



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 07:29 AM UTC

PDB ID : 2WGS / pdb_00002wgs
Title : Crystal structure of Mycobacterium Tuberculosis Glutamine Synthetase in complex with a purine analogue inhibitor.
Authors : Nilsson, M.T.; Krajewski, W.W.; Jones, T.A.; Mowbray, S.L.
Deposited on : 2009-04-27
Resolution : 2.55 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

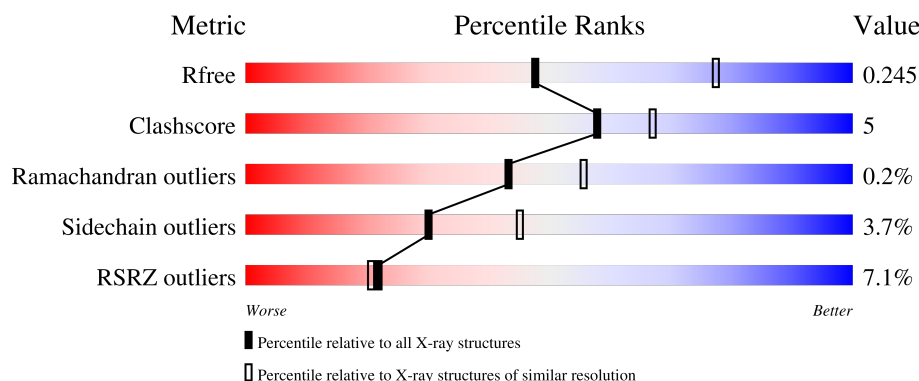
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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.



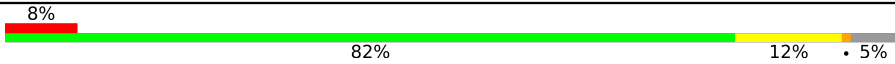
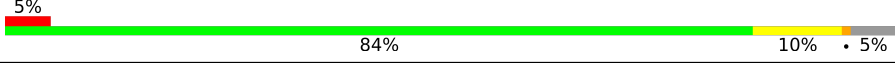
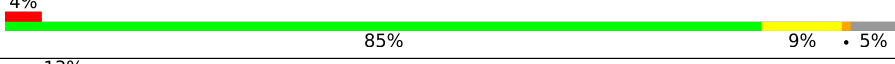
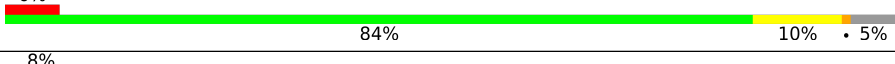
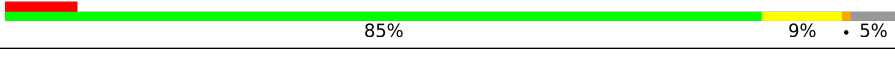
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	486	6% 83% 12% • 5%
1	B	486	4% 84% 10% • 5%
1	C	486	6% 84% 10% • 5%
1	D	486	6% 83% 12% • 5%
1	E	486	8% 84% 10% • 5%

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Mol	Chain	Length	Quality of chain
1	F	486	
1	G	486	
1	H	486	
1	I	486	
1	J	486	
1	K	486	
1	L	486	

2 Entry composition

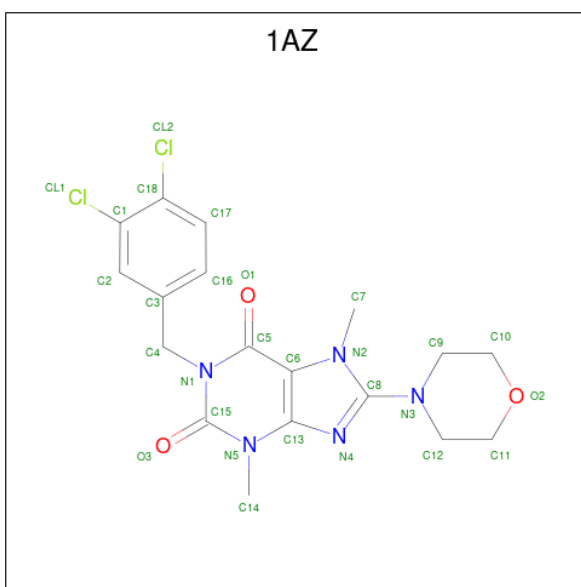
There are 4 unique types of molecules in this entry. The entry contains 45804 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GLUTAMINE SYNTHETASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	463	Total	C	N	O	S	0	0	0
			3660	2331	617	700	12			
1	B	463	Total	C	N	O	S	0	0	0
			3660	2331	617	700	12			
1	C	463	Total	C	N	O	S	0	0	0
			3660	2331	617	700	12			
1	D	463	Total	C	N	O	S	0	0	0
			3660	2331	617	700	12			
1	E	463	Total	C	N	O	S	0	0	0
			3660	2331	617	700	12			
1	F	463	Total	C	N	O	S	0	0	0
			3660	2331	617	700	12			
1	G	463	Total	C	N	O	S	0	0	0
			3660	2331	617	700	12			
1	H	463	Total	C	N	O	S	0	0	0
			3660	2331	617	700	12			
1	I	463	Total	C	N	O	S	0	0	0
			3660	2331	617	700	12			
1	J	463	Total	C	N	O	S	0	0	0
			3660	2331	617	700	12			
1	K	463	Total	C	N	O	S	0	0	0
			3660	2331	617	700	12			
1	L	463	Total	C	N	O	S	0	0	0
			3660	2331	617	700	12			

- Molecule 2 is 1-(3,4-dichlorobenzyl)-3,7-dimethyl-8-morpholin-4-yl-3,7-dihydro-1H-purine-2,6-dione (CCD ID: 1AZ) (formula: C₁₈H₁₉Cl₂N₅O₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			28	18	2	5	3		
2	B	1	Total	C	Cl	N	O	0	0
			28	18	2	5	3		
2	C	1	Total	C	Cl	N	O	0	0
			28	18	2	5	3		
2	D	1	Total	C	Cl	N	O	0	0
			28	18	2	5	3		
2	E	1	Total	C	Cl	N	O	0	0
			28	18	2	5	3		
2	F	1	Total	C	Cl	N	O	0	0
			28	18	2	5	3		
2	G	1	Total	C	Cl	N	O	0	0
			28	18	2	5	3		
2	H	1	Total	C	Cl	N	O	0	0
			28	18	2	5	3		
2	I	1	Total	C	Cl	N	O	0	0
			28	18	2	5	3		
2	J	1	Total	C	Cl	N	O	0	0
			28	18	2	5	3		
2	K	1	Total	C	Cl	N	O	0	0
			28	18	2	5	3		
2	L	1	Total	C	Cl	N	O	0	0
			28	18	2	5	3		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	B	1	Total Cl 1 1	0	0
3	C	1	Total Cl 1 1	0	0
3	D	1	Total Cl 1 1	0	0
3	E	1	Total Cl 1 1	0	0
3	F	1	Total Cl 1 1	0	0
3	G	1	Total Cl 1 1	0	0
3	H	1	Total Cl 1 1	0	0
3	I	1	Total Cl 1 1	0	0
3	J	1	Total Cl 1 1	0	0
3	K	1	Total Cl 1 1	0	0
3	L	1	Total Cl 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	126	Total O 126 126	0	0
4	B	129	Total O 129 129	0	0
4	C	130	Total O 130 130	0	0
4	D	127	Total O 127 127	0	0
4	E	130	Total O 130 130	0	0
4	F	127	Total O 127 127	0	0
4	G	126	Total O 126 126	0	0
4	H	129	Total O 129 129	0	0

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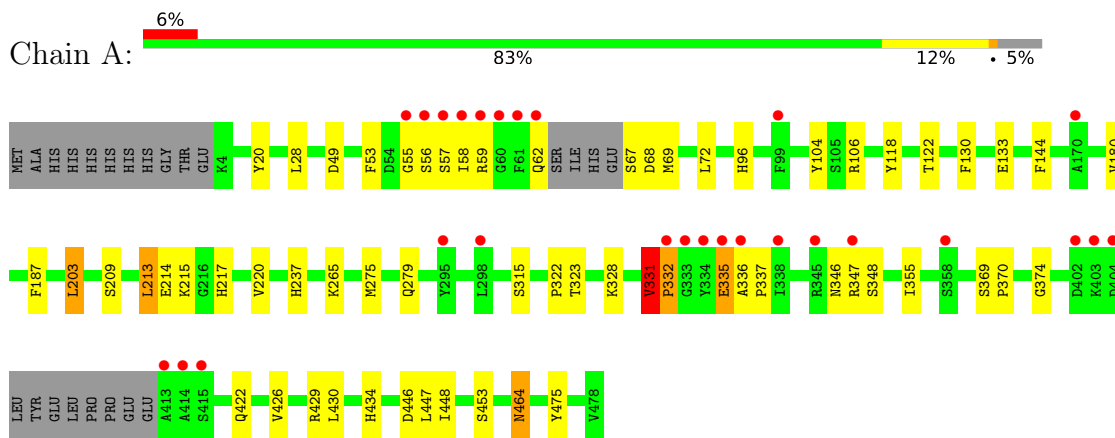
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	126	Total 126	O 126	0	0
4	J	126	Total 126	O 126	0	0
4	K	131	Total 131	O 131	0	0
4	L	129	Total 129	O 129	0	0

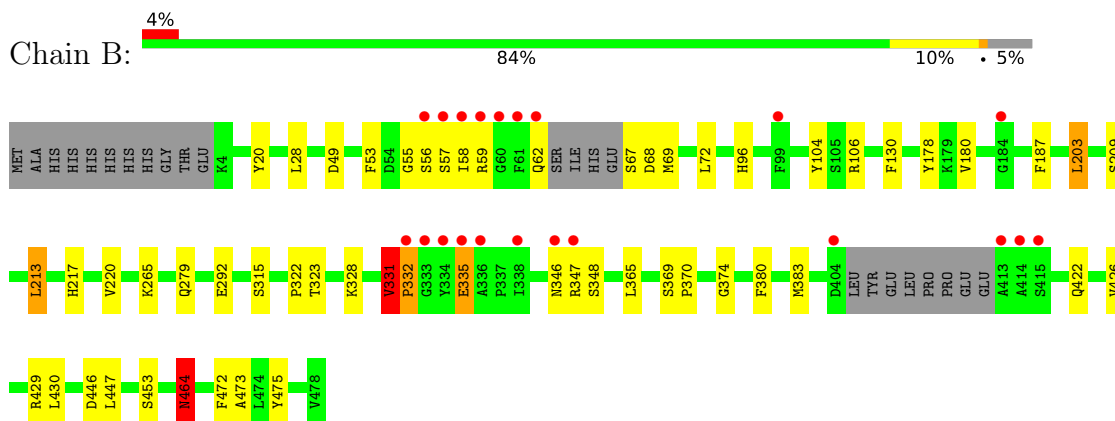
3 Residue-property plots [i](#)

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

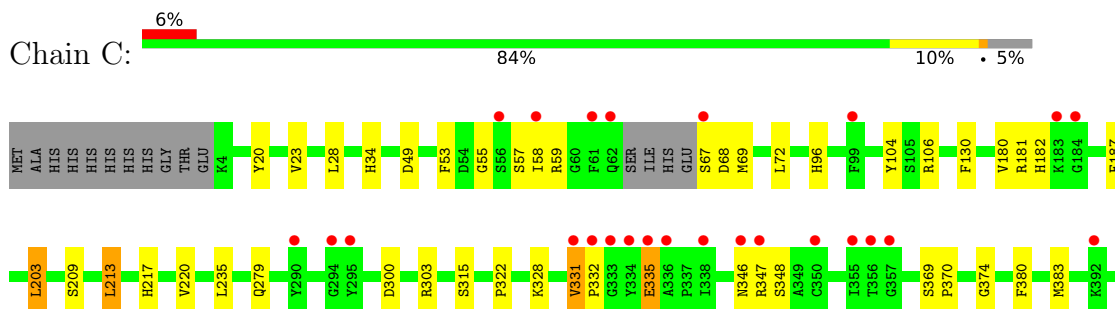
• Molecule 1: GLUTAMINE SYNTHETASE 1

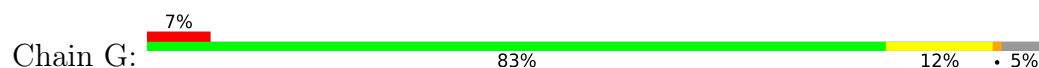
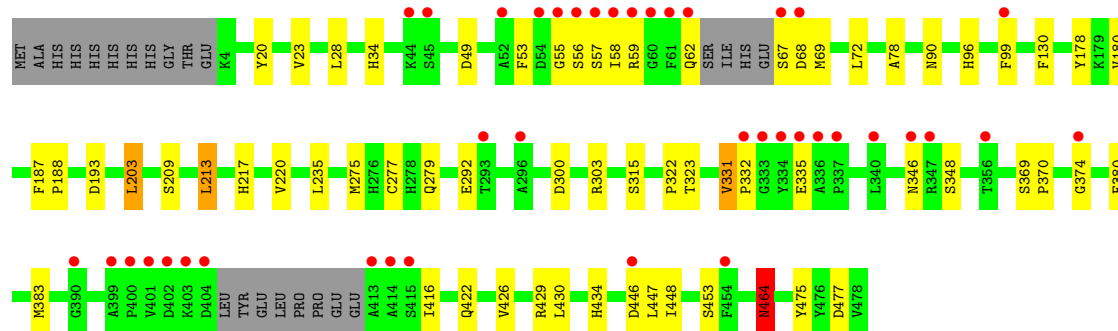
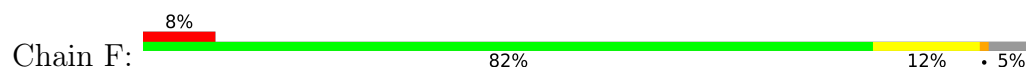
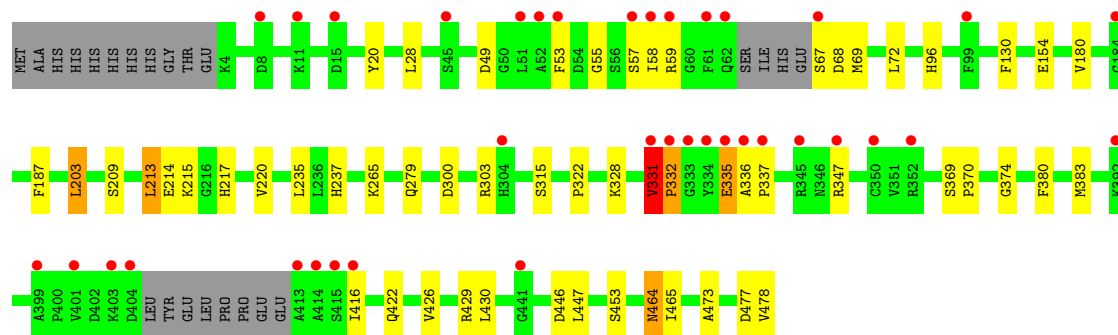
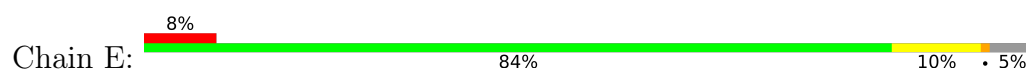
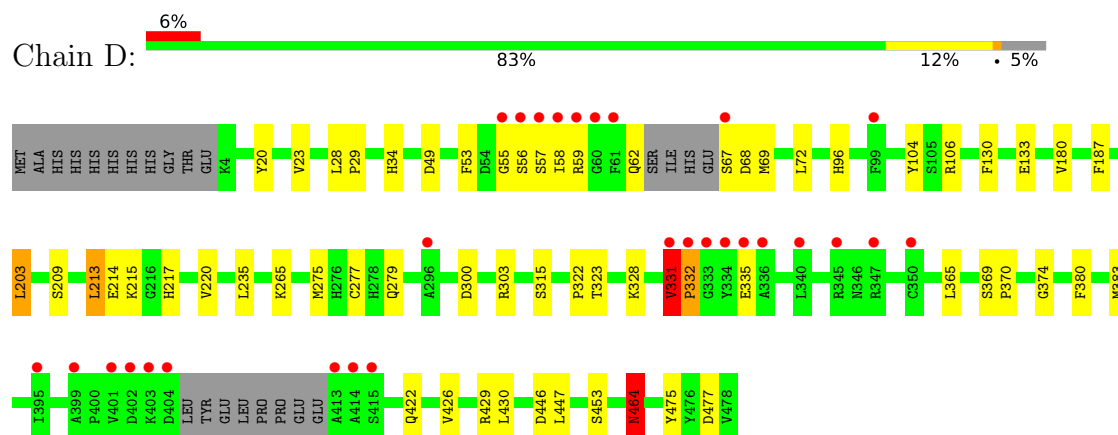
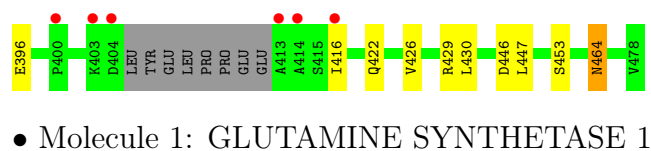


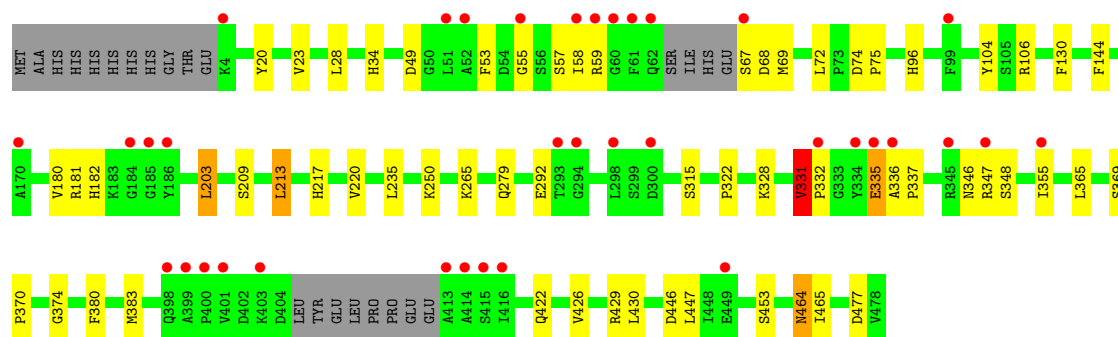
• Molecule 1: GLUTAMINE SYNTHETASE 1



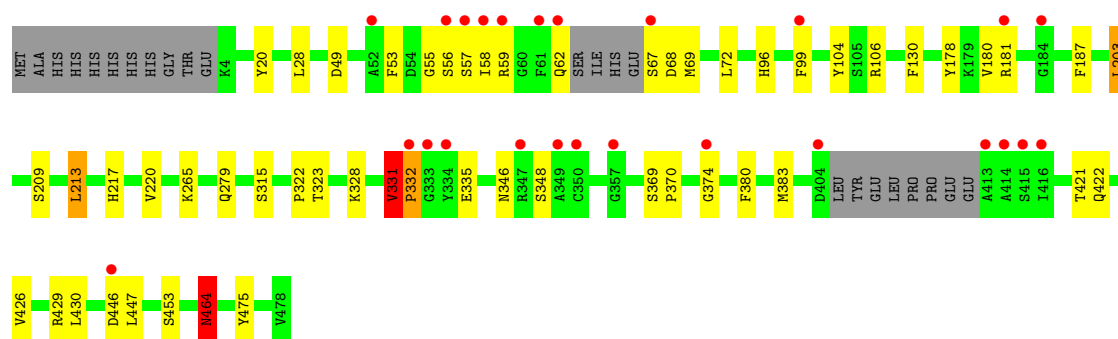
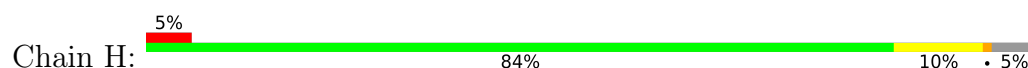
• Molecule 1: GLUTAMINE SYNTHETASE 1



