



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 02:33 pm BST

PDB ID : 3E76  
Title : Crystal structure of Wild-type GroEL with bound Thallium ions  
Authors : Kiser, P.D.; Lorimer, G.H.; Palczewski, K.  
Deposited on : 2008-08-17  
Resolution : 3.94 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.

---

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

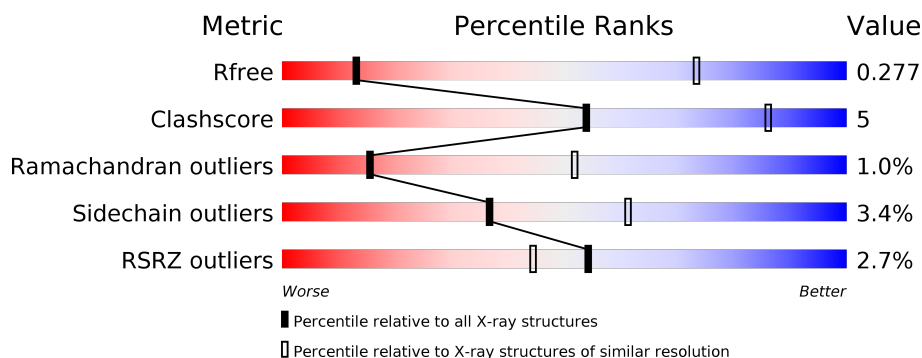
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.94 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.








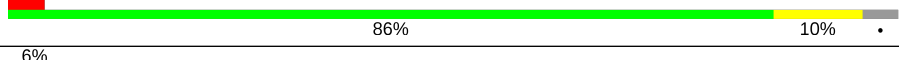


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1036 (4.20-3.68)
Clashscore	141614	1009 (4.18-3.70)
Ramachandran outliers	138981	1057 (4.20-3.68)
Sidechain outliers	138945	1049 (4.20-3.68)
RSRZ outliers	127900	1007 (4.24-3.64)

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	547	<div> <div>78%</div> <div>16%</div> <div>• •</div> </div>
1	B	547	<div> <div>82%</div> <div>14%</div> <div>• •</div> </div>
1	C	547	<div> <div>2%</div> <div>82%</div> <div>13%</div> <div>• •</div> </div>
1	D	547	<div> <div>%</div> <div>81%</div> <div>14%</div> <div>• •</div> </div>
1	E	547	<div> <div>2%</div> <div>82%</div> <div>13%</div> <div>• •</div> </div>
1	F	547	<div> <div>2%</div> <div>79%</div> <div>16%</div> <div>• •</div> </div>

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	G	547	 % 78% 17% • •
1	H	547	 3% 82% 13% • •
1	I	547	 2% 78% 17% • •
1	J	547	 2% 81% 14% • •
1	K	547	 2% 79% 16% • •
1	L	547	 4% 86% 10% •
1	M	547	 6% 84% 12% • •
1	N	547	 7% 86% 10% •

## 2 Entry composition

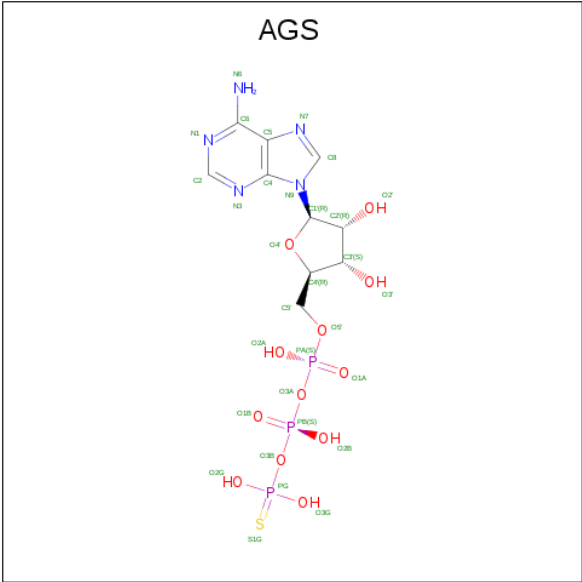
There are 4 unique types of molecules in this entry. The entry contains 54464 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 60 kDa chaperonin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	B	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	C	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	D	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	E	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	F	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	G	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	H	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	I	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	J	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	K	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	L	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	M	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	N	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			

- Molecule 2 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	E	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	F	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	G	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	H	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	I	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	J	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	K	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	L	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	M	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	N	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

- Molecule 3 is THALLIUM (I) ION (three-letter code: Tl) (formula: Tl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	3	Total 3	Tl 3	0	0
3	J	3	Total 3	Tl 3	0	0
3	D	4	Total 4	Tl 4	0	0
3	K	3	Total 3	Tl 3	0	0
3	E	3	Total 3	Tl 3	0	0
3	H	4	Total 4	Tl 4	0	0
3	B	4	Total 4	Tl 4	0	0
3	I	3	Total 3	Tl 3	0	0
3	C	3	Total 3	Tl 3	0	0
3	A	4	Total 4	Tl 4	0	0
3	N	2	Total 2	Tl 2	0	0
3	L	3	Total 3	Tl 3	0	0
3	F	4	Total 4	Tl 4	0	0
3	M	3	Total 3	Tl 3	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: Mg) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total 1	Mg 1	0	0
4	J	1	Total 1	Mg 1	0	0
4	D	1	Total 1	Mg 1	0	0
4	K	1	Total 1	Mg 1	0	0
4	E	1	Total 1	Mg 1	0	0

*Continued on next page...*

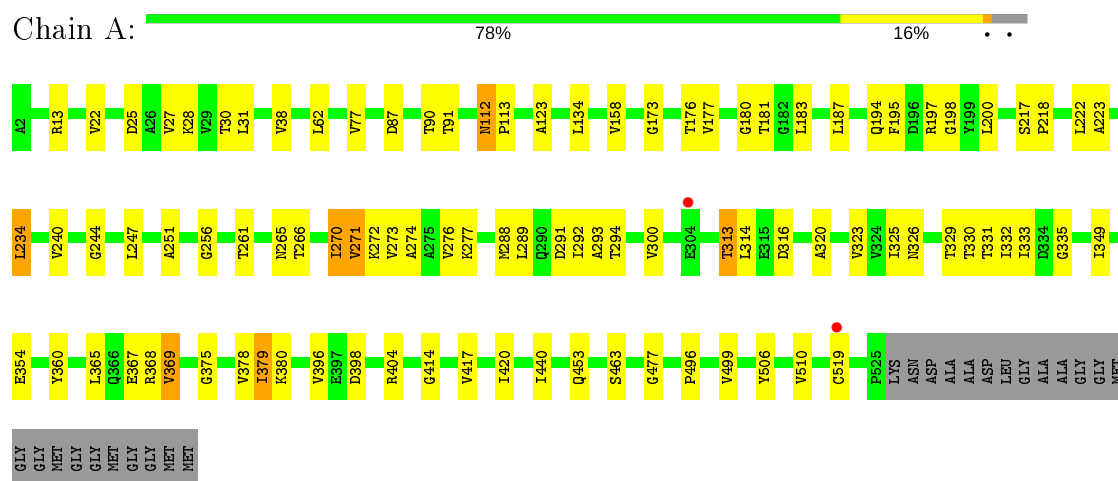
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	1	Total 1	Mg 1	0	0
4	B	1	Total 1	Mg 1	0	0
4	I	1	Total 1	Mg 1	0	0
4	C	1	Total 1	Mg 1	0	0
4	A	1	Total 1	Mg 1	0	0
4	N	1	Total 1	Mg 1	0	0
4	L	1	Total 1	Mg 1	0	0
4	F	1	Total 1	Mg 1	0	0
4	M	1	Total 1	Mg 1	0	0

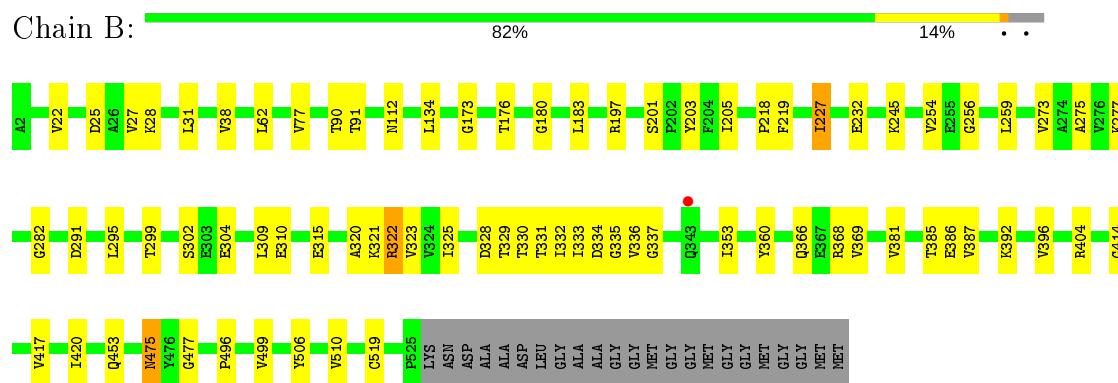
### 3 Residue-property plots [i](#)

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.

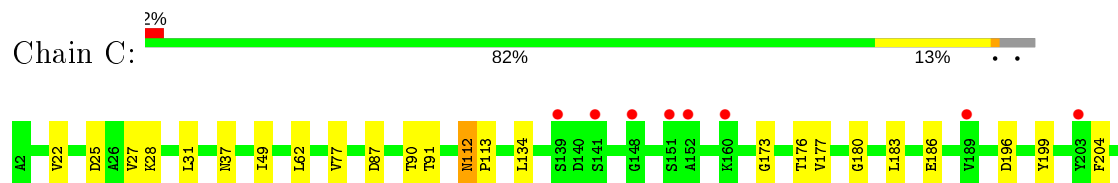
- Molecule 1: 60 kDa chaperonin



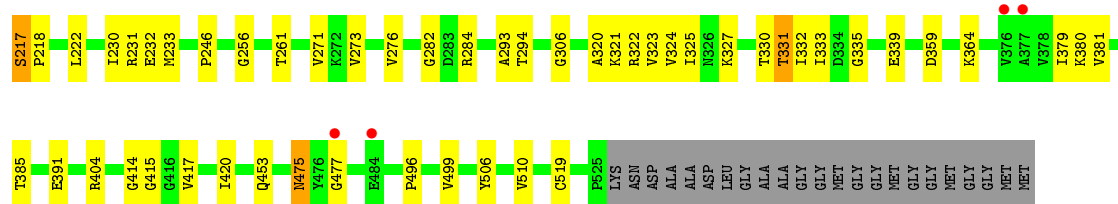
- Molecule 1: 60 kDa chaperonin



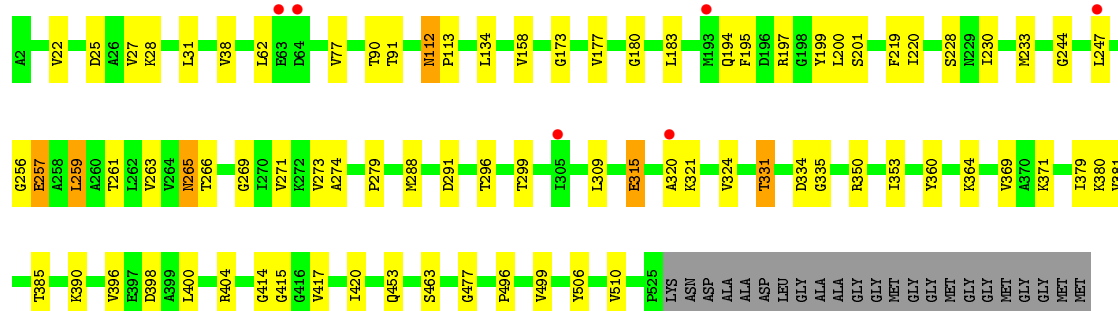
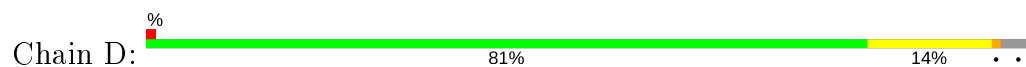
- Molecule 1: 60 kDa chaperonin



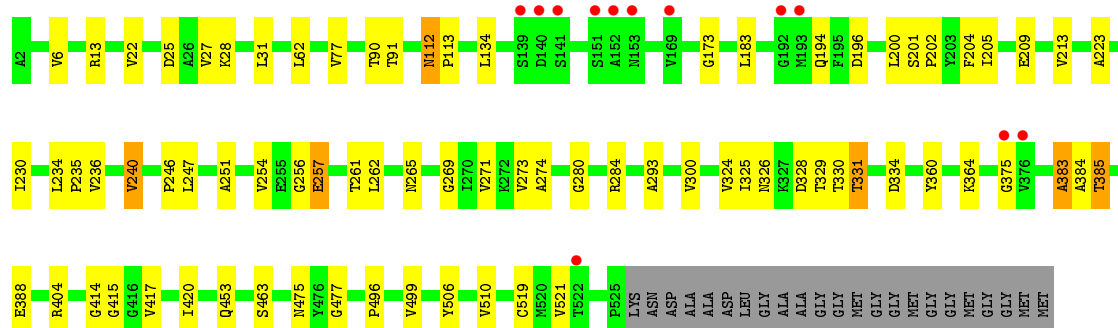
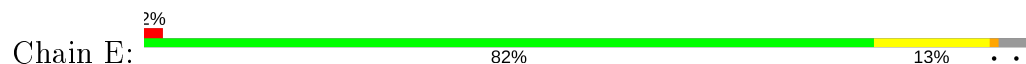




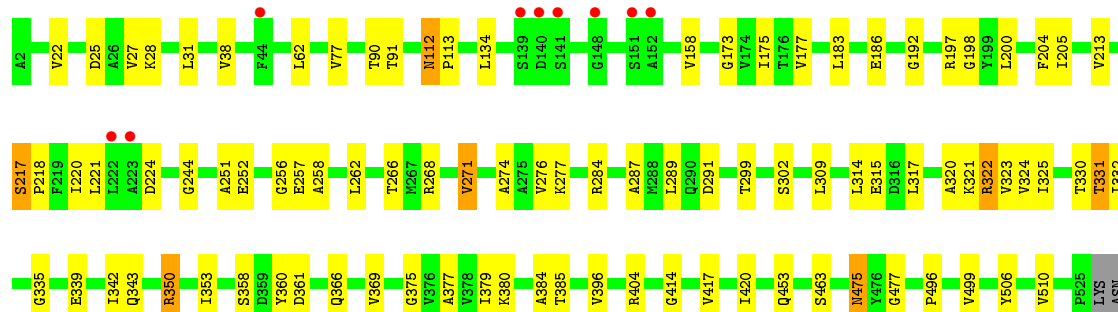
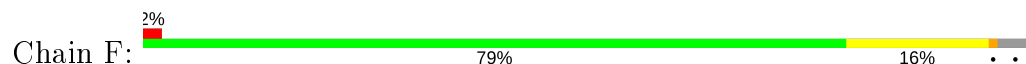
• Molecule 1: 60 kDa chaperonin



• Molecule 1: 60 kDa chaperonin



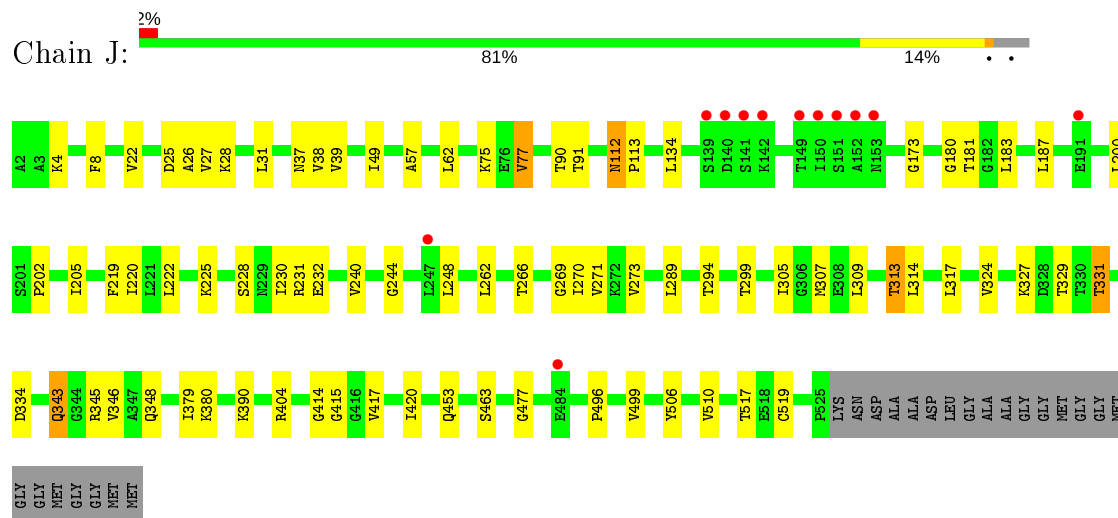
• Molecule 1: 60 kDa chaperonin



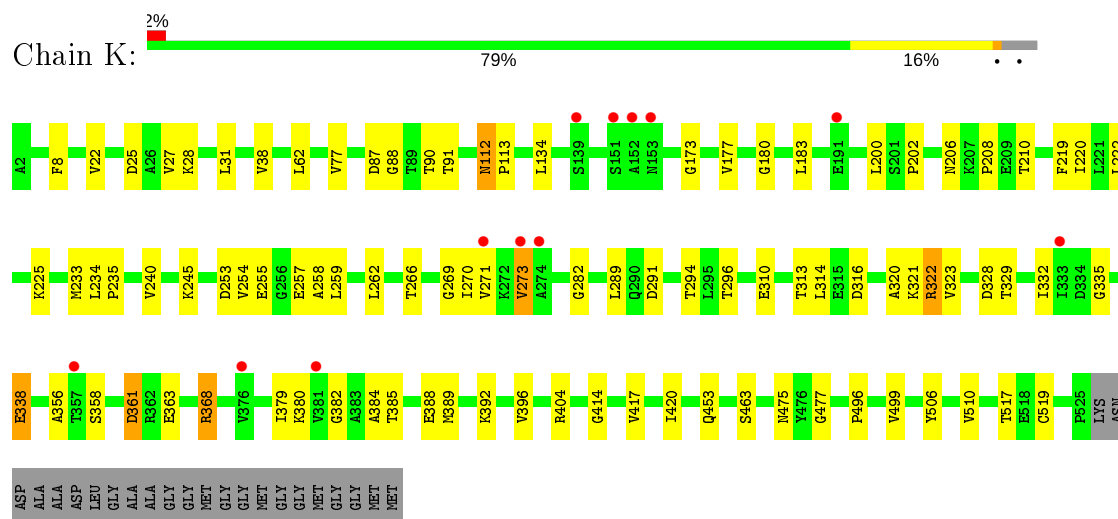


ASN  
ASP  
ALA  
ALA  
ASP  
LEU  
GLY  
ALA  
ALA  
GLY  
GLY  
MET  
MET  
GLY  
GLY  
MET  
MET

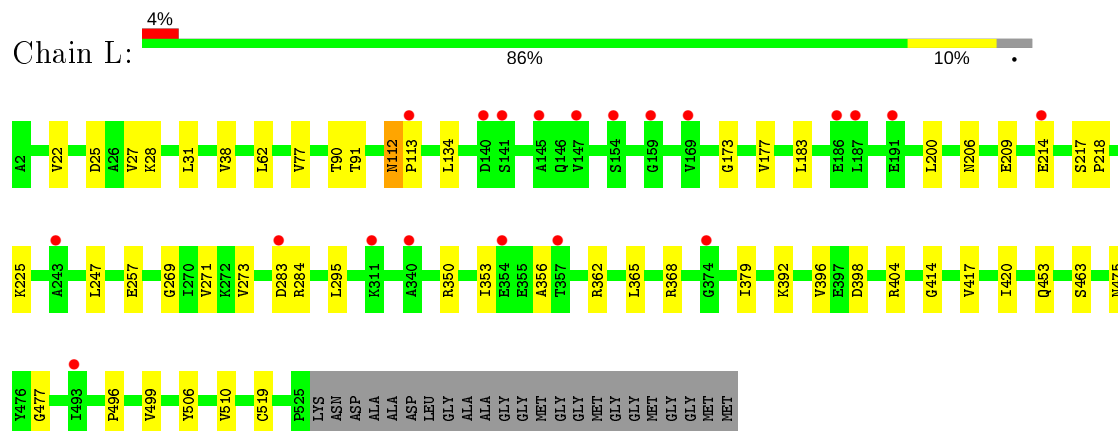
• Molecule 1: 60 kDa chaperonin



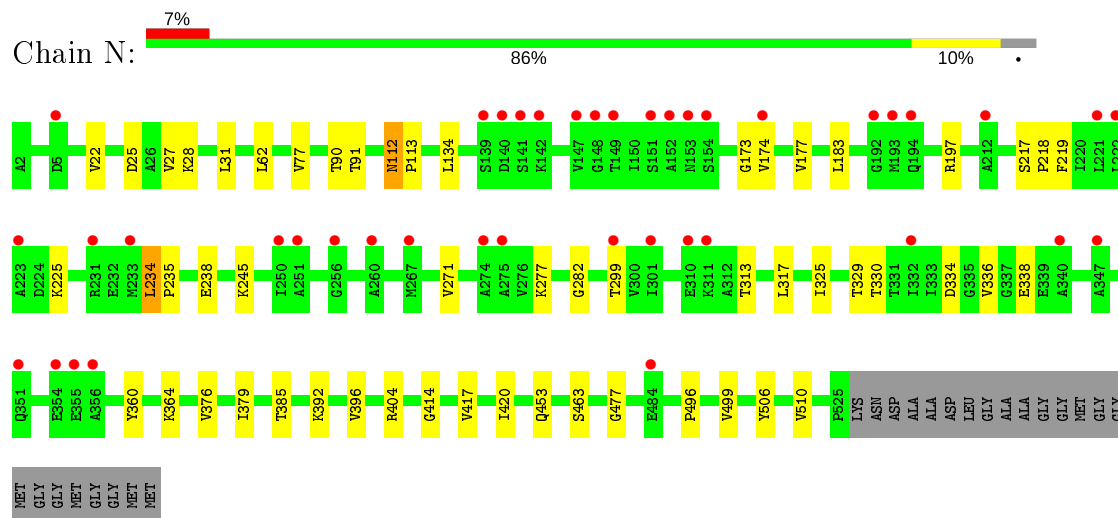
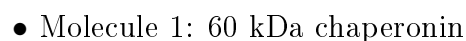
• Molecule 1: 60 kDa chaperonin



• Molecule 1: 60 kDa chaperonin



- Chain M:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.68Å 260.95Å 287.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.39 – 3.94 49.36 – 3.90	Depositor EDS
% Data completeness (in resolution range)	97.7 (49.39-3.94) 96.5 (49.36-3.90)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.37 (at 3.88Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.261 , 0.293 0.249 , 0.277	Depositor DCC
$R_{free}$ test set	4528 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	115.0	Xtriage
Anisotropy	0.482	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 112.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	54464	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, AGS, TL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.38	0/3883	0.63	4/5243 (0.1%)
1	B	0.36	0/3883	0.48	0/5243
1	C	0.46	4/3883 (0.1%)	0.49	0/5243
1	D	0.43	2/3883 (0.1%)	0.50	0/5243
1	E	0.37	0/3883	0.63	4/5243 (0.1%)
1	F	0.36	0/3883	0.50	0/5243
1	G	0.37	0/3883	0.50	0/5243
1	H	0.43	2/3883 (0.1%)	0.50	0/5243
1	I	0.40	2/3883 (0.1%)	0.49	0/5243
1	J	0.36	0/3883	0.49	0/5243
1	K	0.40	2/3883 (0.1%)	0.49	0/5243
1	L	0.34	0/3883	0.47	0/5243
1	M	0.37	2/3883 (0.1%)	0.47	0/5243
1	N	0.44	3/3883 (0.1%)	0.49	1/5243 (0.0%)
All	All	0.39	17/54362 (0.0%)	0.51	9/73402 (0.0%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	232	GLU	CD-OE2	12.24	1.39	1.25
1	N	338	GLU	CD-OE2	11.57	1.38	1.25
1	H	367	GLU	CD-OE2	10.24	1.36	1.25
1	D	315	GLU	CD-OE1	9.77	1.36	1.25
1	H	367	GLU	CD-OE1	9.42	1.36	1.25
1	C	339	GLU	CG-CD	9.28	1.65	1.51
1	D	315	GLU	CD-OE2	9.06	1.35	1.25
1	K	363	GLU	CD-OE1	8.62	1.35	1.25
1	C	232	GLU	CD-OE1	7.40	1.33	1.25
1	N	238	GLU	CD-OE2	7.30	1.33	1.25
1	M	37	ASN	CG-ND2	-6.96	1.15	1.32
1	C	339	GLU	CD-OE1	6.85	1.33	1.25

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	238	GLU	CD-OE1	6.59	1.32	1.25
1	I	209	GLU	CD-OE1	6.18	1.32	1.25
1	M	37	ASN	CG-OD1	-6.08	1.10	1.24
1	I	209	GLU	CD-OE2	5.91	1.32	1.25
1	K	363	GLU	CD-OE2	5.55	1.31	1.25

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	13	ARG	NE-CZ-NH2	-20.52	110.04	120.30
1	A	13	ARG	NE-CZ-NH2	-19.42	110.59	120.30
1	E	13	ARG	NE-CZ-NH1	18.12	129.36	120.30
1	A	13	ARG	NE-CZ-NH1	17.56	129.08	120.30
1	A	13	ARG	CD-NE-CZ	8.14	135.00	123.60
1	E	13	ARG	CD-NE-CZ	7.95	134.73	123.60
1	N	338	GLU	OE1-CD-OE2	5.91	130.39	123.30
1	A	13	ARG	CB-CG-CD	-5.53	97.23	111.60
1	E	13	ARG	CB-CG-CD	-5.40	97.55	111.60

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3855	0	3976	60	0
1	B	3855	0	3974	40	0
1	C	3855	0	3976	41	0
1	D	3855	0	3976	43	0
1	E	3855	0	3974	43	0
1	F	3855	0	3976	50	0
1	G	3855	0	3975	55	0
1	H	3855	0	3976	44	0
1	I	3855	0	3975	56	0
1	J	3855	0	3974	45	0
1	K	3855	0	3975	49	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	3855	0	3976	30	0
1	M	3855	0	3976	36	0
1	N	3855	0	3976	34	0
2	A	31	0	12	0	0
2	B	31	0	12	0	0
2	C	31	0	12	1	0
2	D	31	0	12	1	0
2	E	31	0	12	1	0
2	F	31	0	12	0	0
2	G	31	0	12	2	0
2	H	31	0	12	0	0
2	I	31	0	12	1	0
2	J	31	0	12	1	0
2	K	31	0	12	1	0
2	L	31	0	12	0	0
2	M	31	0	12	0	0
2	N	31	0	12	0	0
3	A	4	0	0	1	0
3	B	4	0	0	0	0
3	C	3	0	0	0	0
3	D	4	0	0	0	0
3	E	3	0	0	0	0
3	F	4	0	0	0	0
3	G	3	0	0	0	0
3	H	4	0	0	0	0
3	I	3	0	0	1	0
3	J	3	0	0	0	0
3	K	3	0	0	0	0
3	L	3	0	0	0	0
3	M	3	0	0	0	0
3	N	2	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	1	0	0	0	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0
All	All	54464	0	55823	586	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 5.

