



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 01:03 am BST

PDB ID : 3F7U  
Title : Crystal Structure of soluble domain of CA4 in complex with small molecule.  
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Deposited on : 2008-11-10  
Resolution : 2.00 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 : 2.11  
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) : 2.11

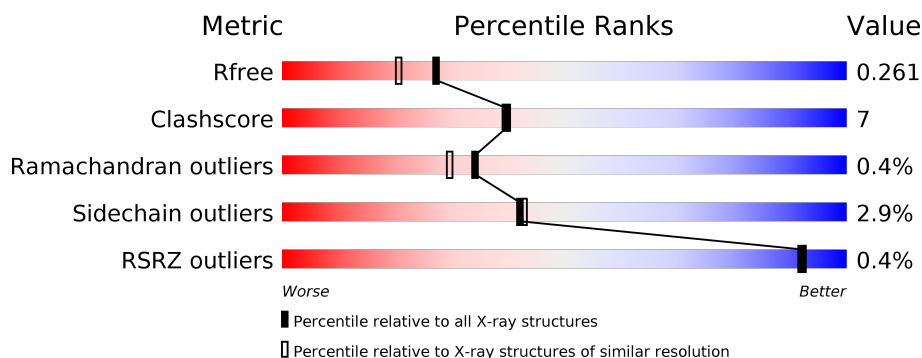
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	266	<div> <div>77%</div> <div>14%</div> <div>7%</div> </div>
1	B	266	<div> <div>74%</div> <div>16%</div> <div>7%</div> </div>
1	C	266	<div> <div>79%</div> <div>12%</div> <div>7%</div> </div>
1	D	266	<div> <div>77%</div> <div>14%</div> <div>7%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8351 atoms, of which 0 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.

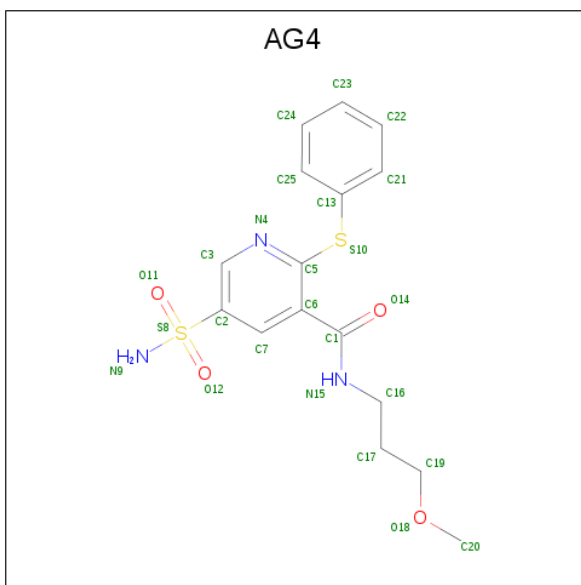
- Molecule 1 is a protein called Carbonic anhydrase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	247	Total	C	N	O	S	0	0	0
			1988	1266	339	372	11			
1	B	247	Total	C	N	O	S	0	0	0
			1988	1266	339	372	11			
1	C	247	Total	C	N	O	S	0	0	0
			1988	1266	339	372	11			
1	D	247	Total	C	N	O	S	0	0	0
			1988	1266	339	372	11			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

- Molecule 3 is N-(3-methoxypropyl)-2-(phenylsulfanyl)-5-sulfamoylpyridine-3-carboxamide (three-letter code: AG4) (formula: C<sub>16</sub>H<sub>19</sub>N<sub>3</sub>O<sub>4</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			25	16	3	4	2		
3	B	1	Total	C	N	O	S	0	0
			25	16	3	4	2		
3	C	1	Total	C	N	O	S	0	0
			25	16	3	4	2		
3	D	1	Total	C	N	O	S	0	0
			25	16	3	4	2		


- Molecule 4 is water.

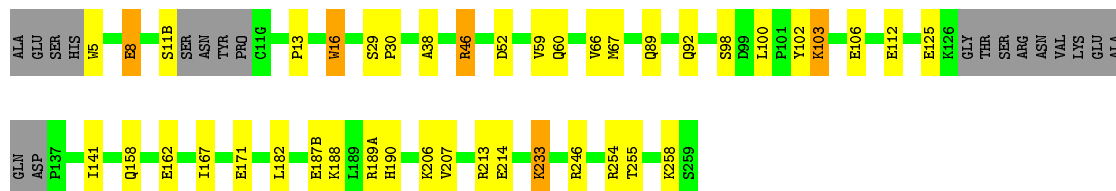
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	68	Total	O	0	0
			68	68		
4	B	88	Total	O	0	0
			88	88		
4	C	79	Total	O	0	0
			79	79		
4	D	60	Total	O	0	0
			60	60		

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


These plots are drawn for all protein, RNA and DNA 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.

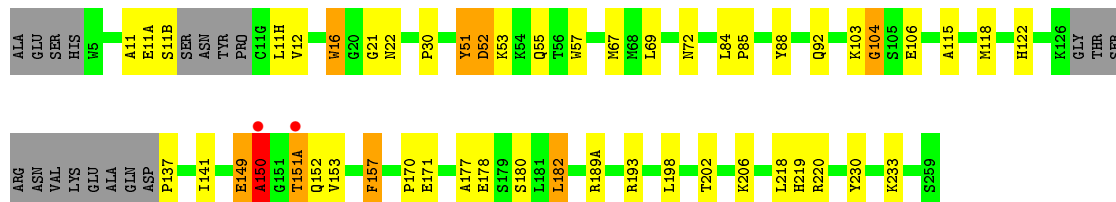
#### • Molecule 1: Carbonic anhydrase 4

Chain A: 




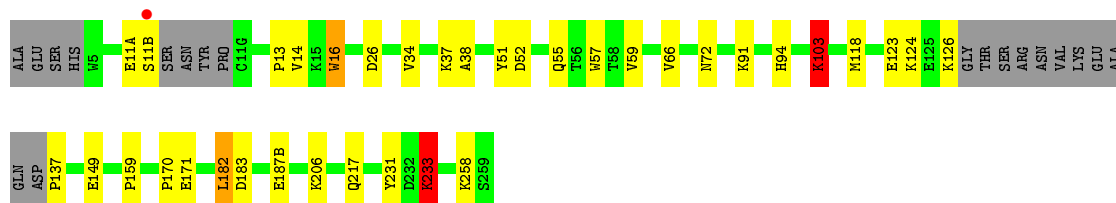
#### • Molecule 1: Carbonic anhydrase 4

Chain B: 



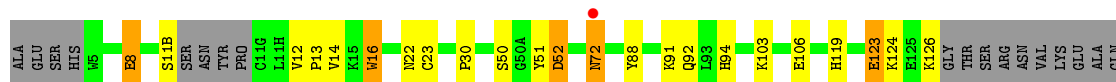
#### • Molecule 1: Carbonic anhydrase 4

Chain C: 



#### • Molecule 1: Carbonic anhydrase 4

Chain D: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.89Å 123.83Å 152.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.45 – 2.00 49.45 – 2.00	Depositor EDS
% Data completeness (in resolution range)	90.2 (49.45-2.00) 90.2 (49.45-2.00)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.38 (at 2.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.212 , 0.264 0.211 , 0.261	Depositor DCC
$R_{free}$ test set	3801 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.6	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 41.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8351	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.30% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, AG4

