Full wwPDB X-ray Structure Validation Report ⓘ

Sep 7, 2023 – 04:39 pm BST

PDB ID	:	8BU3
Title	:	Structure of DDB1 bound to DS19-engaged CDK12-cyclin K
Authors	:	Kozicka, Z.; Kempf, G.; Petzold, G.; Thoma, N.H.
Deposited on	:	2022-11-30
Resolution	:	3.42 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:

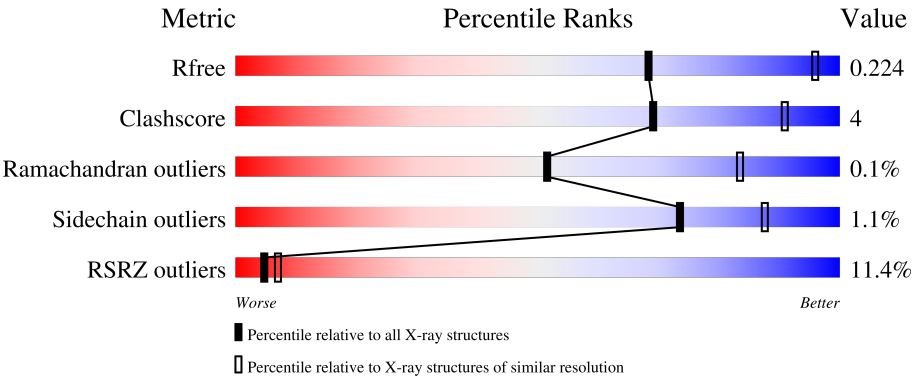
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 3.42 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	1486 (3.50-3.34)
Clashscore	141614	1572 (3.50-3.34)
Ramachandran outliers	138981	1534 (3.50-3.34)
Sidechain outliers	138945	1535 (3.50-3.34)
RSRZ outliers	127900	1395 (3.50-3.34)

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	14% 88% 11% •
1	D	840	13% 87% 11% •
1	G	840	11% 88% 10% •
2	B	344	17% 82% 12% • 5%
2	E	344	10% 81% 13% 6%

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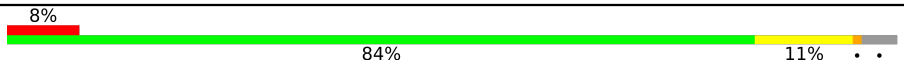
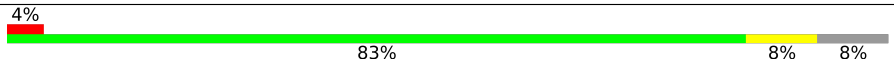
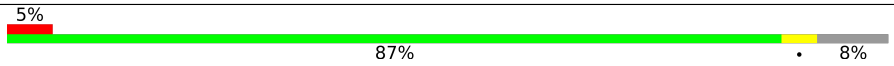
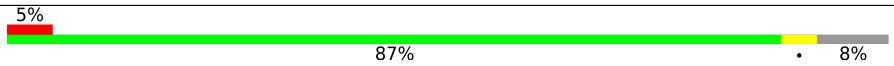
Mol	Chain	Length	Quality of chain
2	H	344	
3	C	271	
3	F	271	
3	I	271	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 67495 atoms, of which 33639 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	826	Total	C	H	N	O	S	6450	0	0
			12937	4105	6450	1094	1252	36			
1	D	827	Total	C	H	N	O	S	6462	0	0
			12957	4111	6462	1095	1253	36			
1	G	826	Total	C	H	N	O	S	6455	0	0
			12941	4106	6455	1093	1251	36			

There are 30 discrepancies between the modelled and reference sequences:

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

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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	ARG	-	expression tag	UNP Q16531
G	700	GLY	-	linker	UNP Q16531
G	701	ASN	-	linker	UNP Q16531
G	702	GLY	-	linker	UNP Q16531
G	703	ASN	-	linker	UNP Q16531
G	704	SER	-	linker	UNP Q16531
G	705	GLY	-	linker	UNP Q16531

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

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
2	B	326	Total	C	H	N	O	P	S	2670	0	0
			5326	1701	2670	450	487	1	17			
2	E	325	Total	C	H	N	O	P	S	2663	0	0
			5309	1695	2663	447	486	1	17			
2	H	330	Total	C	H	N	O	P	S	2702	0	0
			5395	1726	2702	455	494	1	17			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	709	GLY	-	expression tag	UNP Q9NYV4
B	710	GLY	-	expression tag	UNP Q9NYV4
B	711	GLY	-	expression tag	UNP Q9NYV4
B	965	ARG	LYS	engineered mutation	UNP Q9NYV4
B	1052	GLN	-	expression tag	UNP Q9NYV4
E	709	GLY	-	expression tag	UNP Q9NYV4
E	710	GLY	-	expression tag	UNP Q9NYV4
E	711	GLY	-	expression tag	UNP Q9NYV4
E	965	ARG	LYS	engineered mutation	UNP Q9NYV4
E	1052	GLN	-	expression tag	UNP Q9NYV4
H	709	GLY	-	expression tag	UNP Q9NYV4
H	710	GLY	-	expression tag	UNP Q9NYV4
H	711	GLY	-	expression tag	UNP Q9NYV4
H	965	ARG	LYS	engineered mutation	UNP Q9NYV4
H	1052	GLN	-	expression tag	UNP Q9NYV4

- Molecule 3 is a protein called Cyclin-K.

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

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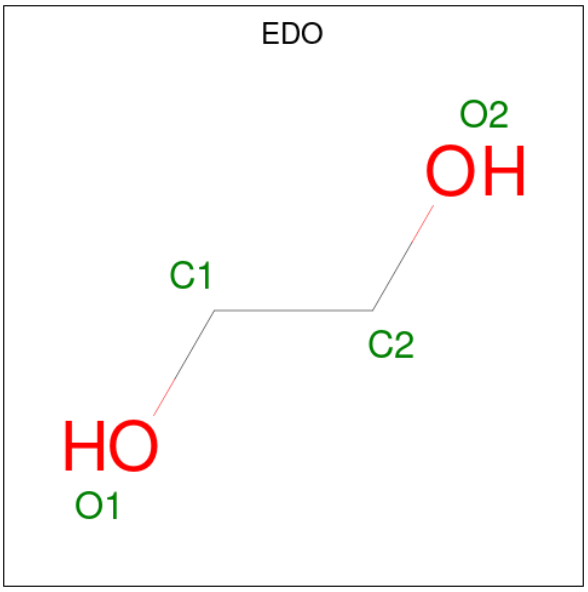
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	F	248	Total	C	H	N	O	S	2048	0	0
			4111	1341	2048	346	363	13			
3	I	248	Total	C	H	N	O	S	2048	0	0
			4111	1341	2048	346	363	13			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	expression tag	UNP O75909
C	-2	GLY	-	expression tag	UNP O75909
C	-1	GLY	-	expression tag	UNP O75909
C	0	ARG	-	expression tag	UNP O75909
F	-3	GLY	-	expression tag	UNP O75909
F	-2	GLY	-	expression tag	UNP O75909
F	-1	GLY	-	expression tag	UNP O75909
F	0	ARG	-	expression tag	UNP O75909
I	-3	GLY	-	expression tag	UNP O75909
I	-2	GLY	-	expression tag	UNP O75909
I	-1	GLY	-	expression tag	UNP O75909
I	0	ARG	-	expression tag	UNP O75909

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	6	0
			10	2	6	2		

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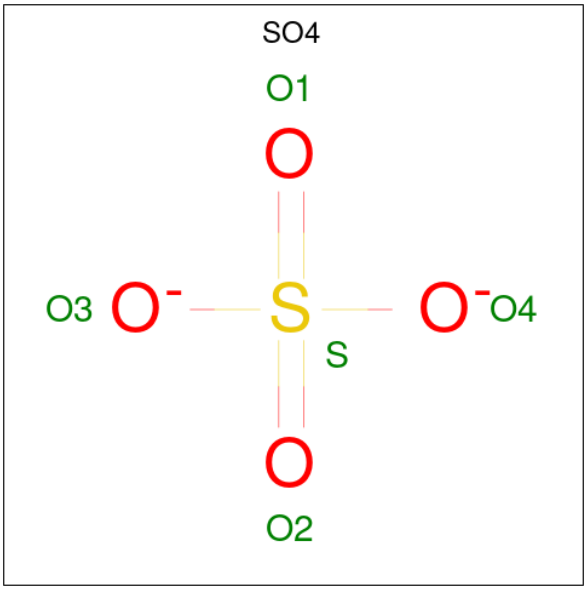
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total C H O 10 2 6 2	6	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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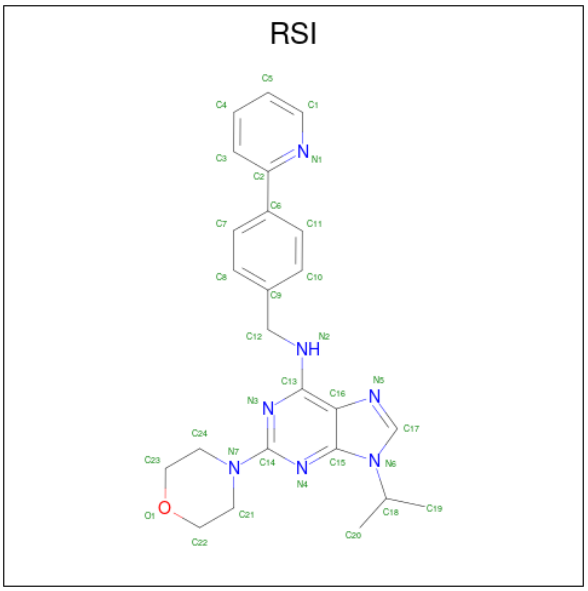
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	F	1	Total O S 5 4 1	0	0
5	G	1	Total O S 5 4 1	0	0
5	G	1	Total O S 5 4 1	0	0
5	G	1	Total O S 5 4 1	0	0
5	G	1	Total O S 5 4 1	0	0
5	H	1	Total O S 5 4 1	0	0
5	H	1	Total O S 5 4 1	0	0
5	I	1	Total O S 5 4 1	0	0
5	I	1	Total O S 5 4 1	0	0
5	I	1	Total O S 5 4 1	0	0

- Molecule 6 is 2-morpholin-4-yl-9-propan-2-yl- {N}-[(4-pyridin-2-ylphenyl)methyl]purin-6-amine (three-letter code: RSI) (formula: $C_{24}H_{27}N_7O$) (labeled as "Ligand of Interest" by depositor).