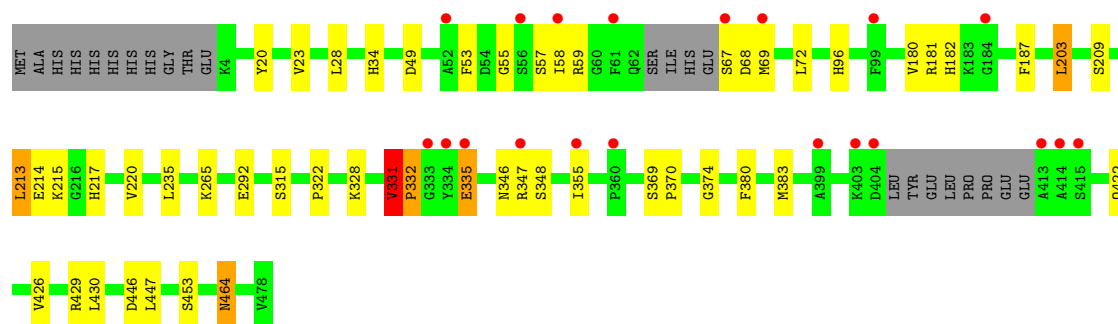
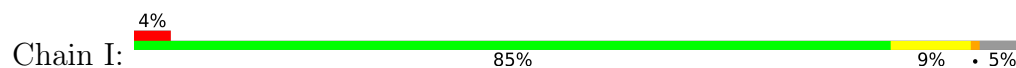




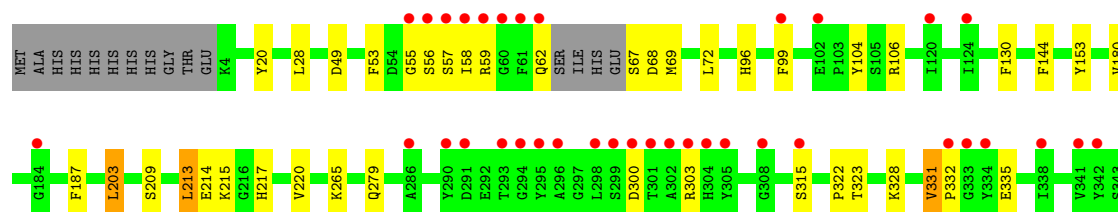
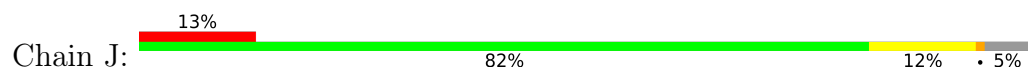
• Molecule 1: GLUTAMINE SYNTHETASE 1

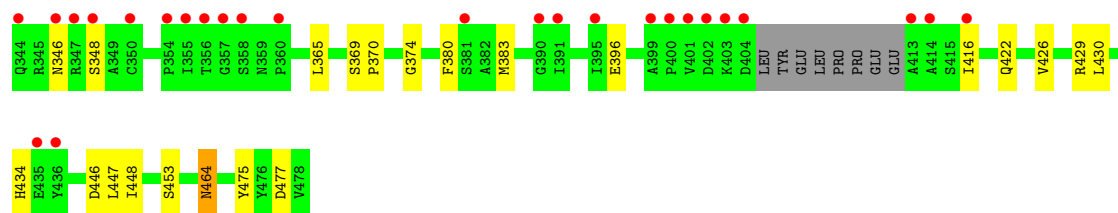


• Molecule 1: GLUTAMINE SYNTHETASE 1



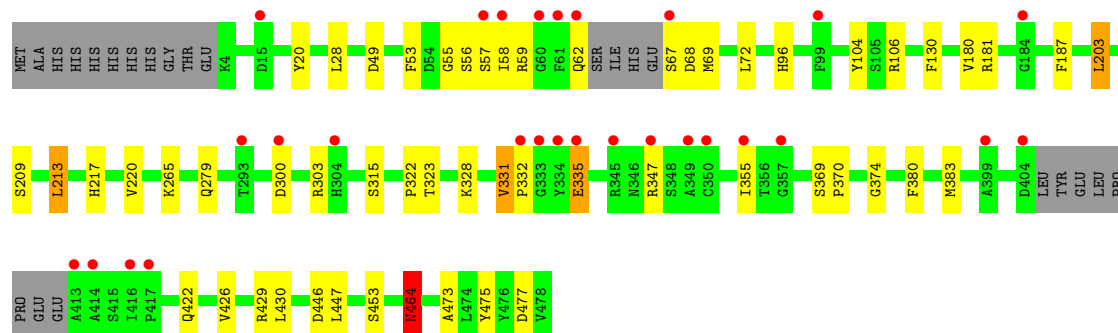
• Molecule 1: GLUTAMINE SYNTHETASE 1





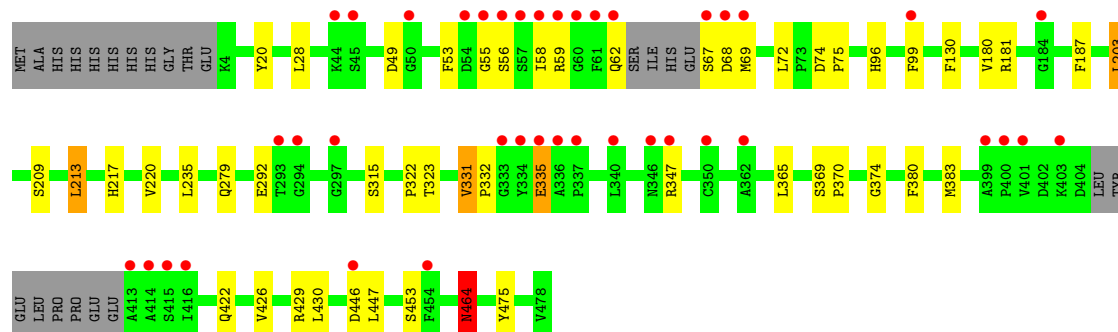
● Molecule 1: GLUTAMINE SYNTHETASE 1

Chain K: 6% 84% 10% 5%



● Molecule 1: GLUTAMINE SYNTHETASE 1

Chain L: 8% 85% 9% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	134.95Å 203.18Å 230.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.95 – 2.55 29.95 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.95-2.55) 99.7 (29.95-2.55)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.35 (at 2.54Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.230 , 0.246 0.229 , 0.245	Depositor DCC
R_{free} test set	10318 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	42.3	Xtrriage
Anisotropy	0.210	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 28.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	45804	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.94 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0653e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 1AZ, CL

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	0.63	0/3760	0.84	3/5105 (0.1%)
1	B	0.63	0/3760	0.83	4/5105 (0.1%)
1	C	0.62	0/3760	0.83	4/5105 (0.1%)
1	D	0.63	0/3760	0.84	4/5105 (0.1%)
1	E	0.63	0/3760	0.85	4/5105 (0.1%)
1	F	0.64	0/3760	0.83	5/5105 (0.1%)
1	G	0.64	0/3760	0.84	3/5105 (0.1%)
1	H	0.64	0/3760	0.82	4/5105 (0.1%)
1	I	0.61	0/3760	0.82	2/5105 (0.0%)
1	J	0.68	0/3760	0.83	4/5105 (0.1%)
1	K	0.63	0/3760	0.84	4/5105 (0.1%)
1	L	0.64	0/3760	0.84	4/5105 (0.1%)
All	All	0.64	0/45120	0.83	45/61260 (0.1%)

There are no bond length outliers.

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	331	VAL	CA-C-N	8.40	130.34	119.84
1	H	331	VAL	C-N-CA	8.40	130.34	119.84
1	G	331	VAL	CA-C-N	8.29	130.20	119.84
1	G	331	VAL	C-N-CA	8.29	130.20	119.84
1	E	331	VAL	CA-C-N	8.22	130.11	119.84
1	E	331	VAL	C-N-CA	8.22	130.11	119.84
1	I	331	VAL	CA-C-N	8.21	130.10	119.84
1	I	331	VAL	C-N-CA	8.21	130.10	119.84
1	L	331	VAL	CA-C-N	8.16	130.04	119.84
1	L	331	VAL	C-N-CA	8.16	130.04	119.84
1	J	331	VAL	CA-C-N	8.09	129.95	119.84
1	J	331	VAL	C-N-CA	8.09	129.95	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	331	VAL	CA-C-N	8.05	129.90	119.84
1	A	331	VAL	C-N-CA	8.05	129.90	119.84
1	F	331	VAL	CA-C-N	8.04	129.89	119.84
1	F	331	VAL	C-N-CA	8.04	129.89	119.84
1	C	331	VAL	CA-C-N	8.04	129.88	119.84
1	C	331	VAL	C-N-CA	8.04	129.88	119.84
1	K	331	VAL	CA-C-N	8.03	129.87	119.84
1	K	331	VAL	C-N-CA	8.03	129.87	119.84
1	D	331	VAL	CA-C-N	7.96	129.79	119.84
1	D	331	VAL	C-N-CA	7.96	129.79	119.84
1	B	331	VAL	CA-C-N	7.74	129.52	119.84
1	B	331	VAL	C-N-CA	7.74	129.52	119.84
1	E	331	VAL	N-CA-C	6.50	115.72	108.05
1	B	331	VAL	N-CA-C	6.30	115.49	108.05
1	L	464	ASN	N-CA-C	6.15	118.78	111.33
1	K	464	ASN	N-CA-C	6.07	118.68	111.33
1	F	464	ASN	N-CA-C	6.05	118.65	111.33
1	C	331	VAL	N-CA-C	5.94	115.06	108.05
1	A	331	VAL	N-CA-C	5.88	114.99	108.05
1	K	331	VAL	N-CA-C	5.81	114.91	108.05
1	L	331	VAL	N-CA-C	5.67	114.74	108.05
1	J	331	VAL	N-CA-C	5.35	114.36	108.05
1	D	331	VAL	N-CA-C	5.25	114.25	108.05
1	G	331	VAL	N-CA-C	5.25	114.25	108.05
1	B	464	ASN	N-CA-C	5.23	117.66	111.33
1	E	416	ILE	N-CA-C	5.19	113.00	107.76
1	H	464	ASN	N-CA-C	5.18	117.59	111.33
1	J	416	ILE	N-CA-C	5.12	112.93	107.76
1	F	331	VAL	N-CA-C	5.12	114.09	108.05
1	F	416	ILE	N-CA-C	5.12	112.93	107.76
1	H	331	VAL	N-CA-C	5.11	114.08	108.05
1	C	416	ILE	N-CA-C	5.04	112.85	107.76
1	D	464	ASN	N-CA-C	5.01	117.40	111.33

