Full wwPDB X-ray Structure Validation Report ⓘ

Sep 7, 2023 – 07:59 pm BST

PDB ID	:	8BUS
Title	:	Structure of DDB1 bound to DS59-engaged CDK12-cyclin K
Authors	:	Kozicka, Z.; Kempf, G.; Focht, V.; Thoma, N.H.
Deposited on	:	2022-11-30
Resolution	:	3.26 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

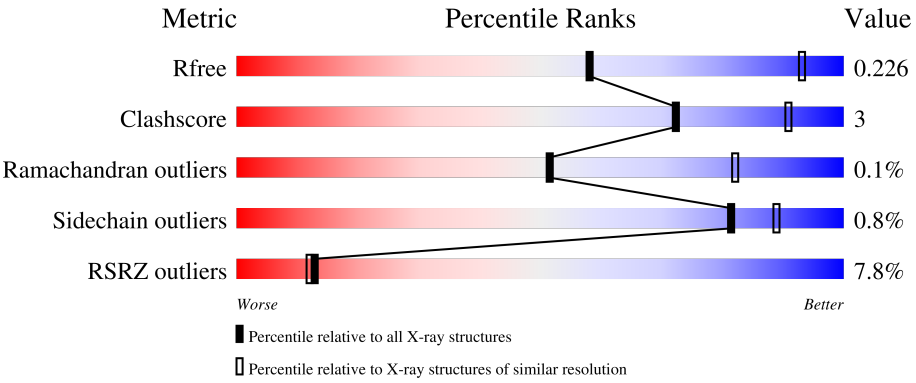
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 3.26 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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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	5% 88% 11% ·
1	D	840	9% 88% 10% ·
1	G	840	8% 84% 14% ·
2	B	344	12% 84% 9% · 6%
2	E	344	14% 87% 8% ·

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Mol	Chain	Length	Quality of chain
2	H	344	7% 89% 7%
3	C	271	% 88% 8%
3	F	271	4% 87% 8%
3	I	271	4% 86% 6% 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
2	TPO	H	893	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 67538 atoms, of which 33668 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	D	826	Total	C	H	N	O	S	6451	0	0
			12938	4105	6451	1094	1252	36			
1	A	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	6453	0	0
			12939	4106	6453	1093	1251	36			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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	E	329	Total	C	H	N	O	P	S	2698	0	0
			5385	1723	2698	454	492	1	17			
2	B	325	Total	C	H	N	O	P	S	2664	0	0
			5310	1695	2664	447	486	1	17			
2	H	330	Total	C	H	N	O	P	S	2703	0	0
			5396	1726	2703	455	494	1	17			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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	F	248	Total	C	H	N	O	S	2049	0	0
			4112	1341	2049	346	363	13			

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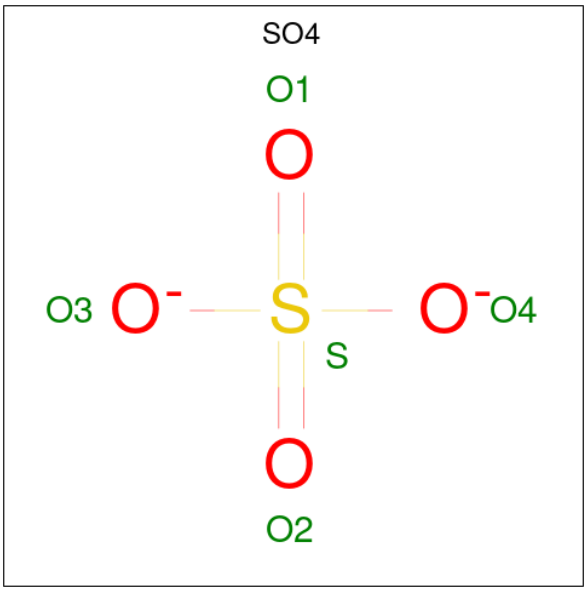
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	248	Total	C	H	N	O	S	2049	0	0
			4112	1341	2049	346	363	13			
3	I	248	Total	C	H	N	O	S	2049	0	0
			4112	1341	2049	346	363	13			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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	D	1	Total	O	S	0	0
			5	4	1		

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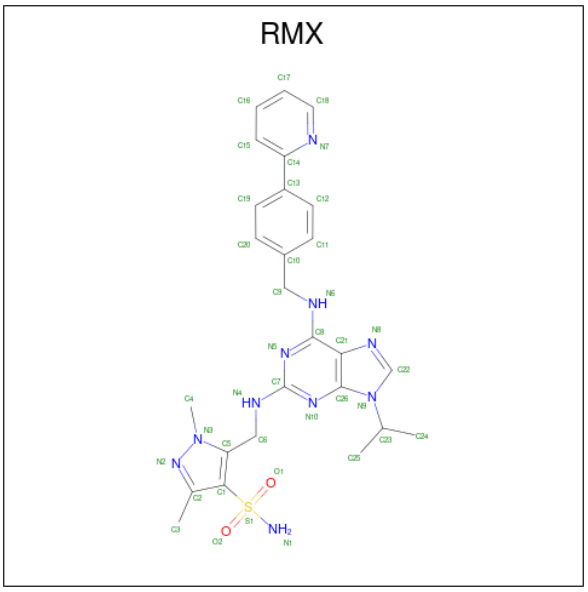
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0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

- Molecule 5 is 1,3-dimethyl-5-[[[9-propan-2-yl-6-[(4-pyridin-2-ylphenyl)methylamino]purin-2-yl]amino]methyl]pyrazole-4-sulfonamide (three-letter code: RMX) (formula: $C_{26}H_{30}N_{10}O_2S$) (labeled as "Ligand of Interest" by depositor).



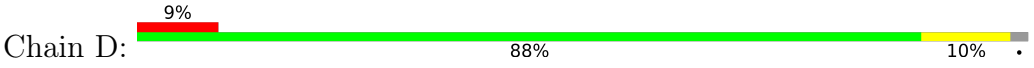
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	E	1	Total	C	H	N	O	S	30	0
			69	26	30	10	2	1		
5	B	1	Total	C	H	N	O	S	30	0
			69	26	30	10	2	1		
5	H	1	Total	C	H	N	O	S	30	0
			69	26	30	10	2	1		

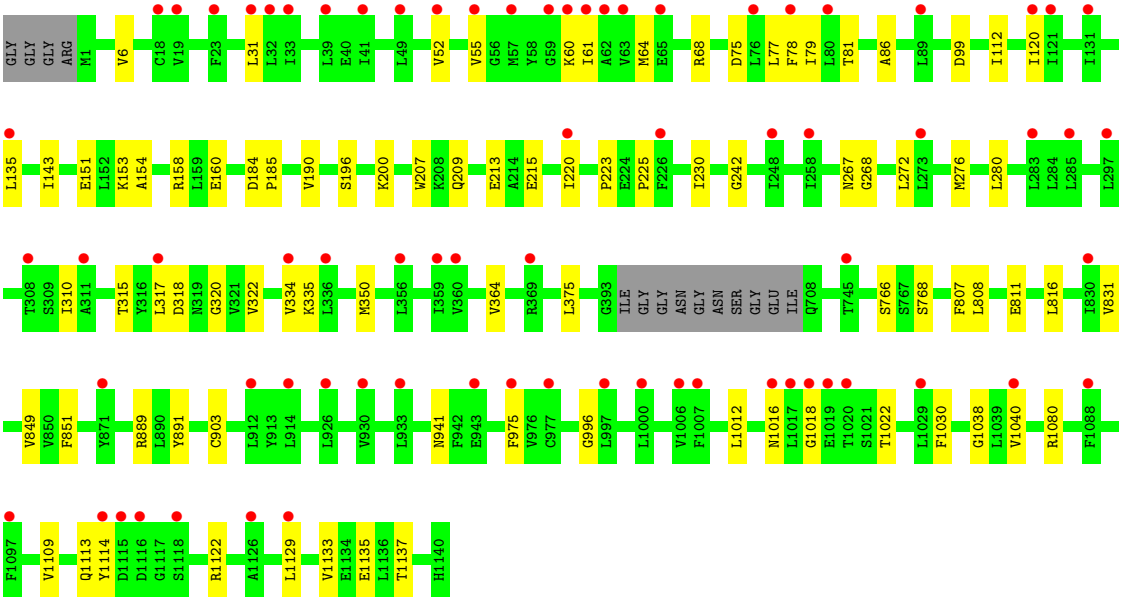
3 Residue-property plots (i)

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

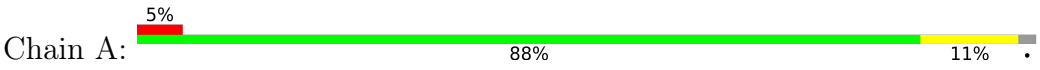
Chain D:

