Full wwPDB X-ray Structure Validation Report (i)

Sep 7, 2023 – 01:31 pm BST

PDB ID	:	8BUF
Title	:	Structure of DDB1 bound to Z12-engaged CDK12-cyclin K
Authors	:	Kozicka, Z.; Kempf, G.; Petzold, G.; Thoma, N.H.
Deposited on	:	2022-11-30
Resolution	:	3.30 Å(reported)

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

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

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

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

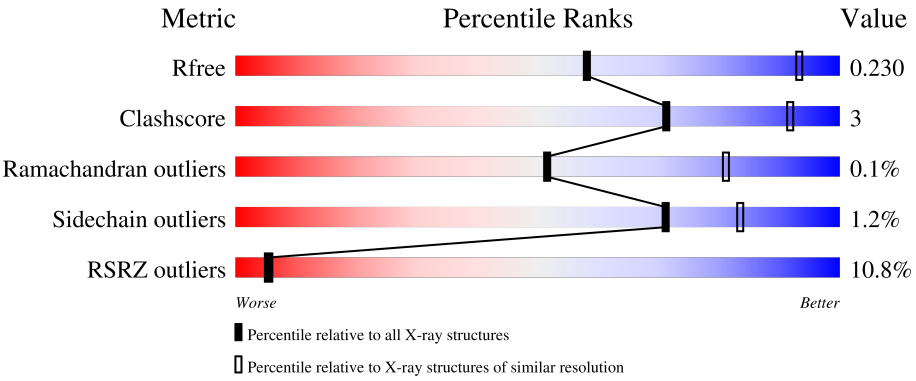
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	13% 89% 9% ·
1	D	840	9% 89% 9% ·
1	G	840	10% 87% 11% ·
2	B	344	12% 79% 14% 7%
2	E	344	15% 82% 13% · ·

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Mol	Chain	Length	Quality of chain
2	H	344	8% 83% 9% 8%
3	C	271	8% 85% 6% 9%
3	F	271	6% 85% 6% 8%
3	I	271	7% 84% 7% 9%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 67286 atoms, of which 33481 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	6500	0	0
			12957	4111	6462	1095	1253	36			
1	G	826	Total	C	H	N	O	S	6454	0	0
			12940	4106	6454	1093	1251	36			

There are 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

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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
2	B	319	Total	C	H	N	O	P	S	2643	0	0
			5214	1661	2622	437	477	1	16			
2	E	329	Total	C	H	N	O	P	S	2697	0	0
			5384	1723	2697	454	492	1	17			
2	H	318	Total	C	H	N	O	P	S	2611	0	0
			5195	1655	2611	436	476	1	16			

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

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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

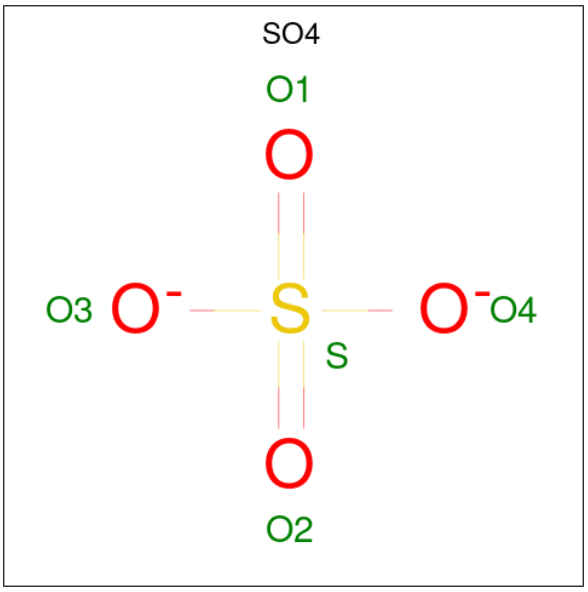
- Molecule 3 is a protein called Cyclin-K.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	247	Total	C	H	N	O	S	2039	0	0
			4092	1335	2039	343	362	13			
3	F	248	Total	C	H	N	O	S	2048	0	0
			4111	1341	2048	346	363	13			
3	I	247	Total	C	H	N	O	S	2041	0	0
			4094	1335	2041	343	362	13			

There are 12 discrepancies between the modelled and reference sequences:

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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

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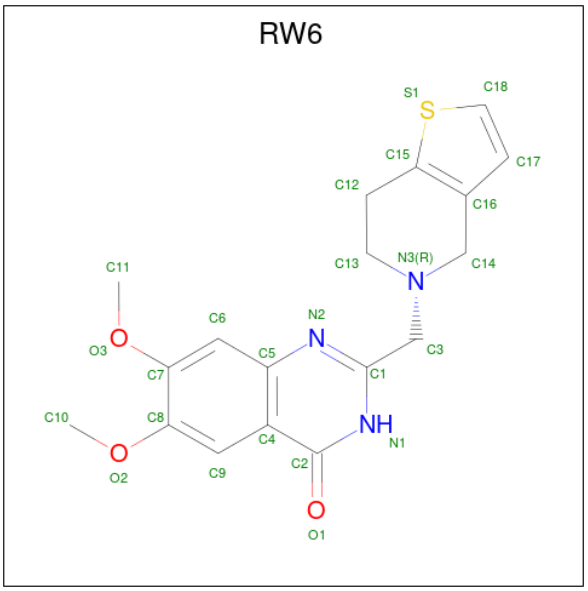
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	I	1	Total O S 5 4 1	0	0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

- Molecule 5 is 2-(6,7-dihydro-4 {H}-thieno[3,2-c]pyridin-5-ylmethyl)-6,7-dimethoxy-3 {H}-quinazolin-4-one (three-letter code: RW6) (formula: $C_{18}H_{19}N_3O_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	B	1	Total	C	H	N	O	S	19	0
			44	18	19	3	3	1		
5	E	1	Total	C	H	N	O	S	19	0
			44	18	19	3	3	1		
5	H	1	Total	C	H	N	O	S	19	0
			44	18	19	3	3	1		

3 Residue-property plots (i)

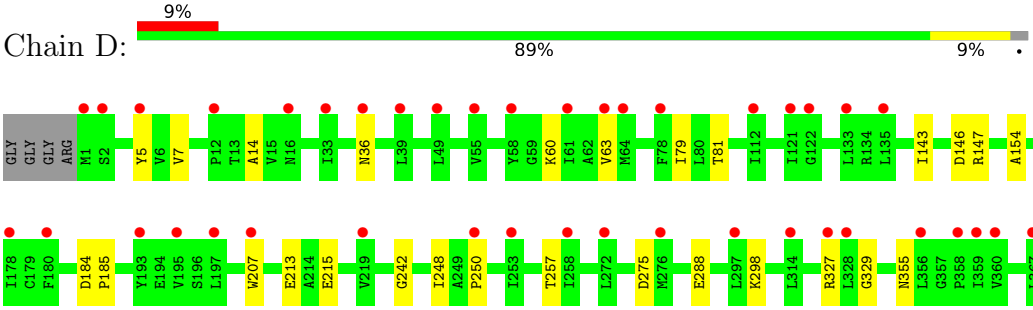
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

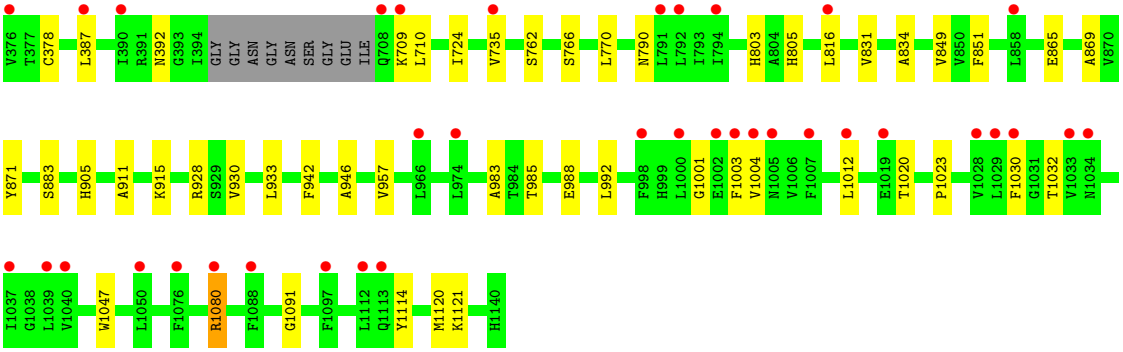
• Molecule 1: DNA damage-binding protein 1

Chain A:

• Molecule 1: DNA damage-binding protein 1

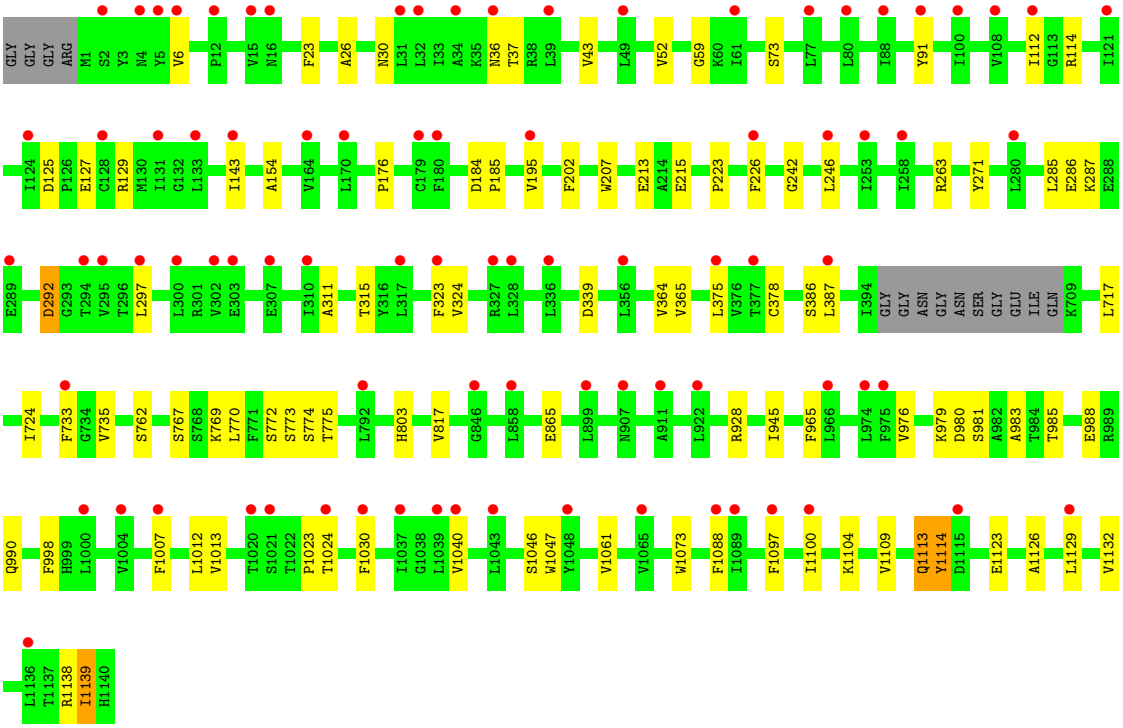
Chain D:





