



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 07:46 PM UTC

PDB ID : 3E76 / pdb_00003e76
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

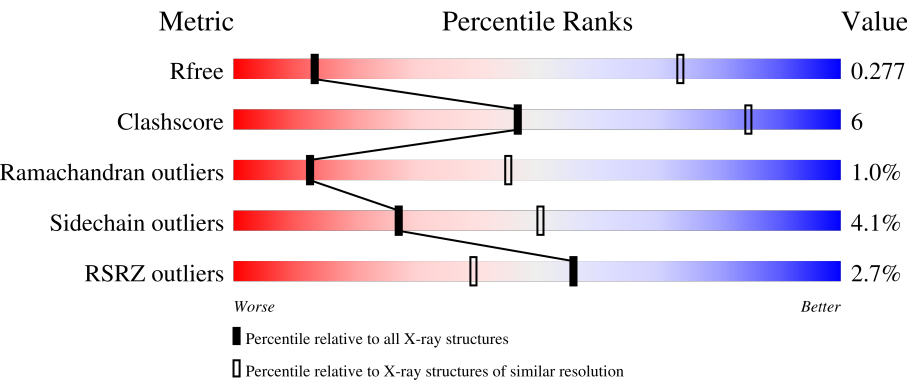
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.94 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}	180053	1022 (4.12-3.76)
Clashscore	190562	1000 (4.10-3.78)
Ramachandran outliers	187476	1009 (4.12-3.76)
Sidechain outliers	187428	1002 (4.12-3.76)
RSRZ outliers	180081	1022 (4.12-3.76)

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

Mol	Chain	Length	Quality of chain
1	A	547	3% 76% 18% • •
1	B	547	% 80% 15% • •
1	C	547	3% 81% 14% • •
1	D	547	3% 79% 16% • •
1	E	547	2% 80% 15% • •

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Mol	Chain	Length	Quality of chain
1	F	547	2% 77% 18% • •
1	G	547	3% 76% 18% • •
1	H	547	3% 80% 14% • •
1	I	547	3% 77% 18% • •
1	J	547	3% 78% 17% • •
1	K	547	% 77% 17% • •
1	L	547	3% 84% 12% •
1	M	547	4% 82% 13% •
1	N	547	3% 85% 11% •

2 Entry composition

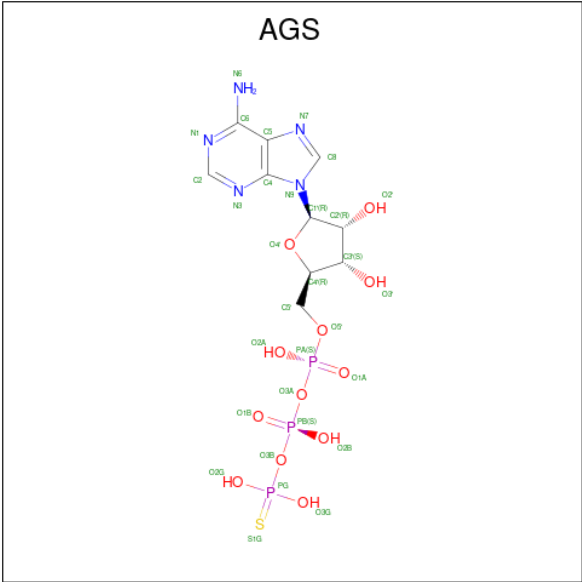
There are 4 unique types of molecules in this entry. The entry contains 54464 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PHOSPHOTHIPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



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 (CCD ID: TL) (formula: Tl).

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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Mg 1	0	0
4	B	1	Total 1	Mg 1	0	0
4	C	1	Total 1	Mg 1	0	0
4	D	1	Total 1	Mg 1	0	0
4	E	1	Total 1	Mg 1	0	0

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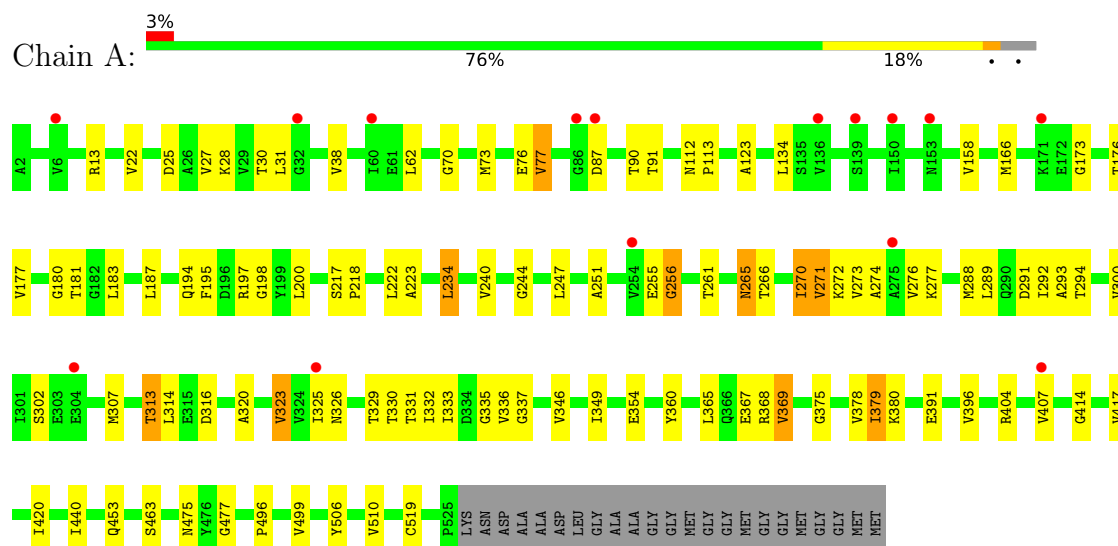
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	1	Total	Mg	0	0
			1	1		
4	G	1	Total	Mg	0	0
			1	1		
4	H	1	Total	Mg	0	0
			1	1		
4	I	1	Total	Mg	0	0
			1	1		
4	J	1	Total	Mg	0	0
			1	1		
4	K	1	Total	Mg	0	0
			1	1		
4	L	1	Total	Mg	0	0
			1	1		
4	M	1	Total	Mg	0	0
			1	1		
4	N	1	Total	Mg	0	0
			1	1		

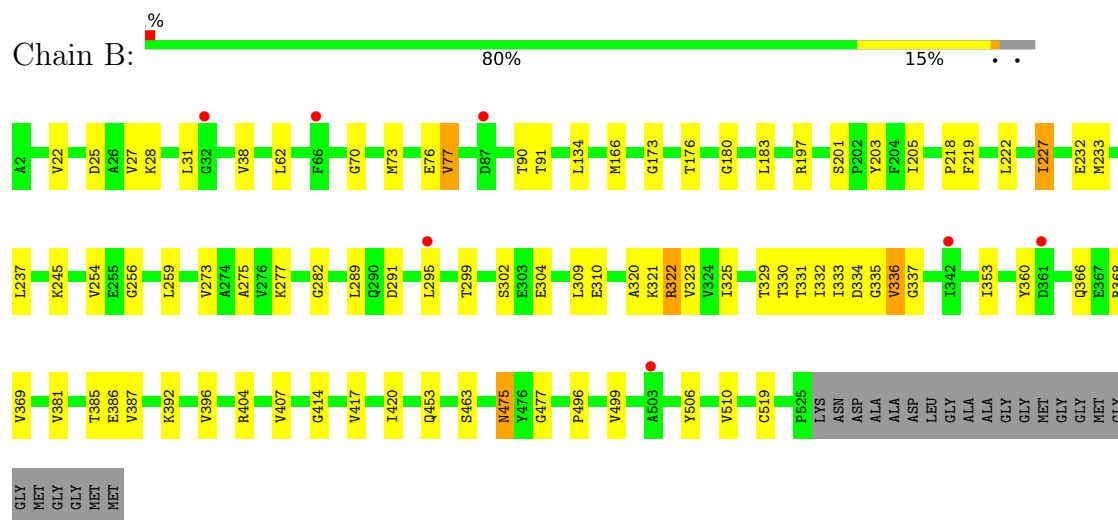
3 Residue-property plots

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

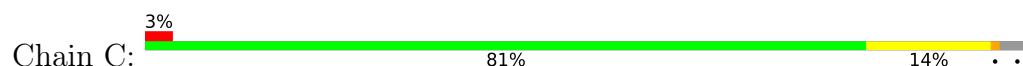
• Molecule 1: 60 kDa chaperonin

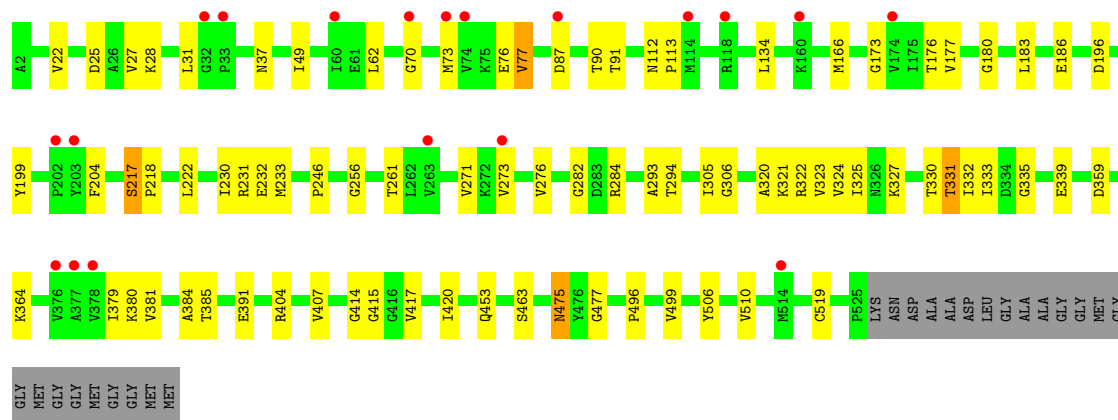


• Molecule 1: 60 kDa chaperonin

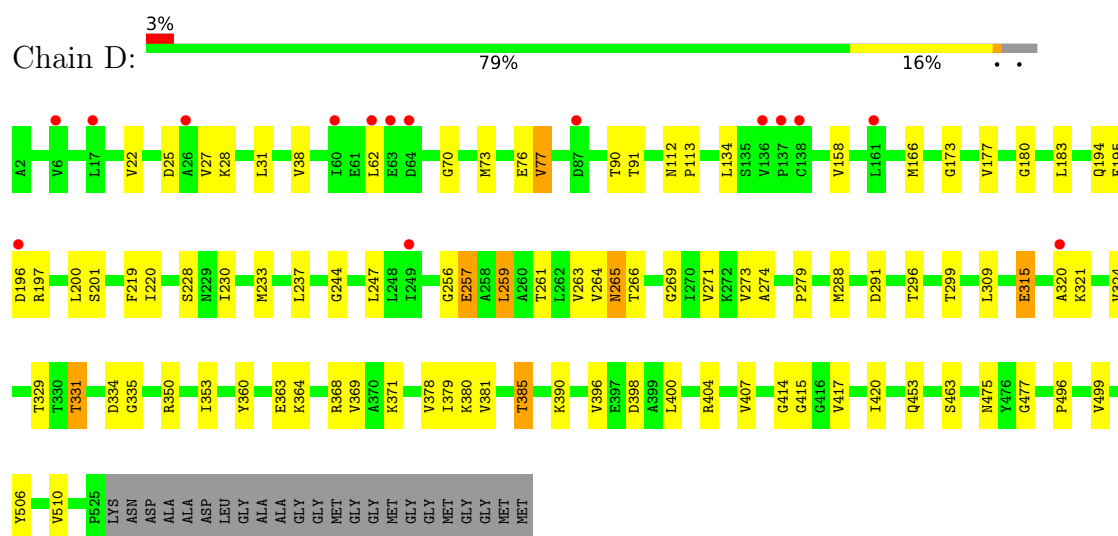


• Molecule 1: 60 kDa chaperonin

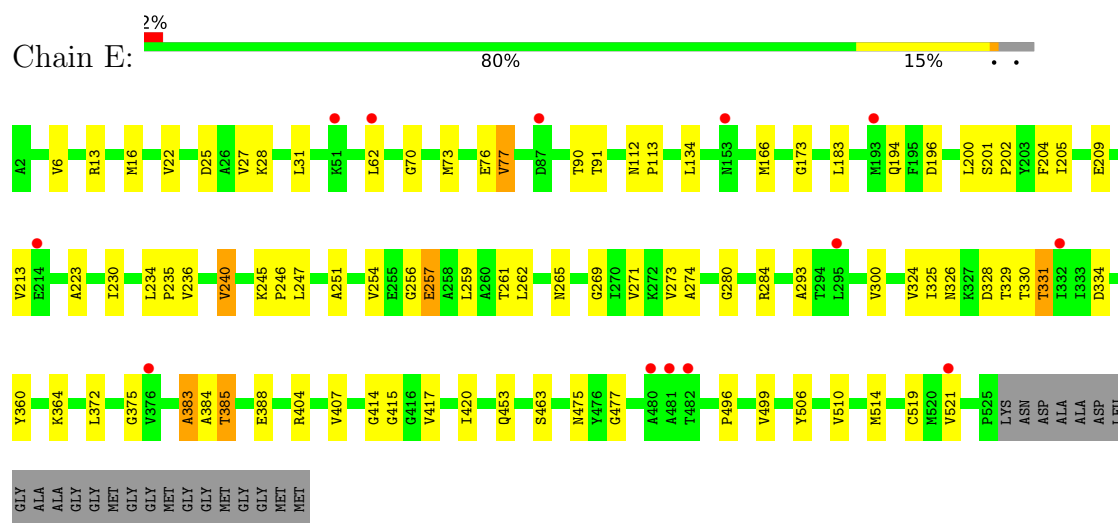




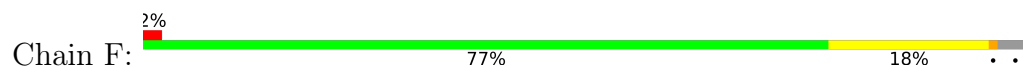
- Molecule 1: 60 kDa chaperonin

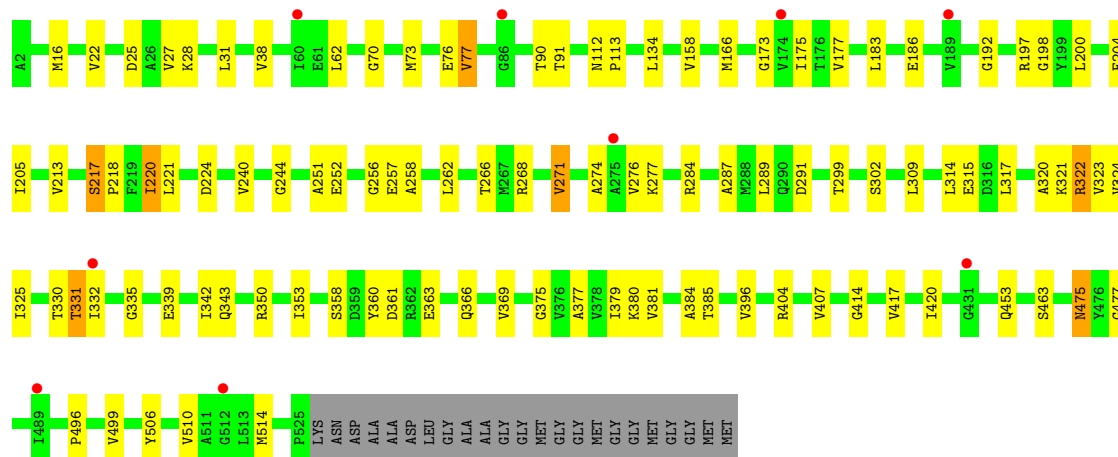


- Molecule 1: 60 kDa chaperonin

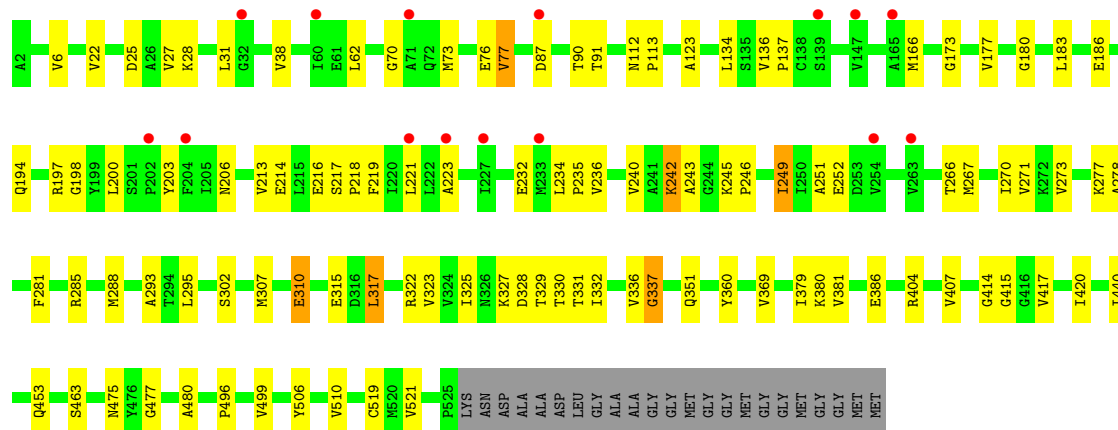
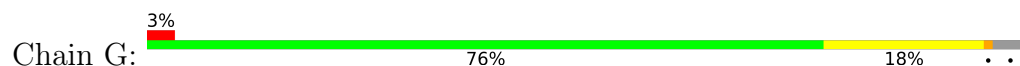


- Molecule 1: 60 kDa chaperonin

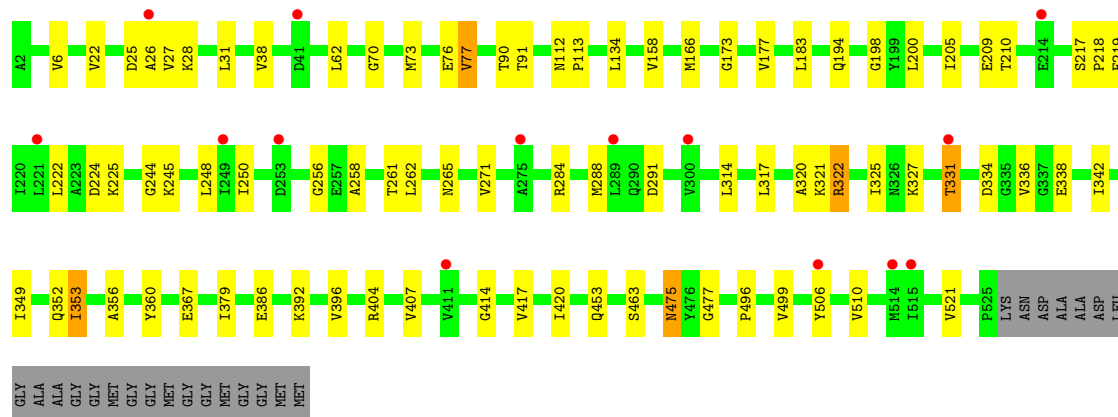
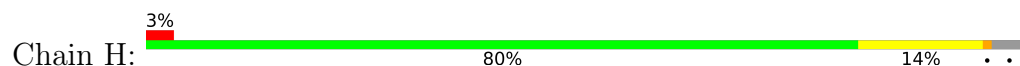