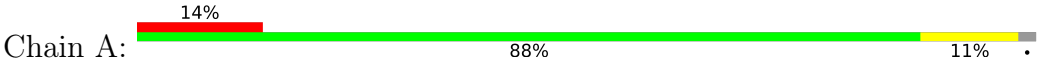
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	H	N	O	27	0
			59	24	27	7	1		
6	E	1	Total	C	H	N	O	27	0
			59	24	27	7	1		
6	H	1	Total	C	H	N	O	27	0
			59	24	27	7	1		

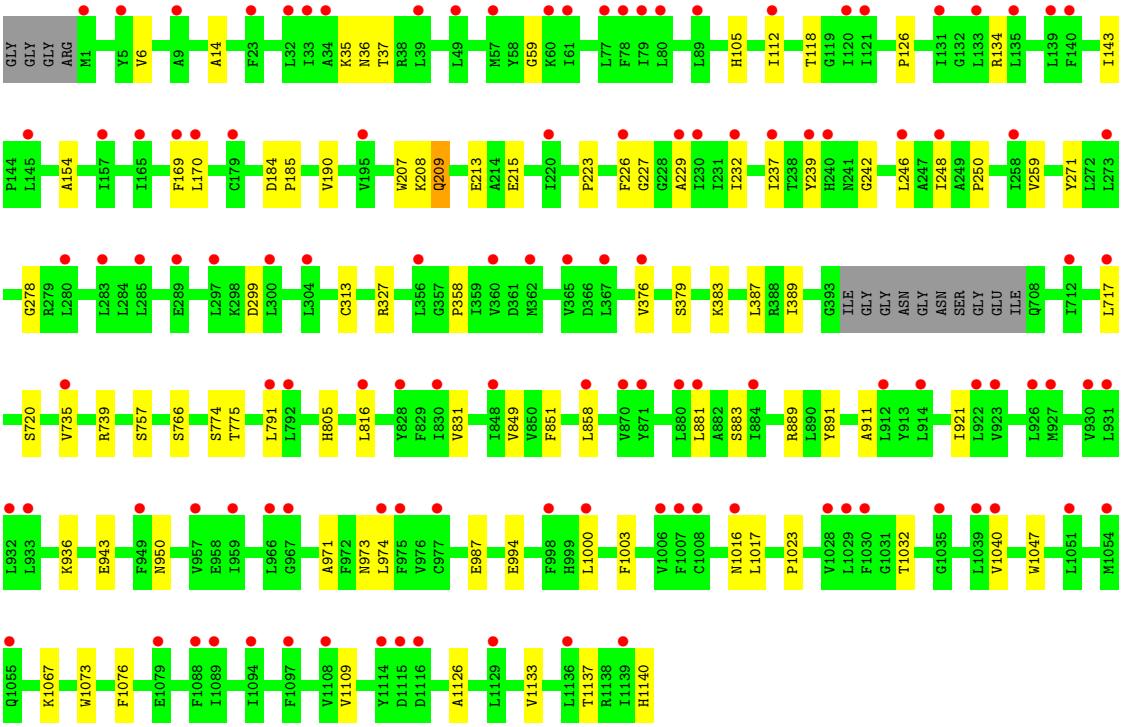
3 Residue-property plots (i)

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

• Molecule 1: DNA damage-binding protein 1

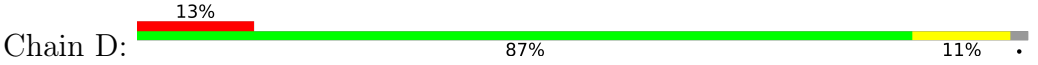
Chain A:

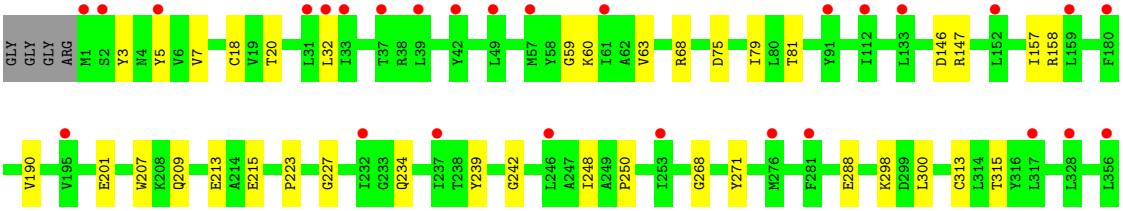


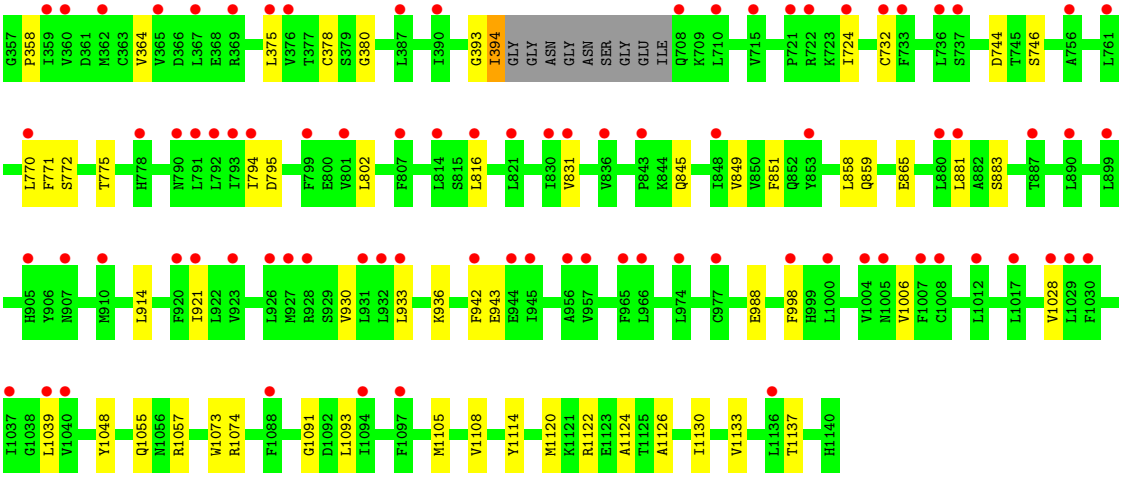


• Molecule 1: DNA damage-binding protein 1

Chain D:





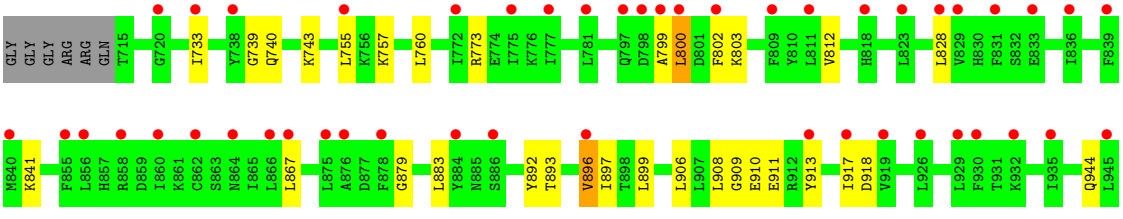


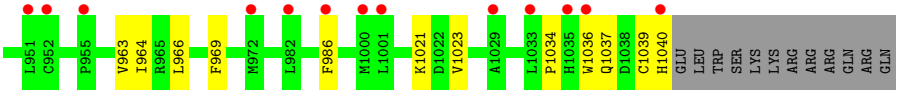
• Molecule 1: DNA damage-binding protein 1

Chain G:

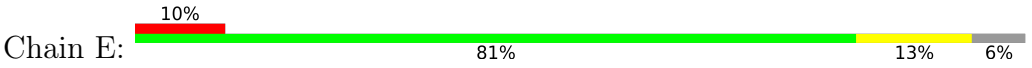
• Molecule 2: Cyclin-dependent kinase 12

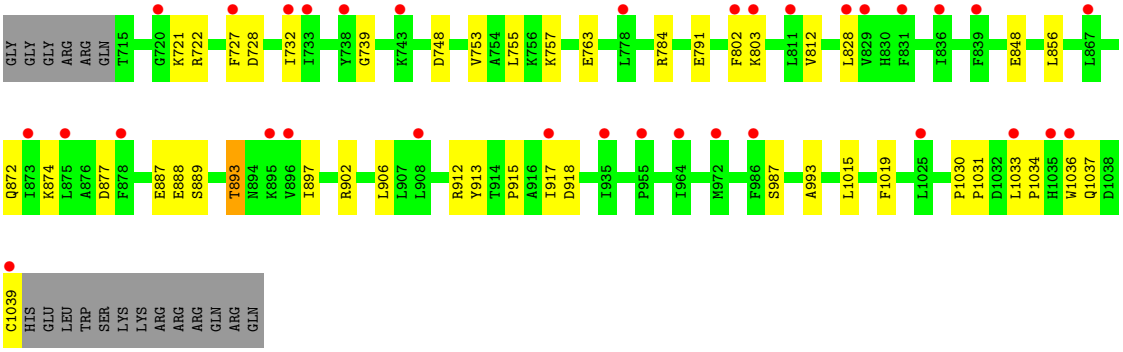
Chain B:



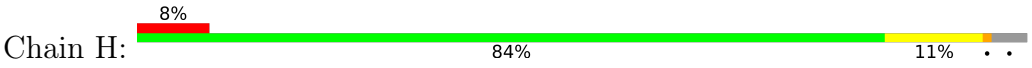


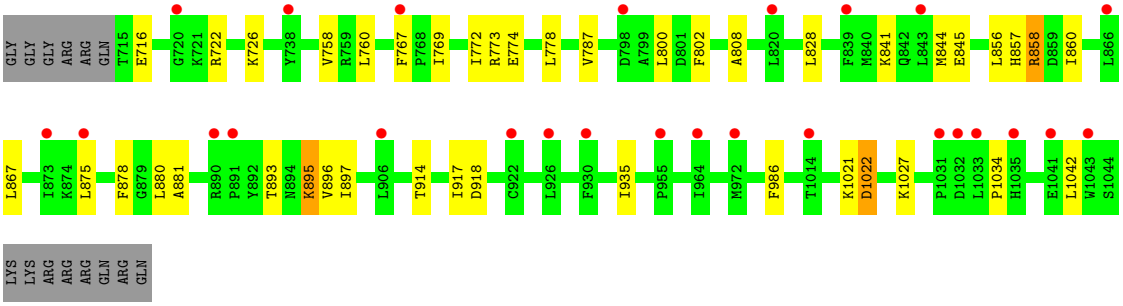
• Molecule 2: Cyclin-dependent kinase 12



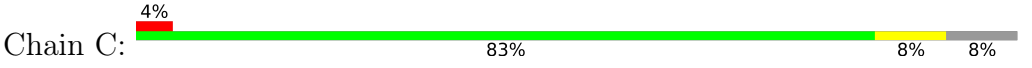


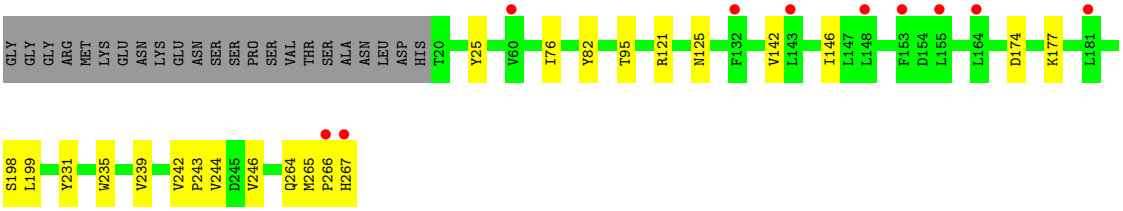
• Molecule 2: Cyclin-dependent kinase 12



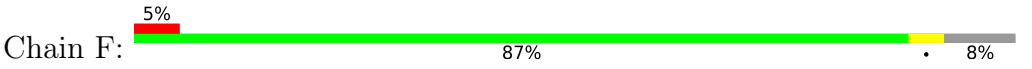


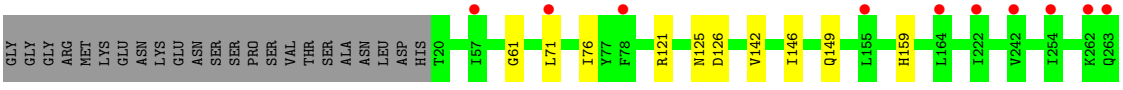
• Molecule 3: Cyclin-K





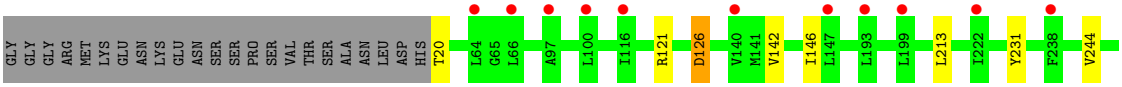
• Molecule 3: Cyclin-K

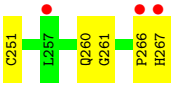




• Molecule 3: Cyclin-K

Chain I:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	249.61Å 249.61Å 217.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	76.73 – 3.42 216.17 – 3.42	Depositor EDS
% Data completeness (in resolution range)	83.4 (76.73-3.42) 83.4 (216.17-3.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.46 (at 3.41Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.185 , 0.213 0.201 , 0.224	Depositor DCC
R_{free} test set	4375 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	137.6	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 102.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.053 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	67495	wwPDB-VP
Average B, all atoms (Å^2)	162.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.56% 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: RSI, EDO, TPO, 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	0.33	0/6604	0.61	0/8931
1	D	0.32	0/6612	0.60	0/8942
1	G	0.33	1/6603 (0.0%)	0.61	0/8930
2	B	0.33	0/2704	0.60	0/3645
2	E	0.32	0/2693	0.60	0/3630
2	H	0.34	0/2743	0.62	0/3699
3	C	0.33	0/2120	0.55	0/2868
3	F	0.33	0/2120	0.56	0/2868
3	I	0.31	0/2120	0.54	0/2868
All	All	0.33	1/34319 (0.0%)	0.60	0/46381

