Full wwPDB X-ray Structure Validation Report (i)

Sep 7, 2023 – 01:37 pm BST

PDB ID	:	8BUL
Title	:	Structure of DDB1 bound to DS11-engaged CDK12-cyclin K
Authors	:	Kozicka, Z.; Kempf, G.; Petzold, G.; Thoma, N.H.
Deposited on	:	2022-11-30
Resolution	:	3.40 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:

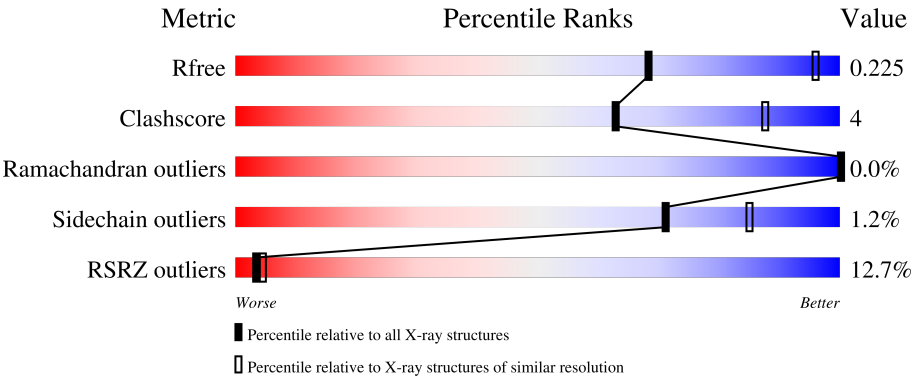
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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% 85% 12% ·
1	D	840	12% 85% 14% ·
1	G	840	12% 83% 15% ·
2	B	344	21% 83% 11% 6%
2	E	344	15% 82% 11% · 6%

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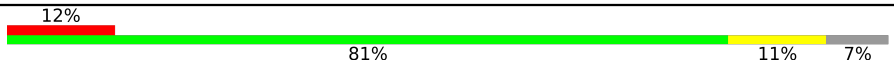
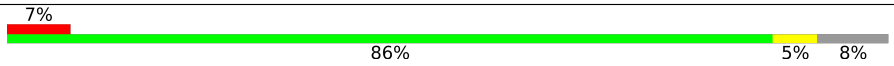
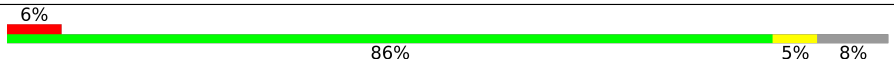
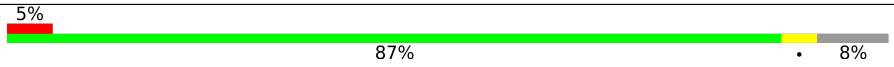
Mol	Chain	Length	Quality of chain
2	H	344	
3	C	271	
3	F	271	
3	I	271	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 67321 atoms, of which 33562 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	6449	0	0
			12936	4105	6449	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	325	Total	C	H	N	O	P	S	2663	0	0
			5309	1695	2663	447	486	1	17			
2	E	324	Total	C	H	N	O	P	S	2658	0	0
			5298	1692	2658	446	485	1	16			
2	H	320	Total	C	H	N	O	P	S	2629	0	0
			5228	1666	2629	438	478	1	16			

There are 12 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	conflict	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	conflict	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	conflict	UNP Q9NYV4

- Molecule 3 is a protein called Cyclin-K.

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

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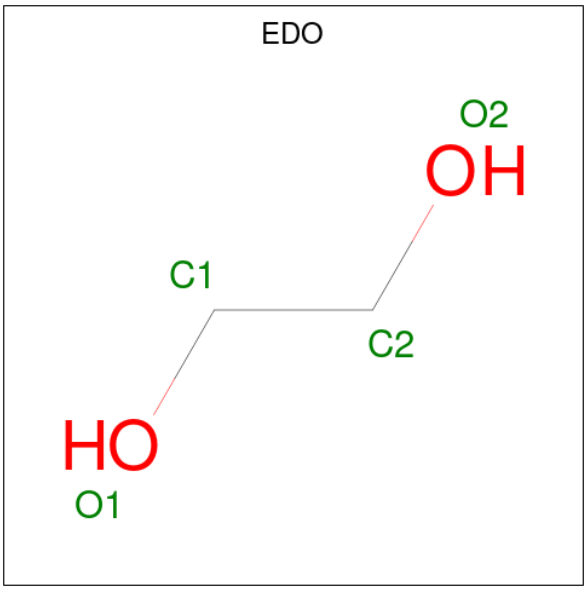
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	I	248	4111	1341	2048	346	363	13	2048	0	0

There are 12 discrepancies between the modelled and reference sequences:

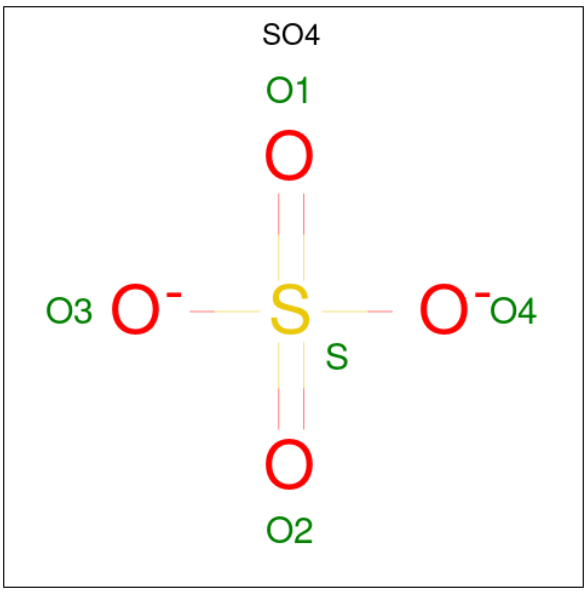
Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	expression tag	UNP O75909
C	-2	GLY	-	expression tag	UNP O75909
C	-1	GLY	-	expression tag	UNP O75909
C	0	ARG	-	expression tag	UNP O75909
F	-3	GLY	-	expression tag	UNP O75909
F	-2	GLY	-	expression tag	UNP O75909
F	-1	GLY	-	expression tag	UNP O75909
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
			Total	C	H	O		
4	A	1	10	2	6	2	6	0
4	D	1	Total	C	H	O	6	0
			10	2	6	2		

- 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	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	D	1	Total O S 5 4 1	0	0
5	E	1	Total O S 5 4 1	0	0

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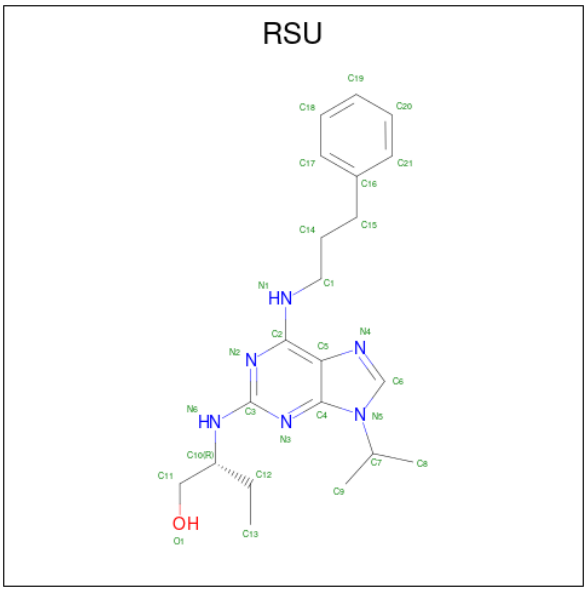
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	F	1	Total O S 5 4 1	0	0
5	F	1	Total O S 5 4 1	0	0
5	F	1	Total O S 5 4 1	0	0
5	G	1	Total O S 5 4 1	0	0
5	G	1	Total O S 5 4 1	0	0
5	G	1	Total O S 5 4 1	0	0
5	G	1	Total O S 5 4 1	0	0
5	H	1	Total O S 5 4 1	0	0
5	H	1	Total O S 5 4 1	0	0
5	I	1	Total O S 5 4 1	0	0
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 {R})-2-[[6-(3-phenylpropylamino)-9-propan-2-yl-purin-2-yl]amino]butan-1-ol (three-letter code: RSU) (formula: $C_{21}H_{30}N_6O$) (labeled as "Ligand of Interest" by depositor).



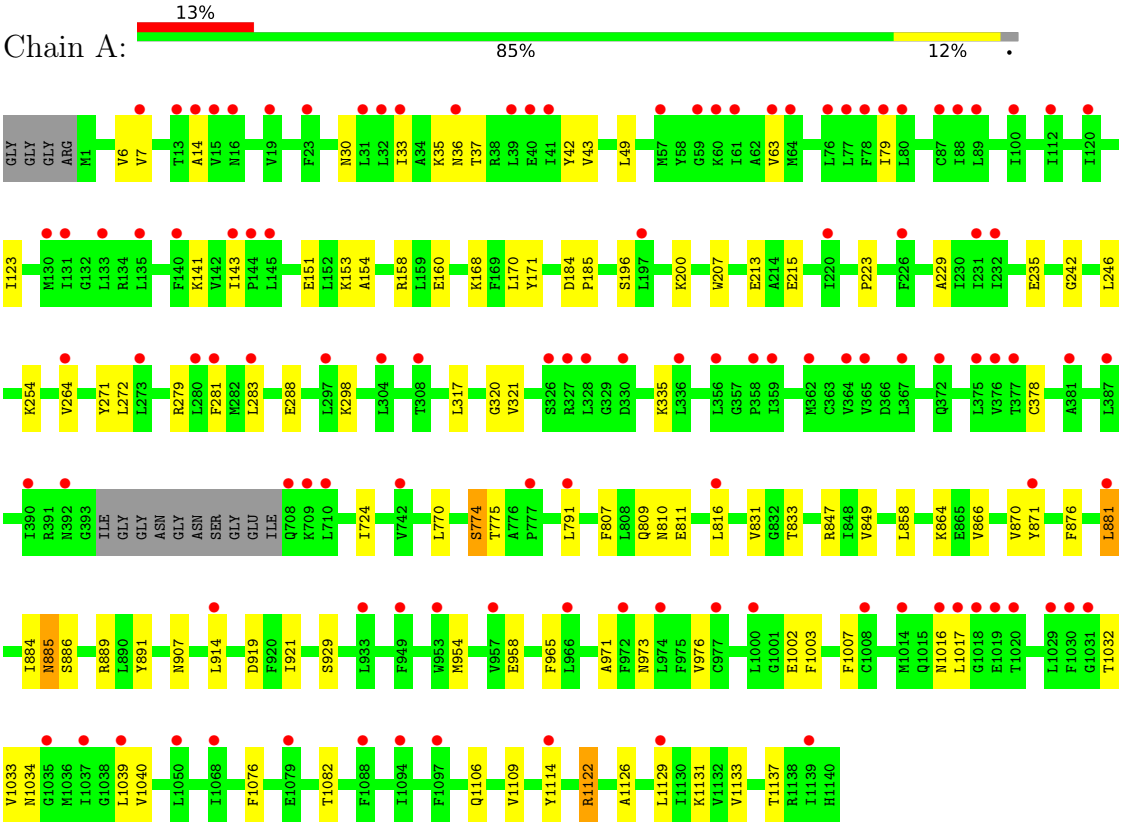
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	H	N	O	30	0
			58	21	30	6	1		
6	E	1	Total	C	H	N	O	30	0
			58	21	30	6	1		
6	H	1	Total	C	H	N	O	30	0
			58	21	30	6	1		

3 Residue-property plots (i)

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

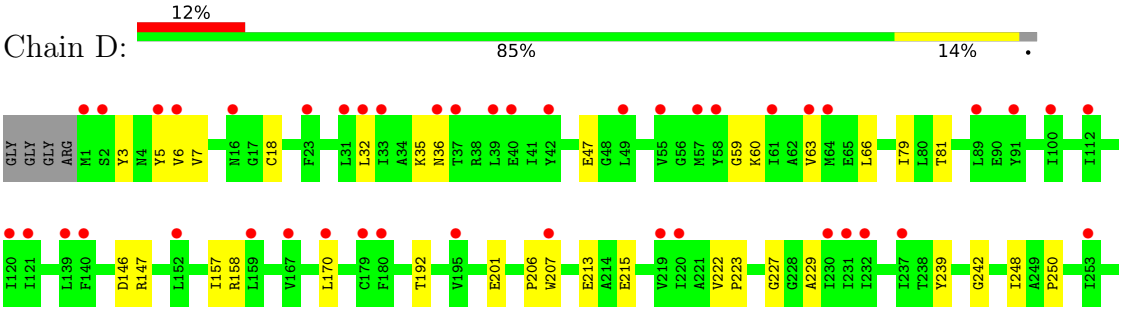
• Molecule 1: DNA damage-binding protein 1