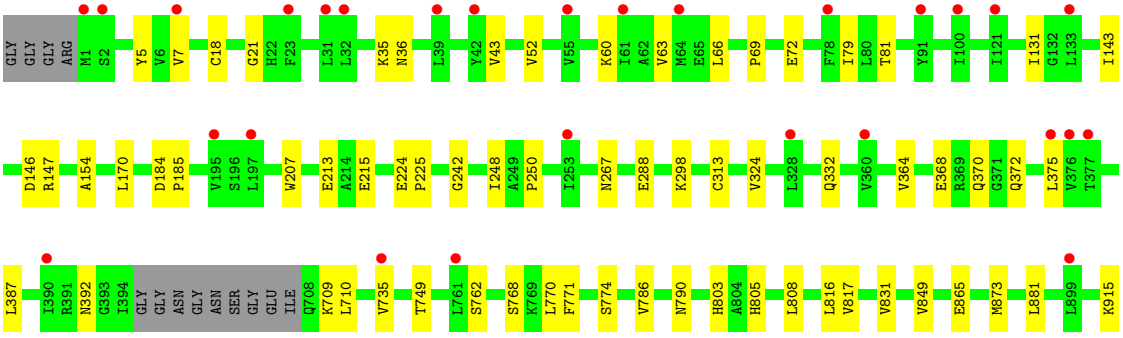


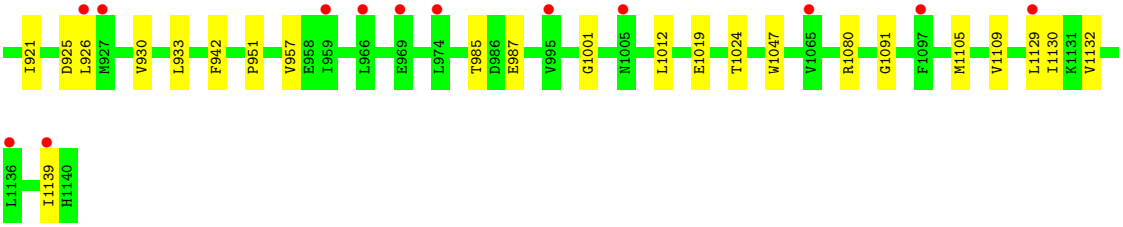


• Molecule 1: DNA damage-binding protein 1

Chain A:

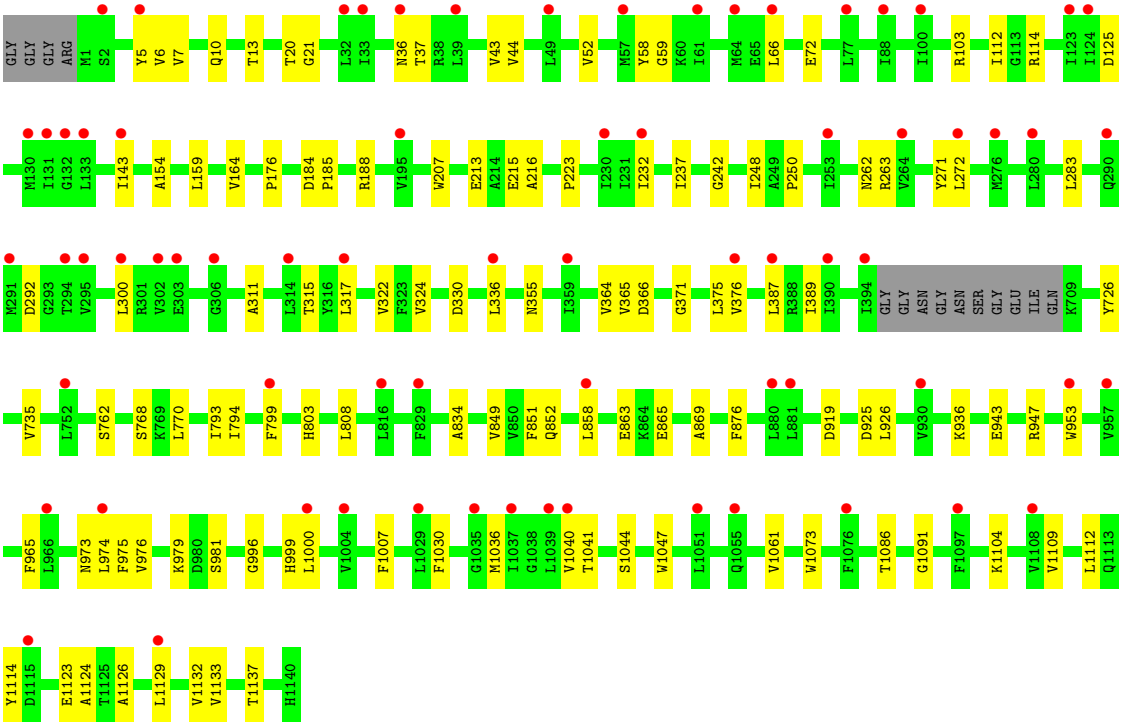






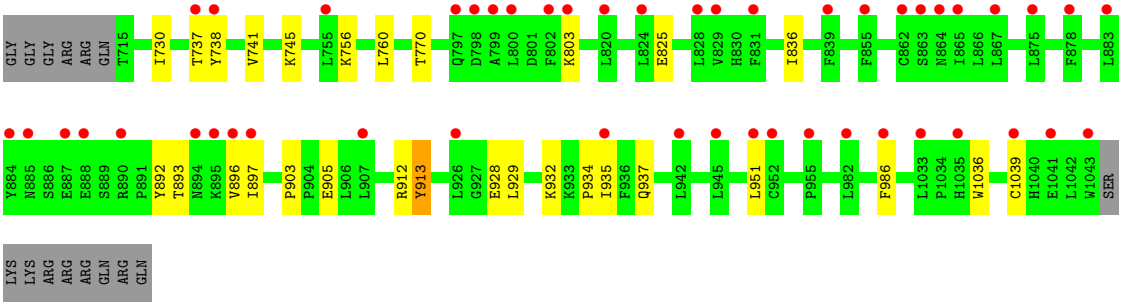
• Molecule 1: DNA damage-binding protein 1

Chain G:



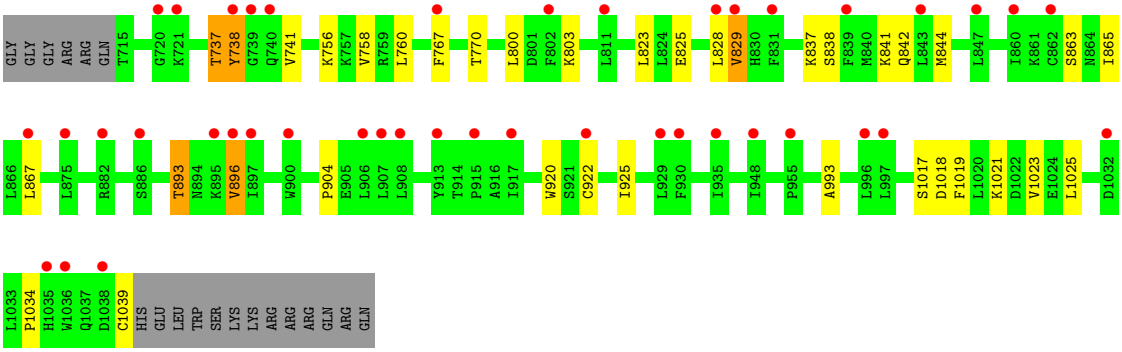
• Molecule 2: Cyclin-dependent kinase 12

Chain E:

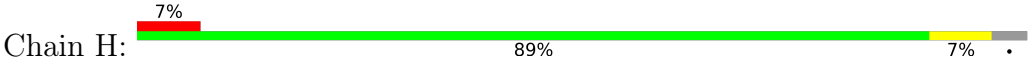


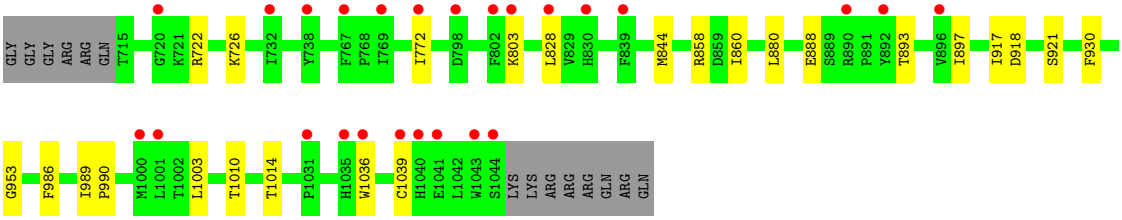
• Molecule 2: Cyclin-dependent kinase 12

Chain B:

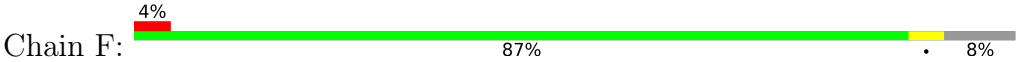


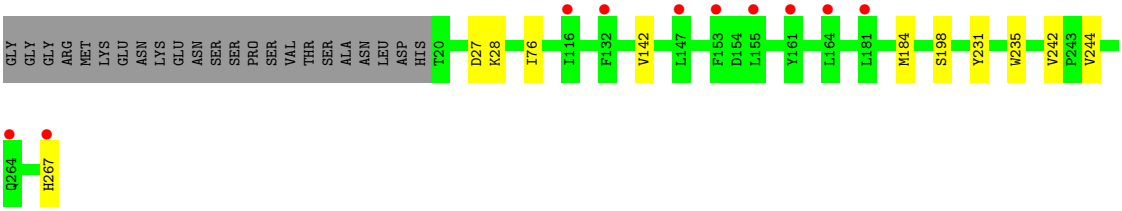
• Molecule 2: Cyclin-dependent kinase 12