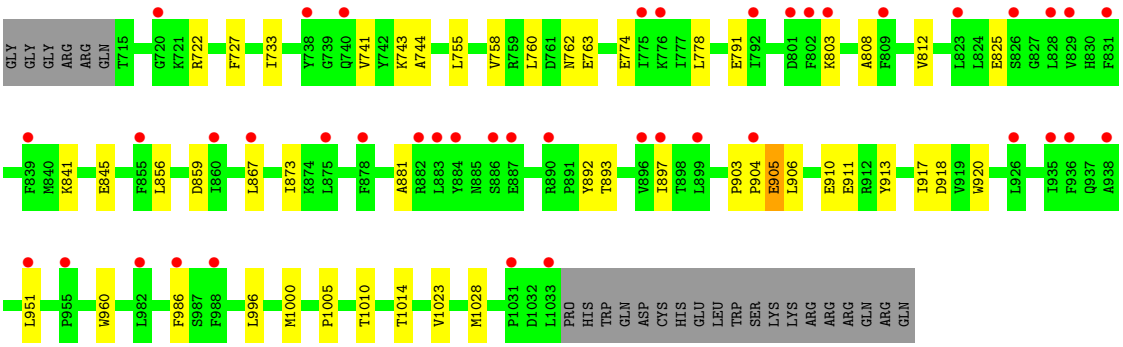
• Molecule 1: DNA damage-binding protein 1

Chain G:



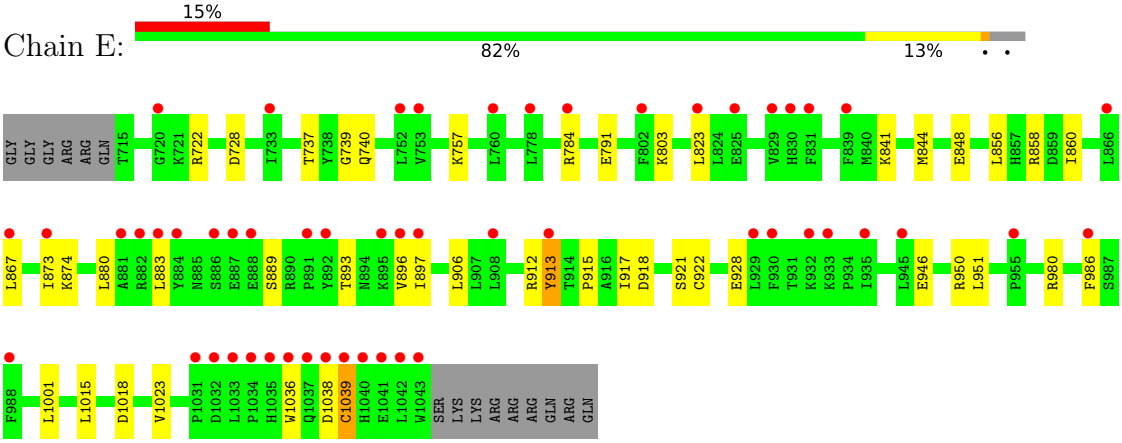
• Molecule 2: Cyclin-dependent kinase 12

Chain B:



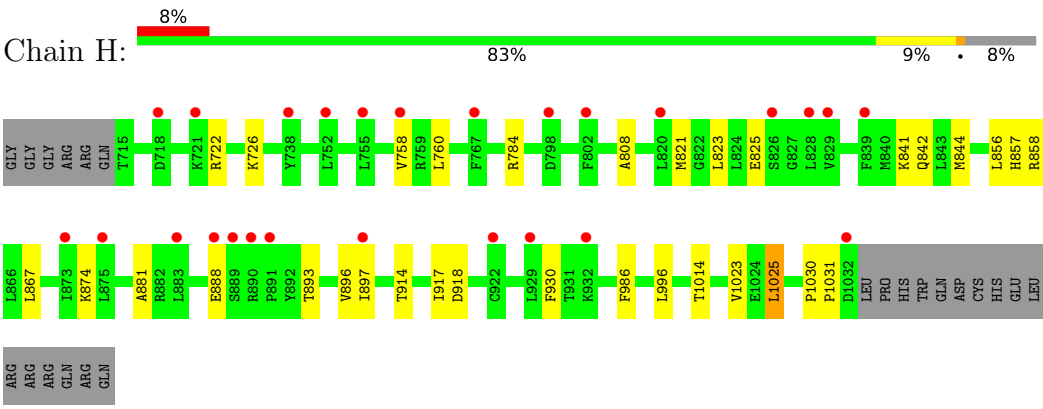
• Molecule 2: Cyclin-dependent kinase 12

Chain E:



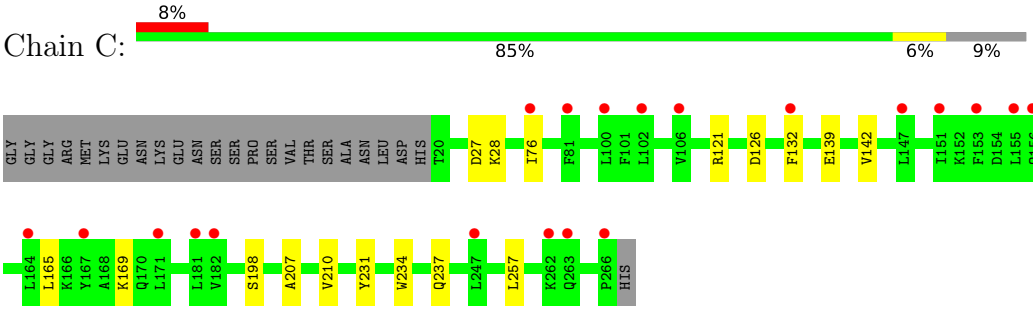
• Molecule 2: Cyclin-dependent kinase 12

Chain H:



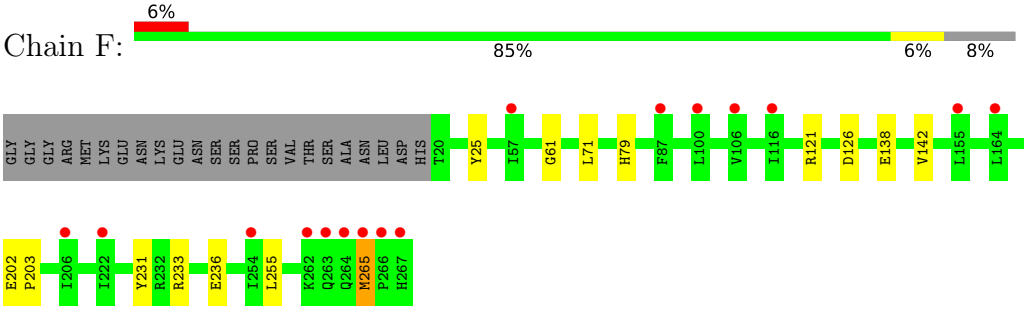
• Molecule 3: Cyclin-K

Chain C:



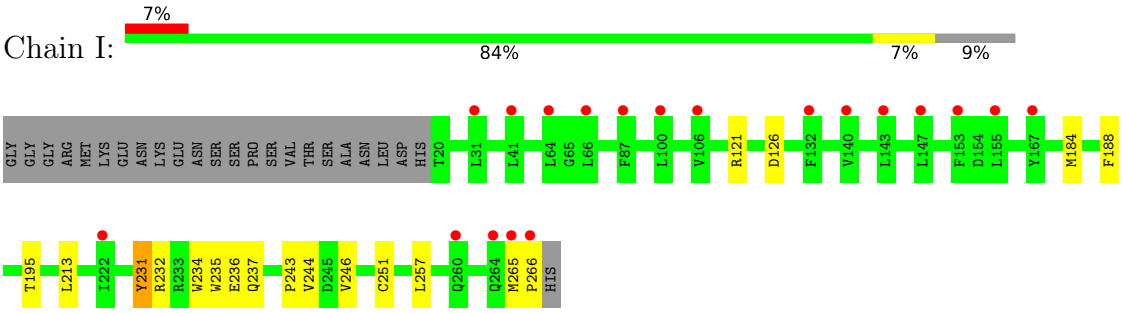
• Molecule 3: Cyclin-K

Chain F:



• 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	249.62Å 249.62Å 220.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	60.33 – 3.30 216.18 – 3.30	Depositor EDS
% Data completeness (in resolution range)	84.5 (60.33-3.30) 84.6 (216.18-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.53 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.184 , 0.220 0.197 , 0.230	Depositor DCC
R_{free} test set	5043 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	135.3	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 100.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.034 for -h,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	67286	wwPDB-VP
Average B, all atoms (Å^2)	156.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% 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: RW6, 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	0.32	0/6604	0.61	0/8931
1	D	0.32	0/6612	0.59	0/8942
1	G	0.33	0/6603	0.61	0/8930
2	B	0.34	0/2635	0.60	0/3549
2	E	0.33	0/2737	0.58	0/3691
2	H	0.35	0/2627	0.61	0/3538
3	C	0.32	0/2109	0.55	0/2853
3	F	0.34	0/2120	0.56	0/2868
3	I	0.33	0/2109	0.55	0/2853
All	All	0.33	0/34156	0.59	0/46155

