



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 7, 2023 – 01:36 pm BST

PDB ID : 8BUP
Title : Structure of DDB1 bound to DS30-engaged CDK12-cyclin K
Authors : Kozicka, Z.; Kempf, G.; Petzold, G.; Thoma, N.H.
Deposited on : 2022-11-30
Resolution : 3.41 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

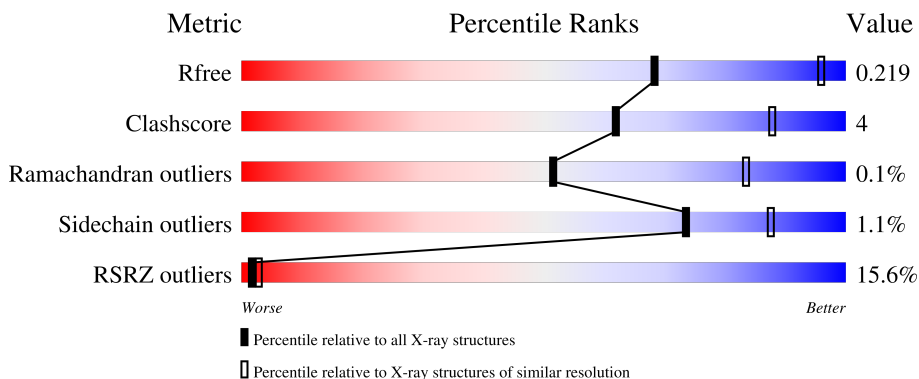
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.41 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1486 (3.50-3.34)
Clashscore	141614	1572 (3.50-3.34)
Ramachandran outliers	138981	1534 (3.50-3.34)
Sidechain outliers	138945	1535 (3.50-3.34)
RSRZ outliers	127900	1395 (3.50-3.34)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	840	 17% 87% 12%
1	D	840	 15% 86% 12%
1	G	840	 15% 82% 16%
2	B	344	 19% 77% 13% 9%
2	E	344	 17% 78% 12% 9%

Continued on next page...

Continued from previous page...

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	F	301	-	-	-	X
4	SO4	H	1103	-	-	-	X
4	SO4	H	1110	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 67034 atoms, of which 33350 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	826	12936	4105	6449	1094	1252	36	6449	0	0
1	D	827	12957	4111	6462	1095	1253	36	6462	0	0
1	G	826	12940	4106	6454	1093	1251	36	6454	0	0

There are 39 discrepancies between the modelled and reference sequences:

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

Continued on next page...

Continued from previous page...

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

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

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
			Total	C	H	N	O	P	S			
2	B	313	Total	C	H	N	O	P	S	2579	0	0
			5128	1633	2579	431	469	1	15			
2	E	313	Total	C	H	N	O	P	S	2579	0	0
			5128	1633	2579	431	469	1	15			
2	H	314	Total	C	H	N	O	P	S	2587	0	0
			5144	1638	2587	432	470	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

Continued on next page...

Continued from previous page...

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

- Molecule 3 is a protein called Cyclin-K.

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

There are 12 discrepancies between the modelled and reference sequences:

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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

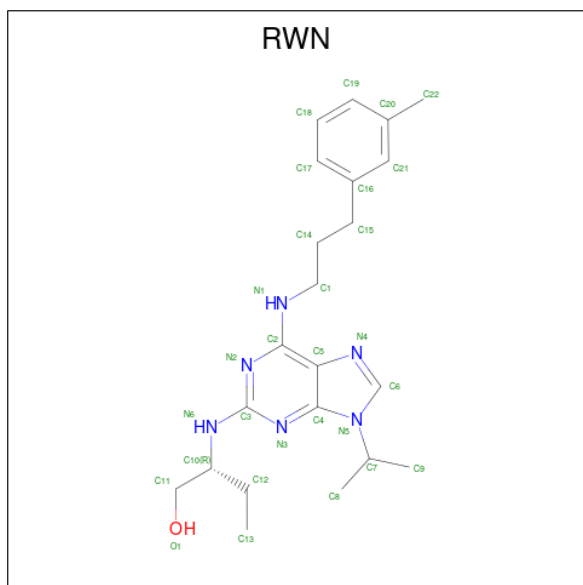
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
4	G	1	5	4	1	0	0
4	G	1	5	4	1	0	0
4	G	1	5	4	1	0	0
4	G	1	5	4	1	0	0
4	G	1	5	4	1	0	0
4	G	1	5	4	1	0	0
4	G	1	5	4	1	0	0
4	G	1	5	4	1	0	0
4	G	1	5	4	1	0	0
4	G	1	5	4	1	0	0
4	H	1	5	4	1	0	0
4	H	1	5	4	1	0	0
4	H	1	5	4	1	0	0
4	H	1	5	4	1	0	0
4	H	1	5	4	1	0	0
4	H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

Continued on next page...

Continued from previous page...

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

- Molecule 5 is (2 {R})-2-[[6-[3-(3-methylphenyl)propylamino]-9-propan-2-yl-purin-2-yl]amino]butan-1-ol (three-letter code: RWN) (formula: C₂₂H₃₂N₆O) (labeled as "Ligand of Interest" by depositor).

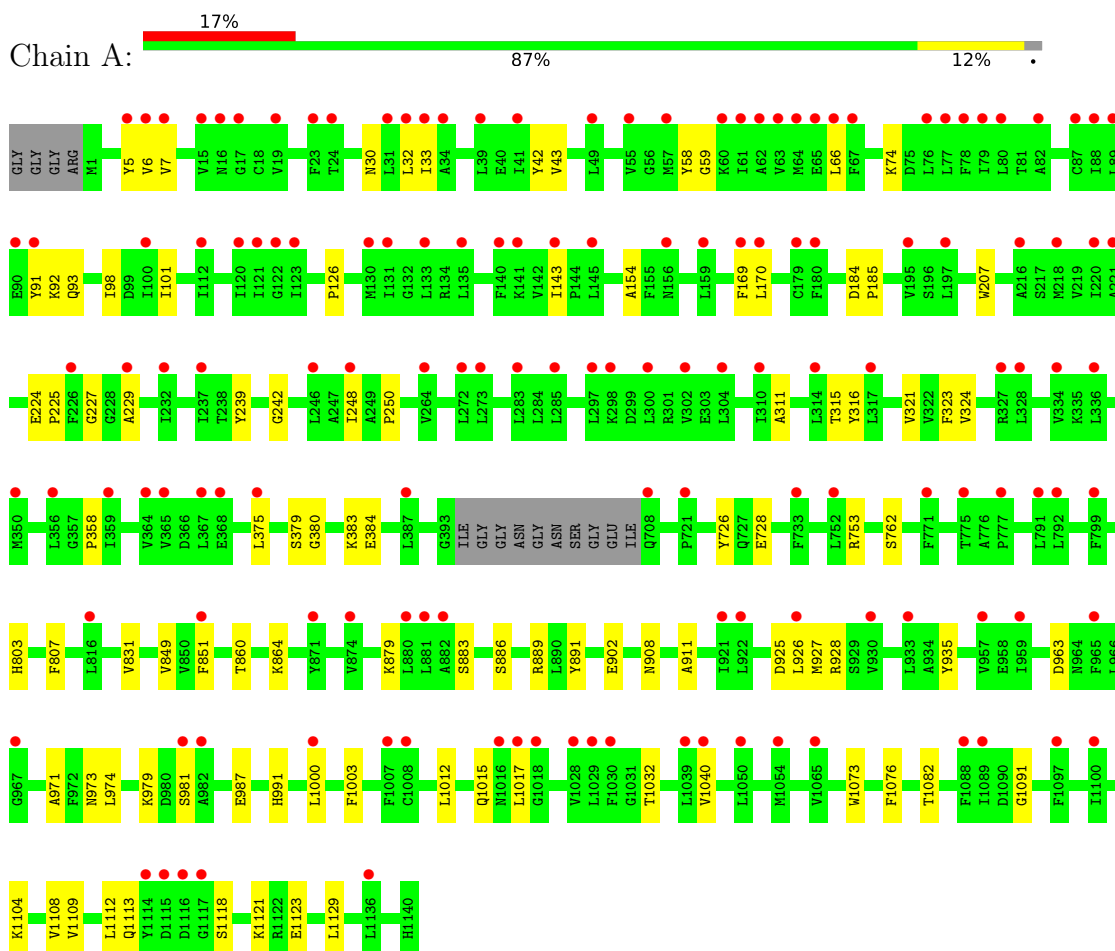


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	H	N	O	32	0
			61	22	32	6	1		
5	E	1	Total	C	H	N	O	32	0
			61	22	32	6	1		
5	H	1	Total	C	H	N	O	32	0
			61	22	32	6	1		

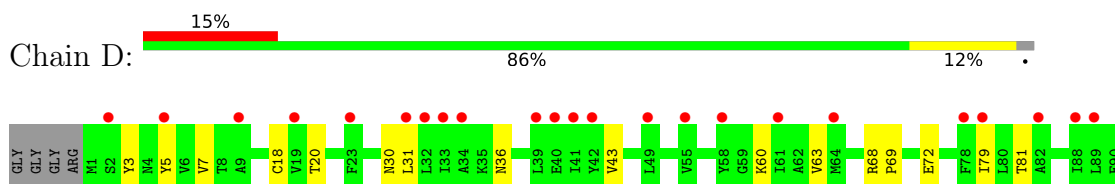
3 Residue-property plots [i](#)

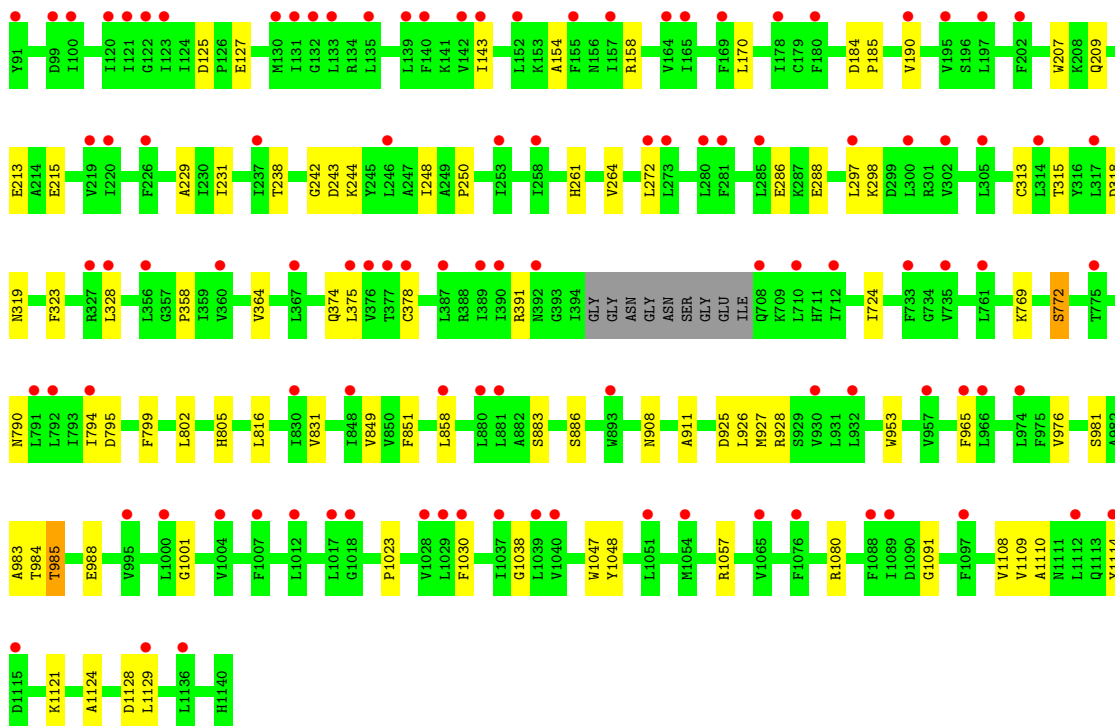
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

