



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 14, 2020 – 02:13 AM BST

PDB ID : 5ZCL  
Title : Crystal structure of OsPP2C50 I267L:OsPYL/RCAR3 with (+)-ABA  
Authors : Lee, S.; Han, S.  
Deposited on : 2018-02-19  
Resolution : 2.66 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.14.4.dev1  
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) : 2.14.4.dev1

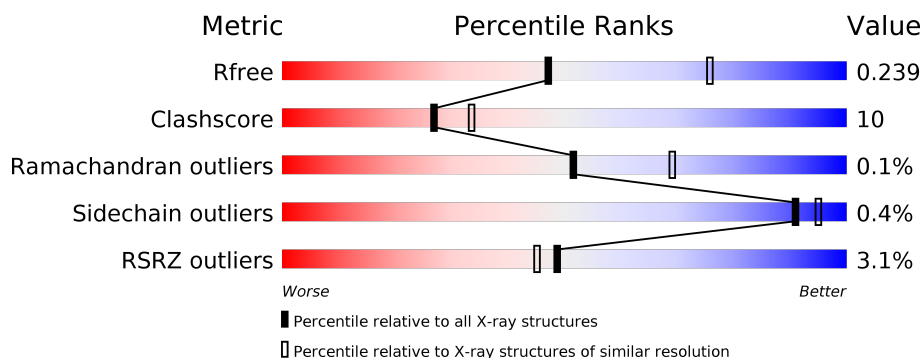
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.66 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	328	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>16%</div> <div>5%</div> </div> </div>
1	B	328	<div> <div>5%</div> <div> <div></div> <div>75%</div> <div>19%</div> <div>6%</div> </div> </div>
2	C	175	<div> <div>%</div> <div> <div></div> <div>71%</div> <div>18%</div> <div>10%</div> </div> </div>
2	D	175	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>19%</div> <div>7%</div> </div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7666 atoms, of which 276 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 Probable protein phosphatase 2C 50.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	312	Total	C	H	N	O	S	0	0	0
			2449	1471	80	439	445	14			
1	B	307	Total	C	H	N	O	S	0	0	0
			2423	1457	80	434	438	14			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	139	ALA	GLU	engineered mutation	UNP Q6L5H6
A	140	ALA	GLU	engineered mutation	UNP Q6L5H6
A	142	ALA	LYS	engineered mutation	UNP Q6L5H6
A	267	LEU	ILE	engineered mutation	UNP Q6L5H6
B	139	ALA	GLU	engineered mutation	UNP Q6L5H6
B	140	ALA	GLU	engineered mutation	UNP Q6L5H6
B	142	ALA	LYS	engineered mutation	UNP Q6L5H6
B	267	LEU	ILE	engineered mutation	UNP Q6L5H6

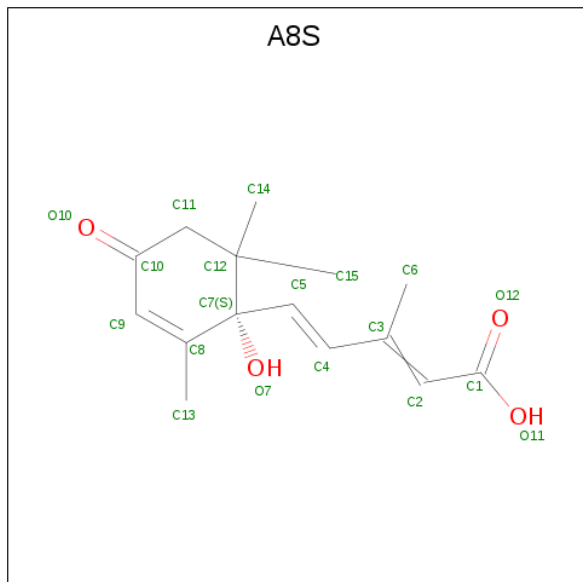
- Molecule 2 is a protein called ABA receptor RCAR3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	158	Total	C	H	N	O	S	0	0	0
			1314	790	58	229	232	5			
2	D	163	Total	C	H	N	O	S	0	0	0
			1366	825	58	240	238	5			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Mg	0	0
			2	2		
3	A	2	Total	Mg	0	0
			2	2		

- Molecule 4 is (2Z,4E)-5-[(1S)-1-hydroxy-2,6,6-trimethyl-4-oxocyclohex-2-en-1-yl]-3-methylpenta-2,4-dienoic acid (three-letter code: A8S) (formula: C<sub>15</sub>H<sub>20</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			19	15	4		
4	D	1	Total	C	O	0	0
			19	15	4		