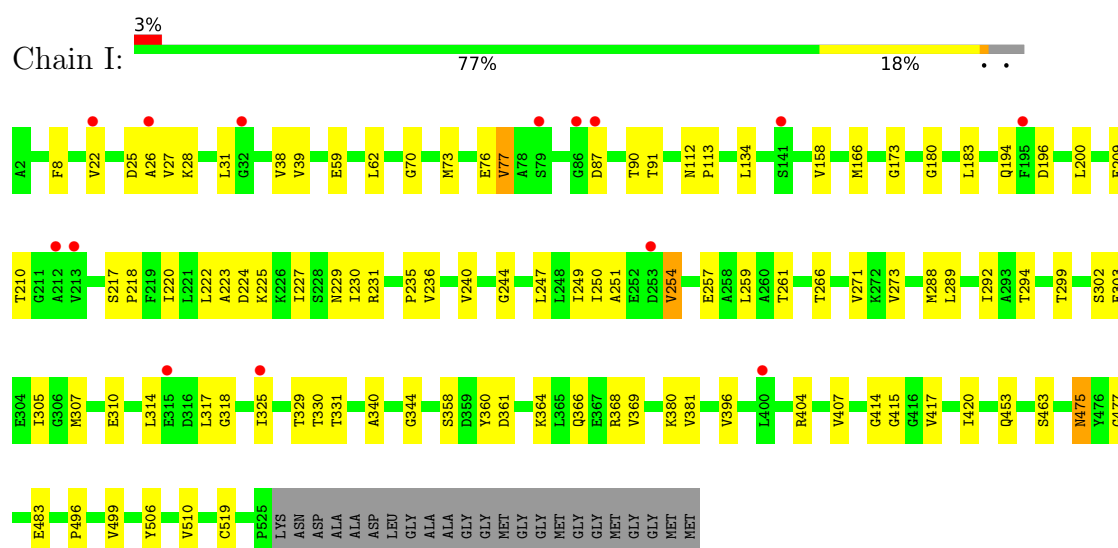
• Molecule 1: 60 kDa chaperonin



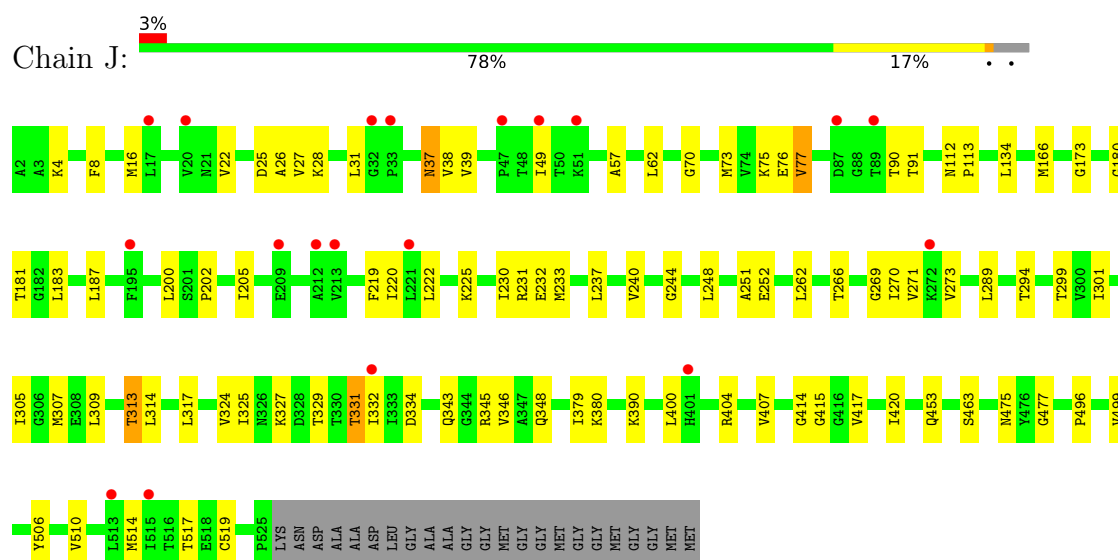
• Molecule 1: 60 kDa chaperonin



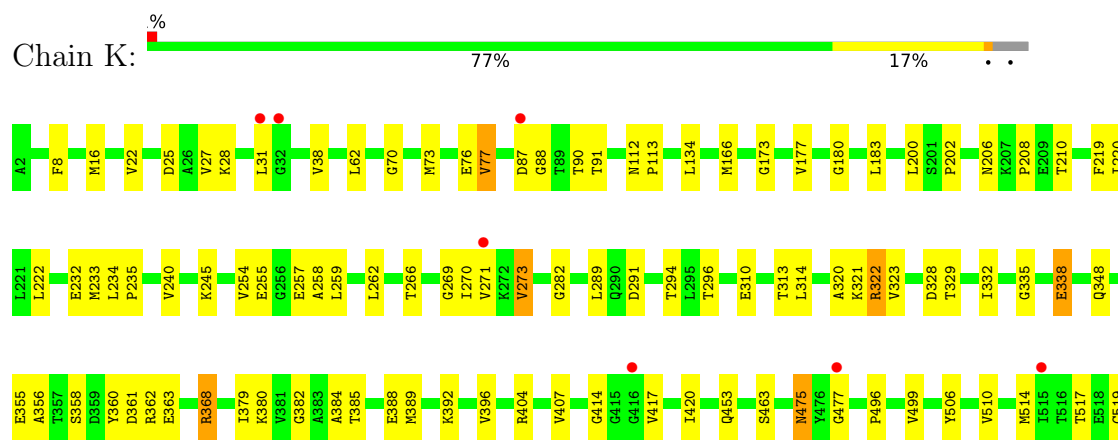
• Molecule 1: 60 kDa chaperonin



- Molecule 1: 60 kDa chaperonin



- Molecule 1: 60 kDa chaperonin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	135.68Å 260.95Å 287.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.39 – 3.94 49.39 – 3.94	Depositor EDS
% Data completeness (in resolution range)	97.7 (49.39-3.94) 98.0 (49.39-3.94)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	115.0	Xtriage
Anisotropy	0.482	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 115.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	54464	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.50	0/3883	0.85	4/5243 (0.1%)
1	B	0.48	0/3883	0.81	0/5243
1	C	0.50	2/3883 (0.1%)	0.80	1/5243 (0.0%)
1	D	0.50	2/3883 (0.1%)	0.84	2/5243 (0.0%)
1	E	0.50	1/3883 (0.0%)	0.84	6/5243 (0.1%)
1	F	0.48	0/3883	0.84	0/5243
1	G	0.48	0/3883	0.82	2/5243 (0.0%)
1	H	0.51	2/3883 (0.1%)	0.82	0/5243
1	I	0.49	2/3883 (0.1%)	0.82	0/5243
1	J	0.48	1/3883 (0.0%)	0.83	1/5243 (0.0%)
1	K	0.49	2/3883 (0.1%)	0.82	1/5243 (0.0%)
1	L	0.46	0/3883	0.79	0/5243
1	M	0.50	2/3883 (0.1%)	0.80	0/5243
1	N	0.52	1/3883 (0.0%)	0.79	0/5243
All	All	0.49	15/54362 (0.0%)	0.82	17/73402 (0.0%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	37	ASN	CG-ND2	-8.47	1.15	1.33
1	C	232	GLU	CD-OE2	7.24	1.39	1.25
1	N	338	GLU	CD-OE2	6.85	1.38	1.25
1	M	37	ASN	CG-OD1	-6.83	1.10	1.23
1	H	367	GLU	CD-OE2	6.08	1.36	1.25
1	D	315	GLU	CD-OE1	5.81	1.36	1.25
1	J	37	ASN	CG-ND2	-5.72	1.21	1.33
1	H	367	GLU	CD-OE1	5.61	1.36	1.25
1	I	196	ASP	CG-OD2	5.58	1.35	1.25
1	C	339	GLU	CG-CD	5.53	1.65	1.52
1	I	196	ASP	CG-OD1	5.46	1.35	1.25
1	D	315	GLU	CD-OE2	5.40	1.35	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	363	GLU	CD-OE1	5.15	1.35	1.25
1	K	348	GLN	CD-OE1	5.12	1.33	1.23
1	E	13	ARG	CD-NE	-5.09	1.39	1.46

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	13	ARG	NE-CZ-NH2	-10.18	110.04	119.20
1	A	13	ARG	NE-CZ-NH2	-9.57	110.59	119.20
1	E	13	ARG	NE-CZ-NH1	7.86	129.36	121.50
1	A	13	ARG	NE-CZ-NH1	7.58	129.08	121.50
1	A	13	ARG	CD-NE-CZ	7.57	135.00	124.40
1	E	13	ARG	CD-NE-CZ	7.38	134.73	124.40
1	A	13	ARG	CB-CG-CD	-6.12	97.23	111.30
1	E	13	ARG	CB-CG-CD	-5.98	97.55	111.30
1	E	245	LYS	CA-C-N	5.90	127.22	119.84
1	E	245	LYS	C-N-CA	5.90	127.22	119.84
1	J	325	ILE	N-CA-C	5.74	114.62	106.53
1	G	278	ALA	CA-C-N	5.51	125.52	119.90
1	G	278	ALA	C-N-CA	5.51	125.52	119.90
1	K	232	GLU	N-CA-C	-5.42	108.44	114.62
1	C	384	ALA	N-CA-C	5.27	117.68	108.52
1	D	196	ASP	N-CA-C	5.26	117.12	109.71
1	D	329	THR	N-CA-C	5.13	115.80	107.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3855	0	3976	65	0
1	B	3855	0	3974	43	0
1	C	3855	0	3976	43	0
1	D	3855	0	3976	47	0
1	E	3855	0	3974	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3855	0	3976	53	0
1	G	3855	0	3975	57	0
1	H	3855	0	3976	46	0
1	I	3855	0	3975	59	0
1	J	3855	0	3974	51	0
1	K	3855	0	3975	53	0
1	L	3855	0	3976	34	0
1	M	3855	0	3976	38	0
1	N	3855	0	3976	36	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	2	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	632	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 6.

All (632) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:L:230:ILE:HG13	1:L:233:MET:HE3	1.80	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:D:233:MET:HE3	1:D:237:LEU:HD11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:K:233:MET:C	1:K:235:PRO:HD2	2.29	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: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:L:206:ASN:HD21	1:L:214:GLU:H	1.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:302:SER:H	1:A:307:MET:HE3	1.73	0.53
1:J:77:VAL:CG1	1:J:506:TYR:HB3	2.38	0.52
1:B:233:MET:HE3	1:B:237:LEU:HD12	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:251:ALA:O	1:G:252:GLU:C	2.52	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:177:VAL:HG22	1:G:379:ILE:HB	1.91	0.52
1:G:323:VAL:HG12	1:G:332:ILE:HA	1.92	0.52
1:B:335:GLY:C	1:B:337:GLY:H	2.17	0.51
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
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:E:70:GLY:HA2	1:E:73:MET:HE3	1.92	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:G:302:SER:H	1:G:307:MET:HE3	1.75	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:F:251:ALA:O	1:F:252:GLU:C	2.54	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:J:230:ILE:C	1:J:232:GLU:H	2.17	0.51
1:I:366:GLN:HA	1:I:369:VAL:HG22	1.93	0.51
1:B:201:SER:C	1:B:203:TYR:H	2.19	0.51
1:B:392:LYS:O	1:B:396:VAL:HG23	2.11	0.51
1:G:336:VAL:O	1:G:337:GLY:C	2.54	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:A:87:ASP:CG	1:A:499:VAL:HG21	2.34	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ARG:NH2	1:G:386:GLU:OE2	2.44	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: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
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: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:C:70:GLY:HA2	1:C:73:MET:HE3	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:305:ILE:HB	1:I:307:MET:HE2	1.95	0.48
1:M:70:GLY:HA2	1:M:73:MET:HE3	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:B:321:LYS:O	1:B:322:ARG:HB2	2.11	0.48
1:D:414:GLY:O	1:D:417:VAL:HG22	2.13	0.48
1:F:70:GLY:HA2	1:F:73:MET:HE3	1.95	0.48
1:H:158:VAL:HG13	1:H:396:VAL:HG22	1.94	0.48
1:J:183:LEU:O	1:J:183:LEU:HG	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
1:D:197:ARG:HE	1:D:279:PRO:HA	1.79	0.48
1:G:70:GLY:HA2	1:G:73:MET:HE3	1.96	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:HG	1:M:183:LEU:O	2.12	0.48
1:A:70:GLY:HA2	1:A:73:MET:HE3	1.97	0.47
1:I:70:GLY:HA2	1:I:73:MET:HE3	1.96	0.47
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:B:38:VAL:HG22	1:C:519:CYS:HB3	1.95	0.47
1:C:186:GLU:HB2	1:C:380:LYS:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:GLY:HA2	1:D:73:MET:HE3	1.97	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:77:VAL:HG12	1:A:506:TYR:HB3	1.96	0.47
1:A:313:THR:H	1:A:316:ASP:HB2	1.79	0.47
1:G:183:LEU:O	1:G:183:LEU:HG	2.13	0.47
1:B:70:GLY:HA2	1:B:73:MET:HE3	1.97	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:N:77:VAL:CG1	1:N:506:TYR:HB3	2.45	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:N:70:GLY:HA2	1:N:73:MET:HE3	1.96	0.47
1:A:87:ASP:OD2	1:A:499:VAL:HG11	2.15	0.47
1:A:414:GLY:O	1:A:417:VAL:HG22	2.15	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:J:70:GLY:HA2	1:J:73:MET:HE3	1.97	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
1:B:166:MET:HE1	1:B:407:VAL:HG21	1.97	0.46
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: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:O	1:E:183:LEU:HG	2.15	0.46
1:G:166:MET:HE1	1:G:407:VAL:HG21	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:31:LEU:HD23	1:N:453:GLN:HB3	1.97	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:J:166:MET:HE1	1:J:407:VAL:HG21	1.97	0.46
1:K:31:LEU:HD23	1:K:453:GLN:HB3	1.98	0.46
1:K:222:LEU:HB3	1:K:289:LEU:HD22	1.98	0.46
1:L:70:GLY:HA2	1:L:73:MET:HE3	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:B:31:LEU:HD23	1:B:453:GLN:HB3	1.97	0.46
1:B:183:LEU:O	1:B:183:LEU:HG	2.15	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:N:166:MET:HE1	1:N:407:VAL:HG21	1.97	0.45
1:C:31:LEU:HD23	1:C:453:GLN:HB3	1.97	0.45
1:C:166:MET:HE1	1:C:407:VAL:HG21	1.98	0.45
1:J:31:LEU:HD23	1:J:453:GLN:HB3	1.99	0.45
1:A:166:MET:HE1	1:A:407:VAL:HG21	1.98	0.45
1:G:219:PHE:CE2	1:G:245:LYS:HB2	2.52	0.45
1:H:70:GLY:HA2	1:H:73:MET:HE3	1.98	0.45
1:L:166:MET:HE1	1:L:407:VAL:HG21	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:313:THR:HG22	1:J:314:LEU:H	1.81	0.45
1:J:415:GLY:H	2:J:549:AGS:HO2'	1.58	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:K:321:LYS:O	1:K:322:ARG:HB2	2.15	0.45
1:M:220:ILE:HG12	1:M:248:LEU:HD23	1.99	0.45
1:D:219:PHE:C	1:D:220:ILE:HG13	2.42	0.45
1:F:166:MET:HE1	1:F:407:VAL:HG21	1.98	0.45
1:I:77:VAL:CG1	1:I:506:TYR:HB3	2.47	0.45
1:M:166:MET:HE1	1:M:407:VAL:HG21	1.98	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:H:360:TYR:CD1	1:N:183:LEU:HD22	2.50	0.45
1:J:26:ALA:HA	1:K:8:PHE:HE1	1.82	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: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:39:VAL:HG23	1:J:517:THR:HG23	1.99	0.44
1:I:166:MET:HE1	1:I:407:VAL:HG21	1.98	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:E:16:MET:SD	1:E:514:MET:HE3	2.58	0.44
1:F:31:LEU:HD23	1:F:453:GLN:HB3	1.99	0.44
1:I:183:LEU:O	1:I:183:LEU:HG	2.16	0.44
1:K:166:MET:HE1	1:K:407:VAL:HG21	1.98	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:336:VAL:O	1:A:337:GLY:C	2.61	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:H:166:MET:HE1	1:H:407:VAL:HG21	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:38:VAL:HG22	1:M:519:CYS:HB3	2.00	0.44
1:L:392:LYS:O	1:L:396:VAL:HG23	2.18	0.44
1:A:112:ASN:HD22	1:A:113:PRO:HD2	1.82	0.44
1:C:37:ASN:HD22	1:C:49:ILE:CG2	2.28	0.44
1:C:217:SER:N	1:C:218:PRO:HD3	2.33	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:K:70:GLY:HA2	1:K:73:MET:HE3	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
1:N:417:VAL:HG11	1:N:477:GLY:HA3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:166:MET:HE1	1:D:407:VAL:HG21	1.99	0.43
1:I:25:ASP:HA	1:I:28:LYS:HG2	2.01	0.43
1:J:251:ALA:O	1:J:252:GLU:C	2.62	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:166:MET:HE1	1:E:407:VAL:HG21	1.99	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:K:360:TYR:C	1:K:362:ARG:H	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:248:LEU:HD13	1:H:325:ILE:HD11	2.00	0.42
1:H:261:THR:O	1:H:265:ASN:HB2	2.18	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:J:305:ILE:HG21	1:J:307:MET:HE2	2.01	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:H	1:K:338:GLU:HG2	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: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: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: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:N	1:I:475:ASN:HD22	2.18	0.42
1:K:16:MET:SD	1:K:514:MET:HE3	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:M:312:ALA:HA	1:M:316:ASP:HB2	2.02	0.42
1:J:233:MET:HE3	1:J:237:LEU:HD21	2.01	0.41
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:6:VAL:HG22	1:G:521:VAL:HG22	2.02	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: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:D:264:VAL:C	1:D:266:THR:H	2.28	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:16:MET:SD	1:L:514:MET:HE3	2.61	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:A:194:GLN:HG3	1:A:330:THR:O	2.21	0.41
1:B:254:VAL:O	1:B:259:LEU:HD12	2.21	0.41
1:E:204:PHE:HD1	1:E:273:VAL:O	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:257:GLU:C	1:E:259:LEU:H	2.28	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:222:LEU:CD1	1:A:293:ALA:HA	2.52	0.41
1:A:255:GLU:O	1:A:256:GLY:C	2.64	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:HD22	1:H:475:ASN:N	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
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:HA	1:I:364:LYS:HD3	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: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:6:VAL:HG22	1:E:521:VAL:HG22	2.03	0.40
1:E:201:SER:O	1:E:204:PHE:HD2	2.05	0.40
1:I:292:ILE:HG13	1:I:292:ILE:H	1.69	0.40
1:M:475:ASN:N	1:M:475:ASN:HD22	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:F:16:MET:SD	1:F:514:MET:HE3	2.62	0.40
1:J:16:MET:SD	1:J:514:MET:HE3	2.62	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:HD3	1:N:364:LYS:HA	1.91	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	522/547 (95%)	494 (95%)	23 (4%)	5 (1%)	12	45
1	B	522/547 (95%)	490 (94%)	25 (5%)	7 (1%)	9	41
1	C	522/547 (95%)	490 (94%)	27 (5%)	5 (1%)	12	45
1	D	522/547 (95%)	487 (93%)	30 (6%)	5 (1%)	12	45
1	E	522/547 (95%)	493 (94%)	22 (4%)	7 (1%)	9	41
1	F	522/547 (95%)	496 (95%)	19 (4%)	7 (1%)	9	41
1	G	522/547 (95%)	490 (94%)	28 (5%)	4 (1%)	16	51
1	H	522/547 (95%)	496 (95%)	18 (3%)	8 (2%)	8	38
1	I	522/547 (95%)	495 (95%)	25 (5%)	2 (0%)	30	65
1	J	522/547 (95%)	496 (95%)	21 (4%)	5 (1%)	12	45
1	K	522/547 (95%)	485 (93%)	33 (6%)	4 (1%)	16	51
1	L	522/547 (95%)	501 (96%)	20 (4%)	1 (0%)	43	75
1	M	522/547 (95%)	495 (95%)	22 (4%)	5 (1%)	12	45
1	N	522/547 (95%)	483 (92%)	32 (6%)	7 (1%)	9	41
All	All	7308/7658 (95%)	6891 (94%)	345 (5%)	72 (1%)	12	45