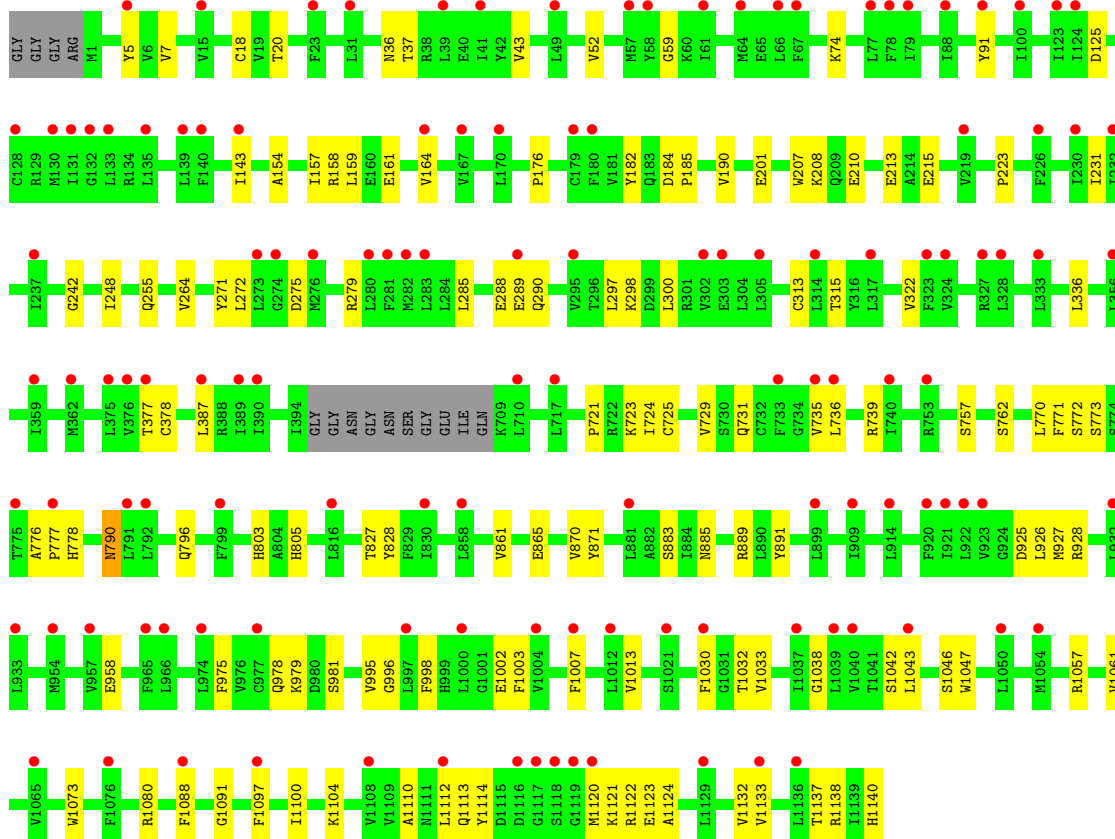
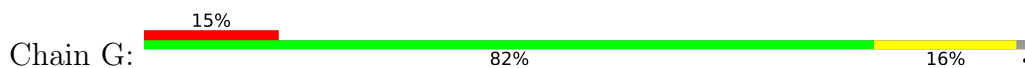


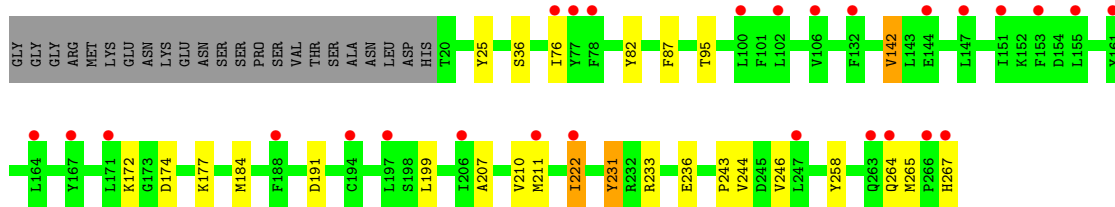
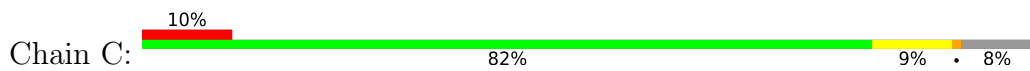
- Molecule 1: DNA damage-binding protein 1



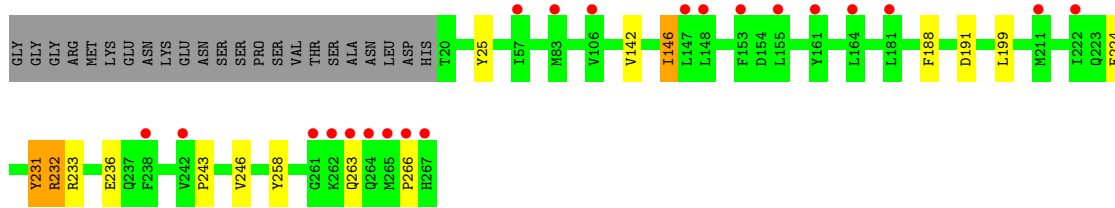
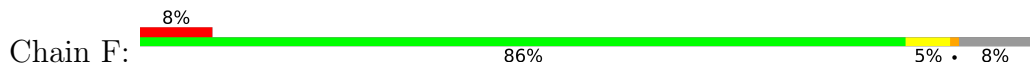


• Molecule 1: DNA damage-binding protein 1

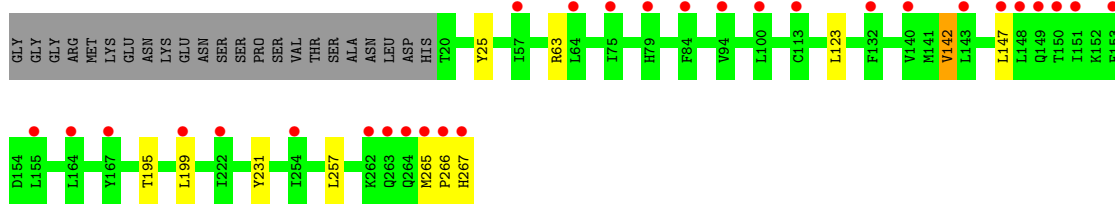
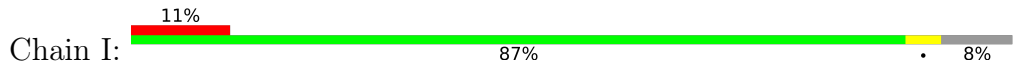




• Molecule 3: Cyclin-K



• 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	248.06Å 248.06Å 221.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	57.53 – 3.41 214.82 – 3.41	Depositor EDS
% Data completeness (in resolution range)	86.6 (57.53-3.41) 86.7 (214.82-3.41)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 3.41Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.200 , 0.223 0.199 , 0.219	Depositor DCC
R_{free} test set	4610 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	143.3	Xtrriage
Anisotropy	0.001	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 106.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	0.044 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	67034	wwPDB-VP
Average B, all atoms (Å ²)	164.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, RWN, 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	0.34	0/6604	0.62	0/8931
1	D	0.33	0/6612	0.59	0/8942
1	G	0.34	0/6603	0.61	0/8930
2	B	0.34	0/2590	0.61	0/3486
2	E	0.35	0/2590	0.61	0/3486
2	H	0.36	0/2598	0.62	0/3496
3	C	0.34	0/2120	0.54	0/2868
3	F	0.35	0/2120	0.54	0/2868
3	I	0.33	0/2120	0.54	0/2868
All	All	0.34	0/33957	0.60	0/45875

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6487	6449	6451	54	1
1	D	6495	6462	6464	57	0
1	G	6486	6454	6456	77	1
2	B	2549	2579	2579	33	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	2549	2579	2579	26	0
2	H	2557	2587	2587	30	1
3	C	2063	2048	2048	16	0
3	F	2063	2048	2048	12	1
3	I	2063	2048	2048	5	0
4	A	30	0	0	2	0
4	B	10	0	0	0	0
4	C	15	0	0	1	0
4	D	65	0	0	0	0
4	E	15	0	0	0	0
4	F	30	0	0	0	0
4	G	60	0	0	0	0
4	H	45	0	0	0	0
4	I	15	0	0	0	0
5	B	29	32	0	0	0
5	E	29	32	0	0	0
5	H	29	32	0	0	0
All	All	33684	33350	33260	296	2