All (586) 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:M:183:LEU:HD22	1:N:360:TYR:CB	1.96	0.95
1:A:87:ASP:OD2	1:A:499:VAL:HG21	1.69	0.91
1:C:87:ASP:OD2	1:C:499:VAL:HG21	1.75	0.86
1:M:183:LEU:HD22	1:N:360:TYR:HB3	1.54	0.86
1:H:360:TYR:CG	1:N:183:LEU:HD22	2.13	0.84
1:D:320:ALA:HA	1:D:335:GLY:HA2	1.60	0.83
1:I:38:VAL:HG22	1:J:519:CYS:HB3	1.63	0.80
1:N:234:LEU:H	1:N:235:PRO:HD2	1.48	0.77
1:H:349:ILE:HA	1:H:352:GLN:HG2	1.68	0.76
1:E:280:GLY:HA2	1:E:284:ARG:HH21	1.51	0.75
1:N:219:PHE:HE2	1:N:245:LYS:HB2	1.52	0.75
1:G:266:THR:HG21	1:G:273:VAL:HB	1.69	0.73
1:H:38:VAL:HG22	1:I:519:CYS:HB3	1.71	0.72
1:H:219:PHE:HE2	1:H:245:LYS:HB2	1.56	0.71
1:J:219:PHE:CD2	1:J:240:VAL:HG13	2.25	0.70
1:A:187:LEU:HD13	1:A:379:ILE:HG23	1.72	0.70
1:G:415:GLY:N	2:G:549:AGS:O2'	2.20	0.70
1:H:219:PHE:CE2	1:H:245:LYS:HB2	2.27	0.70
1:I:247:LEU:HB3	1:I:273:VAL:HG13	1.74	0.69
1:J:77:VAL:HG21	1:J:510:VAL:HG11	1.74	0.69
1:H:321:LYS:O	1:H:322:ARG:HB2	1.90	0.69
1:D:38:VAL:HG22	1:E:519:CYS:HB3	1.76	0.68
1:D:230:ILE:HD12	1:D:261:THR:HG21	1.74	0.68
1:J:38:VAL:HG22	1:K:519:CYS:HB3	1.76	0.68
1:M:365:LEU:HD22	1:M:368:ARG:HH21	1.59	0.67
1:F:339:GLU:HA	1:F:342:ILE:HB	1.76	0.66
1:H:288:MET:HA	1:H:291:ASP:HB2	1.77	0.66
1:A:197:ARG:HD2	1:A:277:LYS:HB2	1.76	0.66
1:F:198:GLY:O	1:F:276:VAL:HG13	1.95	0.65
1:M:325:ILE:HG12	1:M:330:THR:HG23	1.77	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:349:ILE:HA	1:H:352:GLN:CG	2.27	0.65
1:M:183:LEU:HD22	1:N:360:TYR:HB2	1.78	0.65
1:K:219:PHE:CE2	1:K:245:LYS:HB2	2.32	0.65
1:F:220:ILE:HD11	1:F:320:ALA:HB2	1.79	0.65
1:J:37:ASN:HD22	1:J:49:ILE:HG22	1.62	0.65
1:E:417:VAL:HA	1:E:420:ILE:HG22	1.79	0.64
1:E:205:ILE:HA	1:E:213:VAL:HG22	1.78	0.64
1:I:358:SER:HB3	1:I:361:ASP:HB2	1.79	0.64
1:F:38:VAL:HG22	1:G:519:CYS:HB3	1.78	0.64
1:A:291:ASP:OD2	1:A:368:ARG:HD3	1.97	0.64
1:E:77:VAL:HG21	1:E:510:VAL:HG11	1.79	0.64
1:C:37:ASN:HD22	1:C:49:ILE:HG22	1.63	0.64
1:I:417:VAL:HA	1:I:420:ILE:HG22	1.80	0.63
1:J:181:THR:O	1:K:282:GLY:HA3	1.99	0.63
1:N:234:LEU:N	1:N:235:PRO:HD2	2.12	0.63
1:M:27:VAL:HG12	1:M:90:THR:HG23	1.81	0.63
1:I:77:VAL:HG21	1:I:510:VAL:HG11	1.80	0.63
1:F:77:VAL:HG21	1:F:510:VAL:HG11	1.81	0.63
1:H:27:VAL:HG12	1:H:90:THR:HG23	1.81	0.63
1:C:417:VAL:HA	1:C:420:ILE:HG22	1.81	0.63
1:J:202:PRO:O	1:J:205:ILE:HG13	1.99	0.63
1:C:320:ALA:HA	1:C:335:GLY:HA2	1.81	0.62
1:F:417:VAL:HA	1:F:420:ILE:HG22	1.80	0.62
1:A:417:VAL:HA	1:A:420:ILE:HG22	1.80	0.62
1:M:77:VAL:HG21	1:M:510:VAL:HG11	1.80	0.62
1:F:27:VAL:HG12	1:F:90:THR:HG23	1.81	0.62
1:G:417:VAL:HA	1:G:420:ILE:HG22	1.80	0.62
1:B:320:ALA:HA	1:B:335:GLY:HA2	1.80	0.62
1:D:27:VAL:HG12	1:D:90:THR:HG23	1.82	0.62
1:D:77:VAL:HG21	1:D:510:VAL:HG11	1.80	0.62
1:L:417:VAL:HA	1:L:420:ILE:HG22	1.81	0.62
1:L:77:VAL:HG21	1:L:510:VAL:HG11	1.80	0.62
1:J:417:VAL:HA	1:J:420:ILE:HG22	1.82	0.61
1:K:385:THR:HG22	1:L:284:ARG:HH22	1.64	0.61
1:A:30:THR:O	3:A:552:TL:TL	2.22	0.61
1:F:321:LYS:O	1:F:322:ARG:HB2	2.01	0.61
1:B:417:VAL:HA	1:B:420:ILE:HG22	1.82	0.61
1:C:77:VAL:HG21	1:C:510:VAL:HG11	1.82	0.61
1:D:173:GLY:O	1:D:404:ARG:NH2	2.33	0.61
1:A:158:VAL:HG13	1:A:396:VAL:HG22	1.82	0.61
1:J:27:VAL:HG12	1:J:90:THR:HG23	1.83	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:417:VAL:HA	1:D:420:ILE:HG22	1.83	0.61
1:K:77:VAL:HG21	1:K:510:VAL:HG11	1.81	0.61
1:A:195:PHE:CE2	1:A:197:ARG:HB2	2.36	0.61
1:H:417:VAL:HA	1:H:420:ILE:HG22	1.82	0.61
1:C:27:VAL:HG12	1:C:90:THR:HG23	1.83	0.61
1:G:77:VAL:HG21	1:G:510:VAL:HG11	1.83	0.61
1:B:77:VAL:HG21	1:B:510:VAL:HG11	1.82	0.60
1:E:27:VAL:HG12	1:E:90:THR:HG23	1.83	0.60
1:I:483:GLU:OE2	3:I:551:TL:TL	2.23	0.60
1:N:417:VAL:HA	1:N:420:ILE:HG22	1.81	0.60
1:I:288:MET:HG2	1:I:368:ARG:HD3	1.83	0.60
1:E:324:VAL:HB	1:E:331:THR:HG23	1.83	0.60
1:H:77:VAL:HG21	1:H:510:VAL:HG11	1.83	0.60
1:K:417:VAL:HA	1:K:420:ILE:HG22	1.84	0.60
1:G:87:ASP:OD2	1:G:499:VAL:HG21	2.00	0.60
1:K:27:VAL:HG12	1:K:90:THR:HG23	1.84	0.60
1:G:27:VAL:HG12	1:G:90:THR:HG23	1.84	0.59
1:I:325:ILE:HG12	1:I:330:THR:HG23	1.84	0.59
1:F:197:ARG:NE	1:F:277:LYS:HB2	2.17	0.59
1:N:77:VAL:HG21	1:N:510:VAL:HG11	1.84	0.59
1:E:173:GLY:O	1:E:404:ARG:NH2	2.36	0.59
1:F:197:ARG:HE	1:F:277:LYS:HB2	1.67	0.59
1:B:27:VAL:HG12	1:B:90:THR:HG23	1.85	0.59
1:F:186:GLU:HB2	1:F:380:LYS:HB2	1.83	0.59
1:A:200:LEU:HD11	1:A:277:LYS:HG3	1.84	0.59
1:E:204:PHE:CD1	1:E:274:ALA:HA	2.38	0.59
1:K:219:PHE:HE2	1:K:245:LYS:HB2	1.67	0.59
1:A:195:PHE:HE2	1:A:197:ARG:HB2	1.66	0.59
1:D:261:THR:O	1:D:265:ASN:HB2	2.03	0.59
1:I:240:VAL:HG21	1:I:247:LEU:HD22	1.84	0.59
1:L:27:VAL:HG12	1:L:90:THR:HG23	1.85	0.59
1:G:173:GLY:O	1:G:404:ARG:NH2	2.36	0.59
1:I:173:GLY:O	1:I:404:ARG:NH2	2.36	0.59
1:J:266:THR:HG22	1:J:273:VAL:H	1.68	0.59
1:A:261:THR:O	1:A:265:ASN:HB2	2.03	0.58
1:J:262:LEU:O	1:J:266:THR:HG23	2.02	0.58
1:C:284:ARG:HB3	1:C:364:LYS:NZ	2.18	0.58
1:A:173:GLY:O	1:A:404:ARG:NH2	2.36	0.58
1:E:183:LEU:HD22	1:F:360:TYR:CG	2.38	0.58
1:F:350:ARG:HA	1:F:353:ILE:HD12	1.84	0.58
1:N:27:VAL:HG12	1:N:90:THR:HG23	1.86	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:GLY:O	1:B:404:ARG:NH2	2.37	0.58
1:G:221:LEU:HB3	1:G:249:ILE:HG23	1.85	0.58
1:K:358:SER:HB3	1:K:361:ASP:HB2	1.84	0.58
1:M:173:GLY:O	1:M:404:ARG:NH2	2.36	0.58
1:N:392:LYS:O	1:N:396:VAL:HG23	2.02	0.58
1:D:269:GLY:HA3	1:E:257:GLU:HB2	1.86	0.58
1:K:382:GLY:HA2	1:K:389:MET:HG2	1.84	0.58
1:I:27:VAL:HG12	1:I:90:THR:HG23	1.85	0.58
1:K:234:LEU:N	1:K:235:PRO:HD2	2.19	0.58
1:A:326:ASN:HB2	1:A:329:THR:HB	1.85	0.57
1:J:173:GLY:O	1:J:404:ARG:NH2	2.37	0.57
1:A:27:VAL:HG12	1:A:90:THR:HG23	1.86	0.57
1:F:173:GLY:O	1:F:404:ARG:NH2	2.38	0.57
1:H:173:GLY:O	1:H:404:ARG:NH2	2.37	0.57
1:A:313:THR:HG22	1:A:314:LEU:H	1.68	0.57
1:M:417:VAL:HA	1:M:420:ILE:HG22	1.85	0.57
1:A:176:THR:HG21	1:A:333:ILE:HD11	1.85	0.57
1:C:173:GLY:O	1:C:404:ARG:NH2	2.36	0.57
1:L:173:GLY:O	1:L:404:ARG:NH2	2.38	0.57
1:K:173:GLY:O	1:K:404:ARG:NH2	2.38	0.57
1:L:350:ARG:HG3	1:L:353:ILE:HD12	1.87	0.57
1:N:173:GLY:O	1:N:404:ARG:NH2	2.37	0.57
1:F:287:ALA:O	1:F:291:ASP:HB2	2.05	0.57
1:K:323:VAL:HG12	1:K:332:ILE:HA	1.87	0.57
1:A:519:CYS:HB3	1:G:38:VAL:HG22	1.85	0.56
1:G:186:GLU:HB2	1:G:380:LYS:HB2	1.87	0.56
1:A:38:VAL:HG22	1:B:519:CYS:HB3	1.85	0.56
1:E:262:LEU:HD22	1:E:273:VAL:HG11	1.85	0.56
1:G:213:VAL:HB	1:G:325:ILE:HB	1.86	0.56
1:L:206:ASN:HD21	1:L:214:GLU:H	1.52	0.56
1:A:77:VAL:HG21	1:A:510:VAL:HG11	1.85	0.56
1:J:77:VAL:HG12	1:J:506:TYR:HB3	1.87	0.56
1:I:235:PRO:HG3	1:I:310:GLU:HA	1.87	0.56
1:F:358:SER:HB3	1:F:361:ASP:HB2	1.88	0.56
1:B:219:PHE:CE2	1:B:245:LYS:HB2	2.40	0.56
1:K:180:GLY:HA2	1:K:380:LYS:HB3	1.87	0.56
1:M:180:GLY:HA2	1:M:380:LYS:HB3	1.87	0.56
1:E:202:PRO:O	1:E:205:ILE:HG12	2.06	0.56
1:A:325:ILE:HG12	1:A:330:THR:HG23	1.88	0.56
1:F:158:VAL:HG13	1:F:396:VAL:HG22	1.87	0.55
1:K:313:THR:HG22	1:K:314:LEU:HG	1.88	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:235:PRO:HG3	1:M:310:GLU:HG3	1.88	0.55
1:G:223:ALA:O	1:G:251:ALA:HA	2.06	0.55
1:A:180:GLY:HA2	1:A:380:LYS:HB3	1.88	0.55
1:C:180:GLY:HA3	1:C:381:VAL:O	2.06	0.55
1:D:220:ILE:HD13	1:D:296:THR:HG21	1.89	0.55
1:B:325:ILE:HG13	1:B:330:THR:HG23	1.89	0.54
1:H:22:VAL:HG11	1:H:62:LEU:HD21	1.89	0.54
1:E:415:GLY:N	2:E:549:AGS:O2'	2.36	0.54
1:C:496:PRO:O	1:C:499:VAL:HG12	2.08	0.53
1:D:158:VAL:HG13	1:D:396:VAL:HG22	1.90	0.53
1:F:224:ASP:HB3	1:F:302:SER:HA	1.90	0.53
1:J:496:PRO:O	1:J:499:VAL:HG12	2.08	0.53
1:L:247:LEU:HB3	1:L:273:VAL:HG22	1.89	0.53
1:E:496:PRO:O	1:E:499:VAL:HG12	2.07	0.53
1:I:180:GLY:HA2	1:I:380:LYS:HB3	1.90	0.53
1:C:415:GLY:N	2:C:549:AGS:O2'	2.36	0.53
1:D:230:ILE:HA	1:D:233:MET:HB2	1.90	0.53
1:G:496:PRO:O	1:G:499:VAL:HG12	2.08	0.53
1:A:496:PRO:O	1:A:499:VAL:HG12	2.09	0.53
1:D:22:VAL:HG11	1:D:62:LEU:HD21	1.91	0.53
1:C:230:ILE:HD13	1:C:261:THR:HB	1.91	0.53
1:B:323:VAL:HG12	1:B:332:ILE:HA	1.90	0.53
1:I:223:ALA:O	1:I:251:ALA:HA	2.09	0.53
1:I:496:PRO:O	1:I:499:VAL:HG12	2.09	0.53
1:N:22:VAL:HG11	1:N:62:LEU:HD21	1.91	0.53
1:K:233:MET:C	1:K:235:PRO:HD2	2.29	0.52
1:J:77:VAL:CG1	1:J:506:TYR:HB3	2.38	0.52
1:B:385:THR:O	1:B:387:VAL:N	2.40	0.52
1:L:22:VAL:HG11	1:L:62:LEU:HD21	1.91	0.52
1:C:22:VAL:HG11	1:C:62:LEU:HD21	1.92	0.52
1:J:415:GLY:N	2:J:549:AGS:O2'	2.28	0.52
1:D:288:MET:O	1:D:291:ASP:HB2	2.09	0.52
1:I:180:GLY:HA3	1:I:381:VAL:O	2.10	0.52
1:F:22:VAL:HG11	1:F:62:LEU:HD21	1.91	0.52
1:F:258:ALA:O	1:F:262:LEU:HG	2.10	0.52
1:L:183:LEU:HD22	1:M:360:TYR:CG	2.45	0.52
1:L:496:PRO:O	1:L:499:VAL:HG12	2.09	0.52
1:G:323:VAL:HG12	1:G:332:ILE:HA	1.92	0.52
1:G:177:VAL:HG22	1:G:379:ILE:HB	1.91	0.52
1:A:218:PRO:HG3	1:A:323:VAL:HG22	1.92	0.51
1:G:22:VAL:HG11	1:G:62:LEU:HD21	1.91	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:324:VAL:HB	1:J:331:THR:HG23	1.91	0.51
1:M:77:VAL:HG12	1:M:506:TYR:HB3	1.91	0.51
1:N:234:LEU:H	1:N:235:PRO:CD	2.19	0.51
1:I:26:ALA:HA	1:J:8:PHE:HE1	1.75	0.51
1:C:176:THR:HG21	1:C:333:ILE:HD11	1.93	0.51
1:D:266:THR:CG2	1:D:273:VAL:HG12	2.40	0.51
1:J:22:VAL:HG11	1:J:62:LEU:HD21	1.92	0.51
1:K:22:VAL:HG11	1:K:62:LEU:HD21	1.93	0.51
1:D:415:GLY:N	2:D:549:AGS:O2'	2.29	0.51
1:I:288:MET:O	1:I:292:ILE:HG13	2.10	0.51
1:N:496:PRO:O	1:N:499:VAL:HG12	2.10	0.51
1:G:218:PRO:HG3	1:G:323:VAL:HG22	1.92	0.51
1:H:496:PRO:O	1:H:499:VAL:HG12	2.10	0.51
1:I:87:ASP:OD2	1:I:499:VAL:HG21	2.11	0.51
1:I:366:GLN:HA	1:I:369:VAL:HG22	1.93	0.51
1:B:392:LYS:O	1:B:396:VAL:HG23	2.11	0.51
1:H:77:VAL:HG12	1:H:506:TYR:HB3	1.92	0.51
1:M:22:VAL:HG11	1:M:62:LEU:HD21	1.93	0.51
1:N:77:VAL:HG12	1:N:506:TYR:HB3	1.91	0.51
1:H:284:ARG:HH22	1:N:385:THR:HG22	1.76	0.50
1:M:221:LEU:HD23	1:M:249:ILE:HG23	1.92	0.50
1:M:261:THR:O	1:M:265:ASN:HB2	2.11	0.50
1:B:353:ILE:HD13	1:B:366:GLN:HE21	1.76	0.50
1:B:496:PRO:O	1:B:499:VAL:HG12	2.12	0.50
1:F:496:PRO:O	1:F:499:VAL:HG12	2.10	0.50
1:A:197:ARG:NH2	1:G:386:GLU:OE2	2.44	0.50
1:C:177:VAL:HG22	1:C:379:ILE:HB	1.93	0.50
1:D:496:PRO:O	1:D:499:VAL:HG12	2.10	0.50
1:L:77:VAL:HG12	1:L:506:TYR:HB3	1.92	0.50
1:M:496:PRO:O	1:M:499:VAL:HG12	2.11	0.50
1:A:320:ALA:HA	1:A:335:GLY:HA2	1.93	0.50
1:B:219:PHE:HE2	1:B:245:LYS:HB2	1.75	0.50
1:E:325:ILE:HG12	1:E:330:THR:HG23	1.94	0.50
1:G:234:LEU:HB2	1:G:235:PRO:HD3	1.94	0.50
1:C:77:VAL:HG12	1:C:506:TYR:HB3	1.92	0.50
1:J:187:LEU:HD13	1:J:379:ILE:HG12	1.93	0.50
1:A:200:LEU:HD13	1:A:276:VAL:HA	1.93	0.50
1:B:197:ARG:HH11	1:B:277:LYS:HD3	1.77	0.50
1:D:194:GLN:HG3	1:D:331:THR:HB	1.94	0.50
1:K:38:VAL:HG22	1:L:519:CYS:HB3	1.94	0.50
1:E:383:ALA:O	1:E:384:ALA:HB3	2.12	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:22:VAL:HG11	1:I:62:LEU:HD21	1.93	0.50
1:C:222:LEU:HD13	1:C:293:ALA:HA	1.93	0.49
1:K:496:PRO:O	1:K:499:VAL:HG12	2.12	0.49
1:I:225:LYS:HG2	1:I:303:GLU:HG3	1.93	0.49
1:K:270:ILE:HG22	1:K:271:VAL:HG23	1.93	0.49
1:N:183:LEU:O	1:N:183:LEU:HG	2.11	0.49
1:A:183:LEU:HD22	1:B:360:TYR:CD2	2.47	0.49
1:D:360:TYR:CE1	1:D:364:LYS:HE3	2.48	0.49
1:E:22:VAL:HG11	1:E:62:LEU:HD21	1.94	0.49
1:A:22:VAL:HG11	1:A:62:LEU:HD21	1.94	0.49
1:E:194:GLN:HG3	1:E:331:THR:HB	1.92	0.49
1:G:77:VAL:HG12	1:G:506:TYR:HB3	1.93	0.49
1:C:323:VAL:HG12	1:C:332:ILE:HA	1.94	0.49
1:B:321:LYS:O	1:B:322:ARG:HB2	2.11	0.49
1:C:325:ILE:HG12	1:C:330:THR:HG23	1.94	0.49
1:D:266:THR:HG21	1:D:273:VAL:HG12	1.93	0.49
1:H:183:LEU:HD22	1:I:360:TYR:CD2	2.48	0.49
1:M:247:LEU:HB3	1:M:273:VAL:HG22	1.95	0.49
1:A:349:ILE:HG21	1:A:369:VAL:HG13	1.93	0.49
1:L:183:LEU:O	1:L:183:LEU:HG	2.13	0.49
1:F:183:LEU:HD22	1:G:360:TYR:CD2	2.48	0.49
1:H:194:GLN:HG3	1:H:331:THR:HB	1.95	0.49
1:K:269:GLY:HA3	1:L:257:GLU:HB2	1.95	0.49
1:K:320:ALA:HA	1:K:335:GLY:HA2	1.95	0.49
1:F:204:PHE:CD1	1:F:274:ALA:HA	2.48	0.49
1:B:180:GLY:HA3	1:B:381:VAL:O	2.12	0.49
1:E:77:VAL:HG12	1:E:506:TYR:HB3	1.94	0.49
1:F:366:GLN:HA	1:F:369:VAL:HG22	1.94	0.49
1:K:414:GLY:O	1:K:417:VAL:HG22	2.13	0.49
1:M:77:VAL:CG1	1:M:506:TYR:HB3	2.43	0.49
1:F:324:VAL:HB	1:F:331:THR:HG23	1.95	0.48
1:G:219:PHE:HE2	1:G:245:LYS:HB2	1.77	0.48
1:I:224:ASP:HB3	1:I:302:SER:HB3	1.95	0.48
1:D:414:GLY:O	1:D:417:VAL:HG22	2.13	0.48
1:H:158:VAL:HG13	1:H:396:VAL:HG22	1.94	0.48
1:J:183:LEU:HG	1:J:183:LEU:O	2.13	0.48
1:K:77:VAL:HG12	1:K:506:TYR:HB3	1.94	0.48
1:H:31:LEU:HD23	1:H:453:GLN:HB3	1.96	0.48
1:E:223:ALA:O	1:E:251:ALA:HA	2.14	0.48
1:H:392:LYS:O	1:H:396:VAL:HG23	2.13	0.48
1:I:314:LEU:HA	1:I:317:LEU:HD13	1.94	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:ARG:HE	1:D:279:PRO:HA	1.79	0.48
1:H:198:GLY:HA3	1:H:327:LYS:O	2.13	0.48
1:K:384:ALA:HB3	1:K:388:GLU:HB2	1.95	0.48
1:B:366:GLN:HA	1:B:369:VAL:HG22	1.96	0.48
1:C:284:ARG:HB3	1:C:364:LYS:HZ1	1.79	0.48
1:A:222:LEU:HD13	1:A:293:ALA:HA	1.95	0.48
1:I:77:VAL:HG12	1:I:506:TYR:HB3	1.95	0.48
1:A:198:GLY:O	1:A:276:VAL:HG12	2.13	0.48
1:K:183:LEU:HG	1:K:183:LEU:O	2.14	0.48
1:M:183:LEU:O	1:M:183:LEU:HG	2.12	0.48
1:I:220:ILE:N	1:I:318:GLY:O	2.45	0.47
1:L:77:VAL:CG1	1:L:506:TYR:HB3	2.44	0.47
1:F:183:LEU:HG	1:F:183:LEU:O	2.12	0.47
1:C:186:GLU:HB2	1:C:380:LYS:HB2	1.96	0.47
1:B:38:VAL:HG22	1:C:519:CYS:HB3	1.95	0.47
1:D:77:VAL:HG12	1:D:506:TYR:HB3	1.95	0.47
1:G:414:GLY:O	1:G:417:VAL:HG22	2.14	0.47