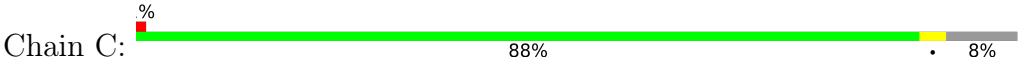


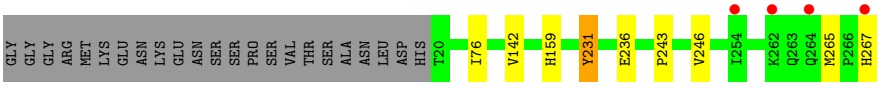
• Molecule 3: Cyclin-K



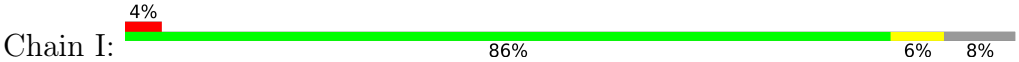


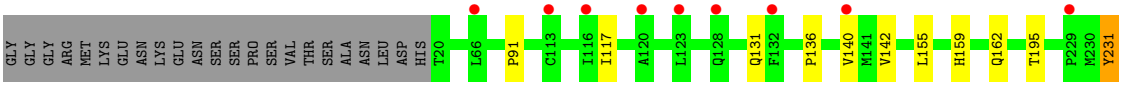
• Molecule 3: Cyclin-K

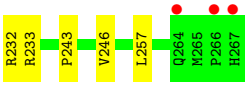




• Molecule 3: Cyclin-K






R232
R233
P243
V246
L257
Q264
M265
P266
H267

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	249.52Å 249.52Å 218.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	60.40 – 3.26 216.09 – 3.26	Depositor EDS
% Data completeness (in resolution range)	83.2 (60.40-3.26) 83.2 (216.09-3.26)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 3.26Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.208 , 0.228 0.208 , 0.226	Depositor DCC
R_{free} test set	5017 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	119.1	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 78.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.034 for -h,-k,l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	67538	wwPDB-VP
Average B, all atoms (Å^2)	142.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.62% 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: SO4, TPO, RMX

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	0.28	0/6612	0.54	0/8942
1	D	0.28	0/6604	0.55	0/8931
1	G	0.28	0/6603	0.54	0/8930
2	B	0.29	0/2693	0.57	0/3630
2	E	0.30	0/2737	0.58	0/3691
2	H	0.28	0/2743	0.52	0/3699
3	C	0.28	0/2120	0.48	0/2868
3	F	0.27	0/2120	0.47	0/2868
3	I	0.28	0/2120	0.50	0/2868
All	All	0.28	0/34352	0.54	0/46427