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

All (296) 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:191:ASP:OD2	3:F:258:TYR:OH	1.98	0.80
1:G:1114:TYR:HB2	1:G:1124:ALA:HB2	1.66	0.78
1:G:208:LYS:NZ	1:G:210:GLU:OE2	2.20	0.74
1:D:1109:VAL:HG12	1:D:1129:LEU:HD12	1.71	0.72
3:F:231:TYR:OH	3:F:236:GLU:OE1	2.07	0.70
1:G:285:LEU:HB3	1:G:297:LEU:HD11	1.73	0.69
2:B:803:LYS:HG2	3:C:142:VAL:HG11	1.75	0.68
2:B:858:ARG:NH1	2:B:893:TPO:O1P	2.25	0.68
2:E:751:GLU:OE1	2:E:790:LYS:NZ	2.29	0.66
1:G:1112:LEU:HD23	1:G:1124:ALA:HB3	1.77	0.65
1:A:1109:VAL:HG12	1:A:1129:LEU:HD12	1.79	0.65
2:B:862:CYS:HG	2:B:901:TYR:HH	1.41	0.65
1:G:43:VAL:HG23	1:G:52:VAL:HG21	1.84	0.60
2:H:934:PRO:HB2	2:H:937:GLN:HG3	1.83	0.60
1:D:851:PHE:HB3	1:D:858:LEU:HD22	1.83	0.60
1:A:207:TRP:HB3	1:A:242:GLY:HA2	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1112:LEU:O	1:G:1123:GLU:HA	2.02	0.59
1:G:158:ARG:HE	2:H:987:SER:HB2	1.68	0.59
1:G:770:LEU:HD21	1:G:865:GLU:HB2	1.84	0.59
2:B:841:LYS:HD3	2:B:1025:LEU:HD13	1.83	0.58
2:H:722:ARG:HE	2:H:726:LYS:HG3	1.67	0.58
1:D:364:VAL:HG22	1:D:375:LEU:HD13	1.84	0.58
2:B:1010:THR:O	2:B:1014:THR:HG23	2.04	0.58
1:G:387:LEU:HD11	1:G:735:VAL:HG21	1.86	0.58
1:G:1120:MET:HG2	1:G:1122:ARG:HE	1.68	0.58
2:B:897:ILE:HD12	2:B:903:PRO:HD3	1.86	0.57
1:G:1113:GLN:HB3	1:G:1121:LYS:HD2	1.86	0.57
2:H:858:ARG:NH1	2:H:913:TYR:OH	2.37	0.57
1:G:1080:ARG:HD3	2:H:825:GLU:HA	1.86	0.57
1:G:377:THR:O	1:G:387:LEU:HD23	2.04	0.57
2:E:858:ARG:NE	2:E:880:LEU:O	2.37	0.57
1:G:143:ILE:HG12	1:G:154:ALA:HB2	1.86	0.56
1:A:170:LEU:HD21	1:A:229:ALA:HB2	1.87	0.56
1:A:1112:LEU:O	1:A:1123:GLU:HA	2.05	0.56
2:B:892:TYR:HB3	2:B:913:TYR:CZ	2.40	0.56
1:A:383:LYS:NZ	1:A:384:GLU:OE2	2.37	0.56
2:H:799:ALA:HB1	2:H:804:LYS:HB2	1.87	0.55
2:B:733:ILE:HG23	2:B:743:LYS:HB2	1.88	0.55
1:A:227:GLY:O	1:A:239:TYR:OH	2.16	0.55
1:G:1047:TRP:HZ3	1:G:1132:VAL:HG13	1.71	0.55
2:H:832:SER:O	2:H:836:ILE:HG13	2.07	0.55
1:D:36:ASN:ND2	1:D:1001:GLY:O	2.40	0.54
1:A:1003:PHE:O	1:A:1032:THR:HA	2.07	0.54
1:D:1080:ARG:HD3	2:E:825:GLU:HA	1.88	0.54
1:A:224:GLU:N	1:A:225:PRO:HD2	2.23	0.54
1:A:991:HIS:HB2	2:B:735:GLU:OE2	2.07	0.54
2:B:722:ARG:HB3	2:B:793:VAL:HG12	1.89	0.54
2:E:1010:THR:O	2:E:1014:THR:HG23	2.09	0.53
2:H:803:LYS:HG2	3:I:142:VAL:HG11	1.89	0.53
2:B:890:ARG:HG2	2:B:891:PRO:HD2	1.90	0.53
1:G:322:VAL:HG21	1:G:336:LEU:HD11	1.91	0.53
2:B:801:ASP:HB2	2:B:804:LYS:HB2	1.91	0.52
2:B:858:ARG:HD2	2:B:896:VAL:HG21	1.91	0.52
2:H:867:LEU:HD13	2:H:873:ILE:HD13	1.90	0.52
1:D:816:LEU:HD13	1:D:831:VAL:HG22	1.91	0.52
1:G:790:ASN:HA	1:G:805:HIS:O	2.09	0.52
1:D:158:ARG:HE	2:E:987:SER:HB2	1.74	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1047:TRP:CZ3	1:G:1132:VAL:HG13	2.45	0.51
2:E:867:LEU:HD13	2:E:873:ILE:HD13	1.91	0.51
1:G:378:CYS:SG	1:G:724:ILE:HB	2.50	0.51
1:D:207:TRP:HB3	1:D:242:GLY:HA2	1.93	0.51
1:A:248:ILE:HG12	1:A:250:PRO:HD3	1.91	0.51
2:H:1025:LEU:O	2:H:1028:MET:HG3	2.11	0.51
3:F:232:ARG:HG2	3:F:233:ARG:N	2.26	0.51
2:E:838:SER:O	2:E:842:GLN:HG3	2.11	0.50
1:A:30:ASN:ND2	1:A:43:VAL:HG22	2.26	0.50
2:B:892:TYR:HB2	2:B:911:GLU:O	2.10	0.50
1:A:1113:GLN:HB3	1:A:1121:LYS:HB3	1.93	0.50
1:D:190:VAL:O	1:D:209:GLN:HA	2.11	0.50
1:D:795:ASP:HB2	1:D:802:LEU:HD21	1.93	0.50
2:H:722:ARG:HH21	2:H:726:LYS:HB3	1.76	0.50
1:D:925:ASP:OD1	1:D:926:LEU:N	2.45	0.50
1:G:74:LYS:NZ	1:G:91:TYR:O	2.36	0.50
1:D:1057:ARG:NH1	1:D:1110:ALA:O	2.45	0.49
1:G:925:ASP:OD1	1:G:926:LEU:N	2.45	0.49
1:A:6:VAL:HG22	1:A:1040:VAL:HG22	1.94	0.49
3:C:231:TYR:OH	3:C:236:GLU:OE1	2.18	0.49
1:A:864:LYS:NZ	4:A:1202:SO4:O4	2.44	0.49
1:A:1015:GLN:C	1:A:1017:LEU:H	2.15	0.49
2:E:802:PHE:CB	3:F:146:ILE:HD11	2.43	0.49
2:H:760:LEU:HD12	2:H:760:LEU:O	2.12	0.49
1:G:288:GLU:HG3	1:G:298:LYS:HB2	1.93	0.49
1:A:59:GLY:HA2	1:A:1073:TRP:CZ3	2.48	0.49
2:B:842:GLN:HG2	2:B:1025:LEU:HD21	1.95	0.49
1:G:870:VAL:HA	1:G:883:SER:O	2.12	0.49
1:A:886:SER:O	1:A:908:ASN:HB2	2.13	0.49
1:G:776:ALA:HB1	1:G:778:HIS:CD2	2.48	0.49
1:G:223:PRO:HD3	1:G:271:TYR:OH	2.12	0.48
1:D:288:GLU:HB2	1:D:298:LYS:HB2	1.93	0.48
1:G:1013:VAL:HG11	1:G:1138:ARG:O	2.13	0.48
1:A:963:ASP:OD1	1:A:979:LYS:HE3	2.13	0.48
2:B:879:GLY:O	2:B:880:LEU:HB2	2.14	0.48
3:C:233:ARG:HD3	3:C:236:GLU:OE2	2.14	0.48
1:D:1114:TYR:CE1	1:D:1128:ASP:HB3	2.49	0.48
3:F:25:TYR:HA	3:F:199:LEU:O	2.13	0.48
2:H:867:LEU:HD13	2:H:873:ILE:CD1	2.43	0.48
3:I:63:ARG:HE	3:I:123:LEU:HD21	1.77	0.48
1:G:762:SER:O	1:G:803:HIS:HA	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:828:TYR:CE1	1:G:861:VAL:HG21	2.49	0.48
2:B:784:ARG:O	2:B:874:LYS:HE2	2.14	0.48
1:D:60:LYS:O	1:D:81:THR:HA	2.13	0.48
1:A:311:ALA:HB2	1:A:324:VAL:HG13	1.94	0.48
1:A:889:ARG:HD2	1:A:891:TYR:CZ	2.48	0.48
2:E:803:LYS:HA	3:F:142:VAL:CG1	2.44	0.48
1:G:771:PHE:O	1:G:773:SER:N	2.47	0.48
2:B:894:ASN:HB2	2:B:911:GLU:HG2	1.95	0.48
1:D:69:PRO:HD2	1:D:72:GLU:HG3	1.95	0.48
1:D:1057:ARG:HD3	1:D:1108:VAL:O	2.14	0.48
1:G:59:GLY:HA2	1:G:1073:TRP:CE3	2.49	0.48
1:G:1003:PHE:O	1:G:1032:THR:HA	2.14	0.47
1:G:378:CYS:HB3	1:G:721:PRO:HB2	1.96	0.47
1:G:1120:MET:HG2	1:G:1122:ARG:NE	2.28	0.47
2:H:733:ILE:HD11	2:H:741:VAL:HG12	1.95	0.47
2:B:858:ARG:NH1	2:B:913:TYR:OH	2.44	0.47
1:D:261:HIS:HA	1:D:272:LEU:O	2.14	0.47
2:E:867:LEU:HD13	2:E:873:ILE:CD1	2.44	0.47
2:H:839:PHE:CZ	2:H:865:ILE:HG21	2.50	0.47
1:D:378:CYS:SG	1:D:724:ILE:HB	2.55	0.47
1:A:849:VAL:HG11	1:A:851:PHE:CZ	2.49	0.47
3:I:195:THR:CG2	3:I:257:LEU:HD11	2.44	0.47
1:A:315:THR:HG23	1:A:323:PHE:HB3	1.96	0.47
3:C:222:ILE:HD12	3:C:222:ILE:H	1.80	0.47
1:G:59:GLY:HA2	1:G:1073:TRP:CZ3	2.50	0.47
1:A:358:PRO:O	1:A:379:SER:HA	2.15	0.47
1:D:315:THR:HG22	1:D:323:PHE:HB3	1.96	0.47
2:H:1010:THR:O	2:H:1014:THR:HG23	2.15	0.47
1:G:184:ASP:HB2	1:G:185:PRO:CD	2.44	0.46
1:G:255:GLN:OE1	1:G:279:ARG:NH1	2.47	0.46
2:B:760:LEU:HD12	2:B:760:LEU:O	2.15	0.46
1:D:1030:PHE:CZ	1:D:1038:GLY:HA3	2.50	0.46
2:E:775:ILE:HD11	2:E:811:LEU:HD21	1.98	0.46
3:C:207:ALA:O	3:C:210:VAL:HG22	2.14	0.46
2:B:899:LEU:O	2:B:944:GLN:NE2	2.48	0.46
2:H:981:ARG:HD2	2:H:984:GLU:OE1	2.16	0.46
1:G:125:ASP:OD2	1:G:176:PRO:HB3	2.16	0.46
2:E:892:TYR:HB2	2:E:911:GLU:O	2.15	0.46
3:F:258:TYR:O	3:F:263:GLN:O	2.34	0.46
1:G:18:CYS:HG	1:G:313:CYS:HG	1.59	0.46
1:A:925:ASP:OD1	1:A:926:LEU:N	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:803:LYS:HG3	3:F:142:VAL:HG21	1.97	0.46
2:B:858:ARG:HB2	2:B:880:LEU:O	2.16	0.46
2:E:760:LEU:HD12	2:E:760:LEU:O	2.16	0.46
2:H:841:LYS:HD2	2:H:1023:VAL:HB	1.98	0.46
1:A:93:GLN:HG3	1:A:98:ILE:HG12	1.98	0.46
2:B:799:ALA:O	2:B:800:LEU:HB2	2.16	0.46
1:D:30:ASN:ND2	1:D:43:VAL:HG22	2.31	0.46
2:E:802:PHE:HB3	3:F:146:ILE:HD11	1.98	0.46
1:G:159:LEU:HD21	1:G:164:VAL:HG21	1.98	0.46
1:G:1097:PHE:O	1:G:1100:ILE:HG12	2.15	0.46
1:A:33:ILE:HD12	1:A:42:TYR:CE1	2.51	0.45
1:D:18:CYS:HG	1:D:313:CYS:HG	1.61	0.45
1:D:983:ALA:O	1:D:985:THR:N	2.49	0.45
1:G:36:ASN:ND2	1:G:1002:GLU:OE2	2.46	0.45
2:H:845:GLU:HA	2:H:1015:LEU:HD11	1.97	0.45
1:A:860:THR:HG21	4:A:1203:SO4:O1	2.16	0.45
1:A:927:MET:O	1:A:928:ARG:HB2	2.15	0.45
3:C:25:TYR:HA	3:C:199:LEU:O	2.16	0.45
3:C:243:PRO:HG2	3:C:246:VAL:HG23	1.98	0.45
1:D:125:ASP:OD2	1:D:127:GLU:HB2	2.16	0.45
1:A:383:LYS:HB3	1:A:753:ARG:HD2	1.98	0.45
1:A:726:TYR:CE2	1:A:728:GLU:HB2	2.51	0.45
2:E:857:HIS:HD2	2:E:878:PHE:HA	1.82	0.45
3:F:243:PRO:HG2	3:F:246:VAL:HG23	1.97	0.45
1:G:207:TRP:HB3	1:G:242:GLY:HA2	1.99	0.45
1:G:1114:TYR:N	1:G:1122:ARG:O	2.47	0.45
3:C:184:MET:CE	3:C:267:HIS:HA	2.47	0.45
1:D:1114:TYR:HB2	1:D:1124:ALA:HB2	1.98	0.45
2:E:841:LYS:HG2	2:E:1025:LEU:HD21	1.98	0.45
1:A:1076:PHE:O	1:A:1082:THR:HA	2.17	0.45
1:A:58:TYR:HB3	1:A:1073:TRP:HB2	1.99	0.45
1:A:184:ASP:HB2	1:A:185:PRO:CD	2.47	0.45
1:A:902:GLU:OE2	1:A:935:TYR:OH	2.25	0.45
2:B:996:LEU:O	2:B:1000:MET:HG3	2.17	0.45
3:C:244:VAL:HG12	4:C:302:SO4:O4	2.16	0.45
1:G:771:PHE:C	1:G:773:SER:H	2.21	0.45
1:A:7:VAL:HG12	1:A:1091:GLY:HA3	1.99	0.45
1:D:231:ILE:HB	1:D:238:THR:OG1	2.18	0.45
1:G:157:ILE:HG23	1:G:201:GLU:HA	1.99	0.45
2:H:951:LEU:HD21	2:H:986:PHE:HE2	1.81	0.45
1:D:769:LYS:O	1:D:772:SER:HB2	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:886:SER:O	1:D:908:ASN:HB2	2.18	0.44
2:E:803:LYS:HA	3:F:142:VAL:HG13	2.00	0.44
1:G:5:TYR:HB2	1:G:1043:LEU:HD11	1.98	0.44
1:A:974:LEU:HD11	1:A:1000:LEU:HD22	1.99	0.44
1:A:987:GLU:HA	2:B:740:GLN:NE2	2.33	0.44
1:A:58:TYR:HB3	1:A:1073:TRP:CB	2.48	0.44
1:D:264:VAL:CG2	1:D:272:LEU:HG	2.47	0.44
1:G:1057:ARG:NH1	1:G:1110:ALA:O	2.50	0.44
2:B:892:TYR:HB3	2:B:913:TYR:CE2	2.53	0.44
1:G:889:ARG:HD2	1:G:891:TYR:CZ	2.52	0.44
1:G:927:MET:O	1:G:928:ARG:HB2	2.18	0.44
1:D:31:LEU:HD13	1:D:315:THR:HG21	1.99	0.44
1:D:318:ASP:O	1:D:319:ASN:HB2	2.18	0.44
1:A:92:LYS:HB2	1:A:101:ILE:CD1	2.47	0.44
1:D:213:GLU:HG2	1:D:215:GLU:H	1.83	0.44
2:H:769:ILE:HA	2:H:772:ILE:HB	1.99	0.44
2:H:858:ARG:O	2:H:896:VAL:O	2.35	0.44
1:A:971:ALA:HB3	1:A:973:ASN:HD22	1.83	0.44
2:E:814:GLU:OE1	2:E:874:LYS:NZ	2.43	0.44
1:G:1030:PHE:CZ	1:G:1038:GLY:HA3	2.53	0.44
1:D:244:LYS:HE2	1:D:297:LEU:O	2.17	0.43
1:D:1114:TYR:CZ	1:D:1128:ASP:HB3	2.53	0.43
1:A:126:PRO:HD3	1:A:169:PHE:HB3	1.99	0.43
1:D:790:ASN:HA	1:D:805:HIS:O	2.17	0.43
1:A:1104:LYS:O	1:A:1108:VAL:HG23	2.19	0.43
1:D:3:TYR:HB3	1:D:1048:TYR:HB2	2.00	0.43
1:D:794:ILE:HG22	1:D:799:PHE:HA	1.99	0.43
1:G:248:ILE:HD12	1:G:300:LEU:O	2.17	0.43
1:G:731:GLN:OE1	1:G:796:GLN:NE2	2.50	0.43
1:A:883:SER:HB2	1:A:911:ALA:HB3	1.99	0.43
1:D:849:VAL:HG11	1:D:851:PHE:CZ	2.54	0.43
1:G:723:LYS:HB2	1:G:736:LEU:HD12	2.00	0.43
3:C:264:GLN:HG2	3:C:265:MET:H	1.83	0.43
2:E:856:LEU:HD21	2:E:915:PRO:HG3	2.01	0.43
1:D:7:VAL:HG12	1:D:1091:GLY:HA3	2.01	0.43
1:G:36:ASN:O	1:G:37:THR:OG1	2.28	0.43
1:G:190:VAL:HG21	1:G:231:ILE:HD11	2.01	0.43
1:A:32:LEU:HD13	1:A:66:LEU:HD11	2.01	0.43
1:D:170:LEU:HD21	1:D:229:ALA:HB2	2.00	0.43
2:E:793:VAL:HG23	2:E:810:TYR:HB2	2.00	0.43
1:G:1080:ARG:NH1	2:H:928:GLU:OE2	2.44	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:TYR:O	1:A:321:VAL:O	2.37	0.42
3:C:82:TYR:CE2	3:C:95:THR:HG21	2.55	0.42
1:D:926:LEU:O	1:D:953:TRP:HA	2.19	0.42
2:B:841:LYS:HD2	2:B:1023:VAL:HB	2.02	0.42
3:C:172:LYS:HA	3:C:172:LYS:HD3	1.88	0.42
1:G:184:ASP:HB2	1:G:185:PRO:HD2	2.02	0.42
1:A:879:LYS:NZ	1:A:935:TYR:OH	2.52	0.42
3:C:174:ASP:OD2	3:C:177:LYS:HG3	2.20	0.42
3:C:191:ASP:OD2	3:C:258:TYR:OH	2.24	0.42
1:D:143:ILE:HG12	1:D:154:ALA:HB2	2.02	0.42
1:D:927:MET:O	1:D:928:ARG:HB2	2.20	0.42
2:E:763:GLU:CG	2:E:763:GLU:O	2.68	0.42
1:G:958:GLU:HB2	1:G:1007:PHE:CB	2.50	0.42
1:G:1061:VAL:HG11	1:G:1104:LYS:HB3	2.01	0.42
2:B:893:TPO:O	2:B:894:ASN:HB3	2.19	0.42
2:E:762:ASN:OD1	2:E:763:GLU:N	2.52	0.42
1:A:5:TYR:CE2	1:A:7:VAL:HG13	2.55	0.41
2:B:763:GLU:CG	2:B:763:GLU:O	2.68	0.41
1:D:985:THR:HB	1:D:988:GLU:HB2	2.00	0.41
1:G:998:PHE:HB2	1:G:1088:PHE:CG	2.54	0.41
1:G:1061:VAL:HG13	1:G:1104:LYS:HD2	2.02	0.41
1:G:1133:VAL:O	1:G:1137:THR:HG23	2.19	0.41
1:D:328:LEU:HA	1:D:358:PRO:HD3	2.03	0.41
1:G:161:GLU:HG2	1:G:182:TYR:CD1	2.55	0.41
1:G:979:LYS:O	1:G:981:SER:N	2.46	0.41
1:A:74:LYS:NZ	1:A:91:TYR:O	2.33	0.41
1:A:358:PRO:HD2	1:A:380:GLY:HA2	2.02	0.41
2:B:856:LEU:HD11	2:B:884:TYR:HB2	2.02	0.41
2:E:755:LEU:HD22	2:E:812:VAL:HG22	2.01	0.41
2:E:857:HIS:ND1	2:E:860:ILE:HG12	2.36	0.41
1:G:20:THR:HG23	1:G:315:THR:OG1	2.20	0.41
1:D:883:SER:HB2	1:D:911:ALA:HB3	2.01	0.41
1:D:1023:PRO:HB3	1:D:1047:TRP:CE2	2.55	0.41
2:E:877:ASP:C	2:E:879:GLY:H	2.24	0.41
3:F:188:PHE:CE1	3:F:266:PRO:HG2	2.56	0.41
1:G:7:VAL:HG12	1:G:1091:GLY:HA3	2.01	0.41
1:A:92:LYS:HB2	1:A:101:ILE:HD11	2.01	0.41
1:A:143:ILE:HG12	1:A:154:ALA:HB2	2.03	0.41
1:G:264:VAL:CG2	1:G:272:LEU:HG	2.50	0.41
1:D:5:TYR:CE2	1:D:7:VAL:HG13	2.56	0.41
1:D:374:GLN:HG2	1:D:391:ARG:HB3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:821:MET:HG2	2:H:825:GLU:HG3	2.02	0.41
3:I:266:PRO:O	3:I:267:HIS:C	2.59	0.41
1:A:762:SER:O	1:A:803:HIS:HA	2.20	0.41
1:D:248:ILE:HG12	1:D:250:PRO:HD3	2.03	0.41
1:G:213:GLU:HG2	1:G:215:GLU:H	1.85	0.41
1:G:729:VAL:HG21	1:G:827:THR:OG1	2.21	0.41
1:G:739:ARG:HD3	1:G:757:SER:OG	2.21	0.41
1:G:871:TYR:HE2	1:G:885:ASN:HA	1.85	0.41
1:G:975:PHE:HA	1:G:996:GLY:O	2.21	0.41
2:H:763:GLU:O	2:H:763:GLU:CG	2.68	0.41
2:H:1021:LYS:HB3	2:H:1021:LYS:HE3	1.89	0.41
1:A:375:LEU:HB2	1:A:1012:LEU:HD21	2.03	0.41
1:A:807:PHE:CZ	1:A:831:VAL:HG11	2.56	0.41
1:G:18:CYS:SG	1:G:313:CYS:SG	3.18	0.41
1:G:925:ASP:HB3	1:G:927:MET:O	2.21	0.41
1:G:978:GLN:HB2	1:G:995:VAL:HG21	2.03	0.41
2:B:980:ARG:NH2	2:B:998:ASP:OD1	2.47	0.40
3:C:207:ALA:O	3:C:211:MET:HG3	2.21	0.40
1:D:286:GLU:O	1:D:297:LEU:HD12	2.20	0.40
1:D:1023:PRO:HB3	1:D:1047:TRP:CZ2	2.56	0.40
1:D:184:ASP:HB2	1:D:185:PRO:CD	2.51	0.40
1:G:275:ASP:OD1	1:G:275:ASP:C	2.60	0.40
2:H:777:ILE:O	2:H:781:LEU:HG	2.22	0.40
3:I:25:TYR:HA	3:I:199:LEU:O	2.21	0.40
1:D:63:VAL:O	1:D:79:ILE:HA	2.22	0.40
2:H:784:ARG:O	2:H:874:LYS:HE2	2.20	0.40
2:B:732:ILE:O	2:B:732:ILE:HG23	2.22	0.40
2:B:760:LEU:HD12	2:B:760:LEU:C	2.41	0.40
1:D:207:TRP:CB	1:D:242:GLY:HA2	2.51	0.40
1:D:965:PHE:O	1:D:976:VAL:HA	2.21	0.40
3:C:36:SER:HG	3:C:87:PHE:HD2	1.69	0.40
1:G:1003:PHE:HB3	1:G:1033:VAL:HG23	2.03	0.40
2:H:839:PHE:HZ	2:H:865:ILE:HG21	1.86	0.40
2:H:903:PRO:HA	2:H:920:TRP:CD1	2.56	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1118:SER:OG	1:G:290:GLN:HE22[2_565]	1.48	0.12
3:F:224:GLU:OE1	2:H:999:HIS:HE2[5_554]	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%)	799 (97%)	22 (3%)	1 (0%)	51	83
1	D	823/840 (98%)	804 (98%)	17 (2%)	2 (0%)	47	80
1	G	822/840 (98%)	795 (97%)	25 (3%)	2 (0%)	47	80
2	B	310/344 (90%)	302 (97%)	8 (3%)	0	100	100
2	E	310/344 (90%)	304 (98%)	6 (2%)	0	100	100
2	H	311/344 (90%)	305 (98%)	6 (2%)	0	100	100
3	C	246/271 (91%)	242 (98%)	4 (2%)	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	4136/4365 (95%)	4035 (98%)	96 (2%)	5 (0%)	51	83