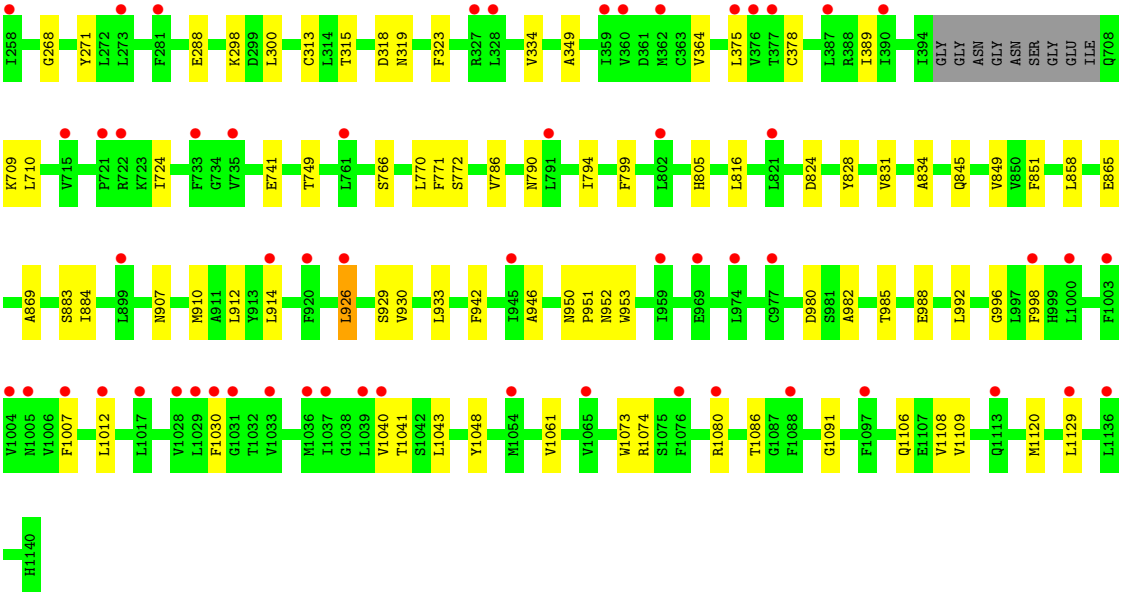
Chain A:



• Molecule 1: DNA damage-binding protein 1

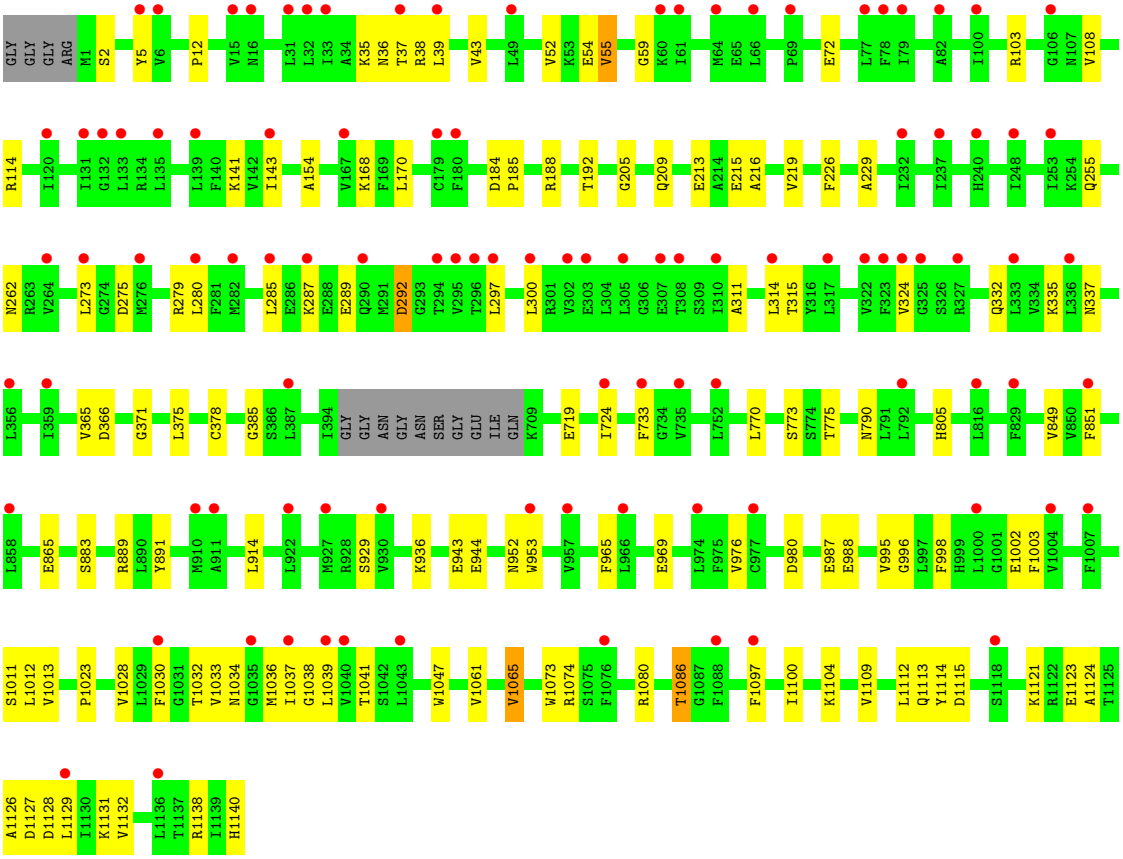
Chain D:





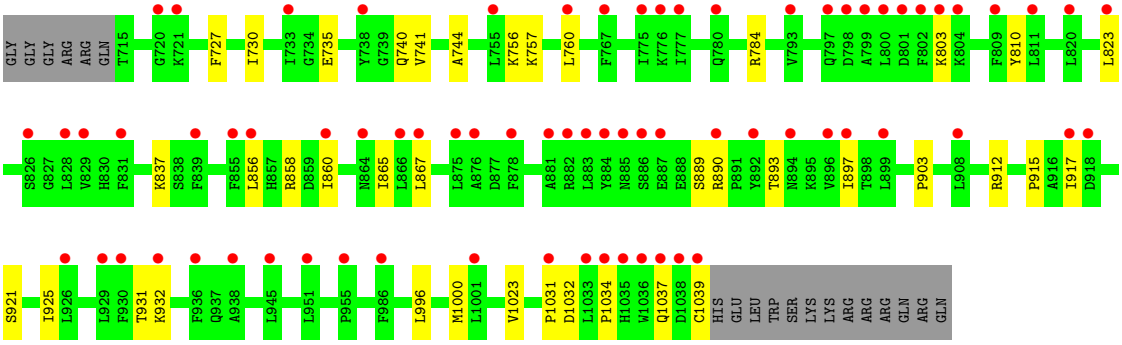
• Molecule 1: DNA damage-binding protein 1

Chain G:



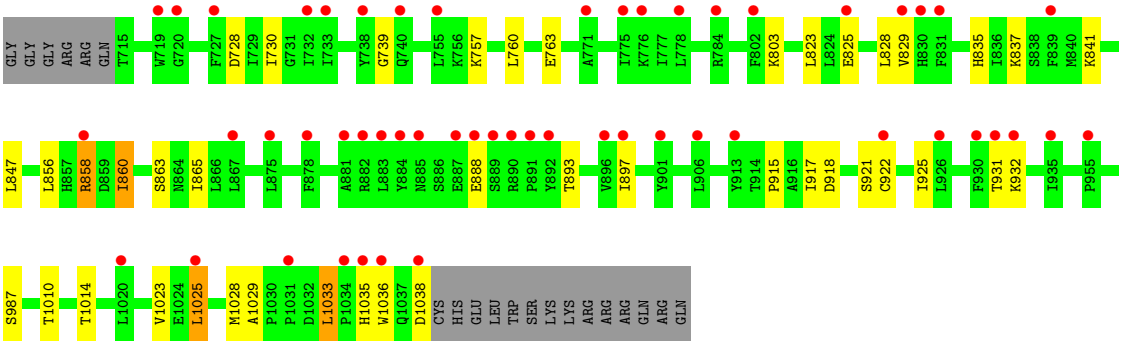
• Molecule 2: Cyclin-dependent kinase 12

Chain B:



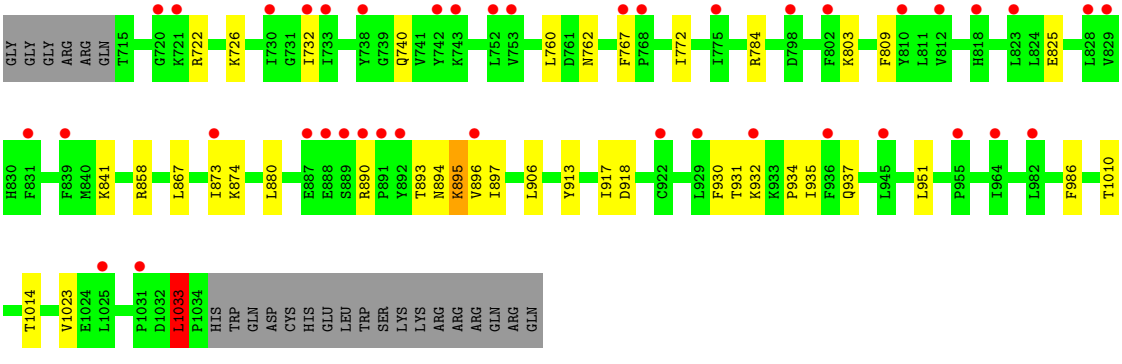
• Molecule 2: Cyclin-dependent kinase 12

Chain E:



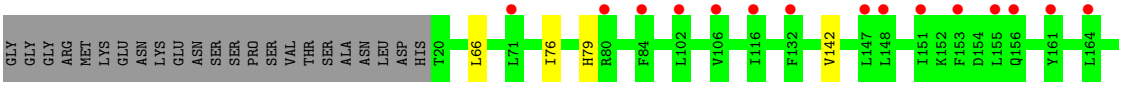
• Molecule 2: Cyclin-dependent kinase 12

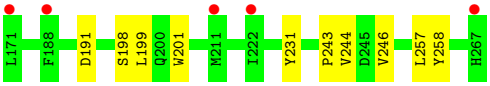
Chain H:



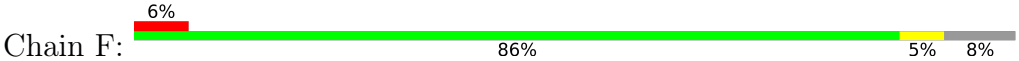
• Molecule 3: Cyclin-K

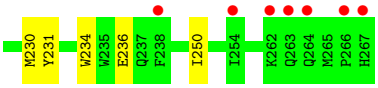
Chain C:



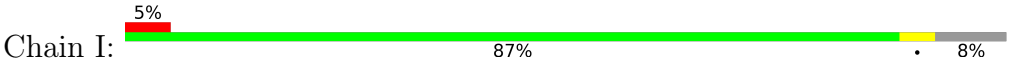


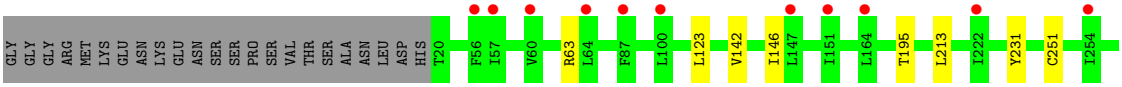
• Molecule 3: Cyclin-K





• Molecule 3: Cyclin-K





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	249.36Å 249.36Å 217.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	54.27 – 3.40 215.95 – 3.40	Depositor EDS
% Data completeness (in resolution range)	85.0 (54.27-3.40) 85.0 (215.95-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.30 (at 3.41Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.177 , 0.215 0.193 , 0.225	Depositor DCC
R_{free} test set	4558 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	130.4	Xtriage
Anisotropy	0.002	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 93.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.043 for -h,-k,l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	67321	wwPDB-VP
Average B, all atoms (Å^2)	154.0	wwPDB-VP

