718	0	0
2	15	991	5425	1734	2718	460	495	1	17	2110	U	0
2	Н	331	Total	С	Н	N	О	Р	S	2718	0	0
2	11	331	5425	1734	2718	460	495	1	17	2710	U	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	709	GLY	-	expression tag	UNP Q9NYV4
В	710	GLY	-	expression tag	UNP Q9NYV4
В	711	GLY	-	expression tag	UNP Q9NYV4
В	965	ARG	LYS	engineered mutation	UNP Q9NYV4
В	1052	GLN	-	expression tag	UNP Q9NYV4
Е	709	GLY	-	expression tag	UNP Q9NYV4
Е	710	GLY	-	expression tag	UNP Q9NYV4
Е	711	GLY	-	expression tag	UNP Q9NYV4
Е	965	ARG	LYS	engineered mutation	UNP Q9NYV4
Е	1052	GLN	-	expression tag	UNP Q9NYV4
Н	709	GLY	-	expression tag	UNP Q9NYV4
Н	710	GLY	-	expression tag	UNP Q9NYV4
Н	711	GLY	-	expression tag	UNP Q9NYV4
Н	965	ARG	LYS	engineered mutation	UNP Q9NYV4
Н	1052	GLN	-	expression tag	UNP Q9NYV4

• Molecule 3 is a protein called Cyclin-K.

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



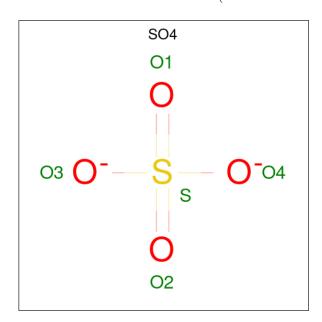
 $Continued\ from\ previous\ page...$

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
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
С	-3	GLY	-	expression tag	UNP O75909
С	-2	GLY	-	expression tag	UNP O75909
С	-1	GLY	-	expression tag	UNP O75909
С	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

 \bullet Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: $\mathrm{O_4S}).$



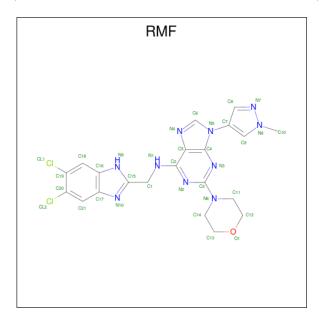
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 5	O 4	S 1	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total O S 5 4 1	0	0
4	Н	1	Total O S 5 4 1	0	0

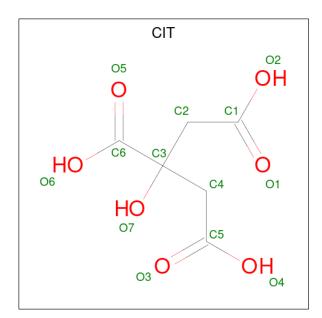
• Molecule 5 is $\{N\}$ -[[5,6-bis(chloranyl)-1 $\{H\}$ -benzimidazol-2-yl]methyl]-9-(1-methylpyrazol -4-yl)-2-morpholin-4-yl-purin-6-amine (three-letter code: RMF) (formula: $C_{21}H_{20}Cl_2N_{10}O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
5	В	1	Total	С	Cl	Н	N	О	20	0
			54	21	2	20	10	1	20	
5	E	1	Total	С	Cl	Η	N	О	20	0
5 E	l Li	1	54	21	2	20	10	1	20	U
5	5 H	1	Total	С	Cl	Н	N	О	20	0
9		П 1	54	21	2	20	10	1	20	

• Molecule 6 is CITRIC ACID (three-letter code: CIT) (formula: C₆H₈O₇).