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	772	SER
1	A	981	SER
1	D	984	THR
1	D	772	SER
1	G	777	PRO

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%)	721 (100%)	0	100	100
1	D	722/728 (99%)	716 (99%)	6 (1%)	81	92
1	G	721/728 (99%)	715 (99%)	6 (1%)	81	92
2	B	281/308 (91%)	277 (99%)	4 (1%)	67	85
2	E	281/308 (91%)	273 (97%)	8 (3%)	43	73
2	H	282/308 (92%)	275 (98%)	7 (2%)	47	75
3	C	223/242 (92%)	219 (98%)	4 (2%)	59	81
3	F	223/242 (92%)	220 (99%)	3 (1%)	69	86
3	I	223/242 (92%)	219 (98%)	4 (2%)	59	81
All	All	3677/3834 (96%)	3635 (99%)	42 (1%)	73	87

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	844	MET
2	B	897	ILE
2	B	905	GLU
2	B	913	TYR
3	C	76	ILE
3	C	142	VAL
3	C	222	ILE
3	C	231	TYR
1	D	20	THR
1	D	68	ARG
1	D	243	ASP
1	D	981	SER
1	D	985	THR
1	D	1121	LYS
2	E	728	ASP
2	E	795	ASP
2	E	797	GLN
2	E	858	ARG
2	E	859	ASP
2	E	883	LEU
2	E	913	TYR
2	E	1025	LEU
3	F	146	ILE
3	F	231	TYR
3	F	232	ARG
1	G	289	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	725	CYS
1	G	790	ASN
1	G	1042	SER
1	G	1046	SER
1	G	1140	HIS
2	H	795	ASP
2	H	865	ILE
2	H	883	LEU
2	H	896	VAL
2	H	897	ILE
2	H	914	THR
2	H	979	ARG
3	I	142	VAL
3	I	147	LEU
3	I	231	TYR
3	I	265	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	952	ASN
1	G	993	GLN
3	I	179	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	TPO	H	893	2	8,10,11	1.80	1 (12%)	10,14,16	1.56	3 (30%)
2	TPO	B	893	2	8,10,11	1.56	1 (12%)	10,14,16	1.42	2 (20%)
2	TPO	E	893	2	8,10,11	1.10	0	10,14,16	1.44	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	-	3/9/11/13	-
2	TPO	B	893	2	-	3/9/11/13	-
2	TPO	E	893	2	-	5/9/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	893	TPO	P-O1P	3.59	1.62	1.50
2	B	893	TPO	P-O1P	3.20	1.60	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	893	TPO	P-OG1-CB	-3.69	112.06	123.21
2	H	893	TPO	P-OG1-CB	-3.59	112.37	123.21
2	B	893	TPO	P-OG1-CB	-3.06	113.95	123.21
2	H	893	TPO	CG2-CB-CA	-2.19	108.84	113.16
2	B	893	TPO	O-C-CA	-2.11	119.24	124.78
2	H	893	TPO	O-C-CA	-2.04	119.43	124.78

There are no chirality outliers.

All (11) torsion outliers are listed below:

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

Continued on next page...

Continued from previous page...

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

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	893	TPO	2	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