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6487	6450	6451	39	0
1	D	6495	6462	6464	42	0
1	G	6486	6454	6456	59	0
2	B	2592	2622	2622	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	2687	2697	2697	23	1
2	H	2584	2611	2611	20	0
3	C	2053	2039	2041	10	0
3	F	2063	2048	2048	10	0
3	I	2053	2041	2041	9	1
4	A	40	0	0	0	0
4	B	10	0	0	0	0
4	C	10	0	0	0	0
4	D	45	0	0	0	0
4	E	20	0	0	0	0
4	F	20	0	0	0	0
4	G	45	0	0	1	0
4	H	30	0	0	0	0
4	I	10	0	0	0	0
5	B	25	19	0	2	0
5	E	25	19	0	0	0
5	H	25	19	0	0	0
All	All	33805	33481	33431	233	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (233) 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:C:121:ARG:NH2	3:C:126:ASP:OD1	1.86	1.08
3:F:231:TYR:OH	3:F:236:GLU:OE1	1.98	0.81
1:A:227:GLY:O	1:A:239:TYR:OH	2.01	0.79
1:G:285:LEU:HB3	1:G:297:LEU:HD11	1.72	0.71
1:G:1114:TYR:HA	1:G:1123:GLU:HA	1.73	0.70
1:G:983:ALA:HB1	1:G:988:GLU:OE1	1.91	0.70
1:G:773:SER:O	1:G:775:THR:N	2.27	0.67
1:G:979:LYS:O	1:G:981:SER:N	2.28	0.67
3:F:121:ARG:NH2	3:F:126:ASP:OD1	2.23	0.63
1:G:364:VAL:HG22	1:G:375:LEU:HD13	1.79	0.63
1:G:226:PHE:CZ	1:G:287:LYS:HG2	2.34	0.63
1:G:1047:TRP:HZ3	1:G:1132:VAL:HG13	1.64	0.62
1:G:226:PHE:CE1	1:G:287:LYS:HG2	2.34	0.61
2:H:841:LYS:HD2	2:H:1023:VAL:HB	1.82	0.61
2:B:906:LEU:HD21	2:B:913:TYR:CD1	2.36	0.60
1:A:1112:LEU:O	1:A:1123:GLU:HA	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:329:GLY:O	1:D:355:ASN:ND2	2.35	0.59
1:A:1109:VAL:HG12	1:A:1129:LEU:HD12	1.83	0.59
1:D:207:TRP:HB3	1:D:242:GLY:HA2	1.85	0.59
3:I:195:THR:CG2	3:I:257:LEU:HD11	2.33	0.59
1:A:775:THR:HG22	1:A:775:THR:O	2.03	0.59
2:E:823:LEU:HD12	2:E:867:LEU:HD23	1.84	0.59
1:G:1109:VAL:HG11	1:G:1126:ALA:HA	1.86	0.58
1:A:889:ARG:HD2	1:A:891:TYR:CZ	2.40	0.57
1:D:816:LEU:HD13	1:D:831:VAL:HG22	1.86	0.57
1:G:773:SER:C	1:G:775:THR:H	2.07	0.57
1:A:59:GLY:HA2	1:A:1073:TRP:CZ3	2.40	0.57
2:B:905:GLU:HA	2:B:960:TRP:HH2	1.69	0.56
1:G:292:ASP:OD1	1:G:292:ASP:N	2.39	0.56
1:G:43:VAL:HG23	1:G:52:VAL:HG21	1.86	0.56
1:D:387:LEU:HD11	1:D:735:VAL:HG21	1.88	0.56
1:A:207:TRP:HB3	1:A:242:GLY:HA2	1.87	0.56
2:E:841:LYS:HD2	2:E:1023:VAL:HB	1.89	0.55
2:B:841:LYS:HD2	2:B:1023:VAL:HB	1.88	0.55
1:G:1023:PRO:HB3	1:G:1047:TRP:CE2	2.42	0.55
1:A:372:GLN:HG3	1:A:1014:MET:HG2	1.89	0.55
1:A:248:ILE:HG12	1:A:250:PRO:HD3	1.88	0.55
3:F:79:HIS:HB3	3:F:199:LEU:HD11	1.88	0.54
2:B:1010:THR:O	2:B:1014:THR:HG23	2.08	0.54
2:E:1036:TRP:HA	2:E:1039:CYS:HB3	1.89	0.54
1:D:288:GLU:HB2	1:D:298:LYS:HB2	1.89	0.53
1:G:387:LEU:HD11	1:G:735:VAL:HG21	1.90	0.53
1:G:770:LEU:HD21	1:G:865:GLU:HB2	1.90	0.53
1:D:213:GLU:HG2	1:D:215:GLU:H	1.73	0.53
1:A:7:VAL:HG12	1:A:1091:GLY:HA3	1.91	0.53
1:G:387:LEU:HG	1:G:717:LEU:HD11	1.89	0.53
1:A:226:PHE:CE2	1:A:287:LYS:HG2	2.44	0.52
1:G:36:ASN:O	1:G:37:THR:OG1	2.24	0.52
2:B:910:GLU:O	2:B:911:GLU:HB3	2.09	0.52
1:D:871:TYR:HE1	2:E:1036:TRP:HZ3	1.56	0.52
2:E:739:GLY:HA3	2:E:757:LYS:O	2.09	0.52
1:D:834:ALA:HB2	1:D:869:ALA:HA	1.90	0.52
1:G:767:SER:N	4:G:1205:SO4:O1	2.43	0.52
2:E:951:LEU:HD21	2:E:986:PHE:HE2	1.75	0.51
3:I:231:TYR:OH	3:I:236:GLU:OE1	2.22	0.51
1:D:1080:ARG:NH1	2:E:928:GLU:OE2	2.44	0.51
2:H:760:LEU:HD12	2:H:760:LEU:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:951:LEU:HD21	2:B:986:PHE:HE2	1.76	0.51
1:A:311:ALA:HB2	1:A:324:VAL:HG13	1.92	0.51
1:D:378:CYS:SG	1:D:724:ILE:HB	2.51	0.50
1:A:1003:PHE:O	1:A:1032:THR:HA	2.12	0.50
1:A:255:GLN:HB2	1:A:279:ARG:HH22	1.77	0.50
2:B:917:ILE:HG13	2:B:918:ASP:N	2.26	0.50
1:D:770:LEU:HD13	1:D:865:GLU:HB2	1.94	0.50
1:D:983:ALA:HB3	1:D:988:GLU:HG3	1.93	0.50
1:G:311:ALA:HB2	1:G:324:VAL:HG13	1.94	0.50
2:E:858:ARG:NE	2:E:880:LEU:O	2.45	0.50
2:H:722:ARG:HE	2:H:726:LYS:HG3	1.77	0.50
2:E:906:LEU:HD21	2:E:913:TYR:CD2	2.47	0.50
3:F:138:GLU:O	3:F:142:VAL:HG13	2.11	0.50
1:D:709:LYS:HG2	1:D:710:LEU:N	2.27	0.49
3:C:76:ILE:CD1	3:C:198:SER:HB3	2.42	0.49
1:G:1113:GLN:HG2	1:G:1114:TYR:H	1.78	0.49
2:E:867:LEU:HD13	2:E:873:ILE:CD1	2.42	0.49
2:H:842:GLN:HG3	2:H:1025:LEU:HD11	1.94	0.49
1:A:928:ARG:HG2	5:B:1101:RW6:C18	2.43	0.49
2:E:856:LEU:HD11	2:E:915:PRO:HG3	1.95	0.49
1:D:7:VAL:HG12	1:D:1091:GLY:HA3	1.94	0.49
1:A:946:ALA:HB1	1:A:992:LEU:HG	1.93	0.48
1:D:375:LEU:HB2	1:D:1012:LEU:HD21	1.95	0.48
1:D:946:ALA:HB1	1:D:992:LEU:HG	1.95	0.48
1:G:6:VAL:HG22	1:G:1040:VAL:HG22	1.95	0.48
1:G:246:LEU:HD12	1:G:297:LEU:HD23	1.96	0.48
2:B:774:GLU:HG2	2:B:778:LEU:HD12	1.96	0.48
1:G:378:CYS:SG	1:G:724:ILE:HB	2.53	0.48
1:A:387:LEU:HD11	1:A:735:VAL:HG21	1.94	0.48
2:E:803:LYS:HG3	3:F:142:VAL:HG11	1.96	0.48
3:I:184:MET:HG3	3:I:266:PRO:HB2	1.95	0.47
1:G:114:ARG:HD3	2:H:930:PHE:O	2.14	0.47
1:A:14:ALA:O	1:A:35:LYS:HG2	2.15	0.47
1:A:43:VAL:HG23	1:A:52:VAL:HG11	1.97	0.47
1:G:143:ILE:HG12	1:G:154:ALA:HB2	1.97	0.47
1:G:1061:VAL:HG11	1:G:1104:LYS:HB3	1.97	0.47
3:I:234:TRP:O	3:I:237:GLN:HG2	2.15	0.47
3:I:243:PRO:HG2	3:I:246:VAL:HG23	1.95	0.47
3:C:27:ASP:OD1	3:C:28:LYS:N	2.48	0.47
2:E:946:GLU:O	2:E:950:ARG:HG2	2.14	0.47
1:G:1024:THR:HG21	1:G:1139:ILE:HD13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:803:LYS:HG3	3:C:142:VAL:HG21	1.97	0.47
1:D:146:ASP:OD1	1:D:147:ARG:N	2.48	0.47
2:B:867:LEU:HG	2:B:873:ILE:HG13	1.95	0.47
1:G:762:SER:O	1:G:803:HIS:HA	2.15	0.47
1:G:184:ASP:HB2	1:G:185:PRO:CD	2.45	0.46
1:D:60:LYS:O	1:D:81:THR:HA	2.15	0.46
2:H:758:VAL:O	2:H:808:ALA:HB1	2.15	0.46
3:C:132:PHE:O	3:C:139:GLU:HG3	2.16	0.46
1:D:63:VAL:O	1:D:79:ILE:HA	2.15	0.46
1:G:207:TRP:HB3	1:G:242:GLY:HA2	1.97	0.46
1:D:849:VAL:HG11	1:D:851:PHE:CZ	2.50	0.46
1:D:1120:MET:HG2	1:D:1121:LYS:H	1.80	0.46
1:D:372:GLN:NE2	1:D:392:ASN:O	2.48	0.46
1:G:59:GLY:HA2	1:G:1073:TRP:CE3	2.51	0.46
1:G:1113:GLN:HG2	1:G:1114:TYR:N	2.30	0.46
2:E:867:LEU:HD13	2:E:873:ILE:HD13	1.98	0.46
1:A:184:ASP:HB2	1:A:185:PRO:CD	2.46	0.46
2:B:758:VAL:O	2:B:808:ALA:HB1	2.16	0.46
2:E:844:MET:HE3	2:E:922:CYS:HB3	1.97	0.45
1:G:30:ASN:ND2	1:G:43:VAL:HG22	2.31	0.45
1:G:365:VAL:HG11	1:G:733:PHE:CZ	2.51	0.45
2:H:917:ILE:HG13	2:H:918:ASP:N	2.31	0.45
1:A:879:LYS:NZ	1:A:935:TYR:OH	2.50	0.45
3:C:234:TRP:O	3:C:237:GLN:HG2	2.16	0.45
3:F:25:TYR:OH	3:F:203:PRO:HD3	2.16	0.45
1:D:915:LYS:HE3	1:D:957:VAL:O	2.17	0.45
1:G:195:VAL:HG22	1:G:202:PHE:HE1	1.82	0.45
1:D:1003:PHE:O	1:D:1032:THR:HA	2.17	0.45
2:E:844:MET:HE2	2:E:844:MET:HA	1.99	0.45
2:H:858:ARG:HG2	2:H:917:ILE:HD11	1.98	0.45
1:A:5:TYR:CE2	1:A:7:VAL:HG13	2.53	0.44
1:A:248:ILE:HD12	1:A:300:LEU:O	2.17	0.44
1:A:1080:ARG:HD3	2:B:825:GLU:HA	1.99	0.44
2:E:722:ARG:NH1	2:E:791:GLU:OE2	2.50	0.44
3:C:76:ILE:HD12	3:C:198:SER:HB3	1.99	0.44
2:E:980:ARG:NH2	2:E:1001:LEU:O	2.46	0.44
1:D:14:ALA:HB1	1:D:327:ARG:HG3	2.00	0.44
1:D:1023:PRO:HB3	1:D:1047:TRP:CZ2	2.53	0.44
1:G:315:THR:HG22	1:G:323:PHE:HB3	2.00	0.44
1:A:92:LYS:HD2	1:A:101:ILE:HD11	1.99	0.44
2:E:917:ILE:HG13	2:E:918:ASP:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:985:THR:HB	1:D:988:GLU:HG2	1.99	0.43
1:G:59:GLY:HA2	1:G:1073:TRP:CZ3	2.53	0.43
1:G:1007:PHE:CD1	1:G:1030:PHE:HB3	2.53	0.43
2:H:856:LEU:O	2:H:881:ALA:HA	2.18	0.43
2:B:904:PRO:HD3	2:B:920:TRP:CE2	2.53	0.43
3:F:255:LEU:HD22	3:F:265:MET:HG2	2.00	0.43
2:H:844:MET:HA	2:H:844:MET:HE2	2.01	0.43
3:C:165:LEU:O	3:C:169:LYS:HG3	2.18	0.43
1:D:36:ASN:ND2	1:D:1001:GLY:O	2.51	0.43
2:B:905:GLU:OE1	2:B:1005:PRO:HB3	2.18	0.43
1:G:1013:VAL:HG11	1:G:1138:ARG:O	2.19	0.43
1:G:127:GLU:HB2	1:G:129:ARG:HG3	2.00	0.43
2:B:903:PRO:HG3	2:B:917:ILE:HG22	2.00	0.43
1:G:773:SER:C	1:G:775:THR:N	2.71	0.43
2:E:860:ILE:HB	2:E:921:SER:CB	2.49	0.42
1:D:7:VAL:CG1	1:D:1091:GLY:HA3	2.50	0.42
2:E:889:SER:HB2	2:E:912:ARG:HD3	2.02	0.42
1:G:286:GLU:O	1:G:297:LEU:HD12	2.19	0.42
2:H:888:GLU:O	2:H:888:GLU:HG3	2.19	0.42
1:A:6:VAL:HG22	1:A:1040:VAL:HG22	2.01	0.42
1:D:834:ALA:HB2	1:D:869:ALA:CB	2.50	0.42
1:G:365:VAL:HG11	1:G:733:PHE:CE2	2.55	0.42
2:B:722:ARG:NH1	2:B:791:GLU:OE2	2.53	0.42
2:B:803:LYS:HG3	3:C:142:VAL:HG11	2.01	0.42
3:C:207:ALA:O	3:C:210:VAL:HG22	2.19	0.42
1:D:933:LEU:HD22	1:D:942:PHE:HB3	2.01	0.42
2:H:914:THR:O	2:H:917:ILE:HG12	2.18	0.42
1:A:378:CYS:SG	1:A:724:ILE:HB	2.60	0.42
2:B:727:PHE:HB3	2:B:744:ALA:HB1	2.02	0.42
1:D:5:TYR:CE2	1:D:7:VAL:HG13	2.55	0.42
1:G:125:ASP:OD2	1:G:176:PRO:HB3	2.18	0.42
2:B:733:ILE:HG23	2:B:743:LYS:HB2	2.01	0.42
1:D:905:HIS:CG	1:D:933:LEU:HD11	2.55	0.42
1:G:375:LEU:HB2	1:G:1012:LEU:HD21	2.02	0.42
2:B:841:LYS:O	2:B:845:GLU:HB2	2.19	0.42
2:B:903:PRO:HB2	2:B:905:GLU:HG3	2.02	0.42
1:D:248:ILE:HG12	1:D:250:PRO:HD3	2.02	0.42
2:B:906:LEU:HD23	2:B:906:LEU:HA	1.79	0.41
1:D:790:ASN:HA	1:D:805:HIS:O	2.20	0.41
3:F:61:GLY:HA3	3:F:71:LEU:CD2	2.50	0.41
3:F:202:GLU:OE1	3:F:202:GLU:N	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:965:PHE:O	1:G:976:VAL:HA	2.20	0.41
2:B:856:LEU:O	2:B:881:ALA:HA	2.20	0.41
2:E:784:ARG:O	2:E:874:LYS:HE2	2.19	0.41
2:E:848:GLU:OE1	2:E:1015:LEU:HD12	2.20	0.41
1:D:883:SER:HB2	1:D:911:ALA:HB3	2.02	0.41
1:G:223:PRO:HD3	1:G:271:TYR:OH	2.19	0.41
1:G:945:ILE:O	1:G:990:GLN:HA	2.20	0.41
2:H:722:ARG:HH21	2:H:726:LYS:HB3	1.85	0.41
1:A:883:SER:HB2	1:A:911:ALA:HB3	2.02	0.41
2:B:892:TYR:O	2:B:911:GLU:HG3	2.21	0.41
1:D:257:THR:O	1:D:275:ASP:HB2	2.20	0.41
2:H:784:ARG:O	2:H:874:LYS:HE2	2.19	0.41
3:I:235:TRP:HZ2	3:I:244:VAL:HG22	1.85	0.41
1:A:222:VAL:HA	1:A:223:PRO:HD3	1.88	0.41
1:D:1004:VAL:HG13	1:D:1030:PHE:HB2	2.01	0.41
1:G:112:ILE:HD13	2:H:986:PHE:CE2	2.56	0.41
1:G:769:LYS:O	1:G:772:SER:HB3	2.21	0.41
1:G:1097:PHE:O	1:G:1100:ILE:HG12	2.21	0.41
2:H:823:LEU:HD12	2:H:867:LEU:HD21	2.03	0.41
1:A:63:VAL:O	1:A:79:ILE:HA	2.21	0.41
1:G:26:ALA:HB2	1:G:73:SER:O	2.21	0.41
1:G:1109:VAL:HG12	1:G:1129:LEU:HD12	2.01	0.41
2:H:1030:PRO:HA	2:H:1031:PRO:HD3	1.90	0.41
3:I:213:LEU:HB2	3:I:251:CYS:SG	2.60	0.41
1:A:971:ALA:HB3	1:A:973:ASN:HD22	1.86	0.41
1:A:1030:PHE:CZ	1:A:1038:GLY:HA3	2.56	0.41
2:B:859:ASP:OD1	2:B:859:ASP:N	2.54	0.41
1:D:143:ILE:HG12	1:D:154:ALA:HB2	2.02	0.41
1:D:170:LEU:HD23	1:D:170:LEU:HA	1.86	0.41
1:G:263:ARG:HA	1:G:271:TYR:CD2	2.55	0.41
2:H:857:HIS:ND1	2:H:860:ILE:HG12	2.36	0.41
2:B:762:ASN:O	2:B:763:GLU:HB3	2.21	0.41
1:A:1076:PHE:O	1:A:1082:THR:HA	2.21	0.40
2:B:755:LEU:HD22	2:B:812:VAL:HG22	2.03	0.40
2:B:996:LEU:O	2:B:1000:MET:HG3	2.21	0.40
1:A:376:VAL:HG21	1:A:733:PHE:CZ	2.57	0.40
1:A:1136:LEU:O	1:A:1139:ILE:HG12	2.21	0.40
2:B:741:VAL:HG21	5:B:1101:RW6:C11	2.51	0.40
1:D:184:ASP:HB2	1:D:185:PRO:CD	2.51	0.40
1:D:762:SER:HB3	1:D:803:HIS:ND1	2.35	0.40
1:G:23:PHE:CE2	1:G:91:TYR:HB2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:121:ARG:NH2	3:I:126:ASP:OD1	2.45	0.40
1:A:143:ILE:HG12	1:A:154:ALA:HB2	2.04	0.40
1:A:963:ASP:OD1	1:A:979:LYS:HE3	2.21	0.40
2:H:821:MET:HG2	2:H:825:GLU:HG3	2.03	0.40
3:I:184:MET:HG2	3:I:188:PHE:CE2	2.57	0.40
1:A:364:VAL:HG22	1:A:375:LEU:HD13	2.04	0.40
1:A:375:LEU:HB2	1:A:1012:LEU:HD21	2.04	0.40
3:F:233:ARG:HB3	3:F:236:GLU:HG3	2.02	0.40
1:G:213:GLU:HG2	1:G:215:GLU:H	1.86	0.40
1:G:998:PHE:HB2	1:G:1088:PHE:CG	2.57	0.40
1:G:226:PHE:HZ	1:G:287:LYS:HG2	1.84	0.40
2:H:996:LEU:HD11	2:H:1014:THR:HG22	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1018:ASP:OD2	3:I:232:ARG:HE[5_554]	1.53	0.07