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6495	6462	6464	49	0
1	D	6487	6451	6451	43	1
1	G	6486	6453	6454	66	1
2	B	2646	2664	2662	25	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	2687	2698	2696	14	0
2	H	2693	2703	2702	15	0
3	C	2063	2049	2048	5	0
3	F	2063	2049	2048	8	0
3	I	2063	2049	2048	13	1
4	A	5	0	0	0	0
4	C	10	0	0	0	0
4	D	15	0	0	0	0
4	F	10	0	0	0	0
4	G	10	0	0	0	0
4	H	5	0	0	0	0
4	I	15	0	0	0	0
5	B	39	30	0	0	0
5	E	39	30	0	0	0
5	H	39	30	0	0	0
All	All	33870	33668	33573	226	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 (226) 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:G:953:TRP:CH2	2:H:828:LEU:HD11	2.25	0.71
2:E:741:VAL:HG22	2:E:756:LYS:HG2	1.70	0.71
1:D:225:PRO:HG2	1:D:267:ASN:HB2	1.76	0.67
1:G:322:VAL:HG21	1:G:336:LEU:HD11	1.77	0.66
1:G:7:VAL:HG22	1:G:1091:GLY:HA3	1.80	0.64
2:E:738:TYR:HD2	2:E:770:THR:HG1	1.48	0.61
1:A:816:LEU:HD13	1:A:831:VAL:HG22	1.83	0.60
2:H:844:MET:HA	2:H:844:MET:HE2	1.84	0.60
1:D:272:LEU:HD22	1:D:280:LEU:HD11	1.84	0.60
1:A:771:PHE:O	1:A:774:SER:HB2	2.03	0.59
3:C:231:TYR:OH	3:C:236:GLU:OE1	2.22	0.58
1:G:159:LEU:HD21	1:G:164:VAL:HG21	1.86	0.58
3:I:117:ILE:HG21	3:I:136:PRO:CB	2.33	0.58
1:A:7:VAL:HG22	1:A:1091:GLY:HA3	1.85	0.58
2:H:1010:THR:O	2:H:1014:THR:HG23	2.03	0.57
1:A:375:LEU:HB2	1:A:1012:LEU:HD21	1.87	0.57
1:A:770:LEU:HD13	1:A:865:GLU:HB2	1.87	0.57
2:B:844:MET:HE3	2:B:922:CYS:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:834:ALA:HB2	1:G:869:ALA:HA	1.88	0.56
2:B:893:TPO:O	2:B:896:VAL:HG13	2.06	0.56
1:A:372:GLN:NE2	1:A:392:ASN:O	2.39	0.55
1:G:858:LEU:HD12	1:G:858:LEU:O	2.06	0.55
1:D:1022:THR:HG22	1:D:1135:GLU:OE2	2.06	0.55
1:D:6:VAL:HG22	1:D:1040:VAL:HG22	1.89	0.55
3:F:235:TRP:CZ2	3:F:244:VAL:HG22	2.41	0.55
1:G:271:TYR:HB2	1:G:283:LEU:HB3	1.87	0.55
2:H:722:ARG:HE	2:H:726:LYS:HG3	1.71	0.55
3:C:243:PRO:HG2	3:C:246:VAL:HG23	1.89	0.55
2:E:803:LYS:HG3	3:F:142:VAL:HG21	1.90	0.54
2:E:951:LEU:HD21	2:E:986:PHE:HE2	1.73	0.54
2:B:993:ALA:HB2	2:B:1019:PHE:CE1	2.43	0.54
1:A:18:CYS:HG	1:A:313:CYS:HG	1.54	0.53
2:H:989:ILE:HG23	2:H:990:PRO:HD2	1.90	0.53
1:G:112:ILE:HD13	2:H:986:PHE:CE2	2.44	0.53
2:H:803:LYS:HA	3:I:142:VAL:HG11	1.91	0.53
1:A:21:GLY:HA3	1:A:66:LEU:HD13	1.90	0.52
1:G:262:ASN:O	1:G:272:LEU:N	2.31	0.52
2:B:738:TYR:HD2	2:B:770:THR:HG1	1.58	0.52
3:I:117:ILE:HG21	3:I:136:PRO:HB2	1.92	0.51
1:D:816:LEU:HD13	1:D:831:VAL:HG22	1.92	0.51
3:I:195:THR:CG2	3:I:257:LEU:HD11	2.40	0.51
1:A:207:TRP:HB3	1:A:242:GLY:HA2	1.92	0.51
1:A:1105:MET:SD	1:A:1130:ILE:HD11	2.50	0.51
1:D:889:ARG:HD2	1:D:891:TYR:CZ	2.45	0.51
1:D:1080:ARG:HD3	2:E:825:GLU:HA	1.92	0.51
3:I:91:PRO:HB3	3:I:131:GLN:HB3	1.92	0.51
1:A:213:GLU:HG2	1:A:215:GLU:H	1.75	0.51
1:G:5:TYR:HB3	1:G:1041:THR:HG23	1.93	0.51
1:A:925:ASP:OD1	1:A:926:LEU:N	2.44	0.51
1:G:925:ASP:OD1	1:G:926:LEU:N	2.44	0.50
2:B:1017:SER:O	2:B:1021:LYS:N	2.41	0.50
1:D:335:LYS:HB2	1:D:350:MET:SD	2.51	0.50
3:F:76:ILE:HD12	3:F:198:SER:HB3	1.93	0.50
1:A:288:GLU:HB2	1:A:298:LYS:HB2	1.93	0.50
1:D:768:SER:HB3	1:D:808:LEU:HD11	1.93	0.50
1:G:143:ILE:HG12	1:G:154:ALA:HB2	1.93	0.50
2:B:737:THR:OG1	2:B:738:TYR:N	2.45	0.50
2:H:772:ILE:HG23	3:I:155:LEU:HD13	1.94	0.50
1:D:364:VAL:HG22	1:D:375:LEU:HD13	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1061:VAL:HG11	1:G:1104:LYS:HB3	1.93	0.49
1:A:768:SER:HB3	1:A:808:LEU:HD11	1.94	0.49
1:G:20:THR:HG23	1:G:315:THR:OG1	2.13	0.49
1:D:112:ILE:HD13	2:E:986:PHE:CE2	2.48	0.49
3:F:76:ILE:CD1	3:F:198:SER:HB3	2.43	0.49
1:D:207:TRP:HB3	1:D:242:GLY:HA2	1.94	0.49
1:A:368:GLU:OE1	1:A:368:GLU:N	2.45	0.49
3:I:117:ILE:HG21	3:I:136:PRO:HB3	1.95	0.49
2:E:730:ILE:HD11	2:E:745:LYS:CG	2.42	0.49
1:D:223:PRO:HD2	1:D:268:GLY:HA3	1.95	0.49
1:G:72:GLU:OE2	1:G:103:ARG:NH2	2.47	0.48
1:G:365:VAL:HG21	1:G:726:TYR:CE2	2.48	0.48
3:F:27:ASP:OD1	3:F:28:LYS:N	2.47	0.48
1:D:375:LEU:HB2	1:D:1012:LEU:HD21	1.95	0.48
3:F:235:TRP:HZ2	3:F:244:VAL:HG22	1.78	0.48
1:A:709:LYS:HG2	1:A:710:LEU:N	2.29	0.48
1:G:974:LEU:HD11	1:G:1000:LEU:HD22	1.94	0.48
1:A:1047:TRP:HZ3	1:A:1132:VAL:HG13	1.78	0.48
1:G:1047:TRP:HZ3	1:G:1132:VAL:HG13	1.78	0.48
1:A:1080:ARG:HD3	2:B:825:GLU:HA	1.95	0.47
3:I:195:THR:HG21	3:I:257:LEU:HD11	1.95	0.47
2:B:865:ILE:HD12	2:B:925:ILE:HD13	1.97	0.47
2:B:841:LYS:HE2	2:B:1025:LEU:HD21	1.96	0.47
1:G:6:VAL:HG22	1:G:1040:VAL:HG22	1.96	0.47
3:F:242:VAL:HG12	3:F:242:VAL:O	2.14	0.47
1:A:224:GLU:N	1:A:225:PRO:HD2	2.30	0.47
1:A:324:VAL:HB	1:A:332:GLN:HB2	1.97	0.47
1:G:125:ASP:OD2	1:G:176:PRO:HB3	2.15	0.47
1:D:276:MET:HA	1:D:310:ILE:HG23	1.97	0.47
2:E:730:ILE:HD11	2:E:745:LYS:HG3	1.97	0.47
1:G:366:ASP:OD2	1:G:371:GLY:N	2.41	0.47
3:I:243:PRO:HG2	3:I:246:VAL:HG23	1.96	0.47
1:G:1109:VAL:HG11	1:G:1126:ALA:HA	1.95	0.47
1:G:979:LYS:O	1:G:981:SER:N	2.44	0.47
2:E:935:ILE:HD12	2:E:986:PHE:HZ	1.80	0.46
2:B:803:LYS:HG3	3:C:142:VAL:HG21	1.97	0.46
1:G:21:GLY:HA3	1:G:66:LEU:HD13	1.97	0.46
1:G:852:GLN:O	1:G:858:LEU:HA	2.15	0.46
2:B:893:TPO:O1P	2:B:893:TPO:HG22	2.15	0.46
1:D:143:ILE:HG12	1:D:154:ALA:HB2	1.97	0.46
1:A:915:LYS:HE3	1:A:957:VAL:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:232:ILE:HD13	1:G:237:ILE:HG23	1.97	0.46
1:G:936:LYS:HE3	1:G:943:GLU:OE1	2.16	0.45
3:I:117:ILE:HD11	3:I:140:VAL:HG21	1.97	0.45
1:D:1133:VAL:O	1:D:1137:THR:HG23	2.16	0.45
1:A:36:ASN:ND2	1:A:1001:GLY:O	2.46	0.45
2:H:858:ARG:NE	2:H:880:LEU:O	2.48	0.45
1:A:1109:VAL:HG12	1:A:1129:LEU:HD12	1.97	0.45
3:C:265:MET:HB2	3:C:267:HIS:ND1	2.31	0.45
1:G:248:ILE:HD12	1:G:300:LEU:O	2.16	0.45
1:G:58:TYR:HB3	1:G:1073:TRP:CB	2.46	0.45
1:G:213:GLU:HG2	1:G:215:GLU:H	1.81	0.45
1:A:370:GLN:C	1:A:372:GLN:H	2.20	0.45
1:G:114:ARG:HD3	2:H:930:PHE:O	2.17	0.45
1:G:975:PHE:HA	1:G:996:GLY:O	2.17	0.45
3:I:231:TYR:CE1	3:I:233:ARG:HB2	2.52	0.45
1:D:1016:ASN:C	1:D:1018:GLY:H	2.19	0.45
1:A:60:LYS:O	1:A:81:THR:HA	2.17	0.45
1:G:364:VAL:HG22	1:G:375:LEU:HD13	1.99	0.45
1:A:951:PRO:HG2	2:B:825:GLU:CB	2.47	0.44
1:G:10:GLN:O	1:G:1036:MET:HG2	2.17	0.44
1:A:63:VAL:O	1:A:79:ILE:HA	2.17	0.44
2:E:892:TYR:HB3	2:E:913:TYR:CZ	2.53	0.44
1:G:13:THR:HB	1:G:355:ASN:HA	1.99	0.44
1:A:146:ASP:OD1	1:A:147:ARG:N	2.51	0.44
1:A:248:ILE:HG12	1:A:250:PRO:HD3	1.99	0.44
1:D:196:SER:O	1:D:200:LYS:N	2.49	0.44
1:G:762:SER:O	1:G:803:HIS:HA	2.18	0.44
1:G:223:PRO:HG3	1:G:263:ARG:HH11	1.82	0.44
1:G:1112:LEU:O	1:G:1123:GLU:HA	2.17	0.44
1:D:64:MET:HG3	1:D:77:LEU:HD11	2.00	0.44
1:D:220:ILE:HB	1:D:230:ILE:HB	2.00	0.44
1:G:770:LEU:HD13	1:G:865:GLU:HB2	2.00	0.44
1:D:213:GLU:HG2	1:D:215:GLU:H	1.82	0.44
1:A:131:ILE:HB	1:A:143:ILE:HB	1.99	0.43
1:G:207:TRP:HB3	1:G:242:GLY:HA2	1.98	0.43
1:G:1133:VAL:O	1:G:1137:THR:HG23	2.18	0.43
2:H:917:ILE:HG13	2:H:918:ASP:N	2.33	0.43
1:A:5:TYR:CE1	1:A:1091:GLY:HA2	2.54	0.43
2:B:828:LEU:O	2:B:1034:PRO:HD3	2.18	0.43
1:D:31:LEU:HD22	1:D:317:LEU:HD21	2.00	0.43
1:G:1007:PHE:CD1	1:G:1030:PHE:HB3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:953:GLY:O	2:H:1003:LEU:HD11	2.19	0.43
1:G:849:VAL:HG11	1:G:851:PHE:CZ	2.54	0.43
1:A:817:VAL:HG22	1:A:873:MET:HE3	2.00	0.43
1:D:849:VAL:HG11	1:D:851:PHE:CZ	2.53	0.43
2:E:928:GLU:O	2:E:932:LYS:HA	2.19	0.43
1:A:184:ASP:HB2	1:A:185:PRO:CD	2.49	0.43
1:G:1109:VAL:HG12	1:G:1129:LEU:HD12	2.00	0.43
1:D:184:ASP:HB2	1:D:185:PRO:CD	2.48	0.43
1:D:903:CYS:CB	1:D:941:ASN:HA	2.48	0.43
1:A:881:LEU:HD21	1:A:921:ILE:HG21	2.01	0.43
1:G:768:SER:HB3	1:G:808:LEU:HD11	2.01	0.43
1:G:973:ASN:OD1	1:G:999:HIS:ND1	2.52	0.43
2:B:844:MET:HE3	2:B:922:CYS:CB	2.48	0.43
2:E:836:ILE:HG23	2:E:929:LEU:HD13	2.01	0.42
1:A:43:VAL:HG23	1:A:52:VAL:HG11	2.01	0.42
1:G:311:ALA:HB2	1:G:324:VAL:HG13	2.00	0.42
1:D:975:PHE:HA	1:D:996:GLY:O	2.19	0.42
1:A:35:LYS:O	1:A:36:ASN:C	2.58	0.42
2:B:738:TYR:HD2	2:B:770:THR:OG1	2.03	0.42
2:B:738:TYR:CD1	2:B:758:VAL:HG22	2.55	0.42
2:B:738:TYR:CE1	2:B:758:VAL:HG22	2.54	0.42
1:D:68:ARG:HB2	1:D:75:ASP:OD1	2.19	0.42
1:A:387:LEU:HD11	1:A:735:VAL:HG21	2.01	0.42
2:B:865:ILE:CD1	2:B:925:ILE:HD13	2.50	0.42
3:C:76:ILE:HD12	3:C:159:HIS:CE1	2.54	0.42
1:A:18:CYS:SG	1:A:313:CYS:SG	3.08	0.42
2:B:760:LEU:HD21	2:B:767:PHE:HD1	1.85	0.42
1:D:807:PHE:HB3	1:D:811:GLU:OE1	2.20	0.42
1:G:376:VAL:HG13	1:G:389:ILE:CD1	2.48	0.42
1:G:996:GLY:HA2	1:G:1086:THR:O	2.20	0.42
1:D:60:LYS:O	1:D:81:THR:HA	2.19	0.42
1:D:120:ILE:HG23	1:D:135:LEU:HD23	2.01	0.42
1:G:248:ILE:HG12	1:G:250:PRO:HD3	2.02	0.42
2:H:888:GLU:OE1	2:H:888:GLU:HA	2.19	0.42
1:A:790:ASN:HA	1:A:805:HIS:O	2.20	0.41
1:G:794:ILE:HG22	1:G:799:PHE:HA	2.01	0.41
1:G:188:ARG:NH1	1:G:216:ALA:O	2.53	0.41
2:E:934:PRO:HD2	2:E:937:GLN:OE1	2.21	0.41
2:B:741:VAL:HG22	2:B:756:LYS:HG3	2.02	0.41
1:G:184:ASP:HB2	1:G:185:PRO:CD	2.49	0.41
1:D:1109:VAL:HG12	1:D:1129:LEU:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:PRO:HG2	1:A:267:ASN:O	2.21	0.41
1:A:985:THR:HG22	1:A:987:GLU:H	1.85	0.41
1:G:44:VAL:HG21	1:G:317:LEU:HD22	2.01	0.41
1:G:387:LEU:HD11	1:G:735:VAL:HG21	2.02	0.41
1:D:1114:TYR:HB2	1:D:1122:ARG:HB3	2.03	0.41
1:A:170:LEU:HD23	1:A:170:LEU:HA	1.93	0.41
1:A:933:LEU:HD22	1:A:942:PHE:HB3	2.03	0.41
2:B:838:SER:O	2:B:842:GLN:HG3	2.20	0.41
1:D:151:GLU:OE1	1:D:153:LYS:HE2	2.21	0.41
1:D:320:GLY:O	1:D:335:LYS:HA	2.20	0.41
1:D:322:VAL:N	1:D:334:VAL:O	2.53	0.41
1:D:1030:PHE:CZ	1:D:1038:GLY:HA3	2.56	0.41
2:B:800:LEU:O	2:B:800:LEU:HG	2.20	0.41
2:B:837:LYS:HB3	2:B:1023:VAL:HG21	2.02	0.41
2:B:904:PRO:HD3	2:B:920:TRP:CE2	2.55	0.41
1:G:876:PHE:CZ	1:G:919:ASP:HA	2.56	0.41
1:G:43:VAL:HG23	1:G:52:VAL:HG21	2.03	0.41
1:D:1113:GLN:HA	1:D:1122:ARG:O	2.20	0.41
1:A:69:PRO:HG2	1:A:72:GLU:HG3	2.03	0.41
1:G:793:ILE:HG13	1:G:858:LEU:HD23	2.03	0.41
1:G:1114:TYR:CD1	1:G:1124:ALA:HB2	2.56	0.41
2:H:860:ILE:HB	2:H:921:SER:CB	2.51	0.41
1:A:364:VAL:HG22	1:A:375:LEU:HD13	2.03	0.41
1:A:749:THR:HG21	1:A:786:VAL:HG11	2.03	0.41
1:G:59:GLY:HA2	1:G:1073:TRP:CE3	2.56	0.41
1:D:320:GLY:HA3	1:D:335:LYS:HG3	2.03	0.40
1:G:768:SER:OG	1:G:863:GLU:OE2	2.26	0.40
2:H:803:LYS:HA	3:I:142:VAL:CG1	2.51	0.40
1:D:61:ILE:HG23	1:D:79:ILE:HG23	2.02	0.40
3:F:184:MET:CE	3:F:267:HIS:HA	2.51	0.40
1:G:965:PHE:O	1:G:976:VAL:HA	2.21	0.40
1:A:143:ILE:HG12	1:A:154:ALA:HB2	2.03	0.40
1:A:1024:THR:HG21	1:A:1139:ILE:HG21	2.03	0.40
2:B:823:LEU:HB3	2:B:829:VAL:CG1	2.52	0.40
1:G:5:TYR:CE1	1:G:1091:GLY:HA2	2.56	0.40
3:I:159:HIS:O	3:I:162:GLN:HG2	2.22	0.40
1:D:78:PHE:HE1	1:D:86:ALA:HB1	1.87	0.40
1:D:158:ARG:HH12	1:D:160:GLU:HG2	1.87	0.40
1:D:190:VAL:O	1:D:209:GLN:HA	2.22	0.40
2:E:903:PRO:HB2	2:E:905:GLU:HG2	2.03	0.40
1:A:762:SER:HG	1:A:803:HIS:CE1	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:36:ASN:O	1:G:37:THR:OG1	2.33	0.40
1:G:43:VAL:HG23	1:G:52:VAL:CG2	2.52	0.40
1:G:330:ASP:HA	1:G:355:ASN:HB3	2.02	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:D:1122:ARG:HE	1:G:292:ASP:OD1[2_565]	1.49	0.11
2:B:1018:ASP:OD2	3:I:232:ARG:H[5_554]	1.58	0.02

