



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 7, 2023 – 01:29 pm BST

PDB ID : 8BUT
Title : Structure of DDB1 bound to DS61-engaged CDK12-cyclin K
Authors : Kozicka, Z.; Kempf, G.; Focht, V.; Thoma, N.H.
Deposited on : 2022-11-30
Resolution : 3.25 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

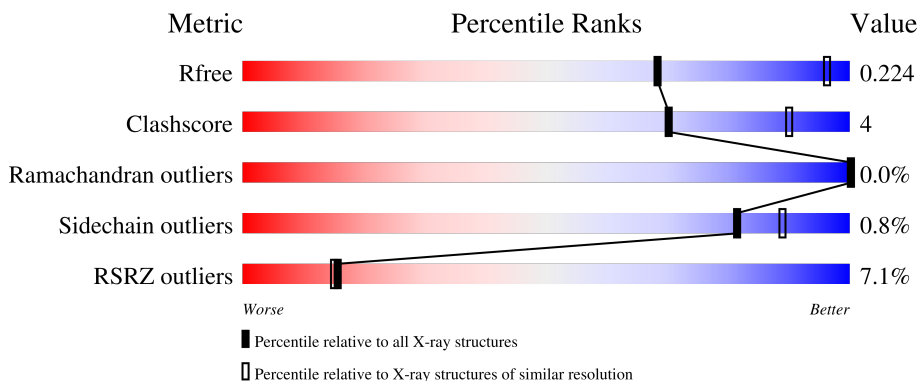
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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.



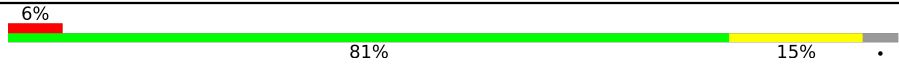

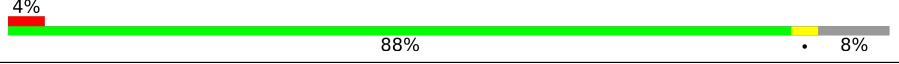
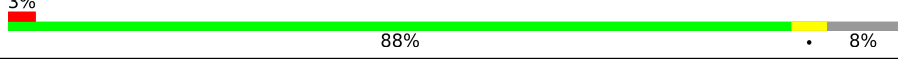
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	840	<div style="display: flex; align-items: center;"> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 89%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">8% 89% 9% .</p>
1	D	840	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 89%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">5% 89% 10% .</p>
1	G	840	<div style="display: flex; align-items: center;"> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 87%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">8% 87% 11% .</p>
2	B	344	<div style="display: flex; align-items: center;"> <div style="width: 12%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 81%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">12% 81% 13% . 6%</p>
2	E	344	<div style="display: flex; align-items: center;"> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 82%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">8% 82% 12% . 6%</p>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	344	 6% 81% 15%
3	C	271	 6% 87% 8%
3	F	271	 4% 88% 8%
3	I	271	 3% 88% 8%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 67451 atoms, of which 33620 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
			Total	C	H	N	O	S			
1	A	826	12937	4105	6450	1094	1252	36	6450	0	0
1	D	827	12957	4111	6462	1095	1253	36	6462	0	0
1	G	826	12938	4106	6452	1093	1251	36	6452	0	0

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q16531
A	-2	GLY	-	expression tag	UNP Q16531
A	-1	GLY	-	expression tag	UNP Q16531
A	0	ARG	-	expression tag	UNP Q16531
A	700	GLY	-	linker	UNP Q16531
A	701	ASN	-	linker	UNP Q16531
A	702	GLY	-	linker	UNP Q16531
A	703	ASN	-	linker	UNP Q16531
A	704	SER	-	linker	UNP Q16531
A	705	GLY	-	linker	UNP Q16531
A	706	GLU	-	linker	UNP Q16531
A	707	ILE	-	linker	UNP Q16531
A	708	GLN	-	linker	UNP Q16531
D	-3	GLY	-	expression tag	UNP Q16531
D	-2	GLY	-	expression tag	UNP Q16531
D	-1	GLY	-	expression tag	UNP Q16531
D	0	ARG	-	expression tag	UNP Q16531
D	700	GLY	-	linker	UNP Q16531
D	701	ASN	-	linker	UNP Q16531
D	702	GLY	-	linker	UNP Q16531
D	703	ASN	-	linker	UNP Q16531
D	704	SER	-	linker	UNP Q16531
D	705	GLY	-	linker	UNP Q16531

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	706	GLU	-	linker	UNP Q16531
D	707	ILE	-	linker	UNP Q16531
D	708	GLN	-	linker	UNP Q16531
G	-3	GLY	-	expression tag	UNP Q16531
G	-2	GLY	-	expression tag	UNP Q16531
G	-1	GLY	-	expression tag	UNP Q16531
G	0	ARG	-	expression tag	UNP Q16531
G	700	GLY	-	linker	UNP Q16531
G	701	ASN	-	linker	UNP Q16531
G	702	GLY	-	linker	UNP Q16531
G	703	ASN	-	linker	UNP Q16531
G	704	SER	-	linker	UNP Q16531
G	705	GLY	-	linker	UNP Q16531
G	706	GLU	-	linker	UNP Q16531
G	707	ILE	-	linker	UNP Q16531
G	708	GLN	-	linker	UNP Q16531

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

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
			Total	C	H	N	O	P	S			
2	B	325	Total	C	H	N	O	P	S	2674	0	0
			5309	1695	2663	447	486	1	17			
2	E	325	Total	C	H	N	O	P	S	2674	0	0
			5309	1695	2663	447	486	1	17			
2	H	329	Total	C	H	N	O	P	S	2707	0	0
			5383	1723	2696	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

Continued on next page...

Continued from previous page...

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

- Molecule 3 is a protein called Cyclin-K.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
3	C	248	Total	C	H	N	O	S	2048	0	0
			4111	1341	2048	346	363	13			
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: O₄S).



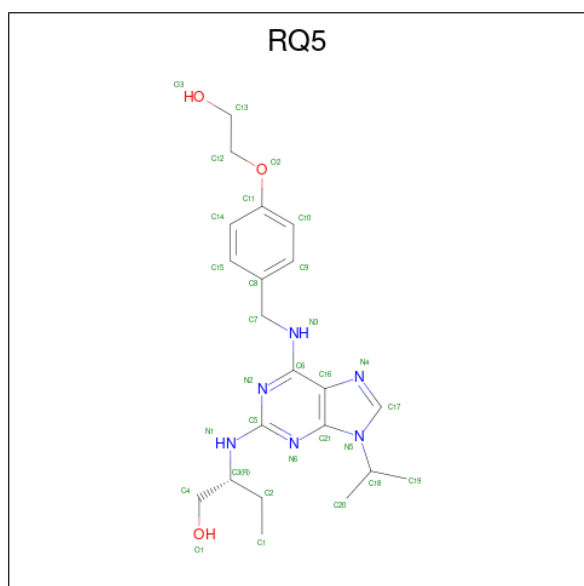
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total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

Continued on next page...

Continued from previous page...

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

- Molecule 5 is 2-[[6-[[4-(2-hydroxyethoxy)phenyl]methylamino]-9-propan-2-yl-purin-2-yl]amino]butan-1-ol (three-letter code: RQ5) (formula: C₂₁H₃₀N₆O₃) (labeled as "Ligand of Interest" by depositor).

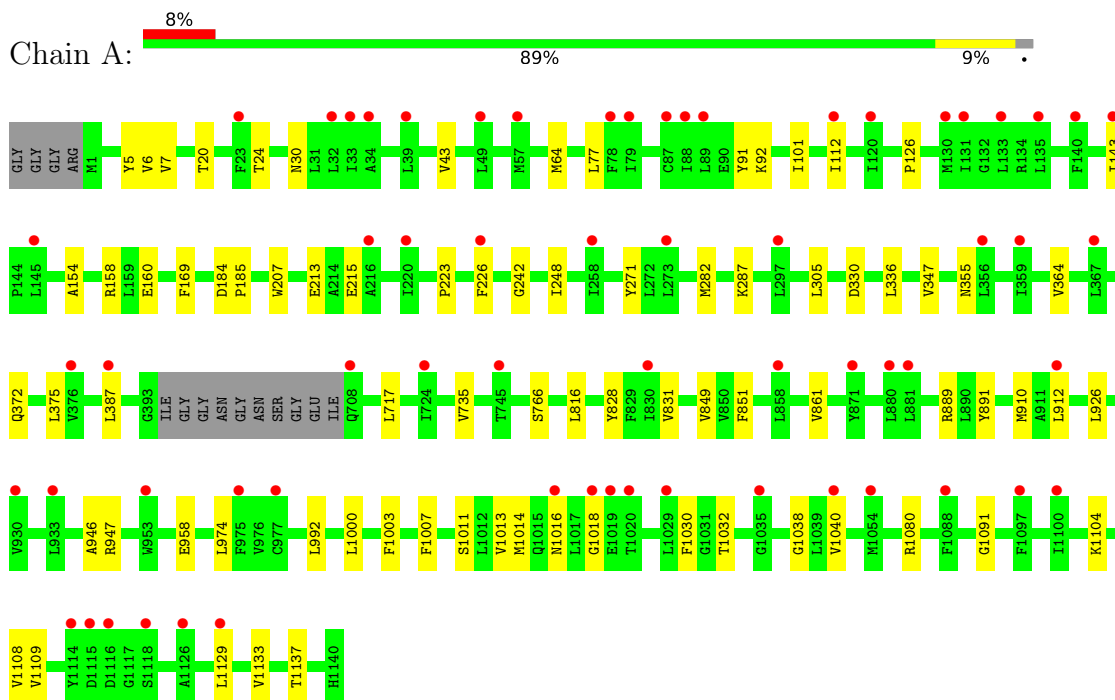


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
5	B	1	Total	C	H	N	O	30	0
			60	21	30	6	3		
5	E	1	Total	C	H	N	O	30	0
			60	21	30	6	3		
5	H	1	Total	C	H	N	O	30	0
			60	21	30	6	3		