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

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, EDO, RSU, TPO

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	0.38	1/6604 (0.0%)	0.65	0/8931
1	D	0.36	0/6612	0.64	0/8942
1	G	0.37	0/6603	0.65	0/8930
2	B	0.38	0/2693	0.64	0/3630
2	E	0.38	0/2687	0.65	1/3622 (0.0%)
2	H	0.40	0/2643	0.66	1/3561 (0.0%)
3	C	0.36	0/2120	0.58	0/2868
3	F	0.38	0/2120	0.60	0/2868
3	I	0.36	0/2120	0.58	0/2868
All	All	0.37	1/34202 (0.0%)	0.63	2/46220 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1122	ARG	CZ-NH2	5.04	1.39	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	828	LEU	CB-CG-CD2	-5.77	101.19	111.00
2	H	1033	LEU	CA-CB-CG	5.74	128.50	115.30

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	6449	6451	63	4
1	D	6495	6462	6464	66	0
1	G	6486	6455	6456	78	4
2	B	2646	2663	2663	23	0
2	E	2640	2658	2658	25	0
2	H	2599	2629	2629	28	0
3	C	2063	2048	2048	9	0
3	F	2063	2048	2048	7	0
3	I	2063	2048	2048	5	0
4	A	4	6	6	0	0
4	D	4	6	6	0	0
5	A	25	0	0	1	0
5	C	15	0	0	0	0
5	D	20	0	0	0	0
5	E	5	0	0	0	0
5	F	15	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	28	30	0	0	0
6	E	28	30	0	0	0
6	H	28	30	0	0	0
All	All	33759	33562	33477	292	4