60 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	H	1105	-	4,4,4	0.30	0	6,6,6	0.09	0
4	SO4	D	1201	-	4,4,4	0.30	0	6,6,6	0.04	0
4	SO4	A	1204	-	4,4,4	0.26	0	6,6,6	0.08	0
4	SO4	G	1204	-	4,4,4	0.33	0	6,6,6	0.07	0
4	SO4	A	1202	-	4,4,4	0.22	0	6,6,6	0.11	0
4	SO4	D	1208	-	4,4,4	0.31	0	6,6,6	0.08	0
4	SO4	G	1212	-	4,4,4	0.33	0	6,6,6	0.07	0
4	SO4	H	1106	-	4,4,4	0.24	0	6,6,6	0.10	0
4	SO4	H	1109	-	4,4,4	0.26	0	6,6,6	0.07	0
4	SO4	D	1211	-	4,4,4	0.28	0	6,6,6	0.05	0
4	SO4	D	1212	-	4,4,4	0.25	0	6,6,6	0.08	0
4	SO4	G	1208	-	4,4,4	0.27	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	H	1103	-	4,4,4	0.34	0	6,6,6	0.08	0
5	RWN	E	1101	-	28,31,31	0.71	1 (3%)	31,42,42	0.89	2 (6%)
4	SO4	D	1203	-	4,4,4	0.29	0	6,6,6	0.09	0
4	SO4	G	1209	-	4,4,4	0.27	0	6,6,6	0.08	0
4	SO4	H	1104	-	4,4,4	0.21	0	6,6,6	0.13	0
4	SO4	I	303	-	4,4,4	0.35	0	6,6,6	0.09	0
4	SO4	B	1103	-	4,4,4	0.37	0	6,6,6	0.06	0
4	SO4	D	1207	-	4,4,4	0.30	0	6,6,6	0.06	0
4	SO4	A	1205	-	4,4,4	0.20	0	6,6,6	0.05	0
4	SO4	G	1203	-	4,4,4	0.30	0	6,6,6	0.04	0
4	SO4	G	1207	-	4,4,4	0.22	0	6,6,6	0.07	0
5	RWN	H	1101	-	28,31,31	0.70	0	31,42,42	0.85	2 (6%)
4	SO4	F	303	-	4,4,4	0.19	0	6,6,6	0.05	0
4	SO4	C	303	-	4,4,4	0.34	0	6,6,6	0.09	0
4	SO4	B	1102	-	4,4,4	0.35	0	6,6,6	0.07	0
4	SO4	F	304	-	4,4,4	0.30	0	6,6,6	0.06	0
4	SO4	F	301	-	4,4,4	0.36	0	6,6,6	0.07	0
4	SO4	D	1213	-	4,4,4	0.36	0	6,6,6	0.06	0
4	SO4	D	1202	-	4,4,4	0.24	0	6,6,6	0.06	0
4	SO4	G	1206	-	4,4,4	0.31	0	6,6,6	0.07	0
4	SO4	D	1210	-	4,4,4	0.35	0	6,6,6	0.04	0
4	SO4	G	1211	-	4,4,4	0.29	0	6,6,6	0.13	0
4	SO4	G	1210	-	4,4,4	0.28	0	6,6,6	0.08	0
4	SO4	I	302	-	4,4,4	0.19	0	6,6,6	0.08	0
4	SO4	G	1202	-	4,4,4	0.27	0	6,6,6	0.05	0
4	SO4	C	302	-	4,4,4	0.36	0	6,6,6	0.08	0
4	SO4	F	305	-	4,4,4	0.26	0	6,6,6	0.09	0
4	SO4	H	1107	-	4,4,4	0.32	0	6,6,6	0.06	0
4	SO4	D	1206	-	4,4,4	0.23	0	6,6,6	0.07	0
4	SO4	E	1104	-	4,4,4	0.29	0	6,6,6	0.10	0
4	SO4	E	1103	-	4,4,4	0.31	0	6,6,6	0.09	0
4	SO4	G	1201	-	4,4,4	0.26	0	6,6,6	0.10	0
4	SO4	G	1205	-	4,4,4	0.35	0	6,6,6	0.07	0
4	SO4	A	1203	-	4,4,4	0.26	0	6,6,6	0.09	0
4	SO4	H	1108	-	4,4,4	0.29	0	6,6,6	0.08	0
4	SO4	I	301	-	4,4,4	0.32	0	6,6,6	0.07	0
4	SO4	F	306	-	4,4,4	0.21	0	6,6,6	0.14	0
4	SO4	D	1204	-	4,4,4	0.27	0	6,6,6	0.07	0
4	SO4	D	1205	-	4,4,4	0.32	0	6,6,6	0.09	0
5	RWN	B	1101	-	28,31,31	0.70	1 (3%)	31,42,42	1.00	3 (9%)
4	SO4	E	1102	-	4,4,4	0.32	0	6,6,6	0.07	0
4	SO4	F	302	-	4,4,4	0.28	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	A	1201	-	4,4,4	0.24	0	6,6,6	0.07	0
4	SO4	H	1110	-	4,4,4	0.32	0	6,6,6	0.06	0
4	SO4	A	1206	-	4,4,4	0.24	0	6,6,6	0.08	0
4	SO4	H	1102	-	4,4,4	0.23	0	6,6,6	0.09	0
4	SO4	D	1209	-	4,4,4	0.35	0	6,6,6	0.06	0
4	SO4	C	301	-	4,4,4	0.27	0	6,6,6	0.05	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	RWN	B	1101	-	-	8/19/19/19	0/3/3/3
5	RWN	H	1101	-	-	8/19/19/19	0/3/3/3
5	RWN	E	1101	-	-	9/19/19/19	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1101	RWN	C2-N2	2.04	1.35	1.32
5	B	1101	RWN	C7-N5	-2.02	1.46	1.49

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1101	RWN	C5-C2-N2	-2.86	118.44	120.81
5	E	1101	RWN	C5-C2-N2	-2.81	118.47	120.81
5	H	1101	RWN	C5-C2-N2	-2.58	118.67	120.81
5	B	1101	RWN	C3-N3-C4	-2.45	112.49	115.28
5	E	1101	RWN	C3-N3-C4	-2.15	112.83	115.28
5	B	1101	RWN	C7-N5-C4	2.04	129.57	127.15
5	H	1101	RWN	C3-N3-C4	-2.00	113.00	115.28

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1101	RWN	N2-C3-N6-C10
5	B	1101	RWN	N3-C3-N6-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	B	1101	RWN	C8-C7-N5-C6
5	B	1101	RWN	C8-C7-N5-C4
5	E	1101	RWN	N2-C3-N6-C10
5	E	1101	RWN	N3-C3-N6-C10
5	E	1101	RWN	C8-C7-N5-C6
5	E	1101	RWN	C8-C7-N5-C4
5	H	1101	RWN	N2-C3-N6-C10
5	H	1101	RWN	N3-C3-N6-C10
5	H	1101	RWN	C9-C7-N5-C6
5	H	1101	RWN	C9-C7-N5-C4
5	E	1101	RWN	C5-C2-N1-C1
5	H	1101	RWN	N1-C1-C14-C15
5	B	1101	RWN	C5-C2-N1-C1
5	H	1101	RWN	C14-C15-C16-C21
5	B	1101	RWN	C14-C15-C16-C17
5	B	1101	RWN	C14-C15-C16-C21
5	H	1101	RWN	C14-C15-C16-C17
5	B	1101	RWN	C9-C7-N5-C6
5	H	1101	RWN	C8-C7-N5-C6
5	E	1101	RWN	C14-C15-C16-C17
5	E	1101	RWN	C14-C15-C16-C21
5	E	1101	RWN	N2-C2-N1-C1
5	E	1101	RWN	C9-C7-N5-C6

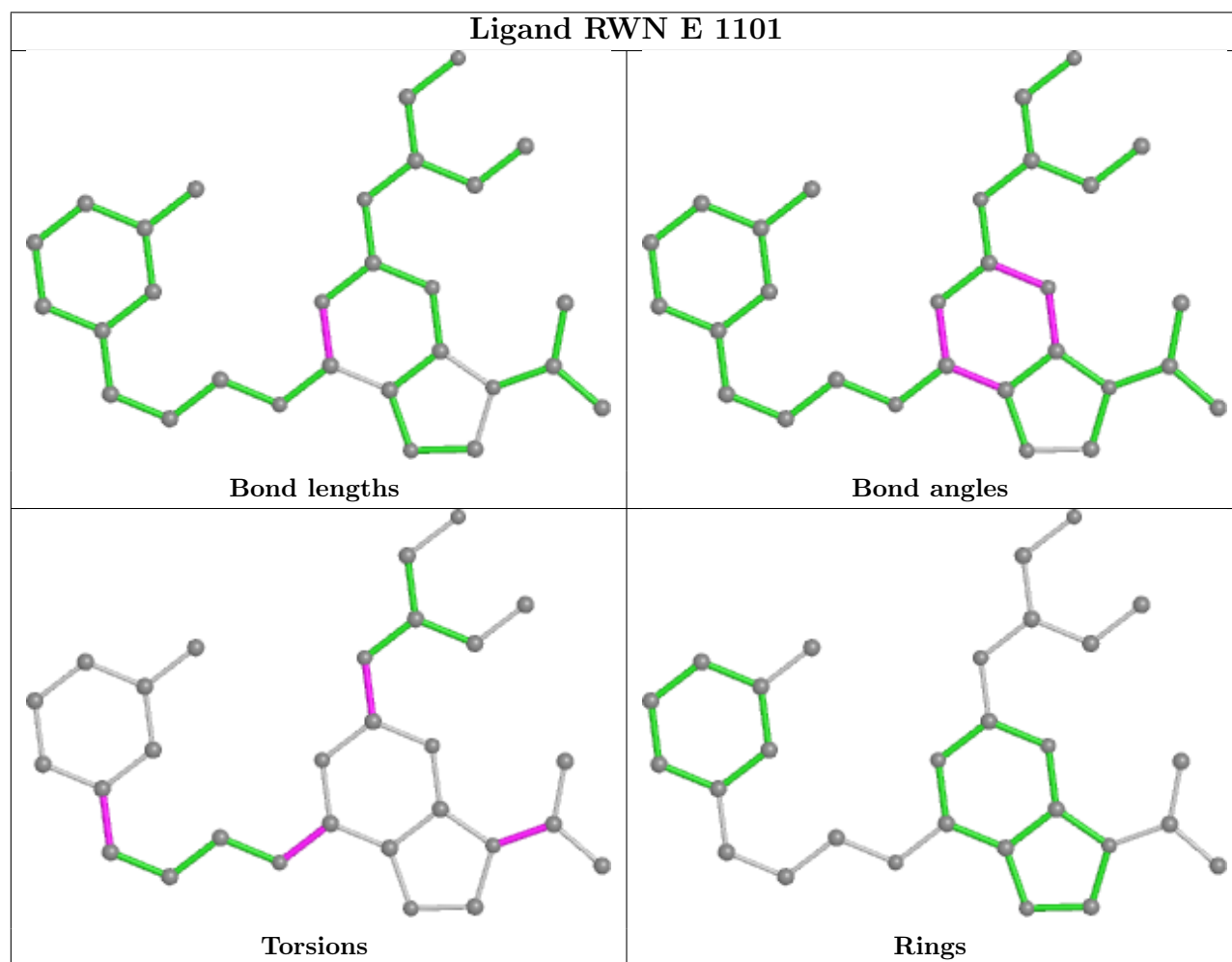
There are no ring outliers.

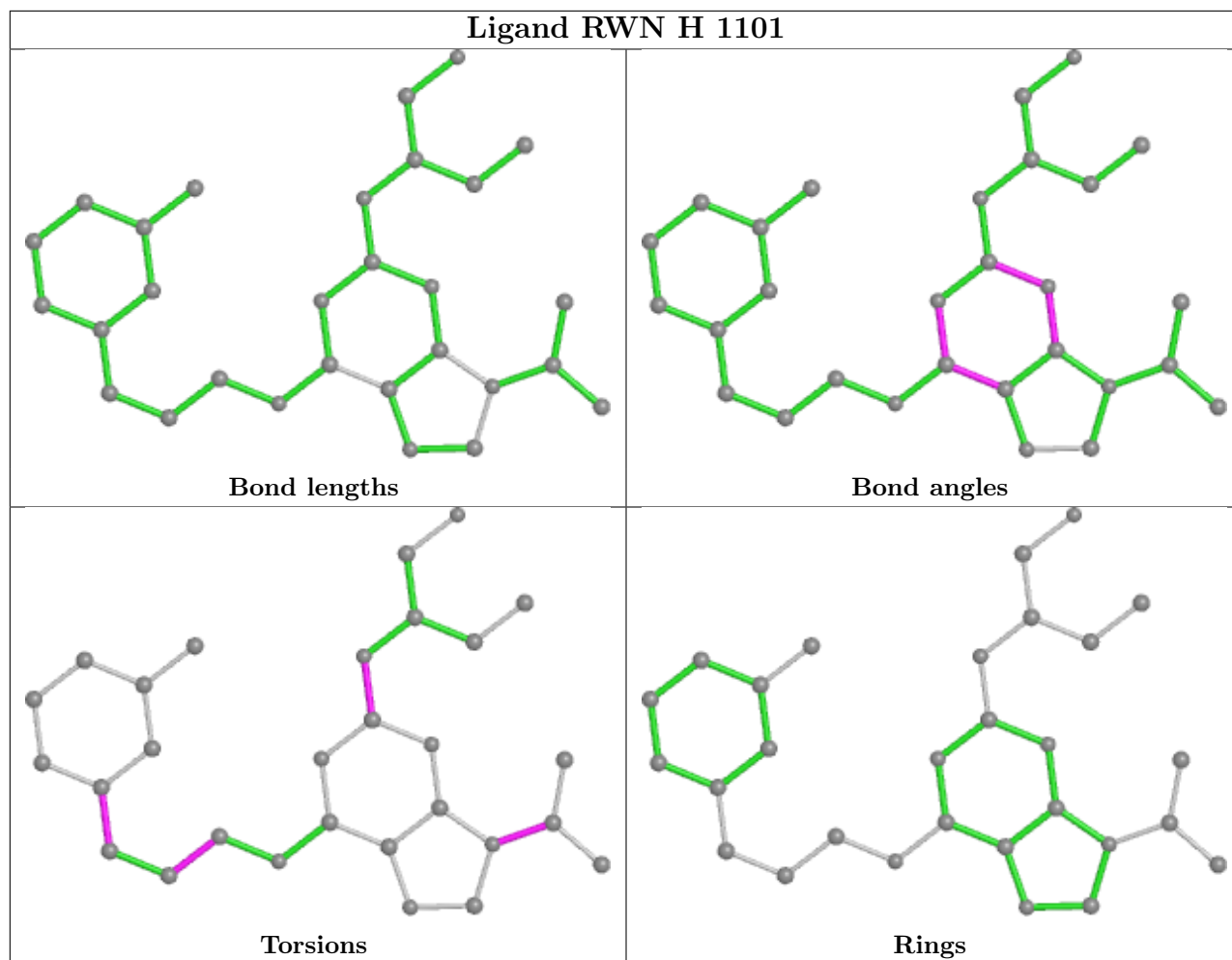
3 monomers are involved in 3 short contacts:

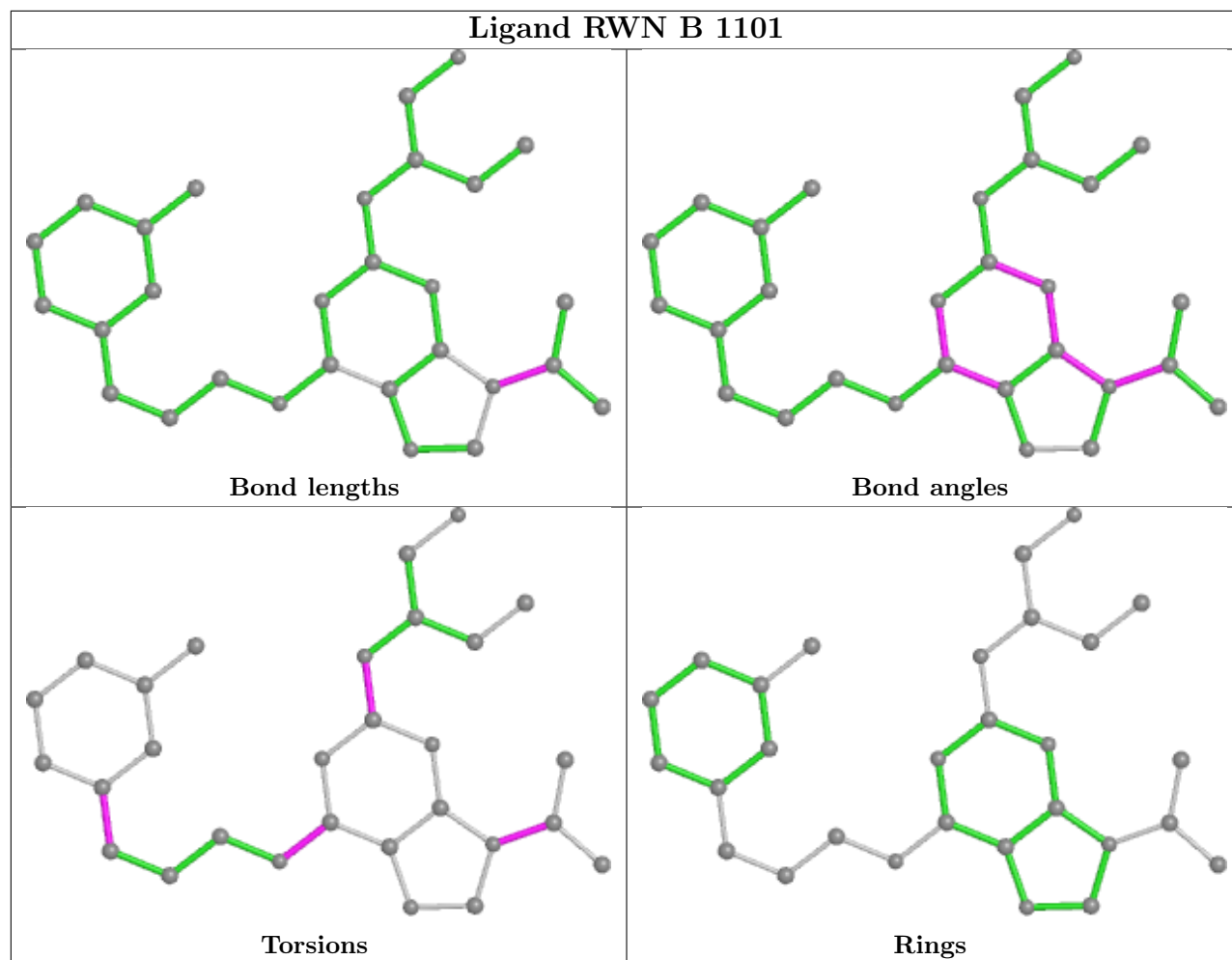
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1202	SO4	1	0
4	C	302	SO4	1	0
4	A	1203	SO4	1	0

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	826/840 (98%)	0.90	146 (17%) 1 2	110, 152, 220, 329	0
1	D	827/840 (98%)	0.83	129 (15%) 2 3	104, 142, 214, 337	0
1	G	826/840 (98%)	0.83	126 (15%) 2 3	110, 144, 225, 306	0
2	B	312/344 (90%)	1.16	67 (21%) 0 1	123, 155, 230, 281	0
2	E	312/344 (90%)	1.06	57 (18%) 1 2	113, 140, 208, 289	0
2	H	313/344 (90%)	0.98	49 (15%) 2 3	102, 130, 192, 272	0
3	C	248/271 (91%)	0.83	27 (10%) 5 8	115, 143, 192, 292	0
3	F	248/271 (91%)	1.04	21 (8%) 10 13	99, 118, 155, 301	0
3	I	248/271 (91%)	0.95	29 (11%) 4 7	113, 134, 176, 292	0
All	All	4160/4365 (95%)	0.92	651 (15%) 2 3	99, 142, 216, 337	0