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	3660	0	3497	47	0
1	B	3660	0	3497	41	0
1	C	3660	0	3497	42	0
1	D	3660	0	3497	42	0
1	E	3660	0	3497	45	0
1	F	3660	0	3497	44	0
1	G	3660	0	3497	47	0
1	H	3660	0	3497	42	0
1	I	3660	0	3497	42	0
1	J	3660	0	3497	44	0
1	K	3660	0	3497	42	0
1	L	3660	0	3497	37	0
2	A	28	0	19	0	0
2	B	28	0	19	0	0
2	C	28	0	19	0	0
2	D	28	0	19	0	0
2	E	28	0	19	0	0
2	F	28	0	19	0	0
2	G	28	0	19	0	0
2	H	28	0	19	0	0
2	I	28	0	19	0	0
2	J	28	0	19	0	0
2	K	28	0	19	0	0
2	L	28	0	19	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
4	A	126	0	0	1	0
4	B	129	0	0	0	0
4	C	130	0	0	0	0
4	D	127	0	0	0	0
4	E	130	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	127	0	0	0	0
4	G	126	0	0	0	0
4	H	129	0	0	0	0
4	I	126	0	0	0	0
4	J	126	0	0	0	0
4	K	131	0	0	0	0
4	L	129	0	0	0	0
All	All	45804	0	42192	391	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 (391) 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:L:55:GLY:HA3	1:L:67:SER:O	1.35	1.26
1:B:55:GLY:HA3	1:B:67:SER:O	1.36	1.23
1:C:55:GLY:HA3	1:C:67:SER:O	1.39	1.22
1:H:55:GLY:HA3	1:H:67:SER:O	1.37	1.22
1:I:55:GLY:HA3	1:I:67:SER:O	1.41	1.20
1:J:55:GLY:HA3	1:J:67:SER:O	1.39	1.19
1:G:55:GLY:HA3	1:G:67:SER:O	1.41	1.19
1:A:55:GLY:HA3	1:A:67:SER:O	1.37	1.18
1:D:55:GLY:HA3	1:D:67:SER:O	1.39	1.18
1:F:55:GLY:HA3	1:F:67:SER:O	1.39	1.18
1:K:55:GLY:HA3	1:K:67:SER:O	1.42	1.17
1:E:55:GLY:HA3	1:E:67:SER:O	1.40	1.16
1:C:464:ASN:HD21	1:I:422:GLN:HE22	1.09	0.99
1:E:422:GLN:HE22	1:G:464:ASN:HD21	1.11	0.98
1:L:55:GLY:CA	1:L:67:SER:O	2.17	0.93
1:A:55:GLY:CA	1:A:67:SER:O	2.18	0.92
1:B:55:GLY:CA	1:B:67:SER:O	2.17	0.91
1:C:422:GLN:HE22	1:I:464:ASN:HD21	1.13	0.91
1:H:55:GLY:CA	1:H:67:SER:O	2.18	0.90
1:J:55:GLY:CA	1:J:67:SER:O	2.20	0.90
1:F:55:GLY:CA	1:F:67:SER:O	2.19	0.90
1:D:55:GLY:CA	1:D:67:SER:O	2.20	0.89
1:G:335:GLU:OE1	1:L:62:GLN:HB3	1.73	0.89
1:E:464:ASN:HD21	1:G:422:GLN:HE22	1.19	0.89
1:C:55:GLY:CA	1:C:67:SER:O	2.20	0.89
1:E:55:GLY:CA	1:E:67:SER:O	2.20	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:55:GLY:CA	1:K:67:SER:O	2.21	0.88
1:I:55:GLY:CA	1:I:67:SER:O	2.21	0.87
1:G:55:GLY:CA	1:G:67:SER:O	2.22	0.87
1:H:62:GLN:HB3	1:I:335:GLU:OE1	1.77	0.85
1:A:335:GLU:OE1	1:F:62:GLN:HB3	1.78	0.82
1:A:464:ASN:HD21	1:K:422:GLN:HE22	1.30	0.79
1:I:57:SER:HB3	1:J:187:PHE:HE2	1.46	0.78
1:D:464:ASN:HD21	1:H:422:GLN:HE22	1.29	0.78
1:G:57:SER:HB3	1:H:187:PHE:HE2	1.50	0.77
1:B:422:GLN:HE22	1:J:464:ASN:HD21	1.33	0.76
1:E:57:SER:HB3	1:F:187:PHE:HE2	1.51	0.76
1:E:422:GLN:NE2	1:G:464:ASN:HD21	1.81	0.75
1:C:20:TYR:CE1	1:D:203:LEU:HD13	2.21	0.75
1:C:464:ASN:HD21	1:I:422:GLN:NE2	1.85	0.75
1:G:347:ARG:HH11	1:L:56:SER:HB3	1.50	0.75
1:H:56:SER:HB3	1:I:347:ARG:HH11	1.52	0.73
1:E:20:TYR:CE1	1:F:203:LEU:HD13	2.22	0.72
1:K:20:TYR:CE1	1:L:203:LEU:HD13	2.23	0.72
1:A:347:ARG:HH11	1:F:56:SER:HB3	1.54	0.72
1:I:57:SER:HB3	1:J:187:PHE:CE2	2.24	0.71
1:B:20:TYR:CE1	1:C:203:LEU:HD13	2.25	0.71
1:B:62:GLN:HB3	1:C:335:GLU:OE1	1.90	0.71
1:G:355:ILE:HG21	1:L:99:PHE:HE1	1.56	0.71
1:E:422:GLN:HE22	1:G:464:ASN:ND2	1.87	0.70
1:A:422:GLN:HE22	1:K:464:ASN:HD21	1.40	0.69
1:G:203:LEU:HD13	1:L:20:TYR:CE1	2.27	0.69
1:C:422:GLN:NE2	1:I:464:ASN:HD21	1.89	0.69
1:A:20:TYR:CE1	1:B:203:LEU:HD13	2.27	0.69
1:A:203:LEU:HD13	1:F:20:TYR:CE1	2.28	0.69
1:G:57:SER:HB3	1:H:187:PHE:CE2	2.28	0.69
1:E:57:SER:HB3	1:F:187:PHE:CE2	2.28	0.69
1:H:20:TYR:CE1	1:I:203:LEU:HD13	2.28	0.68
1:E:464:ASN:HD21	1:G:422:GLN:NE2	1.93	0.67
1:F:422:GLN:HE22	1:L:464:ASN:HD21	1.41	0.67
1:D:422:GLN:HE22	1:H:464:ASN:HD21	1.42	0.67
1:J:62:GLN:HB3	1:K:335:GLU:OE1	1.95	0.66
1:J:20:TYR:CE1	1:K:203:LEU:HD13	2.31	0.66
1:G:20:TYR:CE1	1:H:203:LEU:HD13	2.30	0.65
1:A:59:ARG:HE	1:A:69:MET:HE2	1.61	0.65
1:L:59:ARG:HE	1:L:69:MET:HE2	1.62	0.64
1:F:464:ASN:HD21	1:L:422:GLN:HE22	1.45	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:20:TYR:CE1	1:J:203:LEU:HD13	2.33	0.63
1:E:464:ASN:O	1:G:328:LYS:HE3	1.99	0.63
1:H:59:ARG:HE	1:H:69:MET:HE2	1.62	0.62
1:B:59:ARG:HE	1:B:69:MET:HE2	1.63	0.62
1:E:59:ARG:HE	1:E:69:MET:HE2	1.65	0.62
1:J:57:SER:HB3	1:K:187:PHE:CE2	2.34	0.62
1:K:59:ARG:HE	1:K:69:MET:HE2	1.64	0.62
1:I:59:ARG:HE	1:I:69:MET:HE2	1.65	0.62
1:D:58:ILE:HD12	1:D:69:MET:HB2	1.80	0.61
1:L:58:ILE:HD12	1:L:69:MET:HB2	1.81	0.61
1:E:464:ASN:ND2	1:G:422:GLN:HE22	1.95	0.61
1:C:57:SER:HB3	1:D:187:PHE:HE2	1.65	0.61
1:H:58:ILE:HD12	1:H:69:MET:HB2	1.83	0.61
1:J:56:SER:HB3	1:K:347:ARG:HH11	1.66	0.61
1:D:59:ARG:HE	1:D:69:MET:HE2	1.66	0.61
1:B:56:SER:HB3	1:C:347:ARG:HH11	1.66	0.60
1:B:475:TYR:CZ	1:J:323:THR:HB	2.36	0.60
1:K:62:GLN:HB3	1:L:335:GLU:OE1	2.02	0.60
1:B:58:ILE:HD12	1:B:69:MET:HB2	1.84	0.60
1:E:477:ASP:HB2	1:H:178:TYR:CE1	2.36	0.60
1:C:464:ASN:ND2	1:I:422:GLN:HE22	1.91	0.59
1:K:28:LEU:HD11	1:K:447:LEU:HD11	1.84	0.59
1:F:28:LEU:HD11	1:F:447:LEU:HD11	1.84	0.59
1:I:58:ILE:HD12	1:I:69:MET:HB2	1.84	0.59
1:K:58:ILE:HD12	1:K:69:MET:HB2	1.84	0.59
1:H:28:LEU:HD11	1:H:447:LEU:HD11	1.84	0.58
1:A:59:ARG:NE	1:A:69:MET:HE2	2.17	0.58
1:F:58:ILE:HD12	1:F:69:MET:HB2	1.83	0.58
1:L:28:LEU:HD11	1:L:447:LEU:HD11	1.84	0.58
1:B:464:ASN:HD21	1:J:422:GLN:HE22	1.50	0.58
1:B:422:GLN:NE2	1:J:464:ASN:HD21	2.00	0.58
1:F:59:ARG:HE	1:F:69:MET:HE2	1.68	0.58
1:B:59:ARG:NE	1:B:69:MET:HE2	2.18	0.58
1:D:57:SER:HB3	1:E:187:PHE:HE2	1.69	0.58
1:E:58:ILE:HD12	1:E:69:MET:HB2	1.86	0.58
1:J:59:ARG:HE	1:J:69:MET:HE2	1.69	0.58
1:C:58:ILE:HD12	1:C:69:MET:HB2	1.86	0.57
1:E:328:LYS:HE3	1:G:464:ASN:O	2.03	0.57
1:A:28:LEU:HD11	1:A:447:LEU:HD11	1.87	0.57
1:J:58:ILE:HD12	1:J:69:MET:HB2	1.86	0.57
1:J:315:SER:HB2	1:J:430:LEU:HA	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:SER:HB3	1:E:187:PHE:CE2	2.39	0.57
1:H:99:PHE:HE1	1:I:355:ILE:HG21	1.70	0.57
1:H:59:ARG:NE	1:H:69:MET:HE2	2.20	0.57
1:I:59:ARG:NE	1:I:69:MET:HE2	2.20	0.57
1:G:59:ARG:HE	1:G:69:MET:HE2	1.68	0.56
1:K:57:SER:HB3	1:L:187:PHE:CE2	2.39	0.56
1:K:59:ARG:NE	1:K:69:MET:HE2	2.20	0.56
1:A:57:SER:HB3	1:B:187:PHE:CE2	2.40	0.56
1:C:59:ARG:HE	1:C:69:MET:HE2	1.70	0.56
1:G:58:ILE:HD12	1:G:69:MET:HB2	1.88	0.56
1:K:57:SER:HB3	1:L:187:PHE:HE2	1.70	0.56
1:D:20:TYR:CE1	1:E:203:LEU:HD13	2.41	0.56
1:L:59:ARG:NE	1:L:69:MET:HE2	2.21	0.56
1:B:315:SER:HB2	1:B:430:LEU:HA	1.88	0.56
1:A:464:ASN:HD21	1:K:422:GLN:NE2	1.99	0.56
1:C:57:SER:HB3	1:D:187:PHE:CE2	2.41	0.56
1:J:57:SER:HB3	1:K:187:PHE:HE2	1.70	0.56
1:A:57:SER:HB3	1:B:187:PHE:HE2	1.71	0.56
1:D:59:ARG:NE	1:D:69:MET:HE2	2.21	0.56
1:A:58:ILE:HD12	1:A:69:MET:HB2	1.88	0.55
1:C:315:SER:HB2	1:C:430:LEU:HA	1.88	0.55
1:A:464:ASN:O	1:K:328:LYS:HE3	2.07	0.55
1:C:28:LEU:HD11	1:C:447:LEU:HD11	1.88	0.55
1:D:464:ASN:HD21	1:H:422:GLN:NE2	2.01	0.55
1:G:59:ARG:NE	1:G:69:MET:HE2	2.22	0.55
1:B:28:LEU:HD11	1:B:447:LEU:HD11	1.88	0.54
1:F:323:THR:HB	1:L:475:TYR:CZ	2.42	0.54
1:D:62:GLN:HB3	1:E:335:GLU:OE1	2.08	0.54
1:C:464:ASN:O	1:I:328:LYS:HE3	2.08	0.54
1:K:315:SER:HB2	1:K:430:LEU:HA	1.89	0.54
1:E:59:ARG:NE	1:E:69:MET:HE2	2.21	0.54
1:E:28:LEU:HD11	1:E:447:LEU:HD11	1.89	0.54
1:J:53:PHE:HB3	1:J:58:ILE:HD11	1.89	0.54
1:F:59:ARG:NE	1:F:69:MET:HE2	2.23	0.53
1:F:53:PHE:HB3	1:F:58:ILE:HD11	1.90	0.53
1:F:315:SER:HB2	1:F:430:LEU:HA	1.91	0.53
1:H:56:SER:HB3	1:I:347:ARG:NH1	2.21	0.53
1:I:315:SER:HB2	1:I:430:LEU:HA	1.90	0.53
1:A:53:PHE:HB3	1:A:58:ILE:HD11	1.89	0.53
1:B:53:PHE:HB3	1:B:58:ILE:HD11	1.90	0.53
1:D:323:THR:HB	1:H:475:TYR:CZ	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:GLN:HB3	1:B:335:GLU:OE1	2.08	0.53
1:K:56:SER:HB3	1:L:347:ARG:HH11	1.73	0.53
1:H:315:SER:HB2	1:H:430:LEU:HA	1.90	0.53
1:L:72:LEU:HD12	1:L:96:HIS:CD2	2.43	0.53
1:G:28:LEU:HD11	1:G:447:LEU:HD11	1.90	0.53
1:F:72:LEU:HD12	1:F:96:HIS:CD2	2.44	0.52
1:C:213:LEU:HD13	1:C:217:HIS:HB3	1.91	0.52
1:K:130:PHE:CE1	1:K:279:GLN:HG2	2.44	0.52
1:D:464:ASN:O	1:H:328:LYS:HE3	2.10	0.52
1:J:56:SER:HB3	1:K:347:ARG:NH1	2.25	0.52
1:I:28:LEU:HD11	1:I:447:LEU:HD11	1.91	0.52
1:J:59:ARG:NE	1:J:69:MET:HE2	2.23	0.52
1:J:28:LEU:HD11	1:J:447:LEU:HD11	1.92	0.52
1:D:28:LEU:HD11	1:D:447:LEU:HD11	1.92	0.52
1:D:315:SER:HB2	1:D:430:LEU:HA	1.92	0.52
1:G:347:ARG:NH1	1:L:56:SER:HB3	2.21	0.52
1:A:187:PHE:CE2	1:F:57:SER:HB3	2.45	0.52
1:C:59:ARG:NE	1:C:69:MET:HE2	2.24	0.52
1:E:315:SER:HB2	1:E:430:LEU:HA	1.92	0.52
1:H:213:LEU:HD13	1:H:217:HIS:HB3	1.92	0.51
1:A:213:LEU:HD13	1:A:217:HIS:HB3	1.93	0.51
1:E:53:PHE:HB3	1:E:58:ILE:HD11	1.92	0.51
1:J:130:PHE:CE1	1:J:279:GLN:HG2	2.45	0.51
1:L:53:PHE:HB3	1:L:58:ILE:HD11	1.92	0.51
1:D:477:ASP:OD1	1:I:182:HIS:NE2	2.44	0.51
1:E:331:VAL:HG11	1:G:465:ILE:HG22	1.91	0.51
1:E:465:ILE:HG22	1:G:331:VAL:HG11	1.92	0.51
1:A:347:ARG:NH1	1:F:56:SER:HB3	2.22	0.51
1:G:53:PHE:HB3	1:G:58:ILE:HD11	1.93	0.51
1:A:315:SER:HB2	1:A:430:LEU:HA	1.93	0.51
1:E:265:LYS:HG2	1:E:328:LYS:HB3	1.93	0.51
1:A:335:GLU:CD	1:F:62:GLN:HB3	2.36	0.50
1:K:53:PHE:HB3	1:K:58:ILE:HD11	1.92	0.50
1:F:475:TYR:CZ	1:L:323:THR:HB	2.46	0.50
1:A:355:ILE:HG21	1:F:99:PHE:HE1	1.75	0.50
1:E:72:LEU:HD12	1:E:96:HIS:CD2	2.47	0.50
1:E:473:ALA:HA	1:G:144:PHE:CE1	2.46	0.50
1:H:53:PHE:HB3	1:H:58:ILE:HD11	1.93	0.50
1:B:213:LEU:HD13	1:B:217:HIS:HB3	1.94	0.50
1:D:213:LEU:HD13	1:D:217:HIS:HB3	1.93	0.50
1:J:99:PHE:HE1	1:K:355:ILE:HG21	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:72:LEU:HD12	1:G:96:HIS:CD2	2.47	0.50
1:A:237:HIS:ND1	4:A:2086:HOH:O	2.34	0.49
1:A:323:THR:HB	1:K:475:TYR:CZ	2.47	0.49
1:D:475:TYR:CZ	1:H:323:THR:HB	2.46	0.49
1:K:72:LEU:HD12	1:K:96:HIS:CD2	2.47	0.49
1:A:53:PHE:HD2	1:A:58:ILE:HG13	1.78	0.49
1:F:130:PHE:CE1	1:F:279:GLN:HG2	2.47	0.49
1:B:57:SER:HB3	1:C:187:PHE:CE2	2.47	0.49
1:C:235:LEU:HD23	1:C:235:LEU:C	2.37	0.49
1:D:328:LYS:HE3	1:H:464:ASN:O	2.13	0.49
1:H:130:PHE:CE1	1:H:279:GLN:HG2	2.47	0.49
1:C:53:PHE:HB3	1:C:58:ILE:HD11	1.94	0.49
1:D:53:PHE:HB3	1:D:58:ILE:HD11	1.95	0.49
1:E:130:PHE:CE1	1:E:279:GLN:HG2	2.48	0.49
1:B:130:PHE:CE1	1:B:279:GLN:HG2	2.47	0.49
1:A:328:LYS:HE3	1:K:464:ASN:O	2.13	0.49
1:H:57:SER:HB3	1:I:187:PHE:CE2	2.48	0.48
1:E:237:HIS:ND1	4:E:2085:HOH:O	2.35	0.48
1:I:72:LEU:HD12	1:I:96:HIS:CD2	2.48	0.48
1:H:265:LYS:HG2	1:H:328:LYS:HB3	1.96	0.48
1:A:56:SER:HB3	1:B:347:ARG:HH11	1.78	0.48
1:C:328:LYS:HE3	1:I:464:ASN:O	2.14	0.48
1:F:213:LEU:HD13	1:F:217:HIS:HB3	1.96	0.48
1:H:322:PRO:HG3	1:H:374:GLY:HA3	1.95	0.48
1:I:213:LEU:HD13	1:I:217:HIS:HB3	1.95	0.48
1:J:53:PHE:HD2	1:J:58:ILE:HG13	1.79	0.48
1:K:380:PHE:HA	1:K:383:MET:HE3	1.96	0.48
1:D:130:PHE:CE1	1:D:279:GLN:HG2	2.49	0.48
1:G:315:SER:HB2	1:G:430:LEU:HA	1.96	0.48
1:L:315:SER:HB2	1:L:430:LEU:HA	1.96	0.48
1:B:57:SER:HB3	1:C:187:PHE:HE2	1.79	0.47
1:A:422:GLN:NE2	1:K:464:ASN:HD21	2.10	0.47
1:B:72:LEU:HD12	1:B:96:HIS:CD2	2.49	0.47
1:C:72:LEU:HD12	1:C:96:HIS:CD2	2.50	0.47
1:J:300:ASP:OD1	1:J:303:ARG:NH2	2.47	0.47
1:J:369:SER:N	1:J:370:PRO:CD	2.77	0.47
1:L:53:PHE:HD2	1:L:58:ILE:HG13	1.80	0.47
1:H:72:LEU:HD12	1:H:96:HIS:CD2	2.49	0.47
1:I:369:SER:N	1:I:370:PRO:CD	2.77	0.47
1:E:235:LEU:HD23	1:E:235:LEU:C	2.40	0.47
1:I:53:PHE:HB3	1:I:58:ILE:HD11	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:380:PHE:HA	1:L:383:MET:HE3	1.97	0.47
1:B:472:PHE:CZ	1:J:153:TYR:CE1	3.03	0.47
1:D:72:LEU:HD12	1:D:96:HIS:CD2	2.50	0.47
1:H:104:TYR:CZ	1:H:106:ARG:HB2	2.50	0.47
1:K:213:LEU:HD13	1:K:217:HIS:HB3	1.97	0.47
1:J:72:LEU:HD12	1:J:96:HIS:CD2	2.49	0.47
1:C:369:SER:N	1:C:370:PRO:CD	2.78	0.46
1:K:322:PRO:HG3	1:K:374:GLY:HA3	1.97	0.46
1:G:130:PHE:CE1	1:G:279:GLN:HG2	2.51	0.46
1:K:369:SER:N	1:K:370:PRO:CD	2.78	0.46
1:J:104:TYR:CZ	1:J:106:ARG:HB2	2.50	0.46
1:H:53:PHE:HD2	1:H:58:ILE:HG13	1.80	0.46
1:H:62:GLN:HB3	1:I:335:GLU:CD	2.39	0.46
1:J:265:LYS:HG2	1:J:328:LYS:HB3	1.97	0.46
1:E:213:LEU:HD13	1:E:217:HIS:HB3	1.98	0.46
1:F:53:PHE:HD2	1:F:58:ILE:HG13	1.80	0.46
1:D:331:VAL:HA	1:D:332:PRO:HD3	1.85	0.46
1:F:322:PRO:HG3	1:F:374:GLY:HA3	1.98	0.46
1:A:133:GLU:O	1:A:275:MET:HA	2.16	0.46
1:B:323:THR:HB	1:J:475:TYR:CZ	2.51	0.46
1:C:53:PHE:HD2	1:C:58:ILE:HG13	1.81	0.46
1:D:56:SER:HB3	1:E:347:ARG:HH11	1.80	0.46
1:A:130:PHE:CE1	1:A:279:GLN:HG2	2.51	0.45
1:A:475:TYR:CZ	1:K:323:THR:HB	2.50	0.45
1:F:477:ASP:OD1	1:G:182:HIS:NE2	2.50	0.45
1:K:53:PHE:HD2	1:K:58:ILE:HG13	1.81	0.45
1:G:322:PRO:HG3	1:G:374:GLY:HA3	1.99	0.45
1:B:380:PHE:HA	1:B:383:MET:HE3	1.98	0.45
1:I:181:ARG:HE	1:I:181:ARG:HB2	1.58	0.45
1:L:213:LEU:HD13	1:L:217:HIS:HB3	1.98	0.45
1:I:53:PHE:HD2	1:I:58:ILE:HG13	1.81	0.45
1:I:265:LYS:HG2	1:I:328:LYS:HB3	1.99	0.45
1:D:53:PHE:HD2	1:D:58:ILE:HG13	1.81	0.45
1:D:369:SER:N	1:D:370:PRO:CD	2.79	0.45
1:F:380:PHE:HA	1:F:383:MET:HE3	1.98	0.45
1:I:23:VAL:O	1:I:34:HIS:HA	2.17	0.45
1:A:322:PRO:HG3	1:A:374:GLY:HA3	1.99	0.45
1:J:213:LEU:HD13	1:J:217:HIS:HB3	1.98	0.45
1:B:53:PHE:HD2	1:B:58:ILE:HG13	1.82	0.45
1:B:464:ASN:O	1:J:328:LYS:HE3	2.16	0.45
1:C:380:PHE:HA	1:C:383:MET:HE3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:213:LEU:HD13	1:G:217:HIS:HB3	1.98	0.45
1:E:369:SER:N	1:E:370:PRO:CD	2.80	0.45
1:J:380:PHE:HA	1:J:383:MET:HE3	1.97	0.45
1:L:322:PRO:HG3	1:L:374:GLY:HA3	1.99	0.45
1:E:331:VAL:HA	1:E:332:PRO:HD3	1.83	0.45
1:B:322:PRO:HG3	1:B:374:GLY:HA3	1.99	0.44
1:E:53:PHE:HD2	1:E:58:ILE:HG13	1.82	0.44
1:A:144:PHE:CE1	1:K:473:ALA:HA	2.52	0.44
1:C:181:ARG:HE	1:C:181:ARG:HB2	1.55	0.44
1:C:182:HIS:HE2	1:J:477:ASP:CG	2.25	0.44
1:C:20:TYR:CZ	1:D:203:LEU:HD13	2.51	0.44
1:G:53:PHE:HD2	1:G:58:ILE:HG13	1.81	0.44
1:B:265:LYS:HG2	1:B:328:LYS:HB3	1.99	0.44
1:E:300:ASP:OD1	1:E:303:ARG:NH2	2.51	0.44
1:G:181:ARG:HE	1:G:181:ARG:HB2	1.59	0.44
1:G:335:GLU:CD	1:L:62:GLN:HB3	2.41	0.44
1:B:104:TYR:CZ	1:B:106:ARG:HB2	2.53	0.44
1:E:322:PRO:HG3	1:E:374:GLY:HA3	1.99	0.44
1:G:235:LEU:C	1:G:235:LEU:HD23	2.43	0.44
1:A:72:LEU:HD12	1:A:96:HIS:CD2	2.51	0.44
1:B:328:LYS:HE3	1:J:464:ASN:O	2.18	0.44
1:D:300:ASP:OD1	1:D:303:ARG:NH2	2.50	0.44
1:C:322:PRO:HG3	1:C:374:GLY:HA3	1.99	0.44
1:D:235:LEU:C	1:D:235:LEU:HD23	2.43	0.44
1:F:275:MET:HE3	1:F:277:CYS:SG	2.57	0.44
1:L:130:PHE:CE1	1:L:279:GLN:HG2	2.52	0.44
1:A:331:VAL:HA	1:A:332:PRO:HD3	1.84	0.44
1:A:346:ASN:OD1	1:A:348:SER:HB3	2.18	0.44
1:H:346:ASN:OD1	1:H:348:SER:HB3	2.17	0.44
1:L:235:LEU:C	1:L:235:LEU:HD23	2.43	0.44
1:G:265:LYS:HG2	1:G:328:LYS:HB3	2.00	0.43
1:C:130:PHE:CE1	1:C:279:GLN:HG2	2.53	0.43
1:K:181:ARG:HE	1:K:181:ARG:HB2	1.58	0.43
1:E:477:ASP:HB2	1:H:178:TYR:CD1	2.53	0.43
1:I:380:PHE:HA	1:I:383:MET:HE3	2.00	0.43
1:A:104:TYR:CZ	1:A:106:ARG:HB2	2.53	0.43
1:E:336:ALA:HA	1:E:337:PRO:HD2	1.94	0.43
1:F:323:THR:HB	1:L:475:TYR:CE1	2.53	0.43
1:A:187:PHE:HE2	1:F:57:SER:HB3	1.83	0.43
1:C:346:ASN:OD1	1:C:348:SER:HB3	2.19	0.43
1:J:303:ARG:NH1	1:J:396:GLU:OE2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:346:ASN:OD1	1:G:348:SER:HB3	2.18	0.43
1:H:331:VAL:HA	1:H:332:PRO:HD3	1.86	0.43
1:I:322:PRO:HG3	1:I:374:GLY:HA3	1.99	0.43
1:I:331:VAL:HA	1:I:332:PRO:HD3	1.81	0.43
1:J:346:ASN:OD1	1:J:348:SER:HB3	2.18	0.43
1:L:292:GLU:H	1:L:292:GLU:HG3	1.65	0.43
1:E:380:PHE:HA	1:E:383:MET:HE3	2.00	0.42
1:E:478:VAL:O	1:G:250:LYS:NZ	2.47	0.42
1:B:346:ASN:OD1	1:B:348:SER:HB3	2.19	0.42
1:D:104:TYR:CZ	1:D:106:ARG:HB2	2.54	0.42
1:H:369:SER:N	1:H:370:PRO:CD	2.82	0.42
1:C:422:GLN:HE22	1:I:464:ASN:ND2	1.96	0.42
1:D:380:PHE:HA	1:D:383:MET:HE3	2.01	0.42
1:B:369:SER:N	1:B:370:PRO:CD	2.82	0.42
1:F:292:GLU:H	1:F:292:GLU:HG3	1.69	0.42
1:K:300:ASP:OD1	1:K:303:ARG:NH2	2.52	0.42
1:B:292:GLU:H	1:B:292:GLU:HG3	1.68	0.42
1:L:369:SER:N	1:L:370:PRO:CD	2.82	0.42
1:C:182:HIS:NE2	1:J:477:ASP:OD1	2.53	0.42
1:E:214:GLU:HB3	1:E:215:LYS:H	1.74	0.42
1:I:235:LEU:C	1:I:235:LEU:HD23	2.44	0.42
1:J:322:PRO:HG3	1:J:374:GLY:HA3	2.02	0.42
1:D:322:PRO:HG3	1:D:374:GLY:HA3	2.02	0.42
1:G:104:TYR:CZ	1:G:106:ARG:HB2	2.55	0.42
1:G:380:PHE:HA	1:G:383:MET:HE3	2.02	0.42
1:H:57:SER:HB3	1:I:187:PHE:HE2	1.83	0.42
1:K:265:LYS:HG2	1:K:328:LYS:HB3	2.02	0.42
1:L:74:ASP:HA	1:L:75:PRO:HD2	1.95	0.42
1:D:214:GLU:HB3	1:D:215:LYS:H	1.74	0.41
1:D:275:MET:HE3	1:D:277:CYS:SG	2.60	0.41
1:D:23:VAL:O	1:D:34:HIS:HA	2.20	0.41
1:D:28:LEU:HB3	1:D:29:PRO:HD3	2.02	0.41
1:H:181:ARG:HE	1:H:181:ARG:HB2	1.64	0.41
1:A:336:ALA:HA	1:A:337:PRO:HD2	1.96	0.41
1:C:23:VAL:O	1:C:34:HIS:HA	2.20	0.41
1:F:188:PRO:O	1:F:193:ASP:HB2	2.20	0.41
1:G:292:GLU:H	1:G:292:GLU:HG3	1.66	0.41
1:H:332:PRO:HG3	1:H:421:THR:HG21	2.02	0.41
1:C:104:TYR:CZ	1:C:106:ARG:HB2	2.56	0.41
1:C:303:ARG:NH1	1:C:396:GLU:OE2	2.53	0.41
1:G:336:ALA:HA	1:G:337:PRO:HD2	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:369:SER:N	1:G:370:PRO:CD	2.84	0.41
1:I:214:GLU:HB3	1:I:215:LYS:H	1.74	0.41
1:L:58:ILE:CD1	1:L:69:MET:HB2	2.48	0.41
1:F:346:ASN:OD1	1:F:348:SER:HB3	2.20	0.41
1:H:380:PHE:HA	1:H:383:MET:HE3	2.02	0.41
1:L:181:ARG:HE	1:L:181:ARG:HB2	1.60	0.41
1:A:265:LYS:HG2	1:A:328:LYS:HB3	2.02	0.41
1:I:292:GLU:H	1:I:292:GLU:HG3	1.68	0.41
1:K:20:TYR:CZ	1:L:203:LEU:HD13	2.54	0.41
1:B:56:SER:HB3	1:C:347:ARG:NH1	2.34	0.41
1:F:178:TYR:CE1	1:G:477:ASP:HB2	2.56	0.41
1:A:434:HIS:HB2	1:A:448:ILE:HD13	2.03	0.41
1:D:265:LYS:HG2	1:D:328:LYS:HB3	2.03	0.41
1:H:58:ILE:CD1	1:H:69:MET:HB2	2.49	0.41
1:B:331:VAL:HA	1:B:332:PRO:HD3	1.86	0.41
1:B:473:ALA:HA	1:J:144:PHE:CE1	2.56	0.41
1:F:78:ALA:HA	1:F:90:ASN:O	2.21	0.41
1:I:346:ASN:OD1	1:I:348:SER:HB3	2.20	0.41
1:J:214:GLU:HB3	1:J:215:LYS:H	1.72	0.41
1:J:369:SER:N	1:J:370:PRO:HD3	2.36	0.41
1:A:369:SER:N	1:A:370:PRO:CD	2.84	0.40
1:F:369:SER:N	1:F:370:PRO:CD	2.84	0.40
1:B:178:TYR:CE1	1:K:477:ASP:HB2	2.56	0.40
1:F:23:VAL:O	1:F:34:HIS:HA	2.22	0.40
1:F:434:HIS:HB2	1:F:448:ILE:HD13	2.03	0.40
1:G:23:VAL:O	1:G:34:HIS:HA	2.22	0.40
1:A:335:GLU:OE2	1:F:62:GLN:CB	2.70	0.40
1:D:133:GLU:O	1:D:275:MET:HA	2.21	0.40
1:F:300:ASP:OD1	1:F:303:ARG:NH2	2.54	0.40
1:A:214:GLU:HB3	1:A:215:LYS:H	1.70	0.40
1:E:20:TYR:CZ	1:F:203:LEU:HD13	2.57	0.40
1:F:235:LEU:HD23	1:F:235:LEU:C	2.46	0.40
1:G:74:ASP:HA	1:G:75:PRO:HD2	1.98	0.40
1:A:118:TYR:O	1:A:122:THR:HG23	2.22	0.40
1:C:300:ASP:OD1	1:C:303:ARG:NH2	2.54	0.40
1:J:434:HIS:HB2	1:J:448:ILE:HD13	2.03	0.40
1:K:104:TYR:CZ	1:K:106:ARG:HB2	2.56	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	457/486 (94%)	442 (97%)	14 (3%)	1 (0%)	43	56
1	B	457/486 (94%)	439 (96%)	17 (4%)	1 (0%)	43	56
1	C	457/486 (94%)	439 (96%)	17 (4%)	1 (0%)	43	56
1	D	457/486 (94%)	440 (96%)	16 (4%)	1 (0%)	43	56
1	E	457/486 (94%)	440 (96%)	16 (4%)	1 (0%)	43	56
1	F	457/486 (94%)	440 (96%)	16 (4%)	1 (0%)	43	56
1	G	457/486 (94%)	439 (96%)	17 (4%)	1 (0%)	43	56
1	H	457/486 (94%)	441 (96%)	15 (3%)	1 (0%)	43	56
1	I	457/486 (94%)	439 (96%)	17 (4%)	1 (0%)	43	56
1	J	457/486 (94%)	439 (96%)	17 (4%)	1 (0%)	43	56
1	K	457/486 (94%)	441 (96%)	15 (3%)	1 (0%)	43	56
1	L	457/486 (94%)	440 (96%)	16 (4%)	1 (0%)	43	56
All	All	5484/5832 (94%)	5279 (96%)	193 (4%)	12 (0%)	43	56