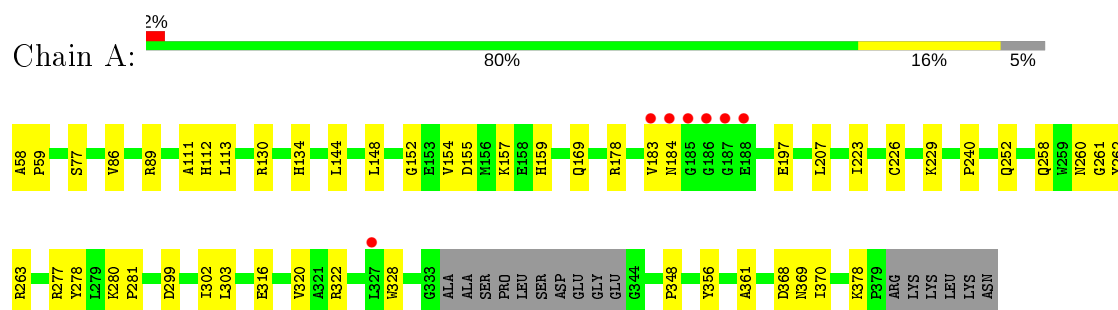
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	32	Total	O	0	0
			32	32		
5	C	18	Total	O	0	0
			18	18		
5	B	15	Total	O	0	0
			15	15		
5	D	7	Total	O	0	0
			7	7		

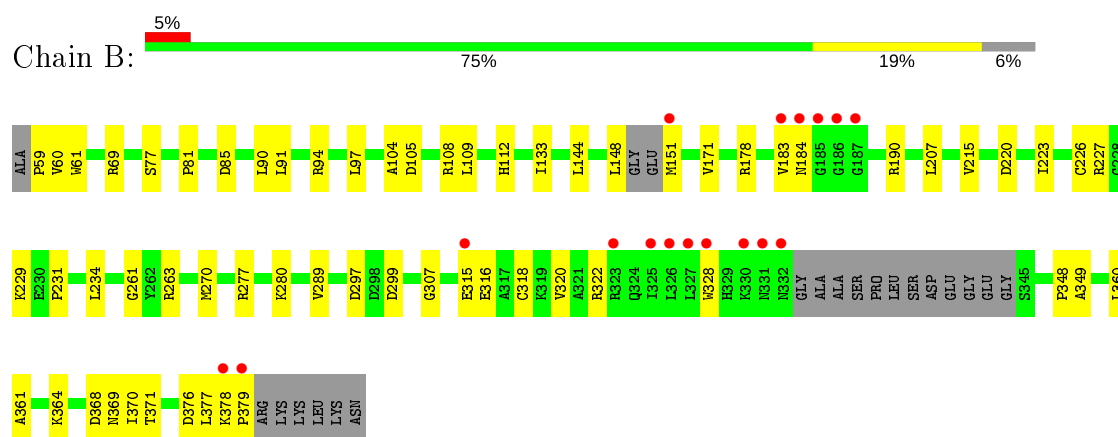
### 3 Residue-property plots [i](#)

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.

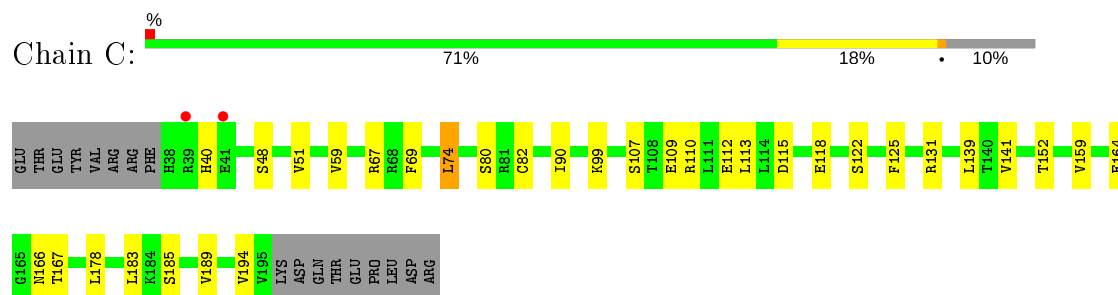
- Molecule 1: Probable protein phosphatase 2C 50



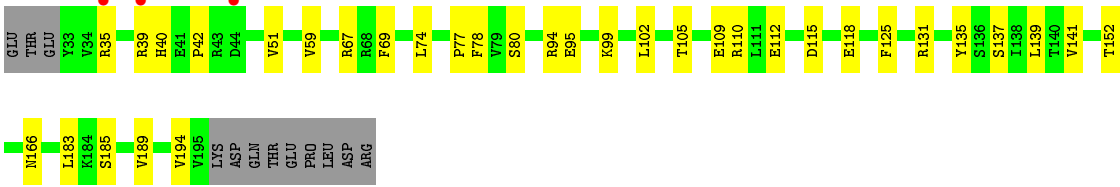
- Molecule 1: Probable protein phosphatase 2C 50



- Molecule 2: ABA receptor RCAR3



- Molecule 2: ABA receptor RCAR3



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.10Å 130.26Å 80.25Å 90.00° 115.99° 90.00°	Depositor
Resolution (Å)	38.15 – 2.66 38.15 – 2.66	Depositor EDS
% Data completeness (in resolution range)	99.3 (38.15-2.66) 99.3 (38.15-2.66)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.53 (at 2.65Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, $R_{free}$	0.195 , 0.240 0.195 , 0.239	Depositor DCC
$R_{free}$ test set	2003 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.1	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 47.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7666	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: A8S, MG