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	1.17	6/2034 (0.3%)	1.03	8/2745 (0.3%)
1	B	1.27	8/2034 (0.4%)	1.12	13/2745 (0.5%)
1	C	1.19	4/2034 (0.2%)	1.03	7/2745 (0.3%)
1	D	1.23	6/2034 (0.3%)	1.02	3/2745 (0.1%)
All	All	1.21	24/8136 (0.3%)	1.05	31/10980 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	3
1	C	0	1
1	D	0	1
All	All	0	7

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	16	TRP	C-N	14.62	1.59	1.33
1	B	104	GLY	N-CA	10.20	1.61	1.46
1	A	103	LYS	CE-NZ	10.10	1.74	1.49
1	D	16	TRP	C-N	9.81	1.50	1.33
1	C	16	TRP	C-N	8.89	1.49	1.33
1	D	8	GLU	CD-OE2	8.53	1.35	1.25
1	C	72	ASN	C-N	8.15	1.52	1.34
1	D	72	ASN	C-N	7.52	1.51	1.34
1	C	52	ASP	CB-CG	6.73	1.65	1.51
1	A	8	GLU	CG-CD	6.20	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	103	LYS	CD-CE	6.06	1.66	1.51
1	B	51	TYR	CD1-CE1	6.04	1.48	1.39
1	A	171	GLU	CG-CD	6.03	1.60	1.51
1	D	103	LYS	CE-NZ	6.02	1.64	1.49
1	B	52	ASP	CB-CG	5.83	1.64	1.51
1	C	187(B)	GLU	CB-CG	5.81	1.63	1.52
1	B	151(A)	THR	CB-CG2	5.80	1.71	1.52
1	A	106	GLU	CD-OE1	-5.79	1.19	1.25
1	B	220	ARG	CZ-NH2	5.47	1.40	1.33
1	D	233	LYS	C-N	5.40	1.46	1.34
1	D	191	TYR	CD1-CE1	5.38	1.47	1.39
1	B	230	TYR	CD1-CE1	5.25	1.47	1.39
1	A	98	SER	CB-OG	5.13	1.49	1.42
1	B	104	GLY	CA-C	5.01	1.59	1.51

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	233	LYS	O-C-N	-12.86	102.12	122.70
1	D	233	LYS	O-C-N	-10.03	106.66	122.70
1	B	16	TRP	C-N-CA	-10.01	101.28	122.30
1	B	103	LYS	C-N-CA	-9.34	102.69	122.30
1	B	52	ASP	CB-CG-OD2	9.19	126.57	118.30
1	C	233	LYS	C-N-CA	9.13	144.52	121.70
1	B	118	MET	CG-SD-CE	-9.10	85.63	100.20
1	C	52	ASP	CB-CG-OD2	8.90	126.31	118.30
1	B	150	ALA	CB-CA-C	-8.30	97.65	110.10
1	B	11(H)	LEU	CA-CB-CG	8.02	133.75	115.30
1	A	103	LYS	CD-CE-NZ	7.88	129.81	111.70
1	A	16	TRP	C-N-CA	7.69	138.45	122.30
1	B	220	ARG	NE-CZ-NH2	-7.56	116.52	120.30
1	B	104	GLY	N-CA-C	7.39	131.58	113.10
1	A	233	LYS	C-N-CA	7.31	139.98	121.70
1	A	233	LYS	O-C-N	-6.94	111.60	122.70
1	D	72	ASN	CA-C-N	-6.86	102.10	117.20
1	B	72	ASN	O-C-N	-6.68	112.01	122.70
1	B	103	LYS	O-C-N	-6.60	111.97	123.20
1	B	103	LYS	CA-C-N	5.95	128.11	116.20
1	D	52	ASP	CB-CG-OD1	5.90	123.61	118.30
1	A	52	ASP	CB-CG-OD2	5.78	123.50	118.30
1	C	233	LYS	CA-C-N	5.76	129.88	117.20
1	C	103	LYS	N-CA-C	5.76	126.55	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	182	LEU	CB-CG-CD1	5.53	120.40	111.00
1	A	246	ARG	NE-CZ-NH1	-5.52	117.54	120.30
1	A	246	ARG	NE-CZ-NH2	5.38	122.99	120.30
1	A	254	ARG	NE-CZ-NH1	-5.35	117.62	120.30
1	B	193	ARG	NE-CZ-NH1	-5.31	117.64	120.30
1	C	183	ASP	CB-CG-OD1	5.06	122.86	118.30
1	C	118	MET	CG-SD-CE	-5.02	92.17	100.20

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	16	TRP	Mainchain
1	A	233	LYS	Mainchain
1	B	149	GLU	Peptide
1	B	150	ALA	Peptide
1	B	16	TRP	Mainchain
1	C	233	LYS	Mainchain
1	D	233	LYS	Mainchain

## 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	1988	0	1967	30	0
1	B	1988	0	1967	38	0
1	C	1988	0	1967	24	0
1	D	1988	0	1967	26	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	25	0	19	0	0
3	B	25	0	19	2	0
3	C	25	0	19	1	0
3	D	25	0	19	3	0
4	A	68	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	88	0	0	0	0
4	C	79	0	0	0	0
4	D	60	0	0	2	0
All	All	8351	0	7944	116	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 7.