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	332	PRO
1	B	332	PRO
1	C	332	PRO
1	D	332	PRO
1	E	332	PRO
1	F	332	PRO
1	G	332	PRO
1	H	332	PRO
1	I	332	PRO
1	J	332	PRO
1	K	332	PRO
1	L	332	PRO

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	390/411 (95%)	376 (96%)	14 (4%)	31	46
1	B	390/411 (95%)	375 (96%)	15 (4%)	29	44
1	C	390/411 (95%)	376 (96%)	14 (4%)	31	46
1	D	390/411 (95%)	375 (96%)	15 (4%)	29	44
1	E	390/411 (95%)	375 (96%)	15 (4%)	29	44
1	F	390/411 (95%)	376 (96%)	14 (4%)	31	46
1	G	390/411 (95%)	375 (96%)	15 (4%)	29	44
1	H	390/411 (95%)	376 (96%)	14 (4%)	31	46
1	I	390/411 (95%)	376 (96%)	14 (4%)	31	46
1	J	390/411 (95%)	375 (96%)	15 (4%)	29	44
1	K	390/411 (95%)	376 (96%)	14 (4%)	31	46
1	L	390/411 (95%)	375 (96%)	15 (4%)	29	44
All	All	4680/4932 (95%)	4506 (96%)	174 (4%)	30	45

All (174) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ASP
1	A	68	ASP
1	A	180	VAL
1	A	203	LEU
1	A	209	SER
1	A	213	LEU
1	A	220	VAL
1	A	331	VAL
1	A	335	GLU
1	A	426	VAL
1	A	429	ARG
1	A	446	ASP
1	A	453	SER
1	A	464	ASN

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Mol	Chain	Res	Type
1	B	49	ASP
1	B	68	ASP
1	B	180	VAL
1	B	203	LEU
1	B	209	SER
1	B	213	LEU
1	B	220	VAL
1	B	331	VAL
1	B	335	GLU
1	B	365	LEU
1	B	426	VAL
1	B	429	ARG
1	B	446	ASP
1	B	453	SER
1	B	464	ASN
1	C	49	ASP
1	C	68	ASP
1	C	180	VAL
1	C	203	LEU
1	C	209	SER
1	C	213	LEU
1	C	220	VAL
1	C	331	VAL
1	C	335	GLU
1	C	426	VAL
1	C	429	ARG
1	C	446	ASP
1	C	453	SER
1	C	464	ASN
1	D	49	ASP
1	D	68	ASP
1	D	180	VAL
1	D	203	LEU
1	D	209	SER
1	D	213	LEU
1	D	220	VAL
1	D	331	VAL
1	D	335	GLU
1	D	365	LEU
1	D	426	VAL
1	D	429	ARG
1	D	446	ASP

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Mol	Chain	Res	Type
1	D	453	SER
1	D	464	ASN
1	E	49	ASP
1	E	68	ASP
1	E	154	GLU
1	E	180	VAL
1	E	203	LEU
1	E	209	SER
1	E	213	LEU
1	E	220	VAL
1	E	331	VAL
1	E	335	GLU
1	E	426	VAL
1	E	429	ARG
1	E	446	ASP
1	E	453	SER
1	E	464	ASN
1	F	49	ASP
1	F	68	ASP
1	F	180	VAL
1	F	203	LEU
1	F	209	SER
1	F	213	LEU
1	F	220	VAL
1	F	331	VAL
1	F	335	GLU
1	F	426	VAL
1	F	429	ARG
1	F	446	ASP
1	F	453	SER
1	F	464	ASN
1	G	49	ASP
1	G	68	ASP
1	G	180	VAL
1	G	203	LEU
1	G	209	SER
1	G	213	LEU
1	G	220	VAL
1	G	331	VAL
1	G	335	GLU
1	G	365	LEU
1	G	426	VAL

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Mol	Chain	Res	Type
1	G	429	ARG
1	G	446	ASP
1	G	453	SER
1	G	464	ASN
1	H	49	ASP
1	H	68	ASP
1	H	180	VAL
1	H	203	LEU
1	H	209	SER
1	H	213	LEU
1	H	220	VAL
1	H	331	VAL
1	H	335	GLU
1	H	426	VAL
1	H	429	ARG
1	H	446	ASP
1	H	453	SER
1	H	464	ASN
1	I	49	ASP
1	I	68	ASP
1	I	180	VAL
1	I	203	LEU
1	I	209	SER
1	I	213	LEU
1	I	220	VAL
1	I	331	VAL
1	I	335	GLU
1	I	426	VAL
1	I	429	ARG
1	I	446	ASP
1	I	453	SER
1	I	464	ASN
1	J	49	ASP
1	J	68	ASP
1	J	180	VAL
1	J	203	LEU
1	J	209	SER
1	J	213	LEU
1	J	220	VAL
1	J	331	VAL
1	J	335	GLU
1	J	365	LEU

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Mol	Chain	Res	Type
1	J	426	VAL
1	J	429	ARG
1	J	446	ASP
1	J	453	SER
1	J	464	ASN
1	K	49	ASP
1	K	68	ASP
1	K	180	VAL
1	K	203	LEU
1	K	209	SER
1	K	213	LEU
1	K	220	VAL
1	K	331	VAL
1	K	335	GLU
1	K	426	VAL
1	K	429	ARG
1	K	446	ASP
1	K	453	SER
1	K	464	ASN
1	L	49	ASP
1	L	68	ASP
1	L	180	VAL
1	L	203	LEU
1	L	209	SER
1	L	213	LEU
1	L	220	VAL
1	L	331	VAL
1	L	335	GLU
1	L	365	LEU
1	L	426	VAL
1	L	429	ARG
1	L	446	ASP
1	L	453	SER
1	L	464	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	398	GLN
1	A	445	ASN
1	A	458	ASN
1	A	464	ASN

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Mol	Chain	Res	Type
1	B	398	GLN
1	B	445	ASN
1	B	458	ASN
1	B	464	ASN
1	C	251	ASN
1	C	398	GLN
1	C	418	GLN
1	C	445	ASN
1	C	458	ASN
1	C	464	ASN
1	D	251	ASN
1	D	398	GLN
1	D	445	ASN
1	D	458	ASN
1	D	464	ASN
1	E	398	GLN
1	E	422	GLN
1	E	445	ASN
1	E	458	ASN
1	E	464	ASN
1	F	398	GLN
1	F	418	GLN
1	F	445	ASN
1	F	458	ASN
1	F	464	ASN
1	G	398	GLN
1	G	422	GLN
1	G	445	ASN
1	G	458	ASN
1	H	251	ASN
1	H	398	GLN
1	H	418	GLN
1	H	445	ASN
1	H	458	ASN
1	H	464	ASN
1	I	251	ASN
1	I	398	GLN
1	I	445	ASN
1	I	458	ASN
1	I	464	ASN
1	J	398	GLN
1	J	418	GLN

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Mol	Chain	Res	Type
1	J	445	ASN
1	J	458	ASN
1	J	464	ASN
1	K	398	GLN
1	K	418	GLN
1	K	445	ASN
1	K	458	ASN
1	K	464	ASN
1	L	398	GLN
1	L	445	ASN
1	L	458	ASN
1	L	464	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 12 are monoatomic - leaving 12 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	1AZ	B	501	-	31,31,31	1.49	6 (19%)	45,46,46	2.43	16 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	1AZ	E	501	-	31,31,31	1.51	5 (16%)	45,46,46	2.50	17 (37%)
2	1AZ	L	501	-	31,31,31	1.48	5 (16%)	45,46,46	2.29	14 (31%)
2	1AZ	H	501	-	31,31,31	1.43	4 (12%)	45,46,46	2.47	17 (37%)
2	1AZ	C	501	-	31,31,31	1.55	7 (22%)	45,46,46	2.34	15 (33%)
2	1AZ	F	501	-	31,31,31	1.44	6 (19%)	45,46,46	2.42	16 (35%)
2	1AZ	J	501	-	31,31,31	1.70	7 (22%)	45,46,46	2.32	15 (33%)
2	1AZ	K	501	-	31,31,31	1.55	8 (25%)	45,46,46	2.36	17 (37%)
2	1AZ	I	501	-	31,31,31	1.54	7 (22%)	45,46,46	2.36	15 (33%)
2	1AZ	G	501	-	31,31,31	1.52	8 (25%)	45,46,46	2.42	14 (31%)
2	1AZ	A	501	-	31,31,31	1.50	6 (19%)	45,46,46	2.41	13 (28%)
2	1AZ	D	501	-	31,31,31	1.53	5 (16%)	45,46,46	2.41	14 (31%)

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	1AZ	B	501	-	-	0/8/16/16	0/4/4/4
2	1AZ	E	501	-	-	0/8/16/16	0/4/4/4
2	1AZ	L	501	-	-	0/8/16/16	0/4/4/4
2	1AZ	H	501	-	-	0/8/16/16	0/4/4/4
2	1AZ	C	501	-	-	0/8/16/16	0/4/4/4
2	1AZ	F	501	-	-	0/8/16/16	0/4/4/4
2	1AZ	J	501	-	-	0/8/16/16	0/4/4/4
2	1AZ	K	501	-	-	0/8/16/16	0/4/4/4
2	1AZ	I	501	-	-	0/8/16/16	0/4/4/4
2	1AZ	G	501	-	-	0/8/16/16	0/4/4/4
2	1AZ	A	501	-	-	0/8/16/16	0/4/4/4
2	1AZ	D	501	-	-	0/8/16/16	0/4/4/4

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	1AZ	C8-N3	4.53	1.50	1.37
2	E	501	1AZ	C8-N3	4.34	1.50	1.37
2	I	501	1AZ	C8-N3	4.28	1.49	1.37
2	K	501	1AZ	C8-N3	4.13	1.49	1.37
2	F	501	1AZ	C8-N3	4.10	1.49	1.37
2	G	501	1AZ	C8-N3	4.05	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	1AZ	C8-N3	4.03	1.49	1.37
2	J	501	1AZ	C8-N3	4.02	1.49	1.37
2	D	501	1AZ	C8-N3	4.01	1.49	1.37
2	H	501	1AZ	C8-N3	3.96	1.49	1.37
2	L	501	1AZ	C8-N3	3.91	1.48	1.37
2	A	501	1AZ	C8-N3	3.86	1.48	1.37
2	J	501	1AZ	C18-CL2	3.60	1.82	1.73
2	J	501	1AZ	C5-N1	-3.24	1.34	1.40
2	F	501	1AZ	C5-N1	-3.18	1.34	1.40
2	L	501	1AZ	C18-CL2	3.06	1.80	1.73
2	B	501	1AZ	C5-N1	-3.02	1.35	1.40
2	A	501	1AZ	C1-CL1	3.01	1.80	1.73
2	H	501	1AZ	C18-CL2	2.87	1.80	1.73
2	D	501	1AZ	C1-CL1	2.86	1.80	1.73
2	L	501	1AZ	C5-N1	-2.86	1.35	1.40
2	G	501	1AZ	C5-N1	-2.83	1.35	1.40
2	I	501	1AZ	C18-CL2	2.79	1.80	1.73
2	K	501	1AZ	C5-N1	-2.78	1.35	1.40
2	D	501	1AZ	C5-N1	-2.78	1.35	1.40
2	H	501	1AZ	C5-N1	-2.73	1.35	1.40
2	I	501	1AZ	C5-N1	-2.72	1.35	1.40
2	A	501	1AZ	C5-N1	-2.68	1.35	1.40
2	J	501	1AZ	C1-CL1	2.68	1.80	1.73
2	K	501	1AZ	C1-CL1	2.66	1.79	1.73
2	E	501	1AZ	C5-N1	-2.63	1.35	1.40
2	B	501	1AZ	C15-N1	2.61	1.43	1.38
2	G	501	1AZ	C1-CL1	2.60	1.79	1.73
2	G	501	1AZ	C15-N1	2.53	1.43	1.38
2	D	501	1AZ	C18-CL2	2.53	1.79	1.73
2	J	501	1AZ	C15-N1	2.52	1.43	1.38
2	C	501	1AZ	C1-CL1	2.49	1.79	1.73
2	E	501	1AZ	C6-N2	-2.49	1.35	1.39
2	H	501	1AZ	C1-CL1	2.45	1.79	1.73
2	D	501	1AZ	C15-N1	2.45	1.43	1.38
2	J	501	1AZ	O3-C15	2.43	1.27	1.22
2	K	501	1AZ	O3-C15	2.39	1.27	1.22
2	C	501	1AZ	C5-N1	-2.36	1.36	1.40
2	B	501	1AZ	C1-CL1	2.36	1.79	1.73
2	C	501	1AZ	C15-N1	2.35	1.42	1.38
2	A	501	1AZ	C15-N5	-2.35	1.34	1.39
2	I	501	1AZ	C15-N1	2.35	1.42	1.38
2	E	501	1AZ	C1-CL1	2.32	1.79	1.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	501	1AZ	C15-N5	-2.30	1.34	1.39
2	A	501	1AZ	C15-N1	2.29	1.42	1.38
2	F	501	1AZ	C18-CL2	2.28	1.79	1.73
2	K	501	1AZ	C15-N1	2.24	1.42	1.38
2	K	501	1AZ	C6-N2	-2.20	1.35	1.39
2	F	501	1AZ	C1-CL1	2.18	1.78	1.73
2	E	501	1AZ	C15-N1	2.17	1.42	1.38
2	A	501	1AZ	C18-CL2	2.16	1.78	1.73
2	I	501	1AZ	C6-N2	-2.15	1.35	1.39
2	J	501	1AZ	C13-N5	-2.14	1.34	1.38
2	K	501	1AZ	C13-N5	-2.14	1.34	1.38
2	B	501	1AZ	O3-C15	2.13	1.26	1.22
2	G	501	1AZ	C15-N5	-2.13	1.34	1.39
2	G	501	1AZ	C18-CL2	2.12	1.78	1.73
2	F	501	1AZ	C6-N2	-2.12	1.35	1.39
2	I	501	1AZ	C15-N5	-2.09	1.34	1.39
2	I	501	1AZ	C1-CL1	2.06	1.78	1.73
2	C	501	1AZ	C18-CL2	2.05	1.78	1.73
2	G	501	1AZ	C6-N2	-2.04	1.36	1.39
2	C	501	1AZ	O3-C15	2.04	1.26	1.22
2	B	501	1AZ	C18-CL2	2.03	1.78	1.73
2	G	501	1AZ	C7-N2	2.03	1.50	1.47
2	F	501	1AZ	C15-N1	2.01	1.42	1.38
2	K	501	1AZ	C7-N2	2.01	1.50	1.47
2	C	501	1AZ	C8-N4	2.01	1.36	1.33
2	L	501	1AZ	C6-N2	-2.00	1.36	1.39