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	292	ASP	CB-CG	-5.64	1.40	1.51

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6487	6450	6451	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	6495	6462	6464	49	0
1	G	6486	6455	6456	55	0
2	B	2656	2670	2670	25	0
2	E	2646	2663	2663	28	0
2	H	2693	2702	2702	27	0
3	C	2063	2048	2048	14	0
3	F	2063	2048	2048	9	0
3	I	2063	2048	2048	6	0
4	A	4	6	6	0	0
4	D	4	6	6	0	0
5	A	15	0	0	0	0
5	C	15	0	0	0	0
5	D	15	0	0	0	0
5	F	10	0	0	0	0
5	G	20	0	0	0	0
5	H	10	0	0	0	0
5	I	15	0	0	0	0
6	B	32	27	0	0	0
6	E	32	27	0	0	0
6	H	32	27	0	0	0
All	All	33856	33639	33562	246	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 (246) 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:292:ASP:OD1	1:G:294:THR:HG22	1.74	0.85
1:D:227:GLY:O	1:D:239:TYR:OH	2.01	0.77
2:B:906:LEU:HD21	2:B:913:TYR:CD2	2.31	0.65
1:D:207:TRP:HB3	1:D:242:GLY:HA2	1.80	0.63
1:G:969:GLU:HG2	1:G:973:ASN:HB2	1.81	0.62
3:I:121:ARG:HH12	3:I:126:ASP:HA	1.64	0.62
1:A:246:LEU:HD21	1:A:299:ASP:HA	1.80	0.62
2:H:758:VAL:O	2:H:808:ALA:HB1	2.00	0.61
2:B:841:LYS:HD2	2:B:1023:VAL:HB	1.83	0.60
2:B:803:LYS:HG3	3:C:142:VAL:HG21	1.83	0.60
1:G:43:VAL:HG23	1:G:52:VAL:HG21	1.84	0.60
1:G:770:LEU:HD21	1:G:865:GLU:HB2	1.84	0.59
1:A:775:THR:HG22	1:A:775:THR:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:213:GLU:HG2	1:D:215:GLU:H	1.67	0.59
1:G:1047:TRP:HZ3	1:G:1132:VAL:HG13	1.67	0.58
2:H:828:LEU:O	2:H:1034:PRO:HD2	2.03	0.58
2:B:828:LEU:O	2:B:1034:PRO:HD2	2.04	0.57
2:E:856:LEU:HD11	2:E:915:PRO:HG3	1.86	0.57
2:B:760:LEU:HD23	2:B:760:LEU:H	1.69	0.57
2:E:803:LYS:HG3	3:F:142:VAL:HG21	1.87	0.56
2:E:802:PHE:HB3	3:F:146:ILE:HD11	1.88	0.56
1:D:849:VAL:HG11	1:D:851:PHE:CZ	2.41	0.56
2:H:1021:LYS:HG2	2:H:1022:ASP:OD1	2.06	0.56
1:A:14:ALA:HB1	1:A:327:ARG:HG3	1.88	0.55
2:H:1022:ASP:OD1	2:H:1022:ASP:N	2.39	0.55
2:B:896:VAL:HG23	2:B:906:LEU:HD13	1.88	0.55
1:G:969:GLU:HG3	1:G:971:ALA:H	1.70	0.55
2:H:1027:LYS:HD2	2:H:1027:LYS:N	2.22	0.54
1:G:773:SER:C	1:G:775:THR:H	2.11	0.54
1:A:207:TRP:HB3	1:A:242:GLY:HA2	1.88	0.54
2:E:802:PHE:CB	3:F:146:ILE:HD11	2.37	0.54
1:A:1133:VAL:O	1:A:1137:THR:HG23	2.07	0.53
1:D:816:LEU:HD13	1:D:831:VAL:HG22	1.89	0.53
1:G:1047:TRP:CZ3	1:G:1132:VAL:HG13	2.43	0.53
1:G:322:VAL:HG21	1:G:336:LEU:HD11	1.91	0.53
1:G:1003:PHE:O	1:G:1032:THR:HA	2.08	0.53
1:G:979:LYS:O	1:G:981:SER:N	2.38	0.52
2:E:897:ILE:HG23	2:E:902:ARG:HG3	1.91	0.52
1:A:387:LEU:HG	1:A:717:LEU:HD11	1.90	0.52
1:D:7:VAL:HG12	1:D:1091:GLY:HA3	1.92	0.52
2:H:917:ILE:HG13	2:H:918:ASP:N	2.25	0.51
1:G:1023:PRO:HB3	1:G:1047:TRP:CE2	2.45	0.51
1:G:159:LEU:HD21	1:G:164:VAL:HG21	1.93	0.51
1:G:213:GLU:HG2	1:G:215:GLU:H	1.76	0.51
1:G:292:ASP:OD1	1:G:292:ASP:C	2.48	0.51
1:D:883:SER:HB3	1:D:914:LEU:HD11	1.93	0.51
1:A:791:LEU:HD23	1:A:858:LEU:HD21	1.94	0.50
1:A:6:VAL:HG22	1:A:1040:VAL:HG22	1.92	0.50
1:A:889:ARG:HD2	1:A:891:TYR:CZ	2.46	0.50
1:D:18:CYS:HG	1:D:313:CYS:HG	1.58	0.50
2:H:844:MET:HA	2:H:844:MET:HE2	1.94	0.50
1:G:112:ILE:HD13	2:H:986:PHE:CE2	2.47	0.50
1:G:292:ASP:OD1	1:G:294:THR:CG2	2.55	0.50
2:H:800:LEU:HD12	2:H:800:LEU:H	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:802:PHE:HB2	3:C:146:ILE:HD11	1.93	0.49
1:G:773:SER:O	1:G:775:THR:N	2.40	0.49
1:G:378:CYS:SG	1:G:724:ILE:HB	2.52	0.49
1:D:158:ARG:HG3	2:E:987:SER:HB2	1.93	0.49
1:D:146:ASP:OD1	1:D:147:ARG:N	2.46	0.49
1:A:36:ASN:O	1:A:37:THR:OG1	2.26	0.49
1:D:1114:TYR:HB2	1:D:1124:ALA:HB2	1.94	0.49
1:D:378:CYS:SG	1:D:724:ILE:HB	2.53	0.49
1:D:770:LEU:HD13	1:D:865:GLU:HB2	1.94	0.49
1:A:184:ASP:HB2	1:A:185:PRO:CD	2.43	0.48
2:B:755:LEU:CD2	2:B:812:VAL:HG22	2.43	0.48
2:B:892:TYR:O	2:B:911:GLU:HG3	2.13	0.48
1:D:60:LYS:O	1:D:81:THR:HA	2.13	0.48
1:D:851:PHE:HB3	1:D:858:LEU:HD22	1.95	0.48
3:C:243:PRO:HG2	3:C:246:VAL:HG23	1.96	0.48
2:E:828:LEU:O	2:E:1034:PRO:HD2	2.14	0.48
1:G:998:PHE:CZ	1:G:1074:ARG:HD2	2.48	0.48
2:E:755:LEU:HD22	2:E:812:VAL:HG22	1.95	0.48
2:E:887:GLU:HG2	2:E:888:GLU:H	1.79	0.48
1:D:5:TYR:CE2	1:D:7:VAL:HG13	2.49	0.47
2:H:857:HIS:ND1	2:H:860:ILE:HG12	2.29	0.47
1:A:170:LEU:HD21	1:A:229:ALA:HB2	1.96	0.47
1:D:393:GLY:O	1:D:394:ILE:HG12	2.15	0.47
1:A:227:GLY:O	1:A:239:TYR:OH	2.31	0.47
2:B:917:ILE:HG13	2:B:918:ASP:N	2.29	0.47
1:G:184:ASP:HB2	1:G:185:PRO:CD	2.45	0.47
1:A:59:GLY:HA2	1:A:1073:TRP:CZ3	2.49	0.47
1:A:974:LEU:HD11	1:A:1000:LEU:HD22	1.97	0.47
1:A:1016:ASN:O	1:A:1017:LEU:HB2	2.15	0.47
2:H:722:ARG:HE	2:H:726:LYS:HG3	1.79	0.47
3:I:260:GLN:HG3	3:I:261:GLY:N	2.29	0.47
1:D:157:ILE:HG23	1:D:201:GLU:HA	1.95	0.47
1:D:288:GLU:HB2	1:D:298:LYS:HB2	1.97	0.47
2:B:733:ILE:HG23	2:B:743:LYS:HB2	1.97	0.47
2:H:935:ILE:HD12	2:H:986:PHE:HZ	1.80	0.47
1:D:1105:MET:SD	1:D:1130:ILE:HD11	2.55	0.47
1:G:59:GLY:HA2	1:G:1073:TRP:CE3	2.50	0.46
1:G:762:SER:O	1:G:803:HIS:HA	2.15	0.46
1:A:278:GLY:HA3	1:A:383:LYS:HE2	1.97	0.46
1:A:376:VAL:HG22	1:A:389:ILE:HG23	1.98	0.46
1:A:387:LEU:HD11	1:A:735:VAL:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:223:PRO:HD3	1:G:271:TYR:OH	2.16	0.46
1:G:360:VAL:HG21	1:G:721:PRO:O	2.16	0.46
1:G:790:ASN:HA	1:G:805:HIS:O	2.15	0.46
1:G:984:THR:O	1:G:984:THR:HG22	2.15	0.46
2:H:767:PHE:HD2	2:H:772:ILE:HG13	1.81	0.46
1:A:1109:VAL:HG11	1:A:1126:ALA:HA	1.98	0.46
2:B:773:ARG:HD2	2:B:879:GLY:O	2.15	0.46
2:E:763:GLU:O	2:E:763:GLU:HG2	2.16	0.46
1:G:1061:VAL:HG11	1:G:1104:LYS:HB3	1.97	0.46
2:H:800:LEU:HD12	2:H:800:LEU:N	2.30	0.46
2:H:895:LYS:HE2	2:H:895:LYS:HB2	1.58	0.46
1:D:190:VAL:O	1:D:209:GLN:HA	2.16	0.46
1:G:43:VAL:HG23	1:G:52:VAL:CG2	2.46	0.46
1:G:1013:VAL:HG11	1:G:1138:ARG:O	2.16	0.46
2:B:910:GLU:O	2:B:911:GLU:HB3	2.16	0.45
1:G:170:LEU:HD21	1:G:229:ALA:HB2	1.99	0.45
2:H:858:ARG:NE	2:H:880:LEU:O	2.49	0.45
2:H:716:GLU:HG3	3:I:20:THR:N	2.32	0.45
2:H:773:ARG:HD3	2:H:881:ALA:O	2.17	0.45
1:D:771:PHE:CE1	1:D:845:GLN:HB3	2.52	0.45
1:G:391:ARG:NH2	1:G:711:HIS:ND1	2.65	0.45
2:E:917:ILE:HG13	2:E:918:ASP:N	2.32	0.45
2:E:803:LYS:HA	3:F:142:VAL:CG1	2.46	0.45
1:G:227:GLY:O	1:G:239:TYR:OH	2.26	0.45
1:A:14:ALA:O	1:A:35:LYS:HG2	2.17	0.45
2:B:799:ALA:O	2:B:800:LEU:HG	2.17	0.45
2:E:1036:TRP:O	2:E:1037:GLN:HB2	2.16	0.45
3:F:121:ARG:HH12	3:F:126:ASP:HA	1.81	0.45
1:G:849:VAL:HG11	1:G:851:PHE:CZ	2.52	0.45
1:G:192:THR:OG1	1:G:206:PRO:HD2	2.17	0.44
1:A:1140:HIS:CG	1:A:1140:HIS:O	2.69	0.44
3:F:61:GLY:HA3	3:F:71:LEU:CD2	2.47	0.44
3:F:76:ILE:HD12	3:F:159:HIS:CE1	2.51	0.44