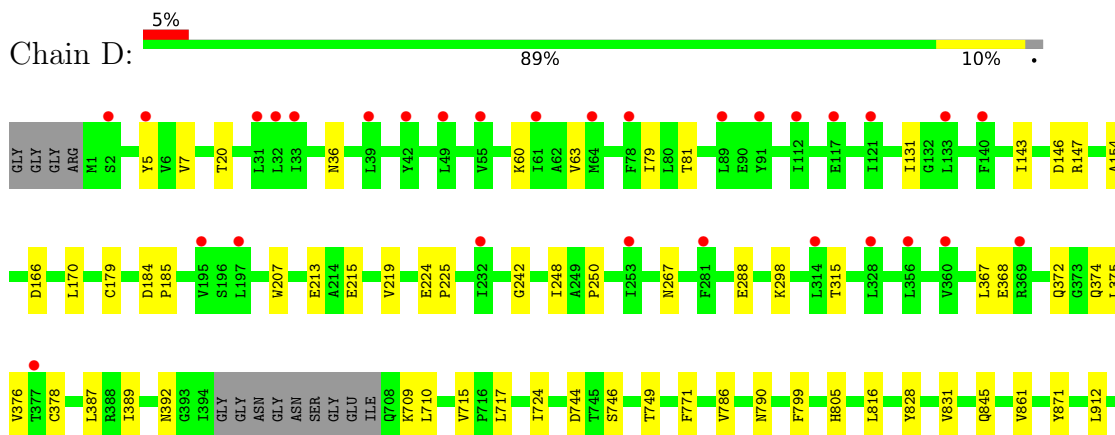
3 Residue-property plots [i](#)

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

- Molecule 1: DNA damage-binding protein 1

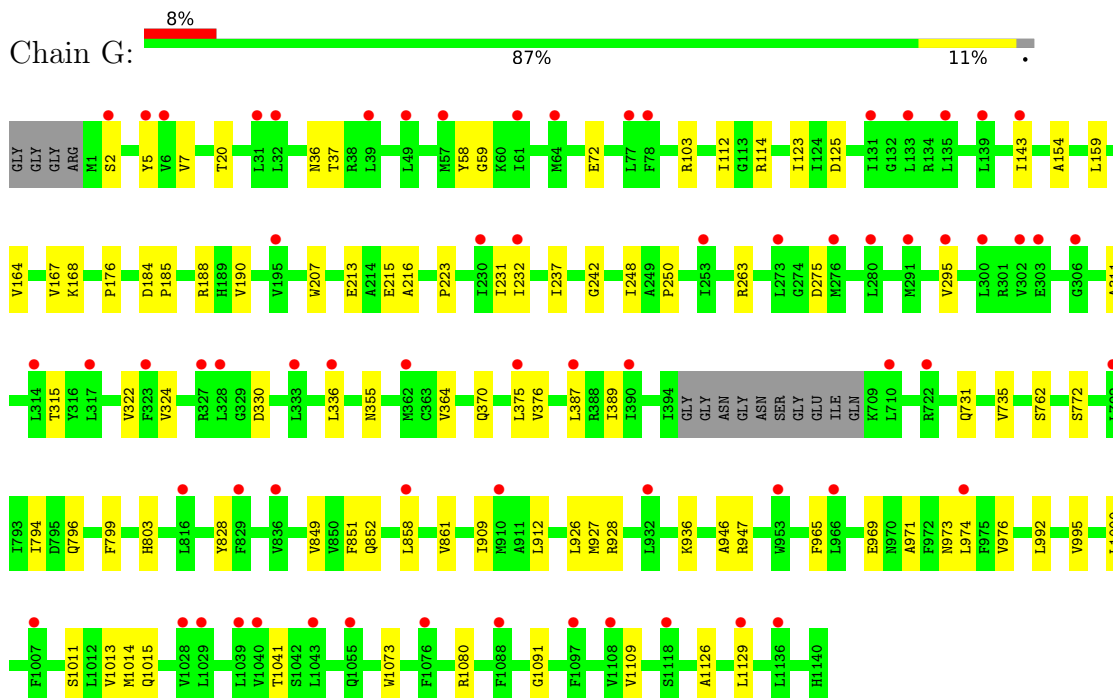


- Molecule 1: DNA damage-binding protein 1

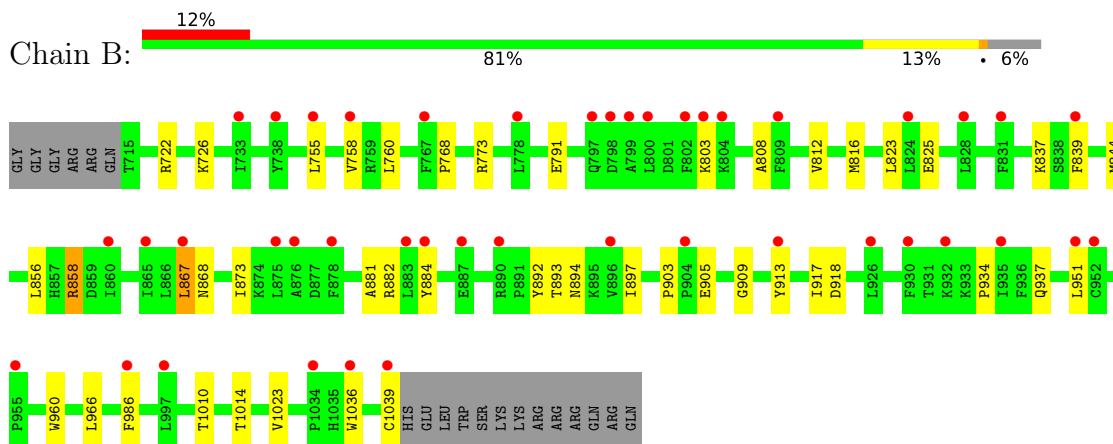




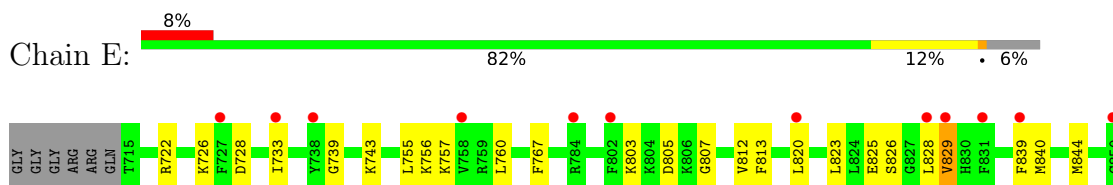
- Molecule 1: DNA damage-binding protein 1

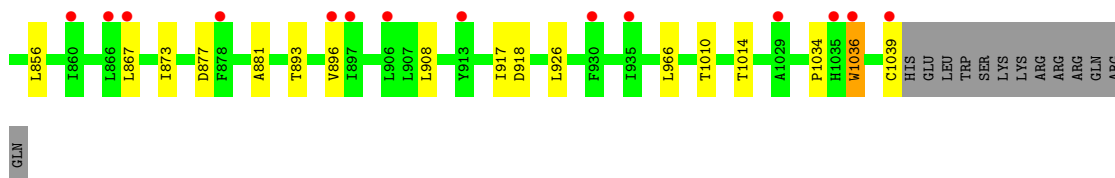


- Molecule 2: Cyclin-dependent kinase 12

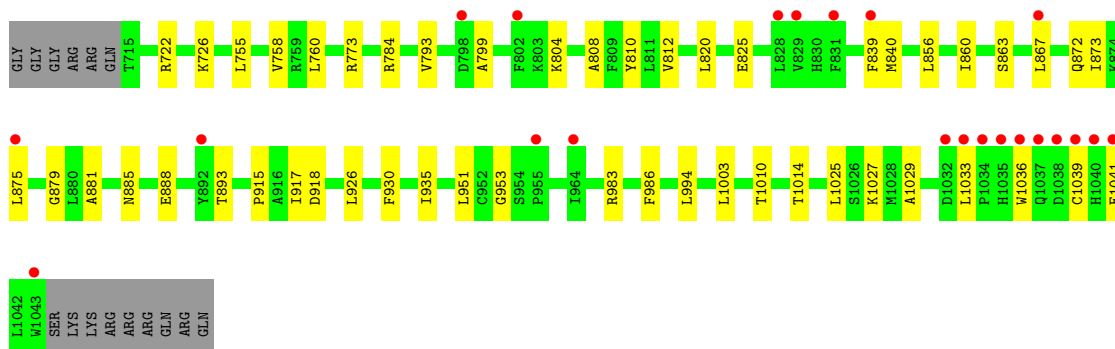
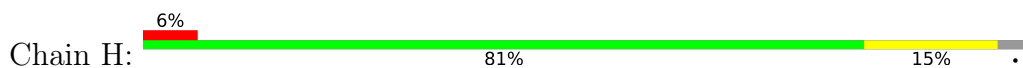


- Molecule 2: Cyclin-dependent kinase 12

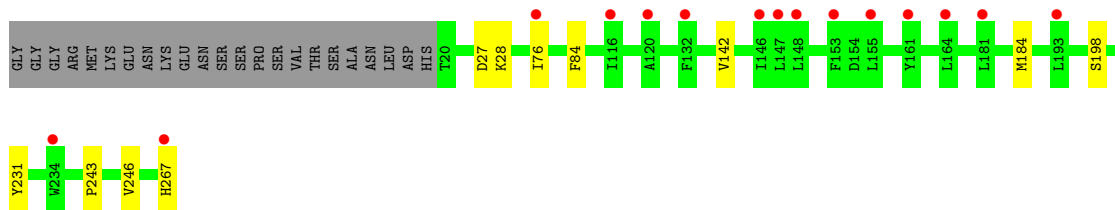
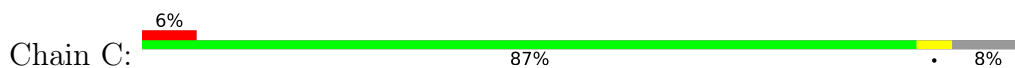




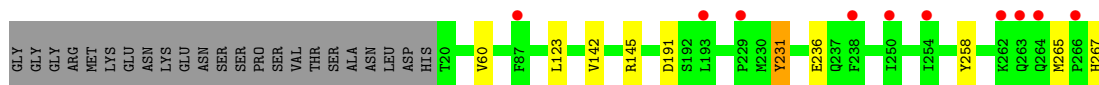
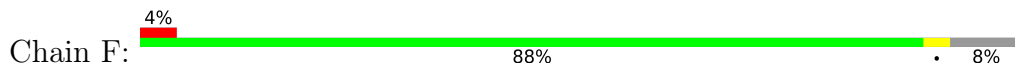
- Molecule 2: Cyclin-dependent kinase 12