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	823/840 (98%)	801 (97%)	22 (3%)	0	100	100
1	D	822/840 (98%)	797 (97%)	24 (3%)	1 (0%)	51	82
1	G	822/840 (98%)	800 (97%)	22 (3%)	0	100	100
2	B	322/344 (94%)	313 (97%)	8 (2%)	1 (0%)	41	72
2	E	326/344 (95%)	315 (97%)	10 (3%)	1 (0%)	41	72
2	H	327/344 (95%)	317 (97%)	10 (3%)	0	100	100
3	C	246/271 (91%)	245 (100%)	1 (0%)	0	100	100
3	F	246/271 (91%)	245 (100%)	1 (0%)	0	100	100
3	I	246/271 (91%)	244 (99%)	2 (1%)	0	100	100
All	All	4180/4365 (96%)	4077 (98%)	100 (2%)	3 (0%)	51	82

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	737	THR
2	E	737	THR
1	D	318	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	722/728 (99%)	719 (100%)	3 (0%)	91	94
1	D	721/728 (99%)	716 (99%)	5 (1%)	84	90
1	G	721/728 (99%)	719 (100%)	2 (0%)	92	96
2	B	292/308 (95%)	286 (98%)	6 (2%)	53	75
2	E	296/308 (96%)	289 (98%)	7 (2%)	49	72
2	H	297/308 (96%)	294 (99%)	3 (1%)	76	85
3	C	223/242 (92%)	222 (100%)	1 (0%)	91	94
3	F	223/242 (92%)	222 (100%)	1 (0%)	91	94
3	I	223/242 (92%)	222 (100%)	1 (0%)	91	94
All	All	3718/3834 (97%)	3689 (99%)	29 (1%)	81	89

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

Mol	Chain	Res	Type
1	D	52	VAL
1	D	55	VAL
1	D	99	ASP
1	D	315	THR
1	D	766	SER
2	E	760	LEU
2	E	896	VAL
2	E	897	ILE
2	E	912	ARG
2	E	913	TYR
2	E	1036	TRP
2	E	1039	CYS

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Mol	Chain	Res	Type
3	F	231	TYR
1	A	849	VAL
1	A	930	VAL
1	A	1019	GLU
2	B	738	TYR
2	B	829	VAL
2	B	863	SER
2	B	867	LEU
2	B	896	VAL
2	B	1039	CYS
3	C	231	TYR
1	G	947	ARG
1	G	1044	SER
2	H	897	ILE
2	H	1036	TRP
2	H	1039	CYS
3	I	231	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1015	GLN
3	I	179	GLN

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	E	893	2	8,10,11	1.65	1 (12%)	10,14,16	1.33	1 (10%)
2	TPO	H	893	2	8,10,11	1.59	1 (12%)	10,14,16	1.28	2 (20%)
2	TPO	B	893	2	8,10,11	1.71	1 (12%)	10,14,16	1.01	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
2	TPO	E	893	2	-	0/9/11/13	-
2	TPO	H	893	2	-	1/9/11/13	-
2	TPO	B	893	2	-	7/9/11/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	893	TPO	P-O1P	3.52	1.61	1.50
2	H	893	TPO	P-O1P	3.51	1.61	1.50
2	B	893	TPO	P-O1P	3.48	1.61	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	893	TPO	P-OG1-CB	-3.01	114.12	123.21
2	H	893	TPO	P-OG1-CB	-2.74	114.92	123.21
2	H	893	TPO	CG2-CB-CA	-2.18	108.87	113.16

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	893	TPO	N-CA-CB-CG2
2	B	893	TPO	N-CA-CB-OG1
2	B	893	TPO	C-CA-CB-CG2
2	B	893	TPO	O-C-CA-CB
2	B	893	TPO	CG2-CB-OG1-P
2	H	893	TPO	CB-OG1-P-O2P
2	B	893	TPO	CA-CB-OG1-P
2	B	893	TPO	CB-OG1-P-O2P

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	893	TPO	2	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	C	301	-	4,4,4	0.13	0	6,6,6	0.13	0
4	SO4	D	1203	-	4,4,4	0.13	0	6,6,6	0.07	0
4	SO4	F	302	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	D	1201	-	4,4,4	0.14	0	6,6,6	0.08	0
4	SO4	F	301	-	4,4,4	0.14	0	6,6,6	0.07	0
5	RMX	E	1101	-	38,43,43	0.92	2 (5%)	45,63,63	1.02	4 (8%)
5	RMX	H	1101	-	38,43,43	0.95	2 (5%)	45,63,63	1.04	4 (8%)
4	SO4	I	303	-	4,4,4	0.15	0	6,6,6	0.07	0
4	SO4	I	301	-	4,4,4	0.14	0	6,6,6	0.12	0
4	SO4	G	1201	-	4,4,4	0.14	0	6,6,6	0.06	0
5	RMX	B	1101	-	38,43,43	0.93	2 (5%)	45,63,63	0.97	4 (8%)
4	SO4	I	302	-	4,4,4	0.13	0	6,6,6	0.10	0
4	SO4	H	1102	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	A	1201	-	4,4,4	0.14	0	6,6,6	0.09	0
4	SO4	G	1202	-	4,4,4	0.15	0	6,6,6	0.06	0
4	SO4	D	1202	-	4,4,4	0.14	0	6,6,6	0.08	0
4	SO4	C	302	-	4,4,4	0.14	0	6,6,6	0.05	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	RMX	H	1101	-	-	2/16/24/24	0/5/5/5
5	RMX	B	1101	-	-	2/16/24/24	0/5/5/5
5	RMX	E	1101	-	-	2/16/24/24	0/5/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	1101	RMX	C1-S1	-3.47	1.73	1.79
5	B	1101	RMX	C1-S1	-3.40	1.73	1.79
5	E	1101	RMX	C1-S1	-3.33	1.73	1.79
5	B	1101	RMX	S1-N1	-2.45	1.55	1.60
5	H	1101	RMX	S1-N1	-2.44	1.55	1.60
5	E	1101	RMX	S1-N1	-2.43	1.55	1.60

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	1101	RMX	C22-N9-C23	3.52	128.87	125.42
5	H	1101	RMX	C22-N9-C23	3.37	128.72	125.42
5	B	1101	RMX	C22-N9-C23	2.89	128.26	125.42
5	H	1101	RMX	C21-C8-N5	-2.58	118.66	120.81
5	E	1101	RMX	C21-C8-N5	-2.52	118.71	120.81
5	B	1101	RMX	C21-C8-N5	-2.52	118.72	120.81
5	E	1101	RMX	C2-N2-N3	2.40	106.42	104.35
5	B	1101	RMX	C2-N2-N3	2.40	106.41	104.35
5	H	1101	RMX	C2-N2-N3	2.38	106.40	104.35
5	H	1101	RMX	C7-N10-C26	-2.20	112.78	115.28
5	B	1101	RMX	C7-N10-C26	-2.12	112.87	115.28
5	E	1101	RMX	C7-N10-C26	-2.10	112.89	115.28

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	1101	RMX	N10-C7-N4-C6
5	E	1101	RMX	N5-C7-N4-C6
5	B	1101	RMX	N10-C7-N4-C6
5	B	1101	RMX	N5-C7-N4-C6