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:231:TYR:OH	3:F:236:GLU:OE1	1.98	0.80
1:D:910:MET:HB3	1:D:926:LEU:HD23	1.72	0.71
1:D:1109:VAL:HG12	1:D:1129:LEU:HD12	1.73	0.69
1:G:43:VAL:HG23	1:G:52:VAL:HG21	1.74	0.69
2:E:803:LYS:HG3	3:F:142:VAL:HG21	1.75	0.68
1:A:816:LEU:HD13	1:A:831:VAL:HG22	1.74	0.67
1:A:871:TYR:HE2	1:A:885:ASN:HB3	1.59	0.67
1:D:213:GLU:HG2	1:D:215:GLU:H	1.58	0.67
1:G:1047:TRP:HZ3	1:G:1132:VAL:HG13	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:GLU:HB2	1:A:298:LYS:HB2	1.78	0.65
1:A:170:LEU:HD21	1:A:229:ALA:HB2	1.79	0.64
1:A:1002:GLU:OE1	1:A:1034:ASN:HB2	1.97	0.64
1:D:851:PHE:HB3	1:D:858:LEU:HD22	1.81	0.63
1:A:1109:VAL:HG11	1:A:1126:ALA:HA	1.82	0.62
1:G:375:LEU:HB2	1:G:1012:LEU:HD21	1.81	0.62
1:A:929:SER:HA	1:A:954:MET:CE	2.30	0.61
1:D:816:LEU:HD13	1:D:831:VAL:HG22	1.83	0.61
1:A:123:ILE:HG21	1:A:168:LYS:HA	1.82	0.61
2:E:858:ARG:O	2:E:897:ILE:HG12	2.00	0.61
1:A:775:THR:HG22	1:A:775:THR:O	2.02	0.59
2:H:867:LEU:HD13	2:H:873:ILE:CD1	2.32	0.59
2:E:835:HIS:HD2	2:E:1029:ALA:HB1	1.67	0.59
1:A:213:GLU:HG2	1:A:215:GLU:H	1.67	0.59
2:E:841:LYS:HG2	2:E:1025:LEU:HD21	1.84	0.58
1:G:1127:ASP:O	1:G:1131:LYS:HG2	2.02	0.58
1:G:770:LEU:HD21	1:G:865:GLU:HB2	1.84	0.58
1:D:709:LYS:HG2	1:D:710:LEU:N	2.18	0.58
1:G:366:ASP:OD2	1:G:371:GLY:N	2.37	0.58
1:A:207:TRP:HB3	1:A:242:GLY:HA2	1.86	0.57
1:D:378:CYS:SG	1:D:724:ILE:HB	2.44	0.57
1:G:1003:PHE:HB3	1:G:1033:VAL:HG23	1.86	0.57
2:E:841:LYS:CG	2:E:1025:LEU:HD21	2.35	0.56
2:B:890:ARG:O	2:B:912:ARG:HG2	2.04	0.56
2:H:894:ASN:HB3	2:H:895:LYS:HD3	1.86	0.56
1:D:907:ASN:HB2	2:E:730:ILE:HG22	1.87	0.56
1:G:55:VAL:HG13	1:G:1065:VAL:HG21	1.87	0.56
2:H:867:LEU:HD13	2:H:873:ILE:HD13	1.88	0.56
1:G:773:SER:C	1:G:775:THR:H	2.10	0.56
2:H:906:LEU:HD21	2:H:913:TYR:CD2	2.41	0.55
1:D:248:ILE:HD12	1:D:300:LEU:O	2.06	0.55
1:G:883:SER:HB3	1:G:914:LEU:HD11	1.88	0.55
2:H:951:LEU:HD21	2:H:986:PHE:HE2	1.71	0.55
2:B:741:VAL:HG22	2:B:756:LYS:HG3	1.87	0.55
1:D:288:GLU:HB2	1:D:298:LYS:HB2	1.88	0.55
1:A:929:SER:HA	1:A:954:MET:HE3	1.89	0.55
1:G:385:GLY:HA3	1:G:719:GLU:O	2.08	0.54
1:A:871:TYR:CE2	1:A:885:ASN:HB3	2.42	0.54
1:D:770:LEU:HD13	1:D:865:GLU:HB2	1.90	0.54
2:H:858:ARG:NE	2:H:880:LEU:O	2.37	0.54
3:C:243:PRO:HG2	3:C:246:VAL:HG23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:ASN:ND2	1:A:43:VAL:HG22	2.23	0.53
2:E:1033:LEU:HD22	2:E:1033:LEU:H	1.72	0.53
1:D:227:GLY:O	1:D:239:TYR:OH	2.20	0.53
3:C:201:TRP:CH2	3:C:246:VAL:HG22	2.44	0.53
1:A:881:LEU:HD13	1:A:914:LEU:HD23	1.90	0.53
1:G:184:ASP:HB2	1:G:185:PRO:CD	2.39	0.53
1:G:1097:PHE:O	1:G:1100:ILE:HG12	2.09	0.53
2:H:722:ARG:HE	2:H:726:LYS:HG3	1.74	0.53
2:E:1025:LEU:O	2:E:1028:MET:HG2	2.09	0.52
1:G:1013:VAL:HG11	1:G:1138:ARG:O	2.09	0.52
3:C:76:ILE:CD1	3:C:198:SER:HB3	2.39	0.52
2:E:856:LEU:HD11	2:E:915:PRO:HG3	1.91	0.52
2:H:1010:THR:O	2:H:1014:THR:HG23	2.09	0.52
1:D:389:ILE:HD12	1:D:389:ILE:N	2.23	0.52
2:E:1010:THR:O	2:E:1014:THR:HG23	2.10	0.52
1:A:6:VAL:HG22	1:A:1040:VAL:HG22	1.92	0.52
1:D:790:ASN:HA	1:D:805:HIS:O	2.08	0.52
2:H:858:ARG:HB3	2:H:896:VAL:HG22	1.92	0.52
1:A:1133:VAL:O	1:A:1137:THR:HG23	2.09	0.52
1:D:334:VAL:HG12	1:D:349:ALA:HA	1.91	0.52
1:D:1080:ARG:HD3	2:E:825:GLU:HA	1.91	0.52
1:G:255:GLN:OE1	1:G:279:ARG:NH1	2.42	0.52
1:G:226:PHE:CZ	1:G:287:LYS:HG3	2.45	0.52
2:H:931:THR:O	2:H:932:LYS:HB2	2.10	0.52
1:A:884:ILE:O	1:A:885:ASN:C	2.47	0.51
2:B:1032:ASP:O	2:B:1034:PRO:HD3	2.10	0.51
1:G:285:LEU:HG	1:G:300:LEU:CD2	2.39	0.51
2:H:858:ARG:HB3	2:H:896:VAL:CG2	2.39	0.51
1:D:318:ASP:O	1:D:319:ASN:HB2	2.11	0.51
1:G:378:CYS:SG	1:G:724:ILE:HB	2.51	0.51
1:G:980:ASP:HB2	1:G:988:GLU:O	2.11	0.51
2:H:841:LYS:NZ	2:H:1023:VAL:O	2.44	0.51
1:A:971:ALA:HB3	1:A:973:ASN:HD22	1.76	0.51
1:D:849:VAL:HG11	1:D:851:PHE:CZ	2.46	0.51
1:D:63:VAL:O	1:D:79:ILE:HA	2.11	0.50
1:G:1115:ASP:HB2	1:G:1121:LYS:HE2	1.93	0.50
1:D:929:SER:OG	1:D:952:ASN:HB2	2.10	0.50
1:G:59:GLY:HA2	1:G:1073:TRP:CZ3	2.46	0.50
1:A:1003:PHE:O	1:A:1032:THR:HA	2.12	0.50
1:D:5:TYR:HB2	1:D:1043:LEU:HD11	1.93	0.50
2:E:837:LYS:HD3	2:E:1023:VAL:CG2	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:170:LEU:HD21	1:G:229:ALA:HB2	1.93	0.50
1:A:811:GLU:HG2	1:A:833:THR:HB	1.94	0.50
1:A:1109:VAL:HG12	1:A:1129:LEU:HD12	1.93	0.50
2:E:858:ARG:HG2	2:E:917:ILE:HD11	1.94	0.50
1:D:7:VAL:HG12	1:D:1091:GLY:HA3	1.94	0.49
2:E:835:HIS:CD2	2:E:1029:ALA:HB1	2.47	0.49
1:A:1003:PHE:HB3	1:A:1033:VAL:HG23	1.94	0.49
1:D:375:LEU:HB2	1:D:1012:LEU:HD21	1.93	0.49
1:D:985:THR:HB	1:D:988:GLU:HB2	1.95	0.49
2:H:896:VAL:HG12	2:H:906:LEU:HD13	1.94	0.49
1:A:184:ASP:HB2	1:A:185:PRO:CD	2.43	0.49
1:D:192:THR:HB	1:D:206:PRO:HD2	1.93	0.49
2:H:722:ARG:HH21	2:H:726:LYS:HB3	1.77	0.49
1:G:59:GLY:HA2	1:G:1073:TRP:CE3	2.47	0.49
1:A:881:LEU:HD11	1:A:921:ILE:HD13	1.94	0.49
1:A:929:SER:HA	1:A:954:MET:HE1	1.94	0.49
1:G:213:GLU:HG2	1:G:215:GLU:H	1.77	0.49
1:G:1061:VAL:HG11	1:G:1104:LYS:HB3	1.94	0.49
1:G:773:SER:O	1:G:775:THR:N	2.41	0.49
1:D:749:THR:HG21	1:D:786:VAL:HG11	1.94	0.49
1:D:5:TYR:CE2	1:D:7:VAL:HG13	2.48	0.48
2:B:823:LEU:HD11	2:B:867:LEU:HD22	1.93	0.48
1:G:262:ASN:HB2	1:G:314:LEU:O	2.13	0.48
1:D:146:ASP:OD1	1:D:147:ARG:N	2.47	0.48
1:G:1080:ARG:HD3	2:H:825:GLU:HA	1.96	0.48
2:B:858:ARG:O	2:B:897:ILE:HG12	2.12	0.48
1:G:365:VAL:HG11	1:G:733:PHE:CZ	2.49	0.48
2:H:934:PRO:HB2	2:H:937:GLN:HG3	1.96	0.48
1:G:929:SER:OG	1:G:952:ASN:HB2	2.14	0.48
1:A:151:GLU:OE1	1:A:153:LYS:HE2	2.14	0.48
1:A:889:ARG:HD2	1:A:891:TYR:CZ	2.49	0.48
2:B:996:LEU:O	2:B:1000:MET:HG3	2.14	0.48
1:G:273:LEU:O	1:G:280:LEU:HD12	2.13	0.47
3:F:222:ILE:HD12	3:F:234:TRP:CZ2	2.49	0.47
1:G:1003:PHE:O	1:G:1032:THR:HA	2.14	0.47
1:D:315:THR:CG2	1:D:323:PHE:HB3	2.45	0.47
1:G:36:ASN:O	1:G:37:THR:OG1	2.25	0.47
1:G:114:ARG:HD3	2:H:930:PHE:O	2.14	0.47
1:G:1112:LEU:HD23	1:G:1129:LEU:HD11	1.95	0.47
1:A:264:VAL:HG22	1:A:272:LEU:HG	1.96	0.47
1:A:1016:ASN:O	1:A:1017:LEU:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:213:LEU:HB2	3:I:251:CYS:SG	2.55	0.47
1:D:18:CYS:SG	1:D:313:CYS:SG	3.12	0.47
3:C:191:ASP:OD2	3:C:258:TYR:OH	2.26	0.47
1:G:143:ILE:HG12	1:G:154:ALA:HB2	1.97	0.47
2:B:1034:PRO:HB2	2:B:1037:GLN:HB2	1.97	0.47
2:B:760:LEU:HD23	2:B:760:LEU:H	1.80	0.46
1:D:6:VAL:HG22	1:D:1040:VAL:HG22	1.96	0.46
1:G:849:VAL:HG11	1:G:851:PHE:CZ	2.50	0.46
1:G:998:PHE:CZ	1:G:1074:ARG:HD2	2.49	0.46
2:E:931:THR:O	2:E:932:LYS:HB2	2.16	0.46
1:D:3:TYR:HB3	1:D:1048:TYR:HB2	1.98	0.46
1:D:1106:GLN:HA	1:D:1109:VAL:HG22	1.96	0.46
2:H:784:ARG:O	2:H:874:LYS:HE2	2.15	0.46
2:B:757:LYS:HG3	2:B:810:TYR:CE2	2.51	0.46
1:D:315:THR:HG22	1:D:323:PHE:HB3	1.97	0.46
3:F:79:HIS:HB3	3:F:199:LEU:HD11	1.98	0.46
1:G:1030:PHE:CZ	1:G:1038:GLY:HA3	2.49	0.46
1:D:248:ILE:HG12	1:D:250:PRO:HD3	1.98	0.46
1:A:320:GLY:O	1:A:335:LYS:HA	2.16	0.46
1:G:39:LEU:HB3	1:G:55:VAL:HG12	1.97	0.46
2:B:867:LEU:HD21	2:B:1031:PRO:HG3	1.98	0.45
1:D:883:SER:HB3	1:D:914:LEU:HD11	1.98	0.45
2:H:917:ILE:HG13	2:H:918:ASP:N	2.30	0.45
1:G:2:SER:HB3	1:G:995:VAL:HG23	1.99	0.45
2:H:767:PHE:HD2	2:H:772:ILE:HG13	1.81	0.45
2:H:1033:LEU:O	2:H:1033:LEU:HD22	2.16	0.45
1:G:72:GLU:OE2	1:G:103:ARG:NH2	2.50	0.45
3:I:63:ARG:HE	3:I:123:LEU:HD21	1.82	0.45
2:B:803:LYS:HG3	3:C:142:VAL:HG21	1.98	0.45
1:D:933:LEU:HD22	1:D:942:PHE:HB3	1.97	0.45
1:D:834:ALA:HB2	1:D:869:ALA:CB	2.47	0.45
1:D:998:PHE:CZ	1:D:1074:ARG:HD2	2.51	0.45
1:G:168:LYS:HG3	1:G:219:VAL:O	2.16	0.45
1:G:297:LEU:HD12	1:G:297:LEU:HA	1.87	0.45
1:G:953:TRP:O	1:G:969:GLU:HA	2.15	0.45
1:D:60:LYS:O	1:D:81:THR:HA	2.17	0.45
1:D:794:ILE:HG22	1:D:799:PHE:HA	1.99	0.45
2:H:896:VAL:HG13	2:H:897:ILE:HG13	1.98	0.45
2:B:735:GLU:HA	2:B:740:GLN:HG2	1.99	0.45
1:G:987:GLU:HA	2:H:740:GLN:NE2	2.31	0.45
1:A:770:LEU:HD12	1:A:847:ARG:HD3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1076:PHE:O	1:A:1082:THR:HA	2.17	0.45
1:D:223:PRO:HD2	1:D:268:GLY:HA3	1.98	0.45
1:G:38:ARG:HD2	1:G:54:GLU:OE2	2.16	0.45
1:G:324:VAL:HB	1:G:332:GLN:HG2	1.98	0.44
2:B:803:LYS:HA	3:C:142:VAL:CG1	2.48	0.44
2:B:865:ILE:HD11	2:B:925:ILE:HD13	2.00	0.44
2:H:858:ARG:NH1	2:H:913:TYR:OH	2.49	0.44
2:H:935:ILE:HD12	2:H:986:PHE:HZ	1.81	0.44
2:B:903:PRO:HG3	2:B:917:ILE:HB	1.99	0.44
1:G:285:LEU:HG	1:G:300:LEU:HD21	2.00	0.44
1:A:965:PHE:O	1:A:976:VAL:HA	2.17	0.44
1:D:1061:VAL:HG21	1:D:1108:VAL:CG2	2.47	0.44
1:G:275:ASP:C	1:G:275:ASP:OD1	2.54	0.44
1:A:907:ASN:HB2	2:B:730:ILE:HG22	1.99	0.44
1:D:926:LEU:O	1:D:953:TRP:HA	2.18	0.44
1:G:188:ARG:NH1	1:G:216:ALA:O	2.50	0.44
1:A:170:LEU:HD23	1:A:170:LEU:HA	1.87	0.44
1:G:996:GLY:HA2	1:G:1086:THR:O	2.17	0.44
2:B:837:LYS:HD3	2:B:1023:VAL:HG22	2.00	0.44
2:E:888:GLU:HG2	2:E:888:GLU:O	2.17	0.44
1:G:192:THR:O	1:G:205:GLY:HA3	2.18	0.44
1:G:311:ALA:HB2	1:G:324:VAL:HG13	2.00	0.44
1:A:866:VAL:HB	1:A:884:ILE:HG12	2.00	0.44
1:G:1036:MET:HG2	1:G:1037:ILE:N	2.31	0.43
1:D:222:VAL:HA	1:D:223:PRO:HD3	1.91	0.43
3:F:206:ILE:HD13	3:F:250:ILE:HD13	2.00	0.43
1:G:365:VAL:HG11	1:G:733:PHE:HZ	1.83	0.43
1:G:889:ARG:HD2	1:G:891:TYR:CZ	2.53	0.43
3:I:195:THR:CG2	3:I:257:LEU:HD11	2.48	0.43
1:D:5:TYR:HB3	1:D:1041:THR:HG23	1.99	0.43
1:G:12:PRO:O	1:G:35:LYS:HD3	2.18	0.43
1:G:1028:VAL:O	1:G:1039:LEU:HA	2.17	0.43
1:G:1113:GLN:HA	1:G:1123:GLU:HA	2.00	0.43
2:E:837:LYS:HD3	2:E:1023:VAL:HG22	2.00	0.43
1:A:7:VAL:HG12	1:A:1039:LEU:HB3	2.00	0.43
1:G:1002:GLU:OE1	1:G:1034:ASN:HB2	2.18	0.43
2:E:847:LEU:HD22	2:E:922:CYS:SG	2.58	0.43
1:G:944:GLU:OE1	2:H:732:ILE:HG22	2.18	0.43
1:A:196:SER:O	1:A:200:LYS:N	2.51	0.43
1:D:1007:PHE:CD1	1:D:1030:PHE:HB3	2.54	0.43
2:H:760:LEU:HD11	2:H:809:PHE:HD2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ILE:HD12	1:A:42:TYR:CE1	2.54	0.43
1:D:32:LEU:HD13	1:D:66:LEU:HD11	2.01	0.43
1:D:771:PHE:CE1	1:D:845:GLN:HB3	2.54	0.43
1:D:824:ASP:OD2	1:D:828:TYR:OH	2.34	0.43
1:G:1112:LEU:O	1:G:1123:GLU:HG3	2.19	0.43
1:D:364:VAL:HG22	1:D:375:LEU:HD13	2.00	0.43
1:A:317:LEU:HB2	1:A:321:VAL:HB	2.00	0.42
1:D:170:LEU:HD21	1:D:229:ALA:HB2	2.00	0.42
1:A:143:ILE:HG12	1:A:154:ALA:HB2	2.01	0.42
1:A:809:GLN:O	1:A:810:ASN:HB2	2.18	0.42
1:G:1023:PRO:HB3	1:G:1047:TRP:CD2	2.53	0.42
1:D:207:TRP:CB	1:D:242:GLY:HA2	2.49	0.42
1:D:207:TRP:HB2	1:D:242:GLY:HA2	2.01	0.42
2:E:917:ILE:HG13	2:E:918:ASP:N	2.34	0.42
2:E:860:ILE:HB	2:E:921:SER:CB	2.49	0.42
1:G:936:LYS:HE3	1:G:943:GLU:OE1	2.18	0.42
1:G:1061:VAL:HG13	1:G:1104:LYS:HD2	2.00	0.42
1:A:36:ASN:O	1:A:37:THR:OG1	2.31	0.42
1:A:864:LYS:NZ	5:A:1203:SO4:O4	2.51	0.42
1:A:14:ALA:O	1:A:35:LYS:HG2	2.19	0.42
2:B:727:PHE:HB3	2:B:744:ALA:HB1	2.01	0.42
3:F:121:ARG:NH2	3:F:126:ASP:OD1	2.50	0.42
1:A:958:GLU:HB2	1:A:1007:PHE:CB	2.49	0.42
2:B:889:SER:HB2	2:B:912:ARG:HD3	2.01	0.42
1:G:335:LYS:HE2	1:G:337:ASN:OD1	2.19	0.42
1:D:996:GLY:HA2	1:D:1086:THR:O	2.20	0.42
1:G:55:VAL:CG1	1:G:1065:VAL:HG21	2.49	0.42
1:A:807:PHE:HB3	1:A:811:GLU:OE1	2.20	0.42
1:G:1114:TYR:HB3	1:G:1124:ALA:HB2	2.01	0.42
1:A:885:ASN:O	1:A:886:SER:HB3	2.20	0.42
2:E:823:LEU:O	2:E:829:VAL:HG22	2.20	0.42
2:E:835:HIS:HD2	2:E:1029:ALA:CB	2.30	0.42
1:G:965:PHE:O	1:G:976:VAL:HA	2.20	0.42
1:A:378:CYS:SG	1:A:724:ILE:HB	2.59	0.41
1:A:791:LEU:HD23	1:A:858:LEU:HD21	2.02	0.41
3:C:66:LEU:HD23	3:C:66:LEU:HA	1.93	0.41
1:A:42:TYR:CD2	1:A:49:LEU:HB3	2.56	0.41
1:A:158:ARG:NH1	1:A:160:GLU:HG2	2.36	0.41
1:A:774:SER:O	1:A:775:THR:HB	2.20	0.41
1:D:884:ILE:HD12	1:D:884:ILE:N	2.35	0.41
3:F:121:ARG:HH12	3:F:126:ASP:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:5:TYR:HB3	1:G:1041:THR:HG23	2.03	0.41
1:G:108:VAL:O	1:G:141:LYS:HE3	2.20	0.41
1:G:1011:SER:OG	1:G:1013:VAL:HG22	2.20	0.41
1:A:775:THR:O	1:A:775:THR:CG2	2.69	0.41
1:D:157:ILE:HG23	1:D:201:GLU:HA	2.02	0.41
1:A:235:GLU:HG2	1:A:254:LYS:HG3	2.02	0.41
2:B:860:ILE:HB	2:B:921:SER:CB	2.50	0.41
2:E:865:ILE:HD12	2:E:925:ILE:HD13	2.02	0.41
1:A:271:TYR:HB2	1:A:283:LEU:HB3	2.02	0.41
3:C:76:ILE:HD12	3:C:198:SER:HB3	2.02	0.41
1:D:741:GLU:HB3	1:D:749:THR:HB	2.01	0.41
1:A:876:PHE:CZ	1:A:919:ASP:HA	2.56	0.41
2:B:865:ILE:CD1	2:B:925:ILE:HD13	2.51	0.41
1:D:158:ARG:HD2	2:E:987:SER:HB2	2.03	0.41
1:D:980:ASP:C	1:D:982:ALA:N	2.74	0.41
1:A:63:VAL:O	1:A:79:ILE:HA	2.21	0.41
1:A:171:TYR:CD2	1:A:223:PRO:HA	2.56	0.41
1:A:279:ARG:NH1	1:A:281:PHE:HZ	2.19	0.41
2:B:856:LEU:HD11	2:B:915:PRO:HG3	2.03	0.41
3:C:79:HIS:HB3	3:C:199:LEU:HD11	2.03	0.41
1:G:184:ASP:HB2	1:G:185:PRO:HD2	2.01	0.41
1:A:1114:TYR:HB2	1:A:1122:ARG:HB3	2.01	0.41
1:G:790:ASN:HA	1:G:805:HIS:O	2.21	0.41
1:D:950:ASN:HA	1:D:951:PRO:HD3	1.91	0.40
2:B:931:THR:O	2:B:932:LYS:HB2	2.21	0.40
1:D:59:GLY:HA2	1:D:1073:TRP:CZ3	2.57	0.40
1:D:946:ALA:HB1	1:D:992:LEU:HG	2.03	0.40
2:E:739:GLY:HA3	2:E:757:LYS:O	2.20	0.40
1:G:1124:ALA:HB1	1:G:1128:ASP:HB2	2.02	0.40
3:I:266:PRO:O	3:I:267:HIS:C	2.60	0.40
1:D:35:LYS:O	1:D:36:ASN:C	2.59	0.40
1:A:141:LYS:HE2	1:A:141:LYS:HB2	1.94	0.40
1:G:1109:VAL:HG11	1:G:1126:ALA:HA	2.04	0.40
1:D:5:TYR:CE2	1:D:7:VAL:CG1	3.05	0.40
1:D:223:PRO:HD3	1:D:271:TYR:OH	2.21	0.40
1:G:170:LEU:HD23	1:G:170:LEU:HA	1.88	0.40
2:H:803:LYS:HG2	3:I:142:VAL:HG11	2.03	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1122:ARG:HH21	1:G:292:ASP:OD1[2_565]	1.36	0.24
1:A:1131:LYS:NZ	1:G:289:GLU:OE2[2_565]	2.03	0.17
1:A:1122:ARG:NH2	1:G:292:ASP:OD1[2_565]	2.17	0.03
1:A:1131:LYS:HZ3	1:G:289:GLU:OE2[2_565]	1.59	0.01