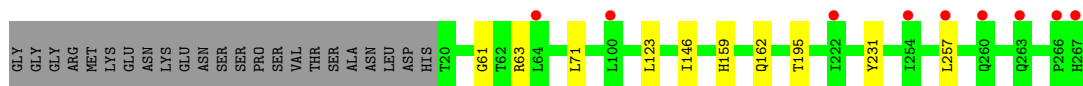
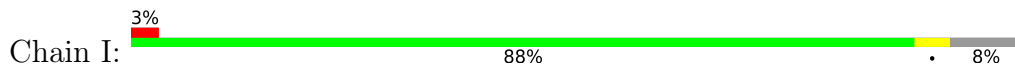
- Molecule 3: Cyclin-K



- 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	249.70Å 249.70Å 218.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	60.41 – 3.25 216.25 – 3.25	Depositor EDS
% Data completeness (in resolution range)	85.2 (60.41-3.25) 85.3 (216.25-3.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 3.26Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.197 , 0.217 0.207 , 0.224	Depositor DCC
R_{free} test set	5198 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	128.7	Xtrriage
Anisotropy	0.002	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 91.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.029 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	67451	wwPDB-VP
Average B, all atoms (Å ²)	149.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, RQ5, 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	0.27	0/6604	0.53	0/8931
1	D	0.27	0/6612	0.53	0/8942
1	G	0.27	0/6603	0.53	0/8930
2	B	0.28	0/2693	0.53	0/3630
2	E	0.27	0/2693	0.52	0/3630
2	H	0.28	0/2737	0.54	0/3691
3	C	0.27	0/2120	0.48	0/2868
3	F	0.27	0/2120	0.48	0/2868
3	I	0.27	0/2120	0.47	0/2868
All	All	0.27	0/34302	0.52	0/46358