2:H:856:LEU:O	2:H:881:ALA:HA	2.17	0.44
2:B:899:LEU:O	2:B:944:GLN:NE2	2.50	0.44
1:D:1120:MET:HG3	1:D:1122:ARG:HG3	1.99	0.44
1:D:1126:ALA:O	1:D:1130:ILE:HG13	2.17	0.44
2:E:739:GLY:HA3	2:E:757:LYS:O	2.18	0.44
1:G:72:GLU:OE2	1:G:103:ARG:NH2	2.50	0.44
1:D:63:VAL:O	1:D:79:ILE:HA	2.18	0.44
1:A:950:ASN:HB2	1:A:994:GLU:OE2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:755:LEU:HD22	2:B:812:VAL:HG22	1.99	0.44
1:D:213:GLU:OE2	1:D:234:GLN:N	2.41	0.44
2:H:769:ILE:HA	2:H:772:ILE:HB	1.98	0.44
1:D:364:VAL:HG22	1:D:375:LEU:HD13	2.00	0.44
1:A:883:SER:HB2	1:A:911:ALA:HB3	2.00	0.44
1:G:768:SER:OG	1:G:863:GLU:OE2	2.26	0.44
1:D:248:ILE:HD12	1:D:300:LEU:O	2.17	0.44
2:B:1036:TRP:CD1	2:B:1037:GLN:HG3	2.53	0.43
2:E:784:ARG:HH21	2:E:872:GLN:HG3	1.82	0.43
1:G:794:ILE:HG22	1:G:799:PHE:HA	2.00	0.43
2:E:889:SER:HB2	2:E:912:ARG:HD3	2.00	0.43
1:G:315:THR:HG22	1:G:323:PHE:HB3	1.99	0.43
1:A:973:ASN:HB3	1:A:1076:PHE:CE2	2.54	0.43
1:G:18:CYS:HG	1:G:313:CYS:HG	1.66	0.43
3:C:76:ILE:HD12	3:C:198:SER:HB3	1.99	0.43
1:D:732:CYS:HB2	1:D:794:ILE:O	2.19	0.43
2:H:778:LEU:HD21	2:H:878:PHE:CD1	2.54	0.43
1:A:248:ILE:HG12	1:A:250:PRO:HD3	1.99	0.43
2:B:909:GLY:O	2:B:910:GLU:C	2.55	0.43
3:C:239:VAL:HG12	3:C:242:VAL:HG23	2.00	0.43
1:D:20:THR:HG23	1:D:315:THR:OG1	2.19	0.43
2:H:787:VAL:HG22	2:H:875:LEU:O	2.19	0.43
1:A:190:VAL:O	1:A:209:GLN:HA	2.19	0.43
1:A:1003:PHE:O	1:A:1032:THR:HA	2.19	0.43
1:G:275:ASP:C	1:G:275:ASP:OD1	2.58	0.43
1:G:6:VAL:HG22	1:G:1040:VAL:HG22	2.00	0.42
1:G:364:VAL:HG22	1:G:375:LEU:HD13	2.01	0.42
2:B:739:GLY:HA3	2:B:757:LYS:O	2.19	0.42
3:C:174:ASP:OD2	3:C:177:LYS:HG3	2.19	0.42
1:D:223:PRO:HD3	1:D:271:TYR:OH	2.19	0.42
1:D:795:ASP:HB2	1:D:802:LEU:HD21	2.00	0.42
1:D:1057:ARG:HD3	1:D:1108:VAL:O	2.19	0.42
2:H:774:GLU:HG3	2:H:878:PHE:HB2	2.01	0.42
1:A:126:PRO:HD3	1:A:169:PHE:HB3	2.00	0.42
1:A:232:ILE:HD13	1:A:237:ILE:HG23	2.01	0.42
1:D:32:LEU:HD12	1:D:32:LEU:N	2.35	0.42
1:D:859:GLN:HA	1:D:859:GLN:OE1	2.18	0.42
1:G:365:VAL:HG11	1:G:733:PHE:CZ	2.55	0.42
2:H:760:LEU:HD21	2:H:767:PHE:HD1	1.84	0.42
1:A:213:GLU:HG2	1:A:215:GLU:H	1.85	0.42
2:E:722:ARG:NH1	2:E:791:GLU:OE2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:59:GLY:HA2	1:G:1073:TRP:CZ3	2.55	0.42
1:G:965:PHE:O	1:G:976:VAL:HA	2.20	0.42
1:A:1023:PRO:HB3	1:A:1047:TRP:CE2	2.55	0.42
1:D:936:LYS:HE2	1:D:943:GLU:HB2	2.02	0.42
2:E:784:ARG:O	2:E:874:LYS:HE2	2.18	0.42
3:C:235:TRP:CH2	3:C:244:VAL:HG22	2.54	0.42
1:D:933:LEU:HD22	1:D:942:PHE:HB3	2.01	0.42
1:A:936:LYS:HE3	1:A:943:GLU:OE1	2.20	0.42
1:D:223:PRO:HD2	1:D:268:GLY:HA3	2.02	0.42
2:E:727:PHE:CE1	2:E:753:VAL:HG21	2.55	0.42
2:E:887:GLU:O	2:E:888:GLU:C	2.59	0.42
2:E:893:TPO:O2P	2:E:893:TPO:HG22	2.20	0.42
1:D:998:PHE:CZ	1:D:1074:ARG:HD2	2.55	0.41
2:E:732:ILE:HG23	2:E:732:ILE:O	2.20	0.41
3:C:121:ARG:HD2	3:C:121:ARG:HA	1.85	0.41
1:D:59:GLY:HA2	1:D:1073:TRP:CZ3	2.55	0.41
1:A:112:ILE:HD13	2:B:986:PHE:CE2	2.55	0.41
1:A:816:LEU:HD13	1:A:831:VAL:HG22	2.02	0.41
3:C:125:ASN:OD1	3:C:125:ASN:C	2.58	0.41
1:D:358:PRO:HD2	1:D:380:GLY:HA2	2.02	0.41
2:E:721:LYS:HE3	3:F:149:GLN:O	2.20	0.41
3:I:266:PRO:O	3:I:267:HIS:C	2.58	0.41
1:A:849:VAL:HG11	1:A:851:PHE:CZ	2.56	0.41
2:B:964:ILE:HA	2:B:969:PHE:CD2	2.56	0.41
3:C:264:GLN:HG2	3:C:265:MET:H	1.86	0.41
3:I:213:LEU:HB2	3:I:251:CYS:SG	2.60	0.41
1:A:143:ILE:HG12	1:A:154:ALA:HB2	2.03	0.41
1:A:223:PRO:HD3	1:A:271:TYR:OH	2.20	0.41
1:D:3:TYR:HB3	1:D:1048:TYR:HB2	2.03	0.41
1:G:10:GLN:O	1:G:1036:MET:HG2	2.20	0.41
2:H:802:PHE:CB	3:I:146:ILE:HD11	2.49	0.41
2:E:1036:TRP:CD1	2:E:1037:GLN:HG3	2.55	0.41
3:F:125:ASN:OD1	3:F:125:ASN:C	2.58	0.41
3:C:266:PRO:O	3:C:267:HIS:C	2.59	0.41
1:D:881:LEU:HD21	1:D:921:ILE:HG21	2.03	0.41
2:E:848:GLU:OE1	2:E:1015:LEU:HD12	2.21	0.41
2:H:841:LYS:O	2:H:845:GLU:HB2	2.21	0.41
1:A:118:THR:OG1	1:A:134:ARG:NH2	2.34	0.41
3:C:25:TYR:HA	3:C:199:LEU:O	2.21	0.41
1:D:1055:GLN:HG2	1:D:1093:LEU:HD23	2.03	0.41
1:A:739:ARG:HD3	1:A:757:SER:OG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:82:TYR:CE2	3:C:95:THR:HG21	2.56	0.41
1:D:744:ASP:OD1	1:D:746:SER:N	2.45	0.41
2:E:993:ALA:HB2	2:E:1019:PHE:CE1	2.56	0.41
1:G:1024:THR:HB	1:G:1041:THR:OG1	2.21	0.41
1:G:1097:PHE:O	1:G:1100:ILE:HG12	2.21	0.41
1:A:105:HIS:CD2	1:A:1067:LYS:HD2	2.56	0.40
1:A:358:PRO:O	1:A:379:SER:HA	2.22	0.40
1:A:881:LEU:HD21	1:A:921:ILE:HG21	2.03	0.40
1:A:971:ALA:HB3	1:A:973:ASN:HD22	1.86	0.40
1:A:987:GLU:HA	2:B:740:GLN:NE2	2.36	0.40
3:C:265:MET:N	3:C:265:MET:SD	2.94	0.40
1:A:766:SER:HB2	1:A:805:HIS:NE2	2.36	0.40
1:D:248:ILE:HG12	1:D:250:PRO:HD3	2.02	0.40
2:E:1030:PRO:HA	2:E:1031:PRO:HD3	1.98	0.40
1:G:255:GLN:OE1	1:G:279:ARG:NH1	2.53	0.40
2:B:963:VAL:HG22	2:B:969:PHE:CD1	2.57	0.40
1:D:1133:VAL:O	1:D:1137:THR:HG23	2.21	0.40
1:G:127:GLU:HB2	1:G:129:ARG:HG3	2.04	0.40
2:B:908:LEU:HB2	2:B:966:LEU:HD13	2.03	0.40
2:B:1021:LYS:HB3	2:B:1021:LYS:HE3	1.94	0.40
1:D:68:ARG:HB2	1:D:75:ASP:OD1	2.22	0.40
1:G:125:ASP:OD1	1:G:127:GLU:N	2.42	0.40
1:G:270:ARG:HG2	1:G:284:LEU:CD2	2.52	0.40
1:G:936:LYS:HD3	1:G:936:LYS:HA	1.86	0.40
1:D:1028:VAL:O	1:D:1039:LEU:HA	2.22	0.40
2:E:906:LEU:HD21	2:E:913:TYR:CD2	2.56	0.40
1:G:773:SER:C	1:G:775:THR:N	2.75	0.40
2:H:914:THR:O	2:H:917:ILE:HG12	2.22	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%)	800 (97%)	21 (3%)	1 (0%)	51 83
1	D	823/840 (98%)	802 (97%)	20 (2%)	1 (0%)	51 83
1	G	822/840 (98%)	798 (97%)	24 (3%)	0	100 100
2	B	323/344 (94%)	312 (97%)	11 (3%)	0	100 100
2	E	322/344 (94%)	314 (98%)	7 (2%)	1 (0%)	41 74
2	H	327/344 (95%)	317 (97%)	10 (3%)	0	100 100
3	C	246/271 (91%)	244 (99%)	2 (1%)	0	100 100
3	F	246/271 (91%)	242 (98%)	4 (2%)	0	100 100
3	I	246/271 (91%)	242 (98%)	4 (2%)	0	100 100
All	All	4177/4365 (96%)	4071 (98%)	103 (2%)	3 (0%)	51 83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	774	SER
1	D	772	SER
2	E	877	ASP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	721/728 (99%)	715 (99%)	6 (1%)	81 92
1	D	722/728 (99%)	717 (99%)	5 (1%)	84 93
1	G	721/728 (99%)	716 (99%)	5 (1%)	84 93
2	B	293/308 (95%)	286 (98%)	7 (2%)	49 76
2	E	292/308 (95%)	288 (99%)	4 (1%)	67 85
2	H	297/308 (96%)	290 (98%)	7 (2%)	49 76
3	C	223/242 (92%)	222 (100%)	1 (0%)	91 96
3	F	223/242 (92%)	222 (100%)	1 (0%)	91 96
3	I	223/242 (92%)	219 (98%)	4 (2%)	59 81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3715/3834 (97%)	3675 (99%)	40 (1%)	73 87