All (183) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	1AZ	C8-N4-C13	6.20	109.29	102.71
2	E	501	1AZ	C8-N4-C13	6.20	109.29	102.71
2	A	501	1AZ	C8-N4-C13	6.19	109.28	102.71
2	B	501	1AZ	C8-N4-C13	6.05	109.13	102.71
2	H	501	1AZ	C8-N4-C13	5.98	109.06	102.71
2	K	501	1AZ	C8-N4-C13	5.91	108.98	102.71
2	F	501	1AZ	C8-N4-C13	5.89	108.96	102.71
2	J	501	1AZ	C8-N4-C13	5.89	108.96	102.71
2	G	501	1AZ	C8-N4-C13	5.85	108.91	102.71
2	C	501	1AZ	C8-N4-C13	5.75	108.81	102.71
2	H	501	1AZ	N3-C8-N2	5.62	127.20	121.42
2	I	501	1AZ	C8-N4-C13	5.48	108.52	102.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	501	1AZ	C8-N4-C13	5.46	108.50	102.71
2	D	501	1AZ	C6-C13-N4	-5.44	106.11	112.77
2	G	501	1AZ	N3-C8-N2	5.34	126.91	121.42
2	A	501	1AZ	C6-C13-N4	-5.31	106.27	112.77
2	E	501	1AZ	C6-C13-N4	-5.19	106.41	112.77
2	F	501	1AZ	N3-C8-N2	5.12	126.68	121.42
2	B	501	1AZ	C1-C2-C3	-5.12	117.15	120.46
2	A	501	1AZ	N3-C8-N2	5.08	126.65	121.42
2	J	501	1AZ	C6-C13-N4	-5.05	106.58	112.77
2	E	501	1AZ	N2-C8-N4	-5.03	108.37	114.64
2	H	501	1AZ	C6-C13-N4	-5.00	106.64	112.77
2	B	501	1AZ	C6-C13-N4	-4.96	106.70	112.77
2	K	501	1AZ	C6-C13-N4	-4.95	106.70	112.77
2	C	501	1AZ	C6-C13-N4	-4.93	106.73	112.77
2	I	501	1AZ	N3-C8-N2	4.89	126.45	121.42
2	C	501	1AZ	N3-C8-N2	4.89	126.44	121.42
2	G	501	1AZ	C6-C13-N4	-4.88	106.79	112.77
2	E	501	1AZ	N3-C8-N2	4.86	126.41	121.42
2	D	501	1AZ	N3-C8-N2	4.83	126.39	121.42
2	I	501	1AZ	C6-C13-N4	-4.80	106.88	112.77
2	F	501	1AZ	N2-C8-N4	-4.79	108.66	114.64
2	L	501	1AZ	C6-C13-N4	-4.79	106.90	112.77
2	G	501	1AZ	C5-N1-C15	-4.75	119.77	125.62
2	A	501	1AZ	N2-C8-N4	-4.75	108.72	114.64
2	K	501	1AZ	N2-C8-N4	-4.75	108.72	114.64
2	F	501	1AZ	C6-C13-N4	-4.74	106.96	112.77
2	F	501	1AZ	C5-N1-C15	-4.74	119.79	125.62
2	H	501	1AZ	N2-C8-N4	-4.72	108.76	114.64
2	D	501	1AZ	N2-C8-N4	-4.66	108.83	114.64
2	L	501	1AZ	C1-C2-C3	-4.63	117.46	120.46
2	G	501	1AZ	N2-C8-N4	-4.62	108.88	114.64
2	H	501	1AZ	C5-N1-C15	-4.61	119.94	125.62
2	B	501	1AZ	N3-C8-N2	4.61	126.16	121.42
2	E	501	1AZ	C5-N1-C15	-4.61	119.95	125.62
2	K	501	1AZ	C5-N1-C15	-4.59	119.97	125.62
2	E	501	1AZ	C1-C2-C3	-4.55	117.51	120.46
2	C	501	1AZ	N2-C8-N4	-4.55	108.96	114.64
2	B	501	1AZ	N2-C8-N4	-4.55	108.96	114.64
2	A	501	1AZ	C5-N1-C15	-4.54	120.03	125.62
2	K	501	1AZ	N3-C8-N2	4.49	126.04	121.42
2	I	501	1AZ	C5-N1-C15	-4.47	120.12	125.62
2	J	501	1AZ	N2-C8-N4	-4.45	109.10	114.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	501	1AZ	N3-C8-N2	4.44	125.99	121.42
2	I	501	1AZ	N2-C8-N4	-4.42	109.13	114.64
2	B	501	1AZ	C5-N1-C15	-4.40	120.21	125.62
2	L	501	1AZ	N2-C8-N4	-4.32	109.25	114.64
2	C	501	1AZ	C5-N1-C15	-4.30	120.33	125.62
2	D	501	1AZ	C5-N1-C15	-4.23	120.41	125.62
2	L	501	1AZ	N3-C8-N2	4.17	125.70	121.42
2	F	501	1AZ	N5-C13-N4	4.16	132.38	125.59
2	H	501	1AZ	N5-C13-N4	4.16	132.38	125.59
2	D	501	1AZ	N5-C13-N4	4.11	132.30	125.59
2	H	501	1AZ	C6-C5-N1	4.10	119.95	112.23
2	A	501	1AZ	N5-C13-N4	4.09	132.27	125.59
2	E	501	1AZ	N5-C13-N4	4.08	132.25	125.59
2	J	501	1AZ	C5-N1-C15	-4.05	120.63	125.62
2	G	501	1AZ	N5-C13-N4	4.00	132.13	125.59
2	F	501	1AZ	C6-C5-N1	3.96	119.69	112.23
2	B	501	1AZ	N5-C13-N4	3.95	132.04	125.59
2	G	501	1AZ	C6-C5-N1	3.95	119.66	112.23
2	J	501	1AZ	N5-C13-N4	3.94	132.03	125.59
2	L	501	1AZ	N5-C13-N4	3.93	132.01	125.59
2	K	501	1AZ	C1-C2-C3	-3.91	117.93	120.46
2	K	501	1AZ	N5-C13-N4	3.91	131.98	125.59
2	I	501	1AZ	N5-C13-N4	3.88	131.93	125.59
2	C	501	1AZ	N5-C13-N4	3.83	131.84	125.59
2	I	501	1AZ	C1-C2-C3	-3.79	118.01	120.46
2	E	501	1AZ	C6-C5-N1	3.78	119.35	112.23
2	B	501	1AZ	C6-C5-N1	3.76	119.31	112.23
2	G	501	1AZ	C1-C2-C3	-3.71	118.06	120.46
2	I	501	1AZ	C6-C5-N1	3.69	119.17	112.23
2	L	501	1AZ	C5-N1-C15	-3.69	121.08	125.62
2	K	501	1AZ	C6-C5-N1	3.69	119.16	112.23
2	J	501	1AZ	C10-C9-N3	-3.64	102.15	109.82
2	A	501	1AZ	C6-C5-N1	3.62	119.05	112.23
2	C	501	1AZ	C1-C2-C3	-3.61	118.12	120.46
2	F	501	1AZ	C1-C2-C3	-3.59	118.14	120.46
2	D	501	1AZ	C6-C5-N1	3.55	118.91	112.23
2	L	501	1AZ	C10-C9-N3	-3.55	102.34	109.82
2	H	501	1AZ	C5-C6-C13	-3.53	118.48	122.92
2	C	501	1AZ	C6-C5-N1	3.52	118.85	112.23
2	J	501	1AZ	C6-C5-N1	3.50	118.82	112.23
2	J	501	1AZ	C1-C2-C3	-3.43	118.24	120.46
2	H	501	1AZ	C10-C9-N3	-3.42	102.61	109.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	1AZ	C10-C9-N3	-3.42	102.62	109.82
2	D	501	1AZ	C10-C9-N3	-3.41	102.63	109.82
2	H	501	1AZ	C1-C2-C3	-3.37	118.28	120.46
2	A	501	1AZ	C10-C9-N3	-3.35	102.76	109.82
2	D	501	1AZ	C1-C2-C3	-3.30	118.33	120.46
2	L	501	1AZ	C6-C5-N1	3.29	118.43	112.23
2	A	501	1AZ	N1-C15-N5	3.29	120.77	116.72
2	B	501	1AZ	C5-C6-C13	-3.24	118.84	122.92
2	A	501	1AZ	C5-C6-C13	-3.22	118.87	122.92
2	F	501	1AZ	N1-C15-N5	3.22	120.68	116.72
2	G	501	1AZ	C10-C9-N3	-3.21	103.05	109.82
2	G	501	1AZ	C5-C6-C13	-3.21	118.88	122.92
2	F	501	1AZ	C5-C6-C13	-3.20	118.89	122.92
2	C	501	1AZ	N1-C15-N5	3.20	120.66	116.72
2	F	501	1AZ	C10-C9-N3	-3.18	103.12	109.82
2	B	501	1AZ	C10-C9-N3	-3.16	103.16	109.82
2	E	501	1AZ	C5-C6-C13	-3.15	118.96	122.92
2	J	501	1AZ	C5-C6-C13	-3.14	118.96	122.92
2	I	501	1AZ	C5-C6-C13	-3.13	118.97	122.92
2	C	501	1AZ	C5-C6-C13	-3.13	118.98	122.92
2	D	501	1AZ	C5-C6-C13	-3.13	118.98	122.92
2	D	501	1AZ	N1-C15-N5	3.07	120.50	116.72
2	I	501	1AZ	C10-C9-N3	-3.06	103.38	109.82
2	H	501	1AZ	O1-C5-C6	-3.04	120.16	126.38
2	H	501	1AZ	N1-C15-N5	3.04	120.47	116.72
2	K	501	1AZ	C5-C6-C13	-3.03	119.11	122.92
2	E	501	1AZ	O1-C5-C6	-3.03	120.18	126.38
2	I	501	1AZ	N1-C15-N5	3.01	120.42	116.72
2	L	501	1AZ	C5-C6-C13	-3.00	119.14	122.92
2	D	501	1AZ	O1-C5-C6	-2.97	120.31	126.38
2	K	501	1AZ	C10-C9-N3	-2.93	103.66	109.82
2	G	501	1AZ	O1-C5-C6	-2.92	120.39	126.38
2	A	501	1AZ	C1-C2-C3	-2.91	118.58	120.46
2	E	501	1AZ	N1-C15-N5	2.87	120.26	116.72
2	I	501	1AZ	O1-C5-C6	-2.85	120.55	126.38
2	K	501	1AZ	N1-C15-N5	2.84	120.22	116.72
2	E	501	1AZ	C10-C9-N3	-2.83	103.86	109.82
2	J	501	1AZ	N1-C15-N5	2.81	120.18	116.72
2	L	501	1AZ	N1-C15-N5	2.81	120.18	116.72
2	A	501	1AZ	O1-C5-C6	-2.78	120.68	126.38
2	G	501	1AZ	N1-C15-N5	2.68	120.02	116.72
2	B	501	1AZ	N1-C15-N5	2.67	120.01	116.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	501	1AZ	C4-N1-C5	2.67	121.48	117.72
2	C	501	1AZ	O1-C5-C6	-2.66	120.94	126.38
2	H	501	1AZ	C11-C12-N3	-2.60	104.35	109.82
2	L	501	1AZ	O1-C5-C6	-2.59	121.07	126.38
2	F	501	1AZ	O1-C5-C6	-2.44	121.39	126.38
2	J	501	1AZ	C12-N3-C8	-2.41	110.32	119.07
2	K	501	1AZ	O1-C5-C6	-2.38	121.51	126.38
2	B	501	1AZ	O1-C5-C6	-2.37	121.53	126.38
2	L	501	1AZ	C11-C12-N3	-2.36	104.84	109.82
2	K	501	1AZ	C11-C12-N3	-2.34	104.89	109.82
2	J	501	1AZ	C11-C12-N3	-2.34	104.90	109.82
2	E	501	1AZ	C12-N3-C8	-2.32	110.67	119.07
2	L	501	1AZ	C12-N3-C8	-2.32	110.67	119.07
2	E	501	1AZ	C13-C6-N2	2.31	108.12	105.37
2	I	501	1AZ	C11-C12-N3	-2.30	104.97	109.82
2	B	501	1AZ	C12-N3-C8	-2.29	110.76	119.07
2	D	501	1AZ	C12-N3-C8	-2.28	110.81	119.07
2	G	501	1AZ	C4-N1-C15	2.26	120.08	116.92
2	H	501	1AZ	O3-C15-N1	-2.26	118.94	121.98
2	K	501	1AZ	O3-C15-N1	-2.26	118.94	121.98
2	F	501	1AZ	C5-C6-N2	2.25	133.89	131.26
2	C	501	1AZ	C13-C6-N2	2.25	108.04	105.37
2	C	501	1AZ	C16-C3-C2	2.22	121.62	118.55
2	J	501	1AZ	O1-C5-C6	-2.22	121.83	126.38
2	F	501	1AZ	C11-C12-N3	-2.21	105.16	109.82
2	J	501	1AZ	C4-N1-C15	2.21	120.00	116.92
2	K	501	1AZ	C12-N3-C8	-2.20	111.08	119.07
2	D	501	1AZ	C13-C6-N2	2.19	107.98	105.37
2	I	501	1AZ	C12-N3-C8	-2.18	111.16	119.07
2	F	501	1AZ	C12-N3-C8	-2.17	111.20	119.07
2	F	501	1AZ	C4-N1-C15	2.17	119.95	116.92
2	H	501	1AZ	C13-C6-N2	2.15	107.93	105.37
2	H	501	1AZ	C12-N3-C8	-2.12	111.37	119.07
2	B	501	1AZ	C4-N1-C15	2.11	119.87	116.92
2	B	501	1AZ	C16-C3-C2	2.11	121.45	118.55
2	A	501	1AZ	C12-N3-C8	-2.11	111.43	119.07
2	E	501	1AZ	C16-C17-C18	-2.08	117.11	119.98
2	E	501	1AZ	C4-N1-C15	2.07	119.82	116.92
2	K	501	1AZ	C16-C3-C2	2.07	121.40	118.55
2	E	501	1AZ	C1-C18-CL2	-2.07	116.00	120.84
2	I	501	1AZ	C13-C6-N2	2.07	107.83	105.37
2	B	501	1AZ	C11-C12-N3	-2.06	105.48	109.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	501	1AZ	C4-N1-C5	2.05	120.61	117.72
2	G	501	1AZ	C12-N3-C8	-2.02	111.76	119.07
2	C	501	1AZ	C12-N3-C8	-2.02	111.76	119.07

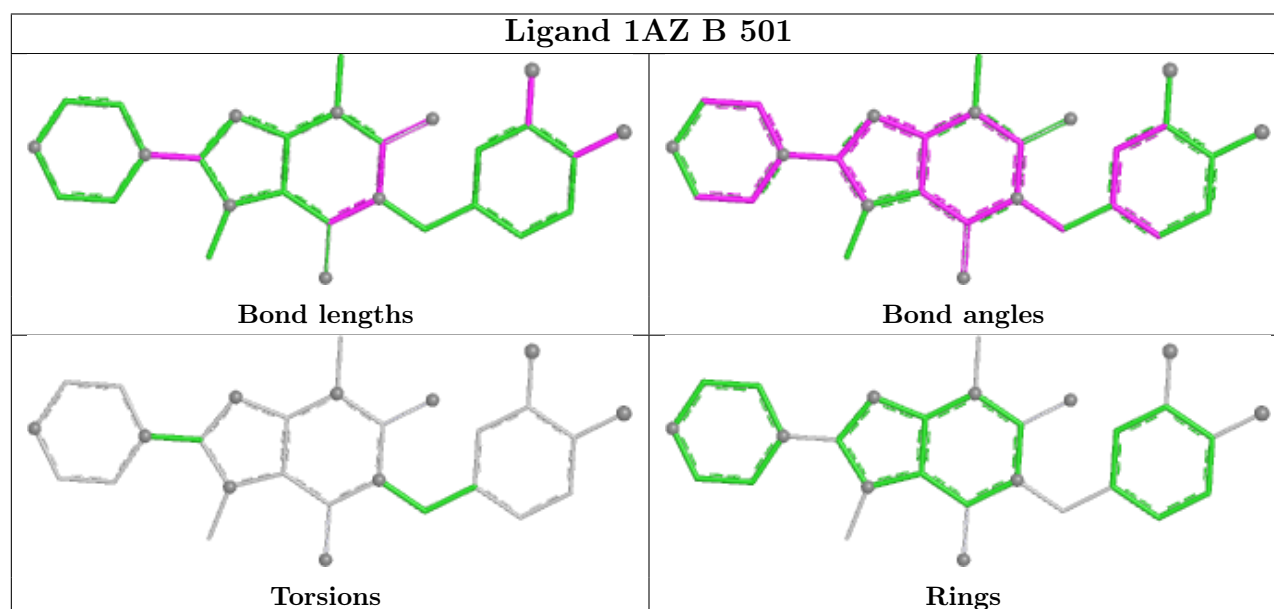
There are no chirality outliers.

There are no torsion outliers.

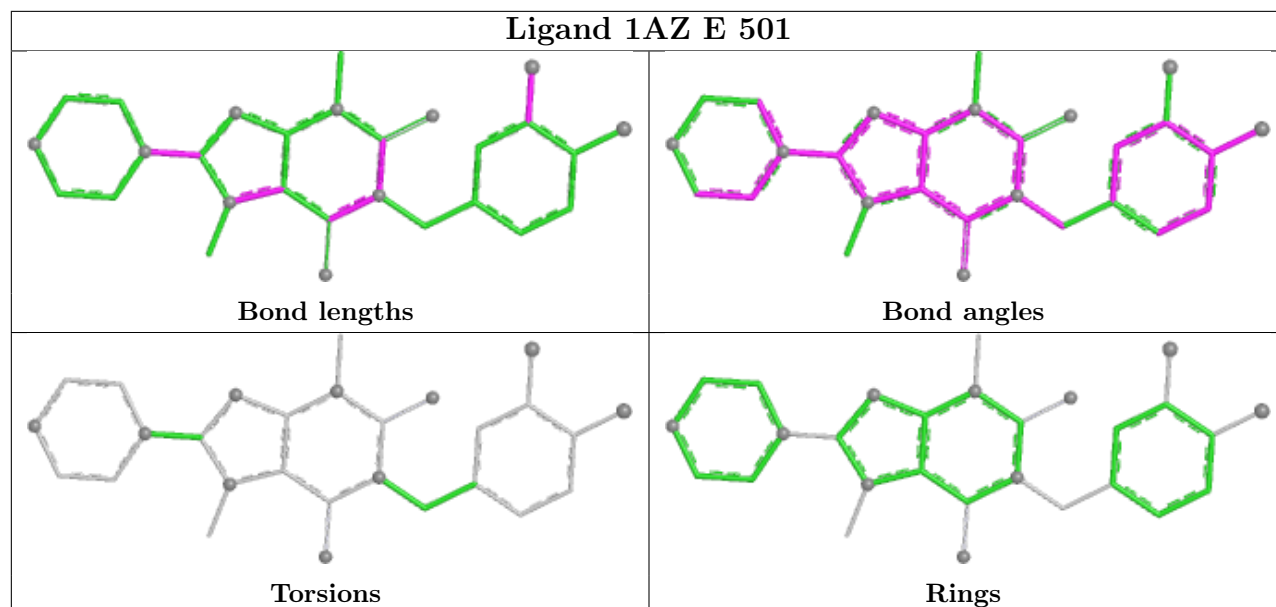
There are no ring outliers.