All (116) 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:A:103:LYS:CE	1:A:103:LYS:NZ	1.74	1.49
1:B:152:GLN:HB3	1:D:14:VAL:O	1.55	1.06
1:B:67:MET:HE2	1:B:69:LEU:HD23	1.41	1.00
1:C:126:LYS:NZ	1:C:137:PRO:HG3	1.76	0.99
1:C:126:LYS:HZ1	1:C:137:PRO:CG	1.86	0.89
1:C:126:LYS:NZ	1:C:137:PRO:CG	2.35	0.88
1:B:67:MET:CE	1:B:69:LEU:CD2	2.52	0.88
1:C:126:LYS:HZ2	1:C:137:PRO:HG3	1.40	0.85
1:B:67:MET:HE2	1:B:69:LEU:CD2	2.05	0.85
1:C:126:LYS:HZ1	1:C:137:PRO:CB	1.90	0.83
1:B:151(A):THR:O	1:B:152:GLN:HG3	1.77	0.83
1:A:103:LYS:O	1:A:103:LYS:CG	2.29	0.79
1:A:59:VAL:CG2	1:A:66:VAL:HG22	2.14	0.77
1:C:51:TYR:HB3	1:C:182:LEU:HD13	1.67	0.77
1:C:103:LYS:O	1:C:103:LYS:HG3	1.82	0.77
1:B:151(A):THR:C	1:B:152:GLN:HG3	2.05	0.76
1:B:198:LEU:HD22	3:B:266:AG4:C3	2.18	0.74
1:C:126:LYS:NZ	1:C:137:PRO:CB	2.51	0.74
1:A:60:GLN:HE21	1:A:67:MET:HE3	1.54	0.72
1:B:67:MET:HE1	1:B:69:LEU:CD2	2.20	0.72
1:C:149:GLU:HG3	1:C:217:GLN:NE2	2.06	0.70
1:B:151(A):THR:HG21	1:D:23:CYS:O	1.94	0.67
1:B:152:GLN:HA	1:B:219:HIS:HD2	1.58	0.67
1:A:59:VAL:CG2	1:A:66:VAL:CG2	2.72	0.67
1:C:103:LYS:O	1:C:103:LYS:CG	2.39	0.66
1:C:124:LYS:HD3	1:C:126:LYS:HG2	1.78	0.65
1:D:123:GLU:OE2	3:D:268:AG4:H23	1.96	0.64
1:B:152:GLN:HA	1:B:219:HIS:CD2	2.32	0.64
1:C:94:HIS:CG	3:C:267:AG4:H20B	2.33	0.64
1:A:60:GLN:HE21	1:A:67:MET:CE	2.11	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:164:LEU:HB2	1:D:228:LYS:HD3	1.81	0.62
1:D:94:HIS:CG	3:D:268:AG4:H20B	2.34	0.62
1:B:67:MET:HE1	1:B:69:LEU:HD21	1.81	0.59
1:A:59:VAL:HG22	1:A:66:VAL:CG2	2.32	0.59
1:A:187(B):GLU:CD	1:A:187(B):GLU:H	2.05	0.59
1:C:170:PRO:O	1:C:171:GLU:HB2	2.02	0.59
1:B:11:ALA:C	1:B:11(B):SER:H	2.05	0.58
1:B:52:ASP:OD1	1:B:53:LYS:N	2.36	0.58
1:A:158:GLN:NE2	1:A:162:GLU:OE2	2.35	0.58
1:A:188:LYS:HB3	1:A:214:GLU:HG3	1.84	0.58
1:D:169:LYS:HE2	1:D:237:GLN:OE1	2.04	0.58
3:B:266:AG4:H20A	3:B:266:AG4:O14	2.04	0.57
1:D:52:ASP:HA	1:D:182:LEU:HD23	1.87	0.57
1:D:126:LYS:HE2	1:D:140:GLU:OE2	2.05	0.56
1:A:103:LYS:O	1:A:103:LYS:HG2	2.04	0.56
1:A:46:ARG:HH11	1:A:189(A):ARG:NH2	2.03	0.56
1:D:51:TYR:C	1:D:182:LEU:HD22	2.28	0.54
1:D:204:ASP:HB3	1:D:206:LYS:HD3	1.88	0.54
1:C:126:LYS:HZ1	1:C:137:PRO:HB2	1.72	0.54
1:D:225:ALA:HB1	1:D:228:LYS:HD2	1.90	0.54
1:A:8:GLU:HG3	1:A:13:PRO:HD2	1.91	0.53
1:A:103:LYS:HG3	1:A:103:LYS:O	2.07	0.53
1:B:151(A):THR:OG1	1:B:152:GLN:CD	2.47	0.52
1:A:38:ALA:O	1:A:258:LYS:HE2	2.09	0.52
1:C:55:GLN:HG3	1:C:57:TRP:CZ2	2.45	0.51
1:B:11:ALA:O	1:B:11(B):SER:N	2.43	0.51
1:A:100:LEU:HD13	1:A:102:TYR:CZ	2.45	0.51
1:A:141:ILE:HD13	1:A:206:LYS:HE3	1.93	0.51
1:B:157:PHE:CG	1:B:218:LEU:HD11	2.46	0.51
1:B:67:MET:CE	1:B:69:LEU:HD21	2.37	0.51
1:C:170:PRO:HG3	1:C:231:TYR:O	2.11	0.51
1:C:59:VAL:HG22	1:C:66:VAL:CG2	2.40	0.51
1:B:152:GLN:CB	1:D:14:VAL:O	2.43	0.50
1:D:51:TYR:HB3	1:D:182:LEU:HD22	1.93	0.50
1:B:157:PHE:CD1	1:B:218:LEU:HD11	2.46	0.50
1:D:14:VAL:HG13	4:D:295:HOH:O	2.12	0.50
1:B:104:GLY:HA3	1:B:115:ALA:O	2.12	0.50
1:D:200:THR:HG21	3:D:268:AG4:H17	1.94	0.49
1:B:11:ALA:C	1:B:11(B):SER:N	2.64	0.49
1:C:38:ALA:O	1:C:258:LYS:HE2	2.13	0.49
1:D:22:ASN:HB2	1:D:202:THR:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:TYR:HB3	1:B:122:HIS:HB3	1.96	0.48
1:B:22:ASN:HB2	1:B:202:THR:O	2.14	0.47
1:C:13:PRO:HA	1:C:16:TRP:CE2	2.49	0.47
1:B:55:GLN:HG3	1:B:57:TRP:CZ2	2.50	0.47
1:D:219:HIS:O	1:D:220:ARG:C	2.53	0.47
1:A:89:GLN:HG3	1:A:125:GLU:CG	2.44	0.47
1:D:30:PRO:HG3	1:D:106:GLU:HB3	1.96	0.47
1:D:8:GLU:HG3	1:D:13:PRO:HD2	1.97	0.47
1:C:149:GLU:CG	1:C:217:GLN:NE2	2.75	0.47
1:D:13:PRO:HA	1:D:16:TRP:CE2	2.51	0.46
1:C:149:GLU:HG3	1:C:217:GLN:HE22	1.78	0.46
1:D:88:TYR:CE2	1:D:124:LYS:HB2	2.50	0.46
1:A:112:GLU:HG2	4:D:563:HOH:O	2.16	0.46
1:B:141:ILE:CD1	1:B:206:LYS:HE3	2.46	0.46
1:B:151(A):THR:O	1:B:152:GLN:CG	2.57	0.45
1:A:190:HIS:ND1	1:A:213:ARG:NH2	2.66	0.44
1:D:91:LYS:HE3	1:D:123:GLU:OE1	2.17	0.44
1:A:60:GLN:NE2	1:A:67:MET:CE	2.81	0.44
1:B:51:TYR:O	1:B:180:SER:HB2	2.18	0.44
1:B:171:GLU:OE1	1:B:233:LYS:HE3	2.18	0.43
1:D:106:GLU:OE1	1:D:119:HIS:HE1	2.01	0.43
1:A:89:GLN:HG3	1:A:125:GLU:HG2	2.00	0.43
1:C:34:VAL:CG1	1:C:37:LYS:HG3	2.48	0.43
1:D:150:ALA:HA	1:D:218:LEU:O	2.19	0.43
1:C:91:LYS:HE3	1:C:123:GLU:CB	2.49	0.43
1:A:141:ILE:O	1:A:207:VAL:HA	2.19	0.42
1:B:30:PRO:HG3	1:B:106:GLU:HB3	2.00	0.42
1:A:66:VAL:CG2	1:A:167:ILE:HD11	2.50	0.42
1:B:152:GLN:HB3	1:B:153:VAL:H	1.47	0.42
1:A:66:VAL:HG23	1:A:167:ILE:HD11	2.01	0.42
1:A:187(B):GLU:N	1:A:187(B):GLU:CD	2.73	0.42
1:C:59:VAL:CG2	1:C:66:VAL:HG22	2.50	0.42
1:A:5:TRP:N	4:A:510:HOH:O	2.53	0.42
1:B:104:GLY:H	1:B:115:ALA:HA	1.84	0.42
1:B:149:GLU:O	1:B:150:ALA:O	2.37	0.42
1:B:151(A):THR:HB	1:B:152:GLN:NE2	2.35	0.42
1:B:84:LEU:HA	1:B:85:PRO:HD3	1.92	0.41
1:A:66:VAL:HG23	1:A:167:ILE:CD1	2.51	0.41
1:B:177:ALA:O	1:B:178:GLU:C	2.58	0.41
1:B:170:PRO:O	1:B:171:GLU:HB2	2.20	0.41
1:D:12:VAL:HB	1:D:13:PRO:CD	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:SER:HB3	1:A:30:PRO:HA	2.04	0.40
1:A:60:GLN:NE2	1:A:67:MET:HE3	2.29	0.40
1:B:11:ALA:HB2	1:B:12:VAL:CG1	2.52	0.40
1:D:170:PRO:HG2	1:D:233:LYS:HG3	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	241/266 (91%)	231 (96%)	10 (4%)	0	100	100
1	B	241/266 (91%)	231 (96%)	7 (3%)	3 (1%)	13	7
1	C	241/266 (91%)	234 (97%)	6 (2%)	1 (0%)	34	30
1	D	241/266 (91%)	235 (98%)	6 (2%)	0	100	100
All	All	964/1064 (91%)	931 (97%)	29 (3%)	4 (0%)	34	30