1:A:313:THR:H	1:A:316:ASP:HB2	1.79	0.47
1:A:77:VAL:HG12	1:A:506:TYR:HB3	1.96	0.47
1:G:183:LEU:HG	1:G:183:LEU:O	2.13	0.47
1:B:77:VAL:HG12	1:B:506:TYR:HB3	1.96	0.47
1:F:323:VAL:HG12	1:F:332:ILE:HA	1.97	0.47
1:G:251:ALA:O	1:G:252:GLU:C	2.52	0.47
1:N:77:VAL:CG1	1:N:506:TYR:HB3	2.45	0.47
1:B:183:LEU:HG	1:B:183:LEU:O	2.15	0.47
1:F:213:VAL:HB	1:F:325:ILE:HB	1.96	0.47
1:H:414:GLY:O	1:H:417:VAL:HG22	2.14	0.47
1:I:236:VAL:O	1:I:240:VAL:HG23	2.15	0.47
1:I:247:LEU:HG	1:I:249:ILE:HD11	1.97	0.47
1:A:414:GLY:O	1:A:417:VAL:HG22	2.15	0.47
1:A:87:ASP:OD2	1:A:499:VAL:HG11	2.15	0.47
1:B:335:GLY:C	1:B:337:GLY:H	2.17	0.47
1:E:326:ASN:HB2	1:E:329:THR:HB	1.97	0.47
1:G:194:GLN:HG3	1:G:330:THR:O	2.14	0.47
1:B:22:VAL:HG11	1:B:62:LEU:HD21	1.96	0.47
1:J:314:LEU:HA	1:J:317:LEU:HD13	1.97	0.47
1:E:230:ILE:HD13	1:E:261:THR:HB	1.97	0.47
1:E:234:LEU:N	1:E:235:PRO:HD2	2.30	0.47
1:F:175:ILE:HA	1:F:377:ALA:HB3	1.96	0.47
1:A:240:VAL:HG11	1:A:247:LEU:HB2	1.97	0.46
1:A:247:LEU:HB3	1:A:273:VAL:HG22	1.97	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:192:GLY:H	1:F:375:GLY:HA2	1.80	0.46
1:N:234:LEU:N	1:N:235:PRO:CD	2.75	0.46
1:A:183:LEU:O	1:A:183:LEU:HG	2.15	0.46
1:D:324:VAL:HB	1:D:331:THR:HG23	1.97	0.46
1:J:269:GLY:HA3	1:K:257:GLU:HB2	1.96	0.46
1:K:258:ALA:O	1:K:262:LEU:HG	2.15	0.46
1:K:321:LYS:O	1:K:322:ARG:HB2	2.15	0.46
1:N:174:VAL:HB	1:N:376:VAL:HG22	1.97	0.46
1:C:77:VAL:CG1	1:C:506:TYR:HB3	2.46	0.46
1:E:183:LEU:HG	1:E:183:LEU:O	2.15	0.46
1:F:251:ALA:O	1:F:252:GLU:C	2.54	0.46
1:J:230:ILE:C	1:J:232:GLU:H	2.17	0.46
1:A:77:VAL:CG1	1:A:506:TYR:HB3	2.45	0.46
1:D:259:LEU:O	1:D:263:VAL:HG23	2.15	0.46
1:K:77:VAL:CG1	1:K:506:TYR:HB3	2.46	0.46
1:N:31:LEU:HD23	1:N:453:GLN:HB3	1.97	0.46
1:G:336:VAL:O	1:G:337:GLY:C	2.54	0.46
1:H:183:LEU:HG	1:H:183:LEU:O	2.15	0.46
1:I:194:GLN:HG3	1:I:331:THR:HB	1.97	0.46
1:C:183:LEU:O	1:C:183:LEU:HG	2.16	0.46
1:E:112:ASN:HD22	1:E:113:PRO:HD2	1.81	0.46
1:G:200:LEU:HD21	1:G:277:LYS:HG3	1.98	0.46
1:K:222:LEU:HB3	1:K:289:LEU:HD22	1.98	0.46
1:K:31:LEU:HD23	1:K:453:GLN:HB3	1.98	0.46
1:H:218:PRO:HD2	1:H:320:ALA:O	2.15	0.46
1:J:180:GLY:HA2	1:J:380:LYS:HB3	1.98	0.46
1:D:77:VAL:CG1	1:D:506:TYR:HB3	2.46	0.46
1:H:25:ASP:HA	1:H:28:LYS:HG2	1.98	0.46
1:H:77:VAL:CG1	1:H:506:TYR:HB3	2.45	0.46
1:H:112:ASN:HD22	1:H:113:PRO:HD2	1.81	0.46
1:A:87:ASP:CG	1:A:499:VAL:HG21	2.34	0.46
1:B:31:LEU:HD23	1:B:453:GLN:HB3	1.97	0.46
1:D:177:VAL:HG22	1:D:379:ILE:HB	1.97	0.46
1:F:414:GLY:O	1:F:417:VAL:HG22	2.16	0.46
1:I:222:LEU:HD21	1:I:250:ILE:HD12	1.97	0.46
1:N:197:ARG:HD2	1:N:277:LYS:HB2	1.97	0.46
1:C:112:ASN:HD22	1:C:113:PRO:HD2	1.81	0.45
1:F:77:VAL:HG12	1:F:506:TYR:HB3	1.97	0.45
1:J:222:LEU:HB3	1:J:289:LEU:HD21	1.97	0.45
1:L:217:SER:N	1:L:218:PRO:HD3	2.32	0.45
1:C:31:LEU:HD23	1:C:453:GLN:HB3	1.97	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:31:LEU:HD23	1:J:453:GLN:HB3	1.99	0.45
1:G:219:PHE:CE2	1:G:245:LYS:HB2	2.52	0.45
1:N:414:GLY:O	1:N:417:VAL:HG22	2.15	0.45
1:B:176:THR:HG21	1:B:333:ILE:HD11	1.98	0.45
1:C:25:ASP:HA	1:C:28:LYS:HG2	1.98	0.45
1:D:180:GLY:HA2	1:D:380:LYS:HB3	1.98	0.45
1:F:77:VAL:CG1	1:F:506:TYR:HB3	2.47	0.45
1:G:77:VAL:CG1	1:G:506:TYR:HB3	2.46	0.45
1:H:338:GLU:O	1:H:342:ILE:HG13	2.15	0.45
1:J:313:THR:HG22	1:J:314:LEU:H	1.81	0.45
1:D:112:ASN:HD22	1:D:113:PRO:HD2	1.82	0.45
1:K:266:THR:HG22	1:K:273:VAL:H	1.80	0.45
1:M:220:ILE:HG12	1:M:248:LEU:HD23	1.99	0.45
1:B:201:SER:C	1:B:203:TYR:H	2.19	0.45
1:I:77:VAL:CG1	1:I:506:TYR:HB3	2.47	0.45
1:E:31:LEU:HD23	1:E:453:GLN:HB3	1.99	0.45
1:F:217:SER:N	1:F:218:PRO:HD3	2.31	0.45
1:F:220:ILE:HD11	1:F:320:ALA:CB	2.46	0.45
1:G:31:LEU:HD23	1:G:453:GLN:HB3	1.98	0.45
1:G:214:GLU:OE2	1:G:322:ARG:NH2	2.50	0.45
1:J:26:ALA:HA	1:K:8:PHE:HE1	1.82	0.45
1:H:360:TYR:CD1	1:N:183:LEU:HD22	2.50	0.45
1:B:414:GLY:O	1:B:417:VAL:HG22	2.17	0.45
1:H:321:LYS:O	1:H:322:ARG:CB	2.62	0.45
1:I:230:ILE:HD13	1:I:261:THR:HB	1.98	0.45
1:L:25:ASP:HA	1:L:28:LYS:HG2	1.99	0.45
1:M:227:ILE:HD12	1:M:254:VAL:HG22	1.98	0.45
1:A:417:VAL:HG11	1:A:477:GLY:HA3	1.99	0.45
1:H:222:LEU:HD23	1:H:250:ILE:HB	1.97	0.45
1:M:112:ASN:HD22	1:M:113:PRO:HD2	1.82	0.45
1:D:183:LEU:O	1:D:183:LEU:HG	2.17	0.45
1:F:325:ILE:HG12	1:F:330:THR:HG23	1.98	0.45
1:G:302:SER:H	1:G:307:MET:HE1	1.81	0.45
1:H:360:TYR:CB	1:N:183:LEU:HD22	2.46	0.45
1:I:158:VAL:HG13	1:I:396:VAL:HG22	2.00	0.44
1:F:218:PRO:HG3	1:F:323:VAL:HG22	1.99	0.44
1:I:183:LEU:O	1:I:183:LEU:HG	2.16	0.44
1:I:39:VAL:HG23	1:J:517:THR:HG23	1.99	0.44
1:L:31:LEU:HD23	1:L:453:GLN:HB3	1.99	0.44
1:C:321:LYS:O	1:C:322:ARG:HB2	2.17	0.44
1:F:31:LEU:HD23	1:F:453:GLN:HB3	1.99	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:220:ILE:HD12	1:K:296:THR:HG21	1.99	0.44
1:L:112:ASN:HD22	1:L:113:PRO:HD2	1.83	0.44
1:B:232:GLU:HB3	1:B:309:LEU:HB2	1.98	0.44
1:D:350:ARG:HG3	1:D:353:ILE:HD11	2.00	0.44
1:I:229:ASN:HB3	1:I:231:ARG:HG3	1.99	0.44
1:J:112:ASN:HD22	1:J:113:PRO:HD2	1.81	0.44
1:C:414:GLY:O	1:C:417:VAL:HG22	2.18	0.44
1:F:221:LEU:HD21	1:F:309:LEU:HD21	1.99	0.44
1:I:112:ASN:HD22	1:I:113:PRO:HD2	1.81	0.44
1:B:417:VAL:HG11	1:B:477:GLY:HA3	1.99	0.44
1:E:360:TYR:OH	1:E:364:LYS:HE3	2.17	0.44
1:G:203:TYR:HB3	1:G:267:MET:SD	2.58	0.44
1:H:417:VAL:HG11	1:H:477:GLY:HA3	2.00	0.44
1:D:31:LEU:HD23	1:D:453:GLN:HB3	1.99	0.44
1:I:227:ILE:HB	1:I:254:VAL:HG13	1.99	0.44
1:C:324:VAL:HB	1:C:331:THR:HG23	2.00	0.44
1:G:180:GLY:HA3	1:G:381:VAL:O	2.18	0.44
1:I:31:LEU:HD23	1:I:453:GLN:HB3	1.99	0.44
1:L:392:LYS:O	1:L:396:VAL:HG23	2.18	0.44
1:L:38:VAL:HG22	1:M:519:CYS:HB3	2.00	0.44
1:A:112:ASN:HD22	1:A:113:PRO:HD2	1.82	0.44
1:C:217:SER:N	1:C:218:PRO:HD3	2.33	0.44
1:C:37:ASN:HD22	1:C:49:ILE:CG2	2.28	0.44
1:D:247:LEU:HB3	1:D:273:VAL:HG23	1.99	0.44
1:J:220:ILE:HG13	1:J:248:LEU:HB3	2.00	0.44
1:D:273:VAL:HG22	1:D:274:ALA:H	1.82	0.43
1:H:258:ALA:O	1:H:262:LEU:HG	2.18	0.43
1:H:353:ILE:H	1:H:353:ILE:HG13	1.66	0.43
1:J:305:ILE:HG21	1:J:307:MET:HE2	2.00	0.43
1:K:177:VAL:HG22	1:K:379:ILE:HB	2.00	0.43
1:B:25:ASP:HA	1:B:28:LYS:HG2	1.99	0.43
1:C:417:VAL:HG11	1:C:477:GLY:HA3	1.99	0.43
1:I:266:THR:HG22	1:I:273:VAL:H	1.82	0.43
1:I:417:VAL:HG11	1:I:477:GLY:HA3	2.01	0.43
1:M:417:VAL:HG11	1:M:477:GLY:HA3	2.00	0.43
1:A:273:VAL:HG12	1:A:274:ALA:N	2.33	0.43
1:B:227:ILE:HD12	1:B:254:VAL:HG22	1.99	0.43
1:E:112:ASN:HD22	1:E:113:PRO:CD	2.31	0.43
1:F:25:ASP:HA	1:F:28:LYS:HG2	1.99	0.43
1:F:177:VAL:HG22	1:F:379:ILE:HB	1.99	0.43
1:J:417:VAL:HG11	1:J:477:GLY:HA3	2.00	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:417:VAL:HG11	1:N:477:GLY:HA3	2.01	0.43
1:A:323:VAL:HG12	1:A:332:ILE:HA	2.00	0.43
1:B:475:ASN:N	1:B:475:ASN:HD22	2.17	0.43
1:E:77:VAL:CG1	1:E:506:TYR:HB3	2.48	0.43
1:I:25:ASP:HA	1:I:28:LYS:HG2	2.01	0.43
1:M:25:ASP:HA	1:M:28:LYS:HG2	2.01	0.43
1:B:77:VAL:CG1	1:B:506:TYR:HB3	2.48	0.43
1:E:25:ASP:HA	1:E:28:LYS:HG2	2.00	0.43
1:F:112:ASN:HD22	1:F:113:PRO:HD2	1.84	0.43
1:G:25:ASP:HA	1:G:28:LYS:HG2	1.99	0.43
1:J:232:GLU:HB3	1:J:309:LEU:HD12	2.01	0.43
1:N:25:ASP:HA	1:N:28:LYS:HG2	2.01	0.43
1:A:31:LEU:HD23	1:A:453:GLN:HB3	2.01	0.43
1:D:180:GLY:HA3	1:D:381:VAL:O	2.18	0.43
1:E:236:VAL:O	1:E:240:VAL:N	2.51	0.43
1:E:414:GLY:O	1:E:417:VAL:HG22	2.18	0.43
1:G:216:GLU:H	1:G:246:PRO:HG3	1.83	0.43
1:G:219:PHE:HB3	1:G:317:LEU:HD23	2.01	0.43
1:K:291:ASP:OD1	1:K:368:ARG:NH1	2.52	0.43
1:K:475:ASN:HD22	1:K:475:ASN:N	2.16	0.43
1:N:112:ASN:HD22	1:N:113:PRO:HD2	1.83	0.43
1:A:177:VAL:HG22	1:A:379:ILE:HG13	2.01	0.43
1:F:314:LEU:HG	1:F:315:GLU:N	2.34	0.43
1:F:320:ALA:HA	1:F:335:GLY:HA2	2.01	0.43
1:G:198:GLY:HA3	1:G:327:LYS:O	2.18	0.43
1:H:224:ASP:O	1:H:225:LYS:HB3	2.19	0.43
1:J:414:GLY:O	1:J:417:VAL:HG22	2.19	0.43
1:B:302:SER:HB2	1:B:304:GLU:HG2	2.01	0.43
1:C:112:ASN:HD22	1:C:113:PRO:CD	2.32	0.43
1:C:199:TYR:HA	1:C:276:VAL:HG12	2.01	0.43
1:D:112:ASN:HD22	1:D:113:PRO:CD	2.32	0.43
1:G:232:GLU:HA	1:G:310:GLU:HG3	2.01	0.43
1:J:112:ASN:HD22	1:J:113:PRO:CD	2.31	0.43
1:K:88:GLY:HA2	2:K:549:AGS:O2B	2.18	0.43
1:G:417:VAL:HG11	1:G:477:GLY:HA3	2.00	0.43
1:A:25:ASP:HA	1:A:28:LYS:HG2	2.00	0.42
1:A:360:TYR:CB	1:G:183:LEU:HD22	2.49	0.42
1:J:496:PRO:O	1:J:499:VAL:CG1	2.67	0.42
1:J:496:PRO:HB2	1:J:499:VAL:HG12	1.99	0.42
1:L:414:GLY:O	1:L:417:VAL:HG22	2.19	0.42
1:M:201:SER:HB3	1:M:204:PHE:CE2	2.54	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:293:ALA:HB2	1:E:300:VAL:HG23	2.01	0.42
1:H:112:ASN:HD22	1:H:113:PRO:CD	2.33	0.42
1:H:261:THR:O	1:H:265:ASN:HB2	2.18	0.42
1:H:248:LEU:HD13	1:H:325:ILE:HD11	2.00	0.42
1:K:417:VAL:HG11	1:K:477:GLY:HA3	2.01	0.42
1:C:496:PRO:O	1:C:499:VAL:CG1	2.68	0.42
1:D:228:SER:O	1:D:257:GLU:HB3	2.19	0.42
1:K:25:ASP:HA	1:K:28:LYS:HG2	2.01	0.42
1:A:112:ASN:HD22	1:A:113:PRO:CD	2.32	0.42
1:A:289:LEU:HD22	1:A:300:VAL:HG23	2.01	0.42
1:I:415:GLY:N	2:I:549:AGS:O2'	2.48	0.42
1:E:200:LEU:HD13	1:E:254:VAL:HB	2.01	0.42
1:E:385:THR:OG1	1:E:388:GLU:HB2	2.20	0.42
1:F:183:LEU:HD22	1:G:360:TYR:CG	2.55	0.42
1:G:236:VAL:HG13	1:G:317:LEU:HD11	2.01	0.42
1:I:414:GLY:O	1:I:417:VAL:HG22	2.19	0.42
1:N:325:ILE:HG13	1:N:330:THR:HG23	2.01	0.42
1:C:204:PHE:HE1	1:C:273:VAL:O	2.03	0.42
1:F:266:THR:HG22	1:F:271:VAL:O	2.20	0.42
1:K:338:GLU:HG2	1:K:338:GLU:H	1.66	0.42
1:L:365:LEU:HD22	1:L:368:ARG:HH21	1.84	0.42
1:G:112:ASN:HD22	1:G:113:PRO:HD2	1.84	0.42
1:J:343:GLN:O	1:J:346:VAL:HB	2.19	0.42
1:J:345:ARG:HA	1:J:348:GLN:HB2	2.01	0.42
1:I:59:GLU:O	1:J:4:LYS:HG3	2.19	0.42
1:J:57:ALA:O	1:J:75:LYS:HD2	2.19	0.42
1:A:181:THR:O	1:B:282:GLY:HA3	2.20	0.42
1:A:223:ALA:O	1:A:251:ALA:HA	2.19	0.42
1:C:475:ASN:N	1:C:475:ASN:HD22	2.18	0.42
1:D:321:LYS:HB2	1:D:334:ASP:HB3	2.02	0.42
1:H:177:VAL:HG22	1:H:379:ILE:HB	2.01	0.42
1:I:112:ASN:HD22	1:I:113:PRO:CD	2.32	0.42
1:I:340:ALA:O	1:I:344:GLY:N	2.49	0.42
1:I:475:ASN:HD22	1:I:475:ASN:N	2.18	0.42
1:K:112:ASN:HD22	1:K:113:PRO:HD2	1.85	0.42
1:K:392:LYS:O	1:K:396:VAL:HG23	2.19	0.42
1:M:177:VAL:HG21	1:M:396:VAL:HG12	2.00	0.42
1:B:254:VAL:HG21	1:B:275:ALA:HB1	2.01	0.42
1:C:218:PRO:HD2	1:C:320:ALA:HB3	2.01	0.42
1:D:195:PHE:HA	1:D:371:LYS:HE3	2.00	0.42
1:I:217:SER:N	1:I:218:PRO:HD3	2.34	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:312:ALA:HA	1:M:316:ASP:HB2	2.02	0.42
1:M:392:LYS:O	1:M:396:VAL:HG23	2.20	0.41
1:A:270:ILE:O	1:A:272:LYS:N	2.47	0.41
1:E:417:VAL:HG11	1:E:477:GLY:HA3	2.01	0.41
1:A:349:ILE:HG23	1:A:365:LEU:HD22	2.02	0.41
1:D:25:ASP:HA	1:D:28:LYS:HG2	2.01	0.41
1:E:240:VAL:HG21	1:E:247:LEU:HD22	2.02	0.41
1:J:39:VAL:HG23	1:K:517:THR:HG23	2.01	0.41
1:K:266:THR:CG2	1:K:273:VAL:H	2.33	0.41
1:M:31:LEU:HD23	1:M:453:GLN:HB3	2.01	0.41
1:N:217:SER:N	1:N:218:PRO:HD3	2.35	0.41
1:D:417:VAL:HG11	1:D:477:GLY:HA3	2.01	0.41
1:F:417:VAL:HG11	1:F:477:GLY:HA3	2.01	0.41
1:G:197:ARG:HD2	1:G:277:LYS:HB2	2.03	0.41
1:G:281:PHE:HA	1:G:285:ARG:HB2	2.02	0.41
1:G:480:ALA:H	2:G:549:AGS:C2	2.33	0.41
1:G:6:VAL:HG22	1:G:521:VAL:HG22	2.02	0.41
1:H:6:VAL:HG22	1:H:521:VAL:HG22	2.03	0.41
1:L:177:VAL:HG22	1:L:379:ILE:HB	2.02	0.41
1:M:112:ASN:HD22	1:M:113:PRO:CD	2.32	0.41
1:E:496:PRO:O	1:E:499:VAL:CG1	2.68	0.41
1:M:414:GLY:O	1:M:417:VAL:HG22	2.19	0.41
1:N:177:VAL:HG22	1:N:379:ILE:HB	2.03	0.41
1:A:360:TYR:CG	1:G:183:LEU:HD22	2.55	0.41
1:G:123:ALA:HB2	1:G:440:ILE:HG23	2.02	0.41
1:J:25:ASP:HA	1:J:28:LYS:HG2	2.02	0.41
1:K:87:ASP:HB3	1:K:499:VAL:HG21	2.03	0.41
1:L:269:GLY:HA3	1:M:257:GLU:HB2	2.03	0.41
1:G:496:PRO:O	1:G:499:VAL:CG1	2.69	0.41
1:M:248:LEU:HD22	1:M:323:VAL:HG11	2.02	0.41
1:B:254:VAL:O	1:B:259:LEU:HD12	2.21	0.41
1:E:269:GLY:HA3	1:F:257:GLU:HB2	2.02	0.41
1:I:496:PRO:O	1:I:499:VAL:CG1	2.69	0.41
1:A:194:GLN:HG3	1:A:330:THR:O	2.21	0.41
1:E:204:PHE:HD1	1:E:273:VAL:O	2.03	0.41
1:A:222:LEU:CD1	1:A:293:ALA:HA	2.52	0.41
1:C:230:ILE:HG13	1:C:233:MET:HG3	2.03	0.41
1:H:26:ALA:HA	1:I:8:PHE:HE1	1.85	0.41
1:H:475:ASN:N	1:H:475:ASN:HD22	2.18	0.41
1:I:254:VAL:O	1:I:259:LEU:HB2	2.20	0.41
1:L:112:ASN:HD22	1:L:113:PRO:CD	2.34	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:THR:HG22	1:A:271:VAL:HG13	2.04	0.40
1:A:496:PRO:O	1:A:499:VAL:CG1	2.69	0.40
1:B:218:PRO:HG3	1:B:323:VAL:HG22	2.03	0.40
1:G:136:VAL:HA	1:G:137:PRO:HD3	1.96	0.40
1:K:240:VAL:HG11	1:K:271:VAL:HG13	2.03	0.40
1:N:112:ASN:HD22	1:N:113:PRO:CD	2.34	0.40
1:C:199:TYR:OH	1:C:327:LYS:HG3	2.20	0.40
1:G:242:LYS:O	1:G:243:ALA:HB3	2.21	0.40
1:I:364:LYS:HD3	1:I:364:LYS:HA	1.94	0.40
1:L:356:ALA:HB3	1:L:362:ARG:NH2	2.37	0.40
1:L:417:VAL:HG11	1:L:477:GLY:HA3	2.03	0.40
1:D:219:PHE:C	1:D:220:ILE:HG13	2.42	0.40
1:F:475:ASN:N	1:F:475:ASN:HD22	2.18	0.40
1:A:123:ALA:HB2	1:A:440:ILE:HG23	2.03	0.40
1:E:201:SER:O	1:E:204:PHE:HD2	2.05	0.40
1:E:6:VAL:HG22	1:E:521:VAL:HG22	2.03	0.40
1:I:292:ILE:HG13	1:I:292:ILE:H	1.69	0.40
1:M:475:ASN:HD22	1:M:475:ASN:N	2.19	0.40
1:B:291:ASP:OD2	1:B:368:ARG:HD2	2.21	0.40
1:D:177:VAL:HG23	1:D:379:ILE:HD12	2.04	0.40
1:K:254:VAL:O	1:K:259:LEU:HB2	2.21	0.40
1:L:496:PRO:O	1:L:499:VAL:CG1	2.69	0.40
1:N:364:LYS:HA	1:N:364:LYS:HD3	1.91	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	522/547 (95%)	494 (95%)	23 (4%)	5 (1%)	15 52
1	B	522/547 (95%)	490 (94%)	25 (5%)	7 (1%)	12 47