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	0/2407	0.52	0/3258
1	B	0.31	0/2380	0.50	0/3220
2	C	0.32	0/1281	0.50	0/1734
2	D	0.32	0/1335	0.50	0/1806
All	All	0.32	0/7403	0.51	0/10018

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	2369	80	2372	43	0
1	B	2343	80	2354	59	0
2	C	1256	58	1265	25	0
2	D	1308	58	1318	24	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	C	19	0	19	2	0
4	D	19	0	19	1	0
5	A	32	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	15	0	0	0	0
5	C	18	0	0	1	0
5	D	7	0	0	1	0
All	All	7390	276	7347	150	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (150) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:CYS:HB3	1:B:322:ARG:HH12	1.26	0.99
1:B:226:CYS:SG	1:B:322:ARG:NH1	2.37	0.97
1:B:227:ARG:HG3	1:B:297:ASP:HB3	1.47	0.95
1:A:154:VAL:HG21	1:A:159:HIS:CE1	2.05	0.92
1:B:178:ARG:HH22	1:B:280:LYS:HD2	1.47	0.79
1:B:318:CYS:HB3	1:B:322:ARG:NH1	1.97	0.78
2:C:167:THR:HB	2:D:95:GLU:HG2	1.65	0.77
1:A:144:LEU:O	1:A:148:LEU:HD23	1.86	0.75
1:B:94:ARG:NH2	1:B:151:MET:O	2.20	0.74
1:A:252:GLN:HG2	1:A:281:PRO:HG2	1.70	0.74
2:D:131:ARG:NH2	2:D:166:ASN:OD1	2.23	0.71
1:A:229:LYS:HA	1:A:322:ARG:CZ	2.23	0.69
1:B:85:ASP:HB3	1:B:108:ARG:HB3	1.75	0.69
1:A:178:ARG:HH22	1:A:280:LYS:CE	2.06	0.68
1:B:229:LYS:HG2	1:B:322:ARG:HD2	1.78	0.66
1:B:60:VAL:HG23	1:B:376:ASP:HB3	1.77	0.65
1:A:260:ASN:OD1	1:B:69:ARG:HD3	1.96	0.65
1:A:316:GLU:OE1	5:A:501:HOH:O	2.14	0.65
1:B:328:TRP:CZ2	1:B:348:PRO:HB2	2.32	0.65
1:B:59:PRO:HG3	1:B:112:HIS:CE1	2.32	0.64
1:B:316:GLU:O	1:B:320:VAL:HG23	1.98	0.63
1:B:328:TRP:CE3	1:B:349:ALA:HB2	2.33	0.63
2:D:51:VAL:HG23	2:D:183:LEU:HD12	1.80	0.62
1:B:361:ALA:HB3	1:B:370:ILE:HD13	1.82	0.62
1:A:183:VAL:HG12	1:A:184:ASN:H	1.66	0.61
1:B:60:VAL:CG2	1:B:376:ASP:HB3	2.30	0.61
2:D:94:ARG:NE	2:D:109:GLU:OE1	2.31	0.60
2:D:185:SER:O	2:D:189:VAL:HG12	2.00	0.60
1:B:361:ALA:CB	1:B:370:ILE:HD13	2.32	0.59
2:D:115:ASP:HB3	2:D:118:GLU:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:59:VAL:HG13	2:D:141:VAL:CG1	2.31	0.59
2:C:110:ARG:HD2	2:C:112:GLU:OE2	2.02	0.59
1:B:277:ARG:HA	1:B:280:LYS:HG3	1.86	0.58
1:A:89:ARG:NH2	1:A:152:GLY:O	2.26	0.58
1:B:378:LYS:N	1:B:379:PRO:HD3	2.18	0.58
1:A:86:VAL:HG23	1:A:111:ALA:HB2	1.86	0.57
1:B:178:ARG:HH12	1:B:280:LYS:HE3	1.69	0.57
1:B:183:VAL:HG12	1:B:184:ASN:H	1.70	0.57
1:B:226:CYS:HB2	1:B:318:CYS:SG	2.44	0.57
4:D:301:A8S:O12	4:D:301:A8S:H4	2.04	0.56
1:A:169:GLN:HB2	5:A:505:HOH:O	2.06	0.56
2:C:131:ARG:NH2	2:C:166:ASN:OD1	2.37	0.56