No monomer is involved in short contacts.

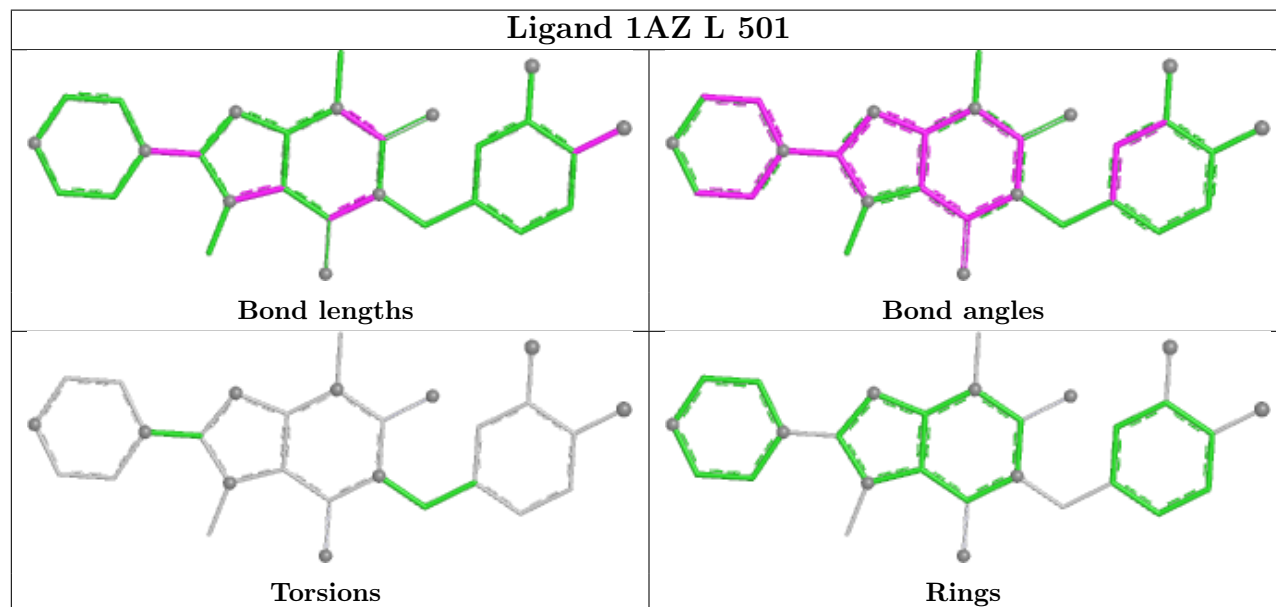
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