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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%)	381 (94%)	23 (6%)	18	44
1	B	404/414 (98%)	389 (96%)	15 (4%)	30	53
1	C	404/414 (98%)	389 (96%)	15 (4%)	30	53
1	D	404/414 (98%)	382 (95%)	22 (5%)	20	45
1	E	404/414 (98%)	390 (96%)	14 (4%)	32	55
1	F	404/414 (98%)	385 (95%)	19 (5%)	23	48
1	G	404/414 (98%)	383 (95%)	21 (5%)	21	46
1	H	404/414 (98%)	389 (96%)	15 (4%)	30	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	404/414 (98%)	389 (96%)	15 (4%)	30	53
1	J	404/414 (98%)	386 (96%)	18 (4%)	24	49
1	K	404/414 (98%)	386 (96%)	18 (4%)	24	49
1	L	404/414 (98%)	391 (97%)	13 (3%)	34	56
1	M	404/414 (98%)	389 (96%)	15 (4%)	30	53
1	N	404/414 (98%)	395 (98%)	9 (2%)	45	65
All	All	5656/5796 (98%)	5424 (96%)	232 (4%)	27	50

All (232) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	GLU
1	A	77	VAL
1	A	91	THR
1	A	134	LEU
1	A	217	SER
1	A	234	LEU
1	A	265	ASN
1	A	270	ILE
1	A	288	MET
1	A	292	ILE
1	A	294	THR
1	A	313	THR
1	A	323	VAL
1	A	331	THR
1	A	346	VAL
1	A	354	GLU
1	A	367	GLU
1	A	369	VAL
1	A	378	VAL
1	A	379	ILE
1	A	391	GLU
1	A	463	SER
1	A	475	ASN
1	B	76	GLU
1	B	77	VAL
1	B	91	THR
1	B	134	LEU
1	B	222	LEU
1	B	227	ILE

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Mol	Chain	Res	Type
1	B	273	VAL
1	B	289	LEU
1	B	295	LEU
1	B	299	THR
1	B	329	THR
1	B	331	THR
1	B	336	VAL
1	B	463	SER
1	B	475	ASN
1	C	76	GLU
1	C	77	VAL
1	C	91	THR
1	C	134	LEU
1	C	196	ASP
1	C	217	SER
1	C	231	ARG
1	C	294	THR
1	C	305	ILE
1	C	331	THR
1	C	359	ASP
1	C	385	THR
1	C	391	GLU
1	C	463	SER
1	C	475	ASN
1	D	76	GLU
1	D	77	VAL
1	D	91	THR
1	D	134	LEU
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	363	GLU
1	D	368	ARG
1	D	369	VAL
1	D	378	VAL
1	D	385	THR
1	D	390	LYS

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Mol	Chain	Res	Type
1	D	398	ASP
1	D	400	LEU
1	D	463	SER
1	D	475	ASN
1	E	76	GLU
1	E	77	VAL
1	E	91	THR
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	372	LEU
1	E	463	SER
1	E	475	ASN
1	F	76	GLU
1	F	77	VAL
1	F	91	THR
1	F	134	LEU
1	F	200	LEU
1	F	217	SER
1	F	220	ILE
1	F	240	VAL
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	363	GLU
1	F	381	VAL
1	F	463	SER
1	F	475	ASN
1	G	76	GLU
1	G	77	VAL
1	G	91	THR
1	G	134	LEU
1	G	206	ASN

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Mol	Chain	Res	Type
1	G	217	SER
1	G	240	VAL
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	317	LEU
1	G	328	ASP
1	G	329	THR
1	G	331	THR
1	G	351	GLN
1	G	369	VAL
1	G	463	SER
1	G	475	ASN
1	H	76	GLU
1	H	77	VAL
1	H	91	THR
1	H	134	LEU
1	H	200	LEU
1	H	209	GLU
1	H	210	THR
1	H	217	SER
1	H	314	LEU
1	H	317	LEU
1	H	331	THR
1	H	353	ILE
1	H	386	GLU
1	H	463	SER
1	H	475	ASN
1	I	76	GLU
1	I	77	VAL
1	I	91	THR
1	I	134	LEU
1	I	200	LEU
1	I	209	GLU
1	I	210	THR
1	I	254	VAL
1	I	257	GLU
1	I	289	LEU
1	I	294	THR

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Mol	Chain	Res	Type
1	I	299	THR
1	I	329	THR
1	I	463	SER
1	I	475	ASN
1	J	76	GLU
1	J	77	VAL
1	J	91	THR
1	J	134	LEU
1	J	200	LEU
1	J	225	LYS
1	J	294	THR
1	J	299	THR
1	J	301	ILE
1	J	313	THR
1	J	327	LYS
1	J	329	THR
1	J	331	THR
1	J	332	ILE
1	J	390	LYS
1	J	400	LEU
1	J	463	SER
1	J	475	ASN
1	K	76	GLU
1	K	77	VAL
1	K	91	THR
1	K	134	LEU
1	K	200	LEU
1	K	206	ASN
1	K	210	THR
1	K	255	GLU
1	K	273	VAL
1	K	294	THR
1	K	310	GLU
1	K	328	ASP
1	K	329	THR
1	K	338	GLU
1	K	355	GLU
1	K	368	ARG
1	K	463	SER
1	K	475	ASN
1	L	76	GLU
1	L	77	VAL

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Mol	Chain	Res	Type
1	L	91	THR
1	L	134	LEU
1	L	200	LEU
1	L	209	GLU
1	L	210	THR
1	L	221	LEU
1	L	283	ASP
1	L	295	LEU
1	L	398	ASP
1	L	463	SER
1	L	475	ASN
1	M	76	GLU
1	M	77	VAL
1	M	91	THR
1	M	134	LEU
1	M	200	LEU
1	M	225	LYS
1	M	234	LEU
1	M	288	MET
1	M	294	THR
1	M	295	LEU
1	M	329	THR
1	M	351	GLN
1	M	398	ASP
1	M	463	SER
1	M	475	ASN
1	N	76	GLU
1	N	77	VAL
1	N	91	THR
1	N	134	LEU
1	N	295	LEU
1	N	299	THR
1	N	329	THR
1	N	463	SER
1	N	475	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	82	ASN
1	A	194	GLN

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Mol	Chain	Res	Type
1	A	265	ASN
1	A	290	GLN
1	A	432	GLN
1	B	68	ASN
1	B	82	ASN
1	B	112	ASN
1	B	194	GLN
1	B	229	ASN
1	B	366	GLN
1	B	432	GLN
1	C	68	ASN
1	C	82	ASN
1	C	112	ASN
1	C	343	GLN
1	C	351	GLN
1	C	432	GLN
1	D	68	ASN
1	D	82	ASN
1	D	112	ASN
1	D	319	GLN
1	D	432	GLN
1	E	68	ASN
1	E	82	ASN
1	E	112	ASN
1	E	194	GLN
1	E	351	GLN
1	E	432	GLN
1	F	68	ASN
1	F	82	ASN
1	F	112	ASN
1	F	432	GLN
1	G	68	ASN
1	G	82	ASN
1	G	112	ASN
1	G	351	GLN
1	G	432	GLN
1	H	68	ASN
1	H	82	ASN
1	H	112	ASN
1	H	229	ASN
1	H	319	GLN
1	H	432	GLN

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Mol	Chain	Res	Type
1	I	68	ASN
1	I	82	ASN
1	I	112	ASN
1	I	194	GLN
1	I	432	GLN
1	J	37	ASN
1	J	68	ASN
1	J	82	ASN
1	J	112	ASN
1	J	194	GLN
1	J	265	ASN
1	J	366	GLN
1	J	432	GLN
1	K	68	ASN
1	K	82	ASN
1	K	194	GLN
1	K	290	GLN
1	K	319	GLN
1	K	432	GLN
1	L	68	ASN
1	L	82	ASN
1	L	194	GLN
1	L	206	ASN
1	L	229	ASN
1	L	351	GLN
1	L	432	GLN
1	M	10	ASN
1	M	68	ASN
1	M	82	ASN
1	M	194	GLN
1	M	351	GLN
1	M	432	GLN
1	N	68	ASN
1	N	82	ASN
1	N	112	ASN
1	N	194	GLN
1	N	229	ASN
1	N	290	GLN
1	N	432	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	J	549	4	32,33,33	1.97	7 (21%)	45,52,52	1.83	10 (22%)
2	AGS	K	549	4	32,33,33	1.78	6 (18%)	45,52,52	1.89	11 (24%)
2	AGS	M	549	4	32,33,33	1.24	3 (9%)	45,52,52	1.84	10 (22%)
2	AGS	F	549	4	32,33,33	1.69	7 (21%)	45,52,52	1.86	11 (24%)
2	AGS	B	549	4	32,33,33	1.60	8 (25%)	45,52,52	1.85	11 (24%)
2	AGS	G	549	4	32,33,33	1.80	7 (21%)	45,52,52	1.86	11 (24%)
2	AGS	D	549	4	32,33,33	1.60	7 (21%)	45,52,52	1.84	11 (24%)
2	AGS	H	549	4	32,33,33	1.70	7 (21%)	45,52,52	1.82	11 (24%)
2	AGS	I	549	4	32,33,33	1.54	7 (21%)	45,52,52	1.87	11 (24%)
2	AGS	L	549	4	32,33,33	1.86	7 (21%)	45,52,52	1.82	11 (24%)
2	AGS	A	549	4	32,33,33	1.63	7 (21%)	45,52,52	1.80	11 (24%)
2	AGS	N	549	4	32,33,33	1.95	7 (21%)	45,52,52	1.82	10 (22%)
2	AGS	E	549	4	32,33,33	1.57	6 (18%)	45,52,52	1.86	11 (24%)
2	AGS	C	549	4	32,33,33	1.68	6 (18%)	45,52,52	1.84	11 (24%)

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	J	549	4	-	3/21/38/38	0/3/3/3
2	AGS	K	549	4	-	3/21/38/38	0/3/3/3
2	AGS	M	549	4	-	5/21/38/38	0/3/3/3
2	AGS	F	549	4	-	4/21/38/38	0/3/3/3
2	AGS	B	549	4	-	3/21/38/38	0/3/3/3
2	AGS	G	549	4	-	5/21/38/38	0/3/3/3
2	AGS	D	549	4	-	3/21/38/38	0/3/3/3
2	AGS	H	549	4	-	4/21/38/38	0/3/3/3
2	AGS	I	549	4	-	4/21/38/38	0/3/3/3
2	AGS	L	549	4	-	4/21/38/38	0/3/3/3
2	AGS	A	549	4	-	4/21/38/38	0/3/3/3
2	AGS	N	549	4	-	3/21/38/38	0/3/3/3
2	AGS	E	549	4	-	4/21/38/38	0/3/3/3
2	AGS	C	549	4	-	4/21/38/38	0/3/3/3

All (92) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	549	AGS	PG-S1G	7.37	2.06	1.90
2	J	549	AGS	PG-S1G	6.91	2.05	1.90
2	K	549	AGS	PG-S1G	5.94	2.03	1.90
2	C	549	AGS	PG-S1G	5.73	2.03	1.90
2	G	549	AGS	PG-S1G	5.52	2.02	1.90
2	L	549	AGS	PG-S1G	5.48	2.02	1.90
2	F	549	AGS	PG-S1G	4.75	2.01	1.90
2	L	549	AGS	PA-O3A	4.36	1.64	1.59
2	J	549	AGS	PB-O3A	4.29	1.64	1.59
2	A	549	AGS	PG-S1G	4.25	1.99	1.90
2	A	549	AGS	PB-O3B	4.10	1.63	1.59
2	H	549	AGS	PB-O3A	3.96	1.63	1.59
2	K	549	AGS	PA-O3A	3.95	1.63	1.59
2	H	549	AGS	PA-O3A	3.87	1.63	1.59
2	H	549	AGS	PB-O3B	3.84	1.63	1.59
2	L	549	AGS	PB-O3B	3.81	1.63	1.59
2	J	549	AGS	PA-O3A	3.74	1.63	1.59
2	B	549	AGS	PA-O3A	3.73	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	549	AGS	PG-S1G	3.70	1.98	1.90
2	E	549	AGS	PG-S1G	3.67	1.98	1.90
2	G	549	AGS	PA-O3A	3.60	1.63	1.59
2	G	549	AGS	PB-O3A	3.59	1.63	1.59
2	D	549	AGS	C5-N7	-3.45	1.32	1.39
2	D	549	AGS	PB-O3B	3.37	1.63	1.59
2	A	549	AGS	C5-N7	-3.36	1.33	1.39
2	I	549	AGS	C5-N7	-3.34	1.33	1.39
2	N	549	AGS	PA-O3A	3.33	1.63	1.59
2	N	549	AGS	PB-O3B	3.32	1.63	1.59
2	B	549	AGS	PB-O3B	3.31	1.63	1.59
2	K	549	AGS	PB-O3A	3.30	1.63	1.59
2	N	549	AGS	C5-N7	-3.30	1.33	1.39
2	B	549	AGS	PB-O3A	3.29	1.63	1.59
2	F	549	AGS	C5-N7	-3.28	1.33	1.39
2	H	549	AGS	C5-N7	-3.27	1.33	1.39
2	J	549	AGS	C5-N7	-3.26	1.33	1.39
2	C	549	AGS	C5-N7	-3.25	1.33	1.39
2	G	549	AGS	C5-N7	-3.22	1.33	1.39
2	L	549	AGS	PB-O3A	3.22	1.63	1.59
2	M	549	AGS	C5-N7	-3.21	1.33	1.39
2	E	549	AGS	C5-N7	-3.20	1.33	1.39
2	D	549	AGS	PG-S1G	3.19	1.97	1.90
2	F	549	AGS	PB-O3B	3.17	1.62	1.59
2	L	549	AGS	C5-N7	-3.17	1.33	1.39
2	B	549	AGS	C5-N7	-3.16	1.33	1.39
2	D	549	AGS	PB-O3A	3.13	1.62	1.59
2	G	549	AGS	PB-O3B	3.12	1.62	1.59
2	F	549	AGS	PB-O3A	3.10	1.62	1.59
2	K	549	AGS	C5-N7	-3.07	1.33	1.39
2	E	549	AGS	PA-O3A	3.06	1.62	1.59
2	F	549	AGS	PA-O3A	3.03	1.62	1.59
2	C	549	AGS	PA-O3A	3.03	1.62	1.59
2	E	549	AGS	PB-O3A	3.01	1.62	1.59
2	D	549	AGS	PA-O3A	2.93	1.62	1.59
2	H	549	AGS	PG-S1G	2.91	1.97	1.90
2	E	549	AGS	PB-O3B	2.87	1.62	1.59
2	N	549	AGS	PB-O3A	2.83	1.62	1.59
2	B	549	AGS	PG-S1G	2.83	1.96	1.90
2	I	549	AGS	PB-O3A	2.76	1.62	1.59
2	J	549	AGS	PB-O3B	2.76	1.62	1.59
2	I	549	AGS	PB-O3B	2.69	1.62	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	549	AGS	PA-O3A	2.60	1.62	1.59
2	D	549	AGS	C4-N9	-2.43	1.32	1.37
2	A	549	AGS	C4-N9	-2.39	1.32	1.37
2	C	549	AGS	C4-N9	-2.38	1.32	1.37
2	N	549	AGS	C4-N9	-2.35	1.32	1.37
2	L	549	AGS	C4-N9	-2.34	1.32	1.37
2	C	549	AGS	PB-O3A	2.32	1.62	1.59
2	G	549	AGS	C4-N9	-2.32	1.32	1.37
2	A	549	AGS	PB-O3A	2.31	1.62	1.59
2	I	549	AGS	C4-N9	-2.31	1.32	1.37
2	F	549	AGS	C4-N9	-2.30	1.32	1.37
2	J	549	AGS	C4-N9	-2.27	1.33	1.37
2	E	549	AGS	C4-N9	-2.26	1.33	1.37
2	H	549	AGS	C4-N9	-2.26	1.33	1.37
2	D	549	AGS	C8-N9	-2.26	1.33	1.37
2	G	549	AGS	C8-N9	-2.23	1.33	1.37
2	B	549	AGS	C4-N9	-2.21	1.33	1.37
2	A	549	AGS	PA-O3A	2.21	1.61	1.59
2	K	549	AGS	C4-N9	-2.19	1.33	1.37
2	I	549	AGS	C8-N9	-2.18	1.33	1.37
2	M	549	AGS	C8-N9	-2.17	1.33	1.37
2	M	549	AGS	C4-N9	-2.11	1.33	1.37
2	A	549	AGS	C8-N9	-2.10	1.34	1.37
2	C	549	AGS	C8-N9	-2.09	1.34	1.37
2	B	549	AGS	C8-N9	-2.08	1.34	1.37
2	K	549	AGS	C8-N9	-2.08	1.34	1.37
2	N	549	AGS	C8-N9	-2.07	1.34	1.37
2	H	549	AGS	C8-N9	-2.07	1.34	1.37
2	J	549	AGS	C8-N9	-2.06	1.34	1.37
2	L	549	AGS	C8-N9	-2.05	1.34	1.37
2	F	549	AGS	C8-N9	-2.05	1.34	1.37
2	B	549	AGS	PG-O2G	-2.03	1.48	1.54