1:A:178:ARG:HH12	1:A:280:LYS:HE3	1.69	0.56
2:C:109:GLU:HG2	2:C:125:PHE:CD1	2.41	0.56
1:A:113:LEU:HD23	1:A:134:HIS:CB	2.37	0.55
2:C:141:VAL:HG13	2:C:152:THR:CG2	2.36	0.55
1:B:183:VAL:HG21	1:B:190:ARG:HD2	1.87	0.55
2:D:59:VAL:HG13	2:D:141:VAL:HG12	1.87	0.55
2:C:115:ASP:HB3	2:C:118:GLU:O	2.07	0.55
2:D:67:ARG:O	2:D:69:PHE:N	2.39	0.55
2:C:82:CYS:HB3	5:C:403:HOH:O	2.07	0.55
1:A:178:ARG:HH22	1:A:280:LYS:HD2	1.72	0.54
2:C:67:ARG:O	2:C:69:PHE:N	2.40	0.54
1:A:178:ARG:HH22	1:A:280:LYS:CD	2.21	0.53
2:D:80:SER:HB3	2:D:99:LYS:HG2	1.90	0.53
1:A:59:PRO:HB3	1:A:112:HIS:CD2	2.44	0.53
2:C:164:GLU:HG3	2:D:105:THR:HG21	1.91	0.52
4:C:301:A8S:H4	4:C:301:A8S:O12	2.09	0.52
1:A:197:GLU:HG3	1:A:278:TYR:HB3	1.92	0.52
1:B:261:GLY:O	1:B:263:ARG:HG3	2.10	0.51
2:C:59:VAL:HG13	2:C:141:VAL:HG12	1.92	0.51
2:C:48:SER:HB2	2:C:159:VAL:HG12	1.93	0.51
1:A:113:LEU:HD23	1:A:134:HIS:HB3	1.93	0.51
1:B:307:GLY:O	1:B:370:ILE:HG12	2.10	0.51
1:B:360:LEU:O	1:B:364:LYS:HG3	2.10	0.51
2:D:125:PHE:HB2	2:D:135:TYR:HB3	1.92	0.51
1:B:97:LEU:HD12	1:B:104:ALA:HB2	1.94	0.50
1:B:60:VAL:HG23	1:B:60:VAL:O	2.12	0.50
1:A:178:ARG:HH22	1:A:280:LYS:HE3	1.76	0.50
1:B:91:LEU:CD1	1:B:109:LEU:HD23	2.42	0.49
2:C:185:SER:O	2:C:189:VAL:HG12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:113:LEU:HB3	2:C:122:SER:HB3	1.93	0.49
1:A:157:LYS:NZ	5:A:503:HOH:O	2.44	0.49
1:B:377:LEU:C	1:B:379:PRO:HD3	2.33	0.49
2:C:90:ILE:HD12	2:C:112:GLU:O	2.13	0.49
1:B:144:LEU:O	1:B:148:LEU:HD23	2.13	0.49
1:B:307:GLY:HA3	1:B:369:ASN:O	2.12	0.48
1:A:316:GLU:O	1:A:320:VAL:HG23	2.13	0.48
1:A:183:VAL:HG12	1:A:184:ASN:N	2.29	0.48
1:B:299:ASP:OD1	1:B:378:LYS:HD2	2.14	0.48
2:C:40:HIS:HB3	2:C:159:VAL:HG11	1.95	0.48
1:B:183:VAL:HG12	1:B:184:ASN:N	2.28	0.48
2:D:51:VAL:HG23	2:D:183:LEU:CD1	2.43	0.48
1:A:178:ARG:NH2	1:A:280:LYS:HD2	2.29	0.48
2:C:194:VAL:HG12	2:C:194:VAL:O	2.14	0.48
1:A:154:VAL:HG22	1:A:155:ASP:N	2.29	0.48
1:A:77:SER:O	1:A:130:ARG:HG3	2.14	0.48
1:B:229:LYS:HA	1:B:322:ARG:NE	2.29	0.48
2:D:194:VAL:O	2:D:194:VAL:HG12	2.13	0.47
1:B:90:LEU:HD11	1:B:144:LEU:HD23	1.96	0.47
2:D:139:LEU:C	2:D:139:LEU:HD23	2.35	0.47
1:A:86:VAL:CG2	1:A:111:ALA:HB2	2.45	0.47
1:A:252:GLN:CG	1:A:281:PRO:HG2	2.42	0.47
1:A:89:ARG:HD3	1:A:148:LEU:HB3	1.97	0.47
1:B:231:PRO:HB3	1:B:318:CYS:SG	2.55	0.47
1:A:361:ALA:HB3	1:A:370:ILE:HD13	1.97	0.46
1:B:207:LEU:HD23	1:B:207:LEU:C	2.35	0.46
1:A:58:ALA:HB3	1:A:59:PRO:HD3	1.98	0.46
2:D:35:ARG:NH1	2:D:39:ARG:HH22	2.13	0.46
2:C:139:LEU:C	2:C:139:LEU:HD23	2.36	0.46
