



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:18 PM UTC

PDB ID : 3Q9B / pdb_00003q9b
Title : Crystal Structure of APAH complexed with M344
Authors : Lombardi, P.M.; Christianson, D.W.
Deposited on : 2011-01-07
Resolution : 2.25 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

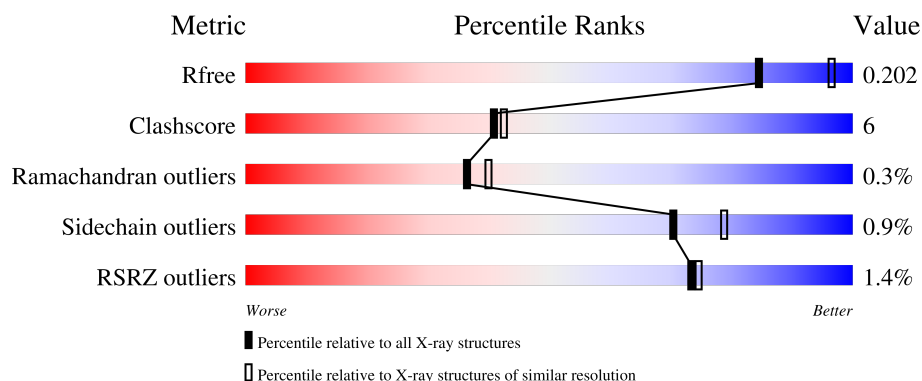
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	341	0% 84% 16%
1	B	341	2% 83% 16%
1	C	341	0% 83% 16%
1	D	341	0% 79% 20%
1	E	341	2% 87% 13%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	341	% 83% 16% .
1	G	341	3% 84% 16%
1	H	341	% 83% 17%
1	I	341	2% 87% 12% .
1	J	341	% 80% 19% .
1	K	341	% 83% 16%
1	L	341	% 84% 16%

2 Entry composition

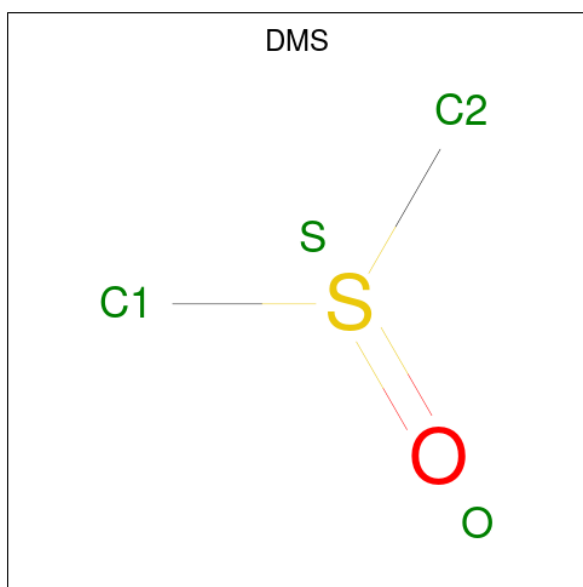
There are 7 unique types of molecules in this entry. The entry contains 33797 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Acetylpolysamine amidohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	0	0	0
			2568	1644	435	480	9			
1	B	341	Total	C	N	O	S	0	0	0
			2568	1644	435	480	9			
1	C	341	Total	C	N	O	S	0	0	0
			2568	1644	435	480	9			
1	D	341	Total	C	N	O	S	0	0	0
			2568	1644	435	480	9			
1	E	341	Total	C	N	O	S	0	0	0
			2568	1644	435	480	9			
1	F	341	Total	C	N	O	S	0	0	0
			2568	1644	435	480	9			
1	G	341	Total	C	N	O	S	0	0	0
			2568	1644	435	480	9			
1	H	341	Total	C	N	O	S	0	0	0
			2568	1644	435	480	9			
1	I	341	Total	C	N	O	S	0	0	0
			2568	1644	435	480	9			
1	J	340	Total	C	N	O	S	0	0	0
			2563	1642	434	478	9			
1	K	341	Total	C	N	O	S	0	0	0
			2568	1644	435	480	9			
1	L	341	Total	C	N	O	S	0	0	0
			2568	1644	435	480	9			