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%)	804 (98%)	17 (2%)	1 (0%)	51	82
1	D	823/840 (98%)	808 (98%)	14 (2%)	1 (0%)	51	82
1	G	822/840 (98%)	803 (98%)	19 (2%)	0	100	100
2	B	322/344 (94%)	313 (97%)	9 (3%)	0	100	100
2	E	321/344 (93%)	316 (98%)	5 (2%)	0	100	100
2	H	317/344 (92%)	310 (98%)	7 (2%)	0	100	100
3	C	246/271 (91%)	243 (99%)	3 (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	4165/4365 (95%)	4081 (98%)	82 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	772	SER
1	A	774	SER

5.3.2 Protein sidechains (i)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	721/728 (99%)	715 (99%)	6 (1%)	81	91
1	D	722/728 (99%)	716 (99%)	6 (1%)	81	91
1	G	721/728 (99%)	714 (99%)	7 (1%)	76	88
2	B	292/308 (95%)	290 (99%)	2 (1%)	84	92
2	E	291/308 (94%)	280 (96%)	11 (4%)	33	61
2	H	287/308 (93%)	283 (99%)	4 (1%)	67	83
3	C	223/242 (92%)	220 (99%)	3 (1%)	69	84
3	F	223/242 (92%)	220 (99%)	3 (1%)	69	84
3	I	223/242 (92%)	221 (99%)	2 (1%)	78	90
All	All	3703/3834 (97%)	3659 (99%)	44 (1%)	71	85

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	246	LEU
1	A	849	VAL
1	A	870	VAL
1	A	881	LEU
1	A	885	ASN
1	A	1106	GLN
2	B	784	ARG
2	B	1039	CYS
3	C	231	TYR
3	C	244	VAL
3	C	257	LEU
1	D	47	GLU
1	D	766	SER
1	D	912	LEU
1	D	926	LEU
1	D	930	VAL
1	D	1120	MET
2	E	728	ASP
2	E	760	LEU
2	E	763	GLU
2	E	858	ARG
2	E	860	ILE

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Mol	Chain	Res	Type
2	E	863	SER
2	E	1025	LEU
2	E	1033	LEU
2	E	1035	HIS
2	E	1036	TRP
2	E	1038	ASP
3	F	146	ILE
3	F	162	GLN
3	F	230	MET
1	G	55	VAL
1	G	209	GLN
1	G	292	ASP
1	G	315	THR
1	G	1065	VAL
1	G	1086	THR
1	G	1140	HIS
2	H	762	ASN
2	H	890	ARG
2	H	895	LYS
2	H	1033	LEU
3	I	146	ILE
3	I	231	TYR

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

Mol	Chain	Res	Type
1	A	991	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	B	893	2	8,10,11	1.44	2 (25%)	10,14,16	1.66	2 (20%)
2	TPO	E	893	2	8,10,11	1.75	1 (12%)	10,14,16	1.53	2 (20%)
2	TPO	H	893	2	8,10,11	1.68	2 (25%)	10,14,16	1.19	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TPO	B	893	2	-	1/9/11/13	-
2	TPO	E	893	2	-	4/9/11/13	-
2	TPO	H	893	2	-	6/9/11/13	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	893	TPO	P-O1P	3.62	1.62	1.50
2	H	893	TPO	CB-CA	3.11	1.60	1.53
2	B	893	TPO	P-OG1	2.26	1.63	1.59
2	B	893	TPO	P-O2P	2.01	1.62	1.54
2	H	893	TPO	P-O2P	2.00	1.62	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	893	TPO	P-OG1-CB	-3.46	112.76	123.21
2	B	893	TPO	CG2-CB-CA	-3.15	106.94	113.16
2	B	893	TPO	P-OG1-CB	-2.82	114.68	123.21
2	E	893	TPO	CG2-CB-CA	-2.01	109.20	113.16

There are no chirality outliers.

All (11) torsion outliers are listed below:

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

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

30 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	I	303	-	4,4,4	0.18	0	6,6,6	0.17	0
5	SO4	A	1204	-	4,4,4	0.28	0	6,6,6	0.15	0
5	SO4	I	302	-	4,4,4	0.32	0	6,6,6	0.09	0
5	SO4	G	1201	-	4,4,4	0.25	0	6,6,6	0.11	0
5	SO4	A	1206	-	4,4,4	0.28	0	6,6,6	0.12	0
4	EDO	D	1201	-	3,3,3	0.68	0	2,2,2	0.07	0
5	SO4	F	301	-	4,4,4	0.29	0	6,6,6	0.12	0
5	SO4	C	303	-	4,4,4	0.37	0	6,6,6	0.06	0
5	SO4	A	1205	-	4,4,4	0.39	0	6,6,6	0.10	0
5	SO4	F	302	-	4,4,4	0.19	0	6,6,6	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	SO4	G	1203	-	4,4,4	0.31	0	6,6,6	0.05	0
4	EDO	A	1201	-	3,3,3	0.49	0	2,2,2	0.33	0
5	SO4	E	1102	-	4,4,4	0.35	0	6,6,6	0.11	0
5	SO4	D	1204	-	4,4,4	0.33	0	6,6,6	0.07	0
5	SO4	H	1103	-	4,4,4	0.38	0	6,6,6	0.11	0
5	SO4	H	1102	-	4,4,4	0.36	0	6,6,6	0.04	0
6	RSU	E	1101	-	27,30,30	0.65	0	29,40,40	1.40	5 (17%)
5	SO4	C	301	-	4,4,4	0.23	0	6,6,6	0.13	0
5	SO4	G	1204	-	4,4,4	0.31	0	6,6,6	0.10	0
6	RSU	H	1101	-	27,30,30	0.66	0	29,40,40	1.06	2 (6%)
5	SO4	F	303	-	4,4,4	0.32	0	6,6,6	0.12	0
5	SO4	G	1202	-	4,4,4	0.31	0	6,6,6	0.11	0
5	SO4	A	1202	-	4,4,4	0.24	0	6,6,6	0.15	0
5	SO4	A	1203	-	4,4,4	0.23	0	6,6,6	0.10	0
6	RSU	B	1101	-	27,30,30	0.75	1 (3%)	29,40,40	1.21	3 (10%)
5	SO4	D	1202	-	4,4,4	0.28	0	6,6,6	0.09	0
5	SO4	D	1205	-	4,4,4	0.27	0	6,6,6	0.16	0
5	SO4	D	1203	-	4,4,4	0.31	0	6,6,6	0.08	0
5	SO4	C	302	-	4,4,4	0.32	0	6,6,6	0.08	0
5	SO4	I	301	-	4,4,4	0.37	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
6	RSU	H	1101	-	-	5/19/19/19	0/3/3/3
6	RSU	B	1101	-	-	7/19/19/19	0/3/3/3
4	EDO	D	1201	-	-	0/1/1/1	-
6	RSU	E	1101	-	-	5/19/19/19	0/3/3/3
4	EDO	A	1201	-	-	0/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1101	RSU	C2-N2	2.14	1.35	1.32

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	1101	RSU	C7-N5-C4	3.28	131.04	127.15
6	B	1101	RSU	C5-C2-N2	-3.19	118.16	120.81
6	H	1101	RSU	C5-C2-N2	-3.11	118.23	120.81
6	B	1101	RSU	C3-N6-C10	3.06	129.48	124.31
6	E	1101	RSU	C3-N6-C10	2.94	129.28	124.31
6	H	1101	RSU	C3-N3-C4	-2.76	112.14	115.28
6	E	1101	RSU	C6-N5-C7	-2.58	122.88	125.42
6	E	1101	RSU	C5-C2-N2	-2.48	118.75	120.81
6	B	1101	RSU	C3-N3-C4	-2.40	112.55	115.28
6	E	1101	RSU	C3-N3-C4	-2.36	112.59	115.28

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	1101	RSU	C12-C10-N6-C3
6	B	1101	RSU	N2-C3-N6-C10
6	B	1101	RSU	N3-C3-N6-C10
6	B	1101	RSU	C8-C7-N5-C4
6	B	1101	RSU	C8-C7-N5-C6
6	E	1101	RSU	C11-C10-N6-C3
6	E	1101	RSU	C9-C7-N5-C4
6	E	1101	RSU	C9-C7-N5-C6
6	H	1101	RSU	N2-C3-N6-C10
6	H	1101	RSU	N3-C3-N6-C10
6	H	1101	RSU	C9-C7-N5-C4
6	H	1101	RSU	C9-C7-N5-C6
6	E	1101	RSU	C1-C14-C15-C16
6	B	1101	RSU	C9-C7-N5-C6
6	B	1101	RSU	C14-C1-N1-C2
6	E	1101	RSU	C14-C1-N1-C2
6	H	1101	RSU	C14-C1-N1-C2

There are no ring outliers.