1:A:368:ASP:OD1	1:A:369:ASN:N	2.48	0.46
2:C:51:VAL:HG23	2:C:183:LEU:HD12	1.97	0.46
1:B:133:ILE:HG12	1:B:171:VAL:HG21	1.97	0.46
1:A:303:LEU:HD12	1:A:303:LEU:N	2.31	0.46
1:B:226:CYS:SG	1:B:299:ASP:HB2	2.56	0.46
2:C:178:LEU:HD13	4:C:301:A8S:H13A	1.96	0.46
1:B:227:ARG:HG3	1:B:297:ASP:CB	2.33	0.46
1:A:320:VAL:CG1	1:A:356:TYR:CD2	3.00	0.45
1:B:97:LEU:CD1	1:B:104:ALA:HB2	2.47	0.45
2:D:141:VAL:HG13	2:D:152:THR:CG2	2.47	0.45
2:D:59:VAL:HG13	2:D:141:VAL:HG11	1.98	0.45
1:A:226:CYS:O	1:A:299:ASP:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ARG:HA	1:A:280:LYS:HG3	1.99	0.45
1:B:226:CYS:SG	1:B:322:ARG:HD3	2.57	0.45
1:A:328:TRP:CZ2	1:A:348:PRO:HB2	2.52	0.44
1:B:94:ARG:NH1	1:B:105:ASP:OD2	2.50	0.44
1:B:229:LYS:HA	1:B:322:ARG:CD	2.47	0.44
2:C:80:SER:HB3	2:C:99:LYS:HG2	1.99	0.44
1:B:229:LYS:HG2	1:B:322:ARG:CD	2.47	0.44
1:B:215:VAL:O	1:B:289:VAL:HA	2.18	0.44
1:B:223:ILE:HG23	1:B:234:LEU:HB2	1.99	0.44
1:A:223:ILE:HA	1:A:302:ILE:O	2.18	0.44
2:C:74:LEU:HD12	2:C:74:LEU:HA	1.85	0.43
1:A:240:PRO:HG2	1:A:262:TYR:O	2.18	0.43
2:D:78:PHE:CD1	2:D:102:LEU:HD11	2.53	0.43
1:B:229:LYS:HA	1:B:322:ARG:HD3	2.01	0.43
1:A:144:LEU:HD11	1:A:159:HIS:HD2	1.84	0.43
1:B:307:GLY:C	1:B:370:ILE:HG12	2.39	0.43
1:B:368:ASP:OD1	1:B:369:ASN:N	2.52	0.43
1:B:229:LYS:HA	1:B:322:ARG:CZ	2.49	0.43
1:A:59:PRO:HG3	1:A:112:HIS:CE1	2.54	0.42
2:C:59:VAL:HG13	2:C:141:VAL:CG1	2.48	0.42
2:D:40:HIS:O	2:D:42:PRO:HD3	2.19	0.42
1:B:77:SER:HB3	1:B:371:THR:HG21	2.02	0.42
2:D:110:ARG:HD2	2:D:112:GLU:OE2	2.20	0.42
1:B:227:ARG:CG	1:B:297:ASP:HB3	2.35	0.42
2:D:135:TYR:CE1	2:D:137:SER:HB3	2.55	0.41
1:B:231:PRO:HG3	1:B:315:GLU:HA	2.03	0.41
2:C:51:VAL:HG23	2:C:183:LEU:CD1	2.50	0.41
1:B:220:ASP:OD2	1:B:270:MET:HE2	2.20	0.41
2:C:141:VAL:HG13	2:C:152:THR:HG23	2.02	0.41
1:A:261:GLY:O	1:A:263:ARG:HG3	2.21	0.41
1:A:229:LYS:HA	1:A:322:ARG:NH1	2.34	0.41
1:B:144:LEU:O	1:B:148:LEU:CD2	2.68	0.41
2:C:107:SER:OG	2:C:109:GLU:OE2	2.38	0.41
1:A:207:LEU:HD23	1:A:207:LEU:C	2.40	0.41
2:D:77:PRO:HG3	2:D:185:SER:HB2	2.04	0.40
1:B:270:MET:HE2	1:B:270:MET:HB3	2.01	0.40
2:D:78:PHE:HB2	5:D:406:HOH:O	2.20	0.40
1:B:61:TRP:CH2	1:B:81:PRO:HG3	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	308/328 (94%)	297 (96%)	10 (3%)	1 (0%)	41	56
1	B	301/328 (92%)	294 (98%)	7 (2%)	0	100	100
2	C	156/175 (89%)	153 (98%)	3 (2%)	0	100	100
2	D	161/175 (92%)	158 (98%)	3 (2%)	0	100	100
All	All	926/1006 (92%)	902 (97%)	23 (2%)	1 (0%)	51	69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	378	LYS