All (651) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	262	LYS	23.5
2	B	886	SER	14.0
3	I	267	HIS	9.3
1	A	1116	ASP	9.3
3	I	266	PRO	9.2
3	F	267	HIS	9.0
3	F	264	GLN	8.9
1	A	1016	ASN	8.8
3	F	263	GLN	8.7
1	A	1115	ASP	8.7
3	C	267	HIS	8.2
3	C	266	PRO	8.0
3	I	264	GLN	7.9
2	B	884	TYR	7.7
2	B	896	VAL	7.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	F	266	PRO	7.2
2	B	887	GLU	7.1
1	A	1017	LEU	7.1
2	E	896	VAL	7.1
2	B	828	LEU	7.0
2	B	800	LEU	6.7
1	D	1114	TYR	6.6
3	I	265	MET	6.1
2	E	882	ARG	5.8
1	G	1116	ASP	5.4
1	A	65	GLU	5.3
1	D	140	PHE	5.2
2	E	884	TYR	5.1
1	G	131	ILE	5.1
3	C	264	GLN	5.1
1	A	367	LEU	5.0
1	D	1115	ASP	4.9
2	B	878	PHE	4.9
2	B	897	ILE	4.9
2	B	802	PHE	4.8
2	E	883	LEU	4.8
3	F	261	GLY	4.7
1	D	31	LEU	4.6
3	F	265	MET	4.6
2	E	720	GLY	4.5
1	A	79	ILE	4.5
2	B	883	LEU	4.5
1	D	89	LEU	4.5
1	G	289	GLU	4.5
2	H	830	HIS	4.5
1	A	57	MET	4.5
1	D	297	LEU	4.4
2	H	828	LEU	4.3
1	A	131	ILE	4.3
1	G	280	LEU	4.2
1	D	32	LEU	4.2
1	A	23	PHE	4.1
1	G	5	TYR	4.1
1	A	64	MET	4.1
1	G	133	LEU	4.1
1	G	49	LEU	4.1
1	G	1117	GLY	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	721	LYS	4.1
1	A	246	LEU	4.1
1	A	130	MET	4.0
2	E	886	SER	4.0
1	A	1097	PHE	4.0
1	A	32	LEU	4.0
2	H	798	ASP	4.0
2	E	878	PHE	4.0
1	A	123	ILE	3.9
2	B	860	ILE	3.9
2	E	831	PHE	3.9
1	A	61	ILE	3.9
1	D	133	LEU	3.9
1	A	63	VAL	3.8
1	D	5	TYR	3.8
1	A	39	LEU	3.8
1	G	1039	LEU	3.8
1	A	34	ALA	3.8
1	G	77	LEU	3.8
2	B	831	PHE	3.8
2	B	885	ASN	3.7
2	B	888	GLU	3.7
1	A	133	LEU	3.7
1	G	966	LEU	3.7
1	A	297	LEU	3.7
2	B	720	GLY	3.7
1	G	302	VAL	3.7
1	A	31	LEU	3.6
1	A	77	LEU	3.6
1	G	274	GLY	3.6
1	G	64	MET	3.6
1	G	1119	GLY	3.6
2	E	1025	LEU	3.6
1	A	33	ILE	3.6
1	A	232	ILE	3.6
1	G	303	GLU	3.6
1	G	143	ILE	3.5
2	E	875	LEU	3.5
1	A	122	GLY	3.5
2	B	829	VAL	3.5
1	D	33	ILE	3.5
1	G	791	LEU	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	801	ASP	3.5
1	A	195	VAL	3.5
2	B	801	ASP	3.5
1	G	1021	SER	3.5
1	D	39	LEU	3.5
2	H	831	PHE	3.5
2	E	888	GLU	3.4
2	E	955	PRO	3.4
1	G	273	LEU	3.4
1	D	1000	LEU	3.4
2	B	889	SER	3.4
1	A	89	LEU	3.4
1	D	131	ILE	3.4
1	A	1114	TYR	3.4
1	A	882	ALA	3.4
2	H	890	ARG	3.4
2	E	887	GLU	3.4
2	B	733	ILE	3.4
3	I	263	GLN	3.4
1	A	285	LEU	3.4
1	A	60	LYS	3.4
2	E	897	ILE	3.3
2	H	878	PHE	3.3
1	G	91	TYR	3.3
2	B	775	ILE	3.3
3	C	100	LEU	3.3
1	A	169	PHE	3.3
2	E	885	ASN	3.3
1	G	914	LEU	3.3
1	A	328	LEU	3.3
2	B	866	LEU	3.3
1	G	328	LEU	3.3
3	I	153	PHE	3.3
1	D	121	ILE	3.3
3	I	262	LYS	3.3
2	B	799	ALA	3.3
1	G	314	LEU	3.2
1	G	100	ILE	3.2
3	C	263	GLN	3.2
1	A	91	TYR	3.2
1	D	1097	PHE	3.2
1	A	49	LEU	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	875	LEU	3.2
1	D	1040	VAL	3.2
1	G	1108	VAL	3.2
1	A	272	LEU	3.2
1	D	100	ILE	3.2
1	A	140	PHE	3.2
2	B	756	LYS	3.2
2	H	955	PRO	3.2
1	G	79	ILE	3.2
1	A	777	PRO	3.2
2	B	781	LEU	3.2
1	G	323	PHE	3.1
1	D	792	LEU	3.1
1	A	930	VAL	3.1
2	H	829	VAL	3.1
1	D	367	LEU	3.1
2	H	826	SER	3.1
1	A	7	VAL	3.1
1	D	1004	VAL	3.1
1	A	135	LEU	3.1
1	A	317	LEU	3.1
1	A	874	VAL	3.1
1	G	1000	LEU	3.1
1	A	112	ILE	3.1
2	H	839	PHE	3.1
1	A	90	GLU	3.1
1	A	120	ILE	3.1
1	D	202	PHE	3.1
1	A	87	CYS	3.1
1	G	1050	LEU	3.1
2	H	865	ILE	3.1
1	G	717	LEU	3.1
2	H	896	VAL	3.0
2	H	929	LEU	3.0
2	B	738	TYR	3.0
1	G	974	LEU	3.0
1	A	179	CYS	3.0
1	D	1065	VAL	3.0
1	A	1029	LEU	3.0
1	G	1129	LEU	3.0
1	G	1088	PHE	3.0
1	A	933	LEU	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	283	LEU	3.0
3	I	100	LEU	3.0
2	E	781	LEU	3.0
1	D	1029	LEU	3.0
1	G	78	PHE	3.0
1	A	957	VAL	3.0
1	D	377	THR	3.0
1	D	23	PHE	3.0
2	B	986	PHE	3.0
1	D	64	MET	3.0
1	D	41	ILE	3.0
1	A	1039	LEU	3.0
3	I	155	LEU	3.0
1	A	100	ILE	2.9
1	G	1004	VAL	2.9
2	B	804	LYS	2.9
1	D	1018	GLY	2.9
1	A	237	ILE	2.9
1	G	124	ILE	2.9
1	G	58	TYR	2.9
1	A	15	VAL	2.9
1	D	1030	PHE	2.9
1	D	1136	LEU	2.9
1	G	775	THR	2.9
2	H	738	TYR	2.9
3	C	132	PHE	2.9
1	D	2	SER	2.9
1	A	229	ALA	2.9
1	D	220	ILE	2.9
1	A	24	THR	2.9
2	B	803	LYS	2.9
1	A	1008	CYS	2.9
1	G	327	ARG	2.9
2	E	829	VAL	2.9
1	A	368	GLU	2.9
1	G	132	GLY	2.9
1	G	317	LEU	2.9
2	H	767	PHE	2.9
1	G	139	LEU	2.9
1	A	799	PHE	2.9
1	A	1054	MET	2.9
1	A	143	ILE	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	167	VAL	2.8
2	E	792	ILE	2.8
1	A	5	TYR	2.8
1	A	387	LEU	2.8
1	A	1089	ILE	2.8
1	D	376	VAL	2.8
2	B	777	ILE	2.8
3	I	222	ILE	2.8
1	G	281	PHE	2.8
1	A	197	LEU	2.8
1	D	122	GLY	2.8
1	D	1017	LEU	2.8
3	I	147	LEU	2.8
1	G	923	VAL	2.8
2	B	839	PHE	2.8
1	D	143	ILE	2.8
1	D	390	ILE	2.8
1	A	881	LEU	2.8
1	G	170	LEU	2.8
1	G	376	VAL	2.8
2	B	865	ILE	2.8
1	G	792	LEU	2.8
2	E	755	LEU	2.8
2	E	828	LEU	2.8
1	D	88	ILE	2.8
1	G	1037	ILE	2.8
1	A	76	LEU	2.8
1	A	170	LEU	2.8
3	F	161	TYR	2.8
2	H	775	ILE	2.8
1	G	736	LEU	2.7
2	B	951	LEU	2.7
1	A	336	LEU	2.7
1	A	310	ILE	2.7
2	E	866	LEU	2.7
1	D	930	VAL	2.7
1	G	356	LEU	2.7
1	G	180	PHE	2.7
1	A	220	ILE	2.7
2	B	929	LEU	2.7
1	D	389	ILE	2.7
1	D	49	LEU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	758	VAL	2.7
1	A	959	ILE	2.7
1	G	830	ILE	2.7
1	G	799	PHE	2.7
1	G	957	VAL	2.7
1	D	61	ILE	2.7
1	A	300	LEU	2.7
1	A	922	LEU	2.7
1	D	1012	LEU	2.7
1	D	195	VAL	2.7
1	G	977	CYS	2.7
2	E	733	ILE	2.7
1	D	387	LEU	2.7
3	I	148	LEU	2.7
2	B	809	PHE	2.7
2	E	930	PHE	2.7
2	H	964	ILE	2.6
1	G	881	LEU	2.6
1	D	78	PHE	2.6
1	A	248	ILE	2.6
1	A	775	THR	2.6
1	D	135	LEU	2.6
1	G	67	PHE	2.6
1	A	6	VAL	2.6
1	G	219	VAL	2.6
1	G	816	LEU	2.6
1	A	180	PHE	2.6
1	A	19	VAL	2.6
1	G	123	ILE	2.6
1	D	775	THR	2.6
1	D	55	VAL	2.6
1	G	164	VAL	2.6
3	C	77	TYR	2.6
1	D	152	LEU	2.6
1	D	237	ILE	2.6
1	G	230	ILE	2.6
1	G	1043	LEU	2.6
1	G	1112	LEU	2.6
1	D	42	TYR	2.6
1	A	356	LEU	2.6
1	A	327	ARG	2.6
2	E	772	ILE	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	780	GLN	2.6
1	A	981	SER	2.6
1	G	295	VAL	2.6
1	G	66	LEU	2.6
1	G	390	ILE	2.6
2	B	836	ILE	2.6
3	C	164	LEU	2.6
1	D	169	PHE	2.6
3	I	132	PHE	2.6
1	D	99	ASP	2.6
3	C	144	GLU	2.6
3	C	194	CYS	2.6
1	D	142	VAL	2.6
1	D	1039	LEU	2.6
2	E	929	LEU	2.6
1	D	79	ILE	2.6
1	G	1054	MET	2.6
2	B	867	LEU	2.6
2	E	922	CYS	2.6
1	A	1088	PHE	2.5
2	B	767	PHE	2.5
1	G	333	LEU	2.5
1	G	41	ILE	2.5
1	G	61	ILE	2.5
1	D	735	VAL	2.5
1	G	39	LEU	2.5
1	A	1030	PHE	2.5
2	H	875	LEU	2.5
1	D	794	ILE	2.5
1	G	237	ILE	2.5
2	B	855	PHE	2.5
3	F	83	MET	2.5
3	F	153	PHE	2.5
2	E	881	ALA	2.5
1	D	300	LEU	2.5
2	E	778	LEU	2.5
2	B	936	PHE	2.5
3	C	188	PHE	2.5
2	B	755	LEU	2.5
1	A	78	PHE	2.5
2	E	802	PHE	2.5
1	G	130	MET	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	264	VAL	2.5
1	D	34	ALA	2.5
1	D	190	VAL	2.5
2	E	787	VAL	2.5
1	A	41	ILE	2.5
1	A	88	ILE	2.5
1	D	258	ILE	2.5
2	E	839	PHE	2.5
1	A	298	LYS	2.5
1	A	66	LEU	2.5
1	A	1000	LEU	2.5
2	B	798	ASP	2.5
2	B	997	LEU	2.5
1	D	157	ILE	2.5
1	G	921	ILE	2.5
2	B	774	GLU	2.5
2	B	772	ILE	2.5
2	E	775	ILE	2.5
1	A	365	VAL	2.5
2	B	1003	LEU	2.5
1	A	1007	PHE	2.5
1	A	921	ILE	2.5
3	C	151	ILE	2.5
1	A	334	VAL	2.5
2	E	823	LEU	2.5
1	A	55	VAL	2.4
1	A	1065	VAL	2.4
1	A	1117	GLY	2.4
2	H	926	LEU	2.4
1	G	282	MET	2.4
2	E	889	SER	2.4
1	D	317	LEU	2.4
1	G	997	LEU	2.4
1	G	1012	LEU	2.4
3	F	181	LEU	2.4
1	G	362	MET	2.4
2	E	752	LEU	2.4
1	A	364	VAL	2.4
1	A	791	LEU	2.4
1	D	974	LEU	2.4
1	G	1136	LEU	2.4
1	D	91	TYR	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	180	PHE	2.4
1	D	1007	PHE	2.4
1	D	858	LEU	2.4
2	B	820	LEU	2.4
2	H	820	LEU	2.4
1	A	226	PHE	2.4
1	A	871	TYR	2.4
1	G	179	CYS	2.4
3	I	167	TYR	2.4
1	D	178	ILE	2.4
3	C	222	ILE	2.4
1	A	159	LEU	2.4
1	A	350	MET	2.4
3	F	164	LEU	2.4
1	D	1088	PHE	2.4
1	A	982	ALA	2.4
1	D	19	VAL	2.4
3	C	171	LEU	2.4
1	D	130	MET	2.4
1	A	733	PHE	2.4
1	A	283	LEU	2.4
1	D	957	VAL	2.4
1	D	1129	LEU	2.4
1	G	1040	VAL	2.4
2	H	811	LEU	2.4
2	B	892	TYR	2.4
1	D	1112	LEU	2.4
2	B	926	LEU	2.4
2	E	847	LEU	2.4
1	G	88	ILE	2.4
2	E	743	LYS	2.4
1	G	375	LEU	2.4
3	I	64	LEU	2.4
2	H	802	PHE	2.4
1	G	232	ILE	2.4
1	G	922	LEU	2.4
3	F	242	VAL	2.3
1	G	140	PHE	2.3
1	G	954	MET	2.3
3	C	153	PHE	2.3
1	G	128	CYS	2.3
2	E	926	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	I	113	CYS	2.3
1	A	17	GLY	2.3
3	F	106	VAL	2.3
1	D	226	PHE	2.3
1	G	1030	PHE	2.3
2	B	918	ASP	2.3
2	E	813	PHE	2.3
2	E	803	LYS	2.3
1	D	272	LEU	2.3
3	I	254	ILE	2.3
1	A	965	PHE	2.3
1	G	1007	PHE	2.3
2	B	930	PHE	2.3
3	C	211	MET	2.3
1	G	31	LEU	2.3
1	G	305	LEU	2.3
1	G	387	LEU	2.3
1	D	155	PHE	2.3
1	G	1097	PHE	2.3
2	B	938	ALA	2.3
2	H	873	ILE	2.3
1	A	145	LEU	2.3
1	A	273	LEU	2.3
1	G	710	LEU	2.3
2	E	738	TYR	2.3
2	E	892	TYR	2.3
3	I	57	ILE	2.3
1	D	1028	VAL	2.3
2	E	844	MET	2.3
3	C	247	LEU	2.3
2	H	922	CYS	2.3
1	G	276	MET	2.3
1	A	792	LEU	2.3
1	D	285	LEU	2.3
1	D	1076	PHE	2.3
1	A	80	LEU	2.3
1	A	880	LEU	2.3
2	B	945	LEU	2.3
3	C	106	VAL	2.3
1	D	273	LEU	2.3
1	A	221	ALA	2.3
1	A	1028	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	164	VAL	2.3
2	E	814	GLU	2.3
2	H	894	ASN	2.3
1	A	752	LEU	2.3
1	D	710	LEU	2.3
1	G	135	LEU	2.3
1	G	733	PHE	2.3
1	G	57	MET	2.3
3	C	102	LEU	2.3
1	A	121	ILE	2.3
1	A	1040	VAL	2.3
2	H	1019	PHE	2.3
3	I	94	VAL	2.3
1	G	777	PRO	2.2
2	H	884	TYR	2.2
1	D	40	GLU	2.2
1	D	1051	LEU	2.2
2	B	823	LEU	2.2
3	C	155	LEU	2.2
2	B	864	ASN	2.2
1	A	359	ILE	2.2
1	G	226	PHE	2.2
2	B	917	ILE	2.2
3	I	75	ILE	2.2
1	A	708	GLN	2.2
1	D	9	ALA	2.2
3	C	161	TYR	2.2
1	A	314	LEU	2.2
1	D	733	PHE	2.2
2	H	718	ASP	2.2
3	C	167	TYR	2.2
1	A	1050	LEU	2.2
1	A	1136	LEU	2.2
1	D	328	LEU	2.2
1	G	1118	SER	2.2
2	H	867	LEU	2.2
2	H	897	ILE	2.2
3	I	149	GLN	2.2
3	I	84	PHE	2.2
1	A	721	PRO	2.2
1	D	761	LEU	2.2
2	B	862	CYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	908	LEU	2.2
3	F	155	LEU	2.2
1	G	1076	PHE	2.2
1	G	15	VAL	2.2
3	F	222	ILE	2.2
2	B	955	PRO	2.2
1	G	377	THR	2.2
1	D	327	ARG	2.2
1	D	1054	MET	2.2
1	G	359	ILE	2.2
2	H	919	VAL	2.2
2	H	1009	CYS	2.2
3	I	140	VAL	2.2
1	G	858	LEU	2.2
3	C	147	LEU	2.2
1	G	1133	VAL	2.2
1	D	965	PHE	2.2
2	H	930	PHE	2.2
2	E	836	ILE	2.2
1	D	893	TRP	2.2
2	H	720	GLY	2.2
1	A	16	ASN	2.2
1	A	156	ASN	2.2
1	D	219	VAL	2.2
1	D	360	VAL	2.2
1	D	830	ILE	2.2
1	G	740	ILE	2.2
1	D	139	LEU	2.2
1	G	965	PHE	2.2
1	G	1120	MET	2.2
3	F	57	ILE	2.2
1	A	304	LEU	2.1
1	A	926	LEU	2.1
1	D	881	LEU	2.1
2	B	811	LEU	2.1
2	E	856	LEU	2.1
3	F	147	LEU	2.1
3	I	199	LEU	2.1
2	B	826	SER	2.1
1	D	848	ILE	2.1
1	G	753	ARG	2.1
3	C	206	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1018	GLY	2.1
1	D	132	GLY	2.1
1	D	378	CYS	2.1
1	A	302	VAL	2.1
1	D	375	LEU	2.1
1	D	880	LEU	2.1
2	E	843	LEU	2.1
1	A	1100	ILE	2.1
1	D	1089	ILE	2.1
1	G	735	VAL	2.1
1	G	909	ILE	2.1
1	A	375	LEU	2.1
1	D	314	LEU	2.1
3	F	148	LEU	2.1
1	A	62	ALA	2.1
1	G	920	PHE	2.1
1	D	246	LEU	2.1
1	D	791	LEU	2.1
1	D	281	PHE	2.1
1	D	995	VAL	2.1
1	A	816	LEU	2.1
1	D	305	LEU	2.1
1	D	356	LEU	2.1
1	D	932	LEU	2.1
1	D	966	LEU	2.1
1	G	932	LEU	2.1
2	H	781	LEU	2.1
3	C	197	LEU	2.1
2	B	932	LYS	2.1
2	H	889	SER	2.1
1	A	82	ALA	2.1
2	E	913	TYR	2.1
1	D	165	ILE	2.1
2	B	729	ILE	2.1
2	E	935	ILE	2.1
1	D	280	LEU	2.1
1	A	216	ALA	2.1
1	D	58	TYR	2.1
2	H	986	PHE	2.1
3	C	78	PHE	2.1
1	G	324	VAL	2.1
1	G	1065	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	873	ILE	2.1
1	A	967	GLY	2.1
1	G	389	ILE	2.1
3	C	76	ILE	2.1
3	I	151	ILE	2.1
1	D	197	LEU	2.1
3	I	143	LEU	2.1
2	E	776	LYS	2.1
1	A	218	MET	2.1
1	A	67	PHE	2.1
3	F	238	PHE	2.1
1	D	712	ILE	2.1
1	G	933	LEU	2.1
2	E	997	LEU	2.1
2	H	951	LEU	2.1
1	D	708	GLN	2.1
2	H	936	PHE	2.1
1	A	141	LYS	2.1
1	D	302	VAL	2.1
2	E	907	LEU	2.1
1	D	82	ALA	2.0
2	B	815	TYR	2.0
1	D	392	ASN	2.0
1	D	120	ILE	2.0
1	D	253	ILE	2.0
1	D	123	ILE	2.0
2	H	847	LEU	2.0
2	H	864	ASN	2.0
1	A	851	PHE	2.0
3	I	79	HIS	2.0
2	H	758	VAL	2.0
1	G	899	LEU	2.0
2	B	843	LEU	2.0
2	H	778	LEU	2.0
2	H	792	ILE	2.0
2	H	906	LEU	2.0
2	E	722	ARG	2.0
3	F	211	MET	2.0
1	D	1037	ILE	2.0
2	H	733	ILE	2.0
1	A	771	PHE	2.0
2	E	986	PHE	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	844	MET	2.0
3	I	150	THR	2.0
2	H	881	ALA	2.0
3	I	164	LEU	2.0
1	G	23	PHE	2.0
2	E	899	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	TPO	H	893	11/12	0.80	0.20	157,170,204,204	5
2	TPO	B	893	11/12	0.83	0.12	193,231,277,282	6
2	TPO	E	893	11/12	0.86	0.20	195,216,260,260	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	F	301	5/5	0.54	0.49	154,157,163,211	0
4	SO4	E	1104	5/5	0.64	0.16	170,173,177,192	0
4	SO4	D	1209	5/5	0.68	0.16	169,170,171,209	0
4	SO4	H	1108	5/5	0.68	0.22	150,152,158,190	0
4	SO4	F	306	5/5	0.71	0.28	153,157,169,188	0
4	SO4	F	305	5/5	0.73	0.33	145,149,162,197	0
4	SO4	H	1106	5/5	0.75	0.17	172,172,174,204	0
4	SO4	H	1103	5/5	0.77	0.47	162,164,169,210	0
4	SO4	H	1110	5/5	0.77	0.78	152,159,166,199	0

Continued on next page...