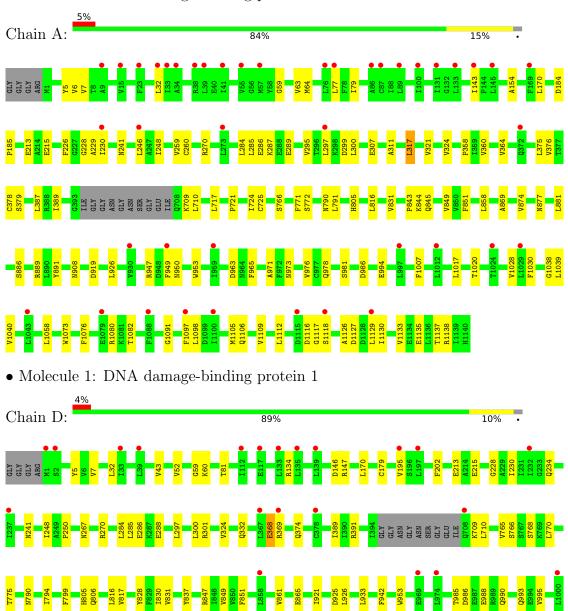
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	С	1	Total 18			5	0
6	F	1	Total 18			5	0
6	I	1	Total 18		H 5	5	0



3 Residue-property plots (i)

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

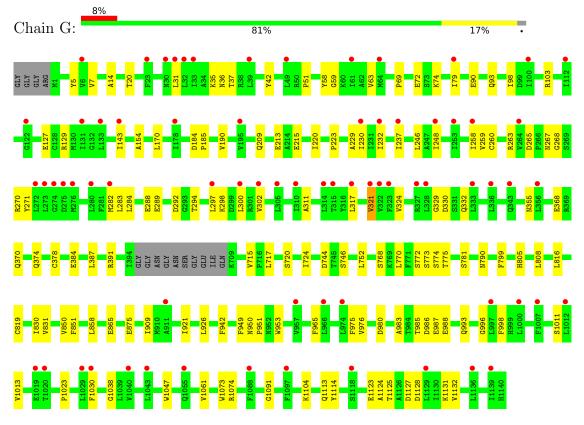
• Molecule 1: DNA damage-binding protein 1



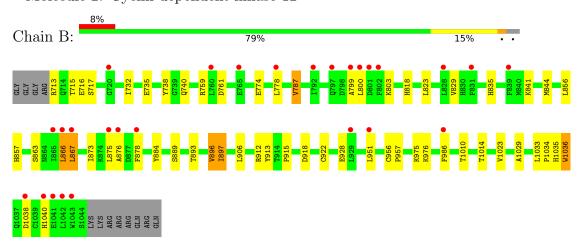




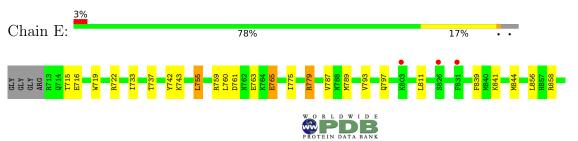
 \bullet Molecule 1: DNA damage-binding protein 1

