Full wwPDB X-ray Structure Validation Report (i)

Sep 7, 2023 – 04:37 pm BST

PDB ID	:	8BUJ
Title	:	Structure of DDB1 bound to DS06-engaged CDK12-cyclin K
Authors	:	Kozicka, Z.; Kempf, G.; Petzold, G.; Thoma, N.H.
Deposited on	:	2022-11-30
Resolution	:	3.62 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 (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 (i)) were used in the production of this report:

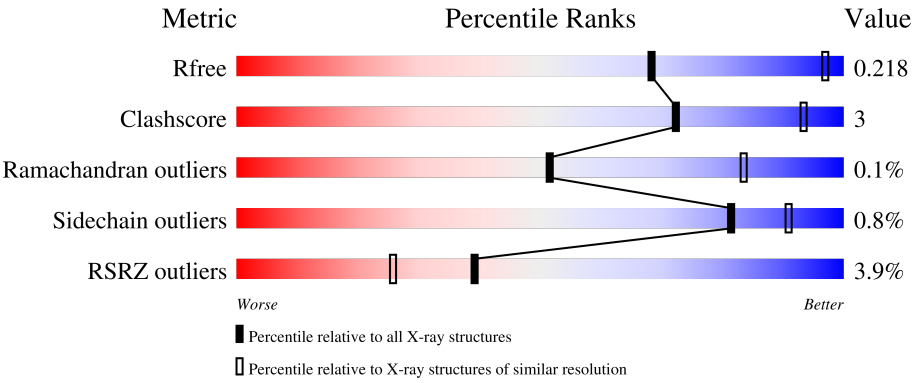
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.62 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	1290 (3.74-3.50)
Clashscore	141614	1387 (3.74-3.50)
Ramachandran outliers	138981	1339 (3.74-3.50)
Sidechain outliers	138945	1339 (3.74-3.50)
RSRZ outliers	127900	1191 (3.74-3.50)

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	6% 88% 10% ·
1	D	840	4% 89% 9% ·
1	G	840	4% 88% 11% ·
2	B	344	6% 83% 11% · 5%
2	E	344	4% 85% 11% ·

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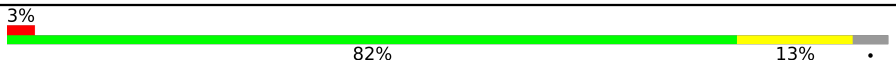
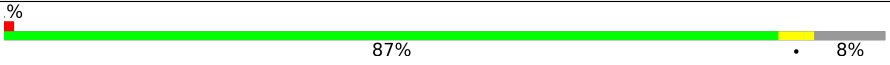
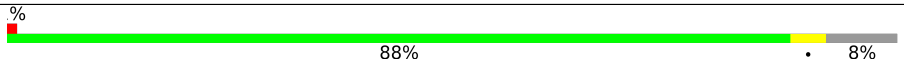
Mol	Chain	Length	Quality of chain
2	H	344	
3	C	271	
3	F	271	
3	I	271	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 67535 atoms, of which 33688 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	C	H	N	O	S	6450	0	0
			12937	4105	6450	1094	1252	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	6454	0	0
			12940	4106	6454	1093	1251	36			

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

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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	B	327	Total	C	H	N	O	P	S	2676	0	0
			5341	1706	2676	451	490	1	17			
2	E	329	Total	C	H	N	O	P	S	2697	0	0
			5384	1723	2697	454	492	1	17			
2	H	329	Total	C	H	N	O	P	S	2697	0	0
			5384	1723	2697	454	492	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

- Molecule 3 is a protein called Cyclin-K.

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

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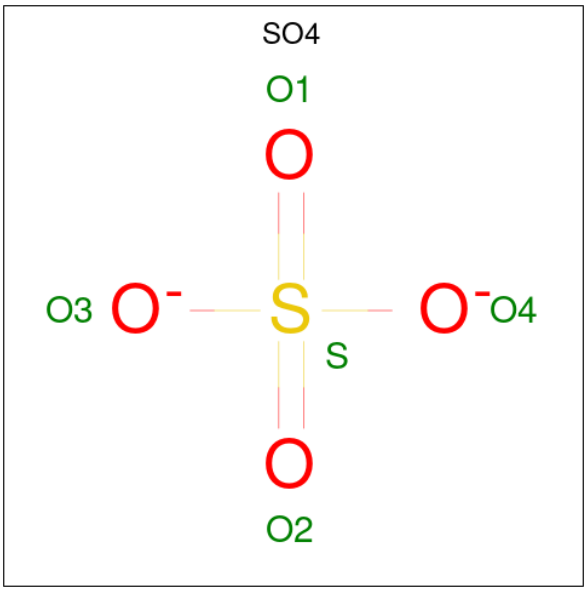
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	F	248	Total	C	H	N	O	S	2048	0	0
			4111	1341	2048	346	363	13			
3	I	248	Total	C	H	N	O	S	2048	0	0
			4111	1341	2048	346	363	13			

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 SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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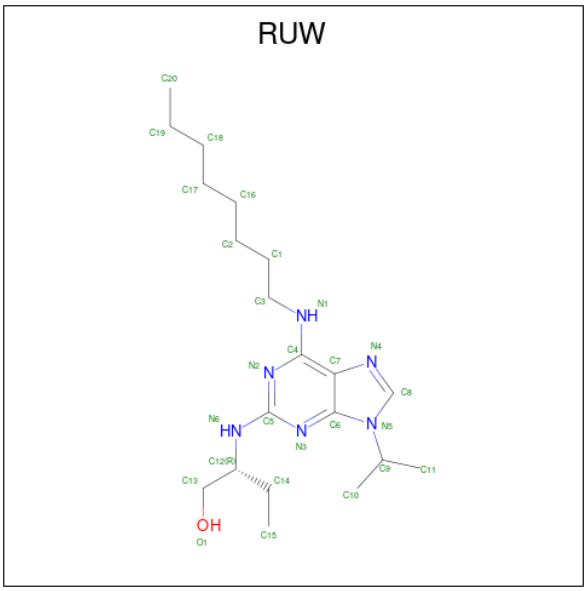
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	I	1	Total O S 5 4 1	0	0
4	I	1	Total O S 5 4 1	0	0

- Molecule 5 is (2 {R})-2-[[6-(octylamino)-9-propan-2-yl-purin-2-yl]amino]butan-1-ol (three-letter code: RUW) (formula: $C_{20}H_{36}N_6O$) (labeled as "Ligand of Interest" by depositor).



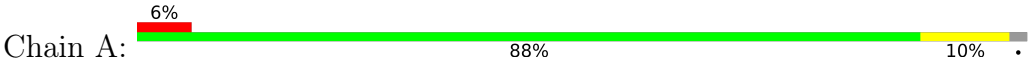
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	H	N	O	43	0
			63	20	36	6	1		
5	E	1	Total	C	H	N	O	43	0
			63	20	36	6	1		
5	H	1	Total	C	H	N	O	43	0
			63	20	36	6	1		

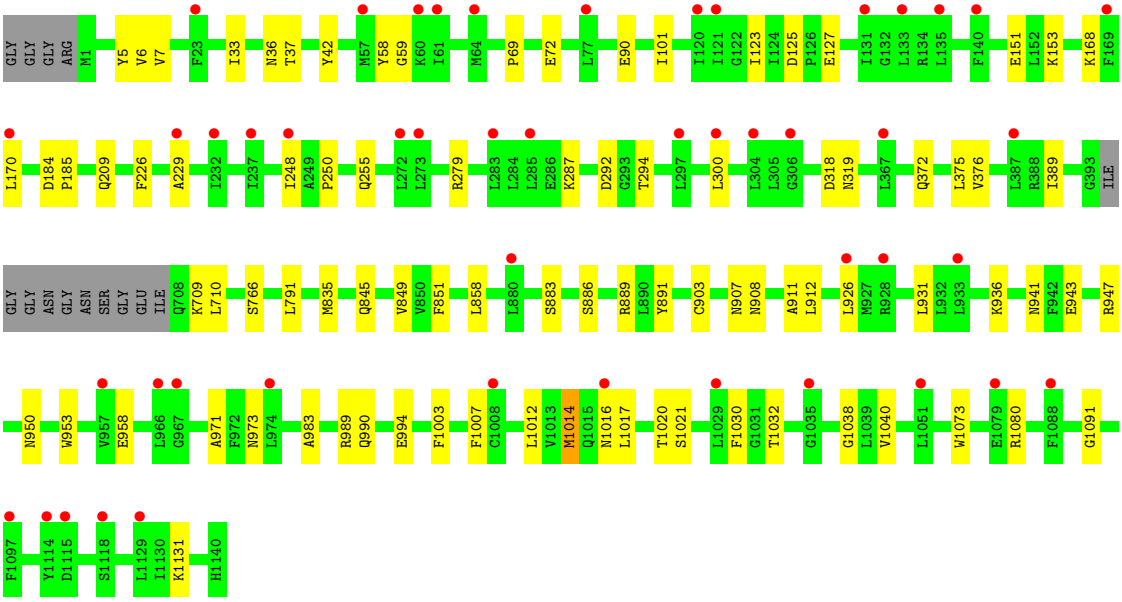
3 Residue-property plots (i)

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

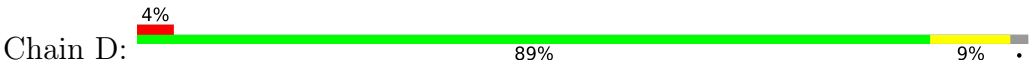
Chain A:

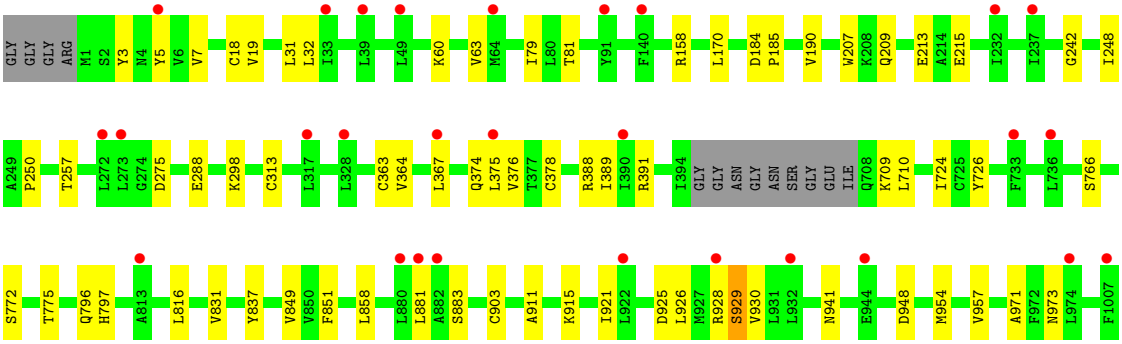




• Molecule 1: DNA damage-binding protein 1

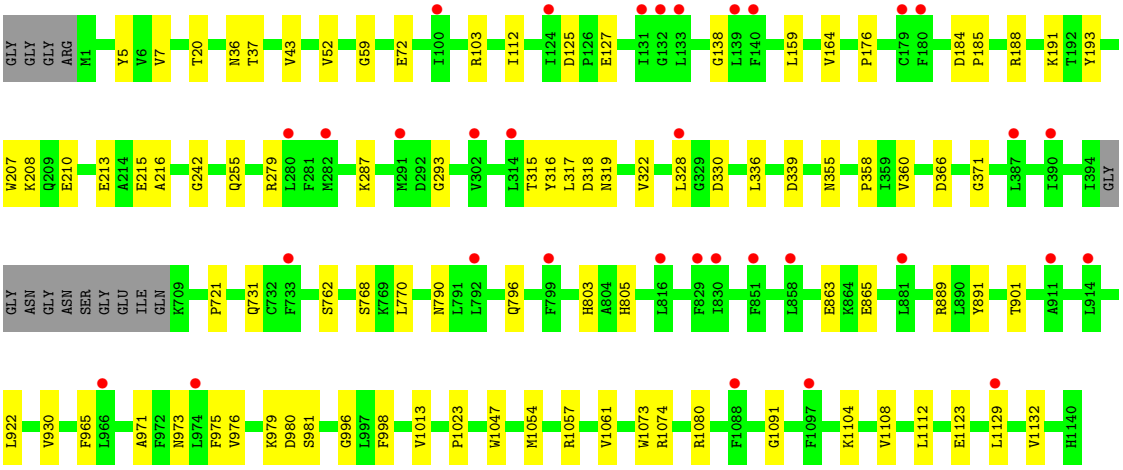
Chain D:





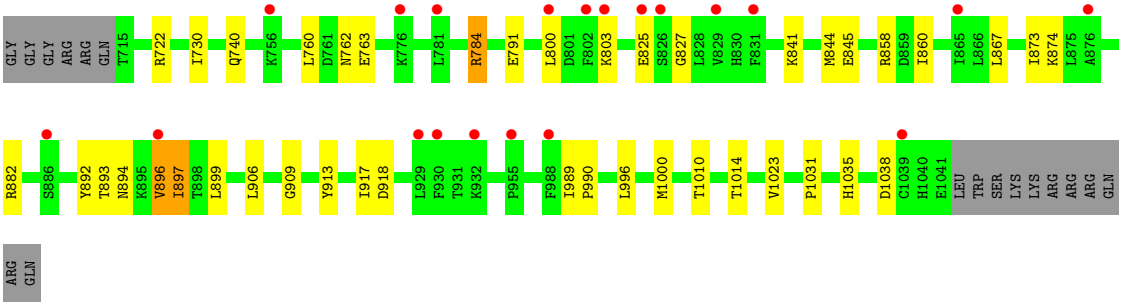
• Molecule 1: DNA damage-binding protein 1

Chain G:



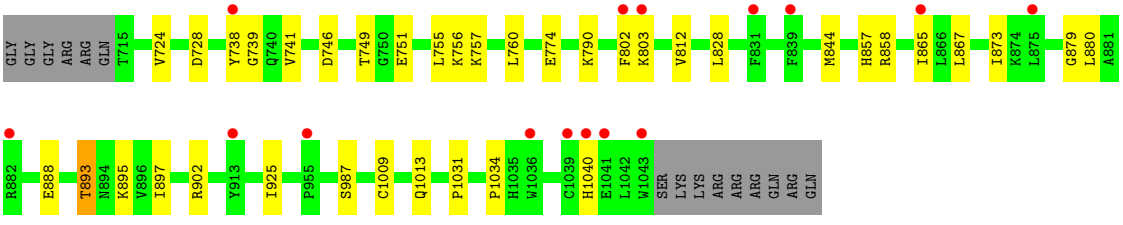
• Molecule 2: Cyclin-dependent kinase 12

Chain B:



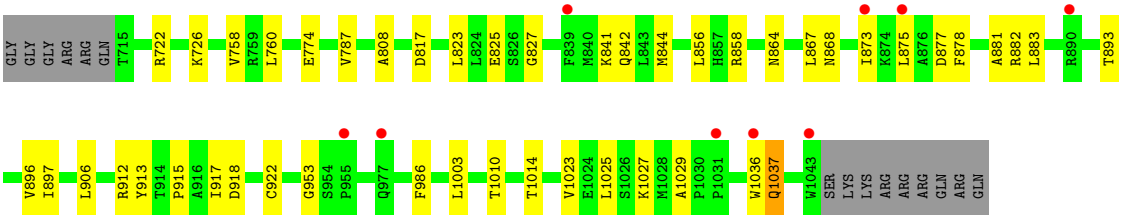
• Molecule 2: Cyclin-dependent kinase 12

Chain E:

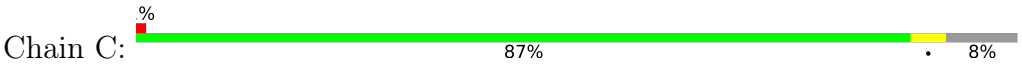


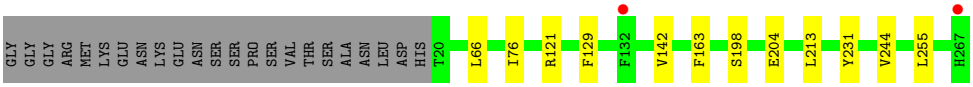
• Molecule 2: Cyclin-dependent kinase 12

Chain H:

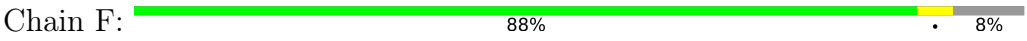


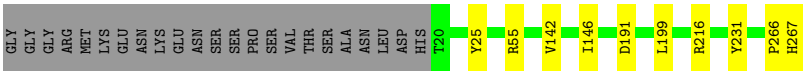
• Molecule 3: Cyclin-K



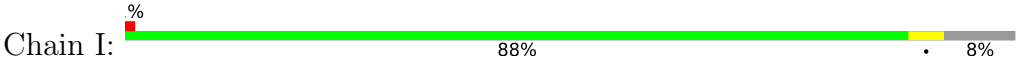


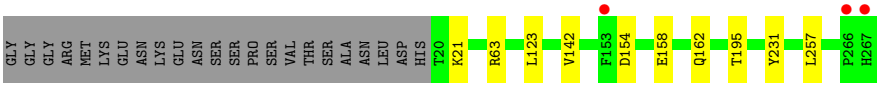
• Molecule 3: Cyclin-K





• Molecule 3: Cyclin-K





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	249.35Å 249.35Å 218.42Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	76.78 – 3.62 215.95 – 3.62	Depositor EDS
% Data completeness (in resolution range)	90.5 (76.78-3.62) 90.5 (215.95-3.62)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.46 (at 3.58Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.164 , 0.206 0.182 , 0.218	Depositor DCC
R_{free} test set	4039 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	150.2	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 119.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.058 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	67535	wwPDB-VP
Average B, all atoms (Å^2)	172.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.60% of the height of the origin peak. No significant pseudotranslation is detected.*

[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, RUW, SO4

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	0.31	0/6604	0.60	0/8931
1	D	0.31	0/6612	0.58	0/8942
1	G	0.32	0/6603	0.59	0/8930
2	B	0.32	0/2713	0.59	0/3657
2	E	0.31	0/2737	0.60	0/3691
2	H	0.38	2/2737 (0.1%)	0.60	0/3691
3	C	0.31	0/2120	0.53	0/2868
3	F	0.32	0/2120	0.55	0/2868
3	I	0.31	0/2120	0.54	0/2868
All	All	0.32	2/34366 (0.0%)	0.58	0/46446

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	912	ARG	CA-CB	-7.19	1.38	1.53
2	H	912	ARG	CG-CD	-5.11	1.39	1.51

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	6451	47	2
1	D	6495	6462	6464	53	0
1	G	6486	6454	6456	51	2
2	B	2665	2676	2676	26	0
2	E	2687	2697	2697	23	0
2	H	2687	2697	2697	26	0
3	C	2063	2048	2048	7	0
3	F	2063	2048	2048	5	0
3	I	2063	2048	2048	5	0
4	A	15	0	0	0	0
4	C	10	0	0	0	0
4	D	15	0	0	0	0
4	F	5	0	0	0	0
4	G	10	0	0	0	0
4	H	5	0	0	0	0
4	I	10	0	0	0	0
5	B	27	36	0	0	0
5	E	27	36	0	0	0
5	H	27	36	0	0	0
All	All	33847	33688	33585	232	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 3.