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	208	LYS
1	A	209	GLN
1	A	226	PHE
1	A	259	VAL
1	A	313	CYS
1	A	720	SER
2	B	800	LEU
2	B	867	LEU
2	B	883	LEU
2	B	896	VAL
2	B	897	ILE
2	B	1039	CYS
2	B	1040	HIS
3	C	231	TYR
1	D	394	ILE
1	D	775	THR
1	D	930	VAL
1	D	988	GLU
1	D	1006	VAL
2	E	728	ASP
2	E	748	ASP
2	E	1033	LEU
2	E	1039	CYS
3	F	267	HIS
1	G	192	THR
1	G	292	ASP
1	G	315	THR
1	G	794	ILE
1	G	1120	MET
2	H	858	ARG
2	H	867	LEU
2	H	895	LYS
2	H	896	VAL
2	H	897	ILE
2	H	1022	ASP
2	H	1042	LEU
3	I	126	ASP

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Mol	Chain	Res	Type
3	I	142	VAL
3	I	231	TYR
3	I	244	VAL

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

Mol	Chain	Res	Type
1	G	261	HIS
2	H	999	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	TPO	E	893	2	8,10,11	1.74	1 (12%)	10,14,16	1.22	1 (10%)
2	TPO	H	893	2	8,10,11	1.88	2 (25%)	10,14,16	1.52	1 (10%)
2	TPO	B	893	2	8,10,11	1.62	1 (12%)	10,14,16	1.23	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	-	4/9/11/13	-
2	TPO	H	893	2	-	2/9/11/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TPO	B	893	2	-	0/9/11/13	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	893	TPO	P-O1P	3.58	1.62	1.50
2	E	893	TPO	P-O1P	3.45	1.61	1.50
2	B	893	TPO	P-O1P	3.44	1.61	1.50
2	H	893	TPO	P-OG1	2.57	1.64	1.59

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	893	TPO	CG2-CB-CA	-3.29	106.67	113.16
2	B	893	TPO	P-OG1-CB	-2.62	115.31	123.21
2	E	893	TPO	CG2-CB-CA	-2.13	108.97	113.16

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	893	TPO	N-CA-CB-CG2
2	E	893	TPO	N-CA-CB-OG1
2	E	893	TPO	C-CA-CB-CG2
2	E	893	TPO	CG2-CB-OG1-P
2	H	893	TPO	CB-OG1-P-O1P
2	H	893	TPO	CB-OG1-P-O2P

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

25 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	$\#\|Z\| > 2$
5	SO4	F	301	-	4,4,4	0.19	0	6,6,6	0.13	0
5	SO4	C	302	-	4,4,4	0.14	0	6,6,6	0.08	0
5	SO4	D	1203	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	F	302	-	4,4,4	0.16	0	6,6,6	0.06	0
5	SO4	H	1103	-	4,4,4	0.15	0	6,6,6	0.06	0
5	SO4	A	1202	-	4,4,4	0.14	0	6,6,6	0.08	0
5	SO4	G	1202	-	4,4,4	0.16	0	6,6,6	0.10	0
5	SO4	C	303	-	4,4,4	0.13	0	6,6,6	0.06	0
5	SO4	D	1202	-	4,4,4	0.13	0	6,6,6	0.07	0
5	SO4	C	301	-	4,4,4	0.15	0	6,6,6	0.16	0
5	SO4	A	1204	-	4,4,4	0.11	0	6,6,6	0.12	0
6	RSI	B	1101	-	33,36,36	1.60	5 (15%)	37,50,50	2.50	9 (24%)
5	SO4	I	303	-	4,4,4	0.17	0	6,6,6	0.08	0
5	SO4	G	1201	-	4,4,4	0.15	0	6,6,6	0.18	0
6	RSI	E	1101	-	33,36,36	1.65	5 (15%)	37,50,50	2.37	10 (27%)
4	EDO	A	1201	-	3,3,3	0.73	0	2,2,2	0.24	0
5	SO4	I	302	-	4,4,4	0.15	0	6,6,6	0.09	0
5	SO4	G	1203	-	4,4,4	0.13	0	6,6,6	0.07	0
5	SO4	I	301	-	4,4,4	0.15	0	6,6,6	0.07	0
6	RSI	H	1101	-	33,36,36	1.55	4 (12%)	37,50,50	2.39	8 (21%)
5	SO4	H	1102	-	4,4,4	0.15	0	6,6,6	0.08	0
5	SO4	G	1204	-	4,4,4	0.11	0	6,6,6	0.06	0
4	EDO	D	1201	-	3,3,3	0.62	0	2,2,2	0.43	0
5	SO4	D	1204	-	4,4,4	0.13	0	6,6,6	0.08	0
5	SO4	A	1203	-	4,4,4	0.13	0	6,6,6	0.11	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
6	RSI	H	1101	-	-	5/17/25/25	0/5/5/5
6	RSI	E	1101	-	-	5/17/25/25	0/5/5/5
4	EDO	A	1201	-	-	0/1/1/1	-
4	EDO	D	1201	-	-	0/1/1/1	-
6	RSI	B	1101	-	-	5/17/25/25	0/5/5/5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1101	RSI	C13-N2	5.78	1.45	1.34
6	E	1101	RSI	C14-N7	5.46	1.45	1.35
6	E	1101	RSI	C13-N2	5.44	1.44	1.34
6	H	1101	RSI	C13-N2	5.33	1.44	1.34
6	H	1101	RSI	C14-N7	4.90	1.44	1.35
6	B	1101	RSI	C14-N7	4.60	1.44	1.35
6	B	1101	RSI	C15-N4	-3.02	1.30	1.35
6	B	1101	RSI	C6-C2	2.72	1.53	1.48
6	E	1101	RSI	C6-C2	2.65	1.53	1.48
6	E	1101	RSI	C18-N6	-2.51	1.45	1.49
6	H	1101	RSI	C6-C2	2.43	1.52	1.48
6	E	1101	RSI	C15-N4	-2.42	1.31	1.35
6	H	1101	RSI	C18-N6	-2.34	1.45	1.49
6	B	1101	RSI	C18-N6	-2.23	1.45	1.49

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	H	1101	RSI	C17-N6-C18	-9.38	116.20	125.42
6	E	1101	RSI	C17-N6-C18	-9.03	116.54	125.42
6	B	1101	RSI	C17-N6-C18	-8.78	116.79	125.42
6	B	1101	RSI	C21-N7-C14	-5.87	111.96	121.69
6	H	1101	RSI	C21-N7-C14	-5.85	111.99	121.69
6	E	1101	RSI	C21-N7-C14	-5.59	112.42	121.69
6	B	1101	RSI	C24-N7-C14	-5.59	112.42	121.69
6	B	1101	RSI	C12-N2-C13	-4.81	116.70	123.11
6	E	1101	RSI	C24-N7-C14	-4.49	114.25	121.69
6	H	1101	RSI	C24-N7-C14	-4.42	114.36	121.69
6	E	1101	RSI	C12-N2-C13	-4.12	117.61	123.11
6	H	1101	RSI	C12-N2-C13	-3.30	118.70	123.11
6	B	1101	RSI	C16-C13-N3	-3.21	118.14	120.81
6	B	1101	RSI	C1-N1-C2	2.87	121.26	117.23
6	H	1101	RSI	C1-N1-C2	2.83	121.20	117.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	1101	RSI	C1-N1-C2	2.68	120.99	117.23
6	H	1101	RSI	C5-C1-N1	-2.68	119.06	123.43
6	E	1101	RSI	C5-C1-N1	-2.65	119.10	123.43
6	B	1101	RSI	C5-C1-N1	-2.40	119.50	123.43
6	B	1101	RSI	C9-C12-N2	-2.37	107.61	113.77
6	E	1101	RSI	C9-C12-N2	-2.31	107.77	113.77
6	H	1101	RSI	N3-C14-N7	-2.30	114.27	117.11
6	B	1101	RSI	C6-C2-N1	2.19	121.12	116.84
6	E	1101	RSI	C6-C2-N1	2.17	121.07	116.84
6	E	1101	RSI	C16-C13-N3	-2.09	119.07	120.81
6	H	1101	RSI	C6-C2-N1	2.06	120.86	116.84
6	E	1101	RSI	C18-N6-C15	-2.04	124.73	127.15

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	1101	RSI	C20-C18-N6-C15
6	B	1101	RSI	C20-C18-N6-C17
6	E	1101	RSI	C20-C18-N6-C15
6	E	1101	RSI	C20-C18-N6-C17
6	H	1101	RSI	C20-C18-N6-C15
6	H	1101	RSI	C20-C18-N6-C17
6	B	1101	RSI	N3-C14-N7-C24
6	E	1101	RSI	N3-C14-N7-C24
6	H	1101	RSI	N3-C14-N7-C24
6	B	1101	RSI	N4-C14-N7-C24
6	E	1101	RSI	N4-C14-N7-C24
6	H	1101	RSI	N4-C14-N7-C24
6	B	1101	RSI	C19-C18-N6-C17
6	E	1101	RSI	C19-C18-N6-C17
6	H	1101	RSI	C19-C18-N6-C17

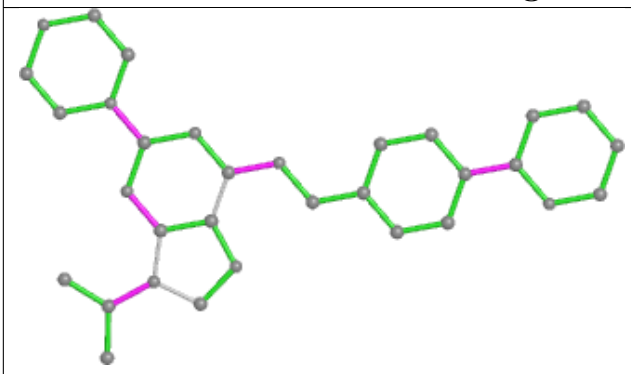
There are no ring outliers.

No monomer is involved in short contacts.

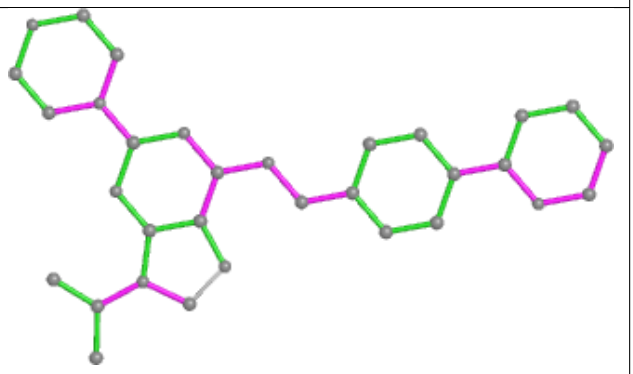
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