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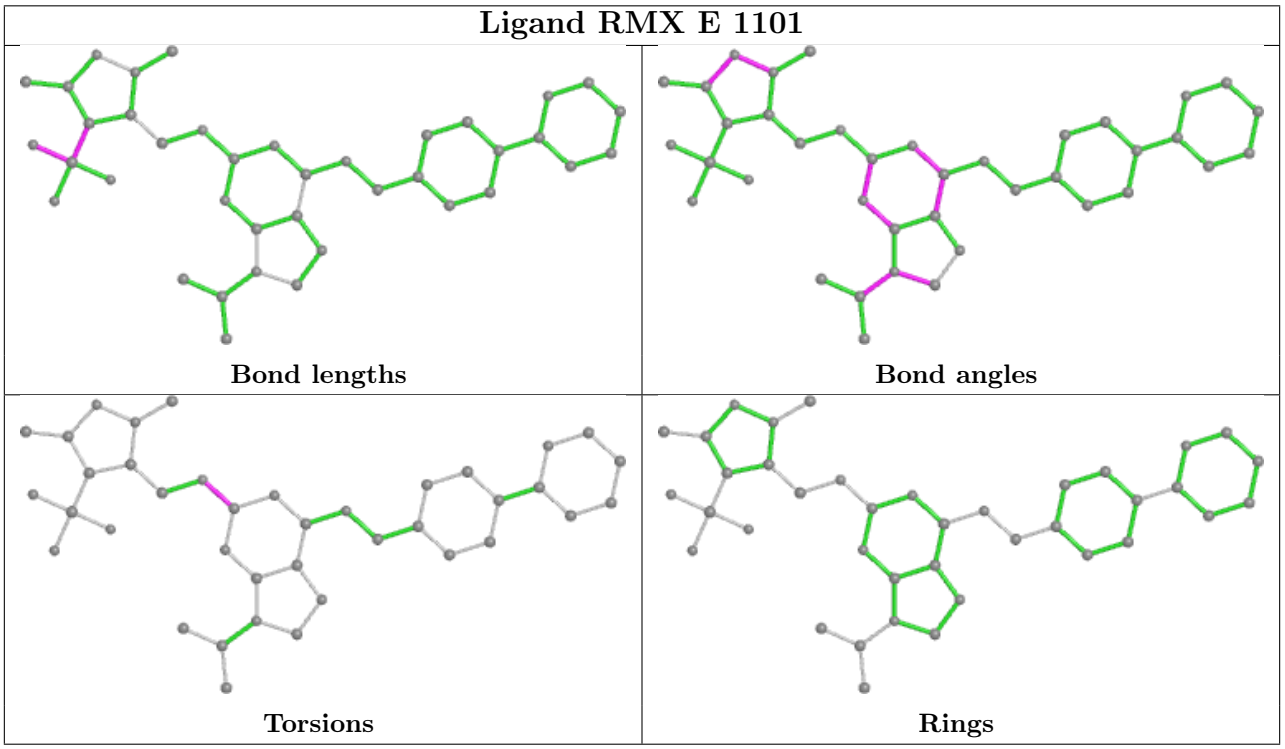
Mol	Chain	Res	Type	Atoms
5	H	1101	RMX	N10-C7-N4-C6
5	H	1101	RMX	N5-C7-N4-C6

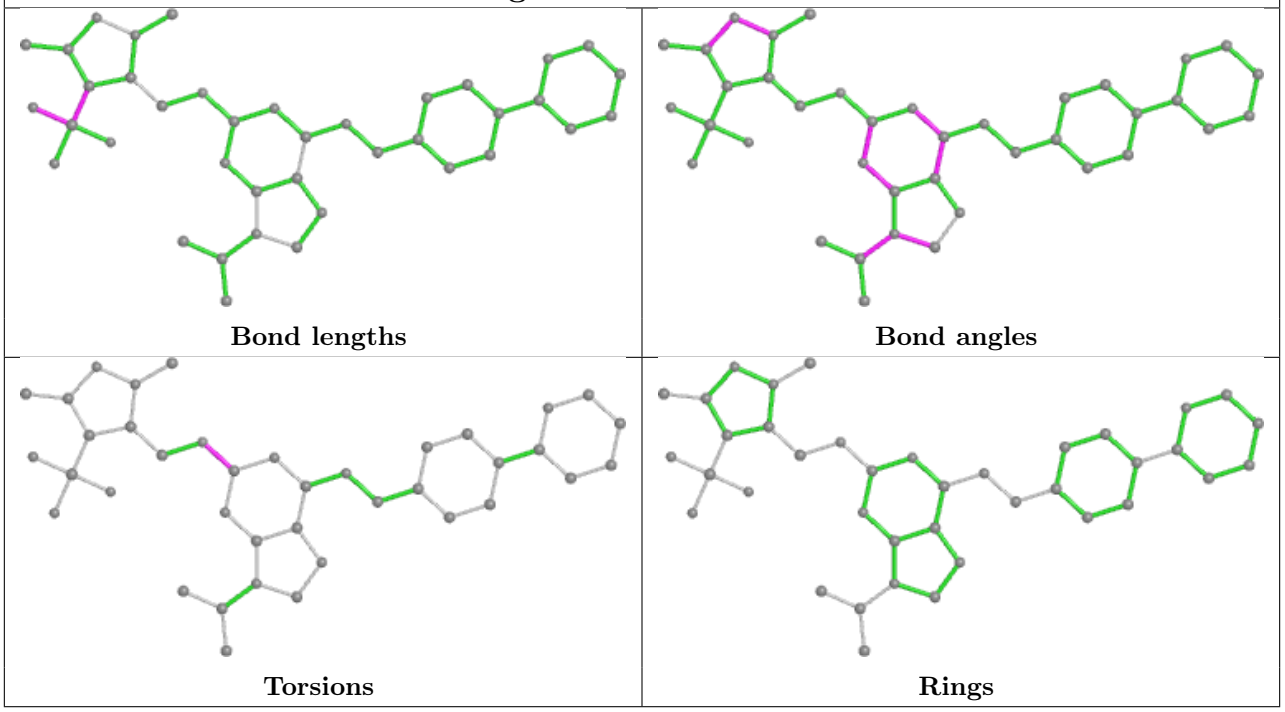
There are no ring outliers.

No monomer is involved in short contacts.

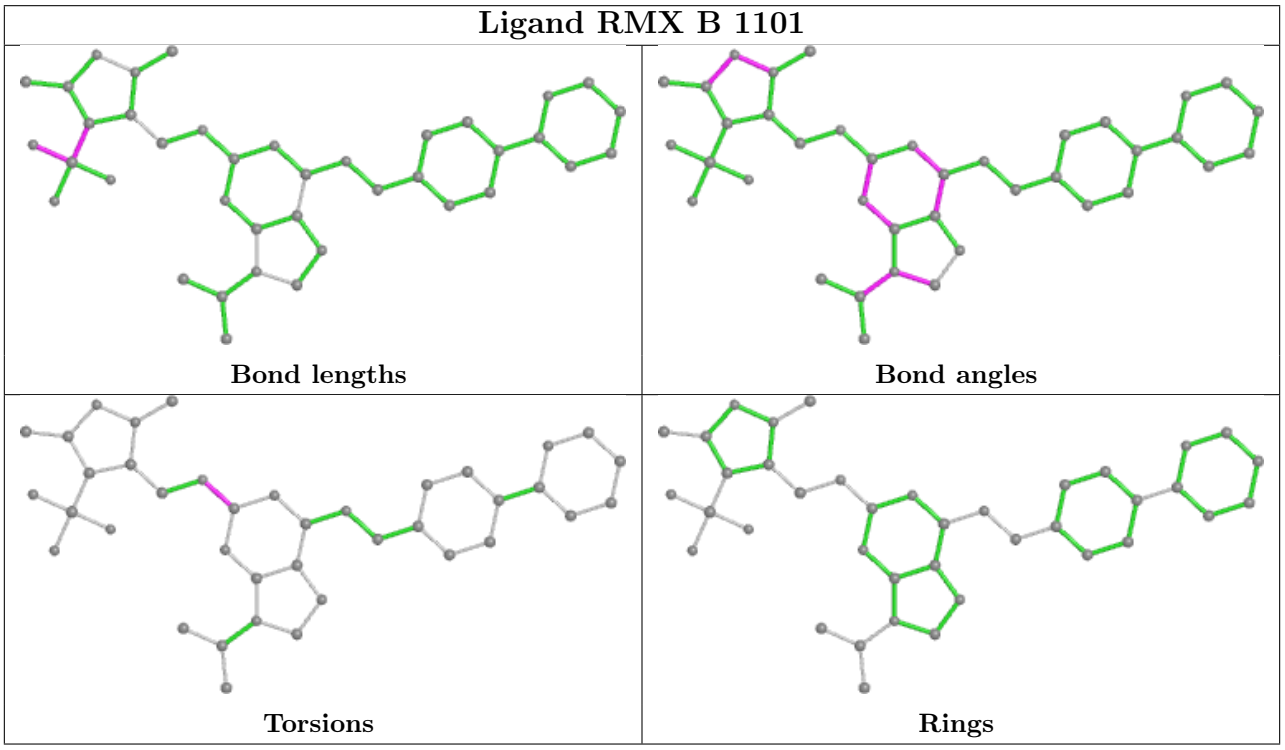
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 RMX H 1101