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6487	6450	6451	43	0
1	D	6495	6462	6464	49	0
1	G	6486	6452	6454	59	0
2	B	2646	2663	2663	32	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	2646	2663	2663	26	0
2	H	2687	2696	2696	26	0
3	C	2063	2048	2048	9	0
3	F	2063	2048	2048	6	0
3	I	2063	2048	2048	5	0
4	A	20	0	0	0	0
4	C	15	0	0	0	0
4	D	20	0	0	0	0
4	F	10	0	0	0	0
4	G	25	0	0	0	0
4	I	15	0	0	0	0
5	B	30	30	0	0	0
5	E	30	30	0	0	0
5	H	30	30	0	1	0
All	All	33831	33620	33535	243	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (243) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:231:TYR:OH	3:F:236:GLU:OE1	2.04	0.75
2:H:867:LEU:HD13	2:H:873:ILE:HD11	1.78	0.66
2:H:1027:LYS:HE2	2:H:1029:ALA:HB2	1.78	0.66
2:B:755:LEU:HD22	2:B:812:VAL:HG22	1.78	0.65
2:B:755:LEU:CD2	2:B:812:VAL:HG22	2.27	0.64
1:G:1109:VAL:HG12	1:G:1129:LEU:HD12	1.79	0.64
1:G:1109:VAL:HG11	1:G:1126:ALA:HA	1.81	0.62
2:B:951:LEU:HD21	2:B:986:PHE:HE2	1.64	0.62
2:B:823:LEU:HD12	2:B:867:LEU:HD13	1.83	0.61
1:G:946:ALA:HB1	1:G:992:LEU:HG	1.82	0.60
1:D:816:LEU:HD13	1:D:831:VAL:HG22	1.82	0.60
2:B:758:VAL:O	2:B:808:ALA:HB1	2.00	0.60
2:B:844:MET:HE2	2:B:844:MET:HA	1.83	0.60
2:E:867:LEU:HD13	2:E:873:ILE:CD1	2.33	0.59
1:G:123:ILE:HG21	1:G:168:LYS:HA	1.84	0.59
2:E:908:LEU:HB2	2:E:966:LEU:HD13	1.84	0.59
3:C:243:PRO:HG2	3:C:246:VAL:HG23	1.83	0.58
1:G:36:ASN:O	1:G:37:THR:OG1	2.19	0.58
1:D:1080:ARG:HD3	2:E:825:GLU:HA	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:722:ARG:HE	2:E:726:LYS:HG3	1.69	0.57
2:E:755:LEU:CD2	2:E:812:VAL:HG22	2.34	0.57
2:B:722:ARG:NH1	2:B:791:GLU:OE2	2.38	0.57
1:D:207:TRP:HB3	1:D:242:GLY:HA2	1.87	0.56
1:D:912:LEU:HD11	1:D:926:LEU:HD13	1.88	0.56
2:H:1010:THR:O	2:H:1014:THR:HG23	2.05	0.56
1:A:828:TYR:CE1	1:A:861:VAL:HG21	2.42	0.55
1:G:858:LEU:HD12	1:G:858:LEU:O	2.07	0.55
2:H:867:LEU:HD13	2:H:873:ILE:CD1	2.36	0.54
2:H:722:ARG:HE	2:H:726:LYS:HG3	1.71	0.54
2:B:722:ARG:HE	2:B:726:LYS:HG3	1.73	0.54
1:G:322:VAL:HG21	1:G:336:LEU:HD11	1.89	0.54
1:A:946:ALA:HB1	1:A:992:LEU:HG	1.90	0.54
1:D:213:GLU:HG2	1:D:215:GLU:H	1.72	0.54
2:B:867:LEU:HD23	2:B:873:ILE:HG13	1.90	0.53
1:G:1011:SER:OG	1:G:1013:VAL:HG22	2.09	0.53
1:D:946:ALA:HB1	1:D:992:LEU:HG	1.89	0.53
1:A:207:TRP:HB3	1:A:242:GLY:HA2	1.91	0.53
3:C:76:ILE:CD1	3:C:198:SER:HB3	2.39	0.53
2:E:1010:THR:O	2:E:1014:THR:HG23	2.08	0.53
2:H:856:LEU:O	2:H:881:ALA:HA	2.08	0.53
2:B:837:LYS:HB3	2:B:1023:VAL:HG21	1.92	0.52
2:E:820:LEU:HD22	2:E:839:PHE:CZ	2.44	0.52
1:G:112:ILE:HD13	2:H:986:PHE:CE2	2.45	0.52
1:G:159:LEU:HD21	1:G:164:VAL:HG21	1.92	0.52
1:G:207:TRP:HB3	1:G:242:GLY:HA2	1.91	0.52
1:A:912:LEU:HD11	1:A:926:LEU:HD13	1.92	0.51
1:D:60:LYS:O	1:D:81:THR:HA	2.10	0.51
1:D:367:LEU:HD12	1:D:374:GLN:OE1	2.10	0.51
2:B:897:ILE:HD12	2:B:903:PRO:HD3	1.92	0.50
2:E:733:ILE:HG21	2:E:743:LYS:HB2	1.93	0.50
2:B:1010:THR:O	2:B:1014:THR:HG23	2.12	0.50
1:D:375:LEU:HB2	1:D:1012:LEU:HD21	1.94	0.50
2:E:739:GLY:HA3	2:E:757:LYS:O	2.11	0.50
1:G:7:VAL:HG12	1:G:1091:GLY:HA3	1.93	0.50
1:A:143:ILE:HG12	1:A:154:ALA:HB2	1.94	0.50
1:G:5:TYR:HB3	1:G:1041:THR:HG23	1.94	0.50
1:G:213:GLU:HG2	1:G:215:GLU:H	1.75	0.50
1:A:30:ASN:ND2	1:A:43:VAL:HG22	2.26	0.50
1:G:20:THR:HG23	1:G:315:THR:OG1	2.12	0.50
1:D:828:TYR:CE1	1:D:861:VAL:HG21	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:709:LYS:HG2	1:D:710:LEU:N	2.27	0.50
1:G:72:GLU:OE2	1:G:103:ARG:NH2	2.45	0.50
1:A:1030:PHE:CZ	1:A:1038:GLY:HA3	2.47	0.50
3:I:195:THR:HG21	3:I:257:LEU:HD11	1.94	0.50
1:G:852:GLN:O	1:G:858:LEU:HA	2.12	0.50
3:I:195:THR:CG2	3:I:257:LEU:HD11	2.42	0.50
1:G:912:LEU:HD11	1:G:926:LEU:HD13	1.93	0.49
3:C:84:PHE:HA	1:D:746:SER:HB2	1.94	0.49
1:D:288:GLU:HB2	1:D:298:LYS:HB2	1.95	0.49
2:E:867:LEU:HD13	2:E:873:ILE:HD11	1.94	0.49
1:A:849:VAL:HG11	1:A:851:PHE:CZ	2.48	0.49
1:A:1109:VAL:HG12	1:A:1129:LEU:HD12	1.94	0.49
1:G:143:ILE:HG12	1:G:154:ALA:HB2	1.95	0.49
2:H:917:ILE:HG13	2:H:918:ASP:N	2.28	0.49
1:G:232:ILE:HD13	1:G:237:ILE:HG23	1.94	0.49
2:H:755:LEU:CD2	2:H:812:VAL:HG22	2.43	0.49
2:B:873:ILE:N	2:B:873:ILE:HD12	2.28	0.49
1:A:6:VAL:HG22	1:A:1040:VAL:HG22	1.95	0.48
1:G:731:GLN:OE1	1:G:796:GLN:NE2	2.46	0.48
1:D:146:ASP:OD1	1:D:147:ARG:N	2.47	0.48
1:A:112:ILE:HD13	2:B:986:PHE:CE2	2.49	0.48
1:A:364:VAL:HG22	1:A:375:LEU:HD13	1.95	0.48
2:E:826:SER:HB2	2:E:828:LEU:HD12	1.94	0.48
1:D:36:ASN:ND2	1:D:1001:GLY:O	2.43	0.48
2:B:960:TRP:CZ2	2:B:966:LEU:HD11	2.49	0.47
2:E:867:LEU:HD13	2:E:873:ILE:HD13	1.96	0.47
2:H:793:VAL:HG23	2:H:810:TYR:HB2	1.96	0.47
1:A:974:LEU:HD11	1:A:1000:LEU:HD22	1.96	0.47
1:D:248:ILE:HG12	1:D:250:PRO:HD3	1.96	0.47
2:E:856:LEU:O	2:E:881:ALA:HA	2.13	0.47
1:G:974:LEU:HD11	1:G:1000:LEU:HD22	1.96	0.47
1:A:30:ASN:HD22	1:A:43:VAL:HG22	1.79	0.47
2:H:773:ARG:HD2	2:H:879:GLY:O	2.13	0.47
1:A:1080:ARG:HD3	2:B:825:GLU:HA	1.96	0.47
1:D:166:ASP:HB3	1:D:219:VAL:HG23	1.97	0.47
1:D:224:GLU:N	1:D:225:PRO:HD2	2.29	0.47
1:G:969:GLU:OE2	1:G:973:ASN:ND2	2.42	0.47
2:B:803:LYS:HG3	3:C:142:VAL:HG21	1.96	0.47
1:D:932:LEU:HD22	1:D:965:PHE:CZ	2.50	0.47
1:D:1030:PHE:CZ	1:D:1038:GLY:HA3	2.50	0.47
2:B:856:LEU:O	2:B:881:ALA:HA	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:755:LEU:HD22	2:E:812:VAL:HG22	1.96	0.46
3:C:76:ILE:HD12	3:C:198:SER:HB3	1.97	0.46
1:A:816:LEU:HD13	1:A:831:VAL:HG22	1.97	0.46
1:D:971:ALA:HB3	1:D:973:ASN:HD22	1.79	0.46
2:E:823:LEU:HB3	2:E:829:VAL:HG11	1.98	0.46
1:G:2:SER:HB2	1:G:995:VAL:HG21	1.97	0.46
2:B:758:VAL:CG1	2:B:768:PRO:HD2	2.46	0.46
1:D:387:LEU:HG	1:D:717:LEU:HD11	1.98	0.46
2:H:820:LEU:HD22	2:H:839:PHE:CZ	2.51	0.46
1:D:315:THR:HG23	1:D:315:THR:O	2.16	0.46
3:I:63:ARG:HE	3:I:123:LEU:HD21	1.81	0.46
1:G:123:ILE:HD13	1:G:167:VAL:HG22	1.97	0.46
1:G:370:GLN:HG2	1:G:1014:MET:HE1	1.98	0.46
2:H:856:LEU:HD22	2:H:915:PRO:HA	1.97	0.46
1:G:59:GLY:HA2	1:G:1073:TRP:CE3	2.51	0.46
2:B:844:MET:HE2	2:B:844:MET:CA	2.46	0.45
1:G:794:ILE:HG22	1:G:799:PHE:HA	1.98	0.45
1:D:974:LEU:HD11	1:D:1000:LEU:HD22	1.98	0.45
1:G:828:TYR:CE1	1:G:861:VAL:HG21	2.51	0.45
2:B:773:ARG:HD3	2:B:881:ALA:O	2.16	0.45
2:B:823:LEU:CD1	2:B:867:LEU:HD13	2.46	0.45
1:G:849:VAL:HG11	1:G:851:PHE:CZ	2.51	0.45
2:H:885:ASN:ND2	2:H:888:GLU:HB3	2.32	0.45
1:D:225:PRO:HG2	1:D:267:ASN:O	2.16	0.45
2:E:917:ILE:HG13	2:E:918:ASP:N	2.32	0.45
1:G:1080:ARG:HD3	2:H:825:GLU:HA	1.98	0.45
1:A:213:GLU:HG2	1:A:215:GLU:H	1.81	0.45
2:E:756:LYS:HD2	2:E:813:PHE:CE1	2.52	0.45
1:G:376:VAL:HG13	1:G:389:ILE:HD13	1.99	0.45
2:H:758:VAL:O	2:H:808:ALA:HB1	2.17	0.45
1:G:315:THR:HG23	1:G:315:THR:O	2.16	0.45
1:A:1016:ASN:C	1:A:1018:GLY:H	2.20	0.45
2:E:828:LEU:O	2:E:1034:PRO:HD2	2.16	0.45
1:G:387:LEU:HD11	1:G:735:VAL:HG21	1.99	0.45
1:A:92:LYS:HD2	1:A:101:ILE:HD11	1.99	0.45
2:E:840:MET:HG3	2:E:926:LEU:HD13	1.99	0.45
2:E:844:MET:HE2	2:E:844:MET:HA	1.99	0.45
1:G:190:VAL:HG21	1:G:231:ILE:HD11	1.99	0.45
2:B:856:LEU:HD11	2:B:884:TYR:HB2	1.99	0.44
1:G:123:ILE:CD1	1:G:167:VAL:HG22	2.47	0.44
1:G:223:PRO:HG3	1:G:263:ARG:HH11	1.81	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:184:MET:CE	3:C:267:HIS:HA	2.47	0.44
2:E:807:GLY:O	3:F:145:ARG:NH1	2.44	0.44
1:G:184:ASP:HB2	1:G:185:PRO:CD	2.47	0.44
3:I:61:GLY:HA3	3:I:71:LEU:HD21	2.00	0.44
1:A:889:ARG:HD2	1:A:891:TYR:CZ	2.52	0.44
3:F:60:VAL:HG22	3:F:123:LEU:HD12	1.99	0.44
2:B:892:TYR:HB3	2:B:913:TYR:CZ	2.53	0.44
1:D:7:VAL:HG12	1:D:1091:GLY:HA3	1.99	0.44
1:D:744:ASP:OD1	1:D:746:SER:HB3	2.18	0.44
2:H:860:ILE:HD11	2:H:875:LEU:HD21	1.99	0.44
1:D:143:ILE:HG12	1:D:154:ALA:HB2	1.99	0.44
1:G:248:ILE:HG12	1:G:250:PRO:HD3	2.00	0.44
2:H:760:LEU:HD12	2:H:760:LEU:N	2.33	0.44
1:A:184:ASP:HB2	1:A:185:PRO:CD	2.47	0.44
2:E:803:LYS:HA	3:F:142:VAL:HG11	1.99	0.44
1:G:762:SER:O	1:G:803:HIS:HA	2.18	0.44
2:H:951:LEU:HD21	2:H:986:PHE:HE2	1.83	0.44
1:A:7:VAL:HG12	1:A:1091:GLY:HA3	2.00	0.44
1:A:1133:VAL:O	1:A:1137:THR:HG23	2.17	0.44
1:A:92:LYS:CD	1:A:101:ILE:HD11	2.48	0.43
1:D:5:TYR:CE2	1:D:7:VAL:HG13	2.53	0.43
2:H:784:ARG:HH21	2:H:872:GLN:HG3	1.83	0.43
1:D:376:VAL:HG22	1:D:389:ILE:HG23	1.99	0.43
1:A:387:LEU:HD11	1:A:735:VAL:HG21	1.99	0.43
1:D:368:GLU:N	1:D:368:GLU:OE1	2.51	0.43
1:G:58:TYR:HB3	1:G:1073:TRP:CB	2.49	0.43
1:G:125:ASP:OD2	1:G:176:PRO:HB3	2.19	0.43
1:G:188:ARG:NH1	1:G:216:ALA:O	2.52	0.43
2:H:983:ARG:HA	2:H:994:LEU:HD11	2.01	0.43
1:G:5:TYR:CE2	1:G:7:VAL:HG13	2.53	0.43
1:G:927:MET:HG3	1:G:928:ARG:HG2	1.99	0.43
1:D:1105:MET:SD	1:D:1130:ILE:HD11	2.58	0.43
1:A:158:ARG:HH12	1:A:160:GLU:HG2	1.84	0.43
1:A:226:PHE:CE1	1:A:287:LYS:HG2	2.53	0.43
2:B:917:ILE:HG13	2:B:918:ASP:N	2.34	0.43
1:G:1011:SER:HB3	1:G:1015:GLN:NE2	2.34	0.43
2:B:858:ARG:NH1	2:B:882:ARG:HD3	2.33	0.43
3:F:265:MET:HB2	3:F:267:HIS:ND1	2.33	0.43
2:H:799:ALA:HB1	2:H:804:LYS:HB2	2.01	0.43
3:F:191:ASP:OD2	3:F:258:TYR:OH	2.27	0.43
1:A:223:PRO:HD3	1:A:271:TYR:OH	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:389:ILE:HG12	1:D:799:PHE:CZ	2.54	0.43
1:G:965:PHE:O	1:G:976:VAL:HA	2.18	0.43
1:A:282:MET:HB2	1:A:305:LEU:HD11	2.00	0.43
2:E:760:LEU:HD21	2:E:767:PHE:HD1	1.84	0.43
1:G:114:ARG:HD3	2:H:930:PHE:O	2.19	0.43
1:D:184:ASP:HB2	1:D:185:PRO:CD	2.49	0.42
1:A:372:GLN:HA	1:A:1014:MET:HA	2.01	0.42
1:D:378:CYS:SG	1:D:724:ILE:HB	2.59	0.42
1:D:971:ALA:HB3	1:D:973:ASN:ND2	2.35	0.42
1:A:387:LEU:HG	1:A:717:LEU:HD11	2.01	0.42
1:D:372:GLN:NE2	1:D:392:ASN:O	2.53	0.42
2:B:934:PRO:HB2	2:B:937:GLN:CG	2.49	0.42
1:A:126:PRO:HD3	1:A:169:PHE:HB3	2.01	0.42
1:G:311:ALA:HB2	1:G:324:VAL:HG13	2.01	0.42
1:G:330:ASP:HA	1:G:355:ASN:HB3	2.02	0.42
2:H:935:ILE:HD12	2:H:986:PHE:HZ	1.85	0.42
3:C:184:MET:HE1	3:C:267:HIS:HA	2.00	0.42
1:D:131:ILE:HB	1:D:143:ILE:HB	2.01	0.42
1:D:936:LYS:HE2	1:D:943:GLU:HB2	2.01	0.42
1:D:985:THR:HB	1:D:988:GLU:HG2	2.02	0.42
1:D:387:LEU:HB2	1:D:715:VAL:HB	2.02	0.42
1:G:971:ALA:HB3	1:G:973:ASN:HD22	1.84	0.42
1:A:330:ASP:HA	1:A:355:ASN:HB3	2.02	0.42
1:G:168:LYS:HE2	1:G:168:LYS:HB3	1.89	0.42
1:G:936:LYS:HD3	1:G:936:LYS:HA	1.91	0.42
1:A:1003:PHE:O	1:A:1032:THR:HA	2.20	0.41
1:G:909:ILE:HD11	5:H:1101:RQ5:C10	2.50	0.41
1:A:5:TYR:CE2	1:A:7:VAL:HG13	2.56	0.41
2:B:894:ASN:OD1	2:B:909:GLY:HA2	2.20	0.41
1:D:816:LEU:CD1	1:D:831:VAL:HG22	2.49	0.41
1:D:20:THR:HG23	1:D:315:THR:OG1	2.20	0.41
1:D:170:LEU:HD11	1:D:179:CYS:HB2	2.02	0.41
1:G:59:GLY:HA2	1:G:1073:TRP:CZ3	2.55	0.41
3:I:159:HIS:O	3:I:162:GLN:HG2	2.21	0.41
1:A:828:TYR:HE1	1:A:861:VAL:HG21	1.84	0.41
1:D:63:VAL:O	1:D:79:ILE:HA	2.21	0.41
1:D:790:ASN:HA	1:D:805:HIS:O	2.20	0.41
1:D:871:TYR:HH	2:E:1036:TRP:HE3	1.69	0.41
3:C:27:ASP:OD1	3:C:28:LYS:N	2.54	0.41
1:G:364:VAL:HG22	1:G:375:LEU:HD13	2.02	0.41
2:H:840:MET:HG3	2:H:926:LEU:HD13	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:910:MET:SD	1:A:912:LEU:HD21	2.61	0.41
2:B:858:ARG:HH12	2:B:882:ARG:HD3	1.86	0.41
1:D:749:THR:HG21	1:D:786:VAL:HG11	2.03	0.41
2:E:823:LEU:HB3	2:E:829:VAL:CG1	2.51	0.41
1:G:7:VAL:CG1	1:G:1091:GLY:HA3	2.50	0.41
1:G:275:ASP:OD1	1:G:275:ASP:C	2.60	0.41
2:H:953:GLY:O	2:H:1003:LEU:HD11	2.21	0.41
1:A:64:MET:HG3	1:A:77:LEU:HD11	2.03	0.40
1:D:771:PHE:CE1	1:D:845:GLN:HB3	2.56	0.40
1:G:946:ALA:CB	1:G:992:LEU:HG	2.51	0.40
1:A:1011:SER:OG	1:A:1013:VAL:HG22	2.22	0.40
1:A:1104:LYS:O	1:A:1108:VAL:HG23	2.20	0.40
2:B:803:LYS:HA	3:C:142:VAL:CG1	2.51	0.40
1:A:24:THR:HA	1:A:91:TYR:CD2	2.57	0.40
2:E:733:ILE:CG2	2:E:743:LYS:HB2	2.51	0.40
1:A:958:GLU:HB2	1:A:1007:PHE:CB	2.51	0.40
2:B:839:PHE:HE2	2:B:867:LEU:HD21	1.87	0.40
1:A:336:LEU:CD2	1:A:347:VAL:HG22	2.52	0.40
2:B:816:MET:HA	2:B:868:ASN:OD1	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	822/840 (98%)	802 (98%)	20 (2%)	0	100	100
1	D	823/840 (98%)	804 (98%)	19 (2%)	0	100	100
1	G	822/840 (98%)	799 (97%)	22 (3%)	1 (0%)	51	82
2	B	322/344 (94%)	311 (97%)	11 (3%)	0	100	100
2	E	322/344 (94%)	312 (97%)	9 (3%)	1 (0%)	41	72