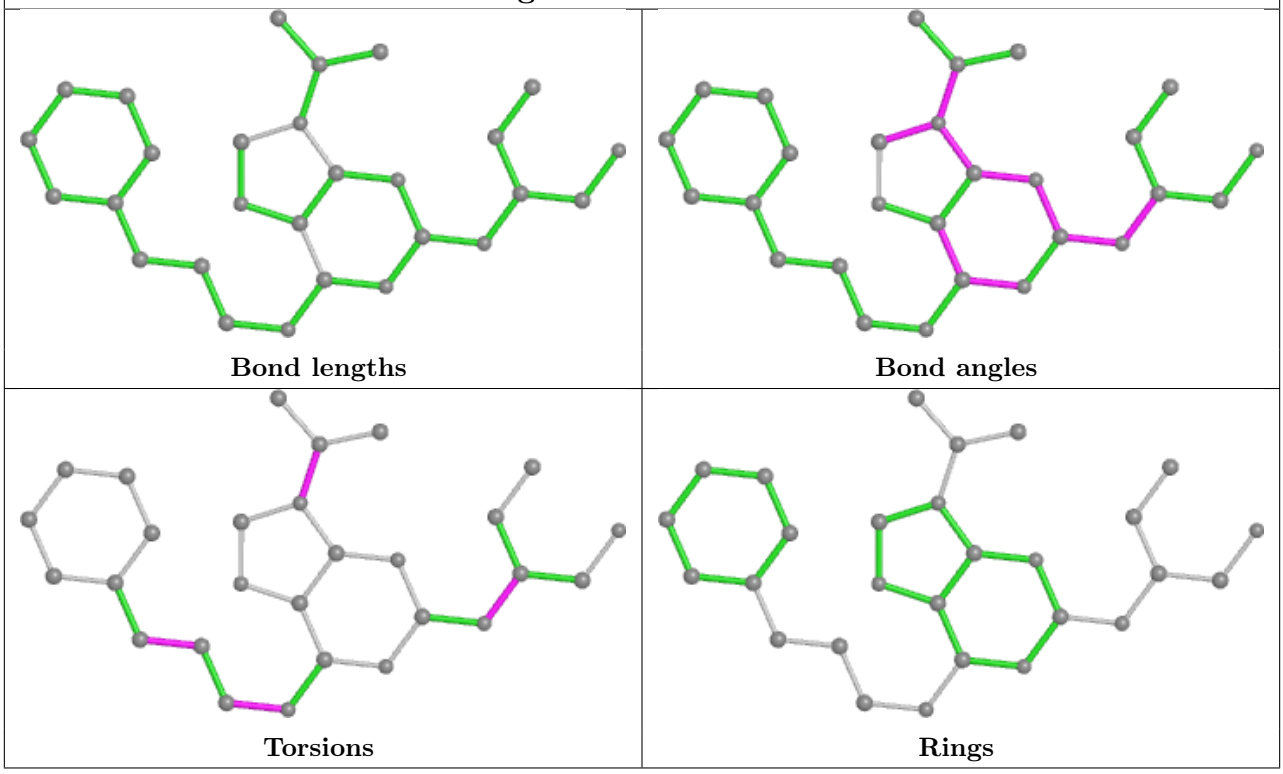
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1203	SO4	1	0

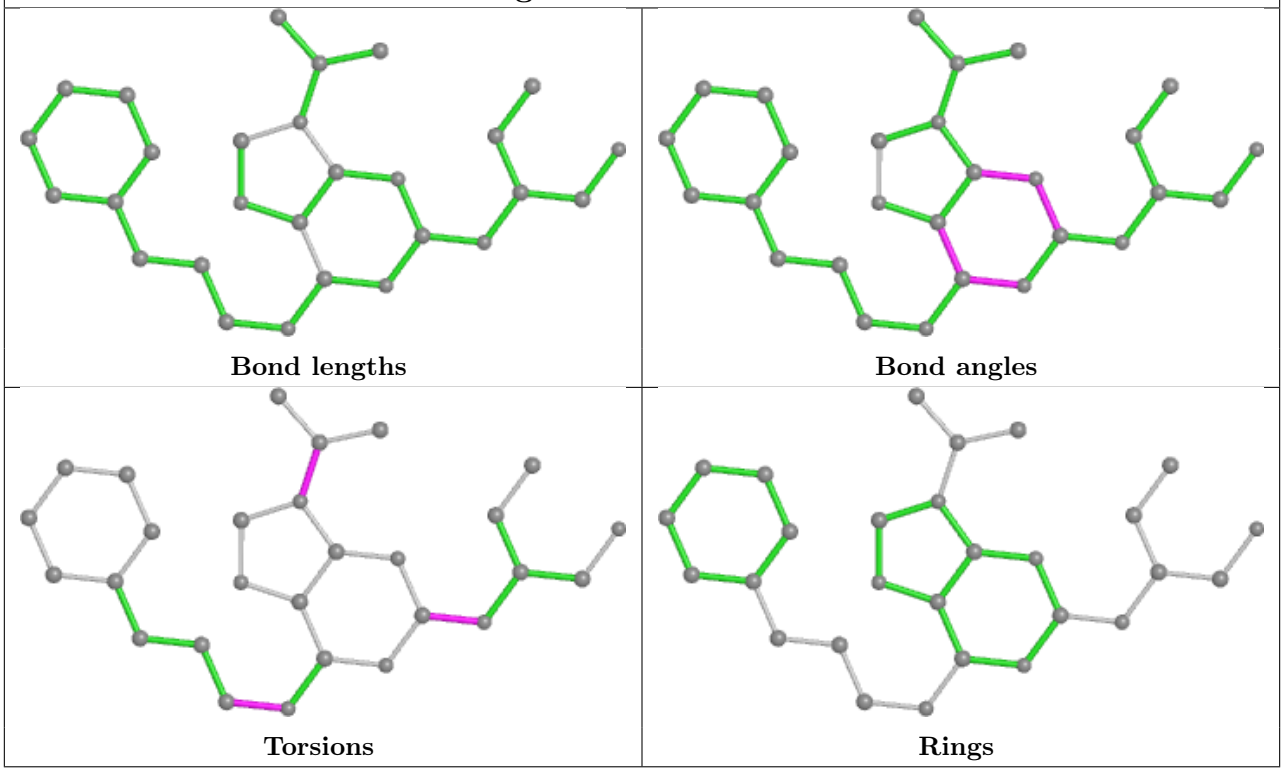
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

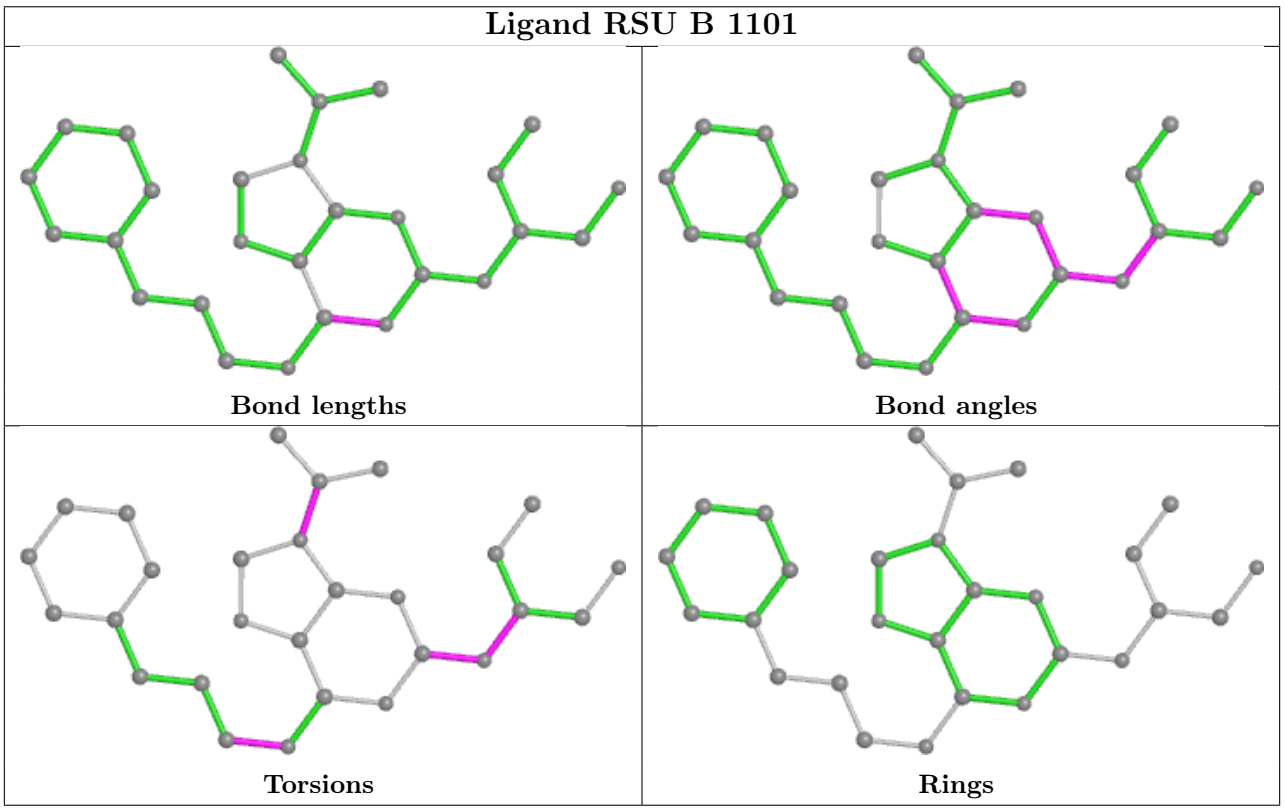
Ligand RSU E 1101



Ligand RSU H 1101



Ligand RSU B 1101



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	826/840 (98%)	0.82	113 (13%) 3 3	99, 136, 208, 286	0
1	D	827/840 (98%)	0.74	101 (12%) 4 5	94, 134, 201, 279	0
1	G	826/840 (98%)	0.74	101 (12%) 4 5	105, 140, 210, 297	0
2	B	324/344 (94%)	1.21	73 (22%) 0 1	115, 145, 216, 256	0
2	E	323/344 (93%)	1.01	53 (16%) 1 2	106, 138, 212, 253	0
2	H	319/344 (92%)	0.99	41 (12%) 3 4	88, 121, 191, 281	0
3	C	248/271 (91%)	0.70	20 (8%) 12 13	104, 132, 170, 227	0
3	F	248/271 (91%)	0.81	17 (6%) 16 18	86, 114, 154, 228	0
3	I	248/271 (91%)	0.75	13 (5%) 27 27	93, 118, 162, 233	0
All	All	4189/4365 (95%)	0.83	532 (12%) 3 4	86, 134, 206, 297	0