All (232) 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)
1:D:796:GLN:HG3	1:D:797:HIS:CE1	2.12	0.84
2:H:844:MET:HE1	2:H:922:CYS:HB3	1.70	0.72
1:G:208:LYS:NZ	1:G:210:GLU:OE2	2.24	0.70
1:D:929:SER:HA	1:D:954:MET:CE	2.27	0.65
1:G:1047:TRP:HZ3	1:G:1132:VAL:HG13	1.61	0.64
2:E:867:LEU:HD21	2:E:1031:PRO:HG3	1.80	0.63
1:A:907:ASN:HB2	2:B:730:ILE:HG22	1.81	0.62
1:D:364:VAL:HG22	1:D:375:LEU:HD13	1.82	0.61
1:A:983:ALA:HB1	1:A:989:ARG:HH11	1.65	0.61
2:B:867:LEU:HD11	2:B:1031:PRO:HG3	1.83	0.61
2:H:844:MET:HE1	2:H:922:CYS:CB	2.30	0.60
1:D:816:LEU:HD13	1:D:831:VAL:HG22	1.83	0.60
1:G:770:LEU:HD21	1:G:865:GLU:HB2	1.84	0.59
1:D:726:TYR:HE1	1:D:796:GLN:OE1	1.86	0.59
1:G:366:ASP:OD2	1:G:371:GLY:N	2.30	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1023:PRO:HB3	1:G:1047:TRP:CE2	2.39	0.58
1:G:43:VAL:HG23	1:G:52:VAL:HG21	1.83	0.58
1:G:1080:ARG:HD3	2:H:825:GLU:HA	1.85	0.58
1:G:1047:TRP:CZ3	1:G:1132:VAL:HG13	2.37	0.57
1:G:7:VAL:HG12	1:G:1091:GLY:HA3	1.87	0.57
1:D:389:ILE:HD12	1:D:389:ILE:N	2.19	0.57
1:D:929:SER:HA	1:D:954:MET:HE3	1.85	0.57
1:D:925:ASP:OD1	1:D:926:LEU:N	2.38	0.57
1:D:709:LYS:HG2	1:D:710:LEU:N	2.20	0.57
1:G:889:ARG:HD3	1:G:901:THR:HG22	1.86	0.57
2:E:755:LEU:HD22	2:E:812:VAL:HG22	1.86	0.56
1:D:374:GLN:HG2	1:D:391:ARG:HB3	1.87	0.56
1:G:731:GLN:OE1	1:G:796:GLN:NE2	2.39	0.56
2:B:803:LYS:HG3	3:C:142:VAL:HG21	1.87	0.56
2:E:828:LEU:O	2:E:1034:PRO:HD2	2.06	0.56
1:D:851:PHE:HB3	1:D:858:LEU:HD22	1.87	0.55
1:G:112:ILE:HD13	2:H:986:PHE:CE2	2.41	0.55
2:H:823:LEU:HD12	2:H:867:LEU:HD23	1.87	0.55
2:H:842:GLN:HG3	2:H:1025:LEU:HD11	1.88	0.55
1:A:375:LEU:HB2	1:A:1012:LEU:HD21	1.89	0.55
1:D:207:TRP:HB3	1:D:242:GLY:HA2	1.89	0.55
2:H:722:ARG:HE	2:H:726:LYS:HG3	1.71	0.55
1:D:726:TYR:CE1	1:D:796:GLN:OE1	2.60	0.55
2:E:879:GLY:O	2:E:880:LEU:HB2	2.08	0.54
1:D:60:LYS:O	1:D:81:THR:HA	2.08	0.54
1:D:796:GLN:HG3	1:D:797:HIS:NE2	2.22	0.53
1:A:6:VAL:HG22	1:A:1040:VAL:HG22	1.90	0.53
1:G:322:VAL:HG21	1:G:336:LEU:HD11	1.90	0.53
2:B:841:LYS:HD2	2:B:1023:VAL:HB	1.91	0.53
1:A:953:TRP:CE3	2:B:827:GLY:HA2	2.44	0.53
1:A:36:ASN:O	1:A:37:THR:OG1	2.23	0.53
1:A:990:GLN:OE1	2:B:740:GLN:NE2	2.39	0.53
1:G:768:SER:OG	1:G:863:GLU:OE2	2.19	0.53
1:A:889:ARG:HD2	1:A:891:TYR:CZ	2.44	0.52
3:C:213:LEU:HD11	3:C:255:LEU:HD11	1.90	0.52
3:I:63:ARG:HE	3:I:123:LEU:HD21	1.74	0.52
2:E:888:GLU:HG2	2:E:888:GLU:O	2.10	0.52
1:A:791:LEU:HD23	1:A:858:LEU:HD21	1.92	0.51
1:D:288:GLU:HB2	1:D:298:LYS:HB2	1.92	0.51
2:H:906:LEU:HD21	2:H:913:TYR:CD2	2.46	0.51
1:A:1003:PHE:O	1:A:1032:THR:HA	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:784:ARG:O	2:B:874:LYS:HE2	2.11	0.50
1:G:36:ASN:O	1:G:37:THR:OG1	2.20	0.50
1:D:158:ARG:HE	2:E:987:SER:HB2	1.77	0.50
1:G:255:GLN:OE1	1:G:279:ARG:NH1	2.41	0.50
2:H:1010:THR:O	2:H:1014:THR:HG23	2.12	0.50
2:E:738:TYR:OH	2:E:774:GLU:OE1	2.29	0.50
1:D:378:CYS:SG	1:D:724:ILE:HB	2.52	0.50
1:D:18:CYS:HG	1:D:313:CYS:HG	1.59	0.50
1:G:979:LYS:C	1:G:981:SER:H	2.15	0.50
1:A:912:LEU:HD11	1:A:926:LEU:HD13	1.93	0.49
1:G:360:VAL:HG21	1:G:721:PRO:O	2.12	0.49
1:A:953:TRP:CZ2	2:B:1038:ASP:HB2	2.48	0.49
2:H:858:ARG:HH12	2:H:882:ARG:HD3	1.78	0.49
1:D:796:GLN:HE21	1:D:797:HIS:CE1	2.30	0.49
1:D:971:ALA:HB3	1:D:973:ASN:ND2	2.28	0.49
2:B:892:TYR:HB3	2:B:913:TYR:CZ	2.47	0.49
2:B:989:ILE:HG23	2:B:990:PRO:HD2	1.94	0.49
1:D:915:LYS:HE3	1:D:957:VAL:O	2.13	0.48
2:H:760:LEU:HD12	2:H:760:LEU:O	2.13	0.48
2:H:1027:LYS:HE2	2:H:1029:ALA:HB2	1.95	0.48
1:A:248:ILE:HG12	1:A:250:PRO:HD3	1.94	0.48
2:H:758:VAL:O	2:H:808:ALA:HB1	2.13	0.48
2:H:841:LYS:HD2	2:H:1023:VAL:HB	1.94	0.48
1:A:248:ILE:HD12	1:A:300:LEU:O	2.14	0.48
2:E:751:GLU:OE1	2:E:790:LYS:NZ	2.35	0.48
1:G:72:GLU:OE2	1:G:103:ARG:NH2	2.47	0.48
1:G:318:ASP:OD1	1:G:319:ASN:N	2.45	0.48
1:A:292:ASP:HB2	1:A:294:THR:HG22	1.96	0.48
1:G:159:LEU:HD21	1:G:164:VAL:HG21	1.94	0.48
1:A:59:GLY:HA2	1:A:1073:TRP:CZ3	2.49	0.48
1:G:43:VAL:HG23	1:G:52:VAL:CG2	2.44	0.48
1:A:950:ASN:HB2	1:A:994:GLU:OE2	2.14	0.47
1:A:226:PHE:CZ	1:A:287:LYS:HG2	2.49	0.47
1:A:318:ASP:OD1	1:A:319:ASN:N	2.46	0.47
1:D:5:TYR:HB2	1:D:1043:LEU:HD11	1.96	0.47
1:D:7:VAL:HG12	1:D:1091:GLY:HA3	1.96	0.47
1:D:929:SER:OG	1:D:948:ASP:HB3	2.13	0.47
1:A:931:LEU:HG	1:A:947:ARG:HG2	1.97	0.47
2:H:867:LEU:HD13	2:H:873:ILE:HD11	1.97	0.47
1:A:5:TYR:CE2	1:A:7:VAL:HG13	2.50	0.46
2:B:722:ARG:NH1	2:B:791:GLU:OE2	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:188:ARG:NH1	1:G:216:ALA:O	2.48	0.46
2:H:842:GLN:CG	2:H:1025:LEU:HD11	2.46	0.46
3:I:158:GLU:OE1	3:I:162:GLN:NE2	2.45	0.46
2:B:906:LEU:HD21	2:B:913:TYR:HD2	1.80	0.46
1:A:184:ASP:HB2	1:A:185:PRO:CD	2.46	0.46
1:A:255:GLN:HB2	1:A:279:ARG:HH22	1.80	0.46
1:A:971:ALA:HB3	1:A:973:ASN:HD22	1.81	0.46
2:B:1010:THR:O	2:B:1014:THR:HG23	2.16	0.46
1:G:20:THR:HG23	1:G:315:THR:OG1	2.16	0.46
1:G:125:ASP:OD1	1:G:127:GLU:N	2.43	0.46
1:A:709:LYS:HG2	1:A:710:LEU:N	2.30	0.45
1:D:374:GLN:HG2	1:D:391:ARG:CB	2.46	0.45
2:B:762:ASN:OD1	2:B:763:GLU:N	2.50	0.45
2:B:858:ARG:HH12	2:B:882:ARG:HD3	1.81	0.45
1:G:922:LEU:HD11	1:G:930:VAL:HG21	1.99	0.45
2:E:857:HIS:O	2:E:858:ARG:HB2	2.17	0.45
2:H:856:LEU:HD22	2:H:915:PRO:HA	1.98	0.45
2:B:760:LEU:HD12	2:B:760:LEU:O	2.16	0.45