Ligand RMX B 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	827/840 (98%)	0.55	41 (4%)	28 26	86, 122, 191, 254	0
1	D	826/840 (98%)	0.69	73 (8%)	10 10	90, 128, 201, 284	0
1	G	826/840 (98%)	0.60	71 (8%)	10 10	94, 128, 198, 287	0
2	B	324/344 (94%)	0.85	42 (12%)	3 3	95, 123, 192, 247	0
2	E	328/344 (95%)	0.93	48 (14%)	2 2	105, 133, 205, 257	0
2	H	329/344 (95%)	0.78	25 (7%)	13 12	84, 108, 196, 243	0
3	C	248/271 (91%)	0.67	4 (1%)	72 69	79, 101, 138, 215	0
3	F	248/271 (91%)	0.55	10 (4%)	38 35	97, 122, 159, 218	0
3	I	248/271 (91%)	0.66	12 (4%)	30 28	83, 104, 150, 219	0
All	All	4204/4365 (96%)	0.67	326 (7%)	13 12	79, 122, 195, 287	0

All (326) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	738	TYR	8.4
2	E	799	ALA	6.8
1	D	1114	TYR	6.2
1	D	1018	GLY	6.1
1	D	1016	ASN	5.7
2	E	738	TYR	5.6
2	E	798	ASP	5.5
3	C	262	LYS	5.5
2	H	738	TYR	5.4
2	E	896	VAL	5.3
2	H	1036	TRP	5.2
2	H	1043	TRP	5.0
1	D	63	VAL	4.8
2	E	887	GLU	4.8
2	H	828	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
2	E	797	GLN	4.5
1	D	1115	ASP	4.4
2	H	1044	SER	4.3
2	E	1043	TRP	4.2
1	D	39	LEU	4.2
1	D	65	GLU	4.1
1	G	131	ILE	4.0
2	E	828	LEU	4.0
2	B	896	VAL	3.9
2	E	737	THR	3.9
1	A	2	SER	3.9
2	E	800	LEU	3.9
2	E	1035	HIS	3.8
2	B	831	PHE	3.8
3	F	267	HIS	3.7
2	B	802	PHE	3.6
1	D	135	LEU	3.6
1	G	295	VAL	3.6
1	D	977	CYS	3.6
3	I	267	HIS	3.6
2	E	803	LYS	3.5
2	B	1036	TRP	3.5
1	D	1019	GLU	3.4
2	H	1035	HIS	3.4
2	H	1041	GLU	3.4
1	D	336	LEU	3.4
1	A	1129	LEU	3.4
2	B	895	LYS	3.4
1	D	926	LEU	3.4
2	E	1039	CYS	3.4
1	D	297	LEU	3.3
2	E	888	GLU	3.3
1	A	91	TYR	3.3
2	E	863	SER	3.2
1	D	57	MET	3.2
1	G	61	ILE	3.2
2	E	884	TYR	3.2
1	D	131	ILE	3.2
2	H	890	ARG	3.2
2	H	839	PHE	3.1
1	A	1	MET	3.1
1	G	133	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	89	LEU	3.1
2	E	839	PHE	3.1
2	E	875	LEU	3.1
1	D	1017	LEU	3.1
1	G	49	LEU	3.1
1	D	283	LEU	3.0
3	I	266	PRO	3.0
1	D	49	LEU	3.0
1	D	23	PHE	3.0
1	D	1097	PHE	3.0
2	B	740	GLN	3.0
1	D	61	ILE	3.0
1	A	376	VAL	3.0
2	B	847	LEU	3.0
2	E	895	LYS	3.0
2	B	862	CYS	3.0
1	G	77	LEU	2.9
1	D	78	PHE	2.9
2	E	883	LEU	2.9
1	D	1118	SER	2.9
3	F	164	LEU	2.9
2	H	1040	HIS	2.9
1	D	369	ARG	2.9
2	E	829	VAL	2.9
2	E	897	ILE	2.9
2	H	798	ASP	2.8
1	D	1000	LEU	2.8
1	G	1097	PHE	2.8
1	D	1116	ASP	2.8
1	A	761	LEU	2.8
3	C	264	GLN	2.8
1	D	18	CYS	2.8
1	A	133	LEU	2.8
1	G	816	LEU	2.8
3	I	123	LEU	2.8
2	B	900	TRP	2.8
1	G	858	LEU	2.8
1	D	1129	LEU	2.8
1	A	328	LEU	2.8
2	B	839	PHE	2.8
1	G	303	GLU	2.7
1	D	273	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	232	ILE	2.7
2	E	862	CYS	2.7
1	G	1039	LEU	2.7
1	G	387	LEU	2.7
1	G	290	GLN	2.7
3	I	120	ALA	2.7
1	G	100	ILE	2.7
3	F	153	PHE	2.7
1	G	1040	VAL	2.7
1	G	314	LEU	2.7
1	G	64	MET	2.7
1	D	62	ALA	2.7
2	B	739	GLY	2.7
3	I	128	GLN	2.7
2	B	907	LEU	2.6
2	B	1035	HIS	2.6
2	B	860	ILE	2.6
2	B	829	VAL	2.6
1	A	1065	VAL	2.6
1	D	121	ILE	2.6
1	A	31	LEU	2.6
1	G	881	LEU	2.6
2	B	917	ILE	2.6
3	F	147	LEU	2.6
1	D	930	VAL	2.6
1	G	66	LEU	2.6
1	G	390	ILE	2.6
2	B	867	LEU	2.5
1	D	248	ILE	2.5
1	D	55	VAL	2.5
1	D	80	LEU	2.5
1	A	78	PHE	2.5
2	H	896	VAL	2.5
1	G	33	ILE	2.5
1	D	1126	ALA	2.5
2	B	882	ARG	2.5
1	D	19	VAL	2.5
1	G	1051	LEU	2.5
1	D	1020	THR	2.5
1	G	124	ILE	2.5
1	G	394	ILE	2.5
2	B	897	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	317	LEU	2.5
2	E	867	LEU	2.5
3	F	155	LEU	2.5
3	F	264	GLN	2.5
1	D	1088	PHE	2.5
1	G	195	VAL	2.5
2	H	1039	CYS	2.5
1	D	943	GLU	2.5
1	A	926	LEU	2.5
1	A	390	ILE	2.5
1	A	927	MET	2.5
1	A	23	PHE	2.5
1	D	59	GLY	2.4
2	H	803	LYS	2.4
2	B	955	PRO	2.4
1	G	291	MET	2.4
2	E	802	PHE	2.4
2	B	913	TYR	2.4
2	H	772	ILE	2.4
1	A	64	MET	2.4
1	D	308	THR	2.4
1	A	42	TYR	2.4
1	A	55	VAL	2.4
2	E	824	LEU	2.4
3	F	181	LEU	2.4
2	B	930	PHE	2.4
1	A	121	ILE	2.4
1	G	123	ILE	2.4
1	D	334	VAL	2.4
3	I	113	CYS	2.4
1	G	143	ILE	2.4
2	B	828	LEU	2.4
2	H	767	PHE	2.4
1	A	1136	LEU	2.4
2	E	951	LEU	2.4
1	D	1007	PHE	2.4
2	E	865	ILE	2.4
2	H	769	ILE	2.4
3	C	267	HIS	2.3
1	G	1037	ILE	2.3
1	G	276	MET	2.3
1	D	31	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	280	LEU	2.3
2	B	935	ILE	2.3
1	G	1000	LEU	2.3
2	E	935	ILE	2.3
2	E	952	CYS	2.3
1	G	130	MET	2.3
1	D	914	LEU	2.3
1	D	933	LEU	2.3
1	D	1029	LEU	2.3
1	G	957	VAL	2.3
2	B	1032	ASP	2.3
1	G	2	SER	2.3
1	D	356	LEU	2.3
2	E	955	PRO	2.3
1	G	799	PHE	2.3
1	D	912	LEU	2.3
1	A	375	LEU	2.3
2	E	926	LEU	2.3
2	B	906	LEU	2.3
3	F	132	PHE	2.2
1	D	311	ALA	2.2
1	G	32	LEU	2.2
1	A	195	VAL	2.2
3	F	161	TYR	2.2
1	D	360	VAL	2.2
2	B	922	CYS	2.2
1	A	197	LEU	2.2
1	G	974	LEU	2.2
1	D	226	PHE	2.2
3	C	254	ILE	2.2
1	G	5	TYR	2.2
2	H	720	GLY	2.2
1	A	899	LEU	2.2
2	H	1001	LEU	2.2
2	H	1000	MET	2.2
1	A	100	ILE	2.2
1	G	88	ILE	2.2
2	B	1038	ASP	2.2
2	B	721	LYS	2.2
1	D	1040	VAL	2.2
2	H	892	TYR	2.2
1	D	975	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	264	VAL	2.2
2	H	732	ILE	2.2
1	D	32	LEU	2.2
1	G	39	LEU	2.2
1	G	829	PHE	2.2
1	D	41	ILE	2.2
1	D	359	ILE	2.2
1	D	1006	VAL	2.2
1	G	1108	VAL	2.2
1	A	1097	PHE	2.2
2	E	986	PHE	2.2
1	D	33	ILE	2.2
1	G	376	VAL	2.2
1	G	1004	VAL	2.2
1	G	272	LEU	2.1
1	G	1129	LEU	2.1
2	E	907	LEU	2.1
2	E	1033	LEU	2.1
2	B	843	LEU	2.1
1	A	61	ILE	2.1
2	H	1031	PRO	2.1
1	D	317	LEU	2.1
1	D	997	LEU	2.1
1	G	36	ASN	2.1
2	H	802	PHE	2.1
1	G	253	ILE	2.1
2	E	1041	GLU	2.1
3	I	229	PRO	2.1
1	A	32	LEU	2.1
1	G	1029	LEU	2.1
2	E	945	LEU	2.1
2	E	885	ASN	2.1
3	I	132	PHE	2.1
1	D	220	ILE	2.1
1	A	974	LEU	2.1
1	G	752	LEU	2.1
2	E	890	ARG	2.1
1	D	285	LEU	2.1
1	G	336	LEU	2.1
1	A	377	THR	2.1
1	G	880	LEU	2.1
1	D	60	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	886	SER	2.1
1	D	52	VAL	2.1
1	D	120	ILE	2.1
1	D	258	ILE	2.1
1	G	294	THR	2.1
1	A	966	LEU	2.1
1	G	1076	PHE	2.1
1	G	230	ILE	2.1
1	A	1005	ASN	2.1
1	G	966	LEU	2.1
2	E	855	PHE	2.1
1	G	930	VAL	2.1
2	B	948	ILE	2.1
1	G	57	MET	2.1
2	E	894	ASN	2.1
2	B	767	PHE	2.1
2	B	915	PRO	2.1
1	A	969	GLU	2.1
1	G	359	ILE	2.1
2	B	720	GLY	2.1
2	B	875	LEU	2.1
2	B	996	LEU	2.1
2	B	997	LEU	2.1
1	A	253	ILE	2.1
2	E	942	LEU	2.1
1	D	745	THR	2.1
3	F	116	ILE	2.1
1	G	306	GLY	2.1
1	A	7	VAL	2.0
1	D	830	ILE	2.0
1	G	1035	GLY	2.0
2	E	755	LEU	2.0
2	E	878	PHE	2.0
1	G	953	TRP	2.0
2	E	864	ASN	2.0
2	E	831	PHE	2.0
3	I	264	GLN	2.0
1	D	76	LEU	2.0
1	A	39	LEU	2.0
1	A	959	ILE	2.0
2	E	982	LEU	2.0
3	I	116	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
2	H	830	HIS	2.0
1	A	1139	ILE	2.0
1	D	871	TYR	2.0
1	A	360	VAL	2.0
1	A	995	VAL	2.0
1	G	1115	ASP	2.0
2	B	908	LEU	2.0
3	I	66	LEU	2.0
1	G	132	GLY	2.0
1	G	1055	GLN	2.0
1	A	735	VAL	2.0
1	G	300	LEU	2.0
1	G	302	VAL	2.0
2	E	820	LEU	2.0
2	B	811	LEU	2.0
2	B	929	LEU	2.0
3	I	140	VAL	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	H	893	11/12	0.65	0.41	154,155,189,189	6
2	TPO	E	893	11/12	0.74	0.21	185,207,251,251	6
2	TPO	B	893	11/12	0.76	0.20	198,214,257,257	6