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	326/344 (95%)	317 (97%)	9 (3%)	0	100	100
3	C	246/271 (91%)	243 (99%)	3 (1%)	0	100	100
3	F	246/271 (91%)	243 (99%)	3 (1%)	0	100	100
3	I	246/271 (91%)	243 (99%)	3 (1%)	0	100	100
All	All	4175/4365 (96%)	4074 (98%)	99 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	877	ASP
1	G	772	SER

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	721/728 (99%)	717 (99%)	4 (1%)	86	91
1	D	722/728 (99%)	721 (100%)	1 (0%)	93	97
1	G	721/728 (99%)	719 (100%)	2 (0%)	92	96
2	B	292/308 (95%)	286 (98%)	6 (2%)	53	75
2	E	292/308 (95%)	286 (98%)	6 (2%)	53	75
2	H	296/308 (96%)	290 (98%)	6 (2%)	55	76
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%)	221 (99%)	2 (1%)	78	87
All	All	3713/3834 (97%)	3684 (99%)	29 (1%)	81	89

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

Mol	Chain	Res	Type
1	A	20	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	248	ILE
1	A	766	SER
1	A	947	ARG
2	B	760	LEU
2	B	858	ARG
2	B	867	LEU
2	B	905	GLU
2	B	1036	TRP
2	B	1039	CYS
3	C	231	TYR
1	D	947	ARG
2	E	728	ASP
2	E	805	ASP
2	E	829	VAL
2	E	896	VAL
2	E	1036	TRP
2	E	1039	CYS
3	F	231	TYR
1	G	295	VAL
1	G	947	ARG
2	H	863	SER
2	H	1025	LEU
2	H	1033	LEU
2	H	1036	TRP
2	H	1039	CYS
2	H	1041	GLU
3	I	146	ILE
3	I	231	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	1.59	1 (12%)	10,14,16	1.35	2 (20%)
2	TPO	B	893	2	8,10,11	1.54	1 (12%)	10,14,16	1.35	1 (10%)
2	TPO	H	893	2	8,10,11	1.53	1 (12%)	10,14,16	1.22	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	E	893	2	-	5/9/11/13	-
2	TPO	B	893	2	-	1/9/11/13	-
2	TPO	H	893	2	-	4/9/11/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	893	TPO	P-O1P	3.41	1.61	1.50
2	H	893	TPO	P-O1P	3.39	1.61	1.50
2	B	893	TPO	P-O1P	3.39	1.61	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	893	TPO	P-OG1-CB	-3.74	111.92	123.21
2	H	893	TPO	P-OG1-CB	-2.97	114.25	123.21
2	E	893	TPO	P-OG1-CB	-2.76	114.87	123.21
2	E	893	TPO	CG2-CB-CA	-2.40	108.43	113.16

There are no chirality outliers.

All (10) torsion outliers are listed below:

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

Continued on next page...

Continued from previous page...

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	E	893	TPO	CA-CB-OG1-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

24 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	G	1205	-	4,4,4	0.15	0	6,6,6	0.09	0
4	SO4	C	301	-	4,4,4	0.16	0	6,6,6	0.11	0
4	SO4	F	302	-	4,4,4	0.15	0	6,6,6	0.09	0
4	SO4	I	301	-	4,4,4	0.15	0	6,6,6	0.12	0
4	SO4	D	1203	-	4,4,4	0.15	0	6,6,6	0.17	0
4	SO4	D	1204	-	4,4,4	0.14	0	6,6,6	0.10	0
4	SO4	G	1204	-	4,4,4	0.14	0	6,6,6	0.13	0
4	SO4	A	1202	-	4,4,4	0.15	0	6,6,6	0.05	0
4	SO4	D	1202	-	4,4,4	0.15	0	6,6,6	0.10	0
4	SO4	G	1203	-	4,4,4	0.15	0	6,6,6	0.11	0
4	SO4	A	1204	-	4,4,4	0.15	0	6,6,6	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	RQ5	B	1101	-	29,32,32	0.63	1 (3%)	32,43,43	1.08	3 (9%)
4	SO4	A	1201	-	4,4,4	0.17	0	6,6,6	0.09	0
4	SO4	D	1201	-	4,4,4	0.17	0	6,6,6	0.08	0
5	RQ5	E	1101	-	29,32,32	0.65	1 (3%)	32,43,43	1.34	5 (15%)
4	SO4	C	303	-	4,4,4	0.15	0	6,6,6	0.09	0
4	SO4	G	1202	-	4,4,4	0.15	0	6,6,6	0.07	0
5	RQ5	H	1101	-	29,32,32	0.63	0	32,43,43	1.10	3 (9%)
4	SO4	I	303	-	4,4,4	0.15	0	6,6,6	0.12	0
4	SO4	A	1203	-	4,4,4	0.15	0	6,6,6	0.08	0
4	SO4	G	1201	-	4,4,4	0.15	0	6,6,6	0.09	0
4	SO4	F	301	-	4,4,4	0.16	0	6,6,6	0.11	0
4	SO4	I	302	-	4,4,4	0.15	0	6,6,6	0.07	0
4	SO4	C	302	-	4,4,4	0.15	0	6,6,6	0.10	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	RQ5	B	1101	-	-	4/21/21/21	0/3/3/3
5	RQ5	E	1101	-	-	5/21/21/21	0/3/3/3
5	RQ5	H	1101	-	-	4/21/21/21	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1101	RQ5	C18-N5	-2.23	1.45	1.49
5	B	1101	RQ5	C18-N5	-2.15	1.45	1.49

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1101	RQ5	C17-N5-C18	4.35	129.69	125.42
5	H	1101	RQ5	C17-N5-C18	3.30	128.66	125.42
5	E	1101	RQ5	C16-C6-N2	-2.84	118.45	120.81
5	H	1101	RQ5	C16-C6-N2	-2.77	118.51	120.81
5	B	1101	RQ5	C16-C6-N2	-2.66	118.60	120.81
5	B	1101	RQ5	C17-N5-C18	2.63	128.00	125.42
5	E	1101	RQ5	C5-N1-C3	-2.57	119.98	124.31
5	E	1101	RQ5	C18-N5-C21	-2.44	124.25	127.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1101	RQ5	C5-N6-C21	-2.42	112.53	115.28
5	B	1101	RQ5	C5-N6-C21	-2.42	112.53	115.28
5	H	1101	RQ5	C5-N6-C21	-2.25	112.72	115.28

There are no chirality outliers.