### 5.3.2 Protein sidechains

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	251/264 (95%)	250 (100%)	1 (0%)	91	95
1	B	250/264 (95%)	250 (100%)	0	100	100
2	C	144/161 (89%)	143 (99%)	1 (1%)	84	91
2	D	149/161 (92%)	148 (99%)	1 (1%)	84	91
All	All	794/850 (93%)	791 (100%)	3 (0%)	91	95

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	258	GLN
2	C	74	LEU
2	D	74	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	159	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](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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	A8S	D	301	-	14,19,19	0.54	0	13,29,29	1.33	3 (23%)
4	A8S	C	301	-	14,19,19	0.56	0	13,29,29	1.26	3 (23%)

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
4	A8S	D	301	-	-	0/8/34/34	0/1/1/1
4	A8S	C	301	-	-	0/8/34/34	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	301	A8S	C6-C3-C2	-2.57	119.27	124.64
4	D	301	A8S	C6-C3-C2	-2.45	119.50	124.64
4	D	301	A8S	C8-C9-C10	-2.39	121.38	123.82
4	C	301	A8S	O7-C7-C12	-2.24	104.99	109.92
4	C	301	A8S	C8-C9-C10	-2.14	121.64	123.82
4	D	301	A8S	O7-C7-C12	-2.04	105.43	109.92

There are no chirality outliers.

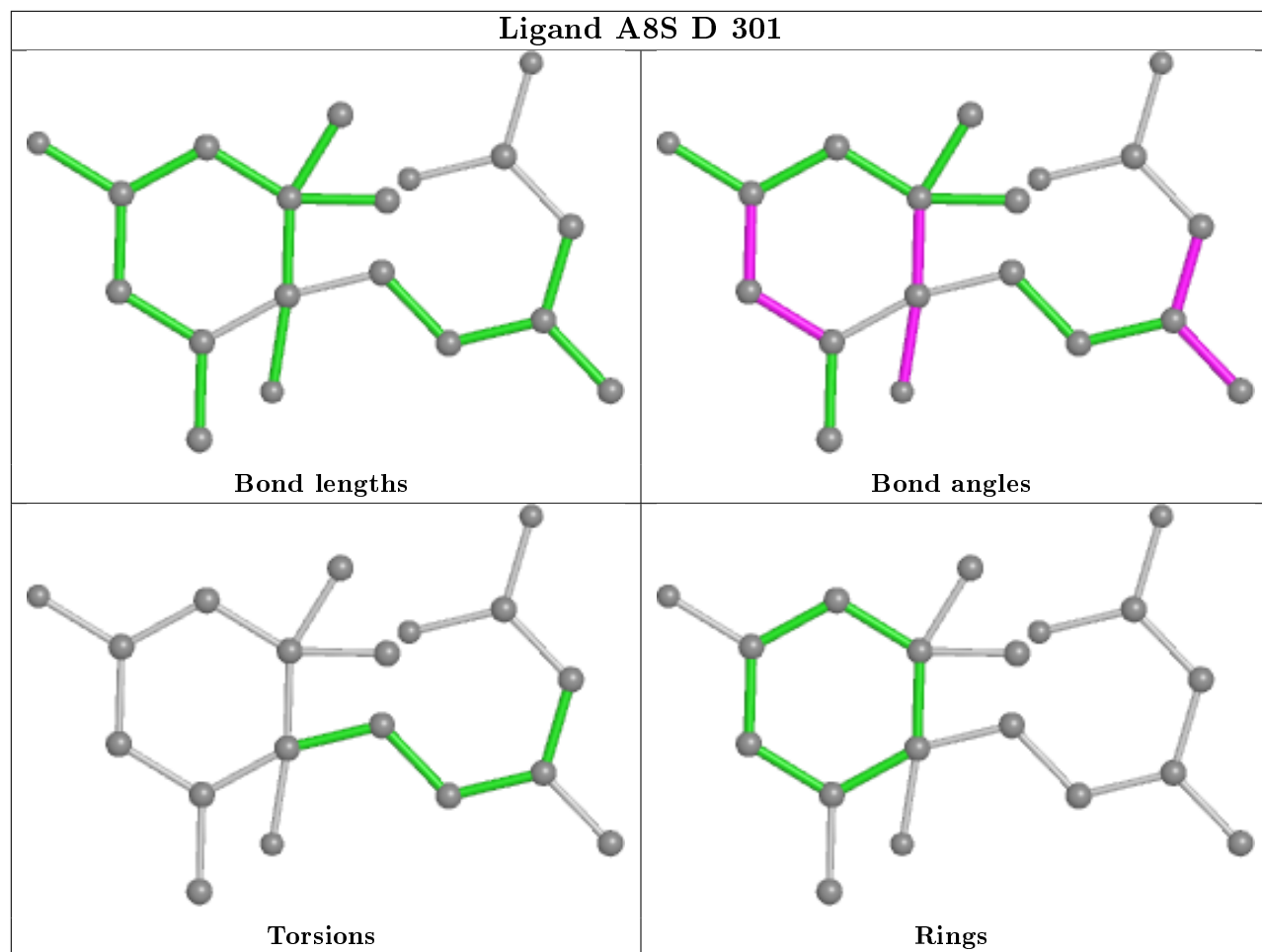
There are no torsion outliers.

There are no ring outliers.