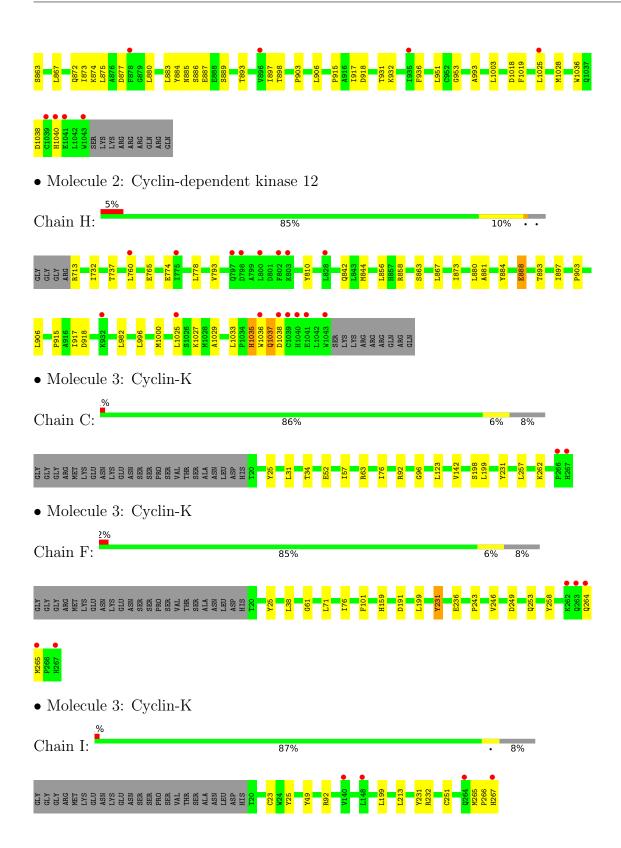


 \bullet Molecule 2: Cyclin-dependent kinase 12



 \bullet Molecule 2: Cyclin-dependent kinase 12







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants	249.94Å 249.94Å 219.30Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	60.58 - 3.13	Depositor
resolution (A)	216.45 - 3.13	EDS
% Data completeness	78.2 (60.58-3.13)	Depositor
(in resolution range)	78.2 (216.45-3.13)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.55 (at 3.13Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.199 , 0.220	Depositor
it, it free	0.208 , 0.227	DCC
R_{free} test set	5407 reflections $(5.00%)$	wwPDB-VP
Wilson B-factor (Å ²)	121.0	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.31, 83.3	EDS
L-test for twinning ²	$< L > = 0.46, < L^2> = 0.29$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	67681	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 1.55% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: SO4, RMF, 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	Bo	nd lengths	Bond	angles
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	0.37	0/6604	0.66	0/8931
1	D	0.36	0/6612	0.64	0/8942
1	G	0.38	0/6603	0.67	0/8930
2	В	0.38	0/2763	0.64	0/3725
2	Е	0.40	0/2757	0.67	0/3717
2	Н	0.42	$1/2757 \ (0.0\%)$	0.66	0/3717
3	С	0.38	0/2120	0.56	0/2868
3	F	0.38	0/2120	0.58	0/2868
3	I	0.37	0/2120	0.57	0/2868
All	All	0.38	$1/34456 \ (0.0\%)$	0.64	0/46566

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(A)	Ideal(A)
2	Н	888	GLU	CG-CD	-5.93	1.43	1.51

There are no bond angle outliers.

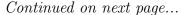
There are no chirality outliers.

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	6487	6449	6451	73	0





Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	6495	6462	6464	46	1
1	G	6486	6452	6454	89	0
2	В	2713	2723	2723	42	0
2	Е	2707	2718	2718	31	1
2	Н	2707	2718	2718	27	1
3	С	2063	2048	2048	10	0
3	F	2063	2048	2048	10	0
3	I	2063	2048	2048	6	1
4	A	5	0	0	0	0
4	G	5	0	0	0	0
4	Н	5	0	0	0	0
5	В	34	20	0	0	0
5	Ε	34	20	0	1	0
5	Н	34	20	0	0	0
6	С	13	5	5	0	0
6	F	13	5	5	0	0
6	I	13	5	5	0	0
All	All	33940	33741	33687	323	2

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 5.

The worst 5 of 323 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	$\operatorname{distance}\ (ext{Å})$	$overlap(\AA)$
3:C:52:GLU:OE1	3:C:92:ARG:NH1	2.12	0.82
1:A:1109:VAL:HG12	1:A:1129:LEU:HD12	1.67	0.77
1:G:768:SER:HB3	1:G:808:LEU:HD11	1.70	0.74
3:F:231:TYR:OH	3:F:236:GLU:OE1	2.05	0.73
1:G:387:LEU:HG	1:G:717:LEU:HD11	1.71	0.72

All (2) 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:368:GLU:O	2:H:888:GLU:OE2[4_565]	2.15	0.05
2:E:1018:ASP:OD2	3:I:232:ARG:HE[5_554]	1.59	0.01