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	11(A)	GLU
1	B	150	ALA
1	C	11(A)	GLU
1	B	21	GLY

### 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	221/237 (93%)	216 (98%)	5 (2%)	50	53
1	B	221/237 (93%)	216 (98%)	5 (2%)	50	53
1	C	221/237 (93%)	213 (96%)	8 (4%)	35	34
1	D	221/237 (93%)	213 (96%)	8 (4%)	35	34
All	All	884/948 (93%)	858 (97%)	26 (3%)	42	43

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11(B)	SER
1	A	46	ARG
1	A	92	GLN
1	A	182	LEU
1	A	255	THR
1	B	92	GLN
1	B	137	PRO
1	B	157	PHE
1	B	182	LEU
1	B	189(A)	ARG
1	C	11(B)	SER
1	C	14	VAL
1	C	26	ASP
1	C	103	LYS
1	C	159	PRO
1	C	182	LEU
1	C	206	LYS
1	C	233	LYS
1	D	11(B)	SER
1	D	50	SER
1	D	72	ASN
1	D	92	GLN
1	D	123	GLU
1	D	182	LEU
1	D	187(B)	GLU
1	D	255	THR

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

Mol	Chain	Res	Type
1	A	60	GLN
1	B	152	GLN
1	C	60	GLN
1	C	217	GLN
1	D	60	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](#)

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\# Z  > 2$
3	AG4	A	265	2	26,26,26	2.50	4 (15%)	30,35,35	2.42	8 (26%)
3	AG4	D	268	2	26,26,26	3.02	6 (23%)	30,35,35	1.88	8 (26%)
3	AG4	C	267	2	26,26,26	2.38	6 (23%)	30,35,35	2.99	13 (43%)
3	AG4	B	266	2	26,26,26	2.46	5 (19%)	30,35,35	1.62	7 (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
3	AG4	A	265	2	-	9/20/20/20	0/2/2/2
3	AG4	D	268	2	-	7/20/20/20	0/2/2/2
3	AG4	C	267	2	-	7/20/20/20	0/2/2/2
3	AG4	B	266	2	-	10/20/20/20	0/2/2/2

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	268	AG4	C2-S8	-10.82	1.60	1.77
3	A	265	AG4	C2-S8	-8.70	1.63	1.77
3	B	266	AG4	C2-S8	-8.31	1.64	1.77
3	C	267	AG4	C2-S8	-6.78	1.66	1.77
3	A	265	AG4	O11-S8	6.34	1.55	1.43
3	D	268	AG4	O12-S8	6.11	1.55	1.43
3	B	266	AG4	O12-S8	5.74	1.54	1.43
3	C	267	AG4	O11-S8	5.61	1.54	1.43
3	B	266	AG4	O11-S8	5.49	1.53	1.43
3	D	268	AG4	O11-S8	5.36	1.53	1.43
3	A	265	AG4	O12-S8	4.67	1.52	1.43
3	C	267	AG4	O12-S8	4.63	1.52	1.43
3	D	268	AG4	C3-C2	4.11	1.42	1.38
3	D	268	AG4	S8-N9	3.98	1.68	1.60
3	A	265	AG4	C13-S10	-3.90	1.69	1.77
3	C	267	AG4	C3-C2	3.50	1.42	1.38
3	C	267	AG4	S8-N9	3.32	1.67	1.60
3	C	267	AG4	C13-S10	-3.19	1.71	1.77
3	D	268	AG4	C13-S10	-3.19	1.71	1.77
3	B	266	AG4	C13-S10	-2.42	1.72	1.77
3	B	266	AG4	S8-N9	2.02	1.64	1.60

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	267	AG4	O11-S8-O12	-9.45	103.23	118.76
3	A	265	AG4	C7-C6-C5	7.08	124.72	117.24
3	A	265	AG4	O12-S8-N9	6.05	116.34	107.36
3	C	267	AG4	O11-S8-N9	5.25	115.15	107.36
3	D	268	AG4	C7-C6-C5	4.91	122.42	117.24
3	C	267	AG4	C6-C1-N15	4.71	126.61	117.36
3	C	267	AG4	O14-C1-N15	-4.56	113.52	122.61
3	A	265	AG4	O11-S8-O12	-4.44	111.46	118.76
3	C	267	AG4	C7-C6-C5	4.44	121.92	117.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	267	AG4	O12-S8-N9	4.35	113.81	107.36
3	A	265	AG4	C6-C5-N4	-4.26	115.96	122.75
3	D	268	AG4	O11-S8-O12	-4.21	111.84	118.76
3	B	266	AG4	C6-C1-N15	4.02	125.26	117.36
3	C	267	AG4	C7-C2-S8	3.63	126.52	119.31
3	C	267	AG4	C7-C2-C3	-3.47	114.91	118.81
3	A	265	AG4	O14-C1-C6	-3.42	114.77	121.01
3	C	267	AG4	C2-S8-N9	3.30	113.05	108.38
3	C	267	AG4	C6-C5-N4	-3.22	117.62	122.75
3	B	266	AG4	O11-S8-O12	-3.20	113.50	118.76
3	D	268	AG4	O11-S8-N9	3.15	112.03	107.36
3	A	265	AG4	C16-N15-C1	-3.14	114.92	122.08
3	B	266	AG4	O12-S8-N9	3.06	111.91	107.36
3	D	268	AG4	C3-C2-S8	-2.99	117.62	120.27
3	B	266	AG4	C7-C6-C5	2.97	120.38	117.24
3	A	265	AG4	C6-C1-N15	2.93	123.11	117.36
3	B	266	AG4	O14-C1-N15	-2.92	116.79	122.61
3	D	268	AG4	C2-S8-N9	2.81	112.36	108.38
3	C	267	AG4	C16-N15-C1	-2.51	116.35	122.08
3	B	266	AG4	O11-S8-N9	2.46	111.00	107.36
3	D	268	AG4	O11-S8-C2	-2.44	104.63	107.35
3	D	268	AG4	C6-C7-C2	-2.34	116.54	120.30
3	B	266	AG4	C6-C5-N4	-2.31	119.06	122.75
3	D	268	AG4	O14-C1-C6	-2.28	116.85	121.01
3	C	267	AG4	O11-S8-C2	-2.20	104.90	107.35
3	A	265	AG4	C6-C7-C2	-2.01	117.07	120.30
3	C	267	AG4	C3-C2-S8	-2.00	118.50	120.27