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	522/547 (95%)	490 (94%)	27 (5%)	5 (1%)	15	52
1	D	522/547 (95%)	487 (93%)	30 (6%)	5 (1%)	15	52
1	E	522/547 (95%)	493 (94%)	22 (4%)	7 (1%)	12	47
1	F	522/547 (95%)	496 (95%)	19 (4%)	7 (1%)	12	47
1	G	522/547 (95%)	490 (94%)	28 (5%)	4 (1%)	19	57
1	H	522/547 (95%)	496 (95%)	18 (3%)	8 (2%)	10	45
1	I	522/547 (95%)	495 (95%)	25 (5%)	2 (0%)	34	70
1	J	522/547 (95%)	496 (95%)	21 (4%)	5 (1%)	15	52
1	K	522/547 (95%)	485 (93%)	33 (6%)	4 (1%)	19	57
1	L	522/547 (95%)	501 (96%)	20 (4%)	1 (0%)	47	79
1	M	522/547 (95%)	495 (95%)	22 (4%)	5 (1%)	15	52
1	N	522/547 (95%)	483 (92%)	32 (6%)	7 (1%)	12	47
All	All	7308/7658 (95%)	6891 (94%)	345 (5%)	72 (1%)	15	52

All (72) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	244	GLY
1	A	375	GLY
1	B	205	ILE
1	H	322	ARG
1	H	336	VAL
1	I	244	GLY
1	K	208	PRO
1	A	256	GLY
1	B	256	GLY
1	B	334	ASP
1	B	336	VAL
1	D	256	GLY
1	E	256	GLY
1	G	271	VAL
1	G	293	ALA
1	G	337	GLY
1	J	270	ILE
1	J	271	VAL
1	K	356	ALA
1	B	310	GLU
1	C	282	GLY

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	E	375	GLY
1	E	385	THR
1	F	322	ARG
1	F	384	ALA
1	F	385	THR
1	H	271	VAL
1	H	334	ASP
1	I	271	VAL
1	J	334	ASP
1	M	334	ASP
1	N	313	THR
1	N	317	LEU
1	B	322	ARG
1	B	386	GLU
1	D	244	GLY
1	D	385	THR
1	E	246	PRO
1	E	334	ASP
1	F	271	VAL
1	H	356	ALA
1	J	231	ARG
1	M	271	VAL
1	N	271	VAL
1	N	334	ASP
1	A	271	VAL
1	D	271	VAL
1	E	271	VAL
1	H	244	GLY
1	K	322	ARG
1	L	271	VAL
1	M	243	ALA
1	A	234	LEU
1	C	246	PRO
1	C	256	GLY
1	C	271	VAL
1	D	259	LEU
1	E	383	ALA
1	G	270	ILE
1	H	205	ILE
1	M	270	ILE
1	N	336	VAL
1	F	205	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	244	GLY
1	F	256	GLY
1	N	282	GLY
1	C	306	GLY
1	H	256	GLY
1	K	202	PRO
1	J	244	GLY
1	M	269	GLY
1	N	234	LEU

### 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	404/414 (98%)	386 (96%)	18 (4%)	27	54
1	B	404/414 (98%)	392 (97%)	12 (3%)	41	64
1	C	404/414 (98%)	392 (97%)	12 (3%)	41	64
1	D	404/414 (98%)	387 (96%)	17 (4%)	30	56
1	E	404/414 (98%)	392 (97%)	12 (3%)	41	64
1	F	404/414 (98%)	389 (96%)	15 (4%)	34	59
1	G	404/414 (98%)	385 (95%)	19 (5%)	26	53
1	H	404/414 (98%)	393 (97%)	11 (3%)	44	66
1	I	404/414 (98%)	389 (96%)	15 (4%)	34	59
1	J	404/414 (98%)	388 (96%)	16 (4%)	31	57
1	K	404/414 (98%)	385 (95%)	19 (5%)	26	53
1	L	404/414 (98%)	393 (97%)	11 (3%)	44	66
1	M	404/414 (98%)	393 (97%)	11 (3%)	44	66
1	N	404/414 (98%)	397 (98%)	7 (2%)	60	78
All	All	5656/5796 (98%)	5461 (97%)	195 (3%)	37	61

All (195) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	THR
1	A	112	ASN
1	A	134	LEU
1	A	217	SER
1	A	234	LEU
1	A	270	ILE
1	A	288	MET
1	A	292	ILE
1	A	294	THR
1	A	313	THR
1	A	331	THR
1	A	354	GLU
1	A	367	GLU
1	A	369	VAL
1	A	378	VAL
1	A	379	ILE
1	A	398	ASP
1	A	463	SER
1	B	91	THR
1	B	112	ASN
1	B	134	LEU
1	B	227	ILE
1	B	273	VAL
1	B	295	LEU
1	B	299	THR
1	B	315	GLU
1	B	328	ASP
1	B	329	THR
1	B	331	THR
1	B	475	ASN
1	C	91	THR
1	C	112	ASN
1	C	134	LEU
1	C	196	ASP
1	C	217	SER
1	C	231	ARG
1	C	294	THR
1	C	331	THR
1	C	359	ASP
1	C	385	THR
1	C	391	GLU
1	C	475	ASN
1	D	91	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	112	ASN
1	D	134	LEU
1	D	199	TYR
1	D	200	LEU
1	D	201	SER
1	D	257	GLU
1	D	265	ASN
1	D	299	THR
1	D	309	LEU
1	D	315	GLU
1	D	331	THR
1	D	369	VAL
1	D	390	LYS
1	D	398	ASP
1	D	400	LEU
1	D	463	SER
1	E	91	THR
1	E	112	ASN
1	E	134	LEU
1	E	196	ASP
1	E	209	GLU
1	E	240	VAL
1	E	257	GLU
1	E	265	ASN
1	E	328	ASP
1	E	331	THR
1	E	463	SER
1	E	475	ASN
1	F	91	THR
1	F	112	ASN
1	F	134	LEU
1	F	200	LEU
1	F	217	SER
1	F	268	ARG
1	F	284	ARG
1	F	289	LEU
1	F	299	THR
1	F	317	LEU
1	F	331	THR
1	F	343	GLN
1	F	350	ARG
1	F	463	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	475	ASN
1	G	91	THR
1	G	112	ASN
1	G	134	LEU
1	G	206	ASN
1	G	217	SER
1	G	242	LYS
1	G	249	ILE
1	G	288	MET
1	G	295	LEU
1	G	310	GLU
1	G	315	GLU
1	G	328	ASP
1	G	329	THR
1	G	331	THR
1	G	351	GLN
1	G	360	TYR
1	G	369	VAL
1	G	463	SER
1	G	475	ASN
1	H	91	THR
1	H	112	ASN
1	H	134	LEU
1	H	200	LEU
1	H	217	SER
1	H	225	LYS
1	H	314	LEU
1	H	317	LEU
1	H	331	THR
1	H	386	GLU
1	H	475	ASN
1	I	91	THR
1	I	112	ASN
1	I	134	LEU
1	I	196	ASP
1	I	199	TYR
1	I	200	LEU
1	I	209	GLU
1	I	210	THR
1	I	225	LYS
1	I	257	GLU
1	I	289	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	I	294	THR
1	I	299	THR
1	I	329	THR
1	I	475	ASN
1	J	77	VAL
1	J	91	THR
1	J	112	ASN
1	J	134	LEU
1	J	200	LEU
1	J	225	LYS
1	J	228	SER
1	J	294	THR
1	J	299	THR
1	J	313	THR
1	J	327	LYS
1	J	329	THR
1	J	331	THR
1	J	343	GLN
1	J	390	LYS
1	J	463	SER
1	K	91	THR
1	K	112	ASN
1	K	134	LEU
1	K	200	LEU
1	K	206	ASN
1	K	210	THR
1	K	225	LYS
1	K	253	ASP
1	K	255	GLU
1	K	273	VAL
1	K	294	THR
1	K	310	GLU
1	K	316	ASP
1	K	328	ASP
1	K	329	THR
1	K	338	GLU
1	K	361	ASP
1	K	368	ARG
1	K	463	SER
1	L	91	THR
1	L	112	ASN
1	L	134	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	L	200	LEU
1	L	209	GLU
1	L	225	LYS
1	L	283	ASP
1	L	295	LEU
1	L	398	ASP
1	L	463	SER
1	L	475	ASN
1	M	91	THR
1	M	112	ASN
1	M	134	LEU
1	M	199	TYR
1	M	200	LEU
1	M	225	LYS
1	M	316	ASP
1	M	329	THR
1	M	398	ASP
1	M	463	SER
1	M	475	ASN
1	N	91	THR
1	N	112	ASN
1	N	134	LEU
1	N	225	LYS
1	N	299	THR
1	N	329	THR
1	N	463	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	290	GLN
1	A	352	GLN
1	B	112	ASN
1	B	366	GLN
1	C	37	ASN
1	C	112	ASN
1	D	112	ASN
1	E	112	ASN
1	E	351	GLN
1	F	112	ASN
1	G	112	ASN
1	H	112	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	H	229	ASN
1	I	112	ASN
1	J	37	ASN
1	J	112	ASN
1	J	265	ASN
1	J	366	GLN
1	L	206	ASN
1	M	351	GLN
1	N	112	ASN

### 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 74 ligands modelled in this entry, 60 are monoatomic - leaving 14 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	$\# Z  > 2$
2	AGS	K	549	4	26,33,33	1.50	2 (7%)	26,52,52	1.55	4 (15%)
2	AGS	H	549	4	26,33,33	1.14	1 (3%)	26,52,52	1.54	4 (15%)
2	AGS	I	549	4	26,33,33	1.26	1 (3%)	26,52,52	1.52	4 (15%)
2	AGS	J	549	4	26,33,33	1.64	1 (3%)	26,52,52	1.56	4 (15%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	AGS	C	549	4	26,33,33	1.50	1 (3%)	26,52,52	1.55	4 (15%)
2	AGS	L	549	4	26,33,33	1.47	2 (7%)	26,52,52	1.48	4 (15%)
2	AGS	M	549	4	26,33,33	1.03	3 (11%)	26,52,52	1.51	3 (11%)
2	AGS	N	549	4	26,33,33	1.75	1 (3%)	26,52,52	1.51	4 (15%)
2	AGS	G	549	4	26,33,33	1.43	1 (3%)	26,52,52	1.55	4 (15%)
2	AGS	A	549	4	26,33,33	1.30	1 (3%)	26,52,52	1.55	4 (15%)
2	AGS	B	549	4	26,33,33	1.15	2 (7%)	26,52,52	1.54	4 (15%)
2	AGS	D	549	4	26,33,33	1.20	2 (7%)	26,52,52	1.57	4 (15%)
2	AGS	E	549	4	26,33,33	1.24	2 (7%)	26,52,52	1.55	4 (15%)
2	AGS	F	549	4	26,33,33	1.39	2 (7%)	26,52,52	1.55	4 (15%)

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	AGS	K	549	4	-	4/17/38/38	0/3/3/3
2	AGS	H	549	4	-	4/17/38/38	0/3/3/3
2	AGS	I	549	4	-	5/17/38/38	0/3/3/3
2	AGS	J	549	4	-	4/17/38/38	0/3/3/3
2	AGS	C	549	4	-	5/17/38/38	0/3/3/3
2	AGS	L	549	4	-	4/17/38/38	0/3/3/3
2	AGS	M	549	4	-	5/17/38/38	0/3/3/3
2	AGS	N	549	4	-	4/17/38/38	0/3/3/3
2	AGS	G	549	4	-	4/17/38/38	0/3/3/3
2	AGS	A	549	4	-	5/17/38/38	0/3/3/3
2	AGS	B	549	4	-	4/17/38/38	0/3/3/3
2	AGS	D	549	4	-	4/17/38/38	0/3/3/3
2	AGS	E	549	4	-	5/17/38/38	0/3/3/3
2	AGS	F	549	4	-	4/17/38/38	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	549	AGS	PG-S1G	7.36	2.06	1.90
2	J	549	AGS	PG-S1G	6.90	2.05	1.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	549	AGS	PG-S1G	5.93	2.03	1.90
2	C	549	AGS	PG-S1G	5.72	2.03	1.90
2	G	549	AGS	PG-S1G	5.51	2.02	1.90
2	L	549	AGS	PG-S1G	5.47	2.02	1.90
2	F	549	AGS	PG-S1G	4.74	2.01	1.90
2	A	549	AGS	PG-S1G	4.25	1.99	1.90
2	I	549	AGS	PG-S1G	3.69	1.98	1.90
2	E	549	AGS	PG-S1G	3.67	1.98	1.90
2	D	549	AGS	PG-S1G	3.18	1.97	1.90
2	H	549	AGS	PG-S1G	2.91	1.97	1.90
2	B	549	AGS	PG-S1G	2.82	1.96	1.90
2	L	549	AGS	O4'-C1'	2.39	1.44	1.41
2	B	549	AGS	PG-O2G	-2.10	1.48	1.54
2	M	549	AGS	O4'-C1'	2.06	1.44	1.41
2	E	549	AGS	PG-O2G	-2.06	1.48	1.54
2	D	549	AGS	PG-O2G	-2.03	1.48	1.54
2	K	549	AGS	PG-O2G	-2.02	1.48	1.54
2	F	549	AGS	PG-O2G	-2.01	1.48	1.54
2	M	549	AGS	PG-O3G	-2.01	1.48	1.54
2	M	549	AGS	PG-O2G	-2.01	1.48	1.54

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	549	AGS	N3-C2-N1	-4.78	121.21	128.68
2	K	549	AGS	N3-C2-N1	-4.74	121.27	128.68
2	C	549	AGS	N3-C2-N1	-4.73	121.29	128.68
2	J	549	AGS	N3-C2-N1	-4.72	121.30	128.68
2	E	549	AGS	N3-C2-N1	-4.67	121.38	128.68
2	B	549	AGS	N3-C2-N1	-4.64	121.42	128.68
2	H	549	AGS	N3-C2-N1	-4.62	121.46	128.68
2	G	549	AGS	N3-C2-N1	-4.60	121.49	128.68
2	D	549	AGS	N3-C2-N1	-4.56	121.55	128.68
2	A	549	AGS	N3-C2-N1	-4.55	121.57	128.68
2	I	549	AGS	N3-C2-N1	-4.51	121.63	128.68
2	L	549	AGS	N3-C2-N1	-4.47	121.69	128.68
2	N	549	AGS	N3-C2-N1	-4.44	121.73	128.68
2	M	549	AGS	N3-C2-N1	-4.44	121.74	128.68
2	M	549	AGS	PA-O3A-PB	-3.74	119.99	132.83
2	D	549	AGS	O4'-C1'-C2'	-3.06	102.46	106.93
2	A	549	AGS	O4'-C1'-C2'	-2.90	102.68	106.93
2	J	549	AGS	O4'-C1'-C2'	-2.86	102.74	106.93

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	549	AGS	O4'-C1'-C2'	-2.83	102.78	106.93
2	E	549	AGS	C5'-C4'-C3'	-2.80	104.70	115.18
2	I	549	AGS	O4'-C1'-C2'	-2.79	102.85	106.93
2	D	549	AGS	C5'-C4'-C3'	-2.77	104.81	115.18
2	J	549	AGS	C5'-C4'-C3'	-2.75	104.86	115.18
2	E	549	AGS	O4'-C1'-C2'	-2.73	102.93	106.93
2	F	549	AGS	O4'-C1'-C2'	-2.73	102.94	106.93
2	F	549	AGS	C5'-C4'-C3'	-2.72	105.00	115.18
2	C	549	AGS	O4'-C1'-C2'	-2.72	102.96	106.93
2	B	549	AGS	C5'-C4'-C3'	-2.70	105.05	115.18
2	B	549	AGS	O4'-C1'-C2'	-2.70	102.98	106.93
2	N	549	AGS	C5'-C4'-C3'	-2.70	105.08	115.18
2	H	549	AGS	O4'-C1'-C2'	-2.69	102.99	106.93
2	G	549	AGS	C5'-C4'-C3'	-2.69	105.10	115.18
2	K	549	AGS	C5'-C4'-C3'	-2.66	105.20	115.18
2	H	549	AGS	C5'-C4'-C3'	-2.63	105.32	115.18
2	C	549	AGS	C5'-C4'-C3'	-2.62	105.38	115.18
2	I	549	AGS	C5'-C4'-C3'	-2.59	105.47	115.18
2	N	549	AGS	O4'-C1'-C2'	-2.57	103.18	106.93
2	A	549	AGS	C5'-C4'-C3'	-2.56	105.60	115.18
2	L	549	AGS	C5'-C4'-C3'	-2.54	105.67	115.18
2	K	549	AGS	O4'-C1'-C2'	-2.53	103.23	106.93
2	A	549	AGS	PA-O3A-PB	-2.46	124.38	132.83
2	L	549	AGS	O4'-C1'-C2'	-2.39	103.43	106.93
2	I	549	AGS	PA-O3A-PB	-2.36	124.73	132.83
2	D	549	AGS	PA-O3A-PB	-2.36	124.74	132.83
2	E	549	AGS	PA-O3A-PB	-2.34	124.81	132.83
2	C	549	AGS	PA-O3A-PB	-2.32	124.87	132.83
2	N	549	AGS	PA-O3A-PB	-2.31	124.91	132.83
2	L	549	AGS	PA-O3A-PB	-2.18	125.33	132.83
2	J	549	AGS	PA-O3A-PB	-2.18	125.36	132.83
2	F	549	AGS	PA-O3A-PB	-2.17	125.38	132.83
2	K	549	AGS	PA-O3A-PB	-2.17	125.39	132.83
2	G	549	AGS	PA-O3A-PB	-2.16	125.40	132.83
2	H	549	AGS	PA-O3A-PB	-2.15	125.45	132.83
2	B	549	AGS	PA-O3A-PB	-2.14	125.50	132.83
2	M	549	AGS	O4'-C1'-C2'	-2.02	103.97	106.93