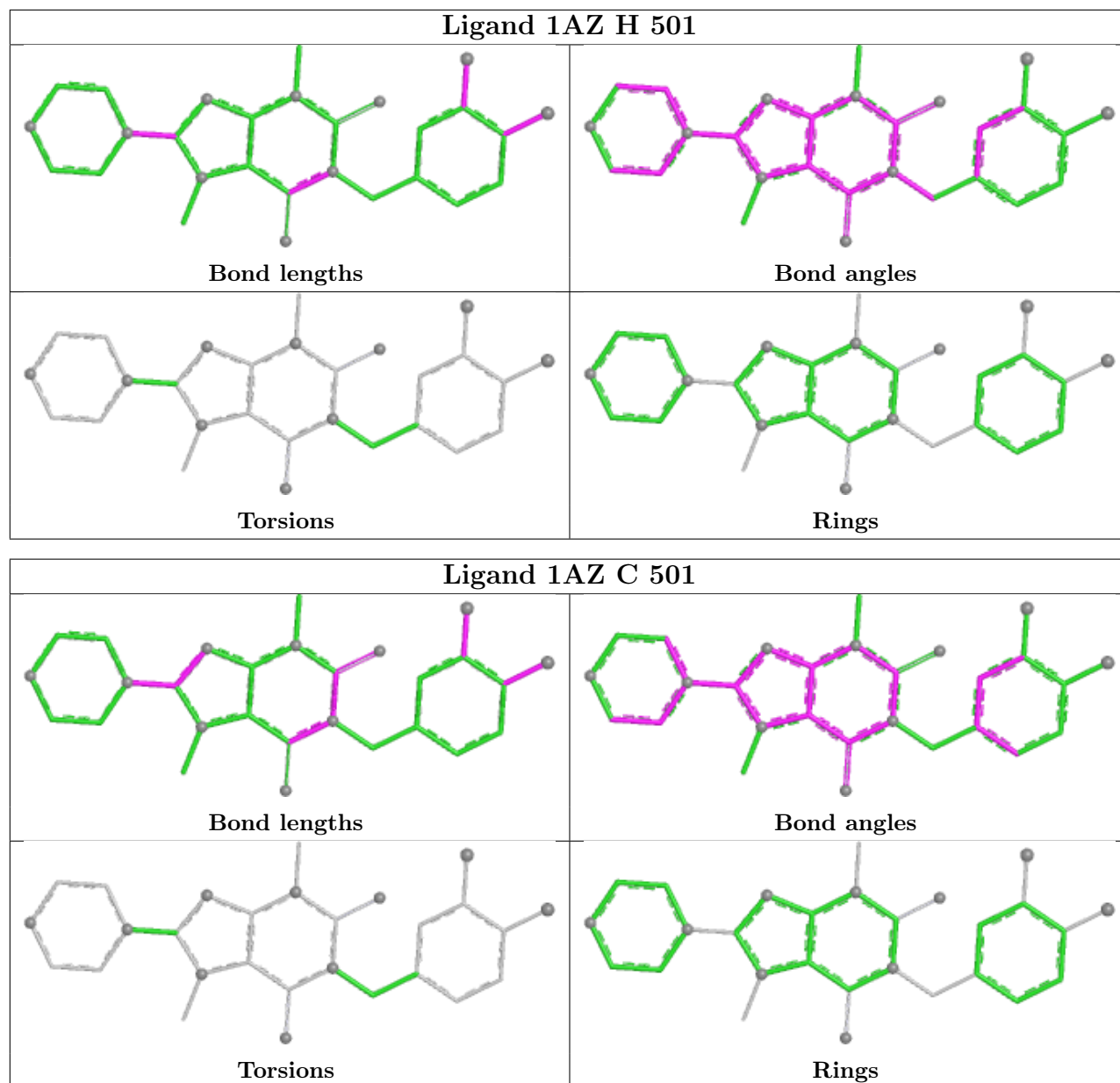


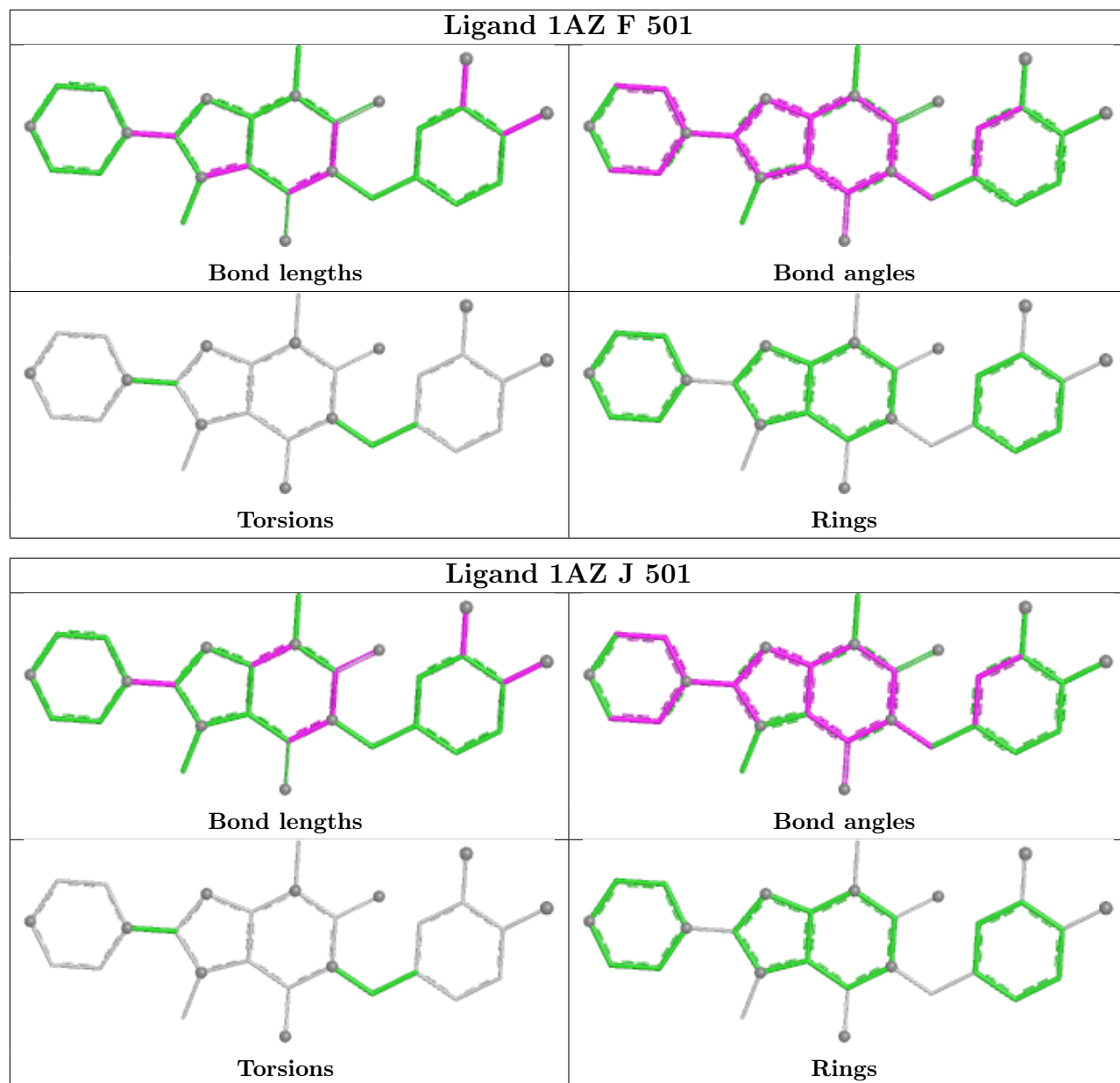
Ligand 1AZ E 501



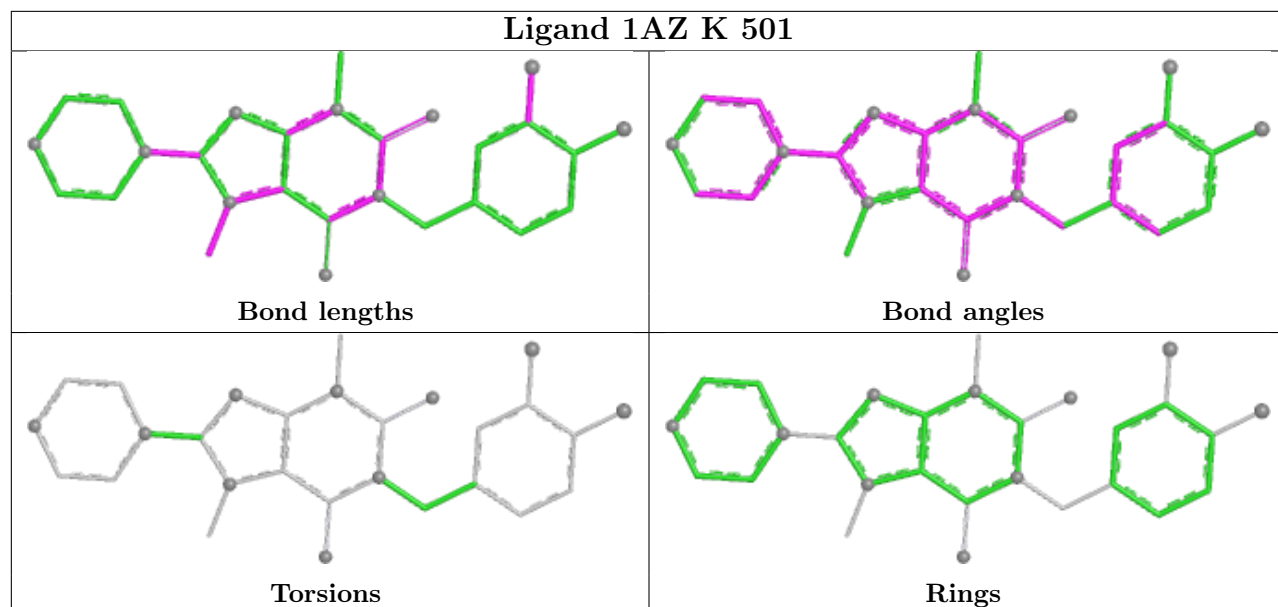
Ligand 1AZ L 501



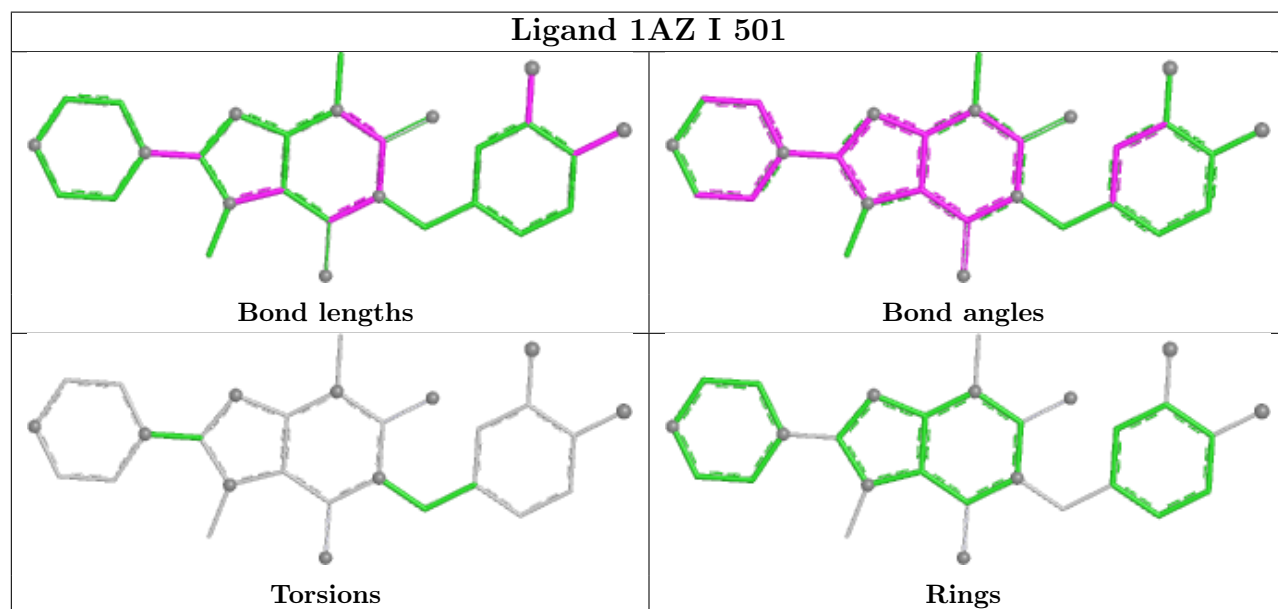




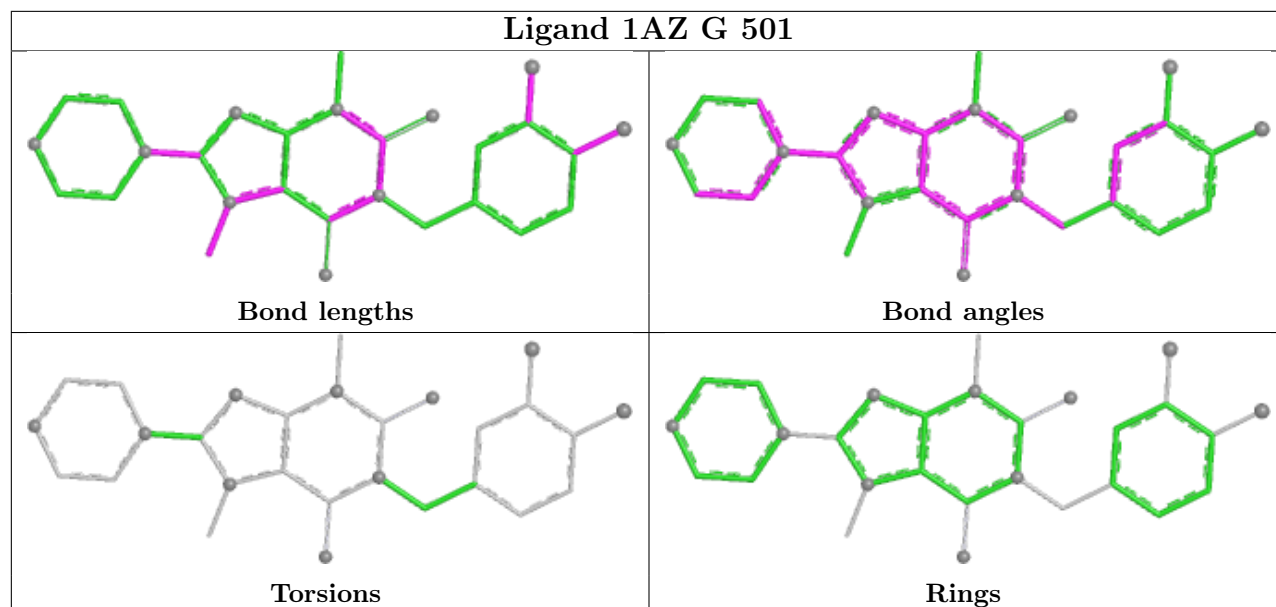
Ligand 1AZ K 501



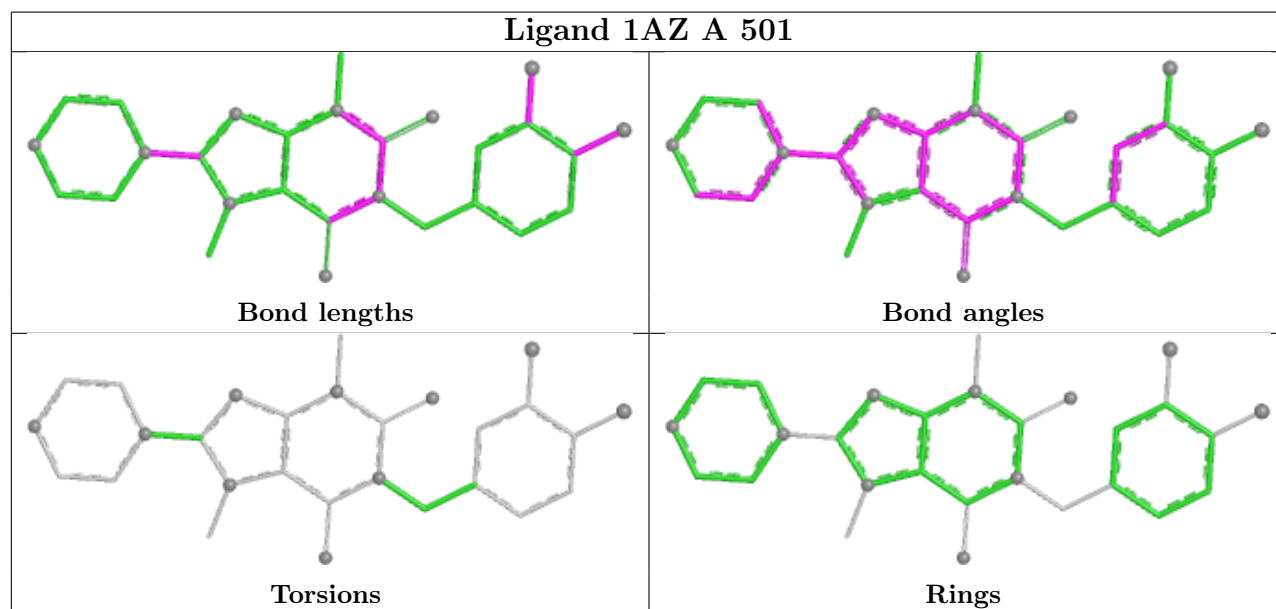
Ligand 1AZ I 501

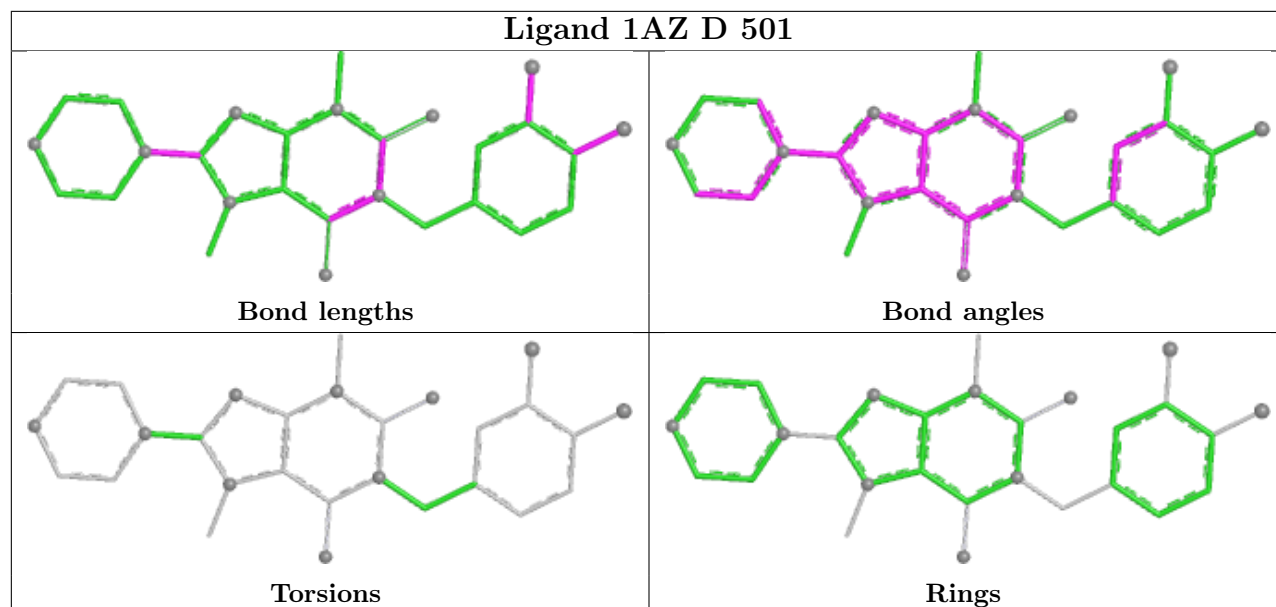


Ligand 1AZ G 501



Ligand 1AZ A 501





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	463/486 (95%)	0.25	27 (5%) 29 28	22, 38, 70, 99	0
1	B	463/486 (95%)	0.26	21 (4%) 38 38	22, 38, 70, 99	0
1	C	463/486 (95%)	0.26	31 (6%) 24 23	22, 39, 70, 99	0
1	D	463/486 (95%)	0.31	29 (6%) 26 25	22, 38, 70, 99	0
1	E	463/486 (95%)	0.40	37 (7%) 18 18	22, 38, 70, 99	0
1	F	463/486 (95%)	0.46	40 (8%) 16 15	22, 38, 70, 99	0
1	G	463/486 (95%)	0.39	36 (7%) 19 18	22, 38, 70, 99	0
1	H	463/486 (95%)	0.33	25 (5%) 31 31	22, 38, 70, 99	0
1	I	463/486 (95%)	0.26	20 (4%) 40 40	22, 39, 70, 99	0
1	J	463/486 (95%)	0.75	62 (13%) 7 5	22, 39, 70, 99	0
1	K	463/486 (95%)	0.37	28 (6%) 27 27	22, 39, 70, 99	0
1	L	463/486 (95%)	0.44	40 (8%) 16 15	22, 38, 70, 99	0
All	All	5556/5832 (95%)	0.37	396 (7%) 22 21	22, 39, 71, 99	0

All (396) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	58	ILE	7.1
1	L	413	ALA	6.3
1	J	296	ALA	6.2
1	L	61	PHE	5.7
1	J	401	VAL	5.6
1	A	58	ILE	5.6
1	H	347	ARG	5.5
1	H	58	ILE	5.2
1	F	58	ILE	5.0
1	F	413	ALA	5.0
1	D	58	ILE	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	413	ALA	4.9
1	E	58	ILE	4.8
1	D	413	ALA	4.8
1	G	413	ALA	4.7
1	J	58	ILE	4.6
1	H	413	ALA	4.6
1	F	401	VAL	4.5
1	K	332	PRO	4.5
1	G	60	GLY	4.4
1	A	347	ARG	4.4
1	K	413	ALA	4.4
1	B	61	PHE	4.4
1	E	334	TYR	4.4
1	J	61	PHE	4.3
1	K	414	ALA	4.3
1	H	61	PHE	4.3
1	L	99	PHE	4.3
1	J	333	GLY	4.2
1	L	60	GLY	4.2
1	A	335	GLU	4.2
1	K	61	PHE	4.2
1	I	334	TYR	4.2
1	D	335	GLU	4.2
1	C	413	ALA	4.1
1	D	347	ARG	4.1
1	J	293	THR	4.1
1	L	57	SER	4.1
1	E	61	PHE	4.1
1	E	336	ALA	4.1
1	J	413	ALA	4.0
1	J	347	ARG	4.0
1	L	414	ALA	4.0
1	E	347	ARG	4.0
1	E	413	ALA	4.0
1	B	404	ASP	4.0
1	I	413	ALA	3.9
1	H	59	ARG	3.9
1	H	67	SER	3.9
1	L	334	TYR	3.9
1	B	184	GLY	3.8
1	C	355	ILE	3.8
1	G	347	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	61	PHE	3.8
1	I	414	ALA	3.7
1	I	184	GLY	3.7
1	C	347	ARG	3.7
1	F	99	PHE	3.7
1	L	68	ASP	3.7
1	B	415	SER	3.6
1	J	298	LEU	3.6
1	J	400	PRO	3.6
1	B	58	ILE	3.6
1	L	54	ASP	3.6
1	A	336	ALA	3.6
1	F	336	ALA	3.6
1	G	67	SER	3.6
1	K	58	ILE	3.6
1	L	335	GLU	3.5
1	L	347	ARG	3.5
1	D	399	ALA	3.5
1	K	350	CYS	3.5
1	K	334	TYR	3.5
1	H	184	GLY	3.5
1	D	99	PHE	3.5
1	A	170	ALA	3.5
1	I	355	ILE	3.5
1	B	347	ARG	3.4
1	J	342	TYR	3.4
1	J	399	ALA	3.4
1	J	59	ARG	3.4
1	H	333	GLY	3.4
1	G	335	GLU	3.4
1	I	61	PHE	3.4
1	G	61	PHE	3.3
1	F	54	ASP	3.3
1	J	357	GLY	3.3
1	D	56	SER	3.3
1	F	56	SER	3.3
1	L	454	PHE	3.3
1	D	334	TYR	3.3
1	J	295	TYR	3.3
1	J	304	HIS	3.3
1	J	334	TYR	3.3
1	J	332	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	414	ALA	3.3
1	E	62	GLN	3.3
1	J	354	PRO	3.3
1	E	335	GLU	3.3
1	F	335	GLU	3.3
1	C	61	PHE	3.2
1	F	347	ARG	3.2
1	C	184	GLY	3.2
1	D	60	GLY	3.2
1	F	333	GLY	3.2
1	G	99	PHE	3.2
1	H	56	SER	3.2
1	L	59	ARG	3.2
1	F	332	PRO	3.2
1	I	333	GLY	3.2
1	J	60	GLY	3.2
1	C	414	ALA	3.2
1	K	62	GLN	3.2
1	J	294	GLY	3.2
1	L	401	VAL	3.2
1	F	414	ALA	3.2
1	E	67	SER	3.2
1	J	348	SER	3.2
1	C	404	ASP	3.2
1	J	350	CYS	3.2
1	E	59	ARG	3.1
1	H	332	PRO	3.1
1	I	58	ILE	3.1
1	F	68	ASP	3.1
1	J	99	PHE	3.1
1	E	416	ILE	3.1
1	B	413	ALA	3.1
1	J	341	VAL	3.1
1	G	334	TYR	3.0
1	A	404	ASP	3.0
1	J	416	ILE	3.0
1	F	356	THR	3.0
1	L	293	THR	3.0
1	J	300	ASP	3.0
1	D	57	SER	3.0
1	I	56	SER	3.0
1	K	333	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	332	PRO	3.0
1	D	59	ARG	3.0
1	D	345	ARG	3.0
1	A	57	SER	3.0
1	J	403	LYS	3.0
1	E	184	GLY	3.0
1	F	399	ALA	3.0
1	F	334	TYR	3.0
1	C	403	LYS	3.0
1	L	67	SER	3.0
1	G	58	ILE	2.9
1	J	290	TYR	2.9
1	F	61	PHE	2.9
1	G	355	ILE	2.9
1	C	334	TYR	2.9
1	C	99	PHE	2.9
1	B	60	GLY	2.9
1	L	184	GLY	2.9
1	D	402	ASP	2.9
1	E	333	GLY	2.9
1	H	99	PHE	2.8
1	G	403	LYS	2.8
1	C	58	ILE	2.8
1	J	346	ASN	2.8
1	B	332	PRO	2.8
1	A	403	LYS	2.8
1	B	414	ALA	2.8
1	A	59	ARG	2.8
1	E	45	SER	2.8
1	E	415	SER	2.8
1	F	67	SER	2.8
1	F	415	SER	2.8
1	C	332	PRO	2.8
1	A	414	ALA	2.8
1	E	350	CYS	2.8
1	E	345	ARG	2.8
1	E	352	ARG	2.8
1	J	57	SER	2.7
1	E	401	VAL	2.7
1	C	336	ALA	2.7
1	G	293	THR	2.7
1	K	349	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	L	400	PRO	2.7
1	I	415	SER	2.7
1	G	52	ALA	2.7
1	F	404	ASP	2.7
1	H	416	ILE	2.7
1	F	346	ASN	2.7
1	J	56	SER	2.7
1	B	336	ALA	2.7
1	J	302	ALA	2.7
1	K	293	THR	2.7
1	L	336	ALA	2.7
1	K	335	GLU	2.7
1	A	62	GLN	2.7
1	K	304	HIS	2.7
1	I	99	PHE	2.7
1	J	391	ILE	2.7
1	A	56	SER	2.7
1	H	334	TYR	2.7
1	G	414	ALA	2.7
1	A	99	PHE	2.6
1	D	61	PHE	2.6
1	E	332	PRO	2.6
1	I	69	MET	2.6
1	G	415	SER	2.6
1	I	67	SER	2.6
1	A	334	TYR	2.6
1	J	356	THR	2.6
1	K	399	ALA	2.6
1	B	333	GLY	2.6
1	F	55	GLY	2.6
1	H	374	GLY	2.6
1	I	404	ASP	2.6
1	J	184	GLY	2.6
1	L	346	ASN	2.6
1	B	56	SER	2.6
1	F	57	SER	2.6
1	J	381	SER	2.6
1	E	414	ALA	2.6
1	F	62	GLN	2.6
1	J	286	ALA	2.6
1	C	295	TYR	2.6
1	J	402	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	K	300	ASP	2.6
1	C	338	ILE	2.6
1	C	62	GLN	2.6
1	H	414	ALA	2.6
1	F	59	ARG	2.6
1	J	360	PRO	2.6
1	L	415	SER	2.6
1	F	403	LYS	2.6
1	A	332	PRO	2.5
1	D	55	GLY	2.5
1	J	62	GLN	2.5
1	A	415	SER	2.5
1	D	336	ALA	2.5
1	H	57	SER	2.5
1	L	56	SER	2.5
1	B	334	TYR	2.5
1	F	374	GLY	2.5
1	J	355	ILE	2.5
1	B	62	GLN	2.5
1	D	401	VAL	2.5
1	J	414	ALA	2.5
1	H	415	SER	2.5
1	J	315	SER	2.5
1	H	350	CYS	2.5
1	K	60	GLY	2.5
1	E	404	ASP	2.5
1	J	338	ILE	2.5
1	B	99	PHE	2.5
1	E	52	ALA	2.5
1	K	347	ARG	2.5
1	J	299	SER	2.5
1	G	62	GLN	2.5
1	J	344	GLN	2.5
1	K	15	ASP	2.4
1	K	357	GLY	2.4
1	E	399	ALA	2.4
1	I	335	GLU	2.4
1	J	55	GLY	2.4
1	J	308	GLY	2.4
1	K	184	GLY	2.4
1	A	345	ARG	2.4
1	G	186	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	53	PHE	2.4
1	F	390	GLY	2.4
1	C	416	ILE	2.4
1	J	395	ILE	2.4
1	A	402	ASP	2.4
1	E	51	LEU	2.4
1	F	402	ASP	2.4
1	J	303	ARG	2.4
1	L	340	LEU	2.4
1	C	331	VAL	2.4
1	C	346	ASN	2.4
1	C	392	LYS	2.4
1	G	170	ALA	2.4
1	I	52	ALA	2.4
1	D	333	GLY	2.3
1	G	398	GLN	2.3
1	G	416	ILE	2.3
1	G	300	ASP	2.3
1	L	350	CYS	2.3
1	E	337	PRO	2.3
1	G	400	PRO	2.3
1	G	59	ARG	2.3
1	G	294	GLY	2.3
1	L	333	GLY	2.3
1	F	446	ASP	2.3
1	J	305	TYR	2.3
1	G	332	PRO	2.3
1	F	293	THR	2.3
1	K	345	ARG	2.3
1	F	45	SER	2.3
1	L	62	GLN	2.3
1	B	338	ILE	2.3
1	H	404	ASP	2.3
1	K	404	ASP	2.3
1	D	350	CYS	2.3
1	G	401	VAL	2.3
1	F	296	ALA	2.3
1	G	185	GLY	2.3
1	L	297	GLY	2.3
1	K	57	SER	2.3
1	L	45	SER	2.3
1	K	355	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	K	416	ILE	2.3
1	E	403	LYS	2.3
1	A	55	GLY	2.2
1	F	60	GLY	2.2
1	H	357	GLY	2.2
1	K	67	SER	2.2
1	L	416	ILE	2.2
1	D	331	VAL	2.2
1	J	390	GLY	2.2
1	J	120	ILE	2.2
1	E	15	ASP	2.2
1	H	52	ALA	2.2
1	E	392	LYS	2.2
1	C	56	SER	2.2
1	D	415	SER	2.2
1	J	404	ASP	2.2
1	L	446	ASP	2.2
1	B	335	GLU	2.2
1	G	345	ARG	2.2
1	H	181	ARG	2.2
1	E	99	PHE	2.2
1	F	400	PRO	2.2
1	F	454	PHE	2.2
1	L	337	PRO	2.2
1	C	183	LYS	2.2
1	D	296	ALA	2.2
1	G	4	LYS	2.2
1	I	399	ALA	2.2
1	I	403	LYS	2.2
1	L	399	ALA	2.2
1	J	301	THR	2.2
1	A	298	LEU	2.2
1	E	57	SER	2.2
1	C	335	GLU	2.2
1	K	99	PHE	2.2
1	L	44	LYS	2.2
1	L	403	LYS	2.2
1	E	304	HIS	2.1
1	B	346	ASN	2.1
1	F	52	ALA	2.1
1	H	349	ALA	2.1
1	L	69	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	340	LEU	2.1
1	G	184	GLY	2.1
1	L	50	GLY	2.1
1	B	59	ARG	2.1
1	J	358	SER	2.1
1	I	360	PRO	2.1
1	E	331	VAL	2.1
1	A	60	GLY	2.1
1	D	395	ILE	2.1
1	I	347	ARG	2.1
1	J	102	GLU	2.1
1	A	358	SER	2.1
1	D	67	SER	2.1
1	F	337	PRO	2.1
1	C	333	GLY	2.1
1	D	340	LEU	2.1
1	G	298	LEU	2.1
1	L	55	GLY	2.1
1	A	338	ILE	2.1
1	G	449	GLU	2.1
1	J	435	GLU	2.1
1	B	57	SER	2.1
1	C	67	SER	2.1
1	H	62	GLN	2.1
1	G	336	ALA	2.1
1	A	333	GLY	2.1
1	L	294	GLY	2.1
1	C	290	TYR	2.1
1	J	291	ASP	2.1
1	C	350	CYS	2.1
1	K	417	PRO	2.1
1	L	362	ALA	2.0
1	G	55	GLY	2.0
1	C	356	THR	2.0
1	D	403	LYS	2.0
1	J	124	ILE	2.0
1	A	295	TYR	2.0
1	D	404	ASP	2.0
1	E	8	ASP	2.0
1	J	436	TYR	2.0
1	G	51	LEU	2.0
1	G	399	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	294	GLY	2.0
1	C	357	GLY	2.0
1	E	11	LYS	2.0
1	E	441	GLY	2.0
1	F	44	LYS	2.0
1	C	400	PRO	2.0
1	H	446	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
2	1AZ	J	501	28/28	0.86	0.12	46,47,49,50	0
2	1AZ	C	501	28/28	0.88	0.12	46,47,49,50	0
3	CL	J	502	1/1	0.88	0.22	57,57,57,57	0
2	1AZ	K	501	28/28	0.89	0.12	46,47,49,50	0
2	1AZ	B	501	28/28	0.89	0.11	46,47,48,50	0
2	1AZ	I	501	28/28	0.90	0.10	46,47,49,50	0
2	1AZ	A	501	28/28	0.90	0.10	46,47,49,49	0
2	1AZ	D	501	28/28	0.90	0.11	46,47,48,49	0
3	CL	I	502	1/1	0.90	0.12	57,57,57,57	0
2	1AZ	H	501	28/28	0.90	0.12	46,47,48,50	0
2	1AZ	E	501	28/28	0.92	0.10	46,47,48,49	0
3	CL	E	502	1/1	0.92	0.13	57,57,57,57	0
3	CL	C	502	1/1	0.93	0.09	57,57,57,57	0
2	1AZ	G	501	28/28	0.93	0.08	46,47,48,50	0
2	1AZ	L	501	28/28	0.93	0.10	46,47,48,49	0
3	CL	A	502	1/1	0.93	0.10	57,57,57,57	0