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	265	AG4	N15-C16-C17-C19
3	A	265	AG4	C3-C2-S8-O11
3	D	268	AG4	C3-C2-S8-O12
3	D	268	AG4	C3-C2-S8-O11
3	C	267	AG4	C3-C2-S8-O11
3	B	266	AG4	C3-C2-S8-O12
3	B	266	AG4	C3-C2-S8-O11
3	A	265	AG4	C16-C17-C19-O18
3	D	268	AG4	C17-C19-O18-C20
3	B	266	AG4	C17-C19-O18-C20

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Mol	Chain	Res	Type	Atoms
3	B	266	AG4	C3-C2-S8-N9
3	A	265	AG4	C7-C2-S8-N9
3	B	266	AG4	C7-C2-S8-N9
3	A	265	AG4	C3-C2-S8-N9
3	D	268	AG4	C7-C2-S8-N9
3	D	268	AG4	C3-C2-S8-N9
3	C	267	AG4	C3-C2-S8-N9
3	C	267	AG4	C7-C2-S8-N9
3	C	267	AG4	C17-C19-O18-C20
3	A	265	AG4	C3-C2-S8-O12
3	A	265	AG4	O14-C1-C6-C5
3	C	267	AG4	O14-C1-C6-C5
3	B	266	AG4	O14-C1-C6-C5
3	B	266	AG4	N15-C1-C6-C5
3	B	266	AG4	C16-C17-C19-O18
3	B	266	AG4	N15-C16-C17-C19
3	A	265	AG4	C7-C2-S8-O11
3	D	268	AG4	O14-C1-C6-C5
3	D	268	AG4	C7-C2-S8-O11
3	C	267	AG4	C7-C2-S8-O11
3	B	266	AG4	C7-C2-S8-O12
3	A	265	AG4	N15-C1-C6-C5
3	C	267	AG4	N15-C1-C6-C5

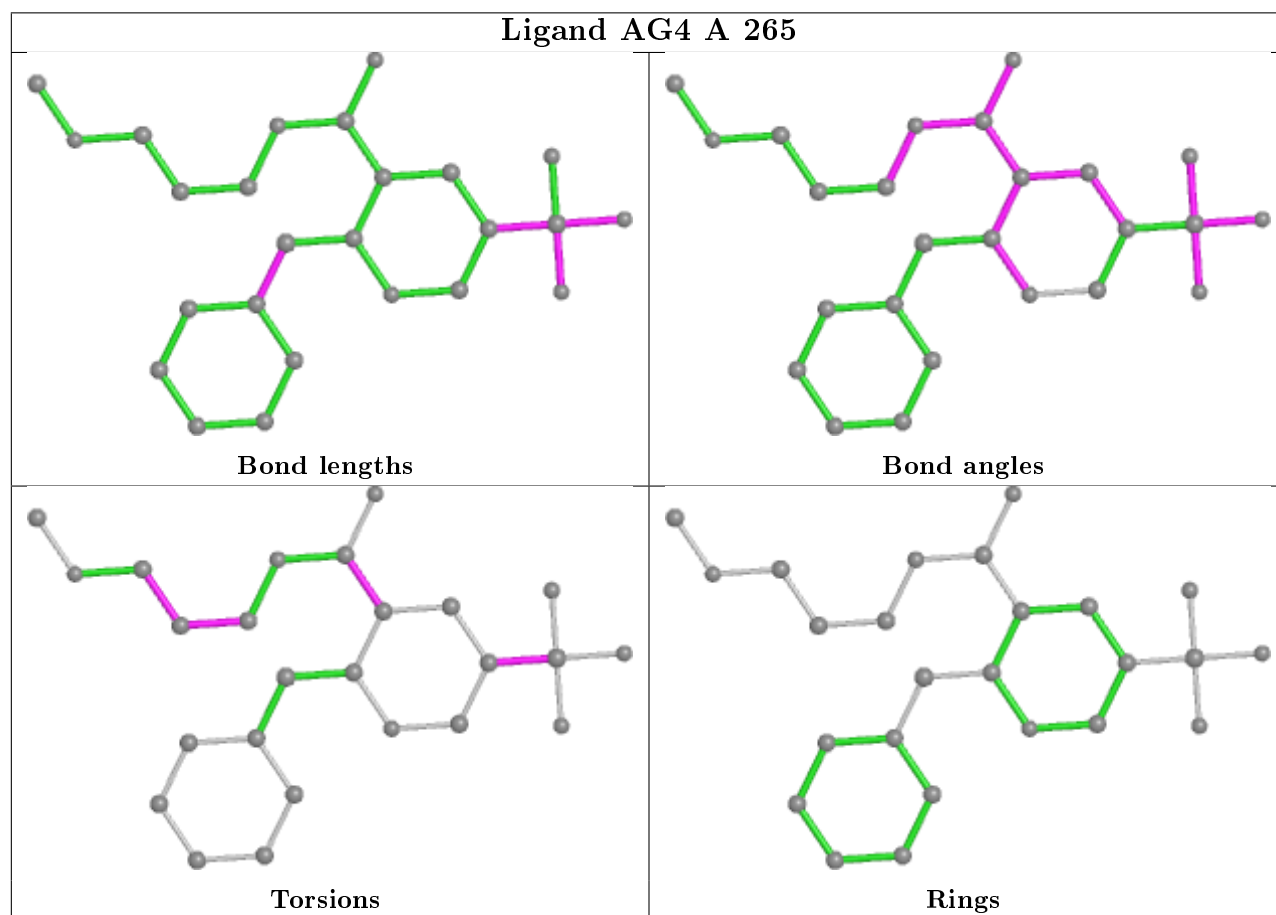
There are no ring outliers.