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	J	549	AGS	C5'-O5'-PA-O2A
2	B	549	AGS	C5'-O5'-PA-O2A
2	G	549	AGS	C5'-O5'-PA-O2A
2	K	549	AGS	C5'-O5'-PA-O2A
2	I	549	AGS	C5'-O5'-PA-O2A
2	C	549	AGS	C5'-O5'-PA-O2A
2	A	549	AGS	C5'-O5'-PA-O2A
2	F	549	AGS	C5'-O5'-PA-O2A
2	M	549	AGS	C5'-O5'-PA-O2A
2	N	549	AGS	C5'-O5'-PA-O2A
2	D	549	AGS	C5'-O5'-PA-O2A
2	E	549	AGS	C5'-O5'-PA-O2A
2	J	549	AGS	C5'-O5'-PA-O3A
2	B	549	AGS	C5'-O5'-PA-O3A
2	H	549	AGS	C5'-O5'-PA-O3A
2	G	549	AGS	C5'-O5'-PA-O3A
2	K	549	AGS	C5'-O5'-PA-O3A
2	I	549	AGS	C5'-O5'-PA-O3A
2	C	549	AGS	C5'-O5'-PA-O3A
2	A	549	AGS	C5'-O5'-PA-O3A
2	F	549	AGS	C5'-O5'-PA-O3A
2	L	549	AGS	C5'-O5'-PA-O3A
2	M	549	AGS	C5'-O5'-PA-O3A
2	D	549	AGS	C5'-O5'-PA-O3A
2	E	549	AGS	C5'-O5'-PA-O3A
2	M	549	AGS	PA-O3A-PB-O1B
2	H	549	AGS	C5'-O5'-PA-O2A
2	L	549	AGS	C5'-O5'-PA-O2A
2	M	549	AGS	C5'-O5'-PA-O1A
2	J	549	AGS	PA-O3A-PB-O1B
2	K	549	AGS	PA-O3A-PB-O1B
2	I	549	AGS	PA-O3A-PB-O1B
2	C	549	AGS	PA-O3A-PB-O1B
2	A	549	AGS	PA-O3A-PB-O1B
2	A	549	AGS	PA-O3A-PB-O2B
2	E	549	AGS	PA-O3A-PB-O1B
2	N	549	AGS	C5'-O5'-PA-O3A
2	B	549	AGS	PA-O3A-PB-O1B
2	H	549	AGS	PA-O3A-PB-O1B
2	G	549	AGS	PA-O3A-PB-O1B
2	I	549	AGS	PA-O3A-PB-O2B
2	C	549	AGS	PA-O3A-PB-O2B
2	F	549	AGS	PA-O3A-PB-O1B

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	L	549	AGS	PA-O3A-PB-O1B
2	M	549	AGS	PA-O3A-PB-O2B
2	N	549	AGS	PA-O3A-PB-O1B
2	D	549	AGS	PA-O3A-PB-O1B
2	E	549	AGS	PA-O3A-PB-O2B
2	J	549	AGS	C5'-O5'-PA-O1A
2	B	549	AGS	C5'-O5'-PA-O1A
2	H	549	AGS	C5'-O5'-PA-O1A
2	G	549	AGS	C5'-O5'-PA-O1A
2	K	549	AGS	C5'-O5'-PA-O1A
2	I	549	AGS	C5'-O5'-PA-O1A
2	C	549	AGS	C5'-O5'-PA-O1A
2	A	549	AGS	C5'-O5'-PA-O1A
2	F	549	AGS	C5'-O5'-PA-O1A
2	L	549	AGS	C5'-O5'-PA-O1A
2	N	549	AGS	C5'-O5'-PA-O1A
2	D	549	AGS	C5'-O5'-PA-O1A
2	E	549	AGS	C5'-O5'-PA-O1A

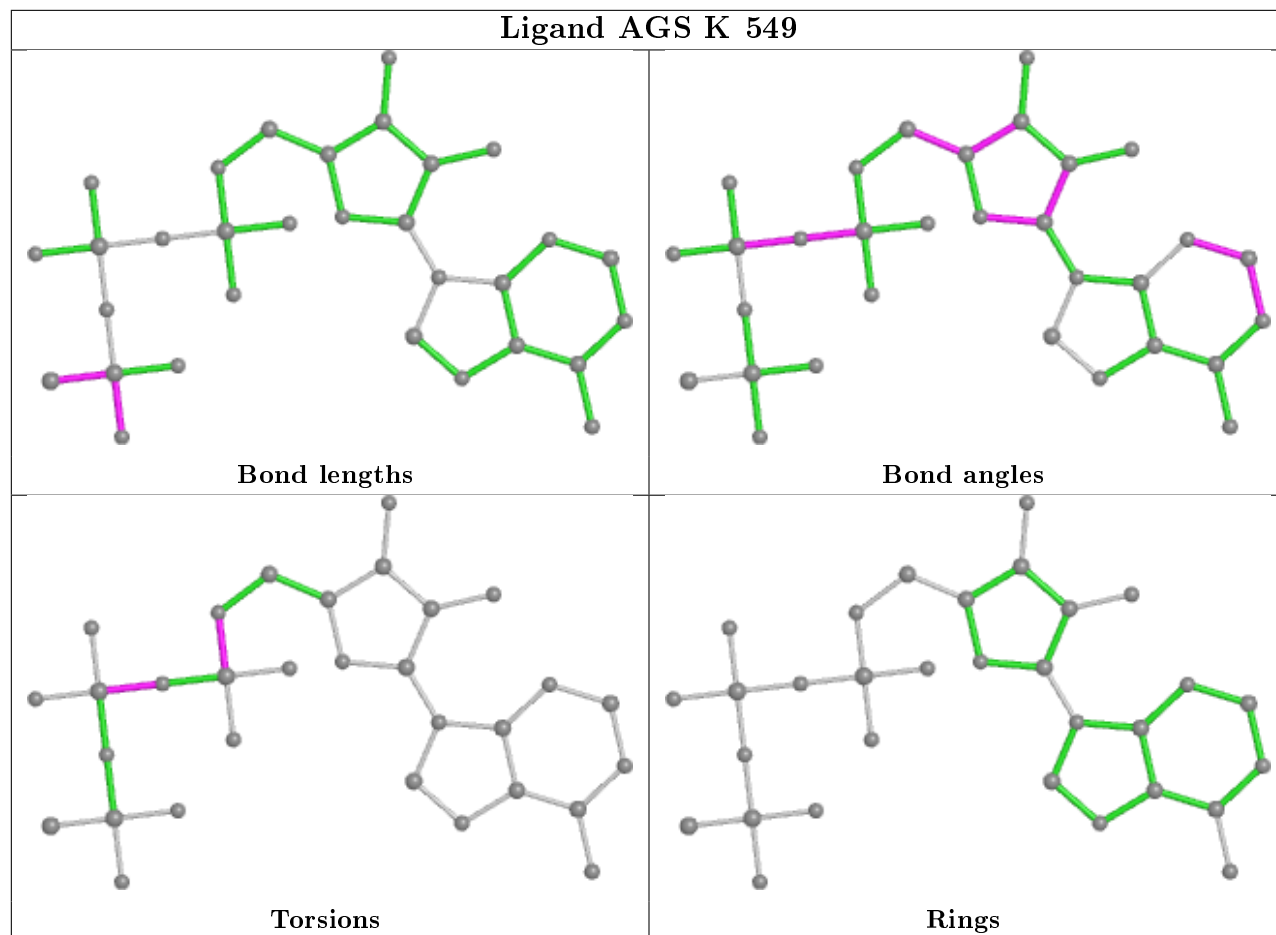
There are no ring outliers.

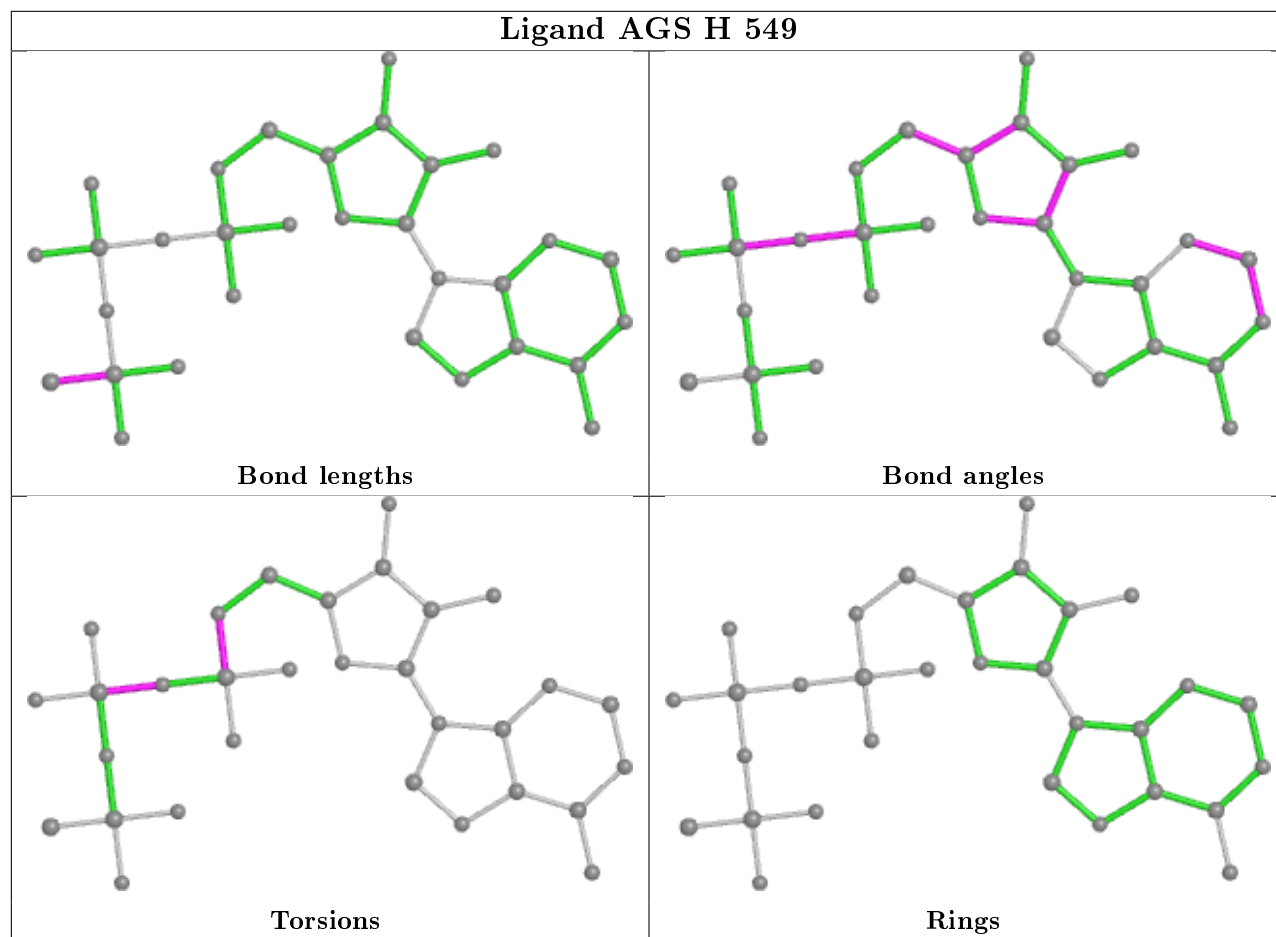
7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	549	AGS	1	0
2	I	549	AGS	1	0
2	J	549	AGS	1	0
2	C	549	AGS	1	0
2	G	549	AGS	2	0
2	D	549	AGS	1	0
2	E	549	AGS	1	0

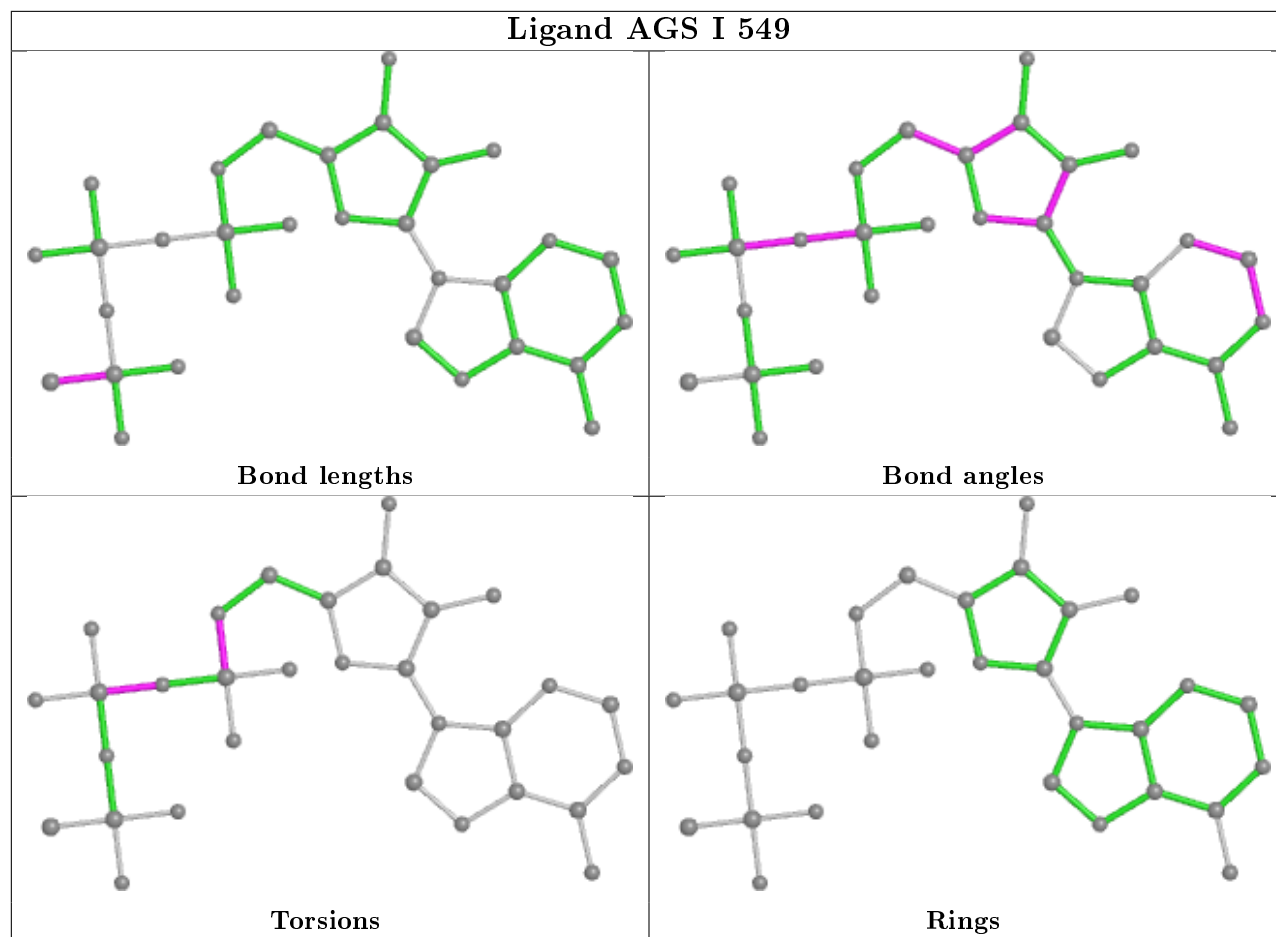
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