All (151) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	549	AGS	C5-C4-N3	-5.31	119.40	126.72
2	I	549	AGS	C5-C4-N3	-5.31	119.41	126.72
2	E	549	AGS	C5-C4-N3	-5.26	119.47	126.72
2	N	549	AGS	C5-C4-N3	-5.21	119.54	126.72
2	D	549	AGS	C5-C4-N3	-5.20	119.56	126.72
2	B	549	AGS	C5-C4-N3	-5.18	119.58	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	549	AGS	C5-C4-N3	-5.17	119.60	126.72
2	F	549	AGS	C5-C4-N3	-5.15	119.63	126.72
2	J	549	AGS	C5-C4-N3	-5.12	119.67	126.72
2	L	549	AGS	C5-C4-N3	-5.11	119.68	126.72
2	G	549	AGS	C5-C4-N3	-5.11	119.68	126.72
2	A	549	AGS	C5-C4-N3	-5.05	119.76	126.72
2	H	549	AGS	C5-C4-N3	-5.04	119.77	126.72
2	K	549	AGS	C5-C4-N3	-5.04	119.77	126.72
2	F	549	AGS	N3-C2-N1	-4.87	121.21	128.58
2	K	549	AGS	N3-C2-N1	-4.83	121.27	128.58
2	C	549	AGS	N3-C2-N1	-4.82	121.29	128.58
2	J	549	AGS	N3-C2-N1	-4.81	121.30	128.58
2	E	549	AGS	N3-C2-N1	-4.76	121.38	128.58
2	B	549	AGS	N3-C2-N1	-4.73	121.42	128.58
2	H	549	AGS	N3-C2-N1	-4.71	121.46	128.58
2	G	549	AGS	N3-C2-N1	-4.68	121.49	128.58
2	D	549	AGS	N3-C2-N1	-4.64	121.55	128.58
2	A	549	AGS	N3-C2-N1	-4.63	121.57	128.58
2	I	549	AGS	N3-C2-N1	-4.59	121.63	128.58
2	L	549	AGS	N3-C2-N1	-4.55	121.69	128.58
2	N	549	AGS	N3-C2-N1	-4.53	121.73	128.58
2	M	549	AGS	N3-C2-N1	-4.52	121.74	128.58
2	C	549	AGS	C2-N3-C4	3.67	120.80	111.83
2	F	549	AGS	C2-N3-C4	3.64	120.72	111.83
2	M	549	AGS	N3-C4-N9	3.64	133.35	127.17
2	E	549	AGS	C2-N3-C4	3.61	120.65	111.83
2	B	549	AGS	C2-N3-C4	3.61	120.65	111.83
2	J	549	AGS	C2-N3-C4	3.61	120.64	111.83
2	K	549	AGS	C2-N3-C4	3.61	120.64	111.83
2	K	549	AGS	N3-C4-N9	3.61	133.30	127.17
2	M	549	AGS	PB-O3B-PG	-3.59	120.02	133.17
2	K	549	AGS	N9-C8-N7	-3.59	108.84	113.94
2	I	549	AGS	C2-N3-C4	3.58	120.58	111.83
2	D	549	AGS	C2-N3-C4	3.58	120.57	111.83
2	G	549	AGS	C2-N3-C4	3.56	120.52	111.83
2	I	549	AGS	N3-C4-N9	3.55	133.21	127.17
2	F	549	AGS	N3-C4-N9	3.55	133.20	127.17
2	B	549	AGS	N3-C4-N9	3.54	133.18	127.17
2	M	549	AGS	C2-N3-C4	3.53	120.45	111.83
2	L	549	AGS	C2-N3-C4	3.50	120.39	111.83
2	N	549	AGS	C2-N3-C4	3.49	120.36	111.83
2	G	549	AGS	N3-C4-N9	3.49	133.11	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	549	AGS	C2-N3-C4	3.49	120.35	111.83
2	E	549	AGS	N3-C4-N9	3.48	133.09	127.17
2	I	549	AGS	N9-C8-N7	-3.48	109.00	113.94
2	H	549	AGS	C2-N3-C4	3.48	120.33	111.83
2	C	549	AGS	N3-C4-N9	3.47	133.07	127.17
2	L	549	AGS	N3-C4-N9	3.46	133.05	127.17
2	J	549	AGS	N3-C4-N9	3.44	133.02	127.17
2	D	549	AGS	N3-C4-N9	3.44	133.02	127.17
2	N	549	AGS	N3-C4-N9	3.40	132.95	127.17
2	G	549	AGS	N9-C8-N7	-3.40	109.12	113.94
2	H	549	AGS	N3-C4-N9	3.39	132.94	127.17
2	A	549	AGS	N3-C4-N9	3.39	132.94	127.17
2	L	549	AGS	N9-C8-N7	-3.39	109.13	113.94
2	B	549	AGS	N9-C8-N7	-3.34	109.20	113.94
2	F	549	AGS	N9-C8-N7	-3.34	109.20	113.94
2	E	549	AGS	N9-C8-N7	-3.30	109.26	113.94
2	M	549	AGS	N9-C8-N7	-3.29	109.27	113.94
2	H	549	AGS	N9-C8-N7	-3.23	109.35	113.94
2	D	549	AGS	N9-C8-N7	-3.23	109.36	113.94
2	I	549	AGS	PB-O3B-PG	-3.19	121.48	133.17
2	A	549	AGS	N9-C8-N7	-3.19	109.42	113.94
2	N	549	AGS	N9-C8-N7	-3.18	109.42	113.94
2	C	549	AGS	N9-C8-N7	-3.17	109.44	113.94
2	K	549	AGS	PB-O3B-PG	-3.16	121.60	133.17
2	J	549	AGS	PB-O3B-PG	-3.13	121.72	133.17
2	G	549	AGS	PB-O3B-PG	-3.06	121.99	133.17
2	C	549	AGS	PB-O3B-PG	-3.05	122.00	133.17
2	F	549	AGS	PB-O3B-PG	-3.03	122.08	133.17
2	E	549	AGS	PB-O3B-PG	-3.02	122.10	133.17
2	J	549	AGS	N9-C8-N7	-3.01	109.66	113.94
2	L	549	AGS	PB-O3B-PG	-2.99	122.23	133.17
2	N	549	AGS	PB-O3B-PG	-2.98	122.27	133.17
2	B	549	AGS	PB-O3B-PG	-2.98	122.27	133.17
2	A	549	AGS	PB-O3B-PG	-2.98	122.28	133.17
2	K	549	AGS	C5-N7-C8	2.96	108.11	103.45
2	H	549	AGS	PB-O3B-PG	-2.96	122.34	133.17
2	I	549	AGS	C5-N7-C8	2.95	108.09	103.45
2	E	549	AGS	C5'-C4'-C3'	-2.92	104.70	115.21
2	D	549	AGS	PB-O3B-PG	-2.90	122.56	133.17
2	D	549	AGS	C5'-C4'-C3'	-2.89	104.81	115.21
2	G	549	AGS	C5-N7-C8	2.88	107.97	103.45
2	J	549	AGS	C5'-C4'-C3'	-2.88	104.86	115.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	549	AGS	C5-N7-C8	2.86	107.94	103.45
2	F	549	AGS	C5'-C4'-C3'	-2.84	105.00	115.21
2	E	549	AGS	C5-N7-C8	2.83	107.90	103.45
2	B	549	AGS	C5'-C4'-C3'	-2.82	105.05	115.21
2	N	549	AGS	C5'-C4'-C3'	-2.82	105.08	115.21
2	L	549	AGS	C5-N7-C8	2.81	107.86	103.45
2	G	549	AGS	C5'-C4'-C3'	-2.81	105.10	115.21
2	B	549	AGS	C5-N7-C8	2.80	107.85	103.45
2	H	549	AGS	C5-N7-C8	2.79	107.83	103.45
2	N	549	AGS	C5-N7-C8	2.79	107.83	103.45
2	K	549	AGS	C5'-C4'-C3'	-2.78	105.20	115.21
2	D	549	AGS	C5-N7-C8	2.78	107.81	103.45
2	I	549	AGS	C4-C5-N7	-2.77	107.41	110.58
2	N	549	AGS	C4-C5-N7	-2.77	107.42	110.58
2	F	549	AGS	C5-N7-C8	2.75	107.77	103.45
2	H	549	AGS	C5'-C4'-C3'	-2.75	105.32	115.21
2	G	549	AGS	C4-C5-N7	-2.74	107.44	110.58
2	C	549	AGS	C5'-C4'-C3'	-2.73	105.38	115.21
2	E	549	AGS	C4-C5-N7	-2.72	107.47	110.58
2	I	549	AGS	C5'-C4'-C3'	-2.71	105.47	115.21
2	M	549	AGS	C4-C5-N7	-2.70	107.50	110.58
2	D	549	AGS	C4-C5-N7	-2.69	107.51	110.58
2	C	549	AGS	C5-N7-C8	2.68	107.66	103.45
2	K	549	AGS	C4-N9-C8	2.67	108.54	105.74
2	A	549	AGS	C5'-C4'-C3'	-2.67	105.60	115.21
2	A	549	AGS	C5-N7-C8	2.67	107.65	103.45
2	L	549	AGS	C4-C5-N7	-2.65	107.55	110.58
2	L	549	AGS	C5'-C4'-C3'	-2.65	105.67	115.21
2	H	549	AGS	C4-C5-N7	-2.63	107.57	110.58
2	K	549	AGS	C4-C5-N7	-2.63	107.58	110.58
2	B	549	AGS	C4-C5-N7	-2.60	107.61	110.58
2	J	549	AGS	C5-N7-C8	2.59	107.52	103.45
2	C	549	AGS	C4-C5-N7	-2.58	107.63	110.58
2	A	549	AGS	C4-C5-N7	-2.51	107.71	110.58
2	J	549	AGS	C4-C5-N7	-2.49	107.74	110.58
2	F	549	AGS	C4-C5-N7	-2.48	107.75	110.58
2	N	549	AGS	C4'-O4'-C1'	-2.45	104.05	109.47
2	K	549	AGS	C4'-O4'-C1'	-2.44	104.08	109.47
2	M	549	AGS	C4'-O4'-C1'	-2.44	104.09	109.47
2	G	549	AGS	C4'-O4'-C1'	-2.40	104.17	109.47
2	G	549	AGS	C4-N9-C8	2.40	108.25	105.74
2	F	549	AGS	C4'-O4'-C1'	-2.39	104.18	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	549	AGS	C4'-O4'-C1'	-2.39	104.18	109.47
2	L	549	AGS	C4'-O4'-C1'	-2.36	104.26	109.47
2	J	549	AGS	C4'-O4'-C1'	-2.33	104.32	109.47
2	L	549	AGS	C4-N9-C8	2.33	108.19	105.74
2	E	549	AGS	C4'-O4'-C1'	-2.30	104.39	109.47
2	I	549	AGS	C4-N9-C8	2.27	108.12	105.74
2	H	549	AGS	C4'-O4'-C1'	-2.26	104.47	109.47
2	F	549	AGS	C4-N9-C8	2.26	108.11	105.74
2	B	549	AGS	C4-N9-C8	2.26	108.11	105.74
2	B	549	AGS	C4'-O4'-C1'	-2.26	104.49	109.47
2	C	549	AGS	C4'-O4'-C1'	-2.25	104.51	109.47
2	D	549	AGS	C4'-O4'-C1'	-2.20	104.61	109.47
2	M	549	AGS	C4-N9-C8	2.20	108.05	105.74
2	C	549	AGS	C4-N9-C8	2.11	107.95	105.74
2	H	549	AGS	C4-N9-C8	2.11	107.95	105.74
2	A	549	AGS	C4'-O4'-C1'	-2.10	104.83	109.47
2	E	549	AGS	C4-N9-C8	2.09	107.93	105.74
2	A	549	AGS	C4-N9-C8	2.08	107.92	105.74
2	D	549	AGS	C4-N9-C8	2.05	107.89	105.74

There are no chirality outliers.

All (53) torsion outliers are listed below:

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

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

There are no ring outliers.

7 monomers are involved in 9 short contacts:

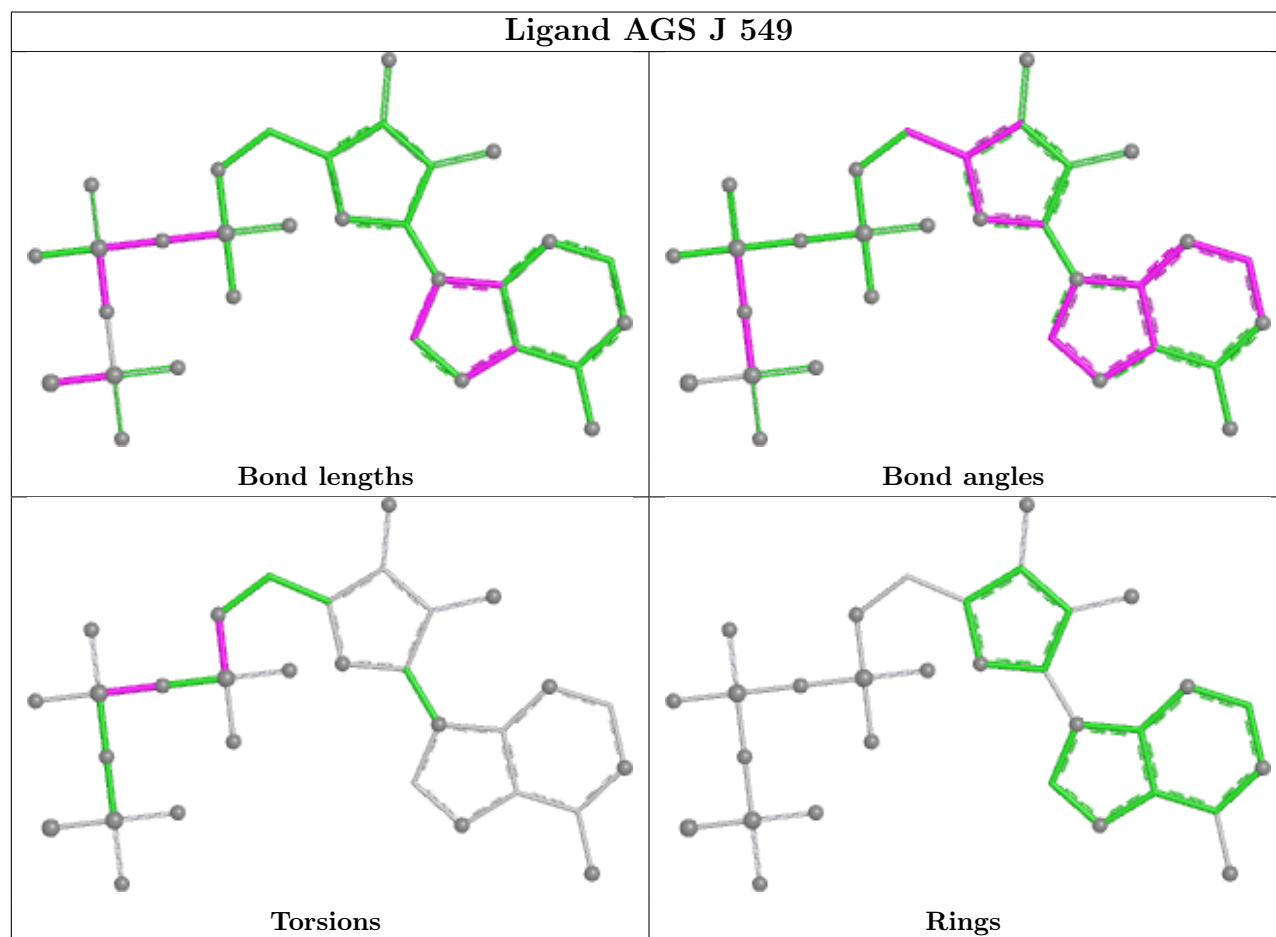
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	549	AGS	2	0
2	K	549	AGS	1	0

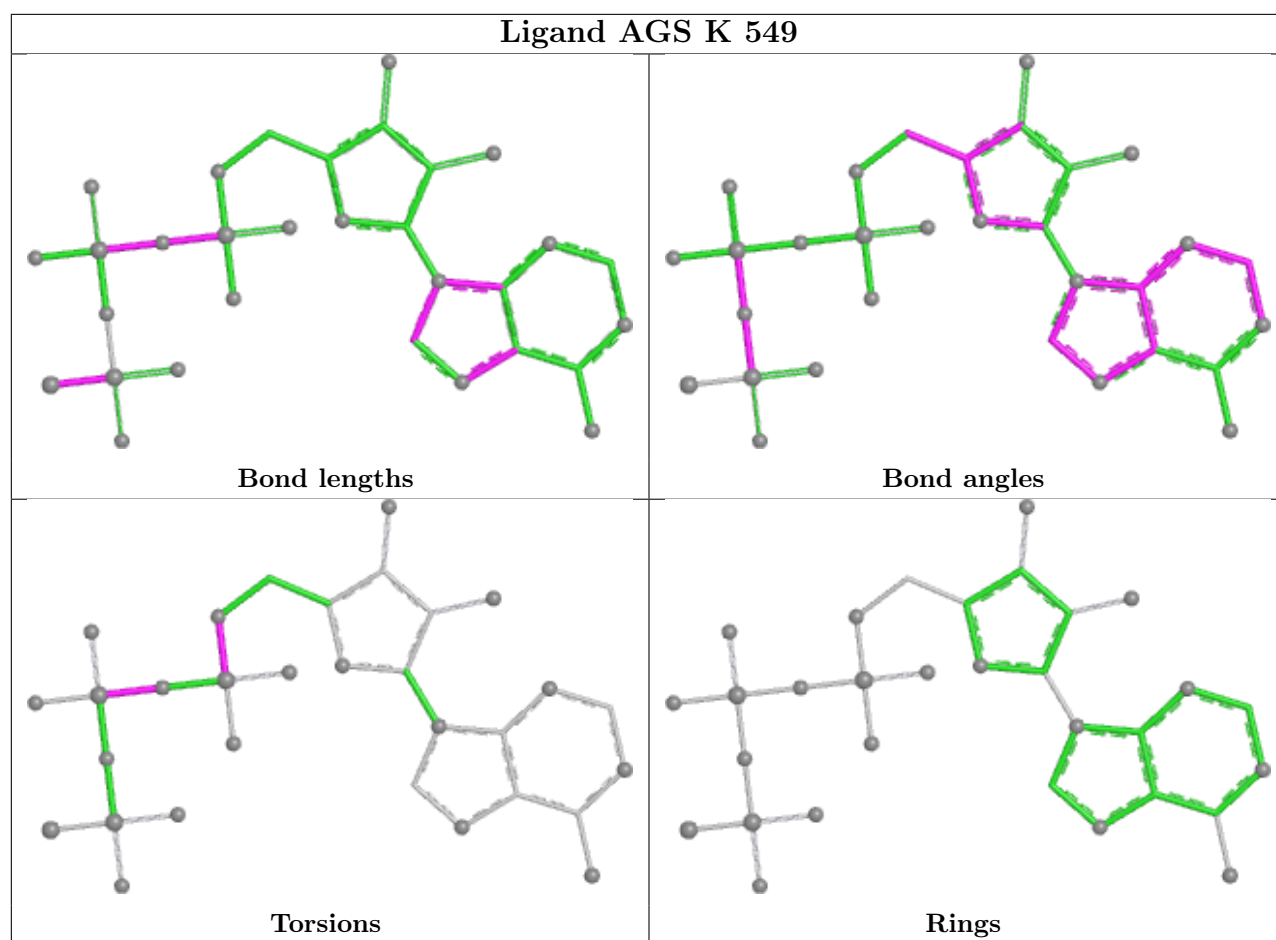
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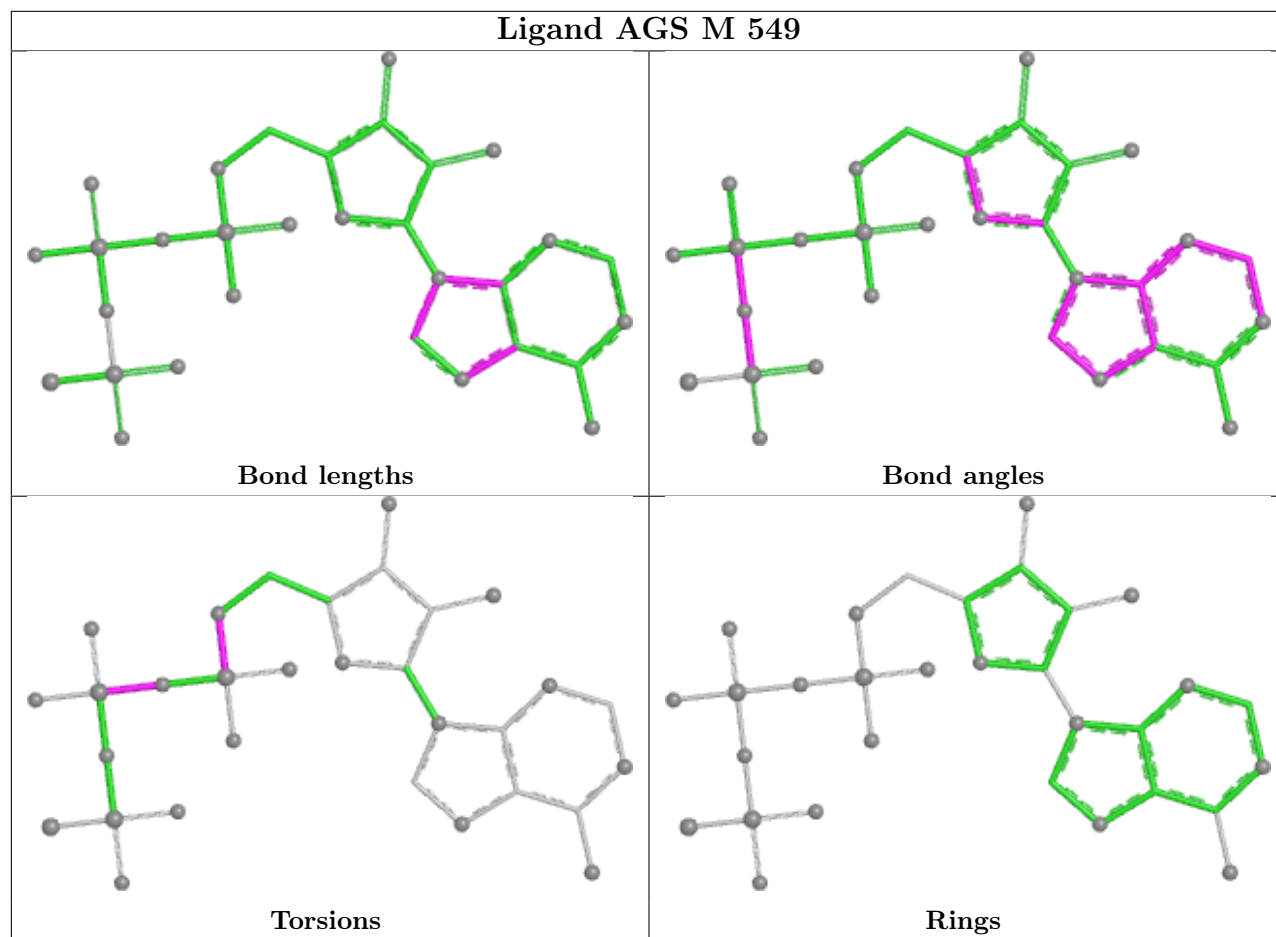
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	549	AGS	2	0
2	D	549	AGS	1	0
2	I	549	AGS	1	0
2	E	549	AGS	1	0
2	C	549	AGS	1	0