All (532) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	1035	HIS	8.7
2	E	1038	ASP	8.3
2	B	800	LEU	8.2
2	B	1035	HIS	7.9
2	B	799	ALA	6.9
2	B	1038	ASP	6.8
2	E	882	ARG	6.4
2	B	883	LEU	6.2
2	E	891	PRO	6.1
1	A	1016	ASN	6.0
2	B	798	ASP	5.9
2	B	886	SER	5.9
2	B	1039	CYS	5.8
2	E	1036	TRP	5.6
2	B	896	VAL	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	1018	GLY	5.5
2	B	802	PHE	5.3
2	H	1031	PRO	5.1
2	H	890	ARG	5.0
2	B	884	TYR	5.0
2	B	797	GLN	4.9
2	B	828	LEU	4.8
2	B	1034	PRO	4.8
1	A	953	TRP	4.6
2	E	896	VAL	4.6
3	I	266	PRO	4.5
3	F	262	LYS	4.5
2	E	890	ARG	4.4
1	G	1118	SER	4.4
3	C	267	HIS	4.4
3	I	267	HIS	4.3
1	A	710	LEU	4.3
1	G	1040	VAL	4.2
1	A	32	LEU	4.2
1	A	61	ILE	4.2
2	H	798	ASP	4.1
3	F	264	GLN	4.1
3	F	267	HIS	4.0
2	E	720	GLY	4.0
1	D	328	LEU	4.0
1	G	1088	PHE	4.0
1	D	37	THR	4.0
2	B	1037	GLN	4.0
1	G	133	LEU	3.9
1	A	708	GLN	3.9
2	E	887	GLU	3.8
2	B	878	PHE	3.8
1	G	5	TYR	3.8
2	B	803	LYS	3.8
1	A	57	MET	3.7
1	G	1129	LEU	3.7
1	A	377	THR	3.6
1	G	131	ILE	3.6
2	H	888	GLU	3.6
1	D	33	ILE	3.6
2	B	804	LYS	3.6
1	D	220	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	860	ILE	3.5
1	A	356	LEU	3.5
1	G	290	GLN	3.5
1	A	79	ILE	3.5
1	D	91	TYR	3.5
2	B	887	GLU	3.5
2	B	733	ILE	3.5
2	B	890	ARG	3.5
2	B	882	ARG	3.4
1	D	195	VAL	3.4
1	G	858	LEU	3.4
1	A	304	LEU	3.4
1	A	336	LEU	3.4
1	G	1043	LEU	3.4
2	B	855	PHE	3.4
2	B	955	PRO	3.4
2	B	867	LEU	3.4
2	E	1034	PRO	3.4
1	A	1097	PHE	3.4
2	H	892	TYR	3.4
1	G	280	LEU	3.4
1	A	1030	PHE	3.4
2	B	831	PHE	3.4
1	A	77	LEU	3.3
2	E	931	THR	3.3
2	H	767	PHE	3.3
2	H	802	PHE	3.3
1	D	237	ILE	3.3
1	G	253	ILE	3.3
1	G	307	GLU	3.3
1	G	1000	LEU	3.3
1	A	64	MET	3.3
2	B	1031	PRO	3.3
1	G	297	LEU	3.3
1	G	300	LEU	3.3
2	B	876	ALA	3.3
1	A	328	LEU	3.2
2	B	1033	LEU	3.2
2	H	896	VAL	3.2
1	A	1014	MET	3.2
2	B	856	LEU	3.2
1	D	1030	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
2	H	829	VAL	3.2
2	H	720	GLY	3.2
1	A	264	VAL	3.2
1	G	232	ILE	3.2
1	G	180	PHE	3.2
2	H	839	PHE	3.2
1	A	33	ILE	3.2
1	A	39	LEU	3.2
2	B	720	GLY	3.2
2	B	875	LEU	3.2
1	D	1004	VAL	3.2
1	G	294	THR	3.2
1	G	143	ILE	3.2
1	A	871	TYR	3.2
2	B	755	LEU	3.1
1	G	303	GLU	3.1
1	D	23	PHE	3.1
1	A	60	LYS	3.1
1	A	36	ASN	3.1
1	D	5	TYR	3.1
1	D	121	ILE	3.1
1	A	1029	LEU	3.1
1	A	1079	GLU	3.1
1	G	953	TRP	3.1
1	G	310	ILE	3.1
1	D	2	SER	3.1
1	D	36	ASN	3.1
1	A	1019	GLU	3.1
1	D	1129	LEU	3.0
1	A	387	LEU	3.0
1	G	64	MET	3.0
1	G	287	LYS	3.0
1	D	64	MET	3.0
1	G	829	PHE	3.0
2	B	829	VAL	3.0
1	A	372	GLN	3.0
2	E	831	PHE	3.0
2	H	738	TYR	3.0
2	E	883	LEU	3.0
1	G	248	ILE	3.0
2	H	828	LEU	3.0
1	D	1040	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	6	VAL	2.9
1	G	356	LEU	2.9
1	G	387	LEU	2.9
2	H	721	LYS	2.9
3	C	161	TYR	2.9
2	E	885	ASN	2.9
2	B	811	LEU	2.9
1	A	135	LEU	2.9
2	B	986	PHE	2.9
1	G	282	MET	2.9
2	B	897	ILE	2.9
1	D	1037	ILE	2.9
1	G	314	LEU	2.9
3	F	57	ILE	2.9
2	E	955	PRO	2.9
1	G	37	THR	2.9
1	D	1076	PHE	2.9
1	A	297	LEU	2.9
1	G	61	ILE	2.9
3	F	263	GLN	2.9
1	D	39	LEU	2.9
1	D	735	VAL	2.9
2	E	878	PHE	2.9
2	E	1031	PRO	2.9
3	C	164	LEU	2.8
1	A	145	LEU	2.8
2	E	802	PHE	2.8
3	I	56	PHE	2.8
1	G	1030	PHE	2.8
1	G	752	LEU	2.8
1	G	1039	LEU	2.8
2	E	875	LEU	2.8
1	D	230	ILE	2.8
2	B	775	ILE	2.8
1	G	240	HIS	2.8
1	G	317	LEU	2.8
2	B	738	TYR	2.8
2	E	867	LEU	2.8
2	E	829	VAL	2.8
1	D	1065	VAL	2.8
1	A	232	ILE	2.8
1	A	89	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	709	LYS	2.8
1	G	15	VAL	2.8
1	A	1129	LEU	2.7
2	H	889	SER	2.7
1	G	32	LEU	2.7
3	F	157	VAL	2.7
1	A	977	CYS	2.7
1	D	791	LEU	2.7
3	C	153	PHE	2.7
1	D	1	MET	2.7
1	G	974	LEU	2.7
1	D	219	VAL	2.7
1	A	1139	ILE	2.7
1	A	881	LEU	2.7
2	H	752	LEU	2.7
1	G	733	PHE	2.7
2	H	742	TYR	2.7
1	A	974	LEU	2.7
1	D	61	ILE	2.7
1	D	57	MET	2.7
2	B	864	ASN	2.7
3	C	132	PHE	2.7
1	A	143	ILE	2.7
1	D	42	TYR	2.7
2	B	885	ASN	2.7
2	E	926	LEU	2.7
1	G	930	VAL	2.7
1	A	327	ARG	2.7
1	A	100	ILE	2.7
1	A	791	LEU	2.7
1	A	1017	LEU	2.7
1	A	777	PRO	2.6
2	E	778	LEU	2.6
1	G	957	VAL	2.6
1	A	949	PHE	2.6
1	G	323	PHE	2.6
2	E	830	HIS	2.6
3	F	78	PHE	2.6
1	D	722	ARG	2.6
1	A	933	LEU	2.6
1	A	80	LEU	2.6
1	D	31	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	66	LEU	2.6
1	G	100	ILE	2.6
1	D	1088	PHE	2.6
1	A	376	VAL	2.6
1	A	140	PHE	2.6
1	G	295	VAL	2.6
1	A	390	ILE	2.6
2	B	926	LEU	2.6
2	E	738	TYR	2.6
2	E	892	TYR	2.6
1	D	1039	LEU	2.6
1	D	1005	ASN	2.6
1	D	1028	VAL	2.6
1	A	326	SER	2.6
1	A	1000	LEU	2.6
1	D	1000	LEU	2.6
2	B	820	LEU	2.6
3	C	155	LEU	2.6
1	A	41	ILE	2.6
1	G	237	ILE	2.6
2	E	733	ILE	2.6
1	D	376	VAL	2.5
1	A	31	LEU	2.5
1	G	910	MET	2.5
2	H	955	PRO	2.5
1	A	23	PHE	2.5
1	D	1033	VAL	2.5
1	D	152	LEU	2.5
1	D	359	ILE	2.5
1	G	78	PHE	2.5
1	A	87	CYS	2.5
1	D	167	VAL	2.5
1	G	49	LEU	2.5
1	G	179	CYS	2.5
1	A	1037	ILE	2.5
1	D	140	PHE	2.5
2	B	929	LEU	2.5
2	H	929	LEU	2.5
2	B	945	LEU	2.5
1	A	226	PHE	2.5
1	D	253	ILE	2.5
1	D	377	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	1037	ILE	2.5
2	E	930	PHE	2.5
2	E	776	LYS	2.5
1	D	49	LEU	2.5
3	C	188	PHE	2.5
2	E	897	ILE	2.5
3	I	57	ILE	2.5
2	E	913	TYR	2.5
2	H	823	LEU	2.5
1	G	911	ALA	2.5
2	B	776	LYS	2.5
1	A	133	LEU	2.5
1	G	77	LEU	2.5
3	I	64	LEU	2.5
1	A	1068	ILE	2.5
1	D	112	ILE	2.5
1	D	232	ILE	2.5
1	G	324	VAL	2.4
1	A	78	PHE	2.4
1	G	724	ILE	2.4
2	B	801	ASP	2.4
1	G	31	LEU	2.4
2	H	1025	LEU	2.4
2	E	922	CYS	2.4
2	H	887	GLU	2.4
1	G	132	GLY	2.4
1	D	16	ASN	2.4
1	A	120	ILE	2.4
1	A	131	ILE	2.4
1	D	387	LEU	2.4
1	G	285	LEU	2.4
1	G	1004	VAL	2.4
2	B	938	ALA	2.4
1	D	390	ILE	2.4
2	H	891	PRO	2.4
1	A	1094	ILE	2.4
2	E	825	GLU	2.4
1	A	392	ASN	2.4
1	A	63	VAL	2.4
1	A	15	VAL	2.4
2	E	755	LEU	2.4
2	H	932	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	1029	LEU	2.4
1	G	135	LEU	2.4
1	D	1097	PHE	2.4
2	H	831	PHE	2.4
1	D	207	TRP	2.4
2	B	1036	TRP	2.4
1	D	998	PHE	2.4
1	G	106	GLY	2.4
1	A	359	ILE	2.4
1	G	79	ILE	2.4
1	G	966	LEU	2.4
2	E	932	LYS	2.4
1	D	55	VAL	2.4
1	D	1113	GLN	2.4
2	H	730	ILE	2.4
3	I	147	LEU	2.4
1	G	167	VAL	2.4
1	A	972	PHE	2.4
1	D	1007	PHE	2.4
2	E	775	ILE	2.4
1	A	914	LEU	2.4
2	E	719	TRP	2.3
3	I	60	VAL	2.3
1	A	112	ILE	2.3
2	E	884	TYR	2.3
3	C	151	ILE	2.3
3	I	222	ILE	2.3
1	G	327	ARG	2.3
3	C	156	GLN	2.3
1	A	1020	THR	2.3
1	G	1097	PHE	2.3
1	A	14	ALA	2.3
1	A	375	LEU	2.3
2	B	866	LEU	2.3
2	H	775	ILE	2.3
2	H	964	ILE	2.3
2	B	932	LYS	2.3
1	A	16	ASN	2.3
1	A	197	LEU	2.3
1	A	283	LEU	2.3
1	G	39	LEU	2.3
2	B	918	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
2	E	858	ARG	2.3
1	G	308	THR	2.3
3	I	87	PHE	2.3
1	D	1054	MET	2.3
1	D	180	PHE	2.3
2	H	768	PRO	2.3
1	G	333	LEU	2.3
1	D	281	PHE	2.3
1	D	362	MET	2.3
1	G	792	LEU	2.3
2	E	935	ILE	2.3
3	F	132	PHE	2.3
2	B	894	ASN	2.3
1	A	367	LEU	2.3
1	D	1012	LEU	2.3
1	G	69	PRO	2.3
1	G	139	LEU	2.3
3	F	181	LEU	2.3
1	G	359	ILE	2.3
1	A	1008	CYS	2.3
1	D	63	VAL	2.3
2	E	839	PHE	2.3
1	D	327	ARG	2.3
2	B	760	LEU	2.3
2	H	982	LEU	2.3
1	A	281	PHE	2.3
2	B	780	GLN	2.3
2	B	809	PHE	2.3
2	B	839	PHE	2.3
1	A	13	THR	2.2
1	D	721	PRO	2.2
1	A	365	VAL	2.2
1	D	761	LEU	2.2
1	D	974	LEU	2.2
2	E	906	LEU	2.2
1	A	19	VAL	2.2
1	D	715	VAL	2.2
2	H	753	VAL	2.2
3	C	84	PHE	2.2
2	E	881	ALA	2.2
1	G	305	LEU	2.2
1	G	922	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	H	936	PHE	2.2
1	A	144	PRO	2.2
1	D	179	CYS	2.2
1	D	170	LEU	2.2
3	F	254	ILE	2.2
1	A	280	LEU	2.2
2	E	727	PHE	2.2
3	F	238	PHE	2.2
1	A	76	LEU	2.2
3	I	164	LEU	2.2
1	A	273	LEU	2.2
1	A	330	ASP	2.2
1	G	816	LEU	2.2
1	A	231	ILE	2.2
1	D	258	ILE	2.2
2	H	732	ILE	2.2
1	A	816	LEU	2.2
1	D	89	LEU	2.2
1	D	926	LEU	2.2
3	F	164	LEU	2.2
3	F	266	PRO	2.2
1	A	220	ILE	2.2
1	G	927	MET	2.2
1	D	977	CYS	2.2
2	H	922	CYS	2.2
1	G	851	PHE	2.2
1	A	364	VAL	2.2
1	D	1036	MET	2.2
2	H	810	TYR	2.2
2	B	930	PHE	2.2
1	A	40	GLU	2.2
1	D	100	ILE	2.2
1	G	1136	LEU	2.1
1	A	957	VAL	2.1
1	G	264	VAL	2.1
2	B	777	ILE	2.1
2	H	873	ILE	2.1
2	E	1020	LEU	2.1
1	A	88	ILE	2.1
2	B	826	SER	2.1
2	B	917	ILE	2.1
1	A	362	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1114	TYR	2.1
2	E	740	GLN	2.1
2	B	951	LEU	2.1
3	I	100	LEU	2.1
1	D	969	GLU	2.1
3	F	158	GLU	2.1
3	I	254	ILE	2.1
1	G	276	MET	2.1
2	B	908	LEU	2.1
3	C	71	LEU	2.1
2	H	818	HIS	2.1
1	G	296	THR	2.1
1	G	322	VAL	2.1
2	H	733	ILE	2.1
1	A	358	PRO	2.1
1	D	899	LEU	2.1
2	B	899	LEU	2.1
2	H	743	LYS	2.1
1	D	360	VAL	2.1
1	G	16	ASN	2.1
1	G	273	LEU	2.1
2	B	1001	LEU	2.1
3	C	147	LEU	2.1
1	A	381	ALA	2.1
2	B	881	ALA	2.1
1	A	7	VAL	2.1
1	G	120	ILE	2.1
1	A	308	THR	2.1
1	A	966	LEU	2.1
1	G	33	ILE	2.1
1	G	302	VAL	2.1
1	G	735	VAL	2.1
2	B	721	LYS	2.1
1	A	59	GLY	2.1
1	A	1050	LEU	2.1
1	D	802	LEU	2.1
1	D	1031	GLY	2.1
3	C	80	ARG	2.1
1	D	58	TYR	2.1
1	G	82	ALA	2.1
1	D	120	ILE	2.1
3	C	222	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
3	I	151	ILE	2.1
1	D	273	LEU	2.1
3	F	155	LEU	2.1
1	A	1088	PHE	2.1
1	G	1076	PHE	2.1
2	B	936	PHE	2.1
1	D	231	ILE	2.1
1	D	945	ILE	2.1
1	A	1039	LEU	2.1
3	F	71	LEU	2.1
1	D	1080	ARG	2.1
1	G	60	LYS	2.1
1	A	1031	GLY	2.1
1	D	32	LEU	2.1
1	D	1017	LEU	2.1
1	D	1136	LEU	2.1
2	E	1025	LEU	2.1
3	C	171	LEU	2.1
1	G	1007	PHE	2.0
2	B	793	VAL	2.0
2	B	892	TYR	2.0
2	E	901	TYR	2.0
2	H	812	VAL	2.0
1	D	159	LEU	2.0
1	D	914	LEU	2.0
3	C	116	ILE	2.0
1	D	40	GLU	2.0
1	D	6	VAL	2.0
1	G	977	CYS	2.0
1	G	1035	GLY	2.0
2	B	767	PHE	2.0
2	E	784	ARG	2.0
2	E	888	GLU	2.0
1	D	959	ILE	2.0
2	E	732	ILE	2.0
1	D	920	PHE	2.0
1	D	1003	PHE	2.0
1	A	742	VAL	2.0
1	D	139	LEU	2.0
1	G	325	GLY	2.0
1	D	733	PHE	2.0
3	C	211	MET	2.0