- Molecule 2 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	B	1	Total	C	O	S	0	0
			4	2	1	1		
2	B	1	Total	C	O	S	0	0
			4	2	1	1		
2	B	1	Total	C	O	S	0	0
			4	2	1	1		
2	B	1	Total	C	O	S	0	0
			4	2	1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total 4	C 2	O 1	S 1	0	0
2	B	1	Total 4	C 2	O 1	S 1	0	0
2	B	1	Total 4	C 2	O 1	S 1	0	0
2	B	1	Total 4	C 2	O 1	S 1	0	0
2	B	1	Total 4	C 2	O 1	S 1	0	0
2	C	1	Total 4	C 2	O 1	S 1	0	0
2	C	1	Total 4	C 2	O 1	S 1	0	0
2	C	1	Total 4	C 2	O 1	S 1	0	0
2	C	1	Total 4	C 2	O 1	S 1	0	0
2	C	1	Total 4	C 2	O 1	S 1	0	0
2	C	1	Total 4	C 2	O 1	S 1	0	0
2	D	1	Total 4	C 2	O 1	S 1	0	0
2	D	1	Total 4	C 2	O 1	S 1	0	0
2	D	1	Total 4	C 2	O 1	S 1	0	0
2	D	1	Total 4	C 2	O 1	S 1	0	0
2	D	1	Total 4	C 2	O 1	S 1	0	0
2	D	1	Total 4	C 2	O 1	S 1	0	0
2	D	1	Total 4	C 2	O 1	S 1	0	0
2	D	1	Total 4	C 2	O 1	S 1	0	0
2	D	1	Total 4	C 2	O 1	S 1	0	0
2	D	1	Total 4	C 2	O 1	S 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total 4	C 2	O 1	S 1	0	0
2	E	1	Total 4	C 2	O 1	S 1	0	0
2	E	1	Total 4	C 2	O 1	S 1	0	0
2	E	1	Total 4	C 2	O 1	S 1	0	0
2	E	1	Total 4	C 2	O 1	S 1	0	0
2	E	1	Total 4	C 2	O 1	S 1	0	0
2	E	1	Total 4	C 2	O 1	S 1	0	0
2	E	1	Total 4	C 2	O 1	S 1	0	0
2	E	1	Total 4	C 2	O 1	S 1	0	0
2	E	1	Total 4	C 2	O 1	S 1	0	0
2	E	1	Total 4	C 2	O 1	S 1	0	0
2	F	1	Total 4	C 2	O 1	S 1	0	0
2	F	1	Total 4	C 2	O 1	S 1	0	0
2	F	1	Total 4	C 2	O 1	S 1	0	0
2	F	1	Total 4	C 2	O 1	S 1	0	0
2	F	1	Total 4	C 2	O 1	S 1	0	0
2	F	1	Total 4	C 2	O 1	S 1	0	0
2	F	1	Total 4	C 2	O 1	S 1	0	0
2	F	1	Total 4	C 2	O 1	S 1	0	0
2	F	1	Total 4	C 2	O 1	S 1	0	0
2	F	1	Total 4	C 2	O 1	S 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	F	1	Total 4	C 2	O 1	S 1	0	0
2	G	1	Total 4	C 2	O 1	S 1	0	0
2	G	1	Total 4	C 2	O 1	S 1	0	0
2	G	1	Total 4	C 2	O 1	S 1	0	0
2	G	1	Total 4	C 2	O 1	S 1	0	0
2	G	1	Total 4	C 2	O 1	S 1	0	0
2	G	1	Total 4	C 2	O 1	S 1	0	0
2	G	1	Total 4	C 2	O 1	S 1	0	0
2	G	1	Total 4	C 2	O 1	S 1	0	0
2	G	1	Total 4	C 2	O 1	S 1	0	0
2	G	1	Total 4	C 2	O 1	S 1	0	0
2	H	1	Total 4	C 2	O 1	S 1	0	0
2	H	1	Total 4	C 2	O 1	S 1	0	0
2	H	1	Total 4	C 2	O 1	S 1	0	0
2	H	1	Total 4	C 2	O 1	S 1	0	0
2	H	1	Total 4	C 2	O 1	S 1	0	0
2	H	1	Total 4	C 2	O 1	S 1	0	0
2	H	1	Total 4	C 2	O 1	S 1	0	0
2	H	1	Total 4	C 2	O 1	S 1	0	0
2	I	1	Total 4	C 2	O 1	S 1	0	0
2	I	1	Total 4	C 2	O 1	S 1	0	0

Continued on next page...

Continued from previous page...