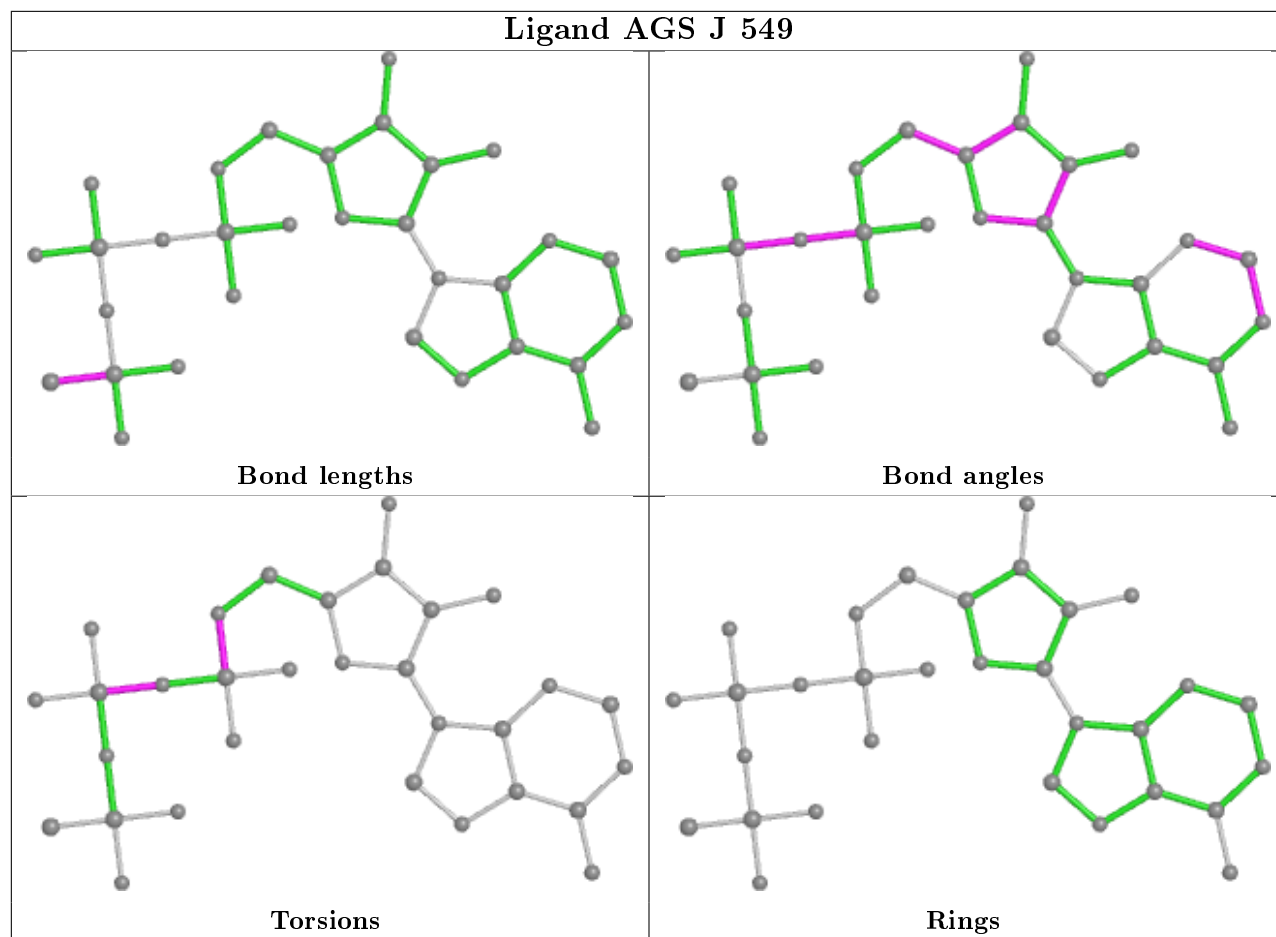


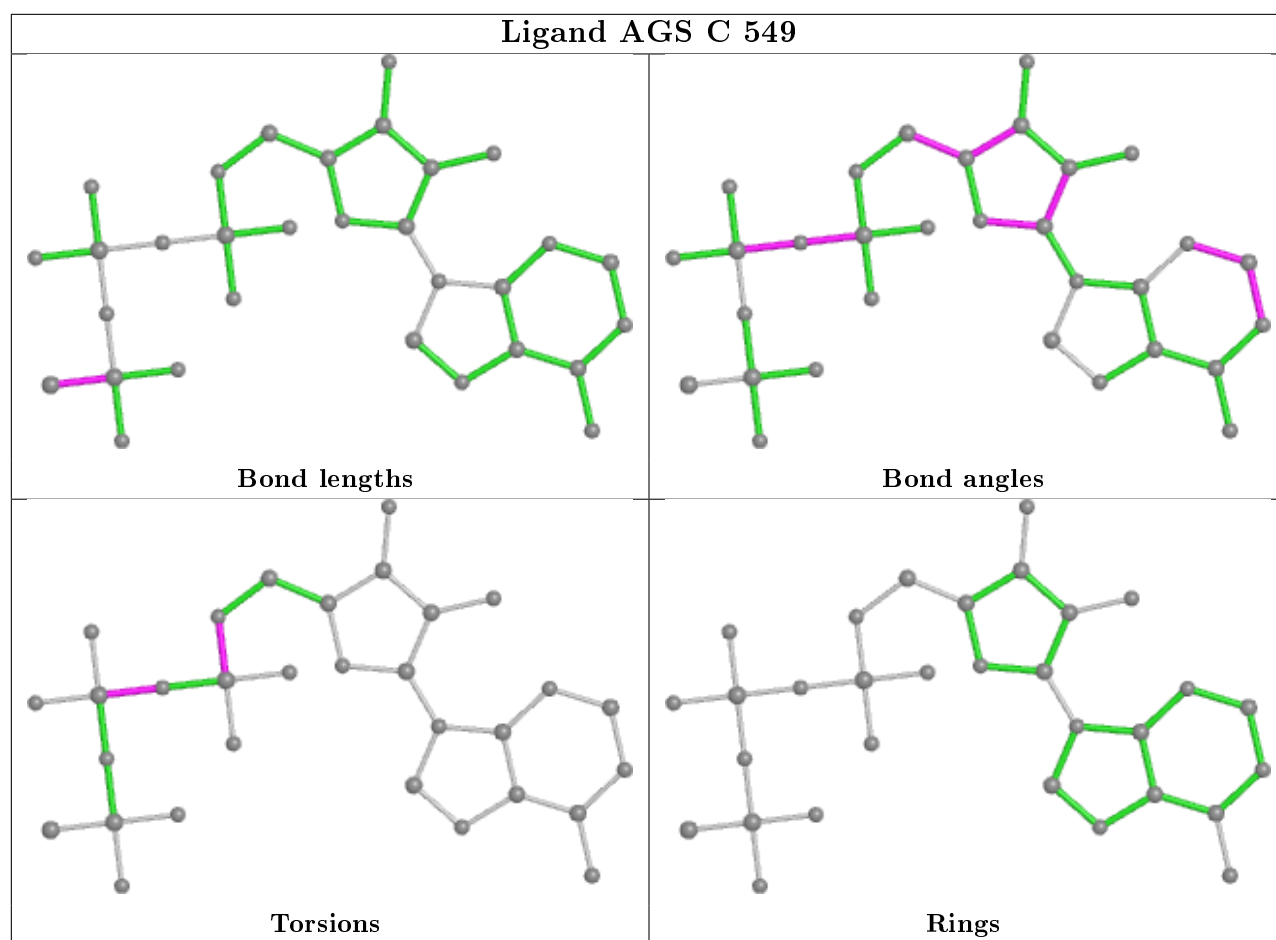
## Ligand AGS I 549

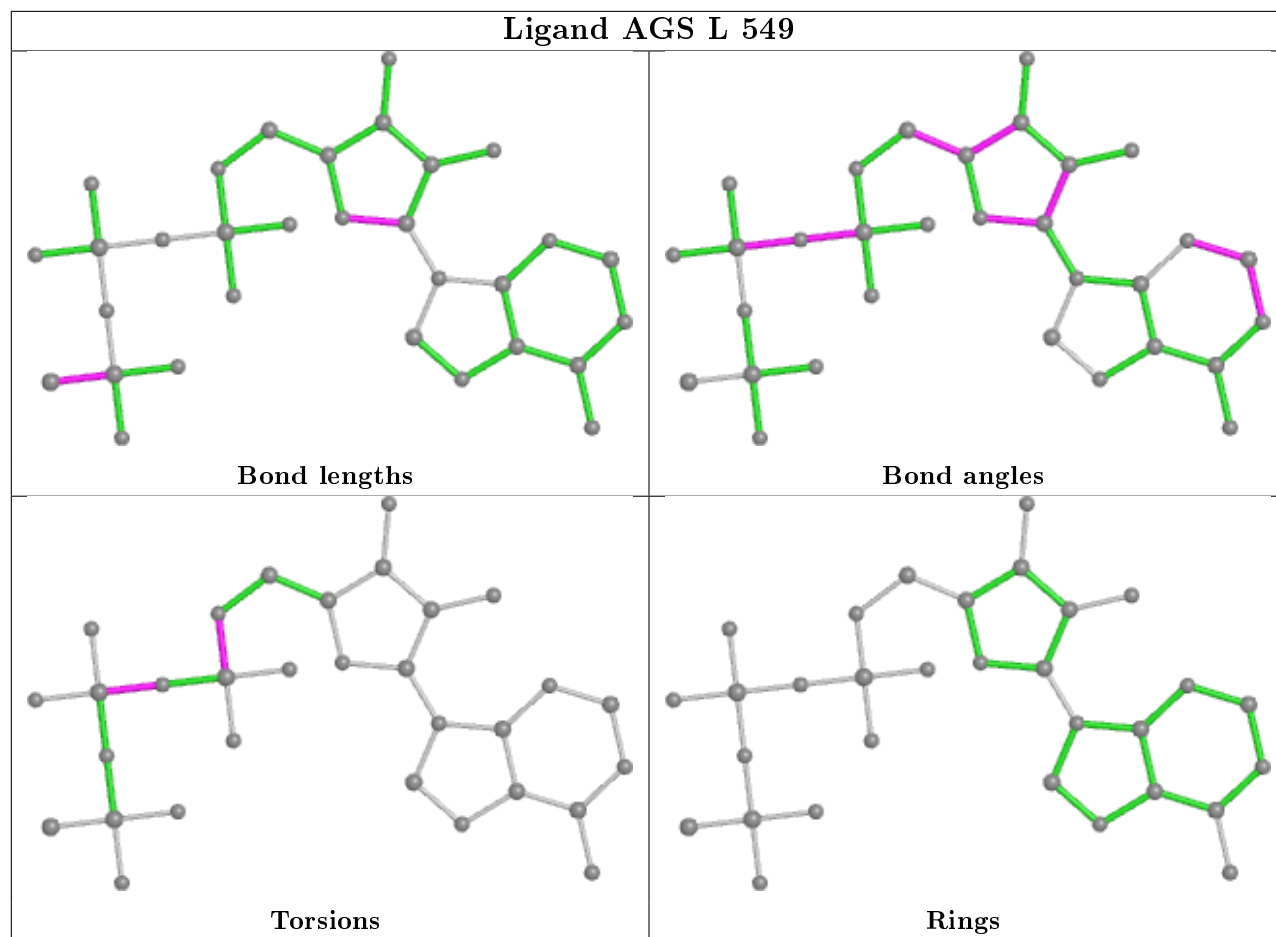


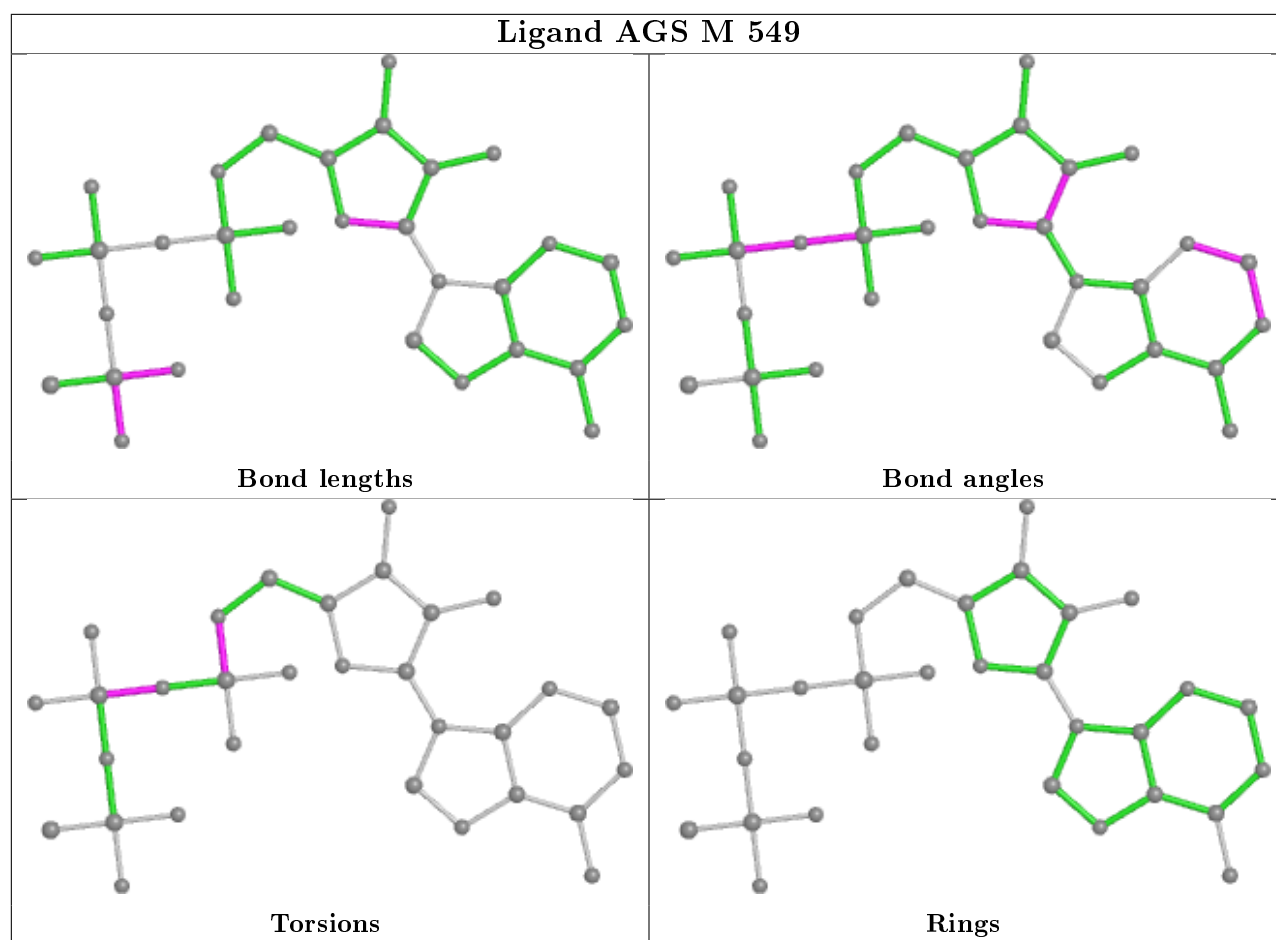


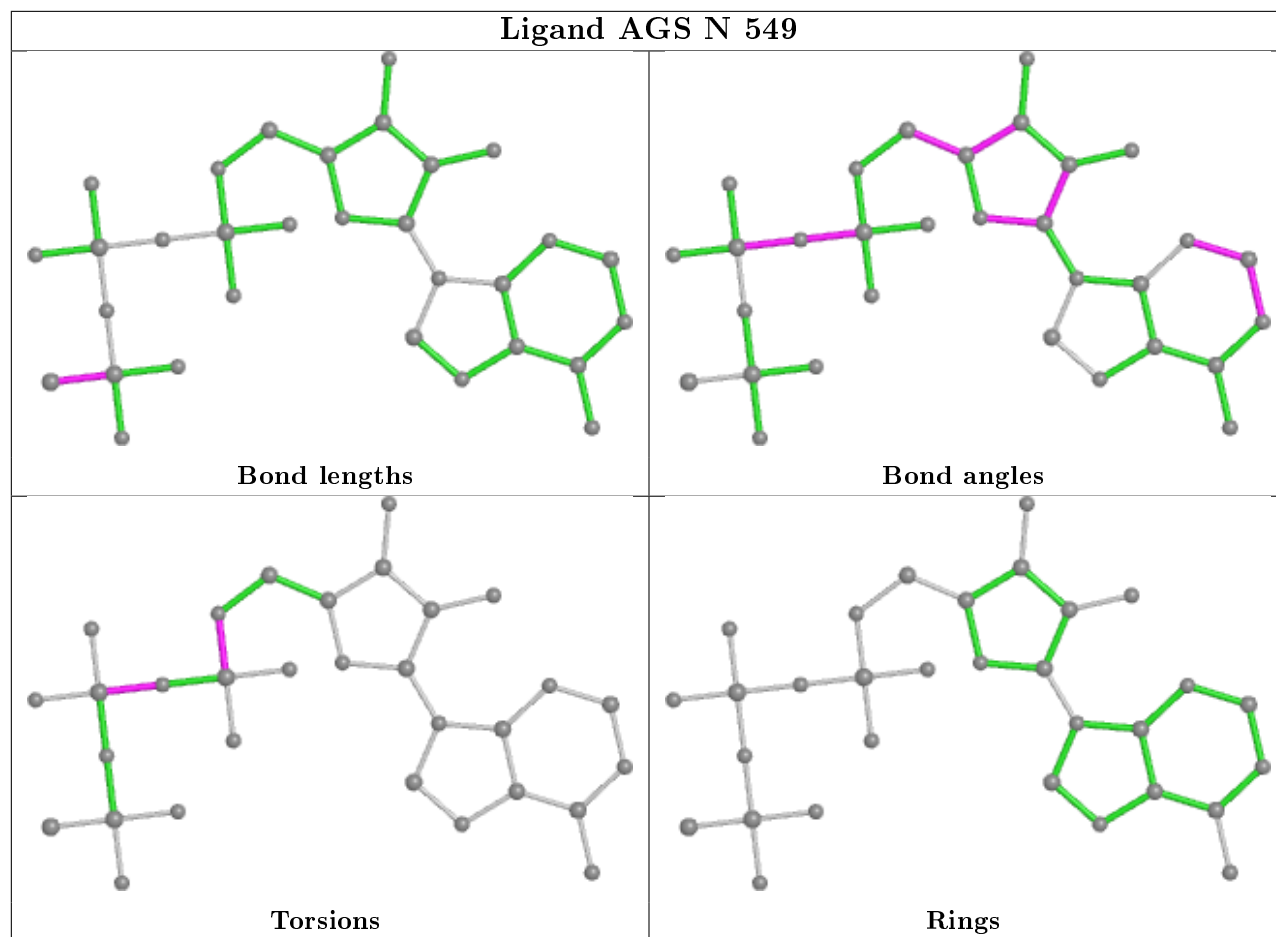
## Ligand AGS J 549

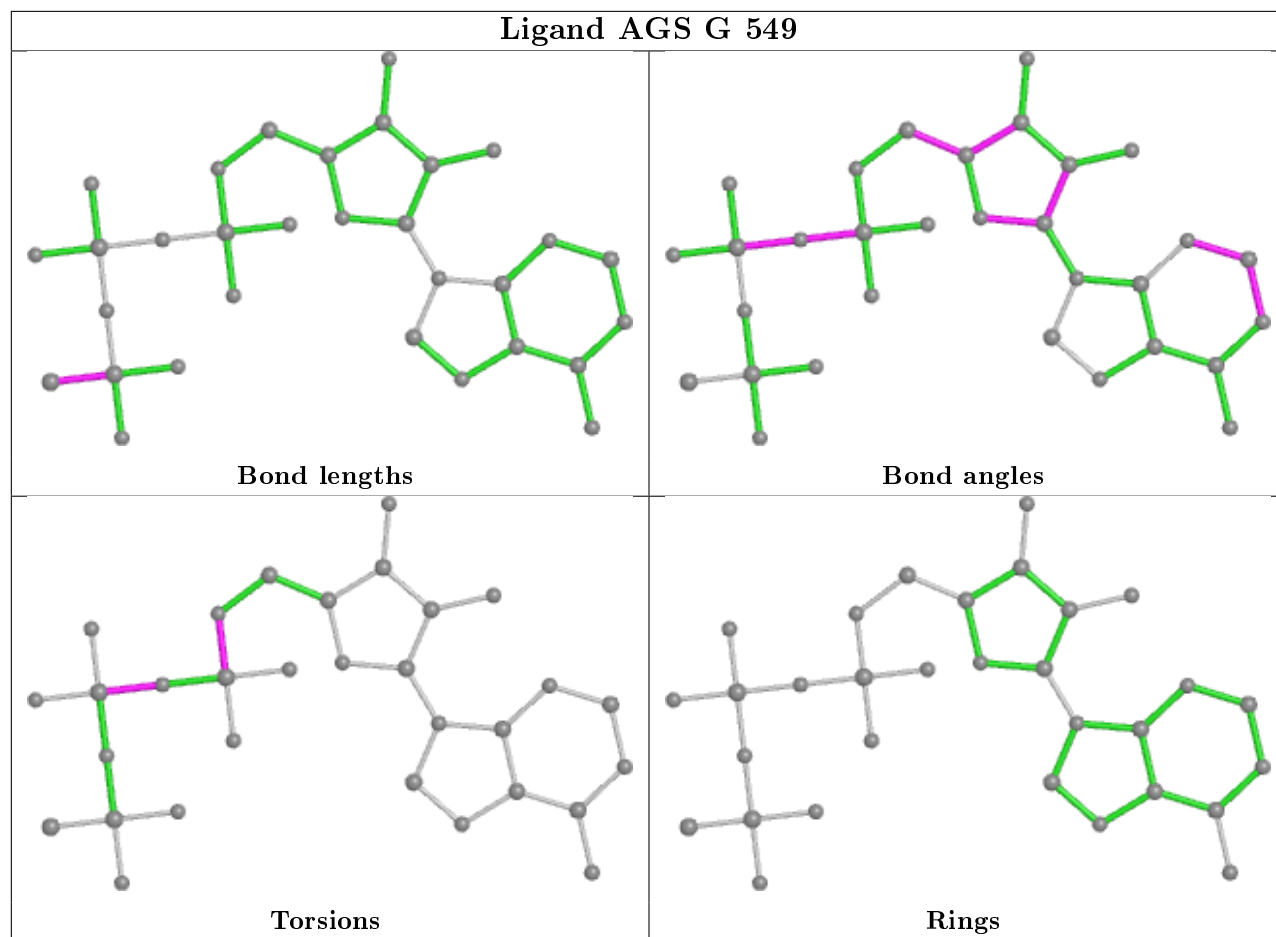


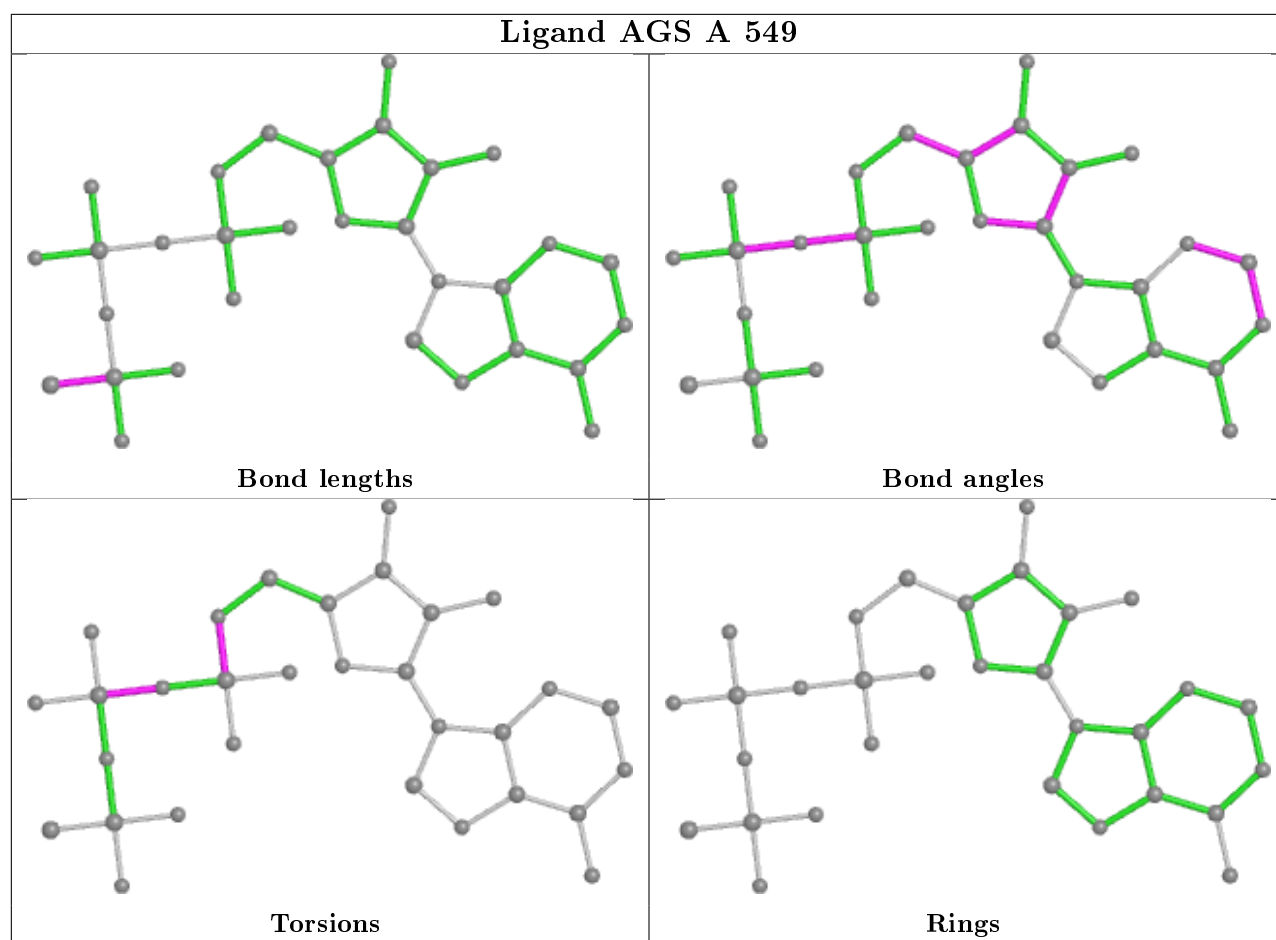




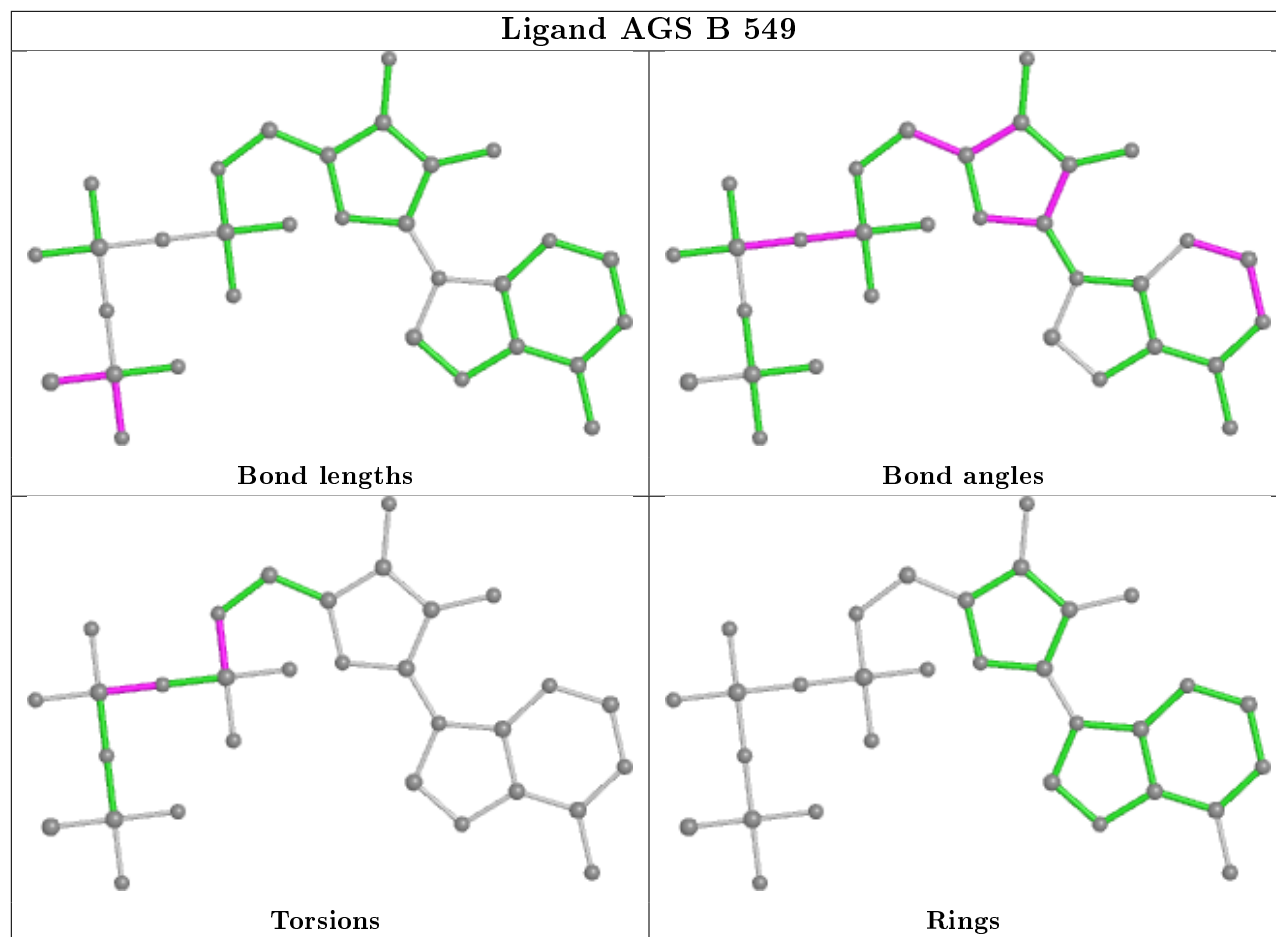




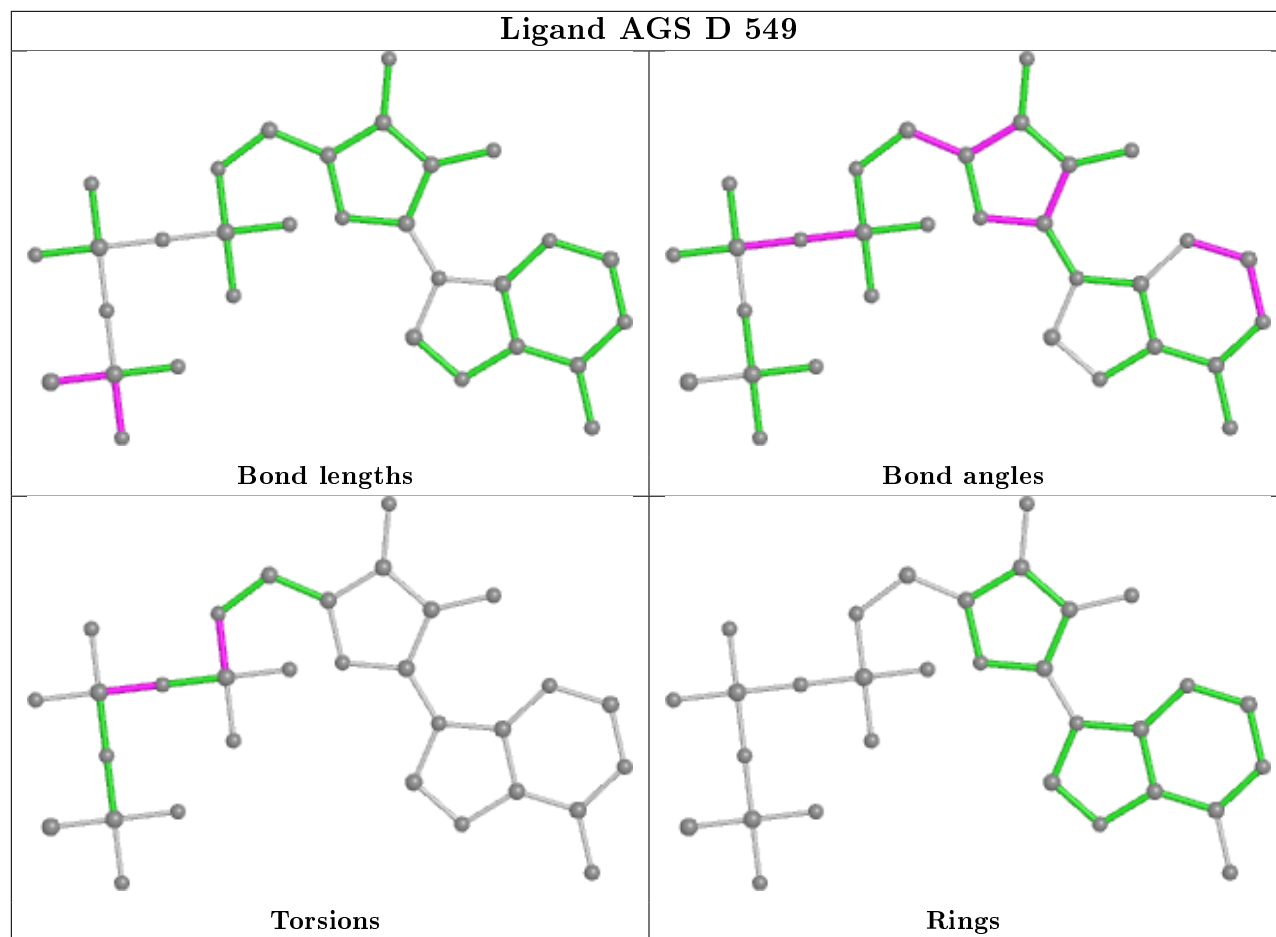




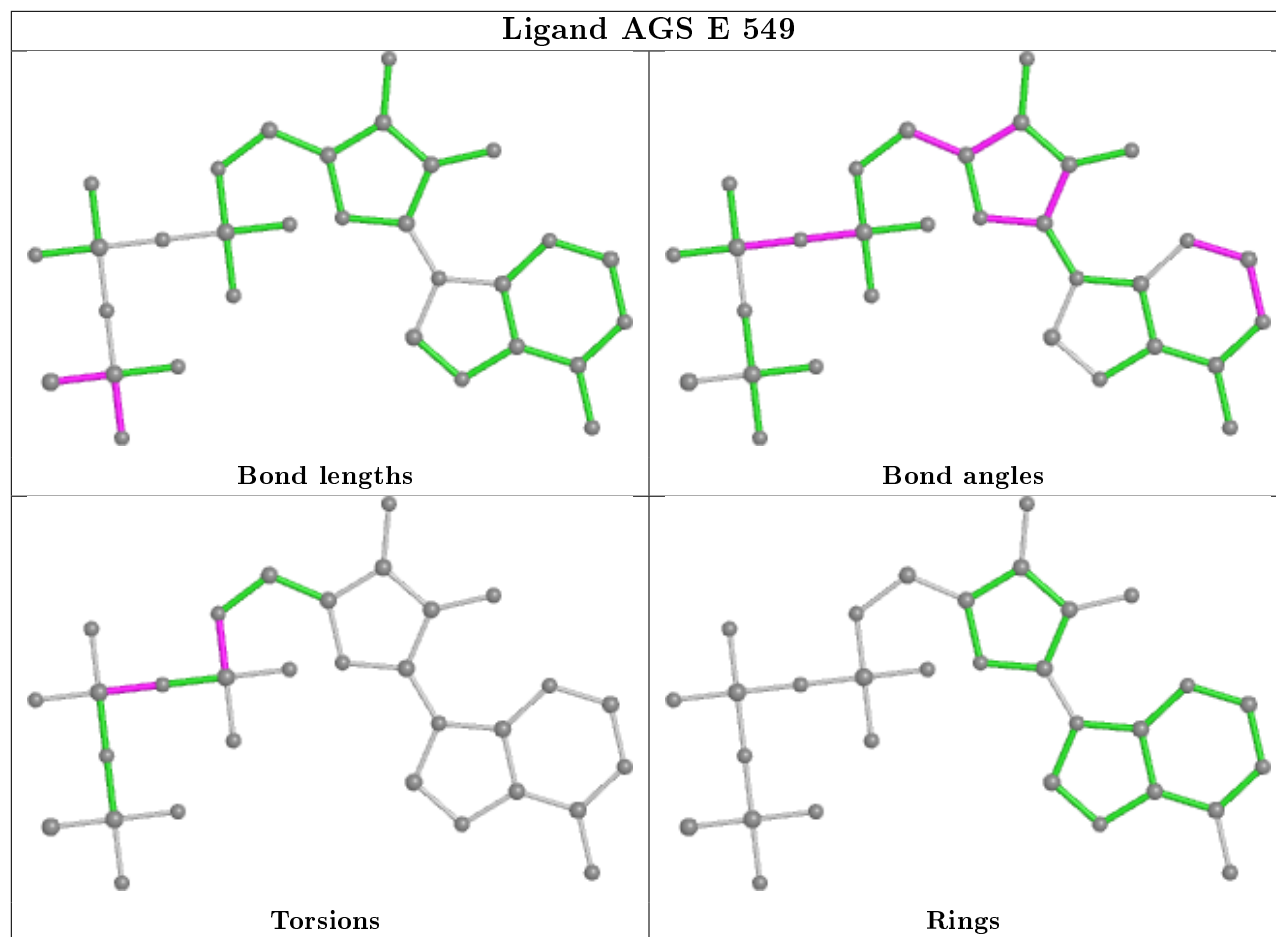
## Ligand AGS B 549

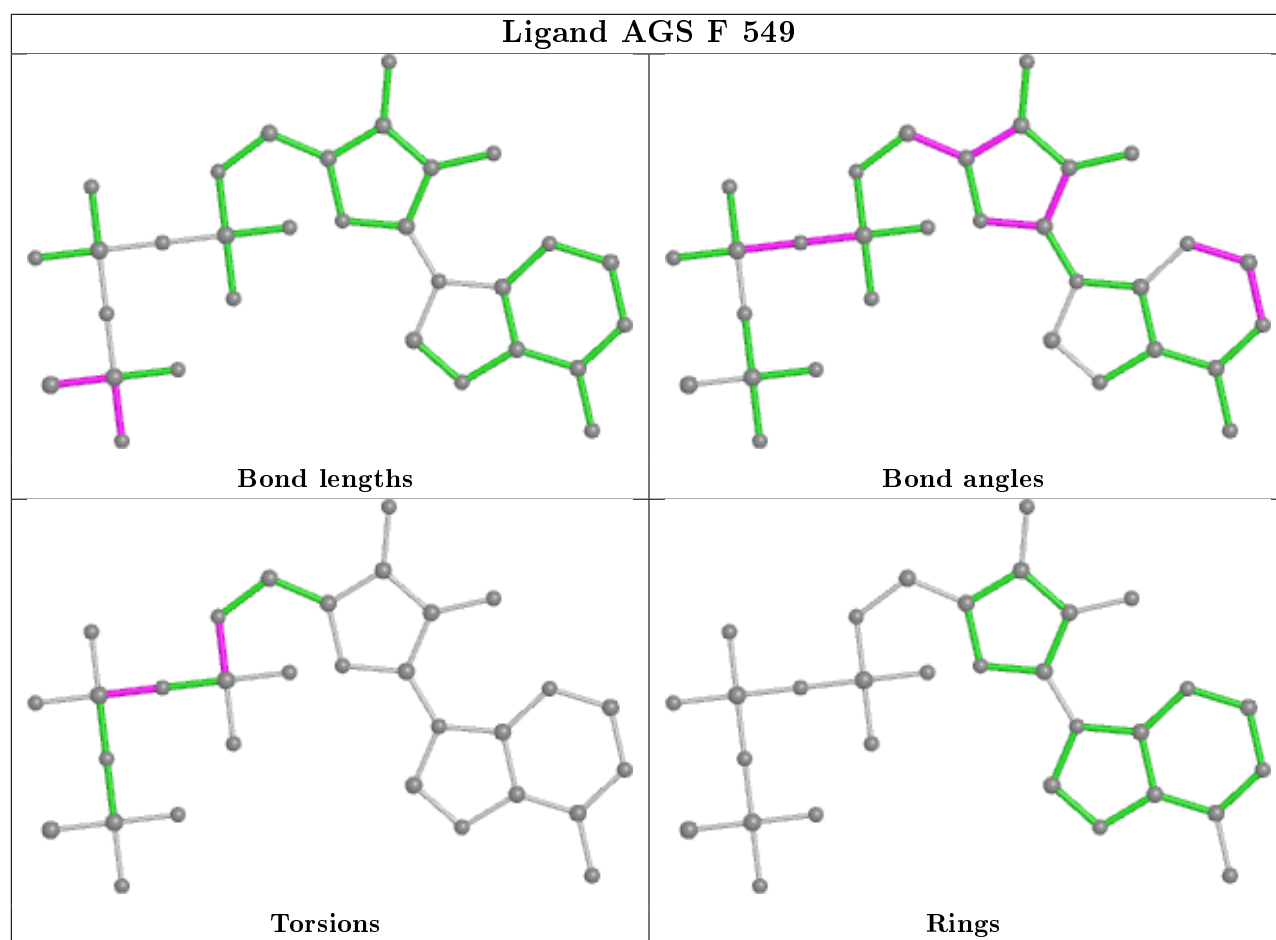






## Ligand AGS E 549





## 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	524/547 (95%)	-0.19	2 (0%) 92 87	125, 125, 125, 125	0
1	B	524/547 (95%)	-0.17	1 (0%) 95 93	125, 125, 125, 125	0
1	C	524/547 (95%)	-0.08	12 (2%) 60 51	125, 125, 125, 125	0
1	D	524/547 (95%)	-0.12	6 (1%) 80 72	125, 125, 125, 125	0
1	E	524/547 (95%)	-0.02	12 (2%) 60 51	125, 125, 125, 125	0
1	F	524/547 (95%)	-0.11	9 (1%) 70 60	125, 125, 125, 125	0
1	G	524/547 (95%)	-0.14	8 (1%) 73 64	125, 125, 125, 125	0
1	H	524/547 (95%)	0.00	15 (2%) 51 41	125, 125, 125, 125	0
1	I	524/547 (95%)	-0.12	12 (2%) 60 51	125, 125, 125, 125	0
1	J	524/547 (95%)	-0.02	12 (2%) 60 51	125, 125, 125, 125	0
1	K	524/547 (95%)	-0.03	12 (2%) 60 51	125, 125, 125, 125	0
1	L	524/547 (95%)	0.05	20 (3%) 40 32	125, 125, 125, 125	0
1	M	524/547 (95%)	0.23	34 (6%) 18 15	125, 125, 125, 125	0
1	N	524/547 (95%)	0.40	41 (7%) 13 11	125, 125, 125, 125	0
All	All	7336/7658 (95%)	-0.02	196 (2%) 54 44	125, 125, 125, 125	0

All (196) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	223	ALA	11.9
1	I	141	SER	7.3
1	N	148	GLY	7.2
1	M	153	ASN	7.1
1	E	152	ALA	6.8
1	N	355	GLU	6.3
1	M	331	THR	6.3
1	N	251	ALA	6.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	M	152	ALA	5.7
1	M	140	ASP	5.4
1	J	152	ALA	5.3
1	M	139	SER	5.2
1	N	152	ALA	5.2
1	N	275	ALA	5.1
1	N	139	SER	5.0
1	N	141	SER	5.0
1	N	151	SER	5.0
1	L	141	SER	4.9
1	I	140	ASP	4.8
1	H	141	SER	4.8
1	E	153	ASN	4.8
1	N	193	MET	4.7
1	M	141	SER	4.5
1	K	153	ASN	4.5
1	H	139	SER	4.5
1	F	223	ALA	4.5
1	E	151	SER	4.4
1	N	301	ILE	4.4
1	N	149	THR	4.4
1	N	310	GLU	4.4
1	N	153	ASN	4.3
1	M	268	ARG	4.2
1	G	147	VAL	4.2
1	D	63	GLU	4.1
1	N	221	LEU	4.1
1	N	222	LEU	4.0
1	K	271	VAL	4.0
1	L	357	THR	4.0
1	N	174	VAL	3.8
1	N	154	SER	3.8
1	N	484	GLU	3.8
1	M	304	GLU	3.8
1	M	275	ALA	3.7
1	L	169	VAL	3.7
1	J	151	SER	3.7
1	N	354	GLU	3.6
1	J	139	SER	3.6
1	I	274	ALA	3.6
1	K	151	SER	3.5
1	N	231	ARG	3.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	G	148	GLY	3.5
1	G	141	SER	3.4
1	C	152	ALA	3.4
1	M	265	ASN	3.4
1	M	212	ALA	3.3
1	M	274	ALA	3.3
1	L	374	GLY	3.3
1	M	273	VAL	3.3
1	E	139	SER	3.3
1	G	140	ASP	3.2
1	L	214	GLU	3.2
1	N	194	GLN	3.2
1	J	247	LEU	3.2
1	E	140	ASP	3.2
1	M	201	SER	3.1
1	N	192	GLY	3.1
1	G	139	SER	3.1
1	N	147	VAL	3.1
1	M	154	SER	3.1
1	H	305	ILE	3.1
1	C	151	SER	3.1
1	C	139	SER	3.0
1	L	191	GLU	3.0
1	N	142	LYS	3.0
1	F	140	ASP	3.0
1	M	206	ASN	3.0
1	L	340	ALA	3.0
1	J	153	ASN	3.0
1	A	519	CYS	3.0
1	N	140	ASP	3.0
1	N	256	GLY	2.9
1	L	186	GLU	2.9
1	M	266	THR	2.9
1	I	153	ASN	2.9
1	M	142	LYS	2.9
1	H	140	ASP	2.9
1	C	376	VAL	2.8
1	N	267	MET	2.8
1	L	311	LYS	2.8
1	F	152	ALA	2.8
1	G	144	ILE	2.8
1	H	275	ALA	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	H	233	MET	2.8
1	M	228	SER	2.8
1	F	151	SER	2.7
1	G	151	SER	2.7
1	J	141	SER	2.7
1	M	186	GLU	2.7
1	N	212	ALA	2.7
1	M	493	ILE	2.7
1	D	320	ALA	2.7
1	N	250	ILE	2.7
1	I	139	SER	2.7
1	C	484	GLU	2.7
1	M	214	GLU	2.6
1	M	189	VAL	2.6
1	J	150	ILE	2.6
1	N	340	ALA	2.6
1	I	204	PHE	2.6
1	H	151	SER	2.6
1	F	148	GLY	2.6
1	N	347	ALA	2.6
1	C	141	SER	2.6
1	J	140	ASP	2.6
1	N	356	ALA	2.6
1	M	181	THR	2.6
1	I	142	LYS	2.6
1	M	227	ILE	2.5
1	L	283	ASP	2.5
1	H	222	LEU	2.5
1	I	275	ALA	2.5
1	L	113	PRO	2.5
1	C	203	TYR	2.5
1	L	145	ALA	2.5
1	B	343	GLN	2.5
1	E	169	VAL	2.5
1	H	300	VAL	2.5
1	F	141	SER	2.4
1	L	154	SER	2.4
1	K	381	VAL	2.4
1	F	222	LEU	2.4
1	L	187	LEU	2.4
1	M	305	ILE	2.4
1	M	354	GLU	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	193	MET	2.4
1	C	189	VAL	2.4
1	J	142	LYS	2.4
1	L	243	ALA	2.4
1	E	376	VAL	2.4
1	L	354	GLU	2.4
1	N	299	THR	2.4
1	N	311	LYS	2.3
1	D	305	ILE	2.3
1	D	193	MET	2.3
1	K	333	ILE	2.3
1	L	140	ASP	2.3
1	H	144	ILE	2.3
1	C	148	GLY	2.3
1	H	143	ALA	2.3
1	N	351	GLN	2.3
1	J	484	GLU	2.3
1	I	183	LEU	2.3
1	K	191	GLU	2.3
1	E	192	GLY	2.3
1	A	304	GLU	2.3
1	N	332	ILE	2.3