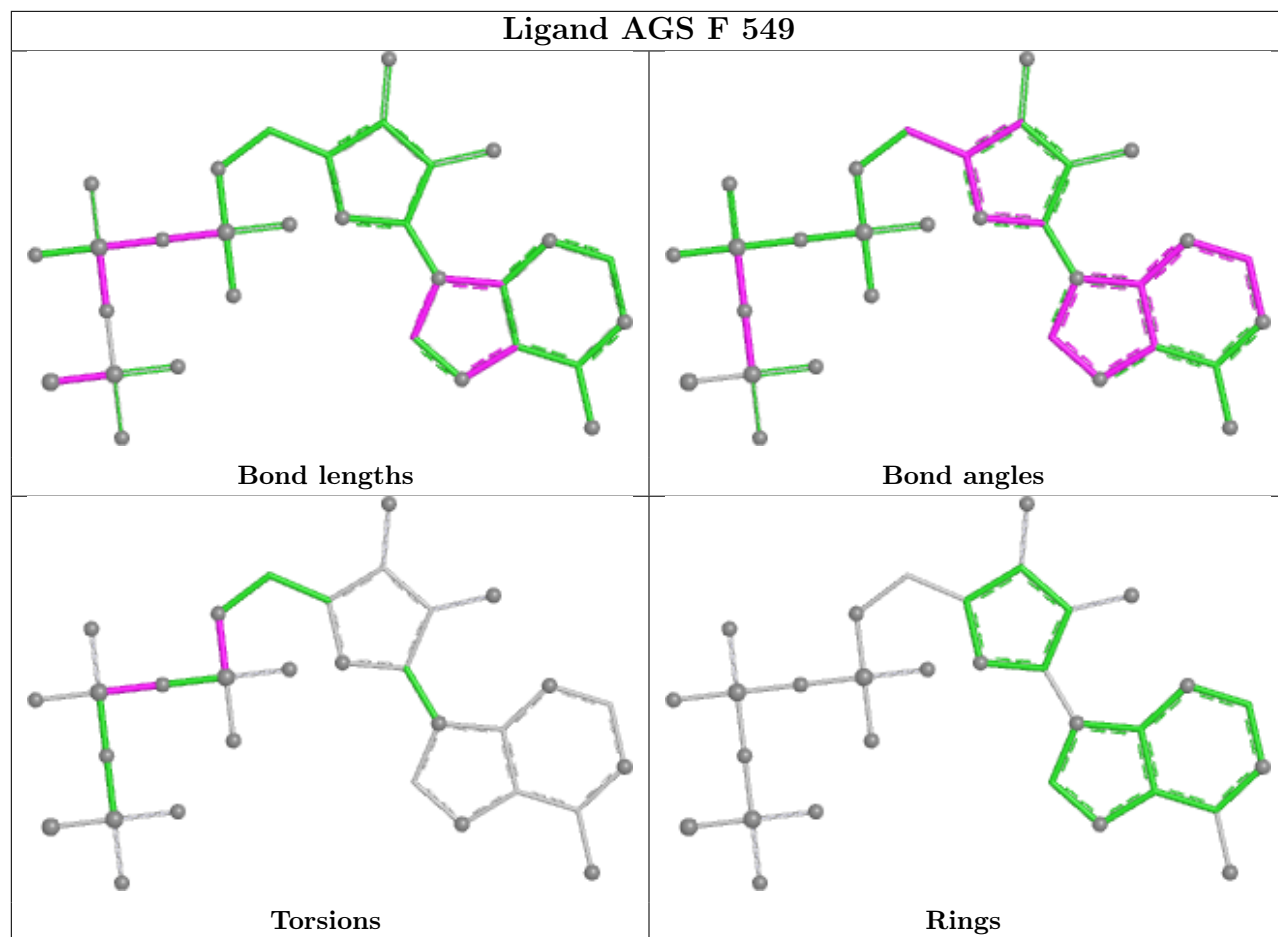
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