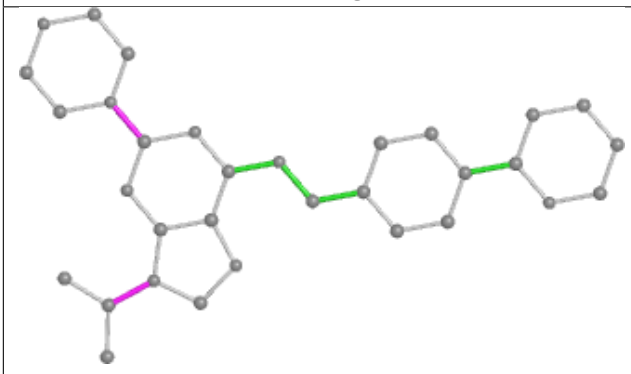
Ligand RSI B 1101



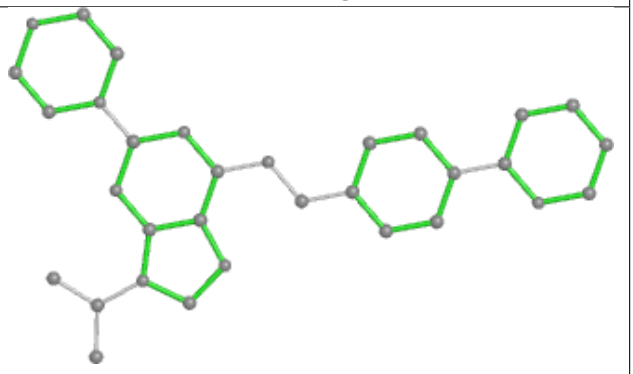
Bond lengths



Bond angles

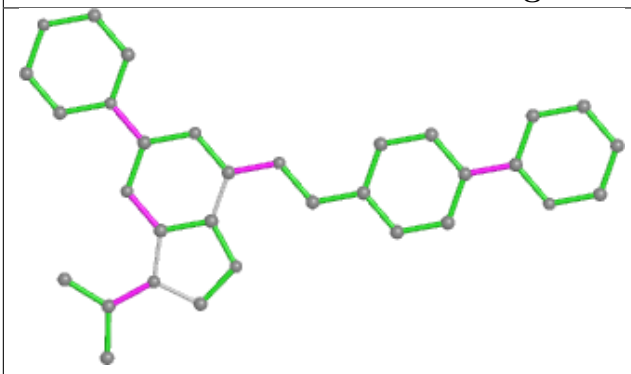


Torsions



Rings

Ligand RSI E 1101



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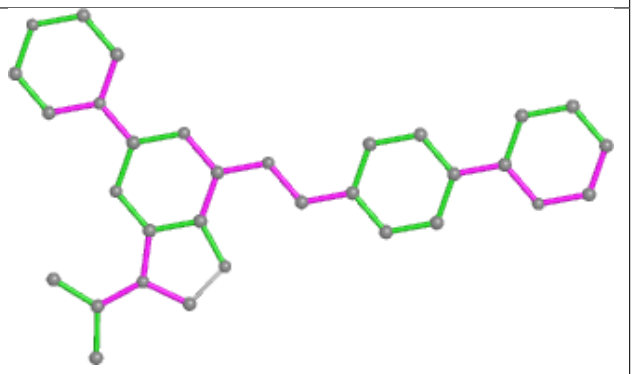
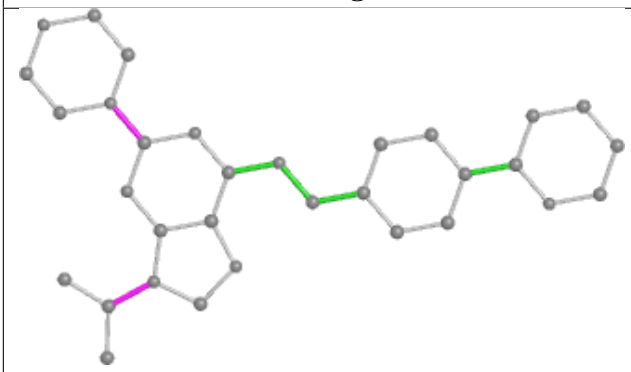


Bond angles



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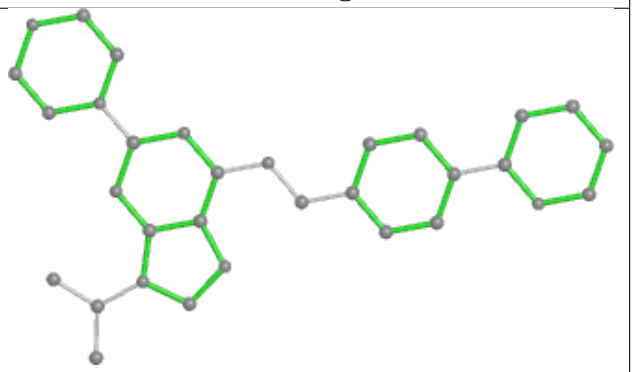
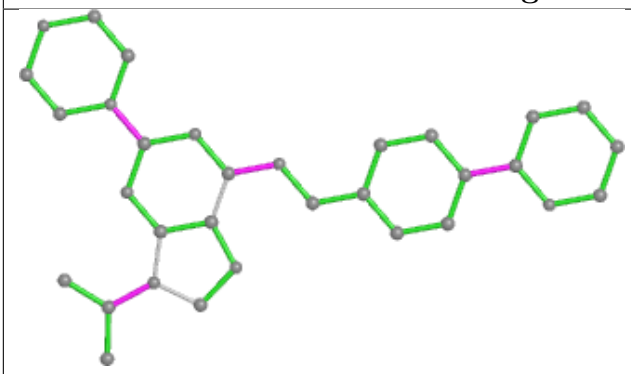
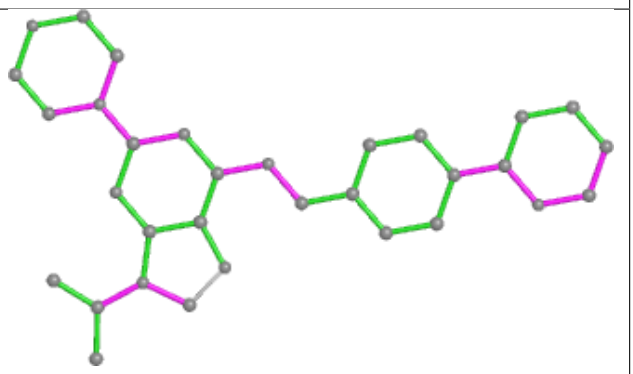


Rings

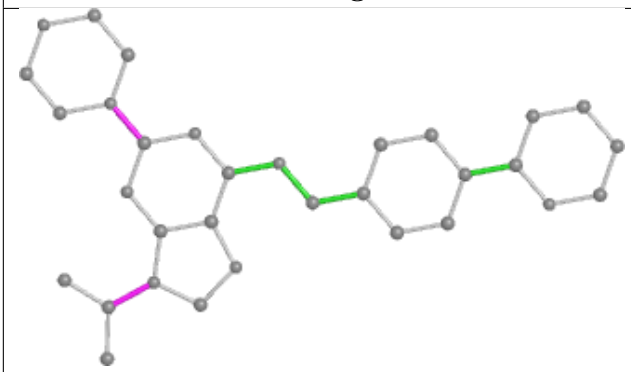
Ligand RSI H 1101



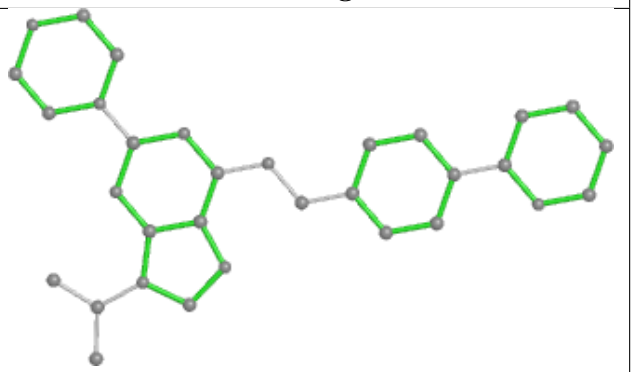
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	826/840 (98%)	0.82	117 (14%) 2 4	107, 148, 222, 310	0
1	D	827/840 (98%)	0.78	113 (13%) 3 4	101, 142, 213, 273	0
1	G	826/840 (98%)	0.63	92 (11%) 5 7	107, 151, 225, 307	0
2	B	325/344 (94%)	1.01	60 (18%) 1 2	116, 150, 222, 267	0
2	E	324/344 (94%)	0.73	33 (10%) 6 9	108, 142, 204, 249	0
2	H	329/344 (95%)	0.86	26 (7%) 12 16	96, 126, 205, 270	0
3	C	248/271 (91%)	0.60	10 (4%) 38 38	110, 140, 175, 252	0
3	F	248/271 (91%)	0.69	13 (5%) 27 28	95, 121, 164, 266	0
3	I	248/271 (91%)	0.77	14 (5%) 24 25	96, 125, 167, 263	0
All	All	4201/4365 (96%)	0.76	478 (11%) 5 7	95, 142, 216, 310	0