3 monomers are involved in 6 short contacts:

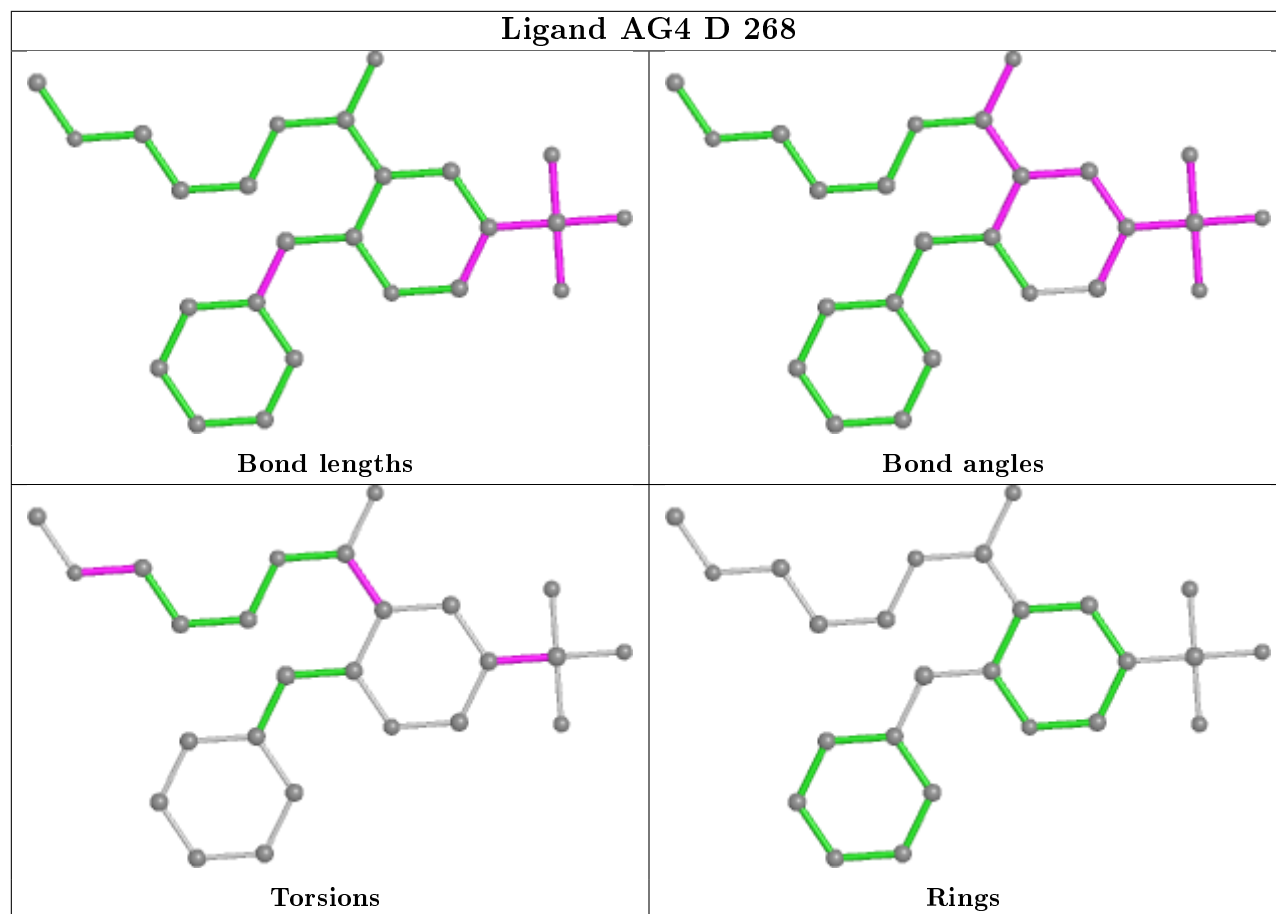
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	268	AG4	3	0
3	C	267	AG4	1	0
3	B	266	AG4	2	0

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.

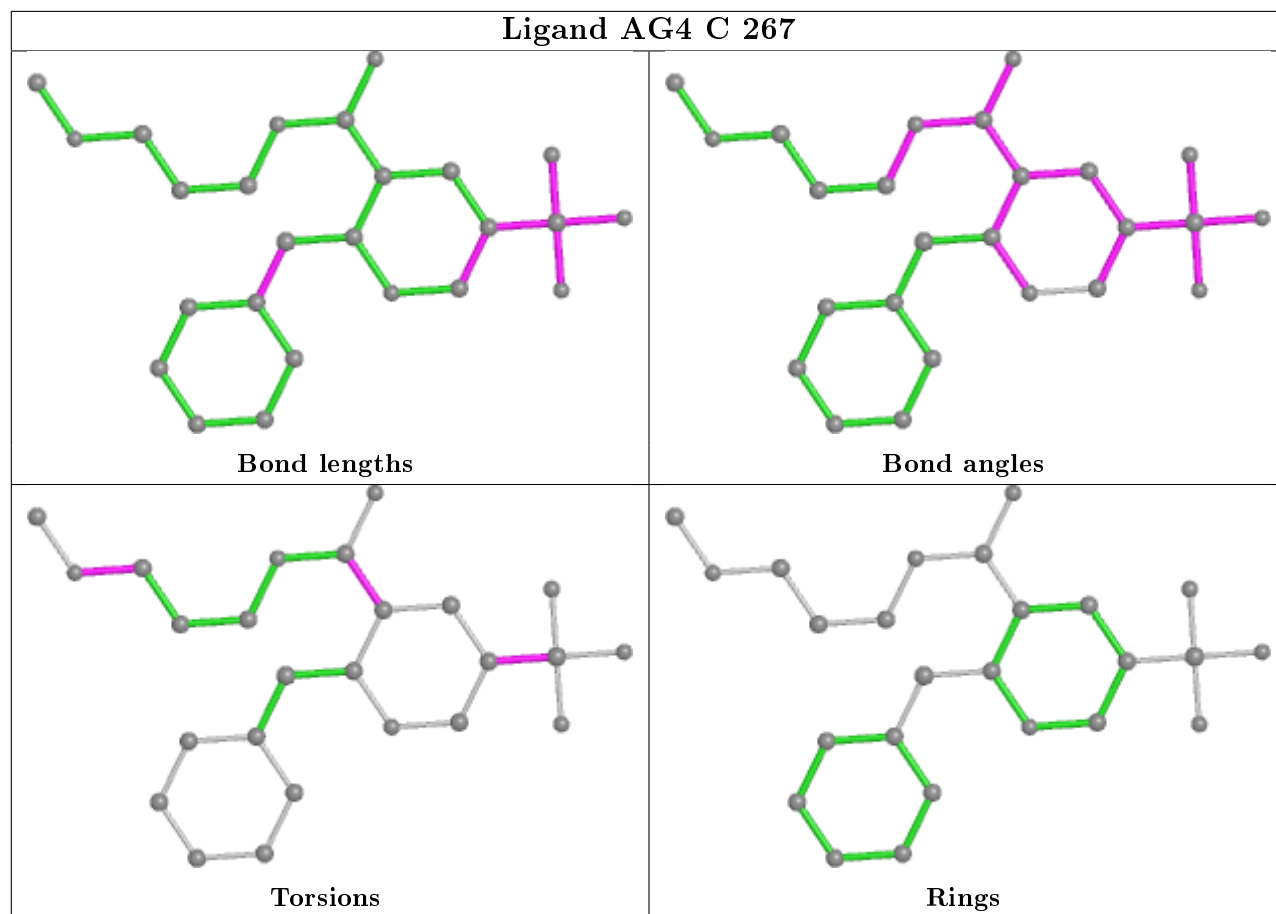
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