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%)	794 (97%)	28 (3%)	0	100	100
1	D	823/840 (98%)	802 (97%)	21 (3%)	0	100	100
1	G	822/840 (98%)	798 (97%)	21 (3%)	3 (0%)	34	66
2	B	316/344 (92%)	306 (97%)	10 (3%)	0	100	100
2	E	326/344 (95%)	316 (97%)	10 (3%)	0	100	100
2	H	315/344 (92%)	308 (98%)	7 (2%)	0	100	100
3	C	245/271 (90%)	244 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	F	246/271 (91%)	243 (99%)	3 (1%)	0	100 100
3	I	245/271 (90%)	242 (99%)	3 (1%)	0	100 100
All	All	4160/4365 (95%)	4053 (97%)	104 (2%)	3 (0%)	51 81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	1113	GLN
1	G	774	SER
1	G	980	ASP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	721/728 (99%)	713 (99%)	8 (1%)	73 85
1	D	722/728 (99%)	716 (99%)	6 (1%)	81 89
1	G	721/728 (99%)	712 (99%)	9 (1%)	71 83
2	B	286/308 (93%)	282 (99%)	4 (1%)	67 82
2	E	296/308 (96%)	287 (97%)	9 (3%)	41 68
2	H	285/308 (92%)	281 (99%)	4 (1%)	67 82
3	C	222/242 (92%)	220 (99%)	2 (1%)	78 87
3	F	223/242 (92%)	221 (99%)	2 (1%)	78 87
3	I	222/242 (92%)	220 (99%)	2 (1%)	78 87
All	All	3698/3834 (96%)	3652 (99%)	46 (1%)	71 83

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	THR
1	A	207	TRP
1	A	290	GLN