1:D:18:CYS:SG	1:D:313:CYS:SG	3.13	0.45
1:A:1030:PHE:CZ	1:A:1038:GLY:HA3	2.52	0.45
3:C:76:ILE:HD12	3:C:198:SER:HB3	1.99	0.45
2:E:739:GLY:HA3	2:E:757:LYS:O	2.16	0.45
1:A:372:GLN:HG3	1:A:1014:MET:HG3	1.97	0.45
1:G:1061:VAL:HG11	1:G:1104:LYS:HB3	1.97	0.45
1:A:849:VAL:HG11	1:A:851:PHE:CZ	2.52	0.44
2:H:774:GLU:HG3	2:H:878:PHE:HB2	1.98	0.44
1:A:170:LEU:HD21	1:A:229:ALA:HB2	1.99	0.44
2:B:867:LEU:HD12	2:B:873:ILE:HD11	1.98	0.44
1:G:979:LYS:O	1:G:981:SER:N	2.49	0.44
1:G:998:PHE:CZ	1:G:1074:ARG:HD2	2.52	0.44
2:E:895:LYS:HG3	2:E:902:ARG:NH1	2.33	0.44
1:G:922:LEU:HD11	1:G:930:VAL:CG2	2.48	0.44
1:A:1020:THR:OG1	1:A:1021:SER:N	2.51	0.44
1:G:125:ASP:OD2	1:G:176:PRO:HB3	2.18	0.44
1:A:835:MET:HB2	1:A:845:GLN:HB2	2.00	0.43
2:E:844:MET:HE2	2:E:844:MET:HA	2.00	0.43
2:H:917:ILE:HG13	2:H:918:ASP:N	2.33	0.43
3:I:195:THR:CG2	3:I:257:LEU:HD11	2.48	0.43
2:B:894:ASN:OD1	2:B:909:GLY:HA2	2.18	0.43
2:B:1035:HIS:O	2:B:1038:ASP:OD1	2.36	0.43
1:D:375:LEU:HB2	1:D:1012:LEU:HD21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:903:CYS:CB	1:D:941:ASN:HA	2.48	0.43
1:G:5:TYR:CE2	1:G:7:VAL:HG13	2.53	0.43
1:A:7:VAL:HG12	1:A:1091:GLY:HA3	2.00	0.43
1:A:69:PRO:HD2	1:A:72:GLU:HG3	2.00	0.43
3:C:121:ARG:HD3	3:C:129:PHE:CG	2.54	0.43
2:E:865:ILE:HD12	2:E:925:ILE:HD13	2.00	0.43
1:G:965:PHE:O	1:G:976:VAL:HA	2.19	0.43
2:H:953:GLY:O	2:H:1003:LEU:HD11	2.19	0.43
2:E:803:LYS:HA	3:F:142:VAL:CG1	2.48	0.43
2:B:917:ILE:HG13	2:B:918:ASP:N	2.33	0.43
3:C:66:LEU:HD23	3:C:66:LEU:HA	1.89	0.43
1:G:191:LYS:HE2	1:G:193:TYR:CE1	2.53	0.43
1:G:207:TRP:HB3	1:G:242:GLY:HA2	2.01	0.43
1:A:936:LYS:HD2	1:A:943:GLU:OE1	2.19	0.43
2:E:741:VAL:HG22	2:E:756:LYS:HG2	2.01	0.43
2:H:817:ASP:HB2	2:H:868:ASN:HA	2.01	0.43
1:D:32:LEU:HD12	1:D:32:LEU:N	2.34	0.43
1:A:883:SER:HB2	1:A:911:ALA:HB3	1.99	0.43
1:A:958:GLU:HB2	1:A:1007:PHE:CB	2.49	0.43
2:B:763:GLU:CG	2:B:763:GLU:O	2.67	0.43
1:G:184:ASP:HB2	1:G:185:PRO:CD	2.48	0.43
3:C:121:ARG:HD3	3:C:129:PHE:CD1	2.54	0.43
1:D:849:VAL:HG11	1:D:851:PHE:CZ	2.54	0.43
1:D:971:ALA:HB3	1:D:973:ASN:HD22	1.82	0.43
1:G:971:ALA:HB3	1:G:973:ASN:HD22	1.84	0.43
1:D:1061:VAL:HG11	1:D:1104:LYS:HB3	2.01	0.42
2:E:738:TYR:OH	2:E:756:LYS:HD3	2.19	0.42
1:G:1023:PRO:HB3	1:G:1047:TRP:CZ2	2.53	0.42
1:G:1112:LEU:O	1:G:1123:GLU:HA	2.19	0.42
2:H:787:VAL:HB	2:H:875:LEU:O	2.19	0.42
2:E:867:LEU:HD13	2:E:873:ILE:CD1	2.49	0.42
1:A:123:ILE:HG21	1:A:168:LYS:HA	2.00	0.42
1:D:367:LEU:HD12	1:D:374:GLN:OE1	2.18	0.42
2:E:760:LEU:HD12	2:E:760:LEU:O	2.19	0.42
1:G:1054:MET:SD	1:G:1129:LEU:HD22	2.59	0.42
1:A:125:ASP:OD2	1:A:127:GLU:HB2	2.20	0.42
1:D:709:LYS:CG	1:D:710:LEU:N	2.82	0.42
1:D:881:LEU:HD21	1:D:921:ILE:HG21	2.01	0.42
1:D:929:SER:HA	1:D:954:MET:HE1	2.00	0.42
2:E:746:ASP:HB3	2:E:749:THR:OG1	2.20	0.42
1:G:213:GLU:HG2	1:G:215:GLU:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:775:THR:HG21	1:D:837:TYR:CE2	2.54	0.42
1:G:59:GLY:HA2	1:G:1073:TRP:CE3	2.54	0.42
1:G:975:PHE:HA	1:G:996:GLY:O	2.20	0.42
3:I:21:LYS:NZ	3:I:154:ASP:OD1	2.47	0.42
1:A:376:VAL:HG22	1:A:389:ILE:CD1	2.49	0.42
1:D:19:VAL:O	1:D:31:LEU:HD12	2.20	0.42
1:D:170:LEU:HD23	1:D:170:LEU:HA	1.90	0.42
1:D:883:SER:HB2	1:D:911:ALA:HB3	2.02	0.42
2:H:856:LEU:O	2:H:881:ALA:HA	2.20	0.42
1:A:886:SER:O	1:A:908:ASN:HB2	2.19	0.42
3:C:163:PHE:CZ	3:C:204:GLU:HG3	2.54	0.42
1:D:257:THR:O	1:D:275:ASP:HB2	2.20	0.42
1:D:363:CYS:O	1:D:375:LEU:HD12	2.20	0.42
1:D:213:GLU:HG2	1:D:215:GLU:H	1.85	0.42
2:E:1009:CYS:HA	2:E:1013:GLN:OE1	2.20	0.42
3:F:266:PRO:O	3:F:267:HIS:C	2.58	0.42
2:H:722:ARG:HH21	2:H:726:LYS:HB3	1.84	0.42
2:H:864:ASN:ND2	2:H:877:ASP:HB3	2.35	0.42
1:A:1080:ARG:HD3	2:B:825:GLU:HA	2.01	0.41
1:G:330:ASP:HA	1:G:355:ASN:HB3	2.01	0.41
2:E:893:TPO:HG22	2:E:893:TPO:O1P	2.20	0.41
2:B:996:LEU:O	2:B:1000:MET:HG3	2.20	0.41
1:D:376:VAL:HA	1:D:388:ARG:O	2.20	0.41
1:A:58:TYR:HB3	1:A:1073:TRP:CB	2.51	0.41
3:I:195:THR:HG21	3:I:257:LEU:HD11	2.03	0.41
1:A:151:GLU:OE1	1:A:153:LYS:HE2	2.20	0.41
3:F:25:TYR:HA	3:F:199:LEU:O	2.21	0.41
1:G:790:ASN:HA	1:G:805:HIS:O	2.20	0.41
1:D:63:VAL:O	1:D:79:ILE:HA	2.21	0.41
1:D:184:ASP:HB2	1:D:185:PRO:CD	2.51	0.41
1:D:248:ILE:HG12	1:D:250:PRO:HD3	2.03	0.41
1:D:3:TYR:HB3	1:D:1048:TYR:HB2	2.02	0.41
1:D:816:LEU:CD1	1:D:831:VAL:HG22	2.49	0.41
1:G:316:TYR:CE2	1:G:317:LEU:O	2.73	0.41
1:A:33:ILE:HD12	1:A:42:TYR:CE1	2.56	0.41
1:D:796:GLN:NE2	1:D:797:HIS:CE1	2.88	0.41
1:D:1057:ARG:HD3	1:D:1108:VAL:O	2.21	0.41
3:F:55:ARG:NH2	3:F:191:ASP:OD1	2.53	0.41
1:G:328:LEU:HA	1:G:358:PRO:HD3	2.02	0.41
1:A:1016:ASN:O	1:A:1017:LEU:HB2	2.20	0.41
2:B:760:LEU:HD12	2:B:760:LEU:C	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:GLU:HB3	1:A:101:ILE:HB	2.04	0.40
2:B:841:LYS:O	2:B:845:GLU:HB2	2.21	0.40
2:E:802:PHE:CB	3:F:146:ILE:HD11	2.51	0.40
1:G:762:SER:O	1:G:803:HIS:HA	2.21	0.40
2:E:724:VAL:O	2:E:724:VAL:HG22	2.22	0.40
1:D:190:VAL:O	1:D:209:GLN:HA	2.21	0.40
1:G:889:ARG:HD2	1:G:891:TYR:CZ	2.56	0.40
1:G:138:GLY:C	1:G:159:LEU:HB3	2.42	0.40
1:G:1057:ARG:HD3	1:G:1108:VAL:O	2.21	0.40
2:H:1037:GLN:HE21	2:H:1037:GLN:HB2	1.80	0.40
1:A:903:CYS:CB	1:A:941:ASN:HA	2.52	0.40
2:B:896:VAL:HG13	2:B:897:ILE:HG12	2.03	0.40