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

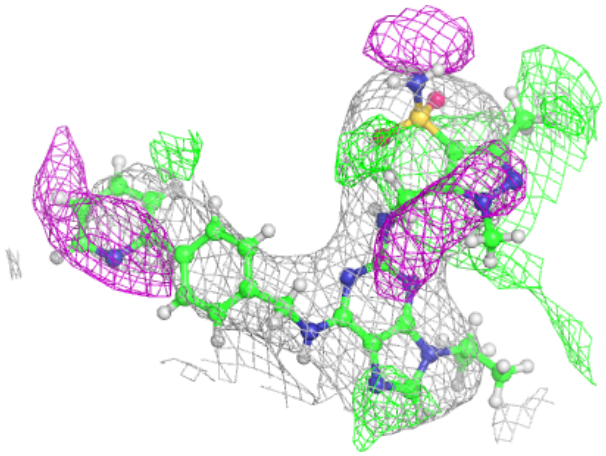
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

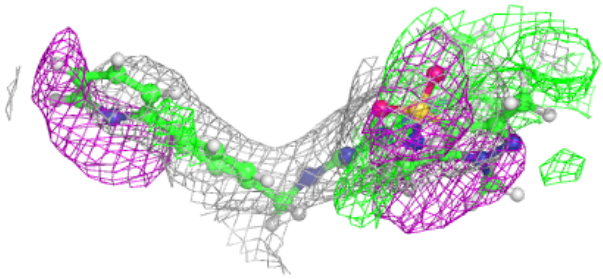
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	F	302	5/5	0.45	0.31	161,177,187,187	0
4	SO4	F	301	5/5	0.73	0.21	142,144,145,145	0
4	SO4	H	1102	5/5	0.74	0.29	153,161,167,177	0
4	SO4	C	302	5/5	0.78	0.27	138,149,156,171	0
4	SO4	D	1203	5/5	0.80	0.17	165,172,176,184	0
4	SO4	D	1202	5/5	0.83	0.20	119,128,137,143	0
4	SO4	I	302	5/5	0.84	0.22	157,167,171,176	0
5	RMX	H	1101	39/39	0.85	0.50	100,126,173,181	30
4	SO4	I	303	5/5	0.88	0.14	136,146,152,164	0
4	SO4	D	1201	5/5	0.88	0.15	136,137,141,141	0
5	RMX	B	1101	39/39	0.89	0.41	101,124,178,185	30
4	SO4	G	1202	5/5	0.90	0.24	132,134,137,138	0
5	RMX	E	1101	39/39	0.92	0.42	112,137,187,190	30
4	SO4	C	301	5/5	0.92	0.17	109,114,116,117	0
4	SO4	A	1201	5/5	0.92	0.12	133,138,140,143	0
4	SO4	I	301	5/5	0.93	0.17	108,110,114,115	0
4	SO4	G	1201	5/5	0.94	0.14	132,138,139,145	0

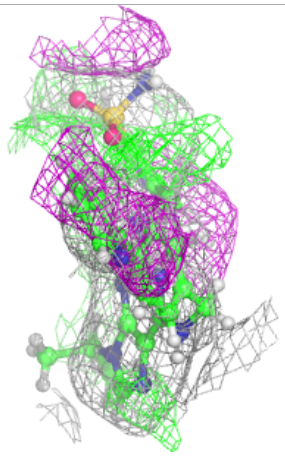
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around RMX 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)

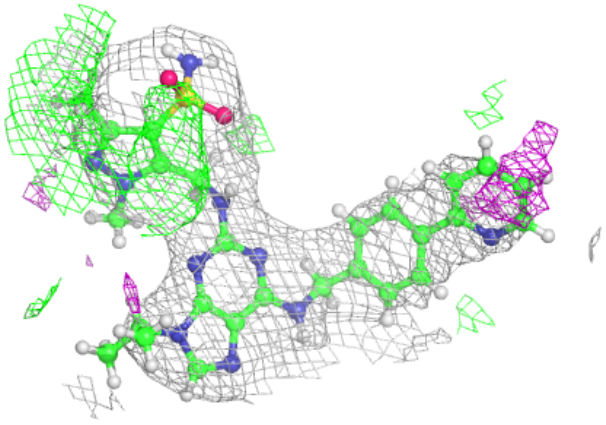


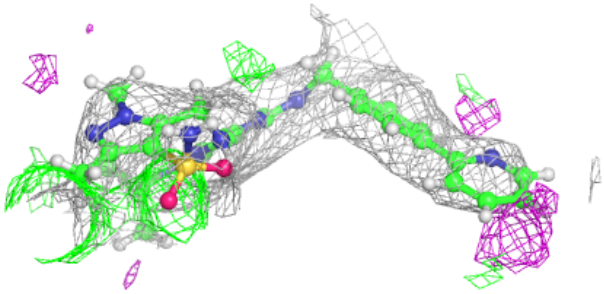


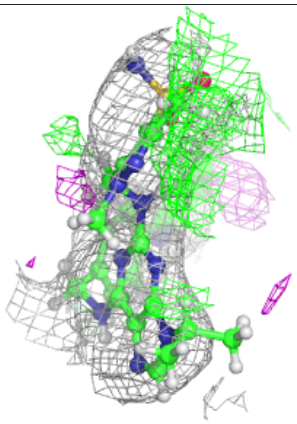


Electron density around RMX B 1101:

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

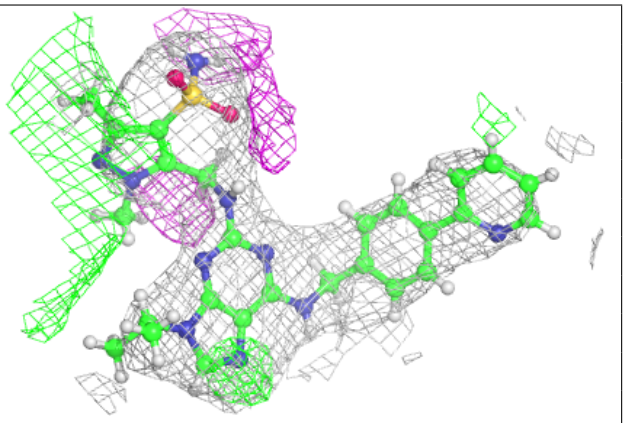


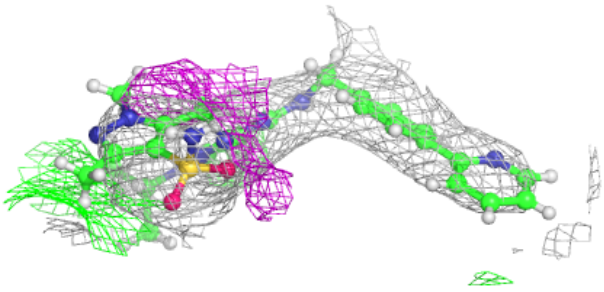


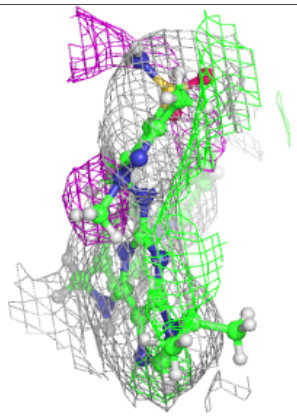


Electron density around RMX E 1101:

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







6.5 Other polymers (i)

There are no such residues in this entry.