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Mol	Chain	Res	Type
1	A	315	THR
1	A	319	ASN
1	A	928	ARG
1	A	1014	MET
1	A	1101	SER
2	B	760	LEU
2	B	897	ILE
2	B	905	GLU
2	B	1028	MET
3	C	231	TYR
3	C	257	LEU
1	D	766	SER
1	D	928	ARG
1	D	930	VAL
1	D	1020	THR
1	D	1080	ARG
1	D	1114	TYR
2	E	728	ASP
2	E	737	THR
2	E	740	GLN
2	E	883	LEU
2	E	896	VAL
2	E	897	ILE
2	E	913	TYR
2	E	1038	ASP
2	E	1039	CYS
3	F	198	SER
3	F	265	MET
1	G	292	ASP
1	G	339	ASP
1	G	386	SER
1	G	817	VAL
1	G	928	ARG
1	G	985	THR
1	G	1046	SER
1	G	1114	TYR
1	G	1139	ILE
2	H	860	ILE
2	H	896	VAL
2	H	897	ILE
2	H	1025	LEU
3	I	231	TYR

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Mol	Chain	Res	Type
3	I	265	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	727	GLN
1	D	261	HIS
2	E	780	GLN
1	G	370	GLN
2	H	999	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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	H	893	2	8,10,11	1.43	1 (12%)	10,14,16	1.40	2 (20%)
2	TPO	E	893	2	8,10,11	1.27	0	10,14,16	1.06	1 (10%)
2	TPO	B	893	2	8,10,11	1.64	1 (12%)	10,14,16	1.30	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	H	893	2	-	2/9/11/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TPO	E	893	2	-	1/9/11/13	-
2	TPO	B	893	2	-	0/9/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	893	TPO	P-O1P	3.44	1.61	1.50
2	H	893	TPO	P-OG1	2.42	1.63	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	893	TPO	P-OG1-CB	-2.98	114.20	123.21
2	E	893	TPO	P-OG1-CB	-2.65	115.21	123.21
2	H	893	TPO	P-OG1-CB	-2.55	115.50	123.21
2	H	893	TPO	CG2-CB-CA	-2.46	108.31	113.16

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	893	TPO	CB-OG1-P-O3P
2	H	893	TPO	CB-OG1-P-O1P
2	H	893	TPO	CB-OG1-P-O3P

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)

49 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SO4	D	1208	-	4,4,4	0.25	0	6,6,6	0.09	0
4	SO4	F	303	-	4,4,4	0.23	0	6,6,6	0.07	0
4	SO4	F	304	-	4,4,4	0.28	0	6,6,6	0.10	0
4	SO4	E	1103	-	4,4,4	0.20	0	6,6,6	0.06	0
4	SO4	A	1203	-	4,4,4	0.23	0	6,6,6	0.10	0
4	SO4	E	1102	-	4,4,4	0.23	0	6,6,6	0.05	0
4	SO4	B	1103	-	4,4,4	0.21	0	6,6,6	0.05	0
4	SO4	D	1201	-	4,4,4	0.18	0	6,6,6	0.08	0
4	SO4	C	301	-	4,4,4	0.18	0	6,6,6	0.07	0
4	SO4	A	1207	-	4,4,4	0.22	0	6,6,6	0.06	0
4	SO4	G	1204	-	4,4,4	0.25	0	6,6,6	0.08	0
4	SO4	D	1205	-	4,4,4	0.25	0	6,6,6	0.06	0
4	SO4	G	1207	-	4,4,4	0.23	0	6,6,6	0.06	0
4	SO4	G	1209	-	4,4,4	0.22	0	6,6,6	0.05	0
4	SO4	D	1202	-	4,4,4	0.23	0	6,6,6	0.05	0
4	SO4	D	1209	-	4,4,4	0.25	0	6,6,6	0.06	0
4	SO4	G	1202	-	4,4,4	0.24	0	6,6,6	0.05	0
4	SO4	H	1104	-	4,4,4	0.23	0	6,6,6	0.08	0
4	SO4	A	1202	-	4,4,4	0.26	0	6,6,6	0.10	0
4	SO4	E	1104	-	4,4,4	0.22	0	6,6,6	0.05	0
4	SO4	H	1107	-	4,4,4	0.28	0	6,6,6	0.06	0
4	SO4	D	1204	-	4,4,4	0.23	0	6,6,6	0.05	0
4	SO4	A	1206	-	4,4,4	0.25	0	6,6,6	0.08	0
4	SO4	H	1106	-	4,4,4	0.22	0	6,6,6	0.06	0
4	SO4	E	1105	-	4,4,4	0.23	0	6,6,6	0.07	0
4	SO4	G	1203	-	4,4,4	0.19	0	6,6,6	0.05	0
4	SO4	H	1103	-	4,4,4	0.28	0	6,6,6	0.08	0
4	SO4	H	1102	-	4,4,4	0.22	0	6,6,6	0.08	0
4	SO4	I	302	-	4,4,4	0.16	0	6,6,6	0.08	0
4	SO4	A	1201	-	4,4,4	0.19	0	6,6,6	0.06	0
5	RW6	B	1101	-	23,28,28	0.79	0	29,40,40	0.89	0
4	SO4	A	1208	-	4,4,4	0.23	0	6,6,6	0.05	0
4	SO4	G	1208	-	4,4,4	0.24	0	6,6,6	0.12	0
4	SO4	D	1207	-	4,4,4	0.23	0	6,6,6	0.06	0
4	SO4	A	1204	-	4,4,4	0.22	0	6,6,6	0.06	0
4	SO4	G	1201	-	4,4,4	0.19	0	6,6,6	0.07	0
4	SO4	D	1206	-	4,4,4	0.21	0	6,6,6	0.05	0
4	SO4	C	302	-	4,4,4	0.26	0	6,6,6	0.04	0
4	SO4	F	302	-	4,4,4	0.17	0	6,6,6	0.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	SO4	B	1102	-	4,4,4	0.23	0	6,6,6	0.07	0
5	RW6	E	1101	-	23,28,28	0.78	0	29,40,40	0.97	1 (3%)
4	SO4	I	301	-	4,4,4	0.26	0	6,6,6	0.06	0
4	SO4	G	1206	-	4,4,4	0.20	0	6,6,6	0.06	0
4	SO4	A	1205	-	4,4,4	0.24	0	6,6,6	0.07	0
4	SO4	D	1203	-	4,4,4	0.22	0	6,6,6	0.11	0
4	SO4	G	1205	-	4,4,4	0.21	0	6,6,6	0.07	0
4	SO4	H	1105	-	4,4,4	0.23	0	6,6,6	0.04	0
5	RW6	H	1101	-	23,28,28	0.78	0	29,40,40	0.98	2 (6%)
4	SO4	F	301	-	4,4,4	0.21	0	6,6,6	0.07	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	RW6	H	1101	-	-	2/6/17/17	0/4/4/4
5	RW6	E	1101	-	-	2/6/17/17	0/4/4/4
5	RW6	B	1101	-	-	4/6/17/17	0/4/4/4

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	1101	RW6	C2-N1-C1	-2.85	122.15	123.81
5	H	1101	RW6	C2-N1-C1	-2.82	122.17	123.81
5	H	1101	RW6	C13-C12-C15	-2.06	108.03	111.32

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1101	RW6	C1-C3-N3-C13
5	B	1101	RW6	C1-C3-N3-C14
5	E	1101	RW6	C1-C3-N3-C14
5	H	1101	RW6	C1-C3-N3-C13
5	H	1101	RW6	C1-C3-N3-C14
5	B	1101	RW6	C6-C7-O3-C11
5	B	1101	RW6	C8-C7-O3-C11

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Mol	Chain	Res	Type	Atoms
5	E	1101	RW6	C1-C3-N3-C13

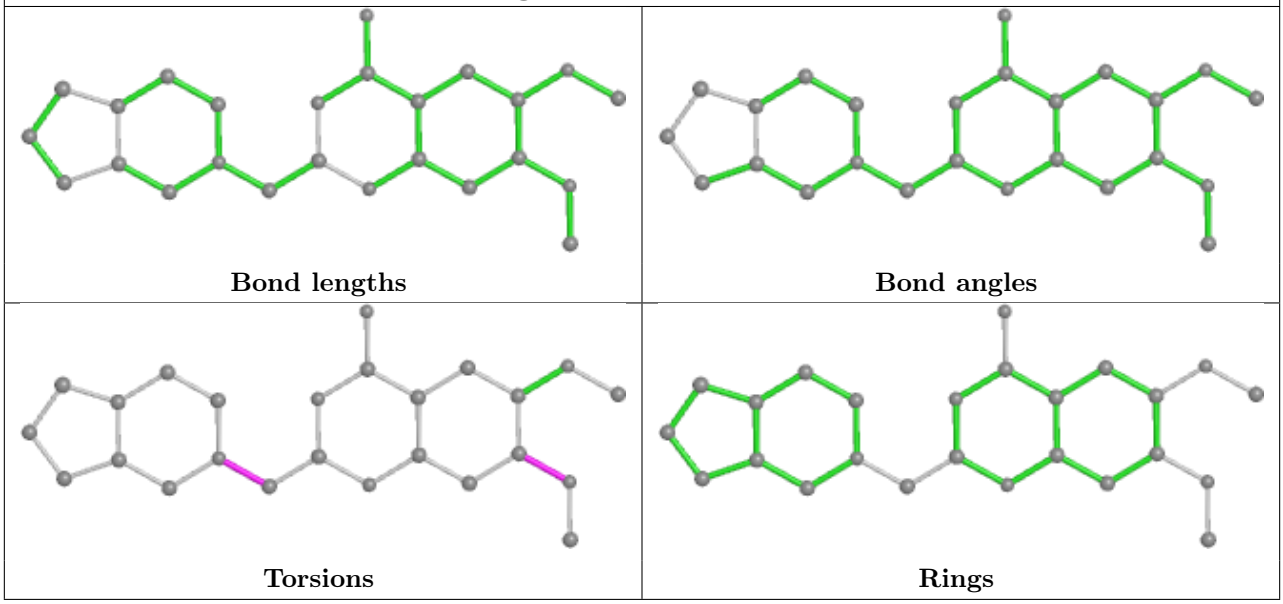
There are no ring outliers.