All (478) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	1035	HIS	6.6
2	B	800	LEU	6.4
2	B	799	ALA	5.7
1	A	1115	ASP	5.4
3	F	267	HIS	5.3
2	H	1043	TRP	5.2
1	A	1016	ASN	5.1
1	A	1097	PHE	5.0
2	B	1035	HIS	5.0
3	I	267	HIS	4.8
2	E	1039	CYS	4.7
3	I	266	PRO	4.7
2	B	828	LEU	4.7
2	B	896	VAL	4.5
1	G	317	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	2	SER	4.3
1	G	394	ILE	4.3
1	G	49	LEU	4.3
1	D	367	LEU	4.2
2	E	802	PHE	4.2
2	B	1040	HIS	4.1
2	B	860	ILE	4.1
1	A	1114	TYR	4.1
1	D	920	PHE	4.0
3	C	267	HIS	4.0
1	A	226	PHE	3.9
1	A	1029	LEU	3.9
1	A	131	ILE	3.8
1	A	1116	ASP	3.7
2	H	839	PHE	3.7
1	A	933	LEU	3.7
1	A	230	ILE	3.7
1	G	733	PHE	3.6
1	A	195	VAL	3.6
1	D	390	ILE	3.6
2	B	867	LEU	3.6
1	A	61	ILE	3.6
1	A	297	LEU	3.6
1	G	306	GLY	3.6
2	B	876	ALA	3.5
1	G	1129	LEU	3.5
1	A	112	ILE	3.5
1	G	195	VAL	3.5
2	H	798	ASP	3.5
1	D	5	TYR	3.5
1	D	1004	VAL	3.5
1	G	858	LEU	3.5
2	B	878	PHE	3.5
1	D	1	MET	3.5
1	A	248	ILE	3.5
2	B	886	SER	3.4
1	D	791	LEU	3.4
1	G	323	PHE	3.4
1	G	133	LEU	3.4
1	A	133	LEU	3.4
2	B	720	GLY	3.4
1	G	387	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	33	ILE	3.3
1	G	131	ILE	3.3
3	F	266	PRO	3.3
1	D	721	PRO	3.3
1	A	289	GLU	3.3
1	A	57	MET	3.3
2	B	1033	LEU	3.3
1	A	1079	GLU	3.3
1	A	926	LEU	3.3
1	D	926	LEU	3.3
1	D	328	LEU	3.3
3	F	262	LYS	3.3
1	G	232	ILE	3.2
2	E	1036	TRP	3.2
1	D	369	ARG	3.2
1	A	957	VAL	3.2
1	D	31	LEU	3.2
1	A	376	VAL	3.2
2	B	733	ILE	3.2
2	E	839	PHE	3.2
2	B	738	TYR	3.2
3	C	164	LEU	3.1
2	B	1000	MET	3.1
2	H	1035	HIS	3.1
2	B	839	PHE	3.1
1	G	829	PHE	3.1
2	B	951	LEU	3.1
1	D	736	LEU	3.1
1	D	359	ILE	3.1
2	B	831	PHE	3.1
1	A	930	VAL	3.1
1	A	32	LEU	3.1
1	A	1129	LEU	3.1
1	D	49	LEU	3.1
1	A	1030	PHE	3.1
1	G	280	LEU	3.1
1	G	180	PHE	3.1
1	G	321	VAL	3.1
1	G	272	LEU	3.1
3	F	264	GLN	3.0
1	A	367	LEU	3.0
1	G	291	MET	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	930	PHE	3.0
2	E	803	LYS	3.0
2	E	831	PHE	3.0
2	E	955	PRO	3.0
1	D	1007	PHE	3.0
1	A	240	HIS	3.0
1	D	881	LEU	3.0
1	G	282	MET	3.0
1	D	387	LEU	3.0
1	D	998	PHE	3.0
1	D	794	ILE	3.0
1	A	927	MET	3.0
2	B	855	PHE	3.0
1	D	237	ILE	3.0
2	B	875	LEU	3.0
1	A	169	PHE	3.0
1	A	1089	ILE	3.0
1	A	914	LEU	3.0
1	D	1029	LEU	3.0
1	G	322	VAL	3.0
1	D	724	ILE	2.9
1	A	39	LEU	2.9
2	H	964	ILE	2.9
1	D	37	THR	2.9
2	B	811	LEU	2.9
1	G	933	LEU	2.9
2	H	873	ILE	2.9
1	A	140	PHE	2.9
1	A	1007	PHE	2.9
1	D	880	LEU	2.9
1	G	253	ILE	2.9
1	A	77	LEU	2.9
1	A	232	ILE	2.9
2	B	755	LEU	2.9
2	B	1036	TRP	2.9
1	A	1008	CYS	2.9
1	A	949	PHE	2.9
1	D	180	PHE	2.9
1	D	821	LEU	2.9
1	D	931	LEU	2.9
2	H	875	LEU	2.9
1	A	79	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	830	ILE	2.8
2	H	1041	GLU	2.8
1	G	61	ILE	2.8
2	B	798	ASP	2.8
1	A	300	LEU	2.8
1	D	761	LEU	2.8
1	G	1051	LEU	2.8
1	G	237	ILE	2.8
1	D	42	TYR	2.8
3	C	153	PHE	2.8
1	G	356	LEU	2.8
2	B	955	PRO	2.8
1	A	220	ILE	2.8
1	D	793	ILE	2.8
1	G	240	HIS	2.8
1	D	91	TYR	2.8
1	D	932	LEU	2.8
1	A	135	LEU	2.8
1	D	710	LEU	2.8
1	D	733	PHE	2.8
1	A	975	PHE	2.8
1	A	792	LEU	2.7
2	E	720	GLY	2.7
1	D	362	MET	2.7
2	H	955	PRO	2.7
1	A	816	LEU	2.7
2	B	1001	LEU	2.7
1	A	1139	ILE	2.7
1	G	289	GLU	2.7
2	E	738	TYR	2.7
2	H	890	ARG	2.7
1	D	830	ILE	2.7
2	B	833	GLU	2.7
1	A	932	LEU	2.7
1	G	1136	LEU	2.7
1	D	945	ILE	2.7
3	F	57	ILE	2.7
1	A	1088	PHE	2.7
2	B	797	GLN	2.7
1	A	923	VAL	2.7
1	G	1000	LEU	2.6
1	A	977	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	281	PHE	2.6
1	D	1040	VAL	2.6
1	A	121	ILE	2.6
1	D	965	PHE	2.6
2	E	829	VAL	2.6
1	G	290	GLN	2.6
1	D	1039	LEU	2.6
1	D	376	VAL	2.6
2	E	828	LEU	2.6
2	E	867	LEU	2.6
1	A	283	LEU	2.6
1	A	959	ILE	2.6
1	D	899	LEU	2.6
3	C	155	LEU	2.6
1	D	1097	PHE	2.6
1	D	360	VAL	2.6
1	A	1055	GLN	2.6
1	D	831	VAL	2.6
1	G	922	LEU	2.6
2	E	873	ILE	2.6
1	D	32	LEU	2.6
1	D	974	LEU	2.6
1	D	1005	ASN	2.6
1	D	905	HIS	2.6
1	D	1037	ILE	2.6
2	B	986	PHE	2.5
2	E	878	PHE	2.5
1	G	305	LEU	2.5
3	C	132	PHE	2.5
1	G	911	ALA	2.5
1	A	89	LEU	2.5
3	C	181	LEU	2.5
1	G	1097	PHE	2.5
1	A	1028	VAL	2.5
2	B	823	LEU	2.5
1	G	78	PHE	2.5
1	D	195	VAL	2.5
1	D	1008	CYS	2.5
1	A	9	ALA	2.5
1	G	861	VAL	2.5
1	G	1040	VAL	2.5
2	B	866	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	858	LEU	2.5
1	G	816	LEU	2.5
2	B	945	LEU	2.5
1	G	124	ILE	2.5
2	E	917	ILE	2.5
1	G	32	LEU	2.5
1	G	851	PHE	2.5
1	A	1	MET	2.5
1	D	928	ARG	2.5
1	D	890	LEU	2.5
1	D	732	CYS	2.5
1	D	977	CYS	2.5
1	A	239	TYR	2.5
1	A	717	LEU	2.5
1	G	328	LEU	2.5
1	G	336	LEU	2.5
2	H	891	PRO	2.5
2	E	972	MET	2.5
2	B	856	LEU	2.5
3	I	100	LEU	2.5
1	D	848	ILE	2.5
1	A	49	LEU	2.4
1	A	304	LEU	2.4
1	D	375	LEU	2.4
1	A	33	ILE	2.4
1	A	139	LEU	2.4
1	G	931	LEU	2.4
1	D	1030	PHE	2.4
1	A	830	ILE	2.4
1	G	273	LEU	2.4
1	G	1039	LEU	2.4
2	B	829	VAL	2.4
2	B	913	TYR	2.4
1	D	790	ASN	2.4
1	A	60	LYS	2.4
1	G	303	GLU	2.4
2	B	972	MET	2.4
1	A	229	ALA	2.4
1	D	317	LEU	2.4
1	G	792	LEU	2.4
1	D	956	ALA	2.4
2	E	935	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	752	LEU	2.4
1	D	356	LEU	2.4
1	D	365	VAL	2.4
1	D	966	LEU	2.4
1	G	930	VAL	2.4
1	G	307	GLU	2.4
2	B	775	ILE	2.4
1	A	273	LEU	2.4
1	A	1108	VAL	2.4
1	G	735	VAL	2.4
1	G	966	LEU	2.4
2	B	809	PHE	2.4
1	A	848	ILE	2.4
1	D	57	MET	2.4
1	D	957	VAL	2.4
2	B	862	CYS	2.4
3	F	263	GLN	2.4
2	B	884	TYR	2.4
3	F	164	LEU	2.4
1	A	870	VAL	2.4
1	G	258	ILE	2.4
2	E	964	ILE	2.4
1	A	145	LEU	2.4
1	A	1040	VAL	2.4
2	E	1025	LEU	2.4
2	H	767	PHE	2.3
1	G	5	TYR	2.3
1	G	724	ILE	2.3
1	G	899	LEU	2.3
1	D	722	ARG	2.3
1	A	912	LEU	2.3
3	I	116	ILE	2.3
1	D	927	MET	2.3
1	G	1054	MET	2.3
1	A	828	TYR	2.3
1	D	253	ILE	2.3
1	G	813	ALA	2.3
1	D	778	HIS	2.3
1	G	33	ILE	2.3
1	G	880	LEU	2.3
3	F	254	ILE	2.3
1	G	923	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	356	LEU	2.3
1	A	922	LEU	2.3
2	B	929	LEU	2.3
1	G	893	TRP	2.3
1	A	246	LEU	2.3
1	G	921	ILE	2.3
2	B	935	ILE	2.3
1	D	715	VAL	2.3
1	G	1088	PHE	2.3
3	F	222	ILE	2.3
2	B	919	VAL	2.3
1	D	910	MET	2.3
2	B	932	LYS	2.3
1	A	120	ILE	2.3
1	D	853	TYR	2.3
3	I	238	PHE	2.3
2	E	908	LEU	2.3
1	G	112	ILE	2.3
1	A	998	PHE	2.3
1	D	923	VAL	2.3
3	I	97	ALA	2.3
1	A	967	GLY	2.3
1	A	1136	LEU	2.3
3	F	71	LEU	2.3
1	D	1028	VAL	2.3
1	G	300	LEU	2.3
3	I	199	LEU	2.3
1	G	794	ILE	2.3
3	I	140	VAL	2.3
1	G	31	LEU	2.2
1	G	932	LEU	2.2
1	D	816	LEU	2.2
1	G	333	LEU	2.2
2	B	917	ILE	2.2
1	G	957	VAL	2.2
1	G	770	LEU	2.2
2	H	1032	ASP	2.2
1	D	159	LEU	2.2
1	G	314	LEU	2.2
2	E	727	PHE	2.2
3	C	266	PRO	2.2
1	A	285	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	926	LEU	2.2
3	I	66	LEU	2.2
1	A	23	PHE	2.2
1	G	715	VAL	2.2
1	G	888	VAL	2.2
1	G	1037	ILE	2.2
1	D	887	THR	2.2
1	D	933	LEU	2.2
3	I	64	LEU	2.2
1	A	258	ILE	2.2
1	A	1094	ILE	2.2
1	D	921	ILE	2.2
2	E	733	ILE	2.2
1	D	756	ALA	2.2
1	A	791	LEU	2.2
1	A	880	LEU	2.2
2	E	732	ILE	2.2
2	E	836	ILE	2.2
3	C	60	VAL	2.2
1	A	1054	MET	2.2
2	B	772	ILE	2.2
1	G	799	PHE	2.2
1	D	61	ILE	2.2
1	A	966	LEU	2.2
1	A	1051	LEU	2.2
3	I	257	LEU	2.2
2	H	930	PHE	2.2
2	B	840	MET	2.2
2	H	972	MET	2.2
1	A	5	TYR	2.2
1	D	942	PHE	2.2
2	B	952	CYS	2.2
2	H	922	CYS	2.2
2	B	858	ARG	2.2
1	A	80	LEU	2.1
1	G	39	LEU	2.1
2	H	820	LEU	2.1
2	H	843	LEU	2.1
1	A	78	PHE	2.1
1	D	737	SER	2.1
1	D	799	PHE	2.1
1	A	165	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1006	VAL	2.1
1	G	945	ILE	2.1
1	A	881	LEU	2.1
2	B	982	LEU	2.1
3	F	155	LEU	2.1
1	A	34	ALA	2.1
1	D	232	ILE	2.1
1	D	792	LEU	2.1
1	G	139	LEU	2.1
2	E	875	LEU	2.1
2	E	743	LYS	2.1
1	A	157	ILE	2.1
1	D	836	VAL	2.1
1	A	362	MET	2.1
2	H	1031	PRO	2.1
1	A	1039	LEU	2.1
1	D	1136	LEU	2.1
2	H	926	LEU	2.1
3	I	193	LEU	2.1
1	G	1076	PHE	2.1
3	F	242	VAL	2.1
1	A	280	LEU	2.1
2	H	1033	LEU	2.1
1	G	140	PHE	2.1
1	A	365	VAL	2.1
2	H	720	GLY	2.1
2	H	906	LEU	2.1
3	C	143	LEU	2.1
2	B	1029	ALA	2.1
1	G	848	ILE	2.1
1	A	170	LEU	2.1
1	A	1035	GLY	2.1
2	H	866	LEU	2.1
3	I	222	ILE	2.1
1	D	907	ASN	2.1
3	I	147	LEU	2.1
1	D	807	PHE	2.1
1	D	1088	PHE	2.1
1	A	735	VAL	2.1
1	D	112	ILE	2.1
1	D	801	VAL	2.1
1	D	708	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	777	ILE	2.1
1	A	974	LEU	2.1
2	B	864	ASN	2.1
1	A	871	TYR	2.1
1	D	1000	LEU	2.1
2	E	895	LYS	2.1
1	A	712	ILE	2.1
1	A	884	ILE	2.1
1	A	1000	LEU	2.1
1	G	297	LEU	2.1
2	B	802	PHE	2.0
1	D	843	PRO	2.0
2	B	781	LEU	2.0
2	H	1014	THR	2.0
1	A	360	VAL	2.0
1	G	853	TYR	2.0
2	E	896	VAL	2.0
3	C	148	LEU	2.0
1	A	179	CYS	2.0
1	G	132	GLY	2.0
1	G	984	THR	2.0
2	E	986	PHE	2.0
1	D	276	MET	2.0
1	D	39	LEU	2.0
1	D	152	LEU	2.0
1	D	246	LEU	2.0
2	E	778	LEU	2.0
2	B	818	HIS	2.0
1	A	237	ILE	2.0
1	A	931	LEU	2.0
1	D	133	LEU	2.0
1	D	770	LEU	2.0
1	D	814	LEU	2.0
1	D	1012	LEU	2.0
1	D	1094	ILE	2.0
1	G	230	ILE	2.0
2	B	836	ILE	2.0
2	E	1033	LEU	2.0
3	F	78	PHE	2.0
1	D	944	GLU	2.0
1	D	1017	LEU	2.0
2	E	811	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
2	H	738	TYR	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	B	893	11/12	0.82	0.18	186,194,233,235	6
2	TPO	E	893	11/12	0.84	0.16	191,204,246,246	6
2	TPO	H	893	11/12	0.87	0.31	146,154,193,193	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	EDO	D	1201	4/4	0.58	0.36	104,125,134,135	6
5	SO4	D	1204	5/5	0.66	0.36	163,163,168,204	0
4	EDO	A	1201	4/4	0.70	0.23	102,122,132,143	6
5	SO4	G	1203	5/5	0.76	0.17	152,155,158,194	0
5	SO4	C	302	5/5	0.77	0.15	165,168,172,209	0
5	SO4	I	302	5/5	0.77	0.17	158,160,166,196	0
5	SO4	G	1201	5/5	0.81	0.19	154,156,158,178	0
5	SO4	C	303	5/5	0.84	0.15	159,163,172,210	0
5	SO4	A	1203	5/5	0.84	0.19	144,145,148,181	0
5	SO4	F	301	5/5	0.84	0.19	153,155,165,200	0
5	SO4	G	1202	5/5	0.85	0.12	157,157,160,195	0
5	SO4	H	1102	5/5	0.86	0.14	164,165,169,210	0
5	SO4	G	1204	5/5	0.88	0.15	154,157,170,205	0
5	SO4	D	1203	5/5	0.88	0.16	143,148,158,191	0