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Mol	Chain	Res	Type	RSRZ
2	E	889	SER	2.0
3	C	106	VAL	2.0
1	D	375	LEU	2.0
1	D	821	LEU	2.0
1	G	336	LEU	2.0
2	B	823	LEU	2.0
2	E	771	ALA	2.0
2	H	945	LEU	2.0
3	F	193	LEU	2.0
1	A	1035	GLY	2.0
1	A	130	MET	2.0
3	C	102	LEU	2.0
3	C	148	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	B	893	11/12	0.72	0.17	192,208,250,253	6
2	TPO	E	893	11/12	0.78	0.22	199,207,248,248	6
2	TPO	H	893	11/12	0.89	0.21	141,158,198,198	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
5	SO4	I	302	5/5	0.69	0.21	154,163,173,195	0
5	SO4	H	1103	5/5	0.70	0.27	156,165,174,207	0

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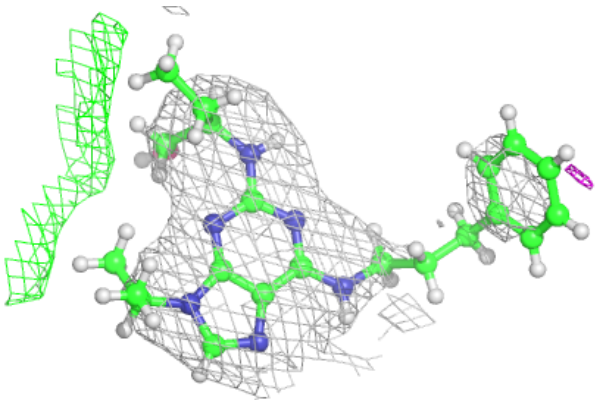
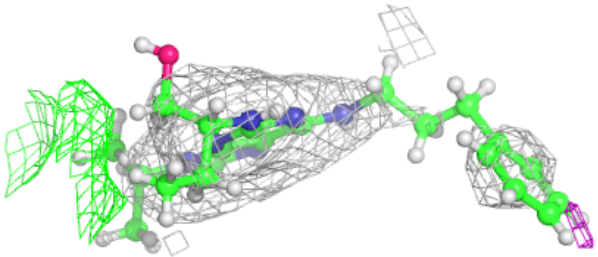
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SO4	G	1203	5/5	0.70	0.21	155,161,170,193	0
4	EDO	D	1201	4/4	0.78	0.32	92,119,144,144	6
5	SO4	A	1205	5/5	0.79	0.14	172,177,186,211	0
5	SO4	A	1204	5/5	0.80	0.31	144,147,162,192	0
5	SO4	C	302	5/5	0.80	0.17	161,168,176,203	0
5	SO4	F	301	5/5	0.80	0.18	149,154,170,197	0
4	EDO	A	1201	4/4	0.81	0.29	88,109,132,132	6
5	SO4	G	1204	5/5	0.82	0.18	145,160,170,195	0
5	SO4	A	1206	5/5	0.83	0.31	148,152,176,200	0
5	SO4	G	1201	5/5	0.83	0.22	144,147,161,164	0
5	SO4	D	1204	5/5	0.83	0.19	148,161,168,199	0
5	SO4	H	1102	5/5	0.84	0.16	171,174,179,209	0
5	SO4	G	1202	5/5	0.86	0.15	150,155,162,182	0
5	SO4	E	1102	5/5	0.86	0.17	164,169,173,205	0
5	SO4	C	303	5/5	0.87	0.11	159,165,172,199	0
5	SO4	D	1202	5/5	0.87	0.17	143,146,147,162	0
5	SO4	A	1202	5/5	0.87	0.21	143,145,156,169	0
5	SO4	I	303	5/5	0.87	0.17	120,133,137,152	0
5	SO4	D	1203	5/5	0.88	0.21	134,151,165,188	0
5	SO4	F	303	5/5	0.88	0.40	139,145,162,188	0
5	SO4	D	1205	5/5	0.89	0.32	133,147,154,187	0
5	SO4	I	301	5/5	0.90	0.14	157,159,168,192	0
5	SO4	A	1203	5/5	0.91	0.21	129,136,145,163	0
5	SO4	C	301	5/5	0.91	0.20	130,141,154,156	0
6	RSU	E	1101	28/28	0.92	0.65	101,131,152,158	30
6	RSU	H	1101	28/28	0.92	0.63	96,126,154,155	30
6	RSU	B	1101	28/28	0.93	0.71	102,130,151,159	30
5	SO4	F	302	5/5	0.95	0.16	109,114,132,136	0

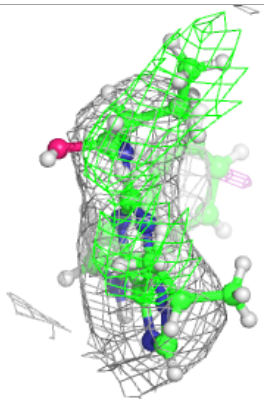
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around RSU 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)

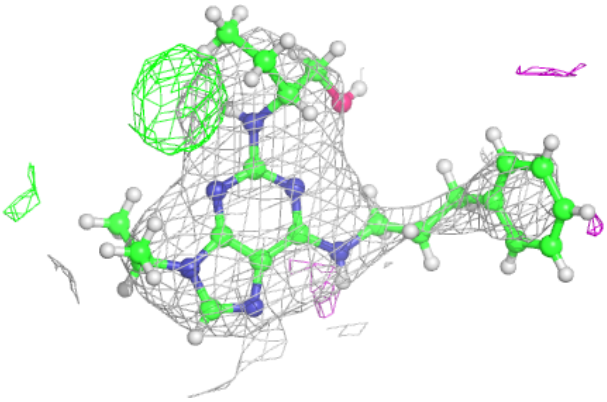


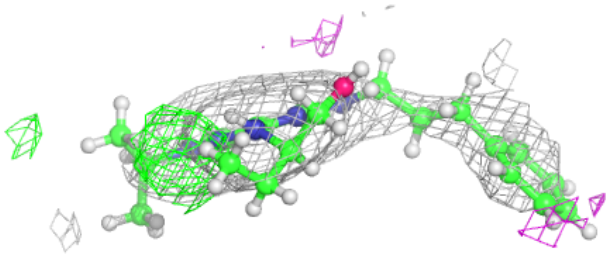


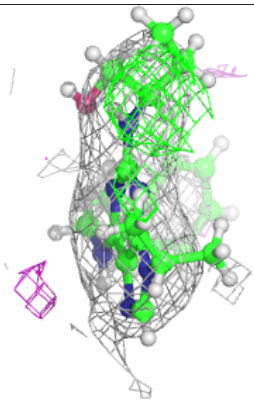


Electron density around RSU H 1101:

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

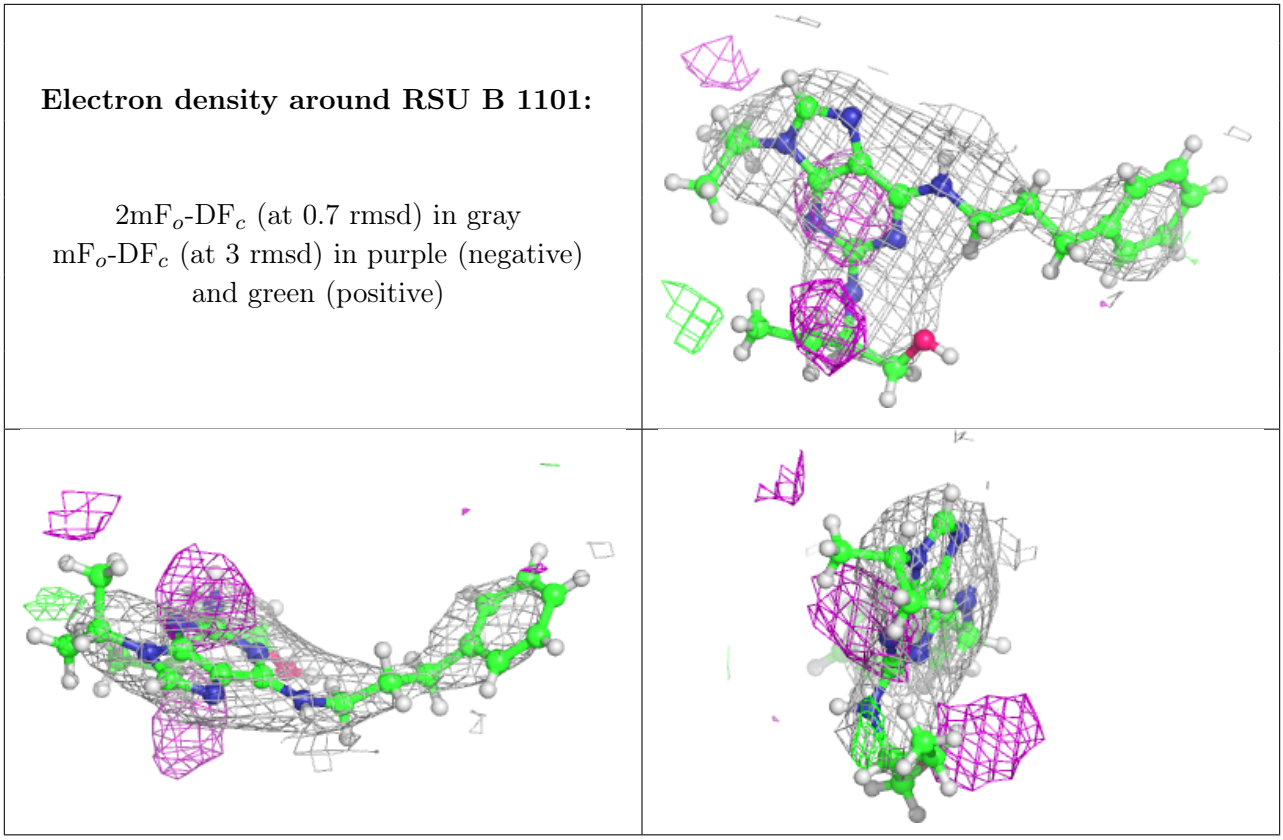






Electron density around RSU B 1101:

$2mF_o$-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

There are no such residues in this entry.