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:A:1131:LYS:NZ	1:G:293:GLY:O[2_565]	1.96	0.24
1:A:1021:SER:OG	1:G:287:LYS:O[2_565]	2.01	0.19

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	822/840 (98%)	801 (97%)	21 (3%)	0	100	100
1	D	823/840 (98%)	802 (97%)	20 (2%)	1 (0%)	51	83
1	G	822/840 (98%)	796 (97%)	25 (3%)	1 (0%)	51	83
2	B	324/344 (94%)	312 (96%)	11 (3%)	1 (0%)	41	74
2	E	326/344 (95%)	318 (98%)	8 (2%)	0	100	100
2	H	326/344 (95%)	318 (98%)	7 (2%)	1 (0%)	41	74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	C	246/271 (91%)	242 (98%)	4 (2%)	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	4181/4365 (96%)	4076 (98%)	101 (2%)	4 (0%)	51 83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	827	GLY
1	D	772	SER
2	B	800	LEU
1	G	980	ASP

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%)	718 (100%)	3 (0%)	91 96
1	D	722/728 (99%)	718 (99%)	4 (1%)	86 94
1	G	721/728 (99%)	719 (100%)	2 (0%)	92 97
2	B	294/308 (96%)	288 (98%)	6 (2%)	55 79
2	E	296/308 (96%)	293 (99%)	3 (1%)	76 88
2	H	296/308 (96%)	291 (98%)	5 (2%)	60 82
3	C	223/242 (92%)	221 (99%)	2 (1%)	78 89
3	F	223/242 (92%)	221 (99%)	2 (1%)	78 89
3	I	223/242 (92%)	221 (99%)	2 (1%)	78 89
All	All	3719/3834 (97%)	3690 (99%)	29 (1%)	81 91

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	209	GLN
1	A	766	SER
1	A	1014	MET
2	B	784	ARG
2	B	844	MET
2	B	860	ILE
2	B	896	VAL
2	B	897	ILE
2	B	899	LEU
3	C	231	TYR
3	C	244	VAL
1	D	766	SER
1	D	928	ARG
1	D	929	SER
1	D	930	VAL
2	E	728	ASP
2	E	897	ILE
2	E	1040	HIS
3	F	216	ARG
3	F	231	TYR
1	G	339	ASP
1	G	1013	VAL
2	H	883	LEU
2	H	896	VAL
2	H	897	ILE
2	H	1036	TRP
2	H	1037	GLN
3	I	142	VAL
3	I	231	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	189	HIS
1	G	189	HIS
2	H	851	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	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	TPO	B	893	2	8,10,11	1.21	0	10,14,16	1.38	1 (10%)
2	TPO	H	893	2	8,10,11	1.51	1 (12%)	10,14,16	1.30	1 (10%)
2	TPO	E	893	2	8,10,11	1.69	1 (12%)	10,14,16	1.16	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	-	1/9/11/13	-
2	TPO	H	893	2	-	5/9/11/13	-
2	TPO	E	893	2	-	4/9/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	893	TPO	P-O1P	3.45	1.61	1.50
2	H	893	TPO	CB-CA	2.67	1.59	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	893	TPO	P-OG1-CB	-3.08	113.91	123.21
2	E	893	TPO	P-OG1-CB	-2.15	116.72	123.21
2	H	893	TPO	O-C-CA	-2.13	119.21	124.78

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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
2	H	893	TPO	N-CA-CB-CG2
2	H	893	TPO	N-CA-CB-OG1
2	H	893	TPO	C-CA-CB-CG2
2	H	893	TPO	CG2-CB-OG1-P
2	H	893	TPO	CB-OG1-P-O3P
2	B	893	TPO	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

17 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	SO4	D	1201	-	4,4,4	0.13	0	6,6,6	0.18	0
4	SO4	A	1201	-	4,4,4	0.13	0	6,6,6	0.11	0
4	SO4	A	1202	-	4,4,4	0.17	0	6,6,6	0.22	0
4	SO4	C	301	-	4,4,4	0.13	0	6,6,6	0.13	0
4	SO4	H	1102	-	4,4,4	0.16	0	6,6,6	0.16	0
4	SO4	I	302	-	4,4,4	0.13	0	6,6,6	0.11	0
5	RUW	B	1101	-	25,28,28	2.11	3 (12%)	25,36,36	1.72	6 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	RUW	E	1101	-	25,28,28	2.42	3 (12%)	25,36,36	1.82	7 (28%)
4	SO4	D	1202	-	4,4,4	0.12	0	6,6,6	0.15	0
5	RUW	H	1101	-	25,28,28	2.30	3 (12%)	25,36,36	1.76	5 (20%)
4	SO4	D	1203	-	4,4,4	0.15	0	6,6,6	0.14	0
4	SO4	G	1201	-	4,4,4	0.16	0	6,6,6	0.08	0
4	SO4	I	301	-	4,4,4	0.15	0	6,6,6	0.20	0
4	SO4	G	1202	-	4,4,4	0.11	0	6,6,6	0.15	0
4	SO4	C	302	-	4,4,4	0.16	0	6,6,6	0.12	0
4	SO4	A	1203	-	4,4,4	0.16	0	6,6,6	0.10	0
4	SO4	F	301	-	4,4,4	0.13	0	6,6,6	0.08	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	RUW	E	1101	-	-	15/21/21/21	0/2/2/2
5	RUW	B	1101	-	-	16/21/21/21	0/2/2/2
5	RUW	H	1101	-	-	13/21/21/21	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1101	RUW	C5-N6	9.60	1.47	1.34
5	H	1101	RUW	C5-N6	9.02	1.46	1.34
5	B	1101	RUW	C5-N6	7.25	1.44	1.34
5	B	1101	RUW	C4-N1	6.73	1.46	1.34
5	E	1101	RUW	C4-N1	6.39	1.46	1.34
5	H	1101	RUW	C4-N1	6.33	1.46	1.34
5	E	1101	RUW	C9-N5	-2.33	1.45	1.49
5	H	1101	RUW	C9-N5	-2.22	1.45	1.49
5	B	1101	RUW	C9-N5	-2.11	1.46	1.49

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	1101	RUW	C5-N3-C6	5.60	121.64	115.28
5	H	1101	RUW	C5-N3-C6	5.55	121.58	115.28
5	B	1101	RUW	C5-N3-C6	5.07	121.03	115.28
5	E	1101	RUW	N3-C5-N2	-3.61	120.51	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	1101	RUW	N3-C5-N2	-3.34	120.94	126.23
5	B	1101	RUW	C3-N1-C4	-3.26	117.40	122.89
5	E	1101	RUW	C3-N1-C4	-3.22	117.47	122.89
5	H	1101	RUW	C6-C7-N4	-2.80	106.48	109.40
5	B	1101	RUW	C6-C7-N4	-2.64	106.64	109.40
5	B	1101	RUW	N3-C5-N2	-2.59	122.13	126.23
5	B	1101	RUW	C5-N6-C12	-2.48	120.13	124.31
5	E	1101	RUW	C6-C7-N4	-2.47	106.83	109.40
5	H	1101	RUW	C3-N1-C4	-2.14	119.28	122.89
5	E	1101	RUW	N6-C5-N2	2.04	120.24	117.18
5	E	1101	RUW	C5-N2-C4	2.03	121.04	116.39
5	E	1101	RUW	O1-C13-C12	-2.01	106.74	111.95
5	B	1101	RUW	O1-C13-C12	-2.01	106.76	111.95
5	H	1101	RUW	C5-N6-C12	-2.01	120.92	124.31

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1101	RUW	C7-C4-N1-C3
5	B	1101	RUW	C14-C12-C13-O1
5	B	1101	RUW	N6-C12-C13-O1
5	B	1101	RUW	C13-C12-C14-C15
5	B	1101	RUW	N6-C12-C14-C15
5	B	1101	RUW	N2-C5-N6-C12
5	B	1101	RUW	N3-C5-N6-C12
5	B	1101	RUW	C10-C9-N5-C6
5	B	1101	RUW	C10-C9-N5-C8
5	E	1101	RUW	C7-C4-N1-C3
5	E	1101	RUW	C13-C12-C14-C15
5	E	1101	RUW	N2-C5-N6-C12
5	E	1101	RUW	N3-C5-N6-C12
5	E	1101	RUW	C11-C9-N5-C6
5	E	1101	RUW	C11-C9-N5-C8
5	H	1101	RUW	C13-C12-C14-C15
5	H	1101	RUW	N6-C12-C14-C15
5	H	1101	RUW	C13-C12-N6-C5
5	H	1101	RUW	N2-C5-N6-C12
5	H	1101	RUW	N3-C5-N6-C12
5	H	1101	RUW	C11-C9-N5-C6
5	H	1101	RUW	C11-C9-N5-C8
5	B	1101	RUW	C2-C1-C3-N1