1	K	376	VAL	2.3
1	J	149	THR	2.2
1	C	160	LYS	2.2
1	F	44	PHE	2.2
1	K	357	THR	2.2
1	J	191	GLU	2.2
1	M	173	GLY	2.2
1	M	323	VAL	2.2
1	M	250	ILE	2.2
1	E	375	GLY	2.2
1	F	139	SER	2.1
1	L	159	GLY	2.1
1	D	64	ASP	2.1
1	I	519	CYS	2.1
1	K	152	ALA	2.1
1	N	260	ALA	2.1
1	H	517	THR	2.1
1	N	274	ALA	2.1
1	L	493	ILE	2.1
1	D	247	LEU	2.1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	N	5	ASP	2.1
1	M	148	GLY	2.1
1	H	323	VAL	2.1
1	N	233	MET	2.1
1	E	522	THR	2.1
1	I	203	TYR	2.1
1	K	139	SER	2.1
1	C	477	GLY	2.1
1	K	273	VAL	2.1
1	H	234	LEU	2.1
1	H	331	THR	2.1
1	C	377	ALA	2.1
1	M	143	ALA	2.1
1	K	274	ALA	2.1
1	G	153	ASN	2.0
1	M	213	VAL	2.0
1	E	141	SER	2.0
1	L	147	VAL	2.0
1	M	324	VAL	2.0
1	I	194	GLN	2.0

## 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(Å <sup>2</sup> )	Q<0.9
3	TL	F	551	1/1	0.73	0.10	125,125,125,125	1
3	TL	G	551	1/1	0.73	0.14	125,125,125,125	1
3	TL	J	551	1/1	0.75	0.18	125,125,125,125	1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	AGS	E	549	31/31	0.76	0.27	125,125,125,125	0
3	TL	H	554	1/1	0.76	0.15	125,125,125,125	1
4	MG	A	553	1/1	0.79	0.25	125,125,125,125	0
2	AGS	L	549	31/31	0.79	0.25	125,125,125,125	0
2	AGS	C	549	31/31	0.80	0.23	125,125,125,125	0
2	AGS	N	549	31/31	0.80	0.23	125,125,125,125	0
4	MG	C	553	1/1	0.81	0.41	125,125,125,125	0
2	AGS	J	549	31/31	0.82	0.27	125,125,125,125	0
2	AGS	M	549	31/31	0.83	0.21	125,125,125,125	0
2	AGS	H	549	31/31	0.83	0.23	125,125,125,125	0
4	MG	I	553	1/1	0.84	0.23	125,125,125,125	0
2	AGS	F	549	31/31	0.84	0.24	125,125,125,125	0
4	MG	G	553	1/1	0.84	0.22	125,125,125,125	0
3	TL	E	550	1/1	0.85	0.13	125,125,125,125	1
3	TL	L	551	1/1	0.85	0.16	125,125,125,125	1
4	MG	H	553	1/1	0.86	0.24	125,125,125,125	0
2	AGS	A	549	31/31	0.86	0.21	125,125,125,125	0
2	AGS	B	549	31/31	0.86	0.19	125,125,125,125	0
4	MG	N	552	1/1	0.86	0.32	125,125,125,125	0
3	TL	B	552	1/1	0.87	0.18	125,125,125,125	1
3	TL	K	552	1/1	0.87	0.18	125,125,125,125	1
2	AGS	G	549	31/31	0.87	0.22	125,125,125,125	0
3	TL	K	550	1/1	0.88	0.10	125,125,125,125	1
3	TL	A	551	1/1	0.88	0.17	125,125,125,125	1
2	AGS	D	549	31/31	0.88	0.18	125,125,125,125	0
2	AGS	K	549	31/31	0.88	0.20	125,125,125,125	0
4	MG	F	553	1/1	0.88	0.25	125,125,125,125	0
3	TL	L	550	1/1	0.89	0.15	125,125,125,125	1
3	TL	C	551	1/1	0.89	0.08	125,125,125,125	1
4	MG	D	553	1/1	0.90	0.21	125,125,125,125	0
2	AGS	I	549	31/31	0.90	0.17	125,125,125,125	0
3	TL	D	552	1/1	0.91	0.05	125,125,125,125	1
4	MG	L	553	1/1	0.92	0.21	125,125,125,125	0
3	TL	N	551	1/1	0.93	0.20	125,125,125,125	1
3	TL	H	552	1/1	0.93	0.16	125,125,125,125	1
3	TL	D	551	1/1	0.93	0.12	125,125,125,125	1
3	TL	H	551	1/1	0.93	0.07	125,125,125,125	1
3	TL	G	552	1/1	0.94	0.12	125,125,125,125	1
3	TL	J	550	1/1	0.94	0.14	125,125,125,125	1
4	MG	M	553	1/1	0.94	0.14	125,125,125,125	0
3	TL	N	550	1/1	0.94	0.07	125,125,125,125	1
3	TL	C	550	1/1	0.94	0.09	125,125,125,125	1

*Continued on next page...*

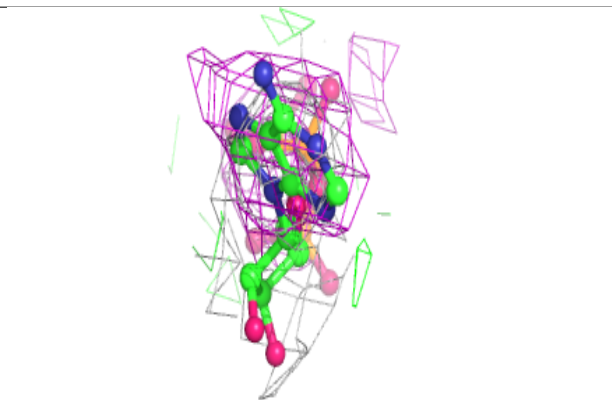
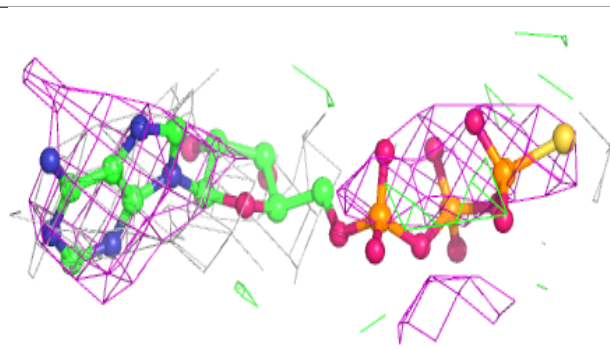
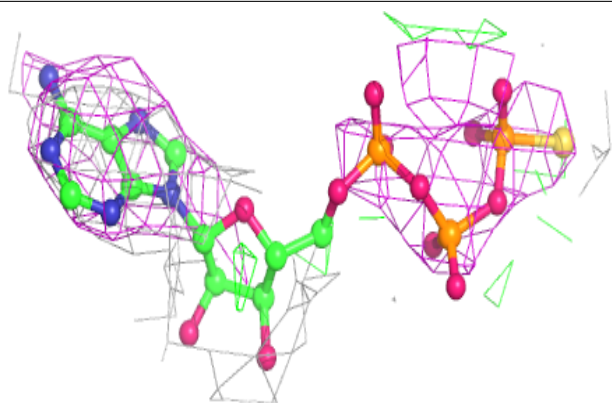
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	TL	H	550	1/1	0.94	0.07	125,125,125,125	1
3	TL	E	551	1/1	0.94	0.06	125,125,125,125	1
4	MG	J	553	1/1	0.94	0.13	125,125,125,125	0
3	TL	A	552	1/1	0.94	0.11	125,125,125,125	1
3	TL	L	552	1/1	0.95	0.04	125,125,125,125	1
4	MG	K	553	1/1	0.95	0.12	125,125,125,125	0
3	TL	G	550	1/1	0.95	0.11	125,125,125,125	1
4	MG	E	553	1/1	0.95	0.34	125,125,125,125	0
3	TL	I	551	1/1	0.95	0.13	125,125,125,125	1
3	TL	M	552	1/1	0.95	0.20	125,125,125,125	1
3	TL	B	550	1/1	0.95	0.11	125,125,125,125	1
4	MG	B	553	1/1	0.95	0.16	125,125,125,125	0
3	TL	B	551	1/1	0.96	0.14	125,125,125,125	1
3	TL	A	550	1/1	0.96	0.08	125,125,125,125	1
3	TL	M	550	1/1	0.96	0.10	125,125,125,125	1
3	TL	M	551	1/1	0.96	0.09	125,125,125,125	1
3	TL	D	550	1/1	0.96	0.11	125,125,125,125	1
3	TL	C	552	1/1	0.96	0.25	125,125,125,125	1
3	TL	F	552	1/1	0.97	0.08	125,125,125,125	1
3	TL	K	551	1/1	0.98	0.11	125,125,125,125	1
3	TL	F	554	1/1	0.98	0.17	125,125,125,125	1
3	TL	I	552	1/1	0.98	0.06	125,125,125,125	1
3	TL	I	550	1/1	0.98	0.08	125,125,125,125	1
3	TL	J	552	1/1	0.98	0.04	125,125,125,125	1
3	TL	A	554	1/1	0.99	0.20	125,125,125,125	1
3	TL	E	552	1/1	0.99	0.25	125,125,125,125	1
3	TL	F	550	1/1	0.99	0.21	125,125,125,125	1
3	TL	D	1	1/1	0.99	0.19	125,125,125,125	1
3	TL	B	554	1/1	1.00	0.19	125,125,125,125	1