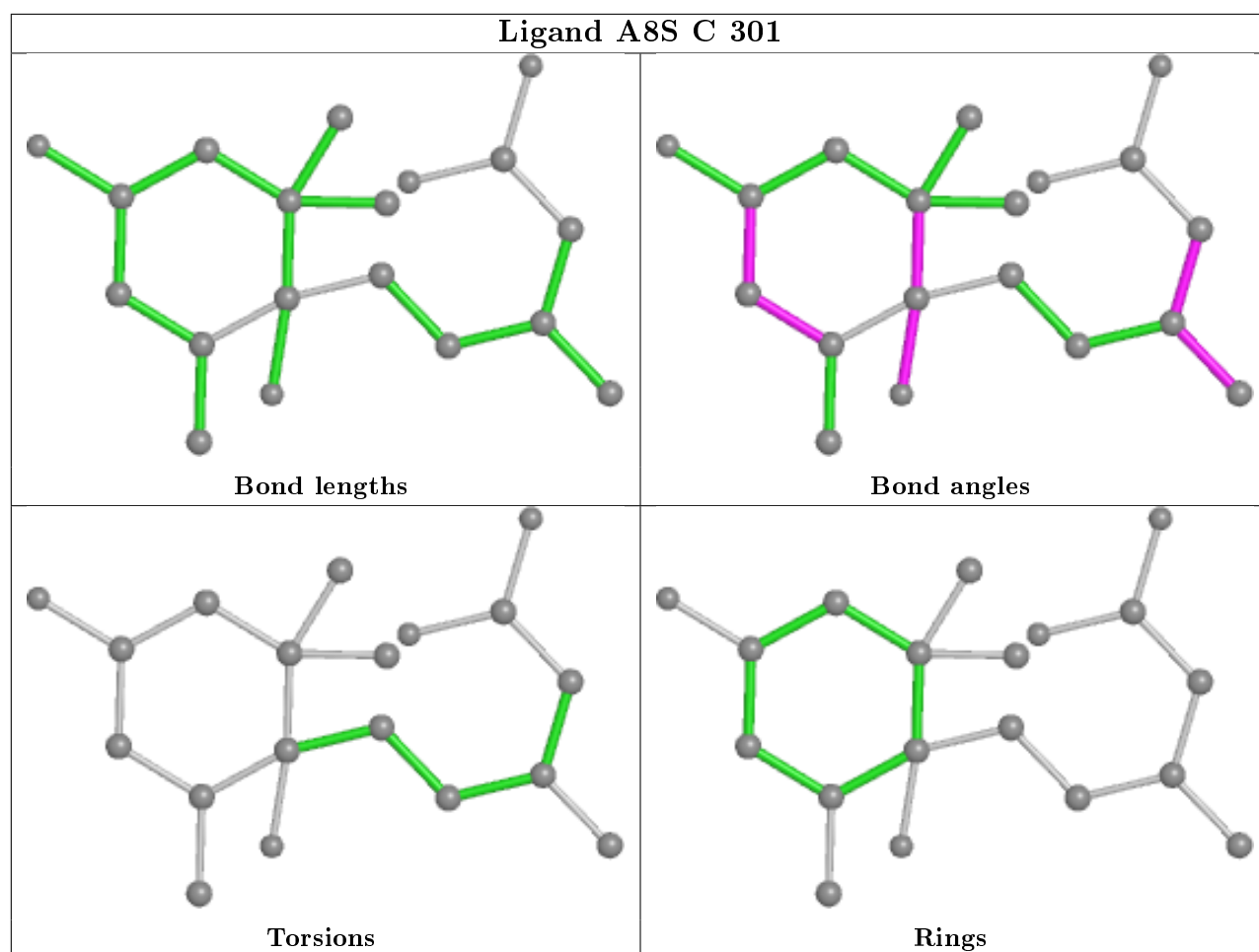
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	301	A8S	1	0
4	C	301	A8S	2	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	312/328 (95%)	-0.15	7 (2%) 62 57	28, 40, 73, 117	0
1	B	307/328 (93%)	0.00	17 (5%) 25 21	33, 50, 94, 118	0
2	C	158/175 (90%)	-0.36	2 (1%) 77 75	30, 40, 67, 105	0
2	D	163/175 (93%)	-0.11	3 (1%) 68 65	34, 49, 76, 102	0
All	All	940/1006 (93%)	-0.13	29 (3%) 49 45	28, 45, 83, 118	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	185	GLY	6.6
1	A	184	ASN	4.6
1	B	151	MET	4.5
1	B	330	LYS	3.8
1	A	187	GLY	3.8
1	B	331	ASN	3.8
1	B	328	TRP	3.6
1	B	184	ASN	3.5
1	B	327	LEU	3.5
2	D	44	ASP	3.4
1	A	186	GLY	3.3
1	B	315	GLU	3.2
1	A	188	GLU	3.0
1	B	185	GLY	2.9
1	B	378	LYS	2.8
1	B	379	PRO	2.7
1	B	332	ASN	2.6
2	D	35	ARG	2.5
1	A	183	VAL	2.5
1	B	323	ARG	2.5
2	C	39	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	186	GLY	2.4
1	B	183	VAL	2.4
1	A	327	LEU	2.3
1	B	187	GLY	2.3
2	D	39	ARG	2.2
1	B	326	LEU	2.2
1	B	325	ILE	2.2
2	C	41	GLU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