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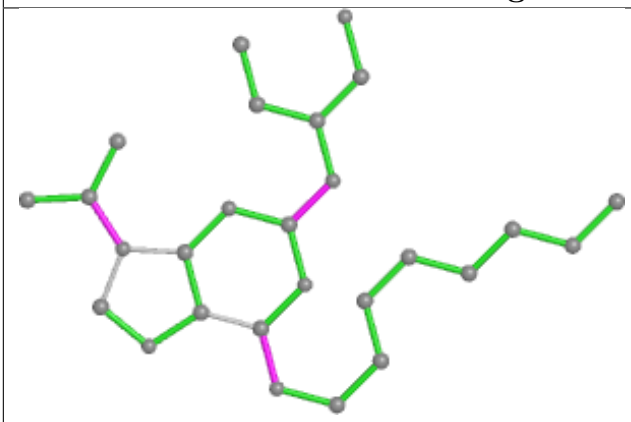
Mol	Chain	Res	Type	Atoms
5	H	1101	RUW	C2-C1-C3-N1
5	H	1101	RUW	C3-C1-C2-C16
5	B	1101	RUW	C3-C1-C2-C16
5	B	1101	RUW	N2-C4-N1-C3
5	E	1101	RUW	C2-C16-C17-C18
5	B	1101	RUW	C17-C18-C19-C20
5	H	1101	RUW	C17-C18-C19-C20
5	E	1101	RUW	C17-C18-C19-C20
5	E	1101	RUW	C3-C1-C2-C16
5	E	1101	RUW	N2-C4-N1-C3
5	B	1101	RUW	C11-C9-N5-C8
5	E	1101	RUW	C10-C9-N5-C8
5	H	1101	RUW	C10-C9-N5-C8
5	E	1101	RUW	N6-C12-C14-C15
5	E	1101	RUW	C16-C17-C18-C19
5	H	1101	RUW	C16-C17-C18-C19
5	B	1101	RUW	C16-C17-C18-C19
5	B	1101	RUW	C17-C16-C2-C1
5	E	1101	RUW	C13-C12-N6-C5
5	H	1101	RUW	C17-C16-C2-C1
5	E	1101	RUW	C17-C16-C2-C1

There are no ring outliers.

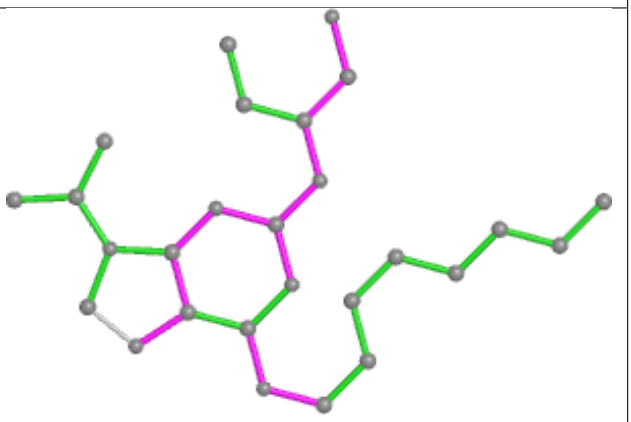
No monomer is involved in short contacts.

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.