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	Perce	ntiles
1	A	822/840 (98%)	798 (97%)	22 (3%)	2 (0%)	47	78
1	D	823/840 (98%)	805 (98%)	17 (2%)	1 (0%)	51	82
1	G	822/840 (98%)	799 (97%)	23 (3%)	0	100	100
2	В	329/344 (96%)	321 (98%)	8 (2%)	0	100	100
2	E	328/344 (95%)	316 (96%)	12 (4%)	0	100	100
2	Н	328/344 (95%)	317 (97%)	10 (3%)	1 (0%)	41	72
3	С	246/271 (91%)	242 (98%)	4 (2%)	0	100	100
3	F	246/271 (91%)	242 (98%)	4 (2%)	0	100	100
3	I	246/271 (91%)	242 (98%)	4 (2%)	0	100	100
All	All	4190/4365 (96%)	4082 (97%)	104 (2%)	4 (0%)	51	82

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	369	ARG
2	Н	1037	GLN
1	A	772	SER
1	A	981	SER

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	721/728 (99%)	711 (99%)	10 (1%)	67	85	
1	D	722/728 (99%)	719 (100%)	3 (0%)	91	96	
1	G	721/728 (99%)	711 (99%)	10 (1%)	67	85	
2	В	299/308 (97%)	290 (97%)	9 (3%)	41	70	
2	E	298/308 (97%)	285 (96%)	13 (4%)	28	59	
2	Н	298/308 (97%)	293 (98%)	5 (2%)	60	82	
3	С	223/242 (92%)	221 (99%)	2 (1%)	78	90	
3	F	223/242 (92%)	222 (100%)	1 (0%)	91	96	
3	I	223/242 (92%)	222 (100%)	1 (0%)	91	96	
All	All	3728/3834 (97%)	3674 (99%)	54 (1%)	67	85	

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type	
2	Е	797	GLN	
2	Е	1038	ASP	
2	Н	863	SER	
2	Е	863	SER	
2	Е	887	GLU	

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	240	HIS
1	G	950	ASN
2	Н	1040	HIS
2	В	944	GLN
2	В	835	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	Dog	Dog	Ros	Ros	Ros	Ros	Link	B	ond leng	$_{ m gths}$	В	ond ang	les
WIOI	Type			Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2						
2	TPO	Н	893	2	8,10,11	1.84	2 (25%)	10,14,16	1.56	1 (10%)						
2	TPO	Е	893	2	8,10,11	1.92	2 (25%)	10,14,16	1.19	1 (10%)						
2	TPO	В	893	2	8,10,11	1.89	3 (37%)	10,14,16	1.38	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	Н	893	2	-	0/9/11/13	-
2	TPO	Е	893	2	-	0/9/11/13	-
2	TPO	В	893	2	-	1/9/11/13	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(A)	$Ideal(\AA)$
2	Е	893	TPO	P-O1P	3.75	1.62	1.50
2	В	893	TPO	P-O1P	3.71	1.62	1.50
2	Н	893	TPO	P-OG1	3.71	1.66	1.59
2	Е	893	TPO	P-OG1	2.68	1.64	1.59
2	В	893	TPO	P-OG1	2.24	1.63	1.59

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
2	Н	893	TPO	CG2-CB-CA	-3.81	105.65	113.16
2	Е	893	TPO	CG2-CB-CA	-2.33	108.56	113.16
2	В	893	TPO	CG2-CB-CA	-2.19	108.84	113.16

There are no chirality outliers.