All (13) torsion outliers are listed below:

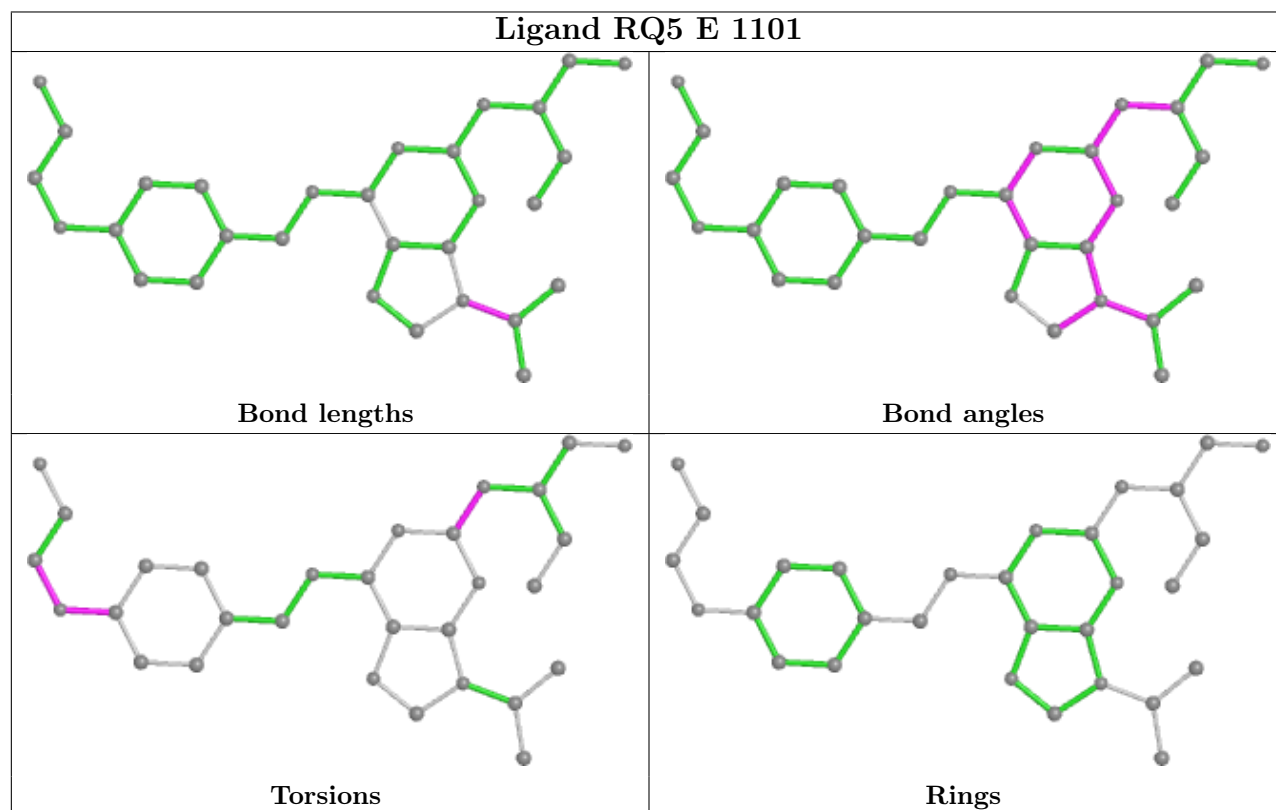
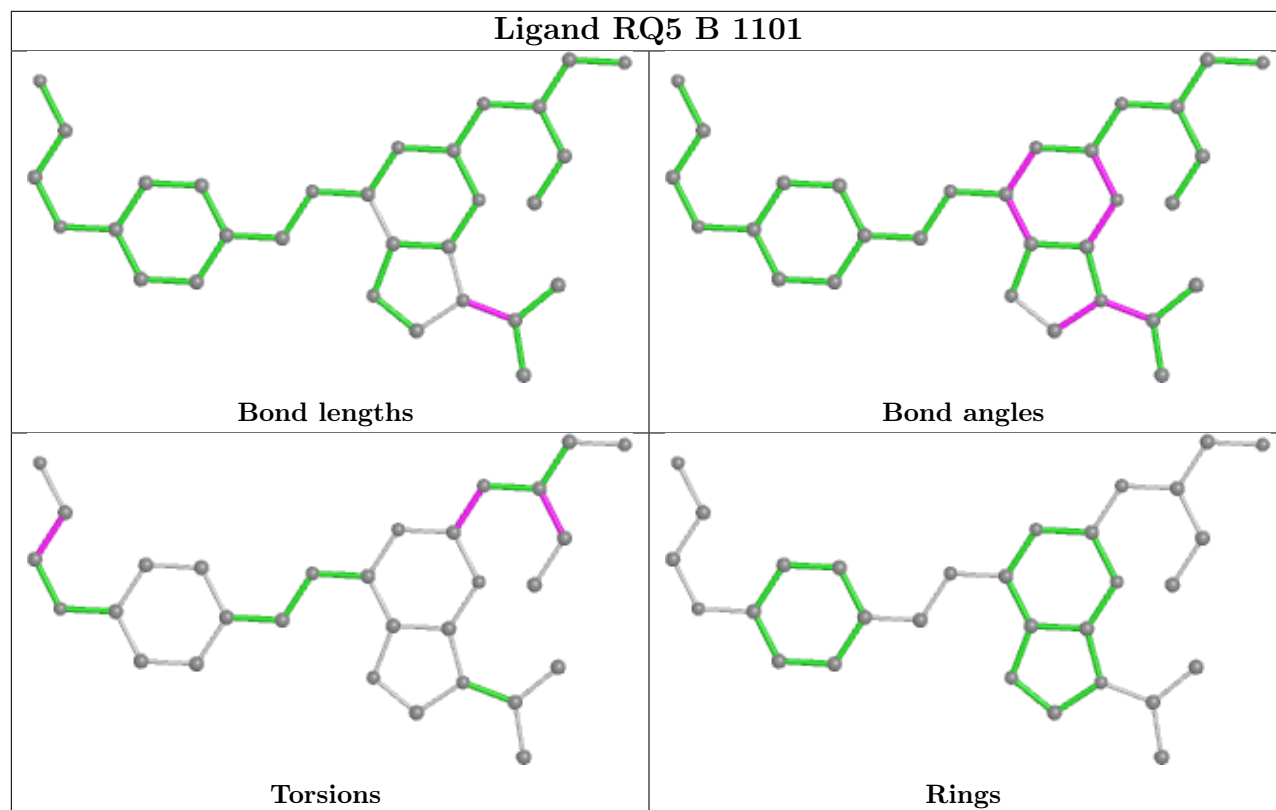
Mol	Chain	Res	Type	Atoms
5	B	1101	RQ5	N2-C5-N1-C3
5	B	1101	RQ5	N6-C5-N1-C3
5	E	1101	RQ5	N2-C5-N1-C3
5	E	1101	RQ5	N6-C5-N1-C3
5	H	1101	RQ5	N2-C5-N1-C3
5	H	1101	RQ5	N6-C5-N1-C3
5	H	1101	RQ5	O2-C12-C13-O3
5	B	1101	RQ5	O2-C12-C13-O3
5	E	1101	RQ5	C14-C11-O2-C12
5	E	1101	RQ5	C10-C11-O2-C12
5	E	1101	RQ5	C13-C12-O2-C11
5	H	1101	RQ5	C1-C2-C3-C4
5	B	1101	RQ5	C1-C2-C3-N1

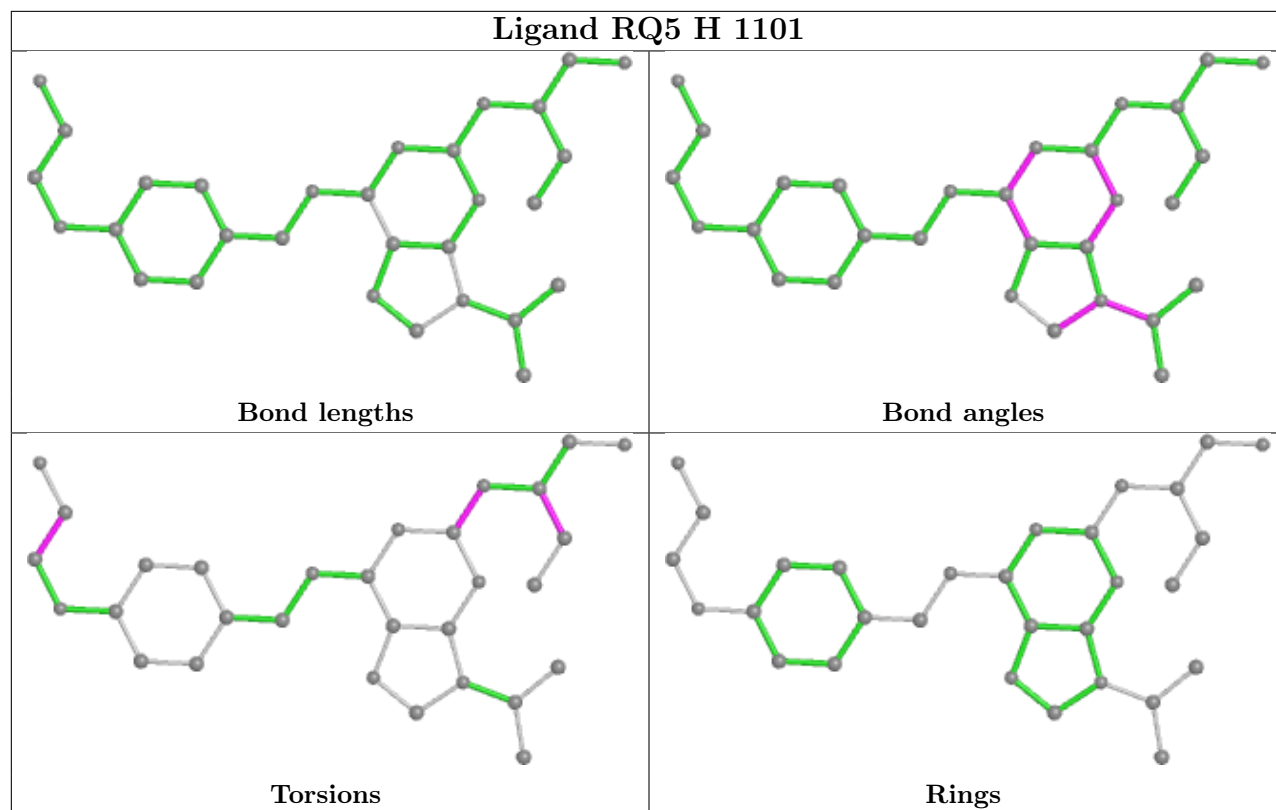
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	1101	RQ5	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	826/840 (98%)	0.62	63 (7%) 13 12	97, 132, 204, 292	0
1	D	827/840 (98%)	0.56	43 (5%) 27 25	95, 130, 198, 285	0
1	G	826/840 (98%)	0.59	67 (8%) 12 11	103, 137, 203, 268	0
2	B	324/344 (94%)	0.89	43 (13%) 3 3	111, 139, 205, 238	0
2	E	324/344 (94%)	0.78	26 (8%) 12 11	101, 133, 201, 251	0
2	H	328/344 (95%)	0.85	22 (6%) 17 17	89, 114, 200, 253	0
3	C	248/271 (91%)	0.59	15 (6%) 21 21	106, 128, 167, 224	0
3	F	248/271 (91%)	0.63	10 (4%) 38 35	86, 109, 146, 217	0
3	I	248/271 (91%)	0.64	9 (3%) 42 39	89, 111, 151, 220	0
All	All	4199/4365 (96%)	0.65	298 (7%) 16 15	86, 129, 201, 292	0