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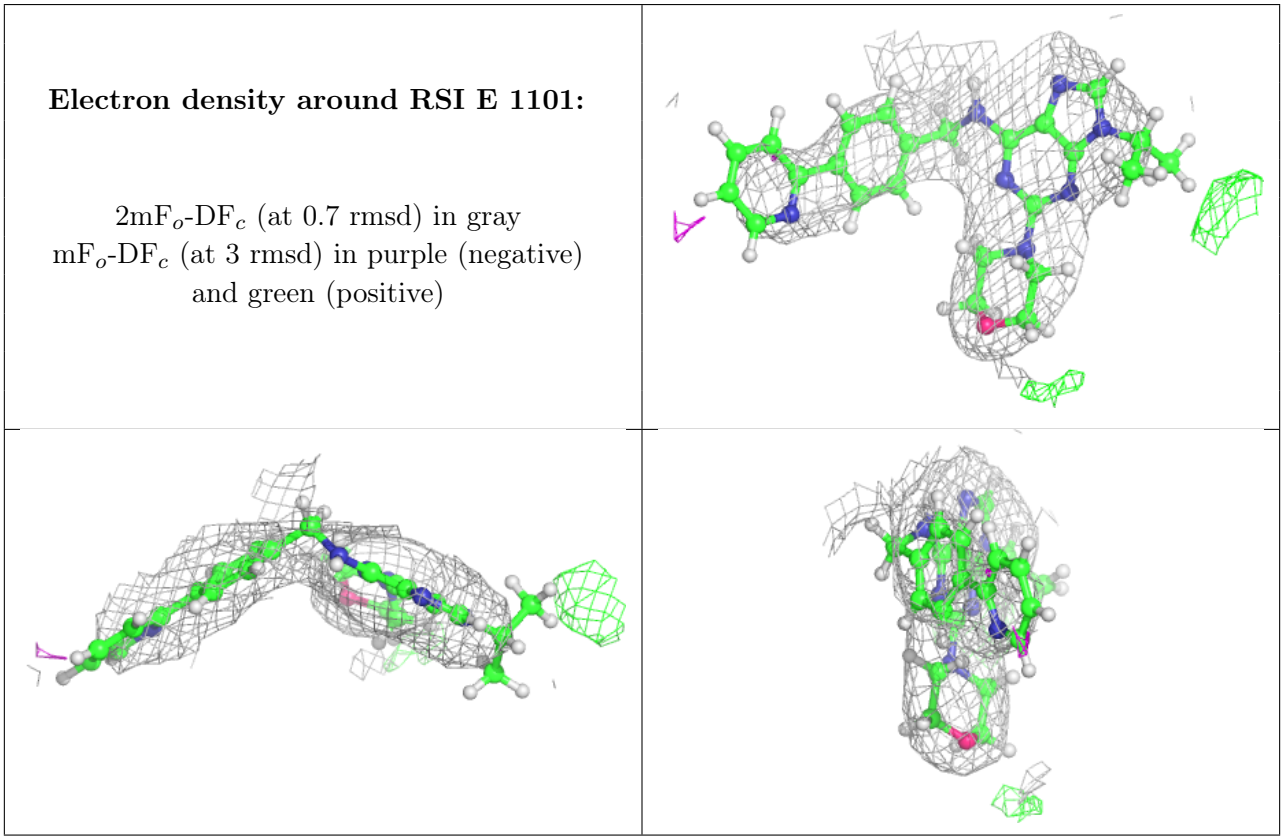
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SO4	A	1202	5/5	0.88	0.22	146,147,147,169	0
5	SO4	I	303	5/5	0.89	0.20	132,133,135,147	0
6	RSI	E	1101	32/32	0.89	0.53	112,125,151,156	27
5	SO4	A	1204	5/5	0.90	0.09	171,178,182,206	0
5	SO4	C	301	5/5	0.90	0.21	152,152,159,186	0
5	SO4	I	301	5/5	0.90	0.15	155,158,160,198	0
5	SO4	D	1202	5/5	0.91	0.16	147,147,154,182	0
5	SO4	H	1103	5/5	0.92	0.13	156,159,169,213	0
5	SO4	F	302	5/5	0.94	0.20	128,128,133,145	0
6	RSI	H	1101	32/32	0.94	0.46	106,121,145,153	27
6	RSI	B	1101	32/32	0.95	0.53	117,129,155,157	27

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

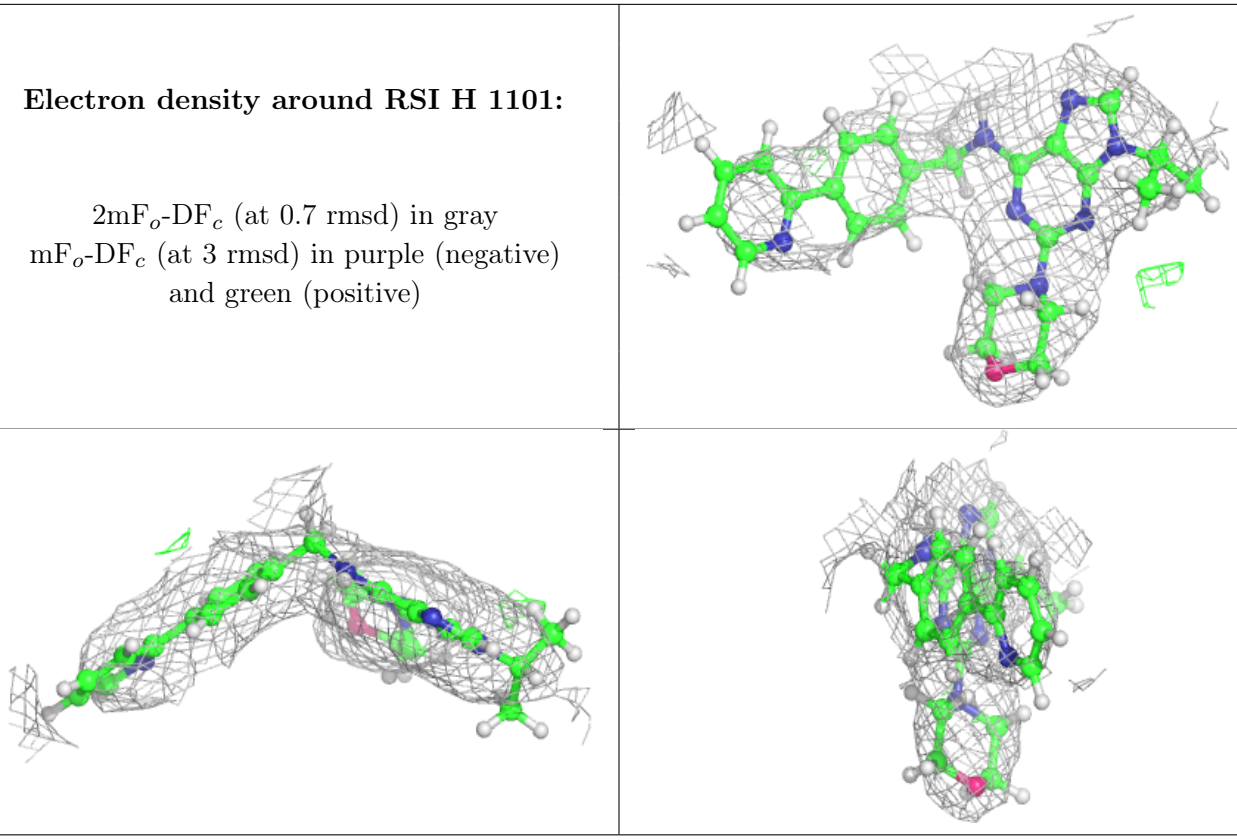
Electron density around RSI E 1101:

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



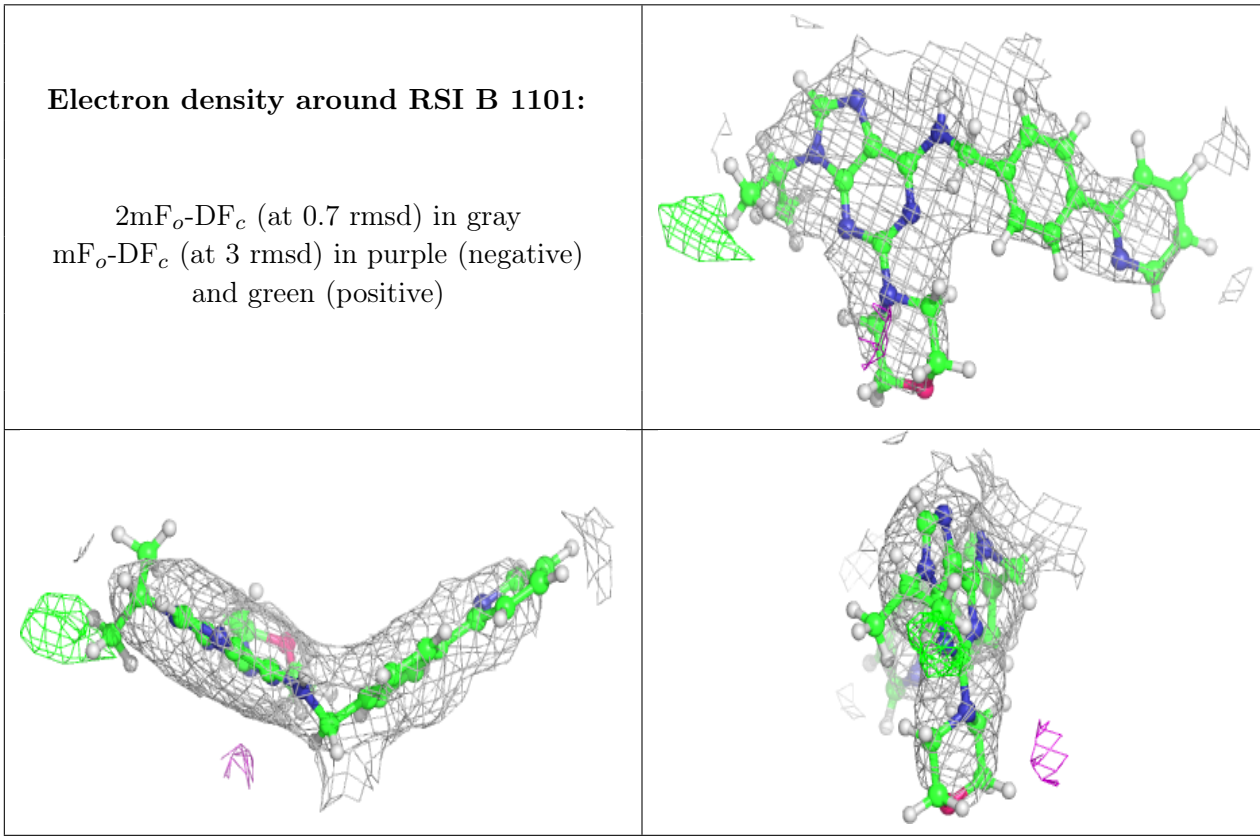
Electron density around RSI H 1101:

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



Electron density around RSI B 1101:

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



6.5 Other polymers (i)

There are no such residues in this entry.