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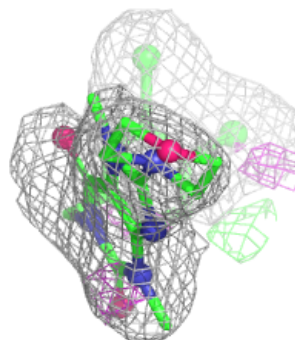
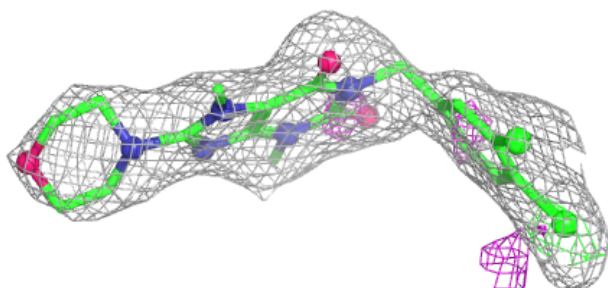
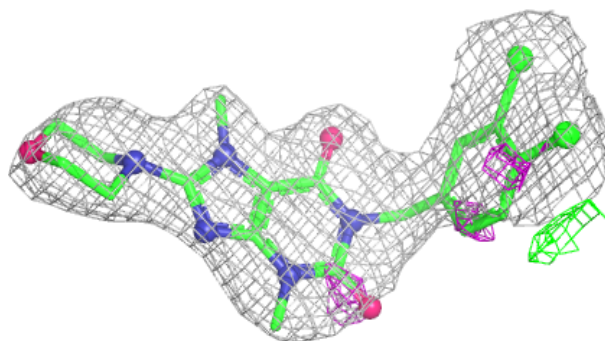
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CL	G	502	1/1	0.94	0.12	57,57,57,57	0
3	CL	B	502	1/1	0.94	0.16	57,57,57,57	0
3	CL	F	502	1/1	0.94	0.22	57,57,57,57	0
3	CL	D	502	1/1	0.95	0.07	57,57,57,57	0
2	1AZ	F	501	28/28	0.95	0.09	46,47,48,49	0
3	CL	H	502	1/1	0.96	0.18	57,57,57,57	0
3	CL	K	502	1/1	0.97	0.21	58,58,58,58	0
3	CL	L	502	1/1	0.97	0.23	57,57,57,57	0

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

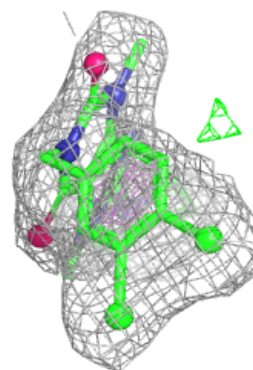
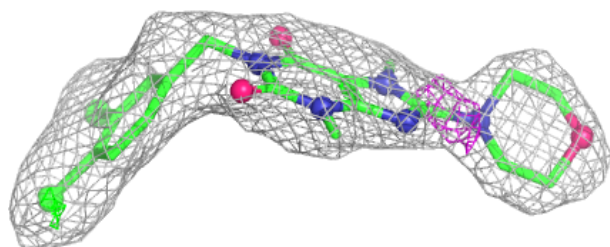
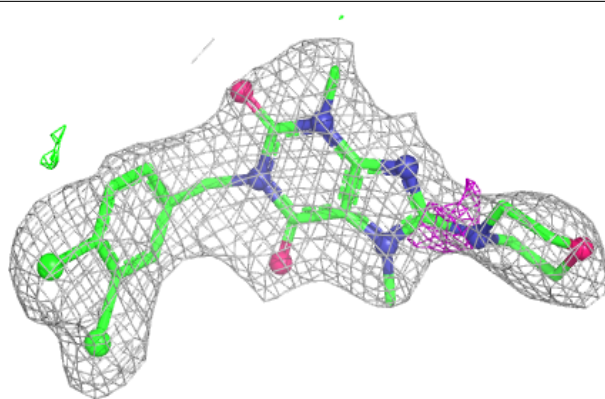
Electron density around 1AZ J 501:

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

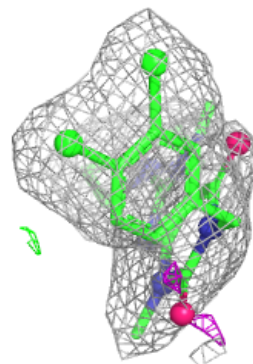
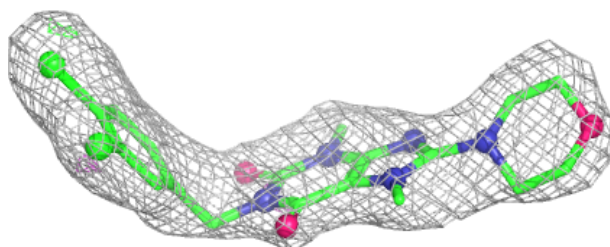
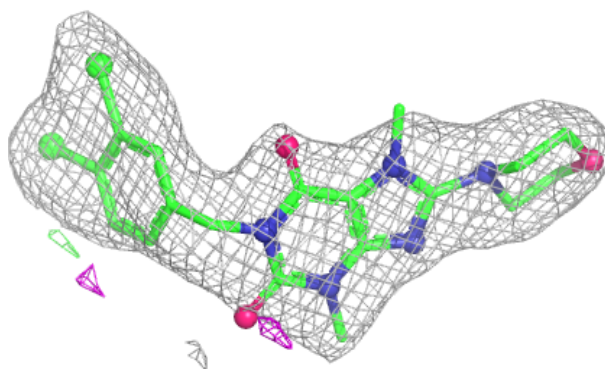


Electron density around 1AZ C 501:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

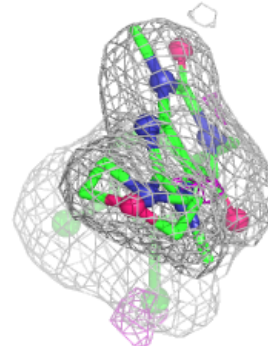
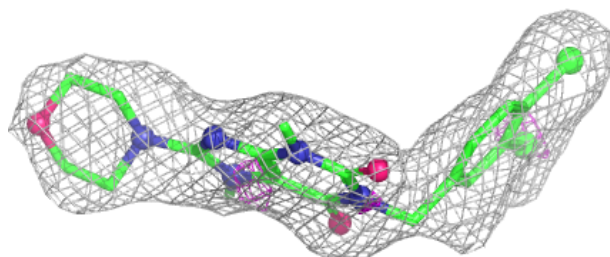
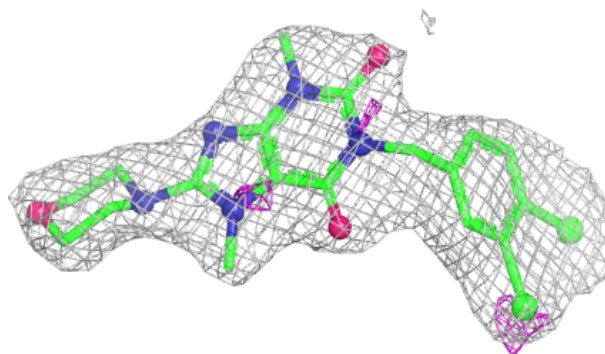
**Electron density around 1AZ K 501:**

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and green (positive)

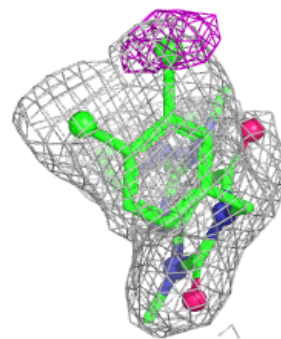
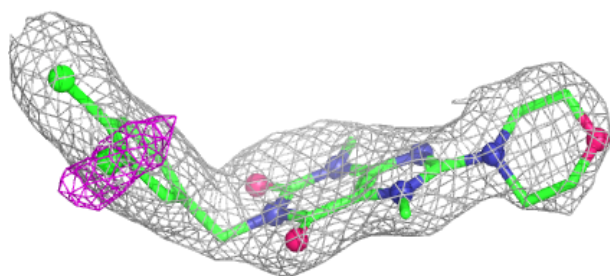
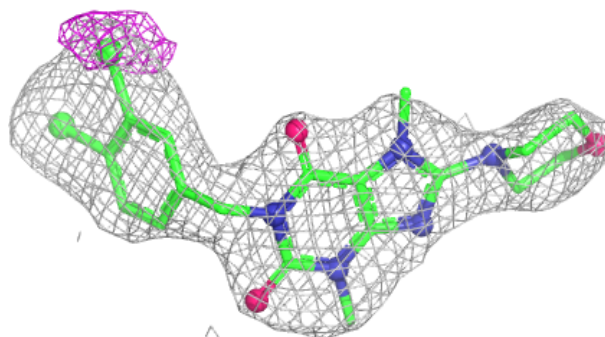


Electron density around 1AZ B 501:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

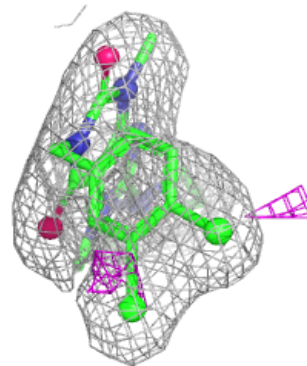
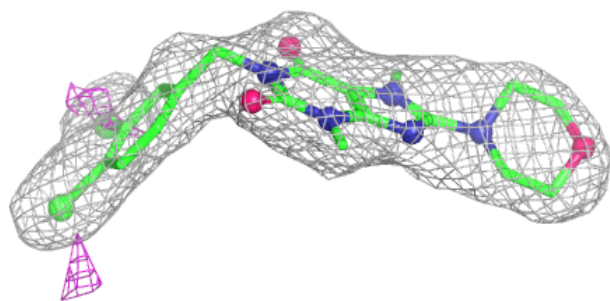
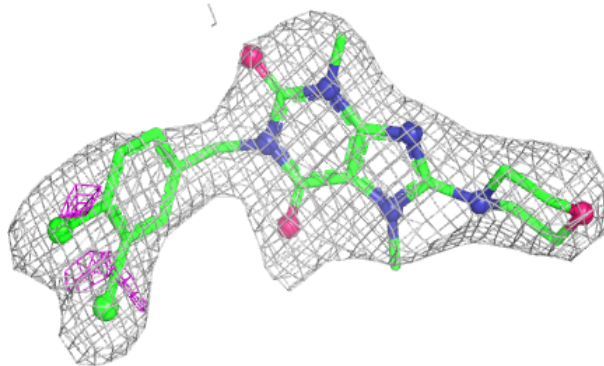
**Electron density around 1AZ I 501:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

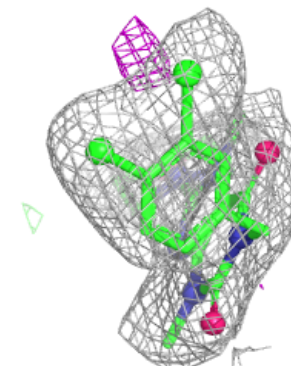
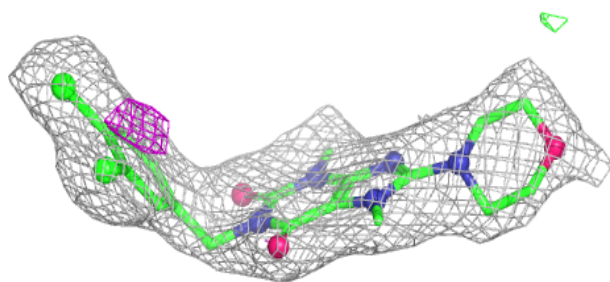
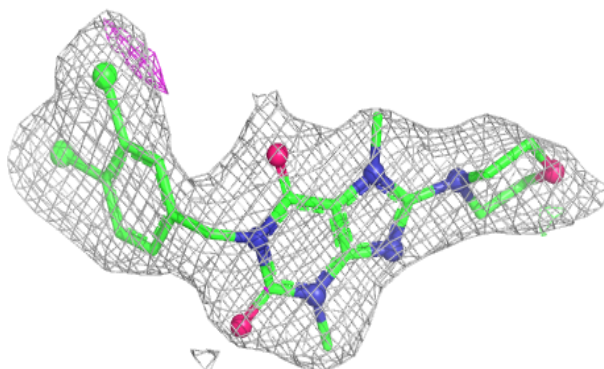


Electron density around 1AZ A 501:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

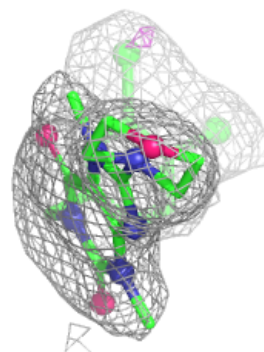
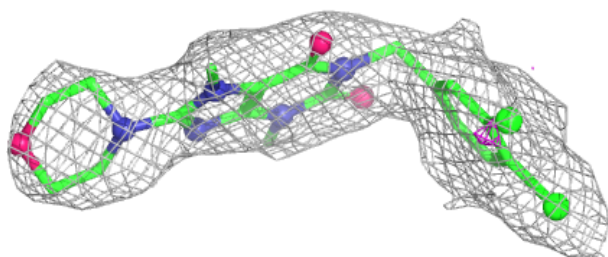
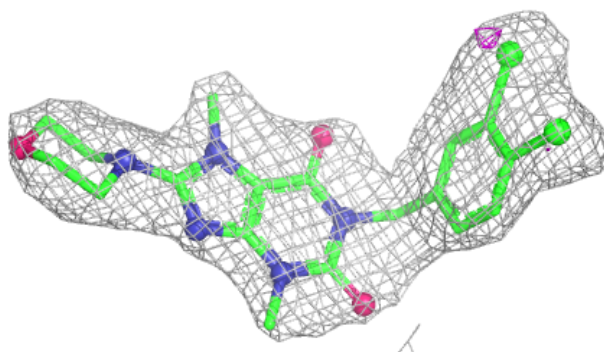
**Electron density around 1AZ D 501:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

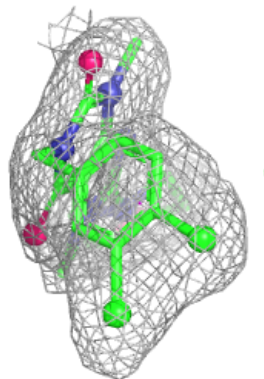
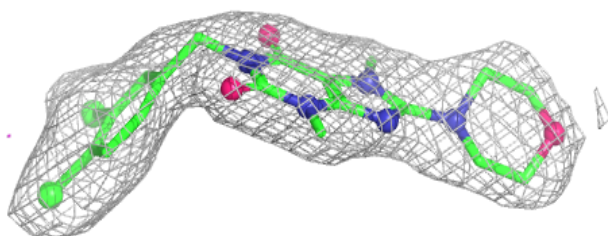
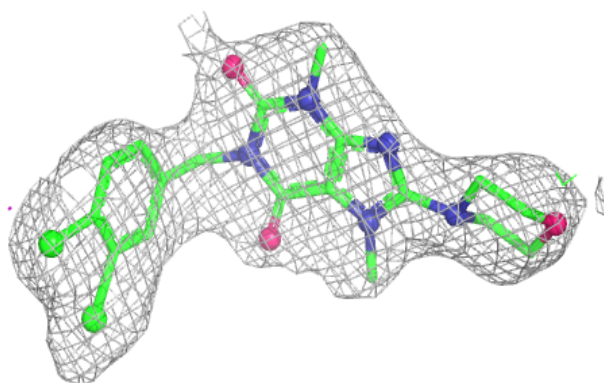


Electron density around 1AZ H 501:

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and green (positive)

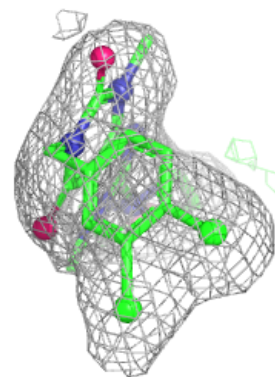
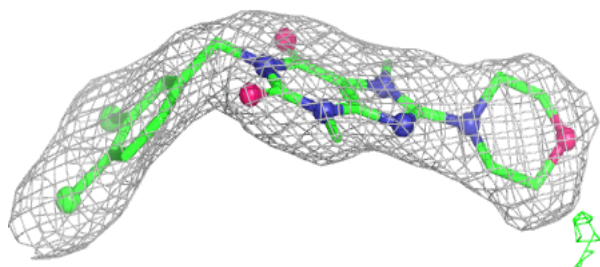
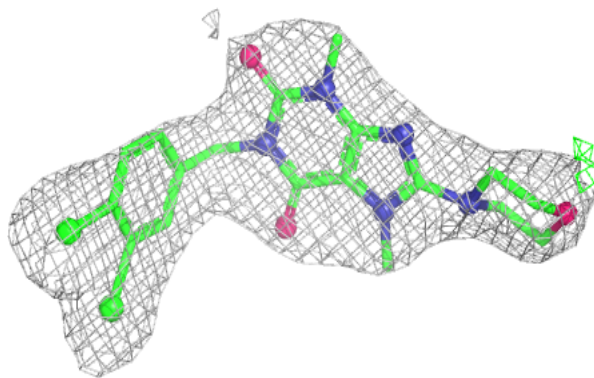
**Electron density around 1AZ E 501:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

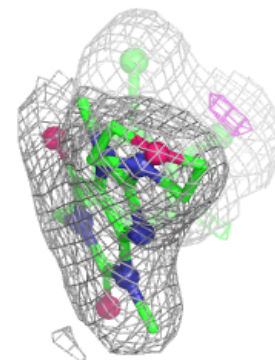
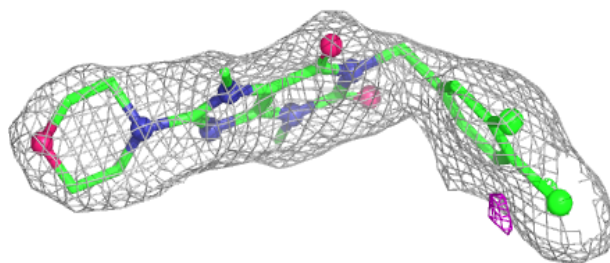
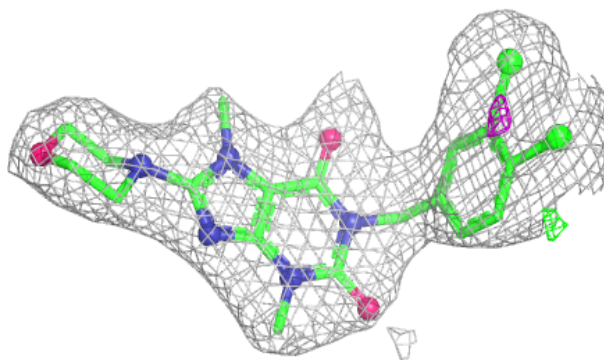


Electron density around 1AZ G 501:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

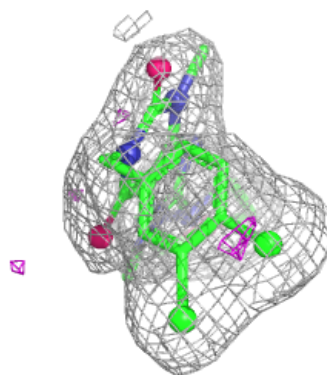
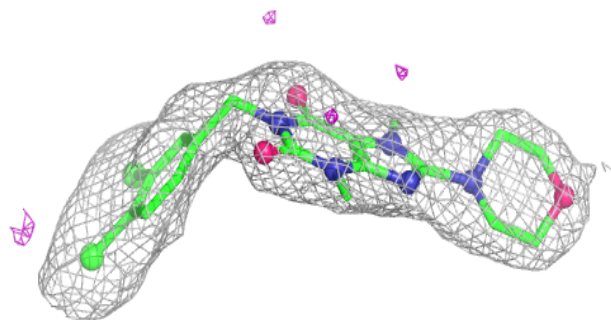
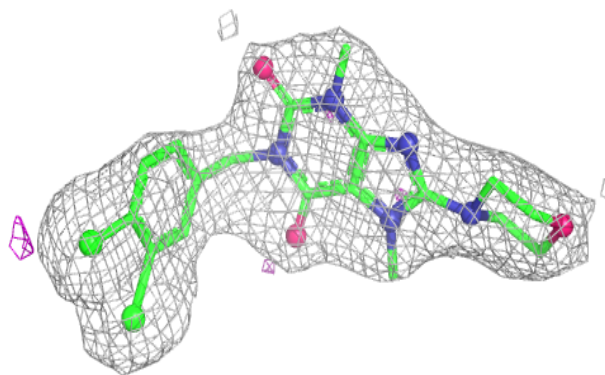
**Electron density around 1AZ L 501:**

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and green (positive)



Electron density around 1AZ F 501:

$2mF_o-DF_c$ (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.