All (298) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	1039	CYS	9.2
2	H	1043	TRP	7.1
2	H	1041	GLU	7.0
2	E	1036	TRP	6.9
2	H	1036	TRP	6.3
2	E	1039	CYS	5.9
2	H	1040	HIS	5.9
2	B	800	LEU	5.4
2	B	1034	PRO	5.3
2	B	798	ASP	5.0
2	B	799	ALA	4.9
2	H	1034	PRO	4.8
2	B	1039	CYS	4.8
2	B	1036	TRP	4.6
2	H	1033	LEU	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	295	VAL	4.4
2	H	798	ASP	4.4
1	D	91	TYR	4.4
2	B	802	PHE	4.3
2	H	828	LEU	4.2
2	B	828	LEU	4.2
3	I	267	HIS	4.1
3	I	266	PRO	4.1
1	A	1118	SER	4.0
1	A	1016	ASN	3.9
1	A	1116	ASP	3.9
2	B	896	VAL	3.7
3	I	260	GLN	3.6
2	H	1038	ASP	3.6
1	A	1097	PHE	3.6
2	B	867	LEU	3.5
2	H	839	PHE	3.5
1	A	23	PHE	3.5
3	F	262	LYS	3.5
1	D	78	PHE	3.5
1	D	1129	LEU	3.4
2	H	1032	ASP	3.4
2	E	802	PHE	3.4
1	D	195	VAL	3.4
1	G	314	LEU	3.4
3	C	181	LEU	3.4
1	D	927	MET	3.4
1	A	131	ILE	3.3
1	G	327	ARG	3.3
2	B	803	LYS	3.3
1	A	1018	GLY	3.3
2	E	829	VAL	3.3
1	A	135	LEU	3.2
1	A	79	ILE	3.2
1	A	145	LEU	3.2
1	D	133	LEU	3.2
2	B	875	LEU	3.2
1	G	858	LEU	3.2
1	A	78	PHE	3.2
1	G	1039	LEU	3.1
1	G	1129	LEU	3.1
2	B	797	GLN	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	809	PHE	3.1
1	A	39	LEU	3.1
2	B	738	TYR	3.1
2	B	839	PHE	3.1
1	A	1035	GLY	3.1
1	G	253	ILE	3.0
1	A	89	LEU	3.0
3	F	254	ILE	3.0
2	E	831	PHE	3.0
1	A	1129	LEU	3.0
1	G	328	LEU	3.0
1	A	1019	GLU	3.0
3	F	264	GLN	2.9
1	A	297	LEU	2.9
1	D	39	LEU	2.9
2	B	878	PHE	2.9
1	G	302	VAL	2.9
2	H	802	PHE	2.9
2	B	952	CYS	2.9
1	A	1114	TYR	2.9
1	G	387	LEU	2.9
2	B	876	ALA	2.9
1	G	1043	LEU	2.9
1	G	306	GLY	2.9
1	G	816	LEU	2.9
1	G	131	ILE	2.8
2	B	755	LEU	2.8
1	G	1118	SER	2.8
1	A	49	LEU	2.8
1	G	49	LEU	2.8
1	A	133	LEU	2.8
1	D	31	LEU	2.8
1	G	323	PHE	2.8
1	D	2	SER	2.8
1	D	328	LEU	2.8
1	G	303	GLU	2.7
1	A	1029	LEU	2.7
1	D	928	ARG	2.7
2	B	860	ILE	2.7
1	G	375	LEU	2.7
2	H	875	LEU	2.7
1	G	5	TYR	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	951	LEU	2.7
2	E	867	LEU	2.7
1	D	931	LEU	2.7
1	A	57	MET	2.7
1	A	32	LEU	2.7
2	E	860	ILE	2.7
1	A	881	LEU	2.7
1	G	966	LEU	2.7
2	E	1035	HIS	2.7
3	C	132	PHE	2.7
1	D	197	LEU	2.6
1	A	1126	ALA	2.6
1	A	140	PHE	2.6
2	H	1035	HIS	2.6
1	A	953	TRP	2.6
3	C	155	LEU	2.6
1	D	281	PHE	2.6
2	B	831	PHE	2.6
1	G	300	LEU	2.6
1	G	953	TRP	2.6
2	H	867	LEU	2.6
1	A	367	LEU	2.6
1	D	232	ILE	2.6
3	C	267	HIS	2.5
1	G	1088	PHE	2.5
2	H	829	VAL	2.5
2	E	839	PHE	2.5
1	G	133	LEU	2.5
2	B	986	PHE	2.5
3	C	153	PHE	2.5
3	C	161	TYR	2.5
1	G	31	LEU	2.5
2	B	865	ILE	2.5
3	I	222	ILE	2.5
1	G	276	MET	2.5
1	A	858	LEU	2.5
3	C	147	LEU	2.5
2	B	932	LYS	2.5
1	A	120	ILE	2.5
2	B	930	PHE	2.5
2	E	935	ILE	2.5
1	D	1004	VAL	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	977	CYS	2.4
1	A	1020	THR	2.4
1	A	33	ILE	2.4
2	H	955	PRO	2.4
2	B	926	LEU	2.4
1	D	89	LEU	2.4
2	E	896	VAL	2.4
1	G	232	ILE	2.4
1	D	1097	PHE	2.4
1	A	912	LEU	2.4
1	D	360	VAL	2.4
1	G	273	LEU	2.4
2	E	866	LEU	2.4
1	A	1115	ASP	2.4
1	G	2	SER	2.4
1	G	195	VAL	2.4
2	E	1029	ALA	2.4
1	D	61	ILE	2.4
3	C	234	TRP	2.4
1	D	1012	LEU	2.4
1	A	930	VAL	2.4
1	D	121	ILE	2.4
1	A	226	PHE	2.4
3	I	263	GLN	2.4
1	D	140	PHE	2.3
1	G	64	MET	2.3
1	G	1007	PHE	2.3
1	G	143	ILE	2.3
1	A	745	THR	2.3
2	E	897	ILE	2.3
3	C	164	LEU	2.3
1	A	273	LEU	2.3
2	B	913	TYR	2.3
2	E	733	ILE	2.3
2	E	828	LEU	2.3
1	G	974	LEU	2.3
1	A	975	PHE	2.3
2	E	878	PHE	2.3
1	D	1039	LEU	2.3
2	H	831	PHE	2.3
1	A	258	ILE	2.3
2	E	727	PHE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	291	MET	2.3
1	D	64	MET	2.3
1	G	57	MET	2.3
1	G	77	LEU	2.3
2	B	767	PHE	2.3
1	D	117	GLU	2.3
1	A	1040	VAL	2.3
1	D	1065	VAL	2.3
1	A	1054	MET	2.3
2	B	733	ILE	2.2
1	D	1126	ALA	2.2
1	A	88	ILE	2.2
2	E	738	TYR	2.2
1	G	1136	LEU	2.2
1	D	253	ILE	2.2
1	G	1097	PHE	2.2
1	A	708	GLN	2.2
1	A	933	LEU	2.2
1	G	39	LEU	2.2
1	A	34	ALA	2.2
3	F	229	PRO	2.2
1	G	135	LEU	2.2
2	B	883	LEU	2.2
2	B	804	LYS	2.2
1	A	356	LEU	2.2
2	E	906	LEU	2.2
1	D	1030	PHE	2.2
1	A	376	VAL	2.2
1	A	724	ILE	2.2
1	D	33	ILE	2.2
1	G	61	ILE	2.2
1	G	910	MET	2.2
2	H	964	ILE	2.2
1	A	871	TYR	2.2
1	G	280	LEU	2.2
2	H	892	TYR	2.2
1	D	369	ARG	2.2
1	A	359	ILE	2.2
1	G	390	ILE	2.2
1	G	1108	VAL	2.2
1	G	722	ARG	2.2
1	G	792	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	F	193	LEU	2.2
2	B	904	PRO	2.2
1	A	387	LEU	2.2
1	D	49	LEU	2.2
3	C	76	ILE	2.2
1	G	1076	PHE	2.1
1	G	1040	VAL	2.1
3	F	250	ILE	2.1
1	D	5	TYR	2.1
1	G	336	LEU	2.1
2	B	884	TYR	2.1
1	D	1007	PHE	2.1
3	F	263	GLN	2.1
2	B	955	PRO	2.1
1	D	32	LEU	2.1
2	E	820	LEU	2.1
1	A	216	ALA	2.1
1	A	830	ILE	2.1
1	D	112	ILE	2.1
2	B	935	ILE	2.1
1	G	1028	VAL	2.1
2	B	887	GLU	2.1
1	A	880	LEU	2.1
1	D	42	TYR	2.1
2	E	913	TYR	2.1
3	F	87	PHE	2.1
1	G	32	LEU	2.1
1	A	87	CYS	2.1
1	A	1100	ILE	2.1
1	D	957	VAL	2.1
3	C	146	ILE	2.1
1	G	1055	GLN	2.1
2	B	890	ARG	2.1
1	G	1029	LEU	2.1
1	G	829	PHE	2.1
2	E	930	PHE	2.1
2	E	784	ARG	2.1
1	G	230	ILE	2.1
1	A	130	MET	2.1
1	G	836	VAL	2.1
3	C	120	ALA	2.1
1	A	143	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	333	LEU	2.1
3	I	64	LEU	2.1
1	G	78	PHE	2.0
2	H	1037	GLN	2.0
1	G	6	VAL	2.0
1	A	220	ILE	2.0
3	I	254	ILE	2.0
2	B	758	VAL	2.0
1	G	317	LEU	2.0
1	G	710	LEU	2.0
1	A	112	ILE	2.0
1	G	139	LEU	2.0
2	B	824	LEU	2.0
3	C	116	ILE	2.0
1	D	377	THR	2.0
1	G	362	MET	2.0
1	D	55	VAL	2.0
2	E	758	VAL	2.0
1	D	314	LEU	2.0
3	C	148	LEU	2.0
3	I	257	LEU	2.0
1	A	1088	PHE	2.0
3	F	238	PHE	2.0
3	F	266	PRO	2.0
1	D	356	LEU	2.0
3	C	193	LEU	2.0
2	E	850	CYS	2.0
1	G	932	LEU	2.0
2	B	778	LEU	2.0
2	B	997	LEU	2.0
3	I	100	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