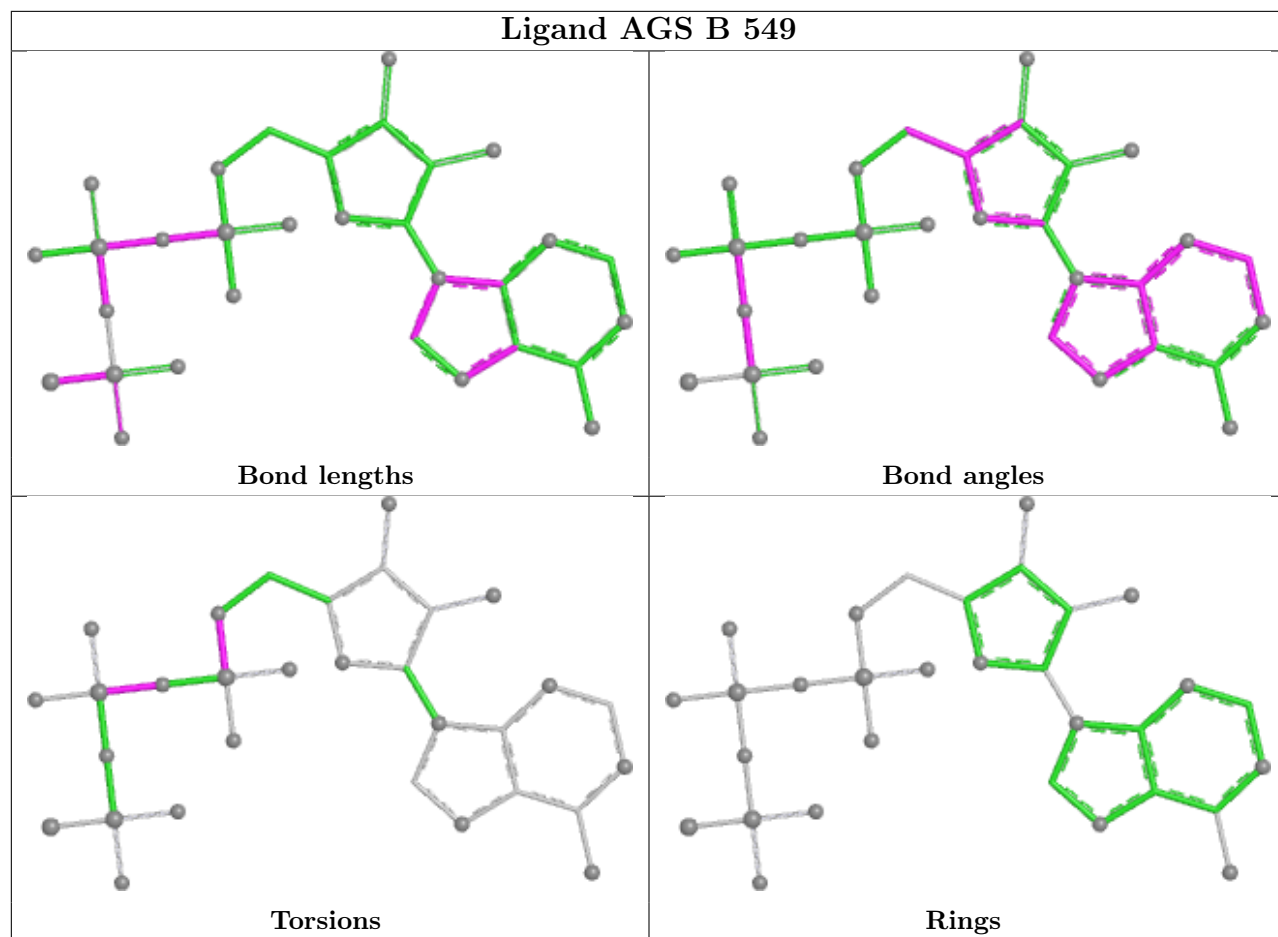


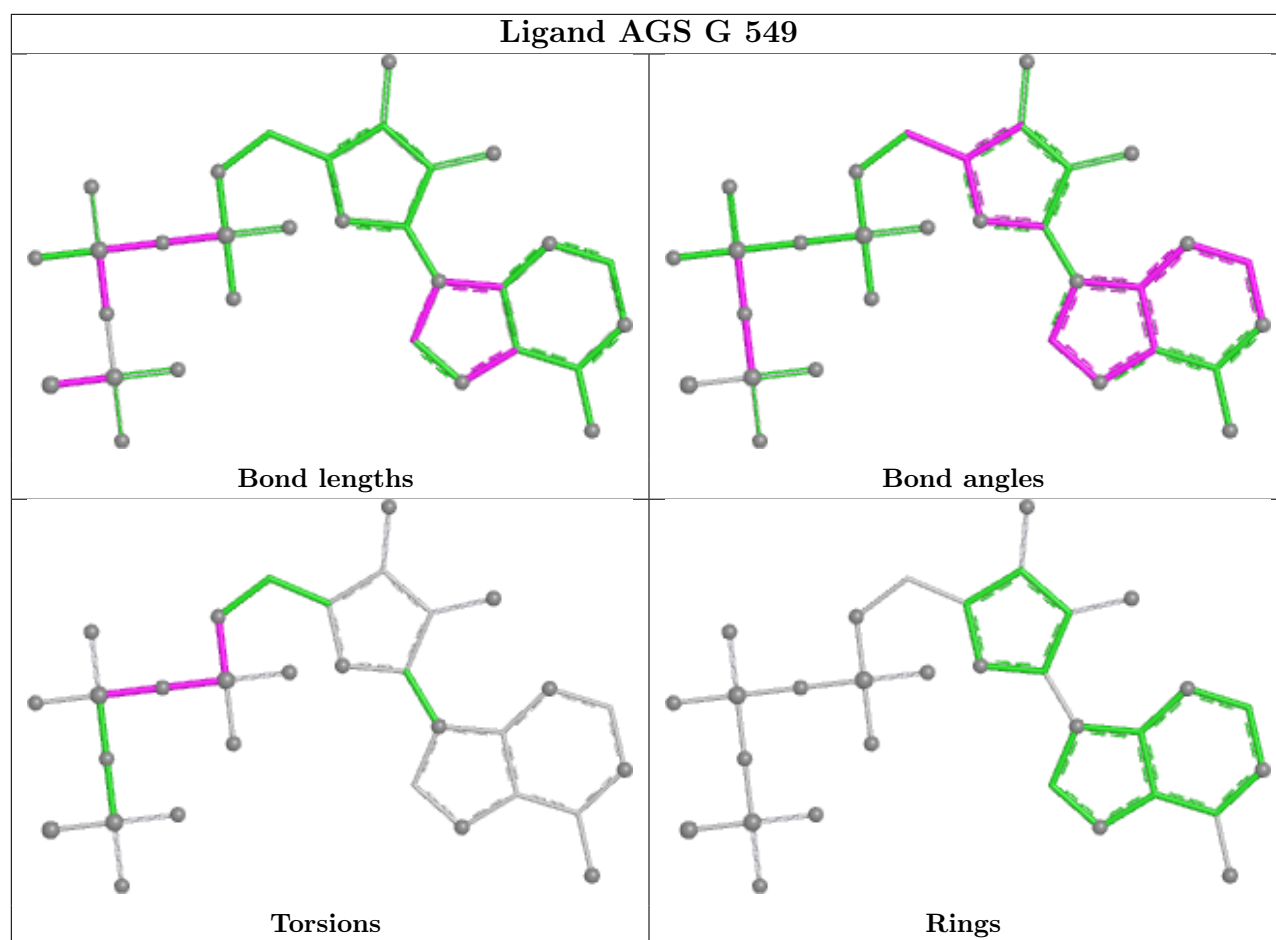


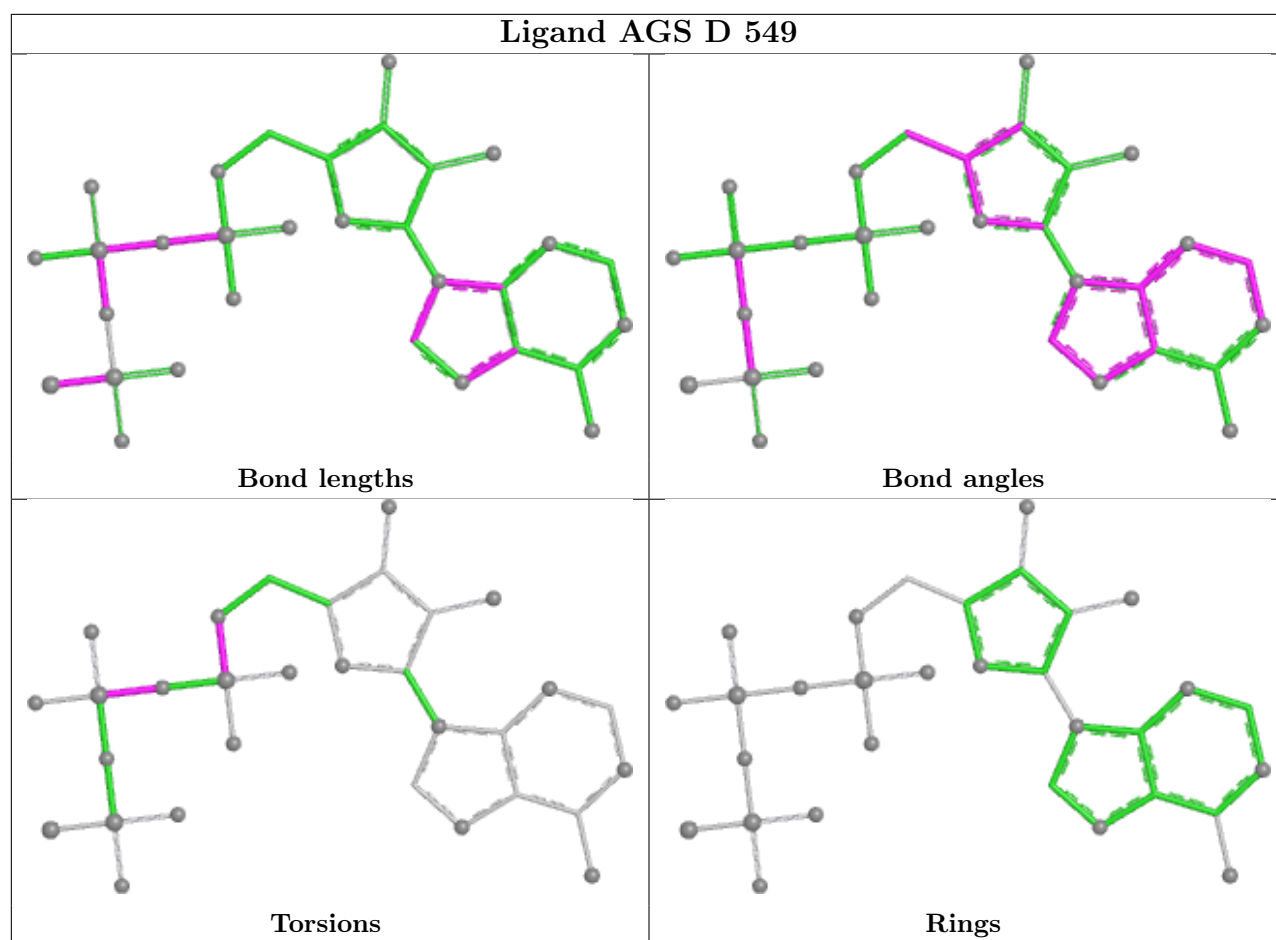
Ligand AGS F 549

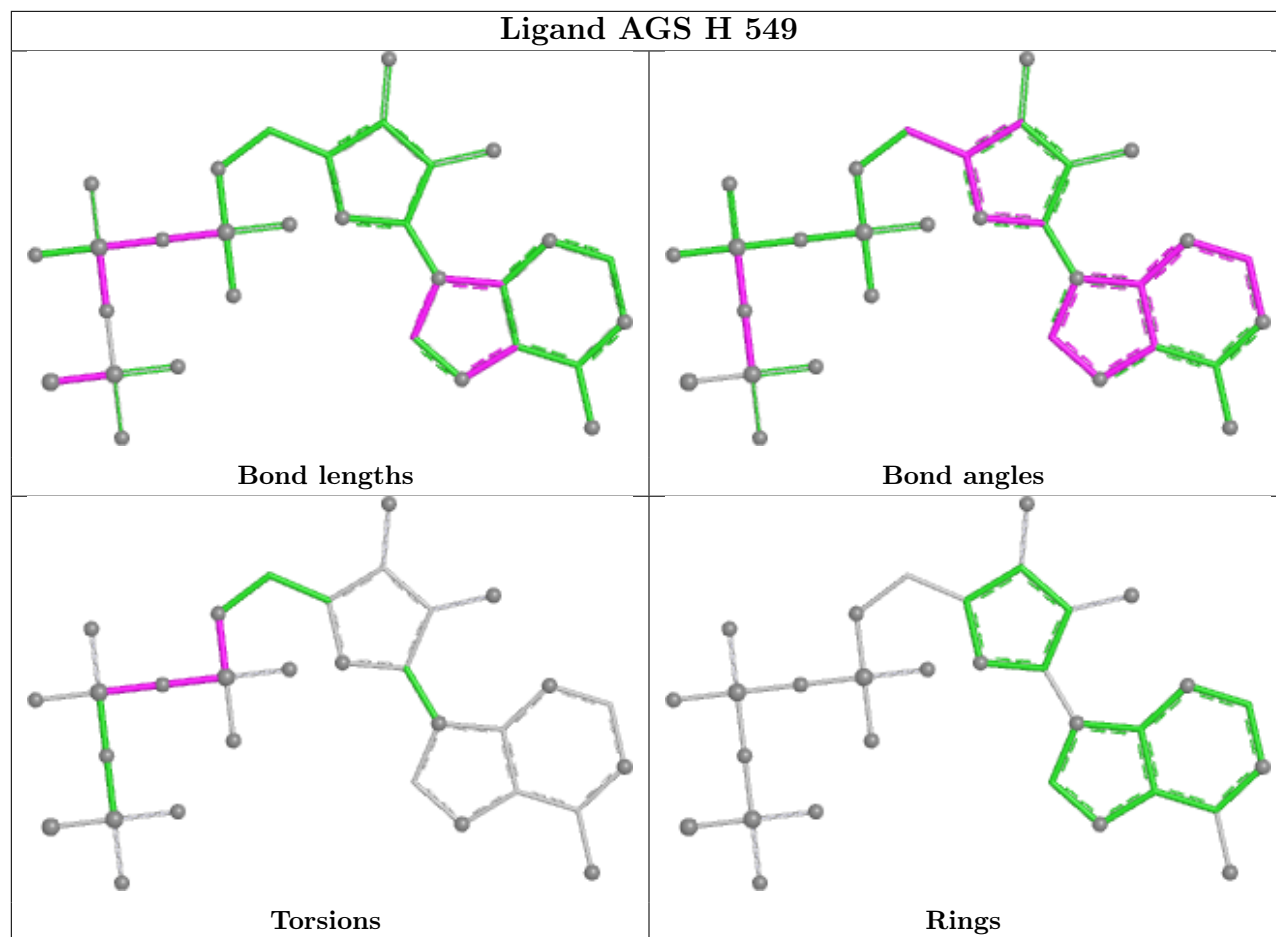


Ligand AGS B 549

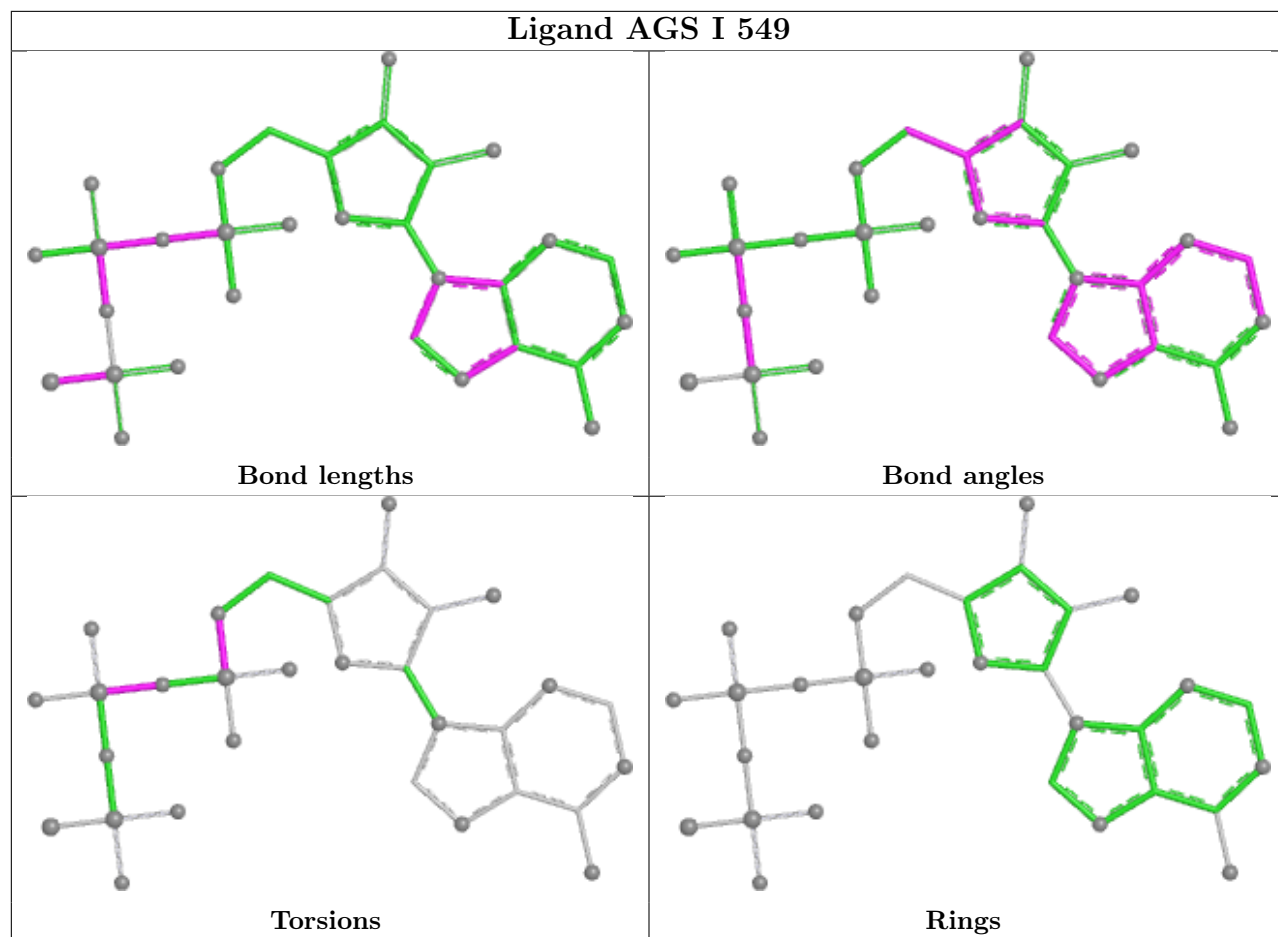




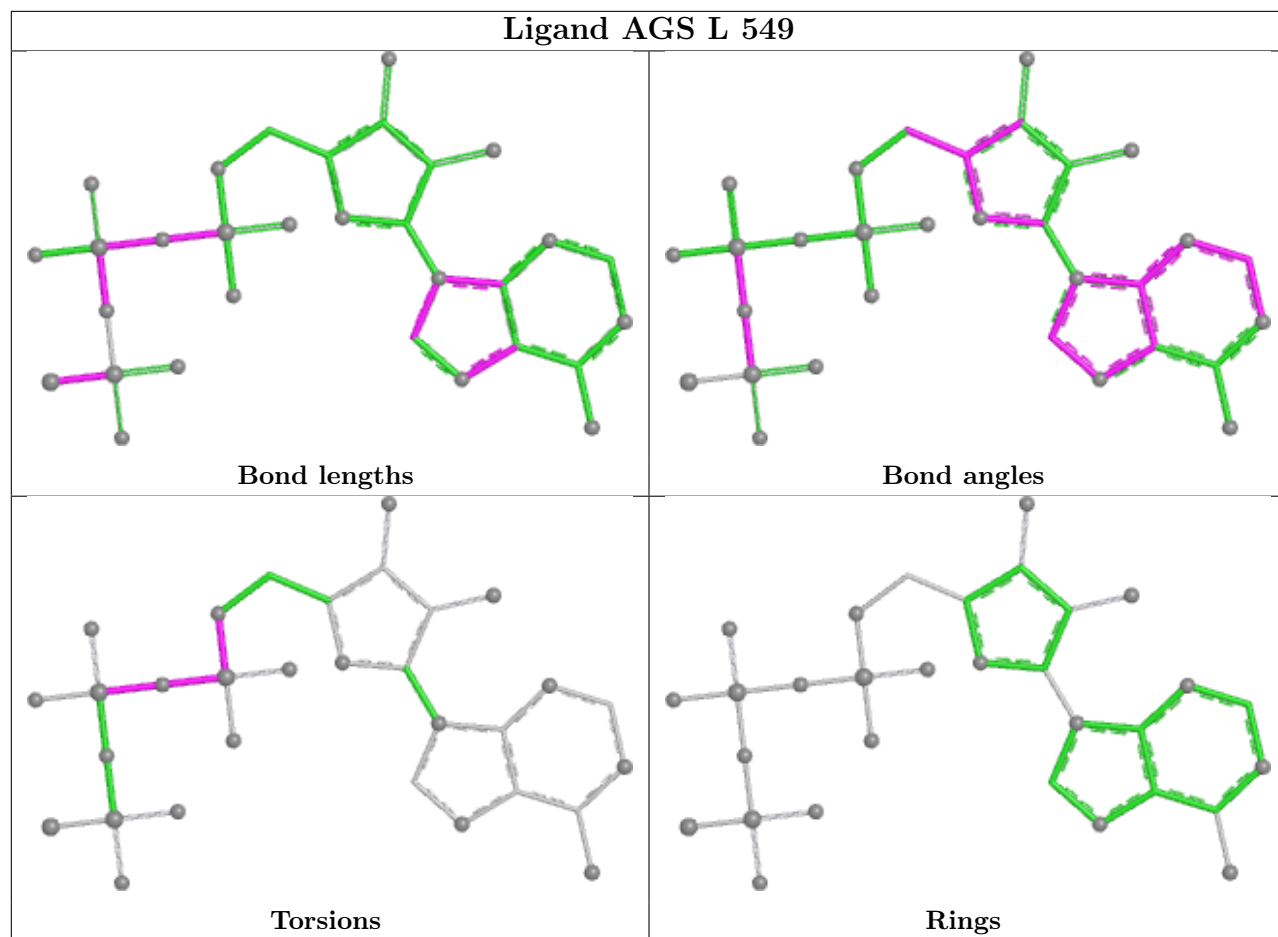


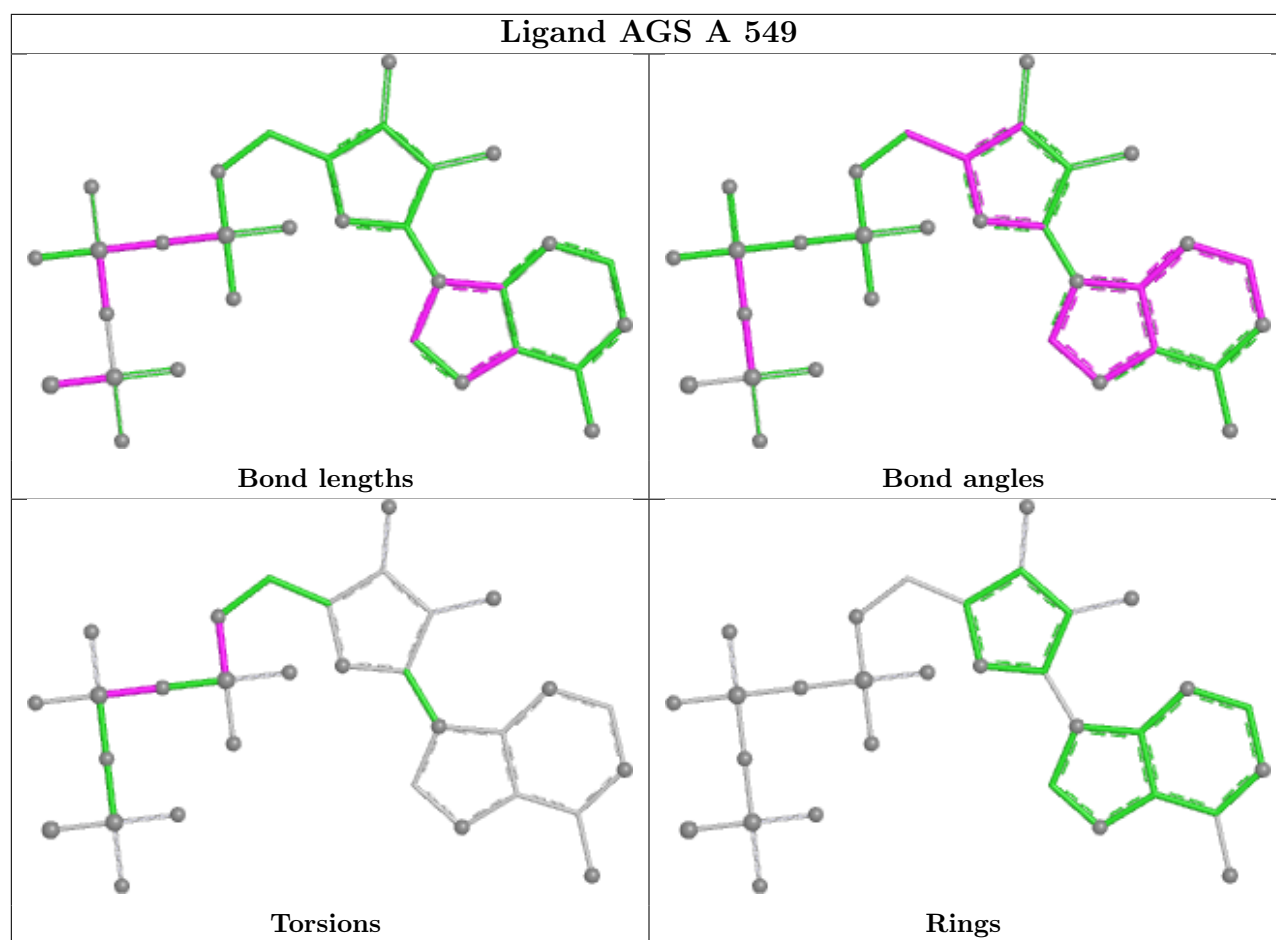


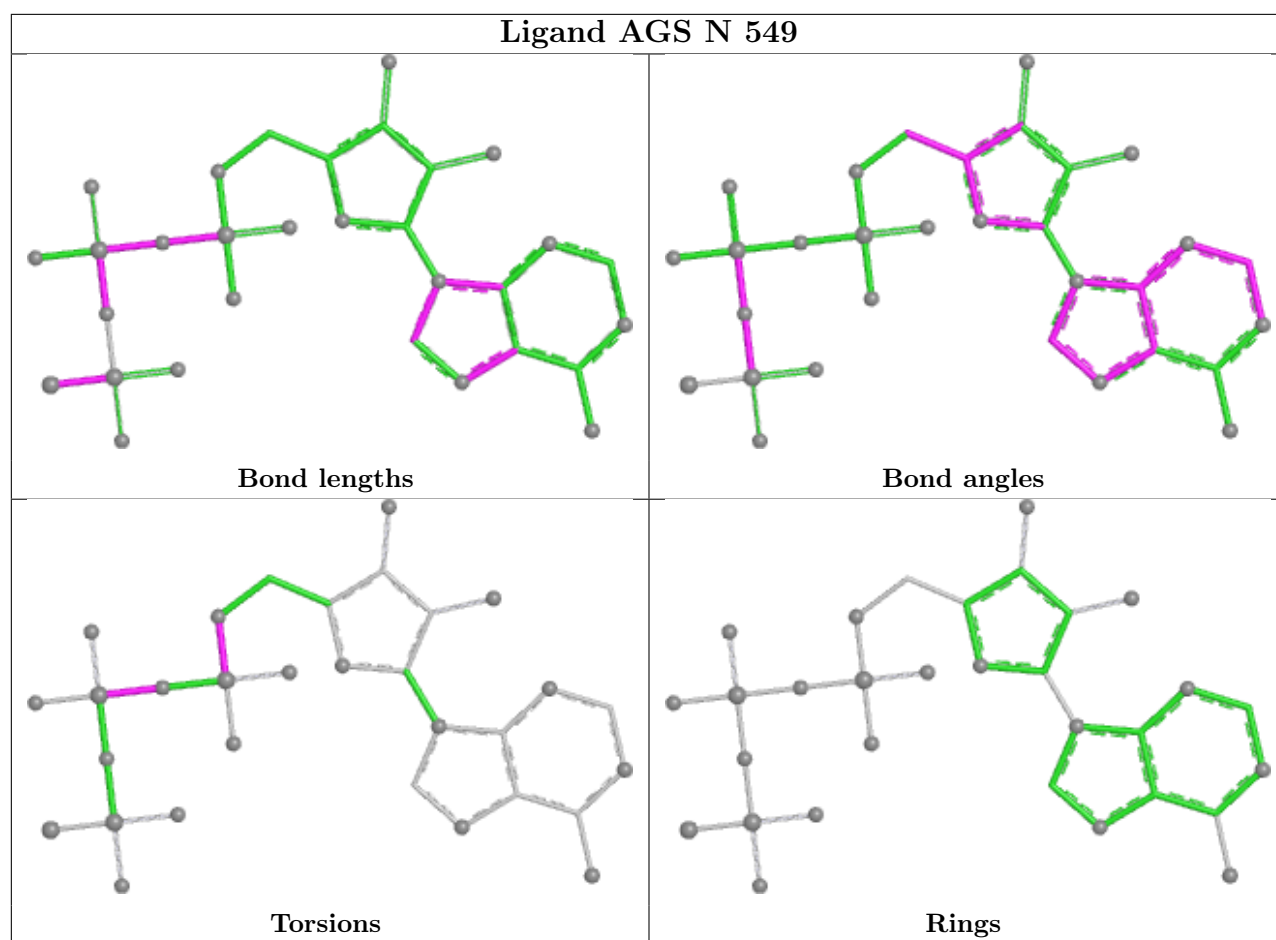
Ligand AGS I 549



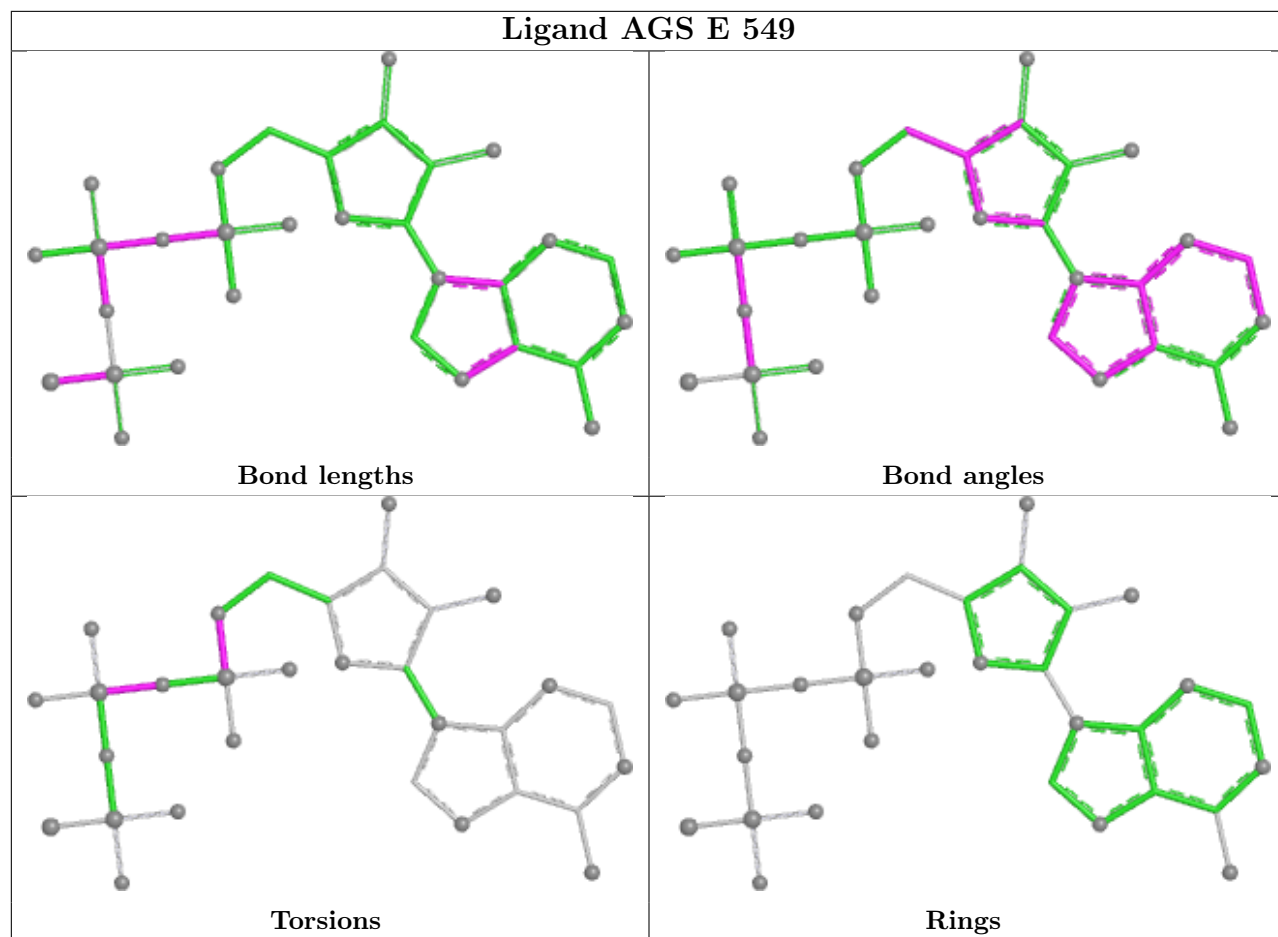
Ligand AGS L 549

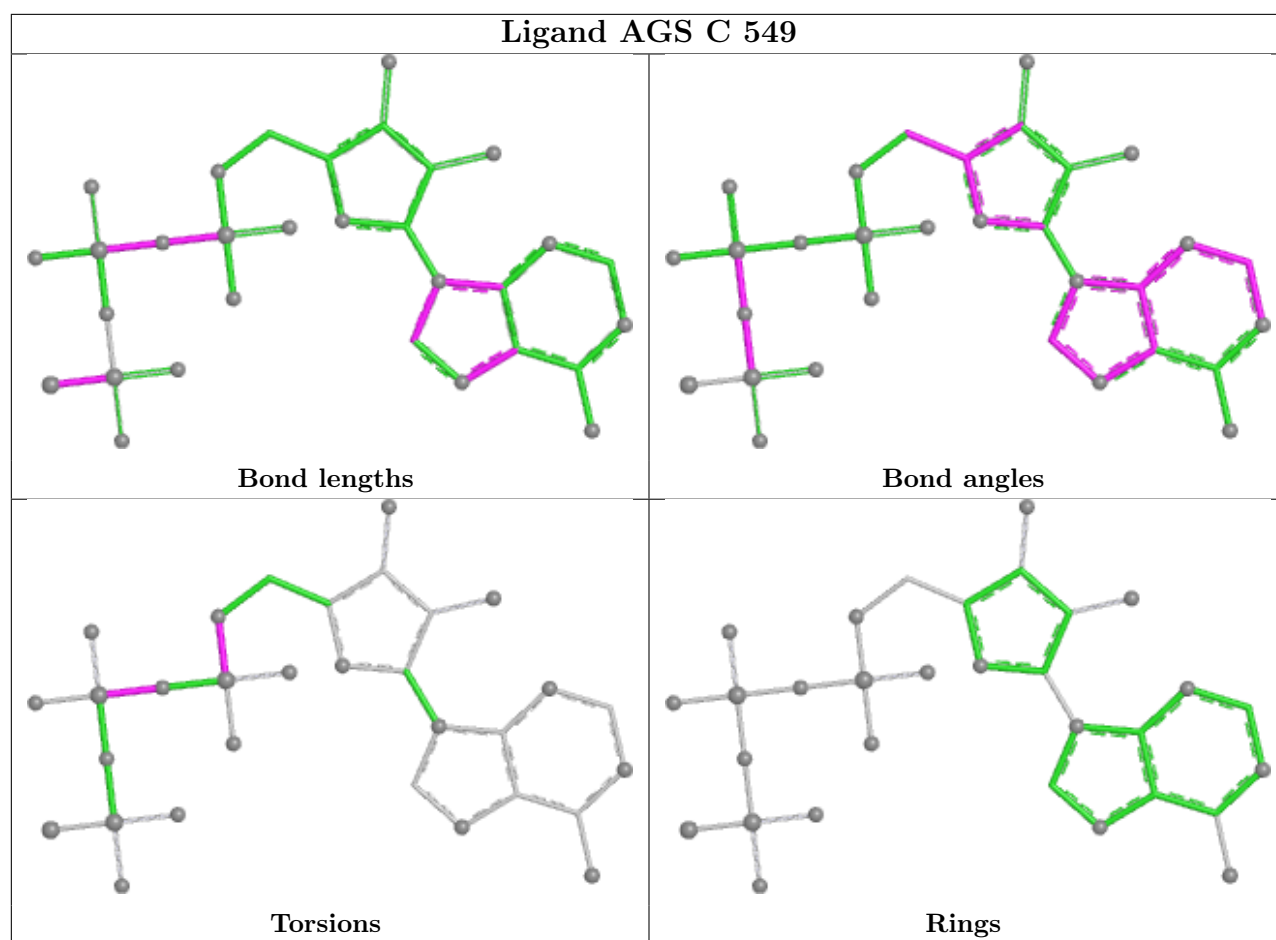






Ligand AGS E 549





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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	524/547 (95%)	0.27	15 (2%)	53	38	125, 125, 125, 125	0
1	B	524/547 (95%)	0.19	7 (1%)	75	55	125, 125, 125, 125	0
1	C	524/547 (95%)	0.28	19 (3%)	46	33	125, 125, 125, 125	0
1	D	524/547 (95%)	0.27	15 (2%)	53	38	125, 125, 125, 125	0
1	E	524/547 (95%)	0.30	13 (2%)	58	41	125, 125, 125, 125	0
1	F	524/547 (95%)	0.23	9 (1%)	69	49	125, 125, 125, 125	0
1	G	524/547 (95%)	0.29	15 (2%)	53	38	125, 125, 125, 125	0
1	H	524/547 (95%)	0.28	14 (2%)	56	39	125, 125, 125, 125	0
1	I	524/547 (95%)	0.26	14 (2%)	56	39	125, 125, 125, 125	0
1	J	524/547 (95%)	0.30	19 (3%)	46	33	125, 125, 125, 125	0
1	K	524/547 (95%)	0.23	7 (1%)	75	55	125, 125, 125, 125	0
1	L	524/547 (95%)	0.22	14 (2%)	56	39	125, 125, 125, 125	0
1	M	524/547 (95%)	0.31	20 (3%)	44	32	125, 125, 125, 125	0
1	N	524/547 (95%)	0.45	17 (3%)	50	36	125, 125, 125, 125	0
All	All	7336/7658 (95%)	0.28	198 (2%)	56	39	125, 125, 125, 125	0

All (198) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	118	ARG	4.9
1	C	74	VAL	4.5
1	H	275	ALA	3.9
1	J	49	ILE	3.9
1	I	79	SER	3.8
1	H	515	ILE	3.8
1	K	477	GLY	3.8
1	J	17	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	M	331	THR	3.7
1	F	332	ILE	3.7
1	K	32	GLY	3.6
1	G	254	VAL	3.6
1	H	214	GLU	3.5
1	G	227	ILE	3.5
1	G	223	ALA	3.5
1	C	70	GLY	3.5
1	M	70	GLY	3.5
1	D	26	ALA	3.4
1	A	275	ALA	3.4
1	M	53	GLY	3.3
1	L	512	GLY	3.2
1	L	62	LEU	3.2
1	M	273	VAL	3.2
1	C	203	TYR	3.2
1	D	60	ILE	3.2
1	E	481	ALA	3.1
1	G	233	MET	3.1
1	L	214	GLU	3.0
1	N	322	ARG	3.0
1	J	332	ILE	3.0
1	F	189	VAL	3.0
1	I	141	SER	3.0
1	N	521	VAL	2.9
1	M	227	ILE	2.9
1	J	33	PRO	2.9
1	C	378	VAL	2.9
1	A	304	GLU	2.8
1	B	295	LEU	2.8
1	M	324	VAL	2.8
1	D	62	LEU	2.8
1	C	174	VAL	2.8
1	J	515	ILE	2.7
1	I	315	GLU	2.7
1	M	20	VAL	2.7
1	N	315	GLU	2.7
1	H	289	LEU	2.7
1	G	60	ILE	2.7
1	K	515	ILE	2.7
1	M	514	MET	2.7
1	J	213	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	L	66	PHE	2.7
1	D	161	LEU	2.7
1	C	376	VAL	2.7
1	D	136	VAL	2.7
1	H	514	MET	2.7
1	G	147	VAL	2.6
1	A	150	ILE	2.6
1	L	515	ILE	2.6
1	A	87	ASP	2.6
1	B	361	ASP	2.6
1	H	221	LEU	2.6
1	C	202	PRO	2.6
1	G	202	PRO	2.6
1	K	271	VAL	2.6
1	E	193	MET	2.6
1	E	214	GLU	2.6
1	M	44	PHE	2.6
1	I	325	ILE	2.6
1	M	17	LEU	2.6
1	I	213	VAL	2.6
1	A	32	GLY	2.6
1	D	249	ILE	2.6
1	I	22	VAL	2.6
1	J	51	LYS	2.6
1	I	195	PHE	2.6
1	E	332	ILE	2.5
1	H	300	VAL	2.5
1	E	295	LEU	2.5
1	G	221	LEU	2.5
1	J	221	LEU	2.5
1	N	514	MET	2.5
1	C	33	PRO	2.5
1	I	32	GLY	2.5
1	C	160	LYS	2.5
1	I	212	ALA	2.5
1	J	195	PHE	2.5
1	J	47	PRO	2.5
1	L	26	ALA	2.5
1	D	196	ASP	2.5
1	L	70	GLY	2.5
1	C	73	MET	2.5
1	N	300	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	L	409	GLU	2.4
1	N	256	GLY	2.4
1	F	489	ILE	2.4
1	N	259	LEU	2.4
1	L	32	GLY	2.4
1	F	174	VAL	2.4
1	J	513	LEU	2.4
1	J	212	ALA	2.4
1	N	251	ALA	2.4
1	M	86	GLY	2.4
1	A	139	SER	2.4
1	N	14	VAL	2.4
1	I	253	ASP	2.4
1	G	165	ALA	2.4
1	I	26	ALA	2.4
1	A	86	GLY	2.3
1	D	138	CYS	2.3
1	A	254	VAL	2.3
1	M	71	ALA	2.3
1	I	87	ASP	2.3
1	K	416	GLY	2.3
1	L	481	ALA	2.3
1	E	87	ASP	2.3
1	J	209	GLU	2.3
1	A	6	VAL	2.3
1	D	17	LEU	2.3
1	H	411	VAL	2.3
1	E	153	ASN	2.3
1	F	275	ALA	2.3
1	A	136	VAL	2.3
1	F	86	GLY	2.3
1	B	342	ILE	2.2
1	F	60	ILE	2.2
1	H	249	ILE	2.2
1	B	32	GLY	2.2
1	G	263	VAL	2.2
1	N	215	LEU	2.2
1	N	515	ILE	2.2
1	C	514	MET	2.2
1	K	31	LEU	2.2
1	J	89	THR	2.2
1	B	87	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	64	ASP	2.2
1	D	87	ASP	2.2
1	C	377	ALA	2.2
1	L	243	ALA	2.2
1	M	16	MET	2.2
1	I	400	LEU	2.2
1	M	411	VAL	2.2
1	G	32	GLY	2.2
1	N	32	GLY	2.2
1	E	482	THR	2.2
1	M	90	THR	2.2
1	C	32	GLY	2.2
1	A	325	ILE	2.2
1	H	331	THR	2.2
1	N	299	THR	2.2
1	B	503	ALA	2.2
1	G	71	ALA	2.2
1	H	26	ALA	2.2
1	N	3	ALA	2.2
1	E	376	VAL	2.2
1	L	86	GLY	2.2
1	L	514	MET	2.2
1	D	320	ALA	2.1
1	E	521	VAL	2.1