2 monomers are involved in 3 short contacts:

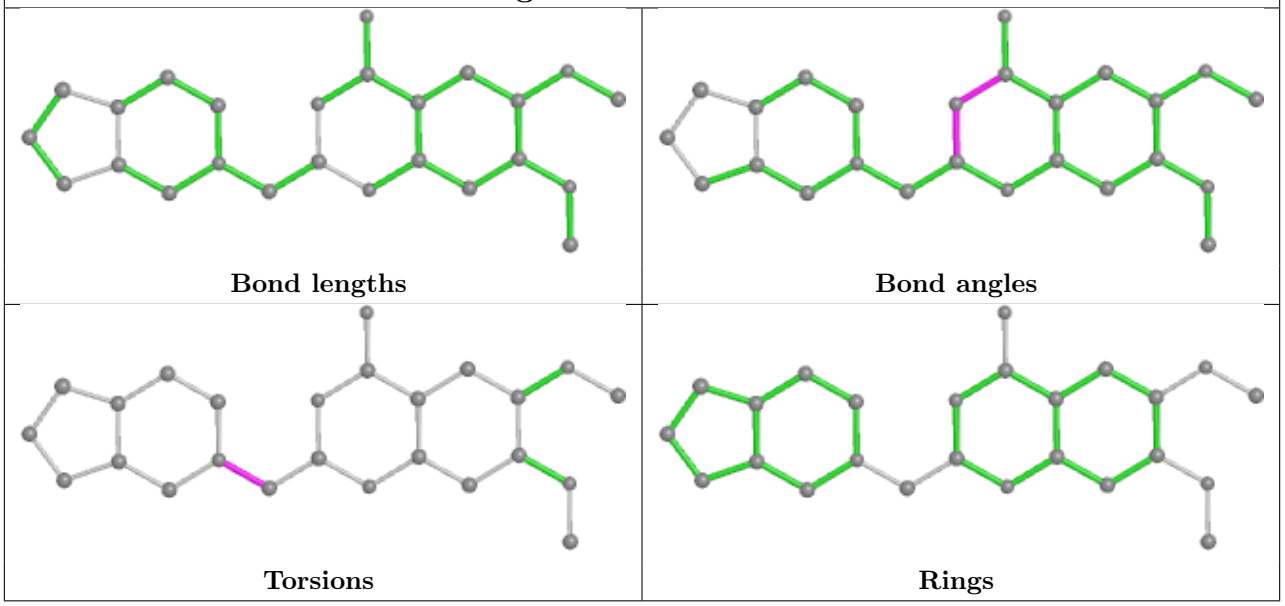
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1101	RW6	2	0
4	G	1205	SO4	1	0

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

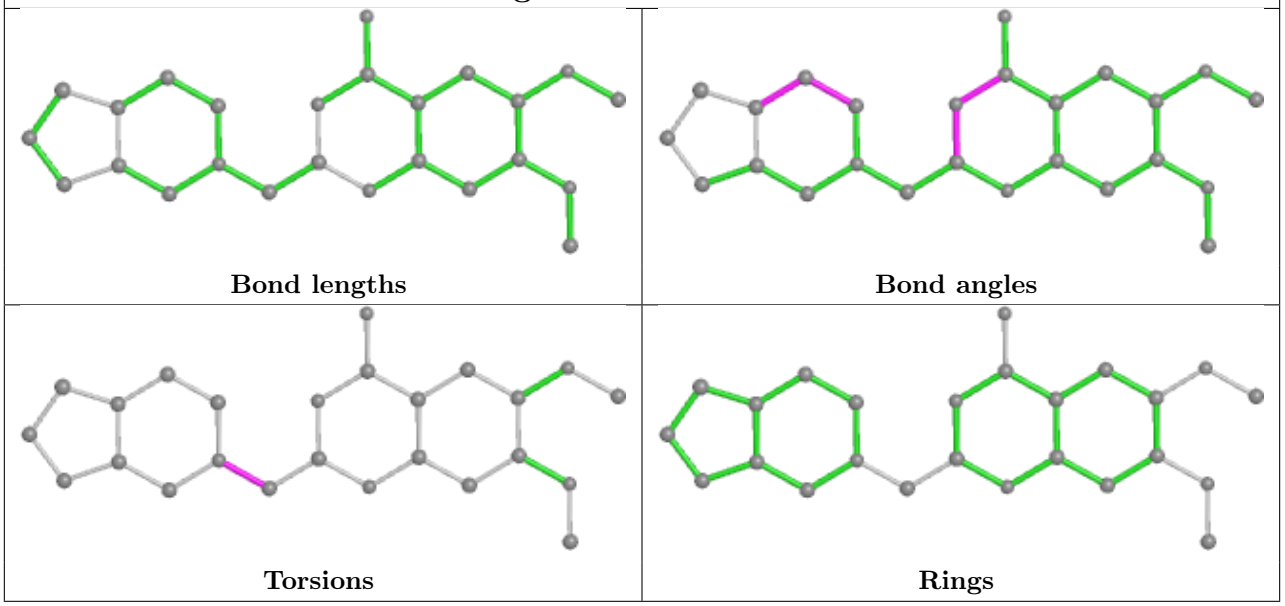
Ligand RW6 B 1101



Ligand RW6 E 1101



Ligand RW6 H 1101



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	826/840 (98%)	0.76	107 (12%) 3 3	101, 141, 214, 295	0
1	D	822/840 (97%)	0.64	79 (9%) 8 8	96, 138, 204, 259	0
1	G	826/840 (98%)	0.66	86 (10%) 6 6	100, 138, 212, 289	0
2	B	315/344 (91%)	0.88	42 (13%) 3 3	114, 147, 213, 244	0
2	E	328/344 (95%)	1.11	53 (16%) 1 2	107, 142, 220, 287	0
2	H	317/344 (92%)	0.85	27 (8%) 10 10	90, 122, 192, 265	0
3	C	247/271 (91%)	0.74	23 (9%) 8 9	109, 133, 178, 256	0
3	F	248/271 (91%)	0.83	17 (6%) 16 16	88, 113, 157, 300	0
3	I	247/271 (91%)	0.72	19 (7%) 13 12	96, 122, 168, 276	0
All	All	4176/4365 (95%)	0.76	453 (10%) 5 5	88, 135, 207, 300	0

All (453) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	1041	GLU	18.0
2	E	1043	TRP	16.0
3	F	264	GLN	16.0
2	E	1042	LEU	12.0
2	E	1040	HIS	8.5
3	F	267	HIS	8.3
3	F	262	LYS	7.3
2	E	1035	HIS	7.2
3	I	266	PRO	7.2
2	B	887	GLU	6.2
2	E	1036	TRP	5.8
2	E	882	ARG	5.7
2	E	896	VAL	5.6
2	B	802	PHE	5.6
3	I	264	GLN	5.5