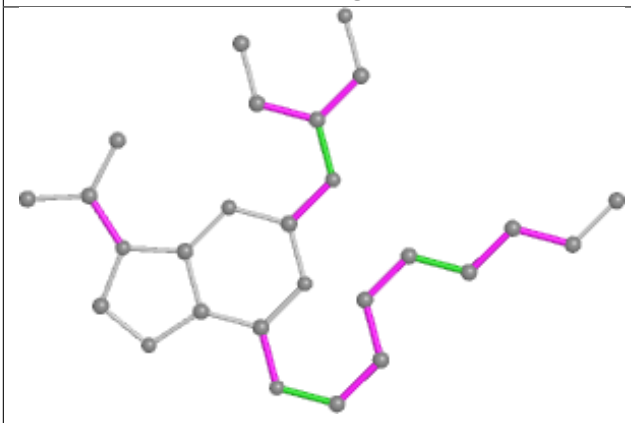
Ligand RUW B 1101



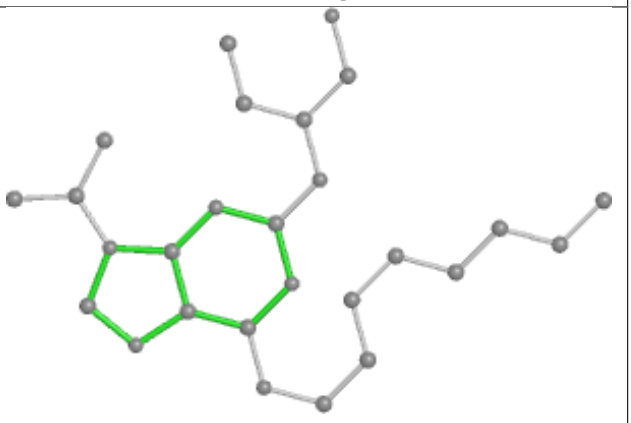
Bond lengths



Bond angles

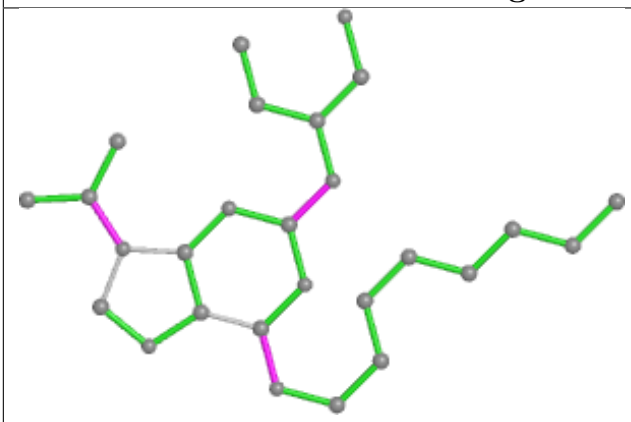


Torsions

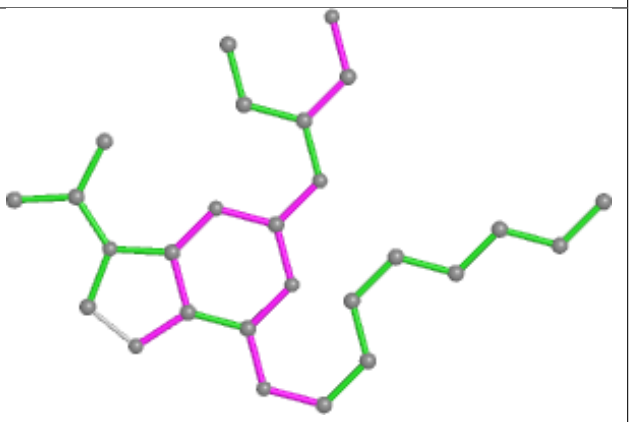


Rings

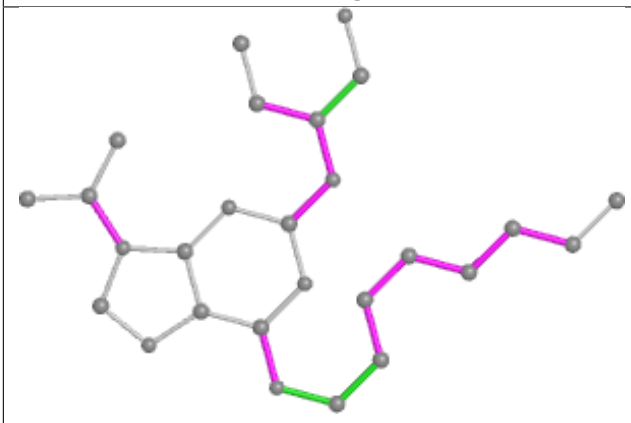
Ligand RUW E 1101



Bond lengths



Bond angles



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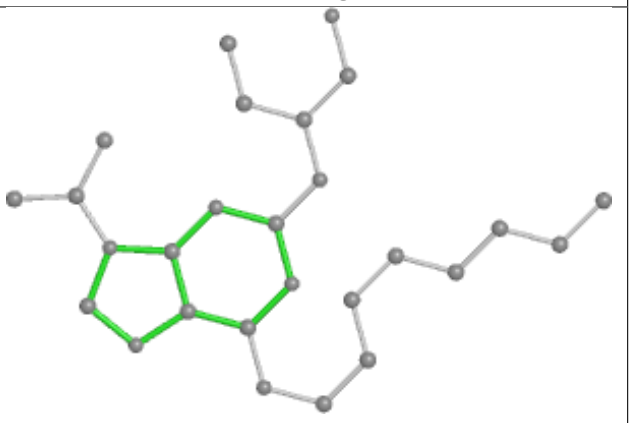
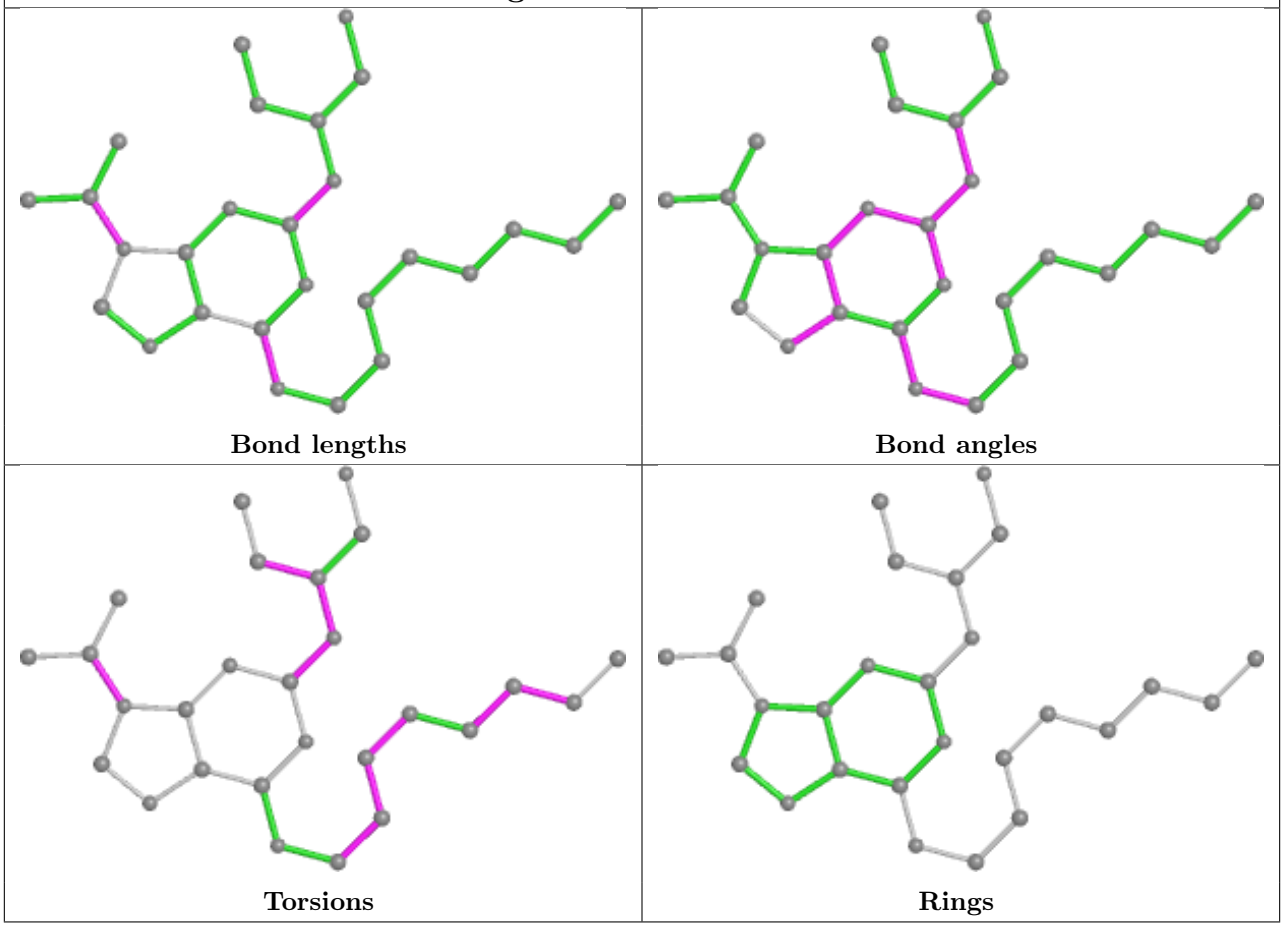


Rings

Ligand RUW H 1101



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, 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>2	OWAB(Å^2)	Q<0.9
1	A	826/840 (98%)	0.41	48 (5%) 23 14	112, 157, 228, 324	0
1	D	827/840 (98%)	0.33	32 (3%) 39 26	106, 152, 228, 310	0
1	G	826/840 (98%)	0.31	33 (3%) 38 25	113, 155, 232, 306	0
2	B	326/344 (94%)	0.45	20 (6%) 21 12	126, 163, 236, 285	0
2	E	328/344 (95%)	0.43	15 (4%) 32 21	116, 154, 230, 269	0
2	H	328/344 (95%)	0.48	9 (2%) 54 39	102, 137, 220, 294	0
3	C	248/271 (91%)	0.18	2 (0%) 86 75	118, 149, 195, 255	0
3	F	248/271 (91%)	0.26	0 100 100	104, 129, 180, 272	0
3	I	248/271 (91%)	0.32	3 (1%) 79 66	106, 132, 186, 252	0
All	All	4205/4365 (96%)	0.36	162 (3%) 39 26	102, 151, 227, 324	0

All (162) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	1043	TRP	7.7
2	B	826	SER	4.8
2	H	1043	TRP	4.7
1	G	133	LEU	3.8
1	A	1114	TYR	3.7
2	E	803	LYS	3.6
1	A	304	LEU	3.5
2	E	1040	HIS	3.5
1	D	928	ARG	3.4
2	B	800	LEU	3.4
1	A	1129	LEU	3.4
3	I	267	HIS	3.2
3	C	267	HIS	3.2
2	E	955	PRO	3.2
2	E	831	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	G	131	ILE	3.1
2	H	1036	TRP	3.1
2	E	802	PHE	3.1
2	B	896	VAL	3.1
2	B	802	PHE	3.0
1	G	816	LEU	3.0
1	A	120	ILE	3.0
1	D	328	LEU	3.0
1	A	1029	LEU	2.9
2	B	1039	CYS	2.9
2	B	876	ALA	2.9
1	A	1118	SER	2.9
2	E	1039	CYS	2.9
2	E	1036	TRP	2.8
1	G	851	PHE	2.8
1	A	133	LEU	2.8
1	A	933	LEU	2.8
1	D	1007	PHE	2.8
2	B	831	PHE	2.8
1	D	733	PHE	2.7
1	D	237	ILE	2.7
3	I	266	PRO	2.7
1	D	390	ILE	2.7
1	A	297	LEU	2.7
1	A	880	LEU	2.6
1	G	966	LEU	2.6
1	A	272	LEU	2.6
1	D	49	LEU	2.6
1	A	57	MET	2.6
1	G	792	LEU	2.5
1	A	1097	PHE	2.5
1	G	733	PHE	2.5
1	G	328	LEU	2.5
1	A	1008	CYS	2.5
1	D	140	PHE	2.5
1	G	1097	PHE	2.5
2	B	930	PHE	2.5
2	B	756	LYS	2.5
2	B	988	PHE	2.5
2	H	1031	PRO	2.5
2	B	929	LEU	2.5
1	A	967	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	77	LEU	2.5
1	A	131	ILE	2.4
2	B	825	GLU	2.4
1	G	140	PHE	2.4
1	D	375	LEU	2.4
1	A	121	ILE	2.4
1	D	1030	PHE	2.4
1	D	1040	VAL	2.4
1	D	1097	PHE	2.4
2	H	955	PRO	2.4
1	G	830	ILE	2.4
2	E	913	TYR	2.4
1	D	33	ILE	2.4
1	A	966	LEU	2.4
1	A	974	LEU	2.4
1	A	64	MET	2.4
1	G	1129	LEU	2.4
1	D	944	GLU	2.4
1	G	390	ILE	2.4
1	D	39	LEU	2.3
1	D	317	LEU	2.3
2	E	839	PHE	2.3
1	G	911	ALA	2.3
1	G	387	LEU	2.3
1	G	139	LEU	2.3
1	A	61	ILE	2.3
1	G	124	ILE	2.3
1	A	367	LEU	2.3
1	G	914	LEU	2.3
1	D	736	LEU	2.3
2	E	738	TYR	2.3
2	E	875	LEU	2.3
1	A	273	LEU	2.3
1	A	232	ILE	2.3
1	G	291	MET	2.3
1	G	858	LEU	2.3
3	I	153	PHE	2.3
1	A	170	LEU	2.3
2	H	873	ILE	2.3
1	G	1088	PHE	2.3
1	D	64	MET	2.2
1	A	1079	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	H	977	GLN	2.2
1	D	880	LEU	2.2
1	A	237	ILE	2.2
2	B	803	LYS	2.2
2	B	932	LYS	2.2
1	A	248	ILE	2.2
1	A	306	GLY	2.2
1	G	132	GLY	2.2
1	G	280	LEU	2.2
1	A	169	PHE	2.2
2	H	839	PHE	2.2
1	A	926	LEU	2.2
1	A	283	LEU	2.2
2	E	865	ILE	2.2
1	D	5	TYR	2.2
1	A	387	LEU	2.2
1	A	957	VAL	2.2
1	A	1016	ASN	2.2
1	A	135	LEU	2.2
1	G	179	CYS	2.2
1	A	23	PHE	2.2
1	G	829	PHE	2.2
1	D	922	LEU	2.1
1	G	881	LEU	2.1
1	A	140	PHE	2.1
1	D	91	TYR	2.1
2	B	829	VAL	2.1
2	H	890	ARG	2.1
1	A	300	LEU	2.1
2	E	1041	GLU	2.1
2	H	875	LEU	2.1
1	G	180	PHE	2.1
1	D	813	ALA	2.1
1	G	799	PHE	2.1
2	B	886	SER	2.1
1	A	1035	GLY	2.1
1	G	100	ILE	2.1
1	D	974	LEU	2.1
1	A	1051	LEU	2.1
1	D	1010	GLY	2.1
1	G	314	LEU	2.1
1	A	229	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	232	ILE	2.1
2	B	865	ILE	2.1
1	D	881	LEU	2.1
1	D	932	LEU	2.1
2	B	776	LYS	2.0
1	A	285	LEU	2.0
1	D	273	LEU	2.0
2	B	781	LEU	2.0
1	D	882	ALA	2.0
1	A	1115	ASP	2.0
1	D	367	LEU	2.0
1	A	928	ARG	2.0
1	D	272	LEU	2.0
1	G	974	LEU	2.0
3	C	132	PHE	2.0
1	A	60	LYS	2.0
1	G	282	MET	2.0
1	G	302	VAL	2.0
1	A	1088	PHE	2.0
2	B	955	PRO	2.0
2	E	882	ARG	2.0