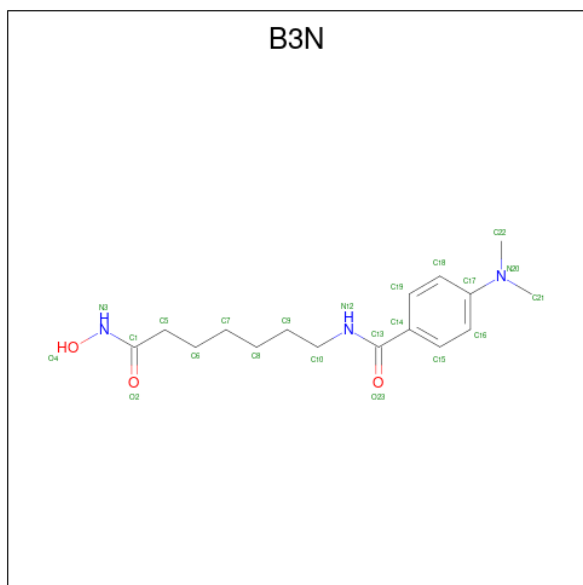
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	I	1	Total 4	C 2	O 1	S 1	0	0
2	I	1	Total 4	C 2	O 1	S 1	0	0
2	I	1	Total 4	C 2	O 1	S 1	0	0
2	I	1	Total 4	C 2	O 1	S 1	0	0
2	I	1	Total 4	C 2	O 1	S 1	0	0
2	I	1	Total 4	C 2	O 1	S 1	0	0
2	J	1	Total 4	C 2	O 1	S 1	0	0
2	J	1	Total 4	C 2	O 1	S 1	0	0
2	J	1	Total 4	C 2	O 1	S 1	0	0
2	J	1	Total 4	C 2	O 1	S 1	0	0
2	J	1	Total 4	C 2	O 1	S 1	0	0
2	J	1	Total 4	C 2	O 1	S 1	0	0
2	J	1	Total 4	C 2	O 1	S 1	0	0
2	J	1	Total 4	C 2	O 1	S 1	0	0
2	K	1	Total 4	C 2	O 1	S 1	0	0
2	K	1	Total 4	C 2	O 1	S 1	0	0
2	K	1	Total 4	C 2	O 1	S 1	0	0
2	K	1	Total 4	C 2	O 1	S 1	0	0
2	K	1	Total 4	C 2	O 1	S 1	0	0
2	K	1	Total 4	C 2	O 1	S 1	0	0
2	K	1	Total 4	C 2	O 1	S 1	0	0
2	K	1	Total 4	C 2	O 1	S 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	K	1	Total	C	O	S	0	0
			4	2	1	1		
2	K	1	Total	C	O	S	0	0
			4	2	1	1		
2	L	1	Total	C	O	S	0	0
			4	2	1	1		
2	L	1	Total	C	O	S	0	0
			4	2	1	1		
2	L	1	Total	C	O	S	0	0
			4	2	1	1		
2	L	1	Total	C	O	S	0	0
			4	2	1	1		
2	L	1	Total	C	O	S	0	0
			4	2	1	1		
2	L	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 3 is 4-(dimethylamino)-N-[7-(hydroxyamino)-7-oxoheptyl]benzamide (CCD ID: B3N) (formula: C₁₆H₂₅N₃O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			22	16	3	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			22	16	3	3		
3	C	1	Total	C	N	O	0	0
			22	16	3	3		
3	D	1	Total	C	N	O	0	0
			22	16	3	3		
3	E	1	Total	C	N	O	0	0
			22	16	3	3		
3	F	1	Total	C	N	O	0	0
			22	16	3	3		
3	G	1	Total	C	N	O	0	0
			22	16	3	3		
3	H	1	Total	C	N	O	0	0
			22	16	3	3		
3	I	1	Total	C	N	O	0	0
			22	16	3	3		
3	J	1	Total	C	N	O	0	0
			22	16	3	3		
3	K	1	Total	C	N	O	0	0
			22	16	3	3		
3	L	1	Total	C	N	O	0	0
			22	16	3	3		

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	K	0	0
			2	2		
4	B	2	Total	K	0	0
			2	2		
4	C	2	Total	K	0	0
			2	2		
4	D	2	Total	K	0	0
			2	2		
4	E	2	Total	K	0	0
			2	2		
4	F	2	Total	K	0	0
			2	2		
4	G	2	Total	K	0	0
			2	2		
4	H	2	Total	K	0	0
			2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	I	1	Total K 1 1	0	0
4	J	2	Total K 2 2	0	0
4	K	2	Total K 2 2	0	0
4	L	2	Total K 2 2	0	0

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Zn 1 1	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	184	Total 184	O 184	0	0
7	B	165	Total 165	O 165	0	0
7	C	192	Total 192	O 192	0	0
7	D	187	Total 187	O 187	0	0
7	E	181	Total 181	O 181	0	0
7	F	196	Total 196	O 196	0	0
7	G	184	Total 184	O 184	0	0
7	H	183	Total 183	O 183	0	0

Continued on next page...