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Mol	Chain	Res	Type	RSRZ
2	B	896	VAL	5.4
2	H	890	ARG	4.9
2	E	1034	PRO	4.9
2	H	1032	ASP	4.8
1	A	1114	TYR	4.6
2	B	803	LYS	4.5
2	E	829	VAL	4.5
1	G	327	ARG	4.4
2	B	897	ILE	4.2
1	A	131	ILE	4.1
1	G	295	VAL	4.1
3	F	265	MET	4.0
1	D	2	SER	4.0
1	A	1020	THR	4.0
2	E	1031	PRO	4.0
2	H	829	VAL	3.9
2	B	884	TYR	3.9
1	A	32	LEU	3.9
2	H	828	LEU	3.9
2	H	888	GLU	3.9
3	F	266	PRO	3.8
2	E	1038	ASP	3.8
3	F	263	GLN	3.8
2	B	1033	LEU	3.8
1	D	1019	GLU	3.8
1	A	39	LEU	3.8
2	E	891	PRO	3.7
1	A	23	PHE	3.7
1	A	64	MET	3.6
1	D	1004	VAL	3.6
1	A	317	LEU	3.6
1	G	49	LEU	3.6
1	A	145	LEU	3.6
1	G	1039	LEU	3.6
2	E	1039	CYS	3.6
1	D	1080	ARG	3.5
2	B	878	PHE	3.5
1	D	974	LEU	3.5
1	A	61	ILE	3.5
2	E	887	GLU	3.4
1	D	49	LEU	3.4
2	B	839	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	232	ILE	3.4
1	A	77	LEU	3.4
1	D	197	LEU	3.4
1	G	297	LEU	3.4
1	G	1021	SER	3.4
1	A	1115	ASP	3.3
2	B	831	PHE	3.3
1	A	367	LEU	3.3
2	H	802	PHE	3.3
3	C	100	LEU	3.3
2	E	831	PHE	3.3
1	A	135	LEU	3.3
1	G	1000	LEU	3.3
3	C	266	PRO	3.3
1	A	1118	SER	3.3
1	G	858	LEU	3.3
1	G	133	LEU	3.3
1	D	367	LEU	3.2
1	G	61	ILE	3.2
1	A	31	LEU	3.2
1	A	89	LEU	3.2
1	A	272	LEU	3.2
2	H	889	SER	3.2
3	C	132	PHE	3.2
1	G	289	GLU	3.2
1	D	708	GLN	3.2
3	C	164	LEU	3.2
1	A	1097	PHE	3.2
1	A	133	LEU	3.2
2	E	784	ARG	3.2
3	C	155	LEU	3.2
1	D	794	ILE	3.1
1	A	57	MET	3.1
1	A	977	CYS	3.1
1	A	1018	GLY	3.1
2	E	752	LEU	3.1
1	A	79	ILE	3.1
2	H	767	PHE	3.1
1	A	60	LYS	3.1
1	G	131	ILE	3.0
1	D	1005	ASN	3.0
1	D	36	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
2	E	1032	ASP	3.0
2	E	892	TYR	3.0
1	G	966	LEU	3.0
1	D	122	GLY	3.0
2	B	801	ASP	3.0
1	A	120	ILE	3.0
2	E	935	ILE	3.0
1	G	1136	LEU	3.0
1	D	1003	PHE	2.9
2	B	860	ILE	2.9
2	B	738	TYR	2.9
2	B	883	LEU	2.9
2	B	720	GLY	2.9
1	A	297	LEU	2.9
3	I	41	LEU	2.9
1	D	709	LYS	2.9
1	G	15	VAL	2.9
3	C	158	GLU	2.9
2	B	776	LYS	2.9
1	D	39	LEU	2.9
1	A	1079	GLU	2.9
1	D	360	VAL	2.9
1	G	1043	LEU	2.9
2	H	721	LYS	2.8
1	A	1035	GLY	2.8
1	A	356	LEU	2.8
1	G	226	PHE	2.8
2	B	890	ARG	2.8
1	G	2	SER	2.8
2	E	1033	LEU	2.8
1	G	128	CYS	2.8
2	H	798	ASP	2.8
3	I	132	PHE	2.8
1	A	13	THR	2.8
1	D	33	ILE	2.8
2	E	955	PRO	2.8
1	D	61	ILE	2.8
1	G	1088	PHE	2.8
1	D	5	TYR	2.8
1	A	829	PHE	2.8
2	E	881	ALA	2.8
2	E	888	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	899	LEU	2.8
2	E	823	LEU	2.8
1	D	359	ILE	2.7
3	C	76	ILE	2.7
1	G	974	LEU	2.7
3	C	181	LEU	2.7
2	B	886	SER	2.7
1	D	314	LEU	2.7
1	D	1007	PHE	2.7
2	H	826	SER	2.7
1	G	39	LEU	2.7
1	G	899	LEU	2.7
2	B	951	LEU	2.7
1	A	949	PHE	2.7
1	A	1068	ILE	2.7
1	A	1029	LEU	2.7
2	E	988	PHE	2.7
1	G	323	PHE	2.7
1	A	63	VAL	2.7
1	A	881	LEU	2.7
2	E	720	GLY	2.7
2	H	839	PHE	2.7
1	A	930	VAL	2.7
1	D	133	LEU	2.7
1	D	792	LEU	2.7
3	F	181	LEU	2.7
1	G	1024	THR	2.6
1	G	112	ILE	2.6
2	H	932	LYS	2.6
1	A	752	LEU	2.6
2	E	884	TYR	2.6
1	D	195	VAL	2.6
1	G	143	ILE	2.6
2	B	867	LEU	2.6
2	H	820	LEU	2.6
1	A	217	SER	2.6
1	G	1089	ILE	2.6
2	H	883	LEU	2.6
1	A	972	PHE	2.6
1	G	328	LEU	2.6
1	A	33	ILE	2.6
2	E	802	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	358	PRO	2.6
3	C	157	VAL	2.6
1	G	91	TYR	2.6
1	G	170	LEU	2.6
1	G	1100	ILE	2.6
1	A	219	VAL	2.6
1	A	220	ILE	2.6
2	E	897	ILE	2.6
1	D	1076	PHE	2.6
2	B	938	ALA	2.6
1	A	975	PHE	2.5
1	A	1116	ASP	2.5
2	E	778	LEU	2.5
1	A	1088	PHE	2.5
1	G	302	VAL	2.5
2	H	752	LEU	2.5
1	G	12	PRO	2.5
1	G	1030	PHE	2.5
1	D	1000	LEU	2.5
2	E	866	LEU	2.5
1	A	80	LEU	2.5
1	D	966	LEU	2.5
1	D	112	ILE	2.5
3	F	57	ILE	2.5
2	E	825	GLU	2.5
2	E	886	SER	2.5
2	H	738	TYR	2.5
1	D	1039	LEU	2.5
2	B	823	LEU	2.5
2	E	1037	GLN	2.5
1	G	1097	PHE	2.5
1	A	365	VAL	2.5
1	G	280	LEU	2.5
1	D	1097	PHE	2.5
3	I	66	LEU	2.5
1	A	86	ALA	2.5
1	D	387	LEU	2.5
2	E	929	LEU	2.5
3	C	167	TYR	2.5
1	A	230	ILE	2.5
1	D	250	PRO	2.4
2	E	913	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	327	ARG	2.4
1	G	32	LEU	2.4
2	E	839	PHE	2.4
3	C	262	LYS	2.4
2	E	883	LEU	2.4
2	H	755	LEU	2.4
1	A	82	ALA	2.4
1	D	135	LEU	2.4
2	B	935	ILE	2.4
1	G	31	LEU	2.4
1	G	246	LEU	2.4
1	G	1020	THR	2.4
2	B	986	PHE	2.4
1	A	124	ILE	2.4
1	A	328	LEU	2.4
1	D	356	LEU	2.4
2	B	936	PHE	2.4
1	G	5	TYR	2.4
1	G	303	GLU	2.4
1	G	336	LEU	2.4
1	G	4	ASN	2.4
1	G	121	ILE	2.4
1	A	933	LEU	2.4
3	C	153	PHE	2.4
1	D	1034	ASN	2.4
1	D	1037	ILE	2.4
2	H	873	ILE	2.4
1	G	317	LEU	2.4
1	D	1040	VAL	2.3
1	D	58	TYR	2.3
1	A	1000	LEU	2.3
1	A	967	GLY	2.3
2	H	718	ASP	2.3
1	A	777	PRO	2.3
1	D	16	ASN	2.3
3	I	140	VAL	2.3
1	G	307	GLU	2.3
1	A	140	PHE	2.3
1	D	1	MET	2.3
1	A	62	ALA	2.3
1	G	733	PHE	2.3
2	B	855	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	276	MET	2.3
1	G	36	ASN	2.3
1	A	34	ALA	2.3
1	G	375	LEU	2.3
3	I	155	LEU	2.3
1	A	19	VAL	2.3
1	D	1030	PHE	2.3
2	H	891	PRO	2.3
1	D	1012	LEU	2.3
1	G	16	ASN	2.3
1	D	1002	GLU	2.3
2	B	955	PRO	2.3
1	D	328	LEU	2.3
1	A	170	LEU	2.3
1	G	922	LEU	2.3
3	C	161	TYR	2.3
1	A	233	GLY	2.3
1	A	130	MET	2.3
1	G	80	LEU	2.3
2	B	792	ILE	2.3
1	D	735	VAL	2.3
1	D	1033	VAL	2.3
3	I	167	TYR	2.3
1	D	63	VAL	2.3
1	G	179	CYS	2.2
1	A	83	LYS	2.2
1	G	124	ILE	2.2
2	B	809	PHE	2.2
1	D	64	MET	2.2
2	B	829	VAL	2.2
2	B	1031	PRO	2.2
1	G	34	ALA	2.2
2	B	826	SER	2.2
3	I	100	LEU	2.2
1	A	143	ILE	2.2
1	A	78	PHE	2.2
1	D	1113	GLN	2.2
1	A	300	LEU	2.2
1	D	207	TRP	2.2
2	E	986	PHE	2.2
1	D	376	VAL	2.2
3	F	254	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	745	THR	2.2
1	G	356	LEU	2.2
1	A	1004	VAL	2.2
1	A	816	LEU	2.2
3	C	156	GLN	2.2
2	B	988	PHE	2.2
2	E	830	HIS	2.2
3	I	153	PHE	2.2
1	A	41	ILE	2.2
2	H	897	ILE	2.2
1	D	791	LEU	2.2
2	B	904	PRO	2.2
3	I	64	LEU	2.2
1	G	195	VAL	2.2
1	G	310	ILE	2.2
3	F	222	ILE	2.2
1	A	336	LEU	2.2
1	D	1029	LEU	2.2
3	F	155	LEU	2.2
3	I	31	LEU	2.2
2	H	758	VAL	2.2
2	H	865	ILE	2.2
3	I	265	MET	2.2
1	A	59	GLY	2.2
1	A	932	LEU	2.2
1	G	792	LEU	2.2
1	D	178	ILE	2.2
3	F	116	ILE	2.2
1	A	283	LEU	2.2
1	G	1129	LEU	2.2
2	H	875	LEU	2.2
1	D	12	PRO	2.2
1	D	78	PHE	2.2
1	A	377	THR	2.2
1	A	304	LEU	2.1
2	B	982	LEU	2.1
1	A	218	MET	2.1
1	D	121	ILE	2.1
1	G	1037	ILE	2.1
2	E	733	ILE	2.1
3	C	151	ILE	2.1
1	D	1050	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
3	I	106	VAL	2.1
1	G	1048	TYR	2.1
3	I	87	PHE	2.1
2	E	932	LYS	2.1
1	A	195	VAL	2.1
3	I	222	ILE	2.1
1	A	1012	LEU	2.1
1	G	77	LEU	2.1
3	C	171	LEU	2.1
3	I	143	LEU	2.1
1	A	87	CYS	2.1
1	G	253	ILE	2.1
3	F	100	LEU	2.1
2	B	882	ARG	2.1
1	A	240	HIS	2.1
1	A	921	ILE	2.1
1	A	923	VAL	2.1
1	D	55	VAL	2.1
1	D	390	ILE	2.1
1	G	294	THR	2.1
1	G	387	LEU	2.1
2	E	933	LYS	2.1
1	D	167	VAL	2.1
1	G	1004	VAL	2.1
2	E	867	LEU	2.1
1	G	1115	ASP	2.1
1	D	1028	VAL	2.1
1	G	6	VAL	2.1
1	A	974	LEU	2.1
1	D	1112	LEU	2.1
1	G	377	THR	2.1
1	A	1094	ILE	2.1
1	D	253	ILE	2.1
1	G	164	VAL	2.1
2	E	895	LYS	2.1
1	D	858	LEU	2.1
1	A	9	ALA	2.1
1	A	65	GLU	2.1
1	A	1008	CYS	2.1
1	D	219	VAL	2.1
2	B	775	ILE	2.1
3	F	106	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	945	LEU	2.1
3	C	102	LEU	2.1
2	E	753	VAL	2.1
1	A	88	ILE	2.1
2	B	875	LEU	2.1
2	B	926	LEU	2.1
2	E	908	LEU	2.1
1	A	882	ALA	2.1
1	G	108	VAL	2.1
3	C	182	VAL	2.1
1	D	258	ILE	2.1
2	E	760	LEU	2.1
1	A	67	PHE	2.0
1	A	978	GLN	2.0
1	A	980	ASP	2.1
1	D	180	PHE	2.0
1	G	975	PHE	2.0
1	A	324	VAL	2.0
1	G	911	ALA	2.0
1	D	816	LEU	2.0
1	G	88	ILE	2.0
1	G	258	ILE	2.0
3	C	247	LEU	2.0
3	F	164	LEU	2.0
1	A	226	PHE	2.0
2	E	930	PHE	2.0
3	I	260	GLN	2.0
1	G	1040	VAL	2.0
3	C	106	VAL	2.0
1	G	300	LEU	2.0
1	G	846	GLY	2.0
2	H	929	LEU	2.0
1	D	1088	PHE	2.0
1	A	1021	SER	2.0
3	C	263	GLN	2.0
1	A	197	LEU	2.0
1	A	1030	PHE	2.0
1	D	998	PHE	2.0
1	G	180	PHE	2.0
1	A	1054	MET	2.0
1	A	1002	GLU	2.0
2	B	740	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	91	TYR	2.0
1	D	193	TYR	2.0
1	D	297	LEU	2.0
2	E	873	ILE	2.0
3	F	206	ILE	2.0
1	A	17	GLY	2.0
1	G	1007	PHE	2.0
3	C	81	PHE	2.0
1	G	907	ASN	2.0
2	H	922	CYS	2.0
1	D	272	LEU	2.0
1	G	100	ILE	2.0
2	B	828	LEU	2.0
3	I	147	LEU	2.0
3	F	87	PHE	2.0
1	A	1024	THR	2.0
1	G	1065	VAL	2.0
3	C	147	LEU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	TPO	E	893	11/12	0.80	0.23	196,207,249,249	6
2	TPO	B	893	11/12	0.84	0.17	190,211,255,259	6
2	TPO	H	893	11/12	0.89	0.20	142,153,187,190	6