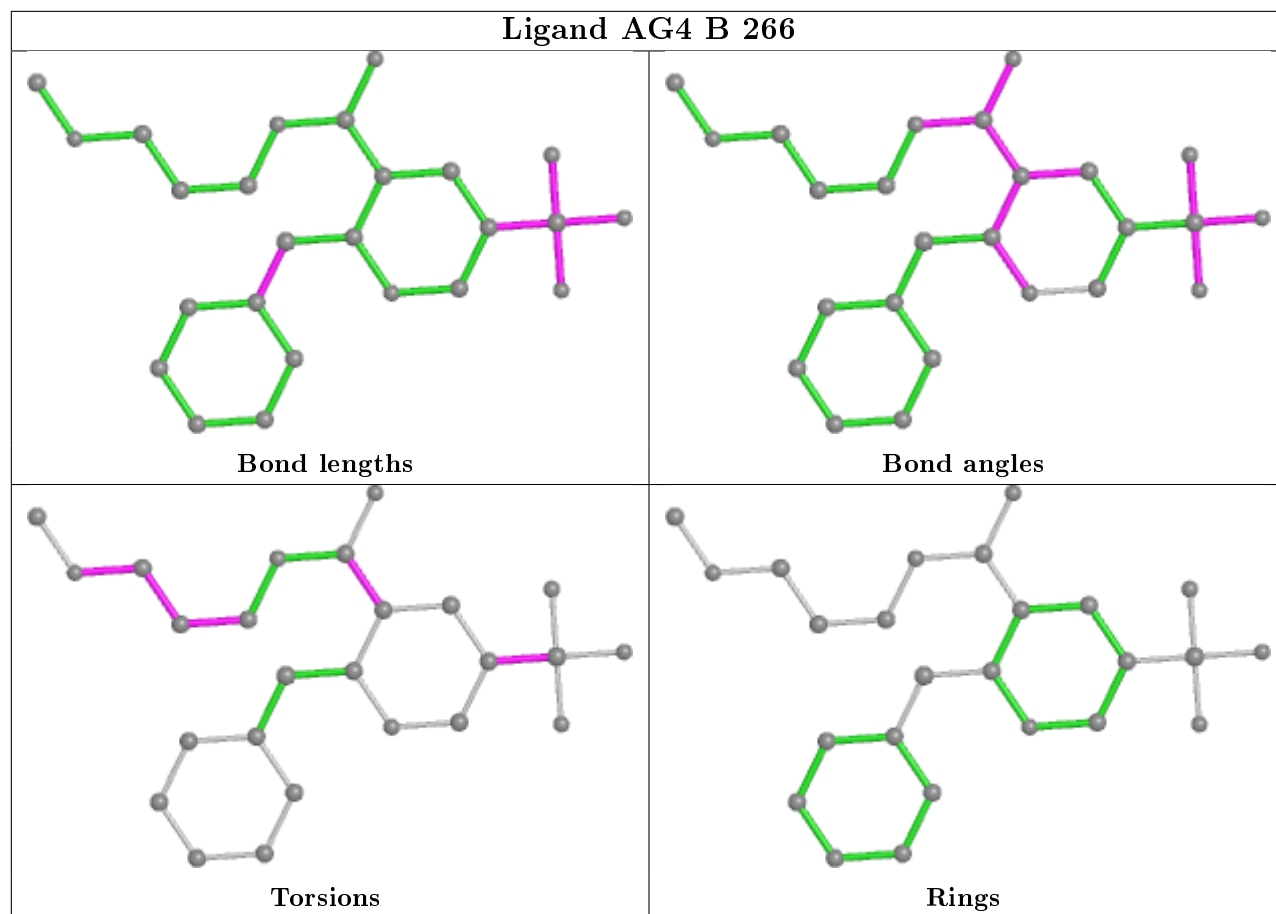


## Ligand AG4 D 268



## Ligand AG4 C 267





## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	247/266 (92%)	-0.53	0 <a href="#">100</a>   <a href="#">100</a>	12, 22, 35, 49	0
1	B	247/266 (92%)	-0.48	2 (0%) <a href="#">86</a>   <a href="#">85</a>	12, 20, 33, 44	0
1	C	247/266 (92%)	-0.53	1 (0%) <a href="#">92</a>   <a href="#">92</a>	12, 21, 34, 42	0
1	D	247/266 (92%)	-0.45	1 (0%) <a href="#">92</a>   <a href="#">92</a>	12, 21, 34, 42	0
All	All	988/1064 (92%)	-0.50	4 (0%) <a href="#">92</a>   <a href="#">92</a>	12, 21, 34, 49	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	151(A)	THR	6.3
1	B	150	ALA	3.6
1	D	72	ASN	2.3
1	C	11(B)	SER	2.1

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

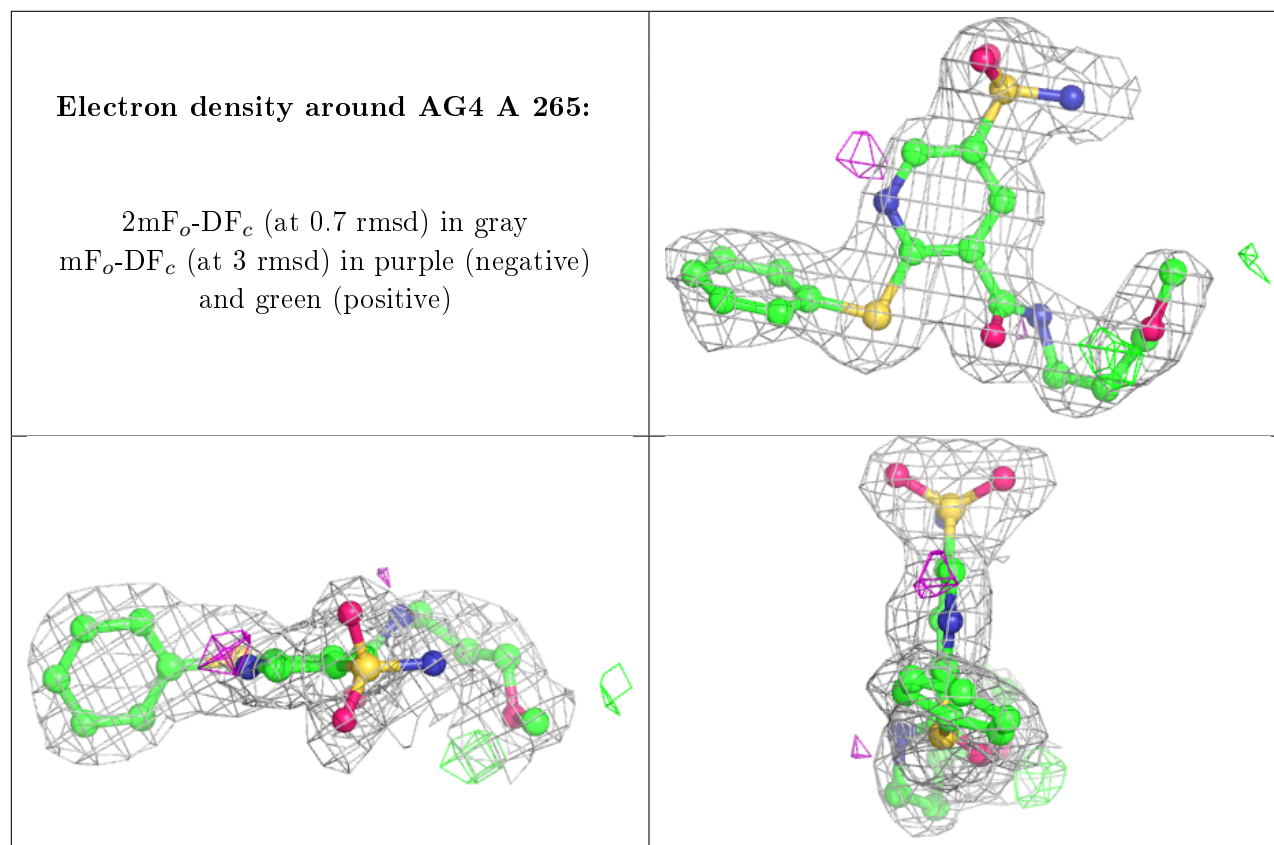
### 6.4 Ligands [i](#)