All (1) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
2	В	893	TPO	O-C-CA-CB

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)

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	Trino	Chain	Dec	Link	Во	ond leng	ths	Bond angles		
MIOI	Mol Type Chain Re	Res	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
5	RMF	Н	1101	-	32,39,39	1.01	3 (9%)	31,57,57	1.86	4 (12%)
5	RMF	Е	1101	-	32,39,39	0.97	3 (9%)	31,57,57	1.86	4 (12%)
6	CIT	I	301	-	12,12,12	1.68	3 (25%)	17,17,17	2.05	8 (47%)
5	RMF	В	1101	-	32,39,39	0.98	3 (9%)	31,57,57	1.96	4 (12%)
4	SO4	G	1201	-	4,4,4	0.51	0	6,6,6	0.18	0
4	SO4	Н	1102	-	4,4,4	0.42	0	6,6,6	0.06	0
6	CIT	F	301	-	12,12,12	1.37	1 (8%)	17,17,17	1.84	5 (29%)
6	CIT	С	301	-	12,12,12	1.22	0	17,17,17	2.32	8 (47%)
4	SO4	A	1201	-	4,4,4	0.52	0	6,6,6	0.09	0

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
5	RMF	Н	1101	-	-	3/7/21/21	0/6/6/6



Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	RMF	E	1101	-	-	4/7/21/21	0/6/6/6
6	CIT	I	301	-	-	12/16/16/16	-
5	RMF	В	1101	-	-	3/7/21/21	0/6/6/6
6	CIT	F	301	-	-	5/16/16/16	-
6	CIT	С	301	-	-	0/16/16/16	-

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	Ideal(Å)
6	I	301	CIT	C2-C3	-3.36	1.49	1.53
5	В	1101	RMF	C7-N5	-2.89	1.40	1.44
5	Е	1101	RMF	C7-N5	-2.80	1.40	1.44
6	I	301	CIT	C4-C3	-2.71	1.50	1.53
5	Н	1101	RMF	C7-N5	-2.65	1.41	1.44

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\mathbf{Ideal}(^o)$
5	В	1101	RMF	C14-N6-C3	-7.00	110.09	121.69
5	В	1101	RMF	C11-N6-C3	-6.72	110.56	121.69
5	Н	1101	RMF	C11-N6-C3	-6.61	110.74	121.69
5	Е	1101	RMF	C14-N6-C3	-6.55	110.83	121.69
5	Ε	1101	RMF	C11-N6-C3	-6.28	111.28	121.69

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	В	1101	RMF	N2-C3-N6-C14
5	В	1101	RMF	N3-C3-N6-C14
5	Е	1101	RMF	N2-C3-N6-C11
5	Е	1101	RMF	N3-C3-N6-C11
5	Н	1101	RMF	N2-C3-N6-C14

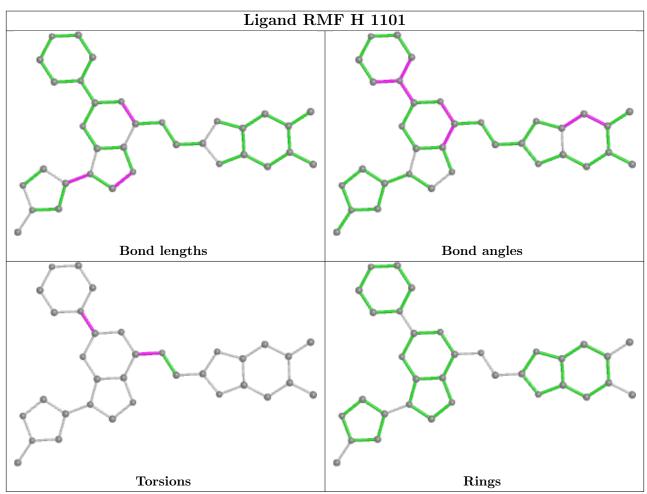
There are no ring outliers.