Continued from previous page...

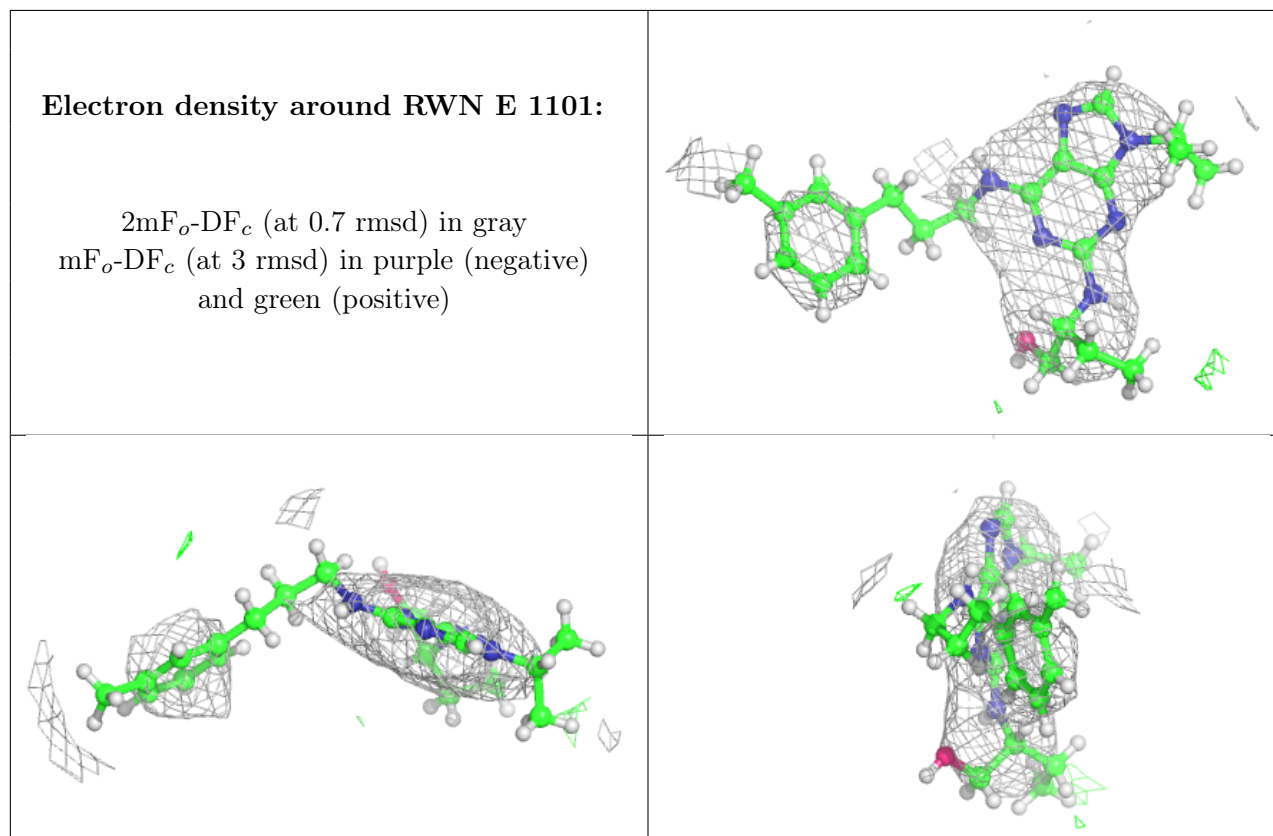
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	D	1212	5/5	0.78	0.18	158,162,163,176	0
4	SO4	G	1204	5/5	0.78	0.28	154,157,164,195	0
4	SO4	D	1201	5/5	0.78	0.19	153,154,159,185	0
4	SO4	H	1105	5/5	0.79	0.22	159,159,161,197	0
4	SO4	G	1205	5/5	0.79	0.29	151,152,160,207	0
4	SO4	D	1207	5/5	0.80	0.20	146,147,158,191	0
4	SO4	H	1109	5/5	0.81	0.25	137,138,153,182	0
4	SO4	G	1211	5/5	0.81	0.19	167,168,170,212	0
4	SO4	F	302	5/5	0.83	0.14	148,151,157,175	0
4	SO4	D	1213	5/5	0.83	0.20	176,182,188,200	0
4	SO4	D	1211	5/5	0.84	0.15	153,155,157,181	0
4	SO4	H	1107	5/5	0.84	0.27	151,158,159,185	0
4	SO4	H	1102	5/5	0.84	0.15	157,159,166,186	0
4	SO4	A	1203	5/5	0.84	0.33	139,145,151,199	0
4	SO4	G	1210	5/5	0.84	0.15	146,151,156,182	0
4	SO4	C	303	5/5	0.85	0.28	148,156,165,212	0
4	SO4	B	1102	5/5	0.85	0.12	173,175,177,203	0
4	SO4	E	1102	5/5	0.85	0.14	158,161,162,203	0
4	SO4	D	1202	5/5	0.85	0.17	137,142,146,172	0
4	SO4	D	1203	5/5	0.86	0.19	137,138,146,184	0
4	SO4	G	1212	5/5	0.86	0.20	168,168,171,214	0
4	SO4	I	303	5/5	0.86	0.14	165,167,170,203	0
4	SO4	D	1204	5/5	0.87	0.15	149,151,160,196	0
5	RWN	E	1101	29/29	0.87	0.65	126,151,169,174	32
4	SO4	G	1202	5/5	0.88	0.15	145,149,151,179	0
4	SO4	D	1210	5/5	0.88	0.13	166,167,168,198	0
4	SO4	G	1208	5/5	0.89	0.20	155,158,167,197	0
4	SO4	G	1207	5/5	0.89	0.18	124,128,130,147	0
4	SO4	D	1205	5/5	0.90	0.12	154,155,159,181	0
4	SO4	G	1209	5/5	0.90	0.14	153,155,157,171	0
4	SO4	A	1204	5/5	0.90	0.13	171,177,178,179	0
4	SO4	I	302	5/5	0.90	0.19	136,137,139,151	0
4	SO4	G	1206	5/5	0.90	0.12	169,171,178,187	0
4	SO4	G	1203	5/5	0.90	0.18	152,155,157,187	0
5	RWN	H	1101	29/29	0.90	0.68	124,149,176,176	32
4	SO4	D	1206	5/5	0.91	0.17	120,121,126,145	0
4	SO4	A	1202	5/5	0.91	0.21	134,137,140,167	0
4	SO4	A	1201	5/5	0.91	0.12	154,155,157,166	0
4	SO4	C	302	5/5	0.91	0.10	164,170,171,209	0
4	SO4	A	1205	5/5	0.92	0.17	127,130,132,144	0
4	SO4	F	304	5/5	0.92	0.19	152,154,157,188	0
4	SO4	E	1103	5/5	0.92	0.11	150,151,156,184	0

Continued on next page...

Continued from previous page...

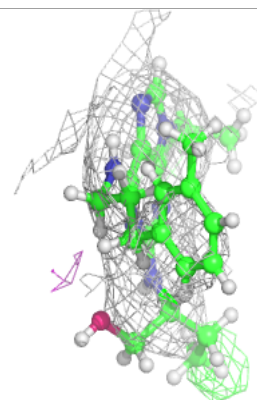
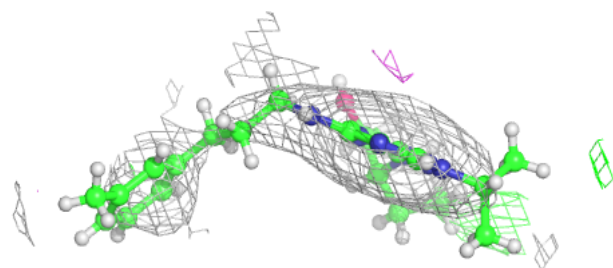
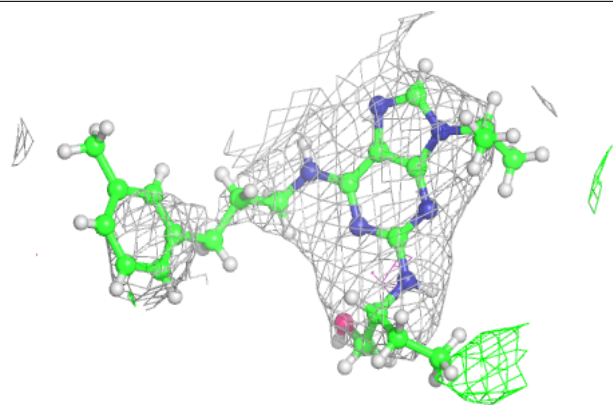
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SO4	A	1206	5/5	0.93	0.11	156,157,157,170	0
5	RWN	B	1101	29/29	0.93	0.83	139,167,196,210	32
4	SO4	G	1201	5/5	0.94	0.23	152,155,158,174	0
4	SO4	B	1103	5/5	0.94	0.07	171,171,172,210	0
4	SO4	D	1208	5/5	0.94	0.11	156,156,160,173	0
4	SO4	C	301	5/5	0.94	0.21	143,143,144,155	0
4	SO4	I	301	5/5	0.94	0.09	150,154,160,193	0
4	SO4	H	1104	5/5	0.95	0.14	141,144,150,177	0
4	SO4	F	303	5/5	0.97	0.23	116,117,121,130	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.

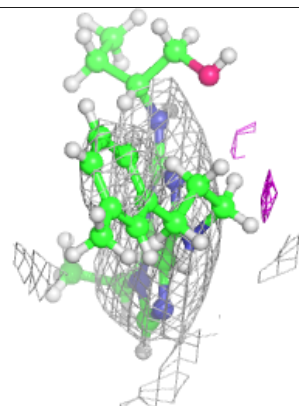
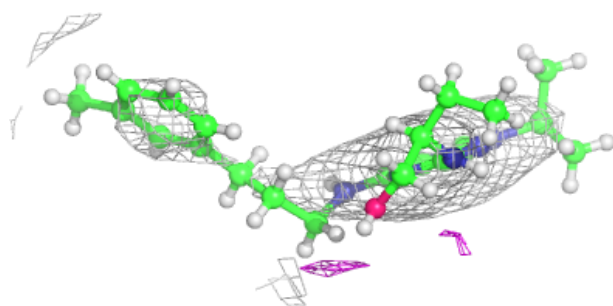
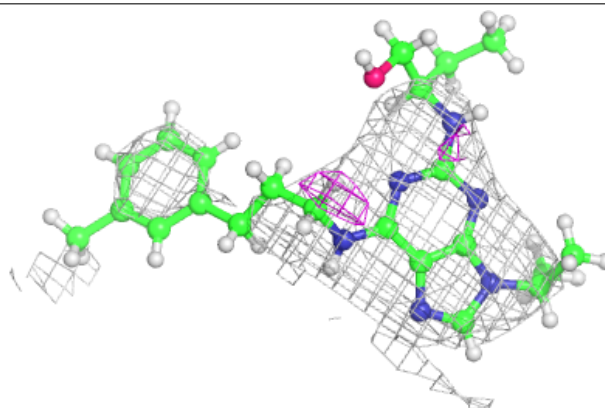


Electron density around RWN H 1101:

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

**Electron density around RWN B 1101:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.