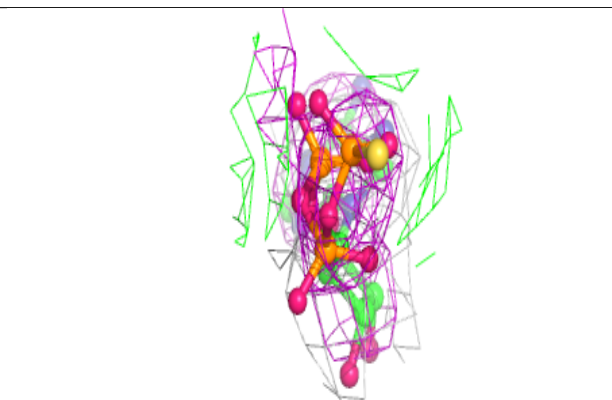
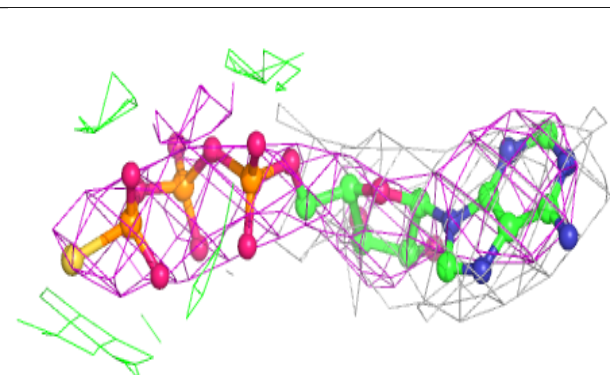
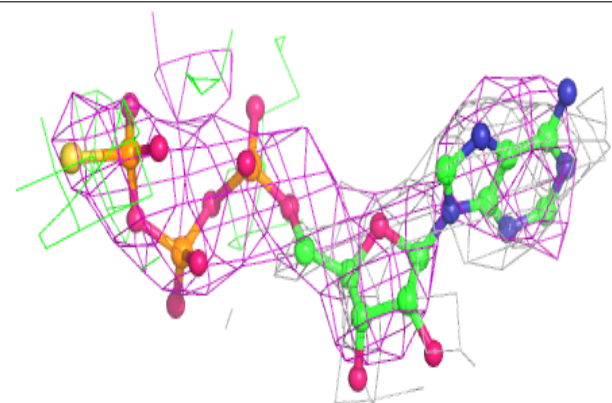
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around AGS E 549:**

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

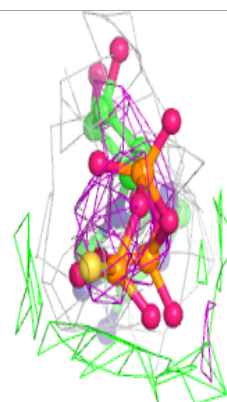
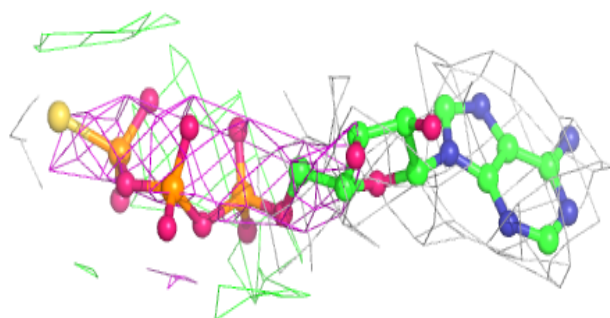
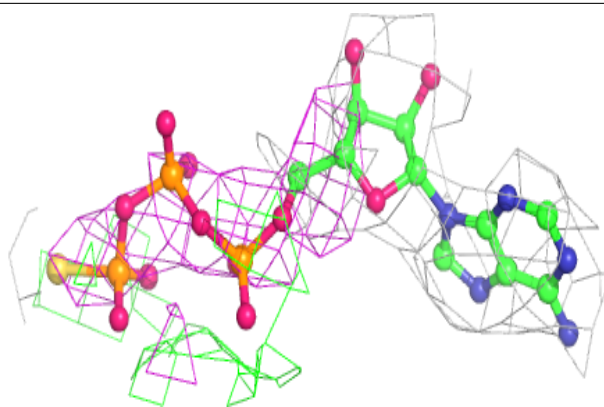
**Electron density around AGS L 549:**

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

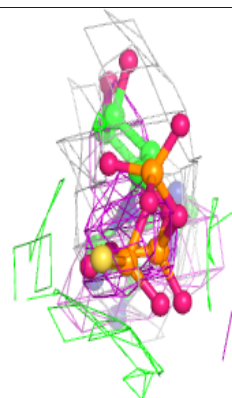
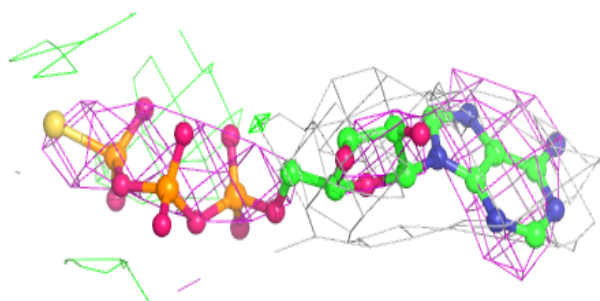
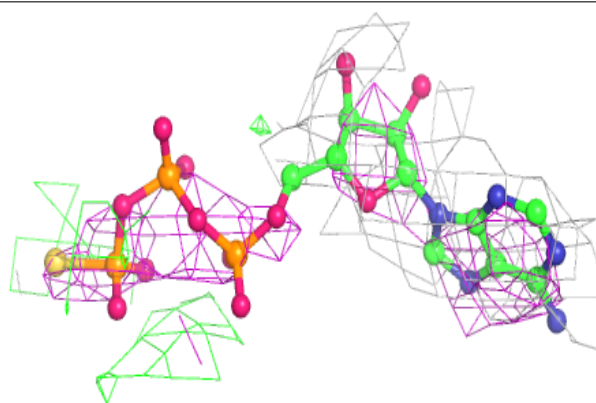


**Electron density around AGS C 549:**

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

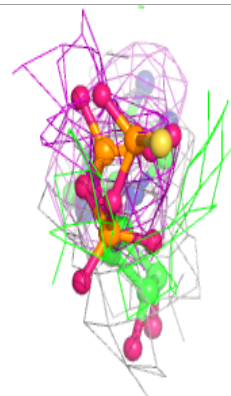
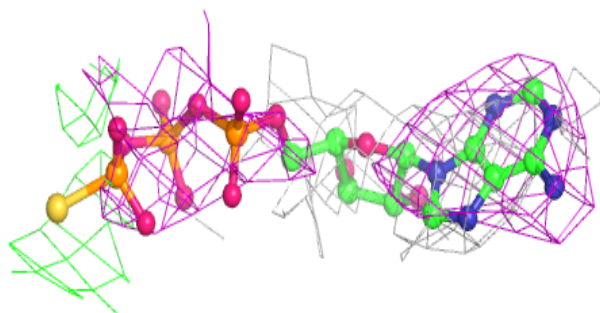
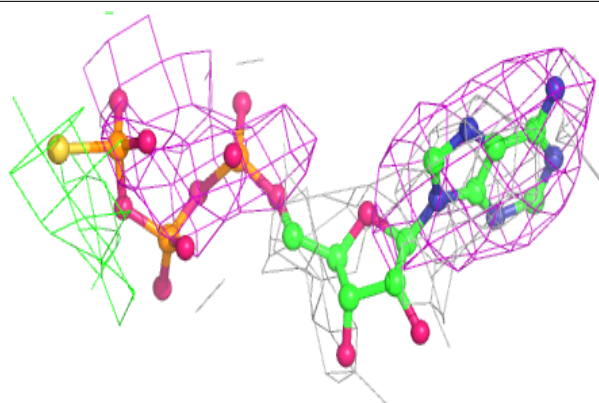
**Electron density around AGS N 549:**

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

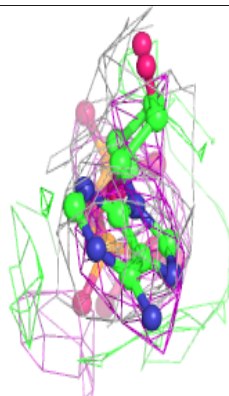
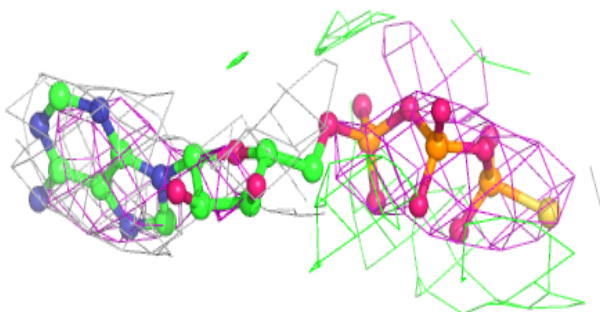
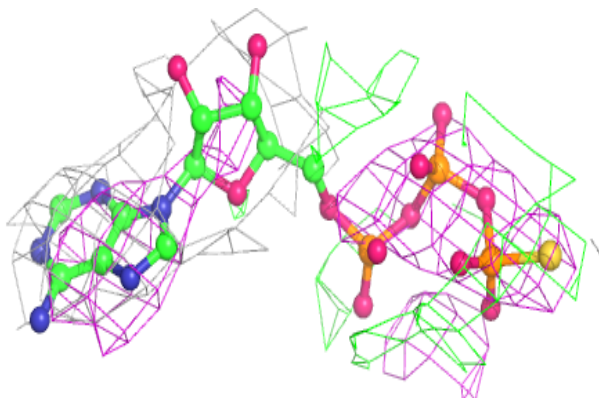


**Electron density around AGS J 549:**

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

**Electron density around AGS M 549:**

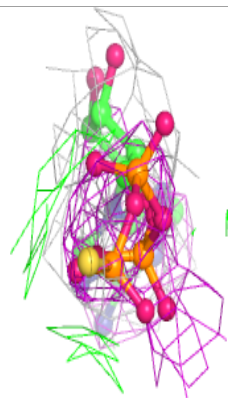
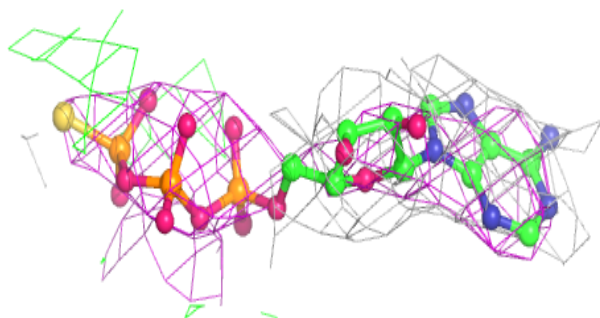
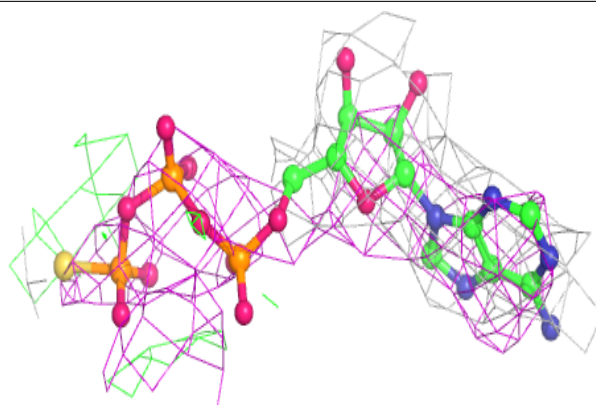
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



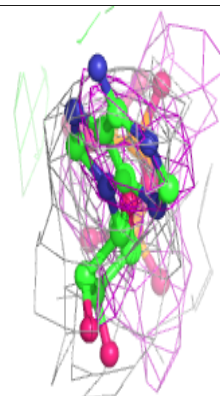
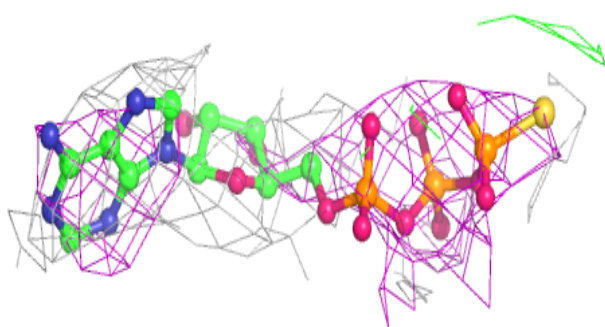
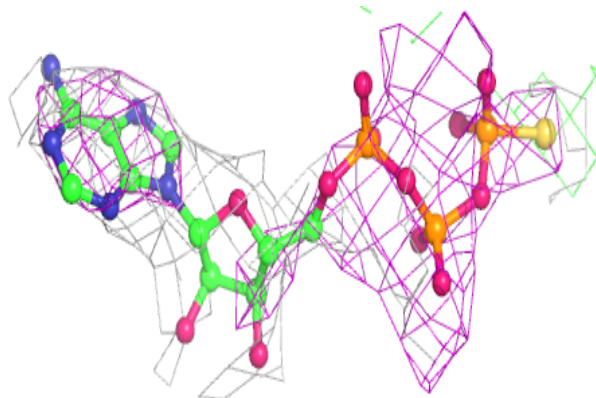


**Electron density around AGS H 549:**

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

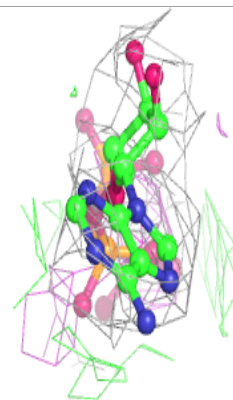
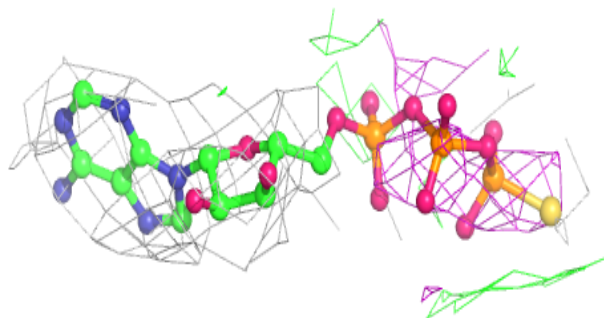
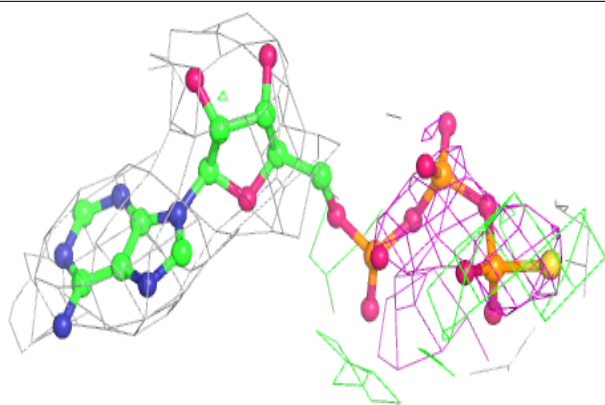
**Electron density around AGS F 549:**

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

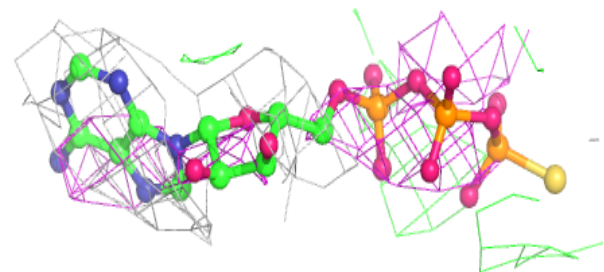
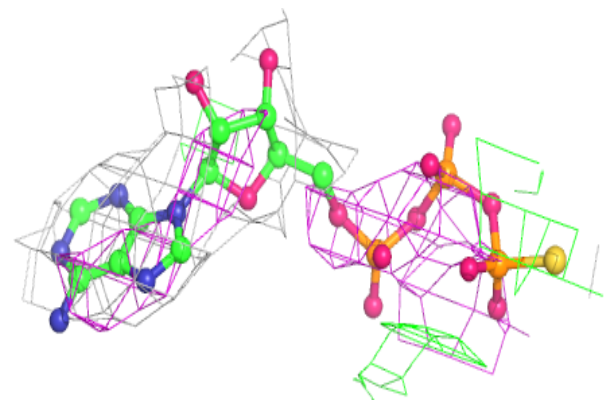


**Electron density around AGS A 549:**

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

**Electron density around AGS B 549:**

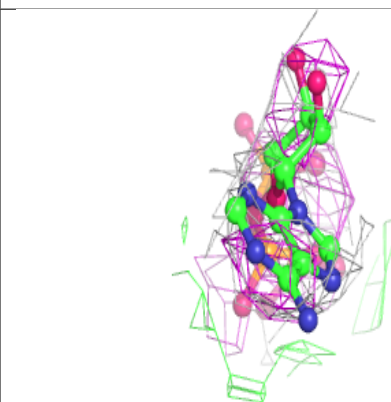
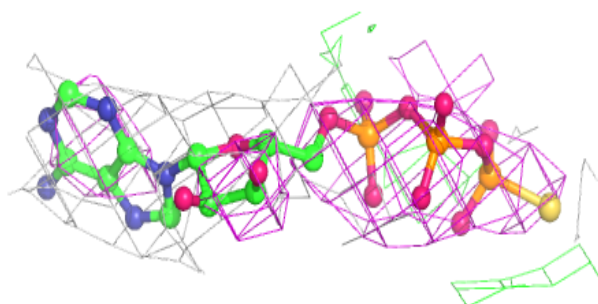
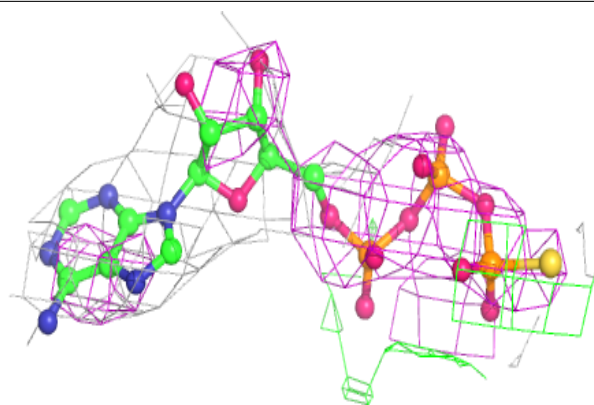
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



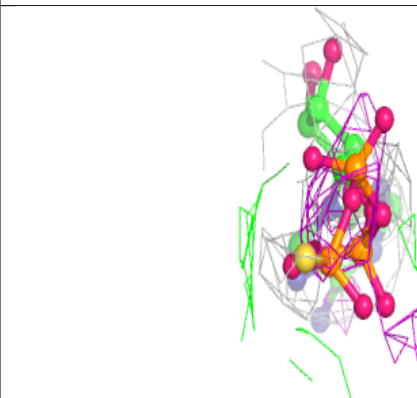
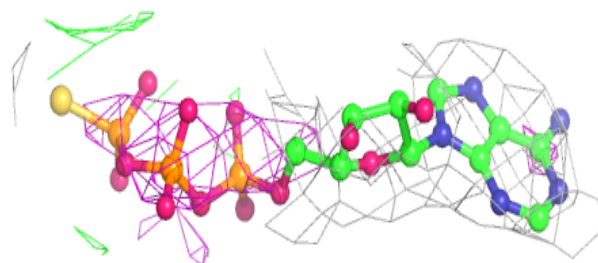
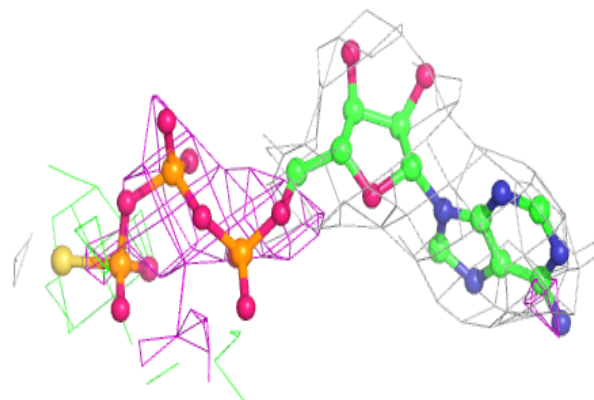


**Electron density around AGS G 549:**

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

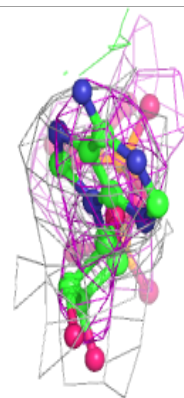
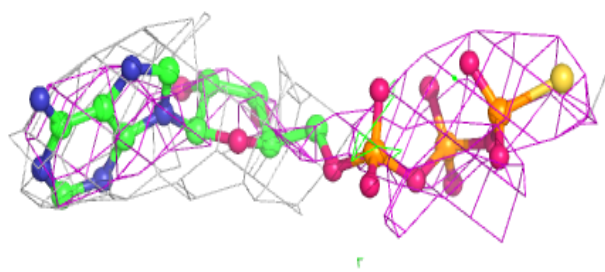
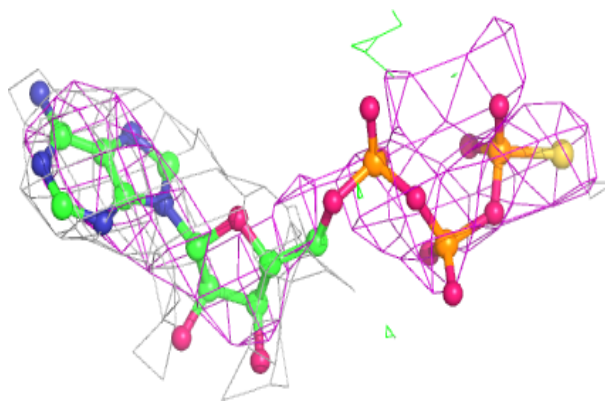
**Electron density around AGS D 549:**

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

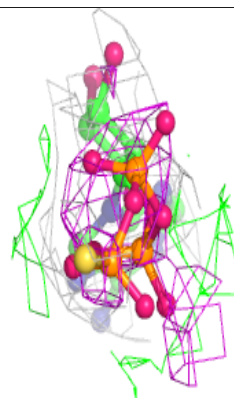
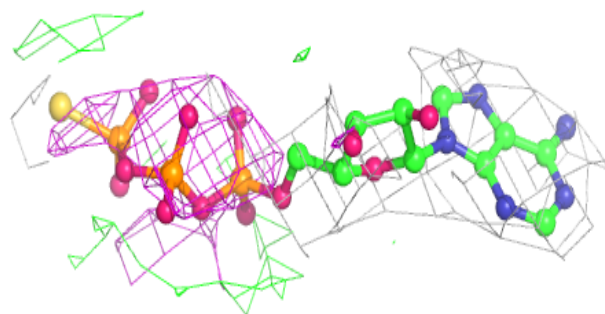
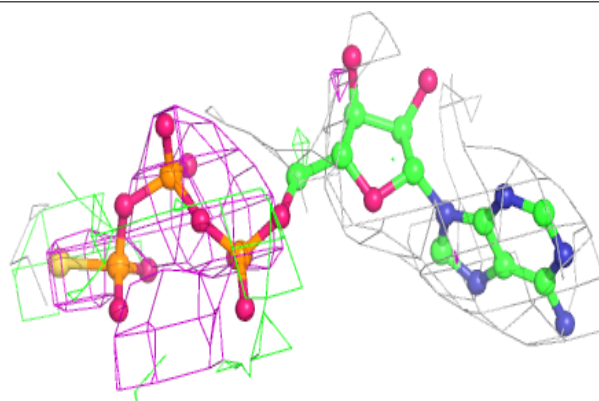


**Electron density around AGS K 549:**

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

**Electron density around AGS I 549:**

$2mF_o-DF_c$  (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.