1 monomer is involved in 1 short contact:

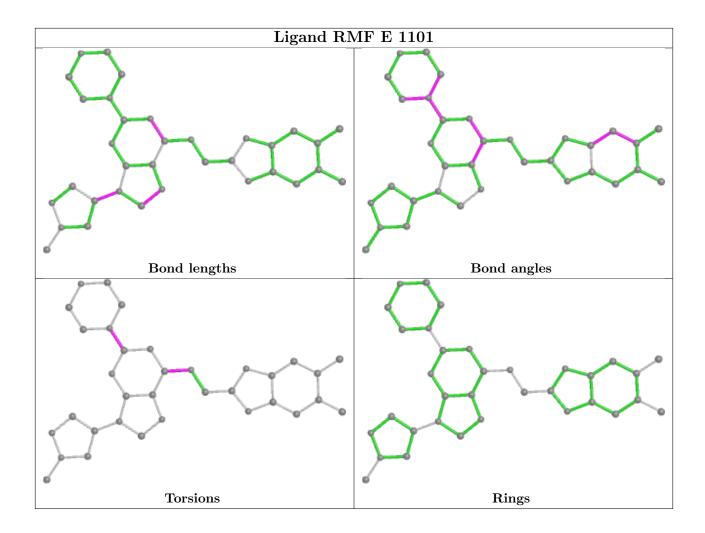
\mathbf{Mol}	Chain	Res	Type	Clashes	Symm-Clashes
5	Е	1101	RMF	1	0



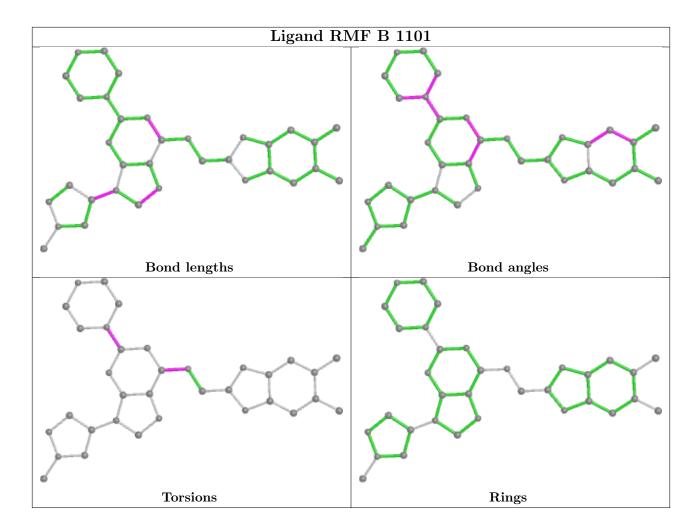
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











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, 95^{th} 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>	$\#\mathrm{RSRZ}{>}2$	$\mathrm{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	A	821/840~(97%)	0.48	42 (5%) 28 13	89, 128, 199, 295	0
1	D	827/840 (98%)	0.39	30 (3%) 42 22	87, 122, 191, 254	0
1	G	826/840 (98%)	0.54	71 (8%) 10 4	99, 146, 226, 288	0
2	В	331/344 (96%)	0.55	27 (8%) 11 5	101, 127, 183, 250	0
2	E	330/344~(95%)	0.55	11 (3%) 46 25	93, 115, 182, 242	0
2	Н	330/344~(95%)	0.58	16 (4%) 30 14	85, 110, 183, 216	0
3	С	248/271 (91%)	0.32	2 (0%) 86 74	93, 117, 160, 243	0
3	F	$248/271 \ (91\%)$	0.47	5 (2%) 65 46	80, 98, 149, 215	0
3	I	248/271 (91%)	0.41	4 (1%) 72 53	86, 106, 150, 238	0
All	All	4209/4365~(96%)	0.48	208 (4%) 29 14	80, 123, 200, 295	0

The worst 5 of 208 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Е	1043	TRP	8.0
2	Н	1043	TRP	7.0
2	Н	1039	CYS	6.4
2	Е	1039	CYS	5.6
1	G	1129	LEU	5.6

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, 95^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	TPO	Е	893	11/12	0.71	0.23	145,156,185,187	6
2	TPO	Н	893	11/12	0.75	0.27	115,127,153,158	6
2	TPO	В	893	11/12	0.86	0.21	150,174,202,207	6

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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.