1	L	33	PRO	2.1
1	M	67	GLU	2.1
1	H	41	ASP	2.1
1	H	253	ASP	2.1
1	K	87	ASP	2.1
1	J	20	VAL	2.1
1	M	323	VAL	2.1
1	G	204	PHE	2.1
1	M	51	LYS	2.1
1	F	431	GLY	2.1
1	M	208	PRO	2.1
1	C	263	VAL	2.1
1	C	87	ASP	2.1
1	J	87	ASP	2.1
1	H	506	TYR	2.1
1	I	86	GLY	2.1
1	A	153	ASN	2.1
1	A	407	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	6	VAL	2.1
1	F	512	GLY	2.1
1	N	480	ALA	2.1
1	J	401	HIS	2.1
1	M	196	ASP	2.1
1	A	60	ILE	2.1
1	N	223	ALA	2.1
1	C	273	VAL	2.1
1	C	60	ILE	2.0
1	D	63	GLU	2.0
1	A	171	LYS	2.0
1	D	137	PRO	2.0
1	E	480	ALA	2.0
1	G	139	SER	2.0
1	N	154	SER	2.0
1	C	114	MET	2.0
1	E	51	LYS	2.0
1	J	32	GLY	2.0
1	J	272	LYS	2.0
1	B	66	PHE	2.0
1	E	62	LEU	2.0
1	G	87	ASP	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	H	553	1/1	0.38	0.19	125,125,125,125	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	G	553	1/1	0.46	0.23	125,125,125,125	0
4	MG	M	553	1/1	0.47	0.23	125,125,125,125	0
4	MG	L	553	1/1	0.48	0.20	125,125,125,125	0
4	MG	E	553	1/1	0.55	0.20	125,125,125,125	0
4	MG	C	553	1/1	0.59	0.18	125,125,125,125	0
4	MG	A	553	1/1	0.61	0.19	125,125,125,125	0
4	MG	I	553	1/1	0.61	0.19	125,125,125,125	0
2	AGS	L	549	31/31	0.69	0.17	125,125,125,125	0
2	AGS	G	549	31/31	0.70	0.15	125,125,125,125	0
4	MG	K	553	1/1	0.70	0.18	125,125,125,125	0
4	MG	D	553	1/1	0.71	0.15	125,125,125,125	0
3	TL	L	551	1/1	0.71	0.20	125,125,125,125	1
2	AGS	M	549	31/31	0.72	0.17	125,125,125,125	0
2	AGS	N	549	31/31	0.74	0.17	125,125,125,125	0
2	AGS	H	549	31/31	0.74	0.16	125,125,125,125	0
2	AGS	K	549	31/31	0.75	0.16	125,125,125,125	0
4	MG	N	552	1/1	0.76	0.14	125,125,125,125	0
2	AGS	E	549	31/31	0.77	0.18	125,125,125,125	0
4	MG	F	553	1/1	0.77	0.13	125,125,125,125	0
2	AGS	F	549	31/31	0.77	0.14	125,125,125,125	0
2	AGS	J	549	31/31	0.78	0.16	125,125,125,125	0
2	AGS	C	549	31/31	0.78	0.14	125,125,125,125	0
2	AGS	B	549	31/31	0.81	0.13	125,125,125,125	0
4	MG	J	553	1/1	0.81	0.18	125,125,125,125	0
4	MG	B	553	1/1	0.81	0.15	125,125,125,125	0
3	TL	M	552	1/1	0.82	0.11	125,125,125,125	1
3	TL	H	554	1/1	0.82	0.14	125,125,125,125	1
2	AGS	I	549	31/31	0.82	0.13	125,125,125,125	0
2	AGS	A	549	31/31	0.83	0.13	125,125,125,125	0
2	AGS	D	549	31/31	0.84	0.14	125,125,125,125	0
3	TL	G	551	1/1	0.87	0.10	125,125,125,125	1
3	TL	J	551	1/1	0.90	0.10	125,125,125,125	1
3	TL	F	551	1/1	0.91	0.08	125,125,125,125	1
3	TL	H	550	1/1	0.92	0.09	125,125,125,125	1
3	TL	K	550	1/1	0.92	0.08	125,125,125,125	1
3	TL	E	552	1/1	0.93	0.08	125,125,125,125	1
3	TL	N	550	1/1	0.94	0.12	125,125,125,125	1
3	TL	B	550	1/1	0.94	0.07	125,125,125,125	1
3	TL	D	551	1/1	0.94	0.09	125,125,125,125	1
3	TL	M	550	1/1	0.94	0.13	125,125,125,125	1
3	TL	E	550	1/1	0.94	0.10	125,125,125,125	1
3	TL	C	552	1/1	0.95	0.14	125,125,125,125	1

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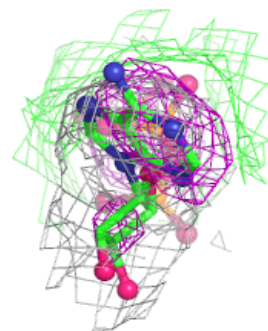
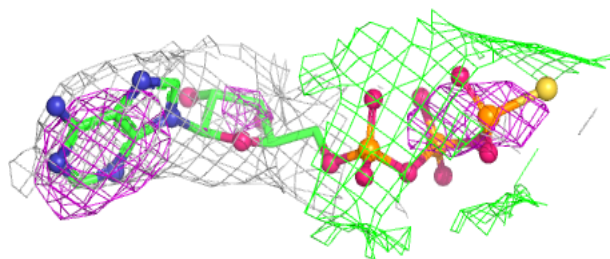
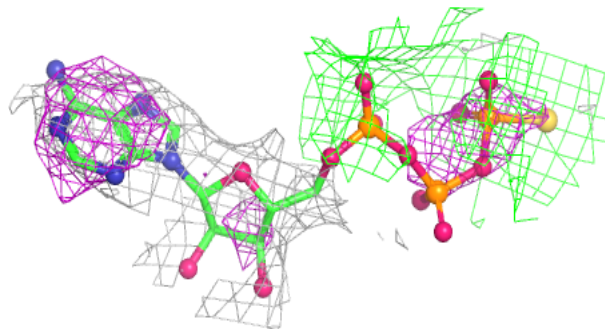
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	TL	C	550	1/1	0.95	0.06	125,125,125,125	1
3	TL	L	550	1/1	0.96	0.06	125,125,125,125	1
3	TL	A	551	1/1	0.96	0.11	125,125,125,125	1
3	TL	L	552	1/1	0.96	0.07	125,125,125,125	1
3	TL	I	551	1/1	0.96	0.08	125,125,125,125	1
3	TL	K	552	1/1	0.96	0.12	125,125,125,125	1
3	TL	K	551	1/1	0.97	0.07	125,125,125,125	1
3	TL	I	550	1/1	0.97	0.06	125,125,125,125	1
3	TL	B	552	1/1	0.97	0.09	125,125,125,125	1
3	TL	N	551	1/1	0.97	0.11	125,125,125,125	1
3	TL	H	552	1/1	0.97	0.07	125,125,125,125	1
3	TL	C	551	1/1	0.97	0.06	125,125,125,125	1
3	TL	H	551	1/1	0.98	0.05	125,125,125,125	1
3	TL	E	551	1/1	0.98	0.05	125,125,125,125	1
3	TL	D	550	1/1	0.98	0.03	125,125,125,125	1
3	TL	A	552	1/1	0.98	0.06	125,125,125,125	1
3	TL	M	551	1/1	0.98	0.06	125,125,125,125	1
3	TL	F	552	1/1	0.98	0.06	125,125,125,125	1
3	TL	J	550	1/1	0.98	0.06	125,125,125,125	1
3	TL	G	550	1/1	0.98	0.05	125,125,125,125	1
3	TL	D	552	1/1	0.98	0.07	125,125,125,125	1
3	TL	G	552	1/1	0.98	0.06	125,125,125,125	1
3	TL	B	551	1/1	0.98	0.08	125,125,125,125	1
3	TL	F	554	1/1	0.99	0.10	125,125,125,125	1
3	TL	I	552	1/1	0.99	0.05	125,125,125,125	1
3	TL	A	550	1/1	0.99	0.03	125,125,125,125	1
3	TL	F	550	1/1	0.99	0.11	125,125,125,125	1
3	TL	J	552	1/1	0.99	0.03	125,125,125,125	1
3	TL	A	554	1/1	1.00	0.13	125,125,125,125	1
3	TL	B	554	1/1	1.00	0.11	125,125,125,125	1
3	TL	D	1	1/1	1.00	0.15	125,125,125,125	1