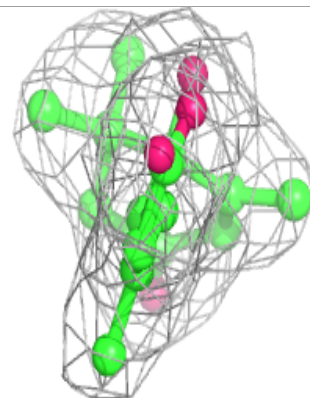
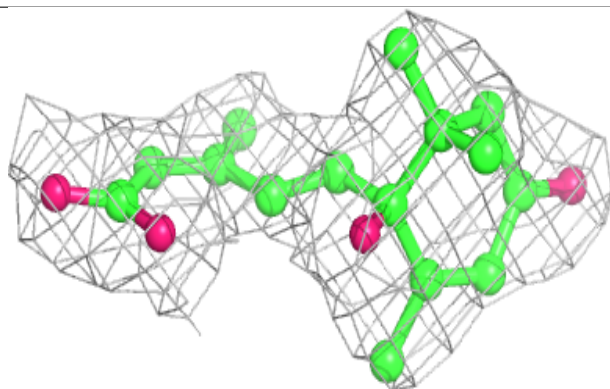
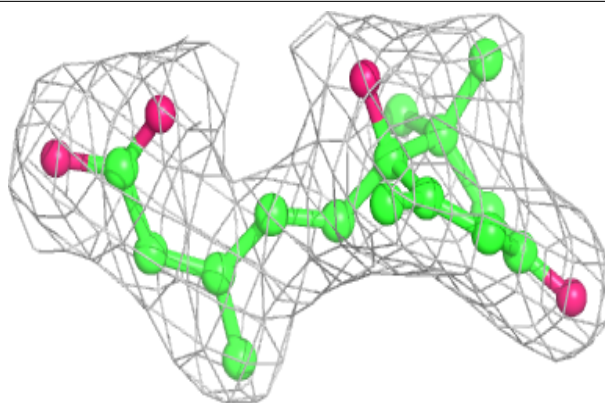
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	MG	A	401	1/1	0.82	0.17	44,44,44,44	0
3	MG	A	402	1/1	0.91	0.36	39,39,39,39	0
4	A8S	C	301	19/19	0.97	0.13	27,38,45,46	0
4	A8S	D	301	19/19	0.97	0.14	33,40,50,51	0
3	MG	B	402	1/1	0.98	0.17	47,47,47,47	0
3	MG	B	401	1/1	0.98	0.25	45,45,45,45	0

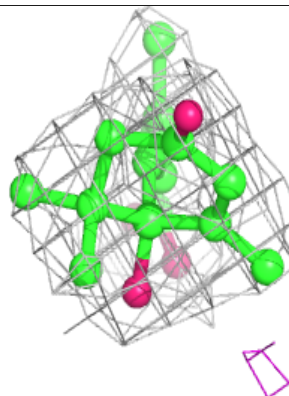
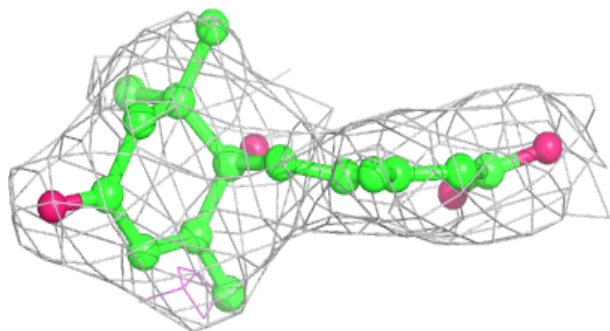
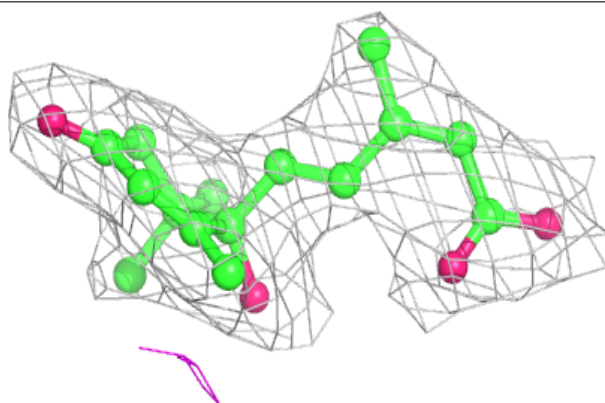
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around A8S C 301:**

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

**Electron density around A8S D 301:**

$2mF_o-DF_c$  (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.