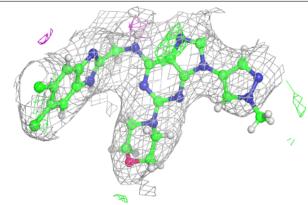
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\operatorname{\textbf{B-factors}}(\mathring{\mathbf{A}}^2)$	Q < 0.9
4	SO4	A	1201	5/5	0.77	0.16	149,153,163,229	0
4	SO4	Н	1102	5/5	0.83	0.21	127,128,135,191	0
6	CIT	I	301	13/13	0.83	0.28	107,114,138,138	5
4	SO4	G	1201	5/5	0.85	0.27	171,172,175,234	0
6	CIT	F	301	13/13	0.86	0.17	101,104,125,125	5
6	CIT	С	301	13/13	0.90	0.15	114,117,140,140	5
5	RMF	Н	1101	34/34	0.94	0.28	94,111,138,152	20
5	RMF	В	1101	34/34	0.94	0.29	101,111,136,153	20
5	RMF	E	1101	34/34	0.95	0.28	94,106,131,152	20

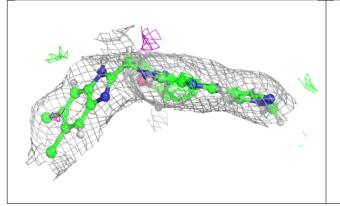
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

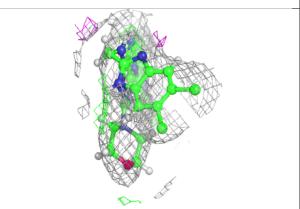


Electron density around RMF H 1101:

 $2 {
m mF}_o {
m -DF}_c$ (at 0.7 rmsd) in gray ${
m mF}_o {
m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

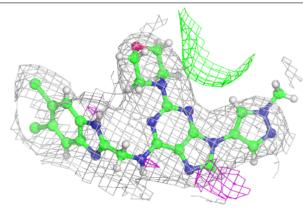


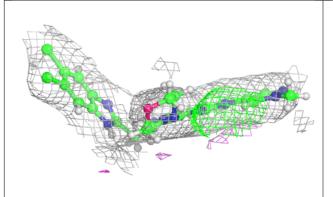


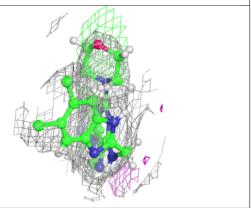


Electron density around RMF B 1101:

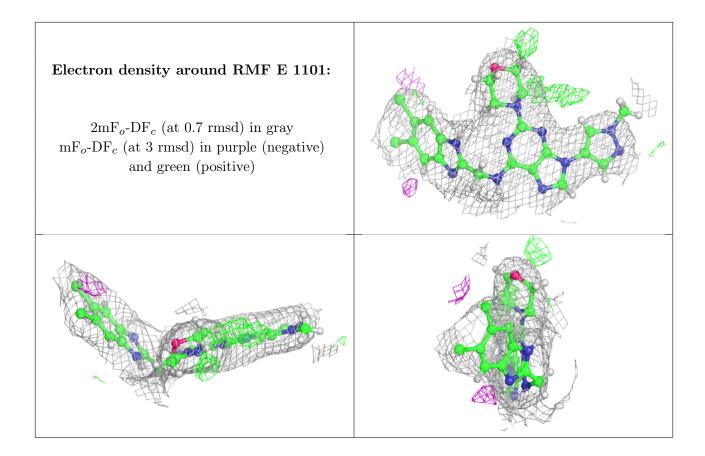
 $2 {
m mF}_o {
m -DF}_c$ (at 0.7 rmsd) in gray ${
m mF}_o {
m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)











6.5 Other polymers (i)

There are no such residues in this entry.