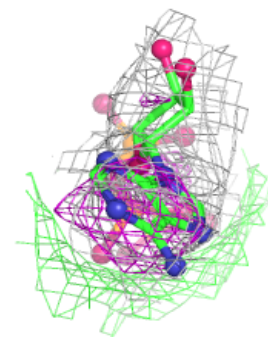
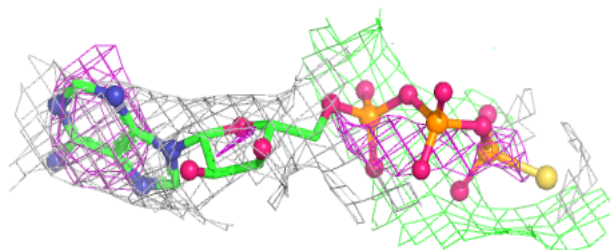
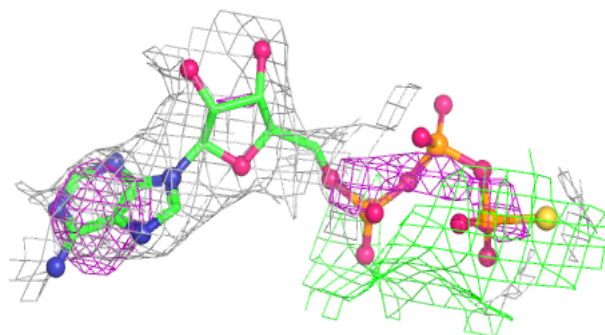
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AGS 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)

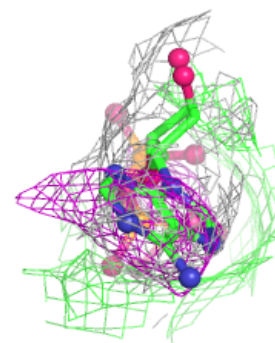
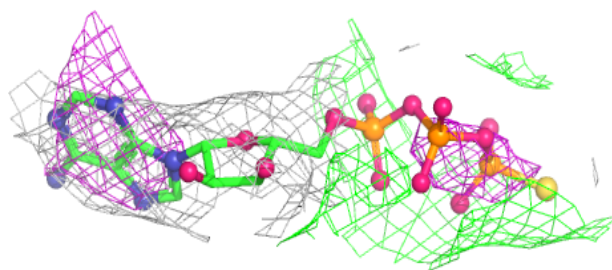
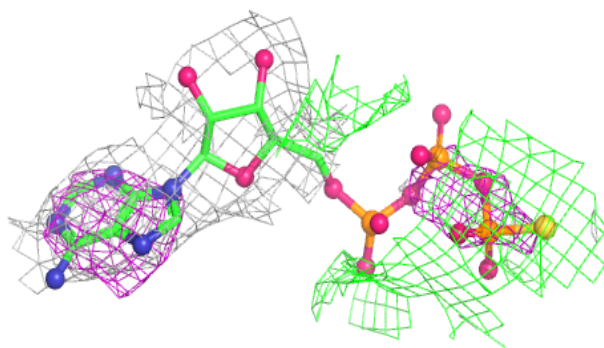
**Electron density around AGS G 549:**

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

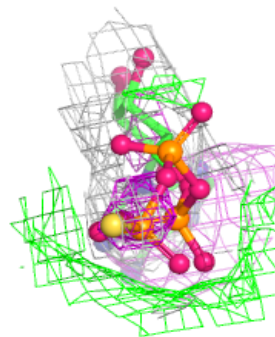
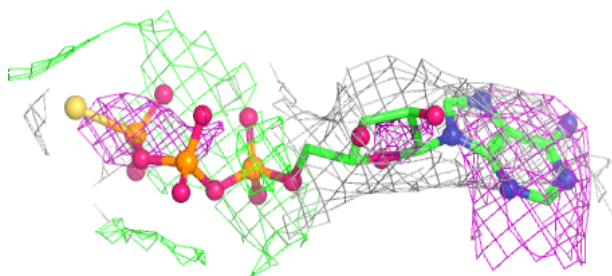
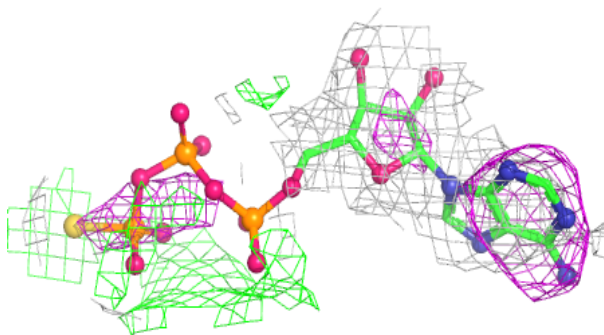


Electron density around AGS M 549:

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

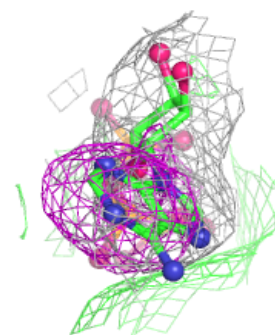
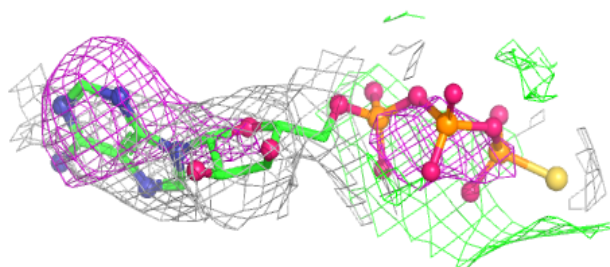
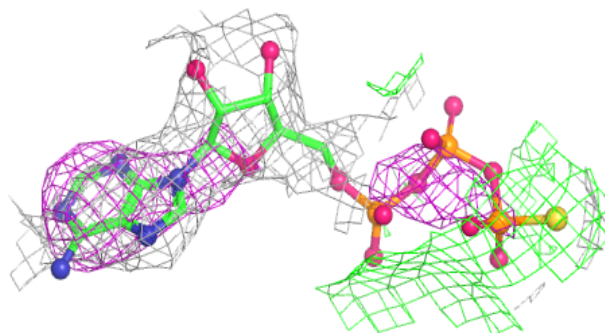
**Electron density around AGS N 549:**

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

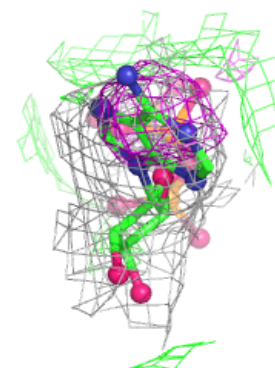
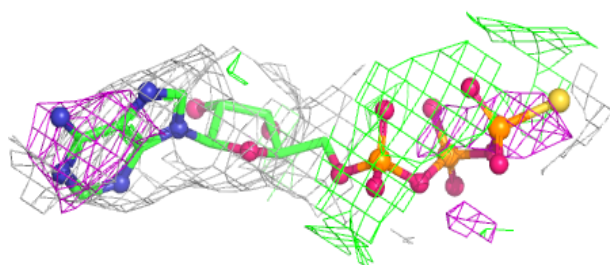
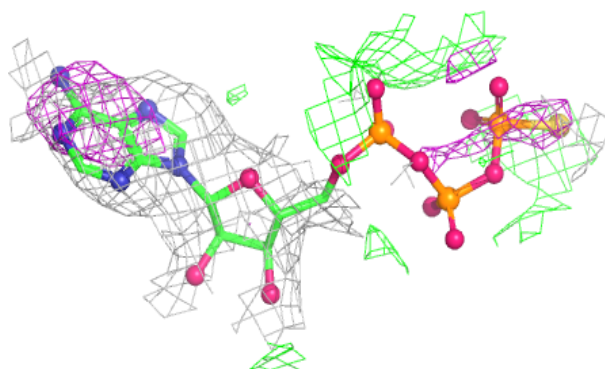


Electron density around AGS H 549:

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

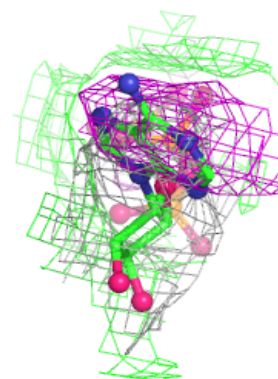
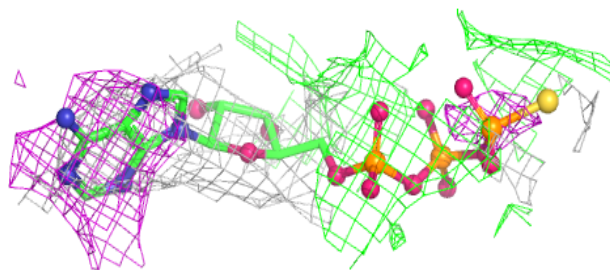
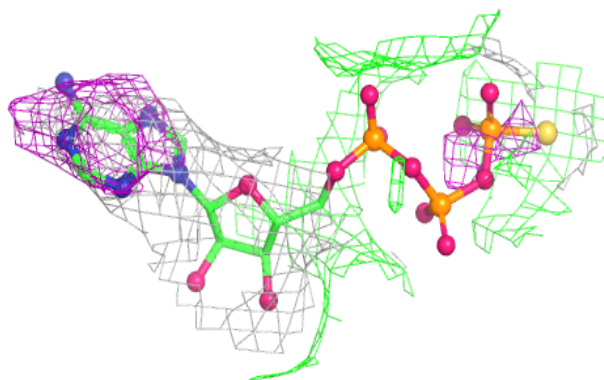
**Electron density around AGS K 549:**

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

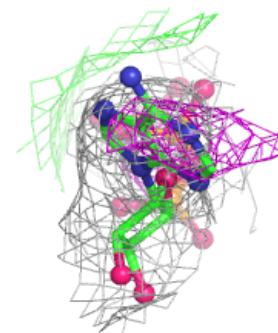
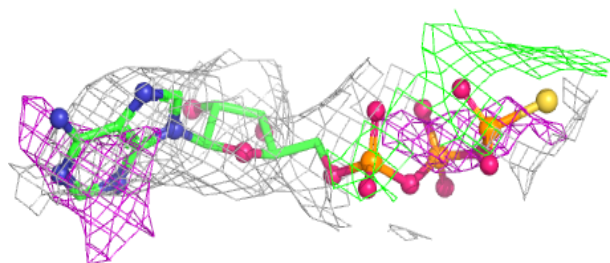
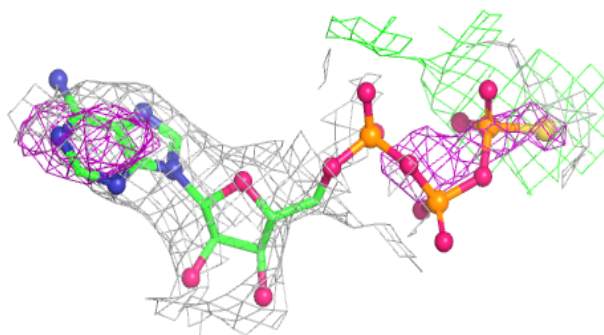


Electron density around AGS E 549:

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

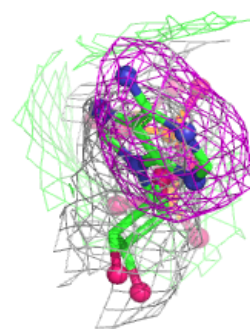
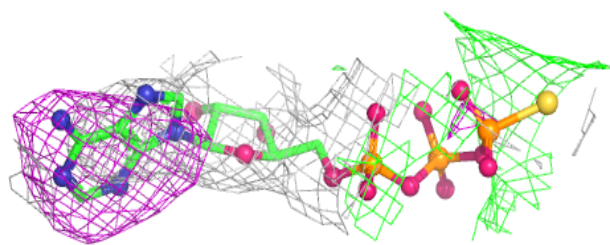
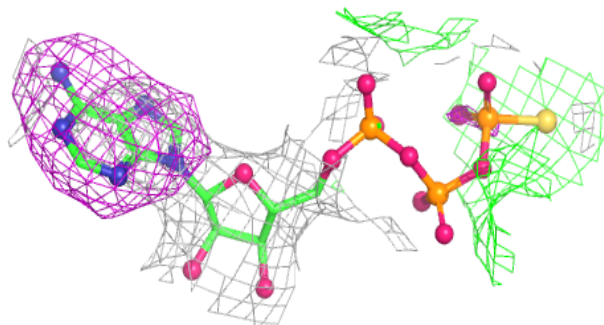
**Electron density around AGS F 549:**

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

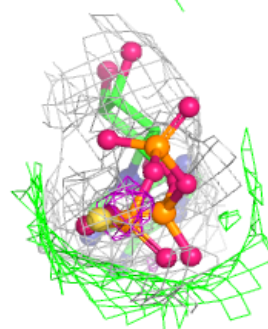
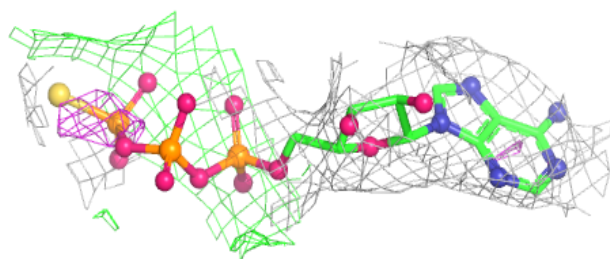
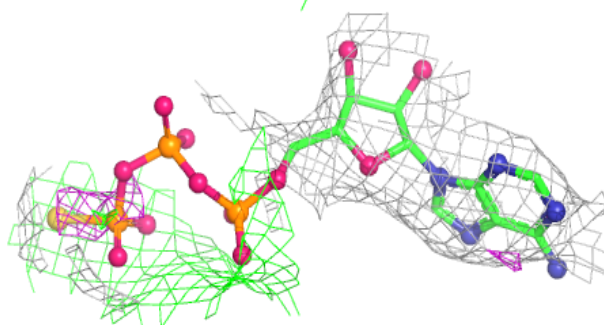


Electron density around AGS J 549:

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

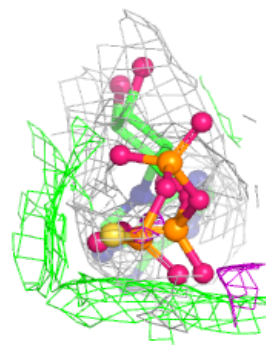
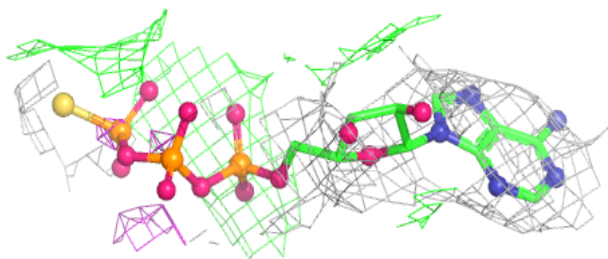
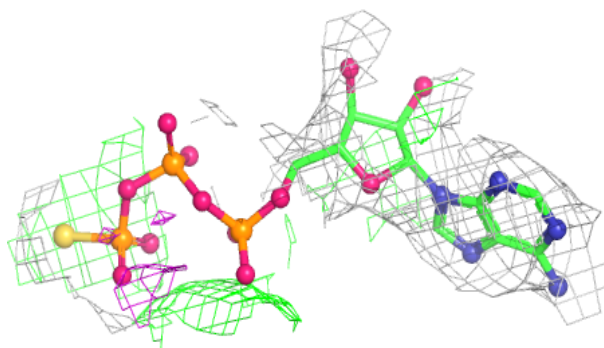
**Electron density around AGS C 549:**

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

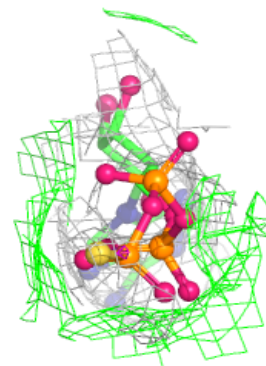
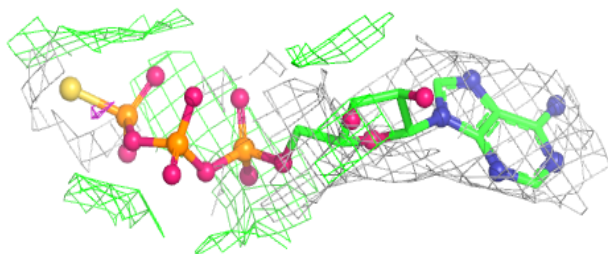
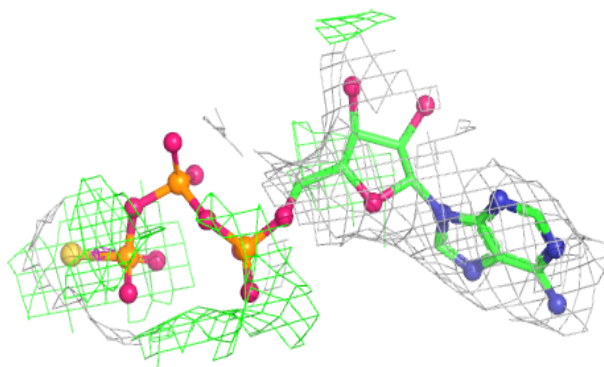


Electron density around AGS B 549:

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

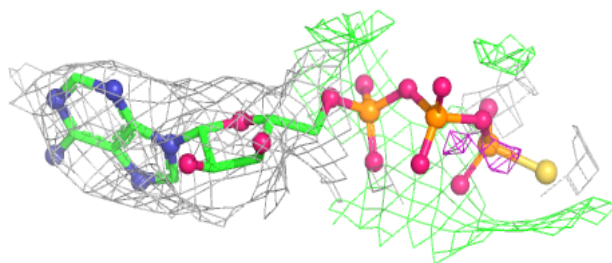
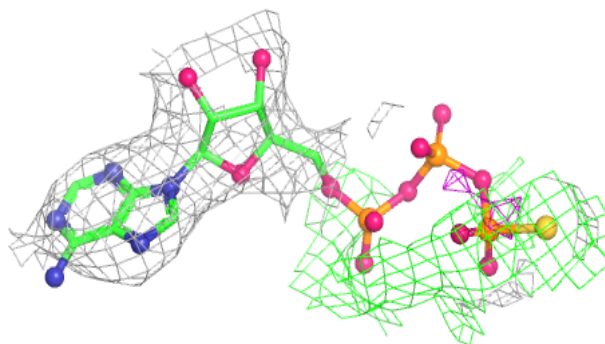
**Electron density around AGS I 549:**

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

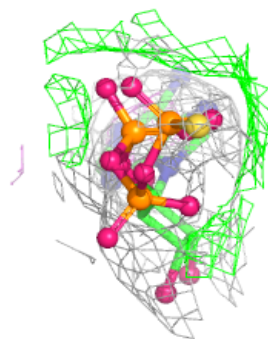
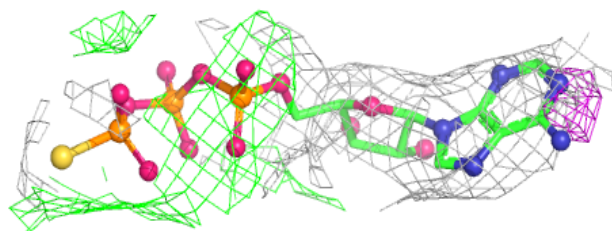
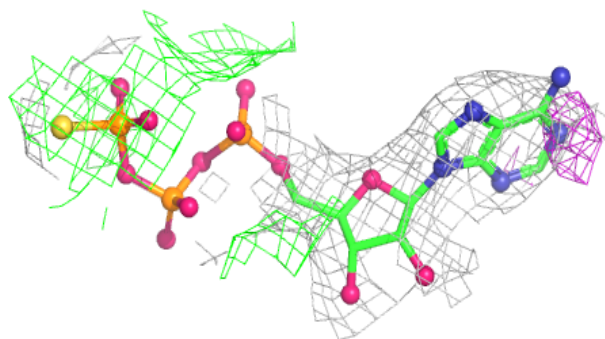


Electron density around AGS A 549:

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

**Electron density around AGS 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.