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	F	304	5/5	0.59	0.19	156,165,179,202	0
4	SO4	E	1105	5/5	0.66	0.17	170,174,177,202	0
4	SO4	D	1205	5/5	0.80	0.21	157,161,171,196	0
4	SO4	D	1207	5/5	0.80	0.18	143,150,166,189	0
4	SO4	D	1209	5/5	0.81	0.17	164,166,170,194	0
4	SO4	G	1204	5/5	0.81	0.15	154,158,169,197	0
4	SO4	H	1107	5/5	0.83	0.35	156,159,176,201	0
4	SO4	D	1202	5/5	0.84	0.21	144,158,169,194	0
4	SO4	F	303	5/5	0.84	0.16	158,161,166,197	0
4	SO4	A	1207	5/5	0.84	0.12	153,156,161,182	0
4	SO4	G	1202	5/5	0.84	0.11	149,153,161,182	0
4	SO4	A	1208	5/5	0.84	0.43	163,165,171,199	0
4	SO4	G	1207	5/5	0.84	0.17	144,148,153,177	0
4	SO4	C	302	5/5	0.84	0.12	161,165,167,194	0
4	SO4	G	1203	5/5	0.85	0.19	144,151,155,171	0
4	SO4	F	301	5/5	0.85	0.14	153,153,160,181	0
4	SO4	E	1102	5/5	0.86	0.13	152,167,170,195	0
4	SO4	D	1208	5/5	0.86	0.13	163,165,165,190	0
4	SO4	E	1104	5/5	0.87	0.11	174,175,180,205	0
4	SO4	A	1202	5/5	0.87	0.19	141,142,143,165	0
4	SO4	A	1206	5/5	0.87	0.18	162,164,169,194	0
4	SO4	D	1204	5/5	0.87	0.14	146,151,163,185	0
4	SO4	H	1105	5/5	0.87	0.19	154,154,162,192	0
4	SO4	B	1102	5/5	0.87	0.14	172,172,180,203	0
4	SO4	A	1203	5/5	0.89	0.20	131,141,154,169	0
4	SO4	A	1205	5/5	0.89	0.13	140,143,161,183	0
4	SO4	D	1203	5/5	0.89	0.20	138,152,154,179	0
4	SO4	H	1103	5/5	0.89	0.13	167,167,177,212	0
4	SO4	A	1201	5/5	0.89	0.17	148,148,164,169	0
4	SO4	C	301	5/5	0.89	0.22	135,139,150,159	0
4	SO4	A	1204	5/5	0.90	0.19	178,178,180,200	0
4	SO4	H	1106	5/5	0.90	0.25	145,147,156,178	0
4	SO4	B	1103	5/5	0.90	0.12	163,164,175,199	0
4	SO4	I	301	5/5	0.90	0.10	160,160,163,189	0
4	SO4	H	1102	5/5	0.91	0.11	168,170,173,198	0
4	SO4	G	1206	5/5	0.91	0.09	172,174,179,203	0
4	SO4	D	1206	5/5	0.91	0.19	138,138,146,171	0
5	RW6	B	1101	25/25	0.91	0.47	110,134,161,169	19
4	SO4	G	1205	5/5	0.92	0.20	142,157,159,175	0
4	SO4	G	1208	5/5	0.92	0.19	148,151,165,175	0
4	SO4	E	1103	5/5	0.92	0.13	157,158,164,191	0
4	SO4	G	1201	5/5	0.93	0.20	136,136,146,149	0
4	SO4	D	1201	5/5	0.93	0.15	144,148,152,162	0

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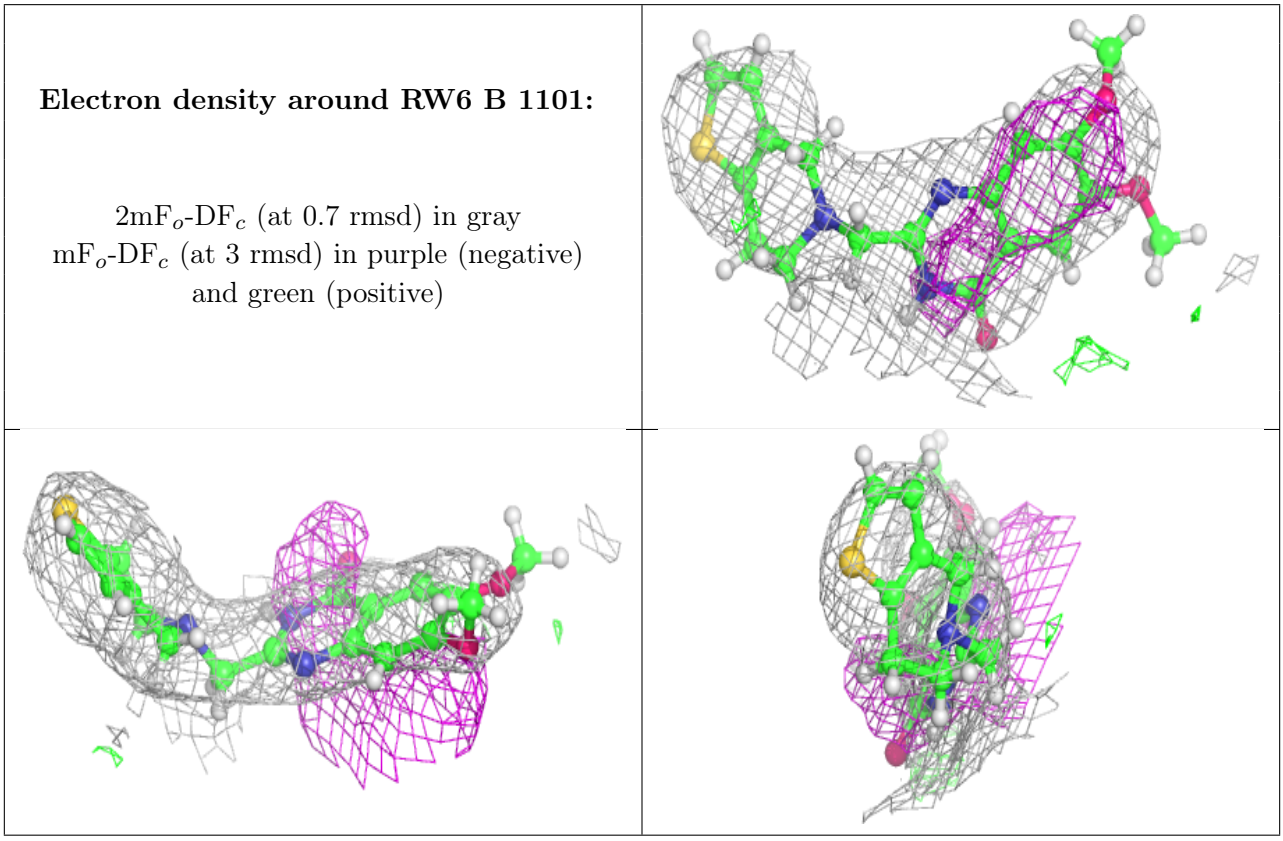
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	H	1104	5/5	0.93	0.13	142,152,159,183	0
4	SO4	I	302	5/5	0.93	0.19	118,130,143,150	0
4	SO4	G	1209	5/5	0.93	0.19	148,152,163,181	0
5	RW6	E	1101	25/25	0.94	0.50	112,139,166,174	19
5	RW6	H	1101	25/25	0.94	0.40	111,134,161,201	19
4	SO4	F	302	5/5	0.95	0.18	113,121,138,139	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.

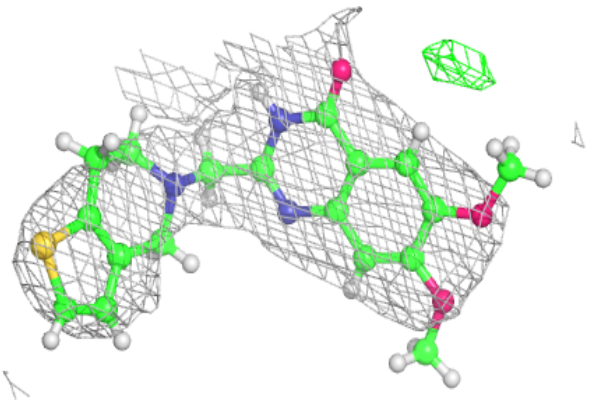
Electron density around RW6 B 1101:

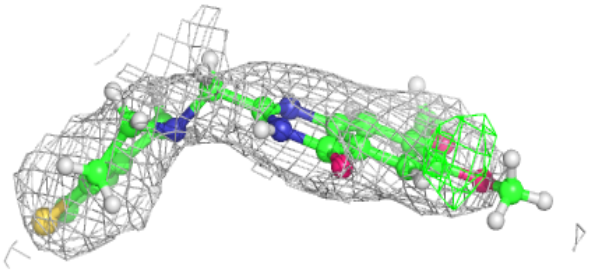
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

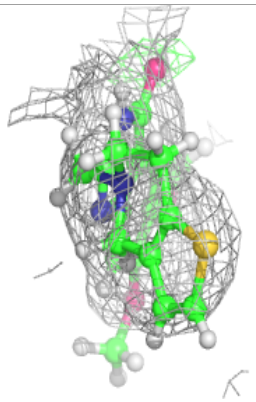


Electron density around RW6 E 1101:

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

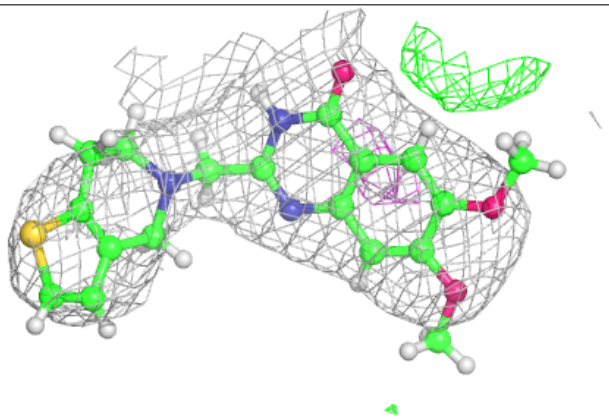


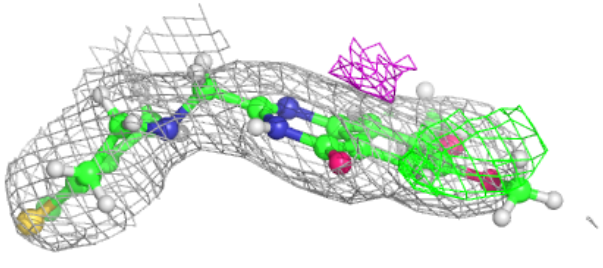


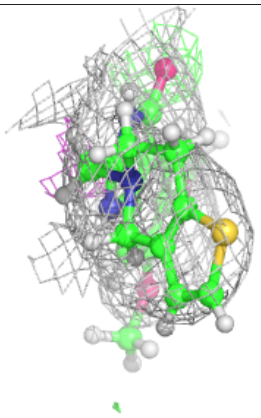


Electron density around RW6 H 1101:

$2mF_o$-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.