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	B-factors(Å^2)	Q<0.9
2	TPO	E	893	11/12	0.72	0.20	206,238,287,299	6
2	TPO	B	893	11/12	0.78	0.16	193,228,280,280	6
2	TPO	H	893	11/12	0.85	0.26	121,181,204,221	6

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

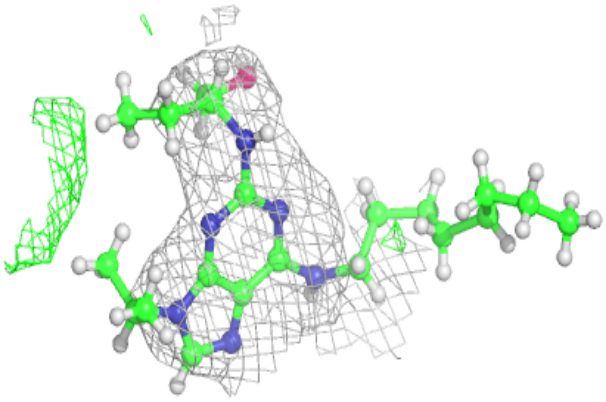
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

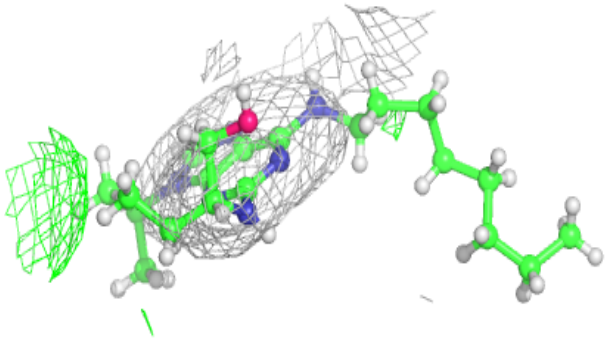
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	G	1201	5/5	0.65	0.29	147,159,180,230	0
4	SO4	D	1203	5/5	0.75	0.21	157,172,197,251	0
4	SO4	C	302	5/5	0.79	0.25	186,188,196,261	0
4	SO4	A	1202	5/5	0.79	0.20	148,156,170,212	0
4	SO4	C	301	5/5	0.79	0.23	130,148,174,211	0
4	SO4	D	1202	5/5	0.80	0.18	148,167,174,236	0
4	SO4	I	302	5/5	0.83	0.20	100,151,161,185	0
4	SO4	H	1102	5/5	0.85	0.18	182,188,196,259	0
4	SO4	A	1201	5/5	0.85	0.16	160,169,195,236	0
4	SO4	I	301	5/5	0.86	0.13	166,167,185,234	0
4	SO4	D	1201	5/5	0.86	0.16	155,155,176,226	0
4	SO4	G	1202	5/5	0.89	0.12	165,172,196,246	0
5	RUW	E	1101	27/27	0.89	0.62	116,164,189,197	43
5	RUW	H	1101	27/27	0.89	0.65	115,161,184,211	43
5	RUW	B	1101	27/27	0.90	0.69	127,167,205,220	43
4	SO4	F	301	5/5	0.93	0.22	116,134,163,180	0
4	SO4	A	1203	5/5	0.94	0.10	178,191,195,252	0

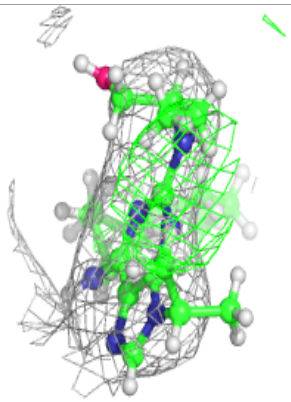
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around RUW 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)

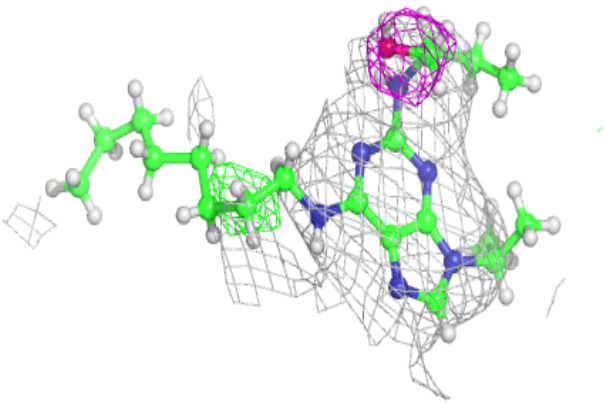


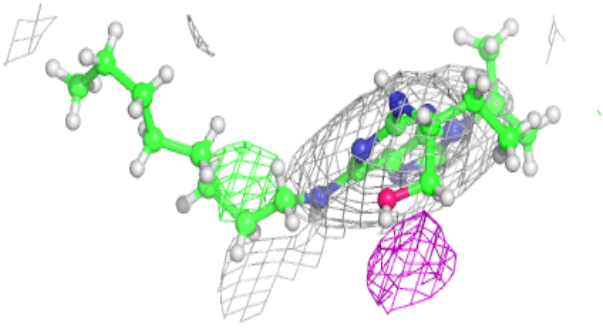


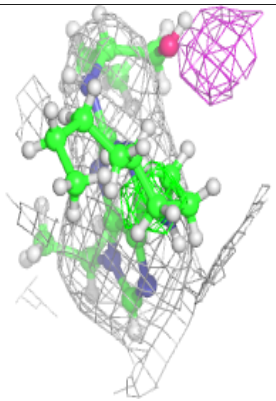


Electron density around RUW H 1101:

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

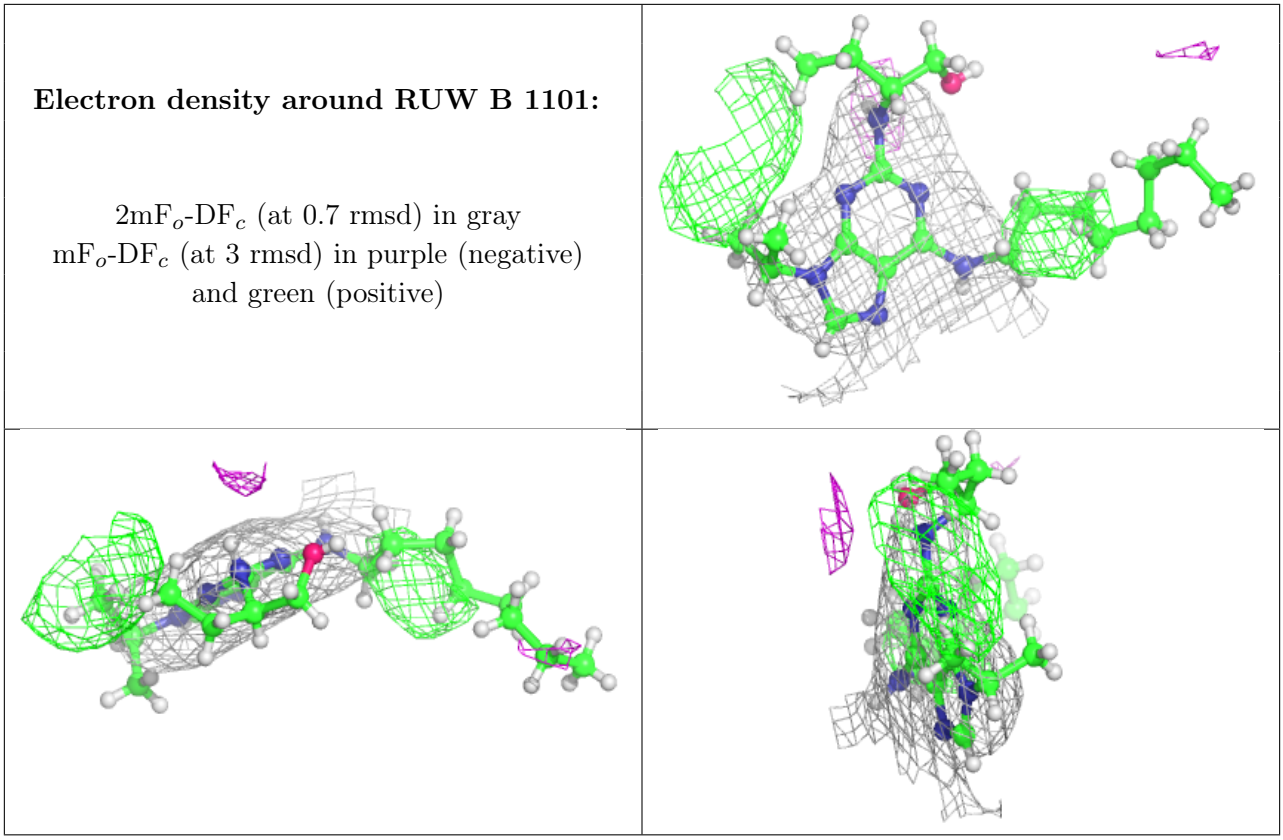






Electron density around RUW B 1101:

$2mF_o$-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.