MODRES-RSR INFOmissingINFO

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands

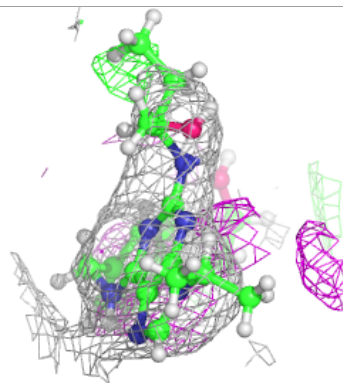
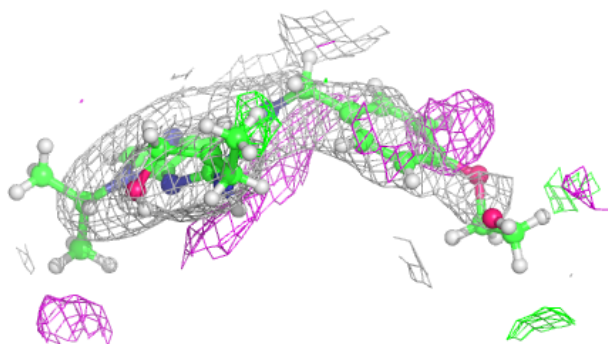
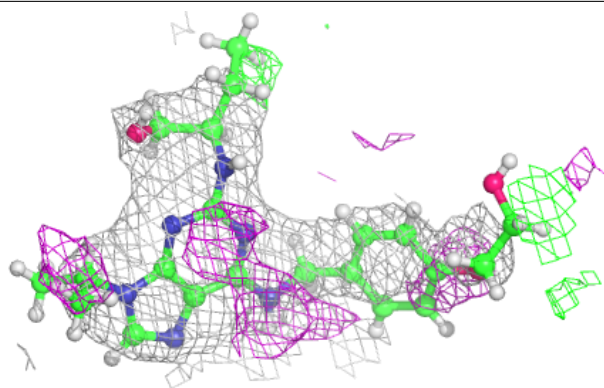
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SO4	D	1204	5/5	0.62	0.24	144,155,166,212	0
4	SO4	I	303	5/5	0.63	0.24	149,153,158,201	0
4	SO4	C	303	5/5	0.71	0.15	158,159,166,209	0
4	SO4	A	1204	5/5	0.74	0.17	140,149,155,197	0
4	SO4	G	1202	5/5	0.77	0.19	153,158,159,198	0
4	SO4	G	1205	5/5	0.78	0.21	143,145,153,195	0
4	SO4	D	1202	5/5	0.80	0.19	135,143,149,193	0
4	SO4	G	1204	5/5	0.80	0.20	155,155,166,213	0
4	SO4	C	302	5/5	0.81	0.15	149,150,157,196	0
4	SO4	D	1203	5/5	0.84	0.21	132,137,142,200	0
4	SO4	A	1202	5/5	0.84	0.22	130,135,142,185	0
4	SO4	C	301	5/5	0.85	0.19	146,148,150,179	0
5	RQ5	E	1101	30/30	0.85	0.60	115,142,185,189	30
4	SO4	F	302	5/5	0.86	0.13	140,144,150,195	0
5	RQ5	H	1101	30/30	0.87	0.52	111,139,185,189	30
4	SO4	D	1201	5/5	0.89	0.25	134,136,139,162	0
5	RQ5	B	1101	30/30	0.89	0.50	120,145,185,189	30
4	SO4	G	1201	5/5	0.90	0.20	140,140,146,157	0
4	SO4	A	1203	5/5	0.91	0.23	127,129,135,186	0
4	SO4	G	1203	5/5	0.92	0.14	149,152,158,193	0
4	SO4	I	302	5/5	0.92	0.12	147,150,158,195	0
4	SO4	A	1201	5/5	0.92	0.19	136,136,137,155	0
4	SO4	I	301	5/5	0.95	0.19	126,127,130,146	0
4	SO4	F	301	5/5	0.95	0.22	123,125,129,148	0

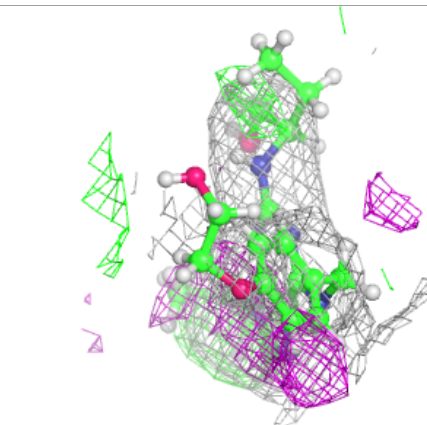
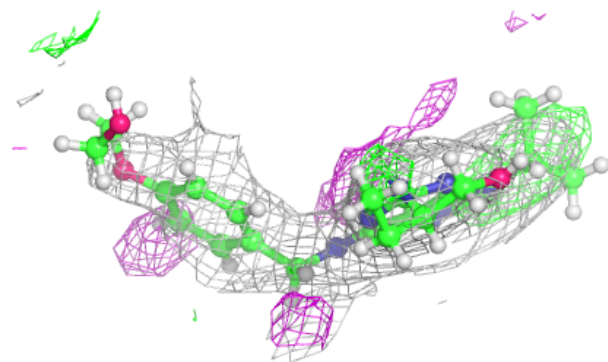
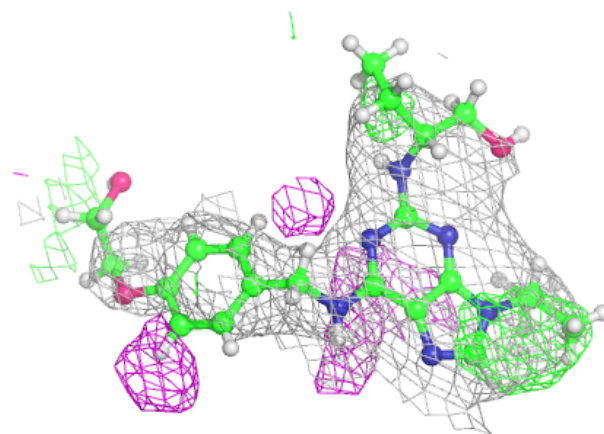
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

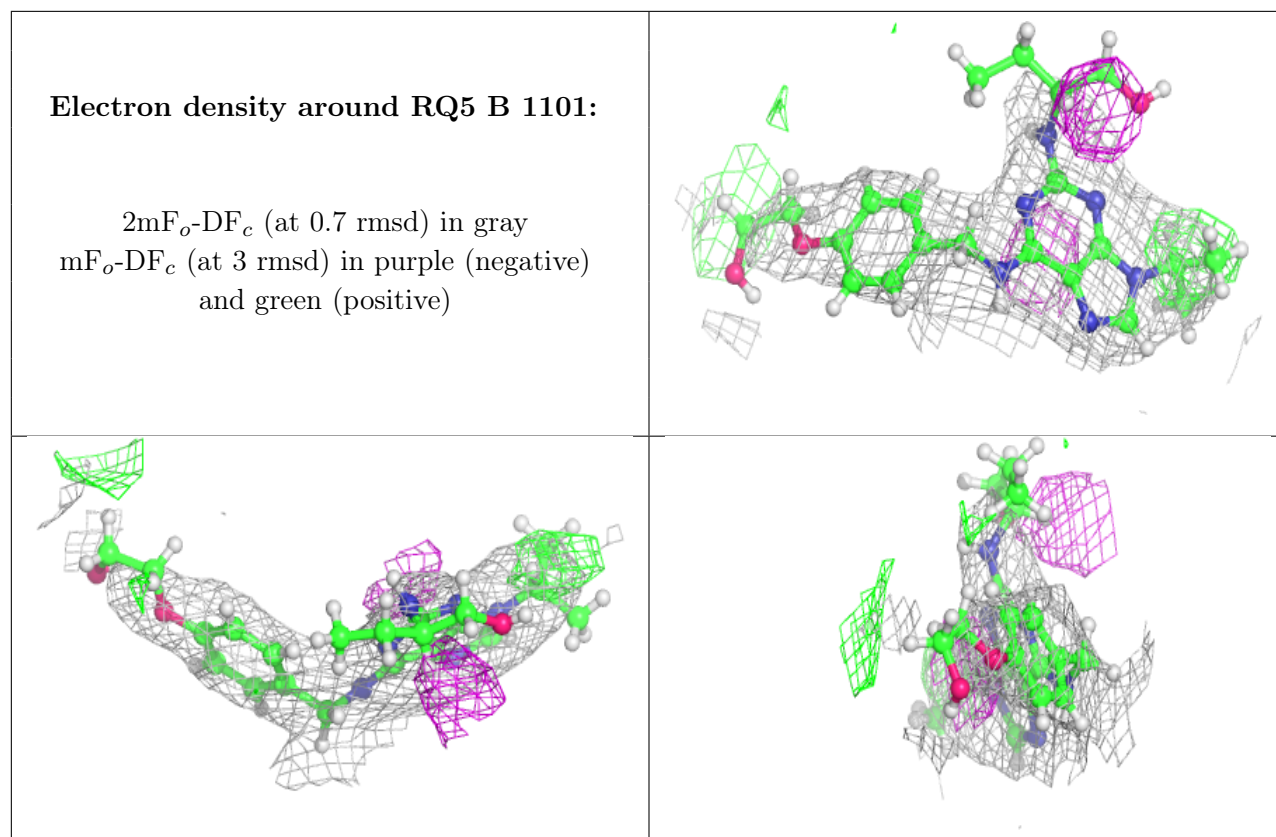
Electron density around RQ5 E 1101:

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

**Electron density around RQ5 H 1101:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.