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<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.



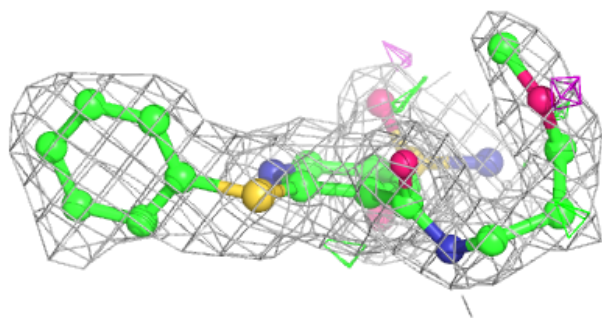
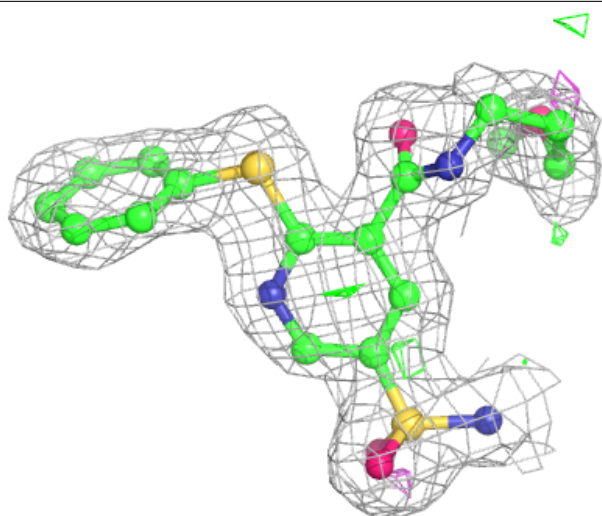
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	AG4	A	265	25/25	0.94	0.14	21,34,40,41	0
3	AG4	C	267	25/25	0.94	0.14	20,30,38,40	0
3	AG4	D	268	25/25	0.95	0.11	21,32,40,42	0
3	AG4	B	266	25/25	0.95	0.15	24,31,47,48	0
2	ZN	A	260	1/1	1.00	0.09	16,16,16,16	0
2	ZN	C	262	1/1	1.00	0.07	16,16,16,16	0
2	ZN	D	263	1/1	1.00	0.07	16,16,16,16	0
2	ZN	B	261	1/1	1.00	0.09	15,15,15,15	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.



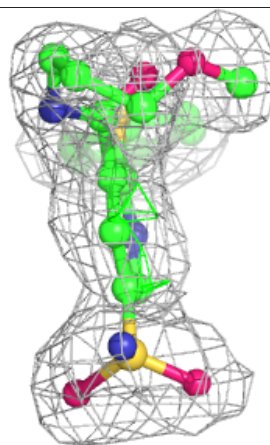
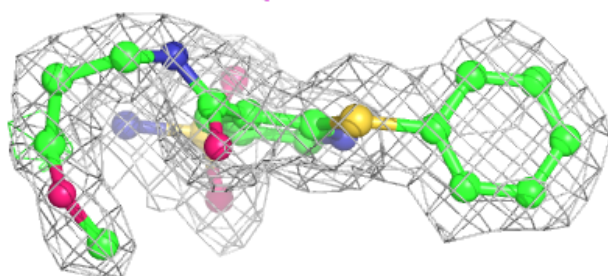
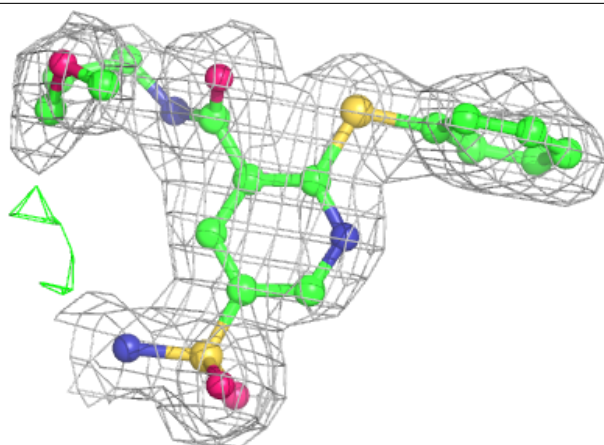
**Electron density around AG4 C 267:**

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

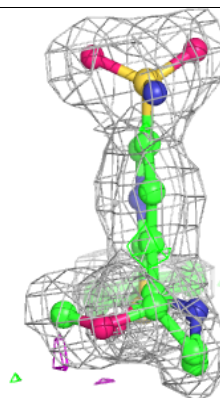
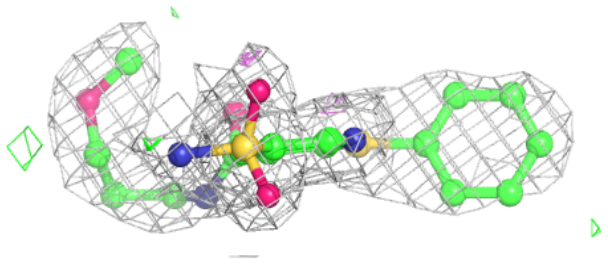
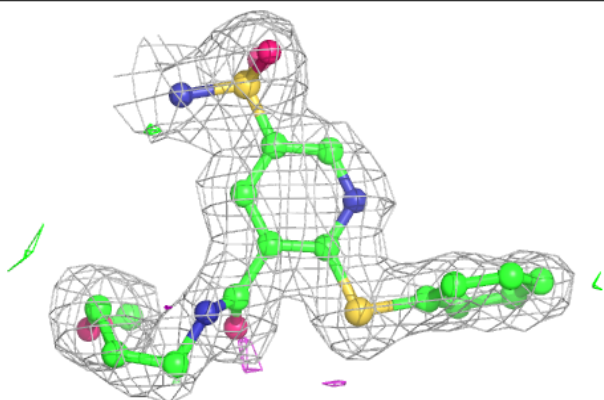


**Electron density around AG4 D 268:**

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

**Electron density around AG4 B 266:**

$2mF_o - DF_c$  (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.