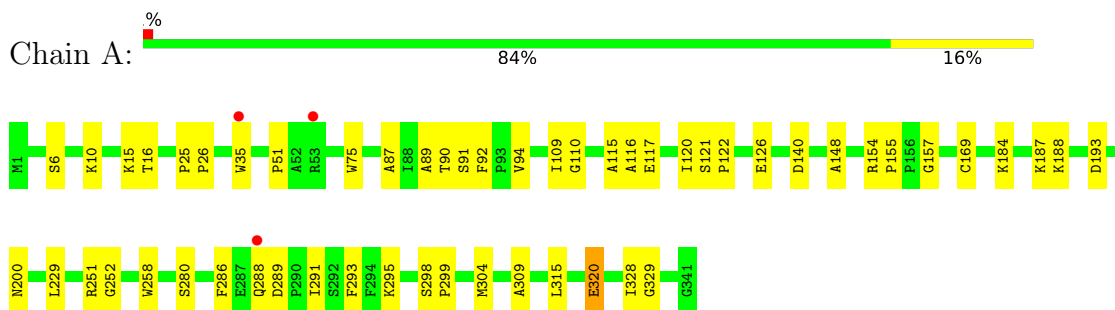
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	I	204	Total 204	O 204	0	0
7	J	174	Total 174	O 174	0	0
7	K	211	Total 211	O 211	0	0
7	L	182	Total 182	O 182	0	0

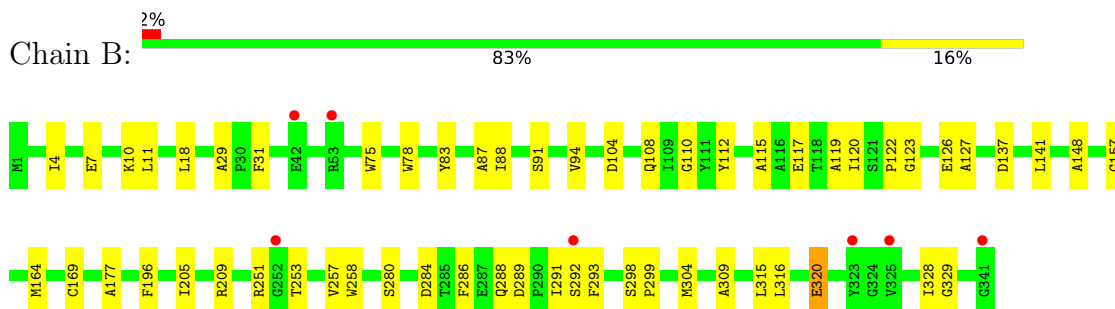
3 Residue-property plots [i](#)

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.

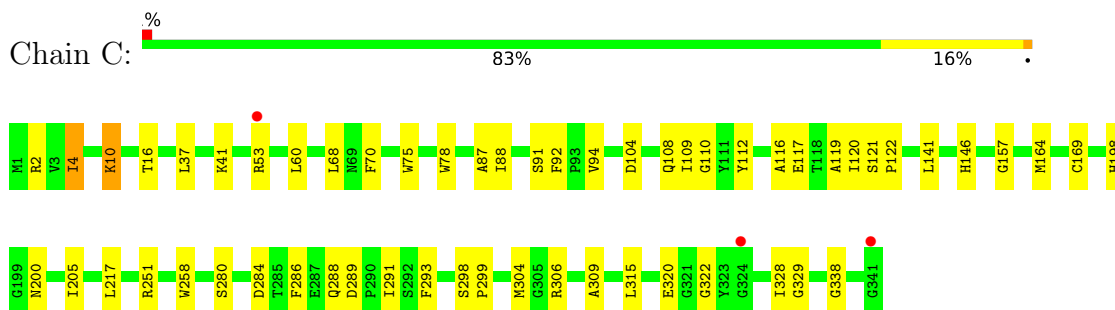
- Molecule 1: Acetypolyamine amidohydrolase



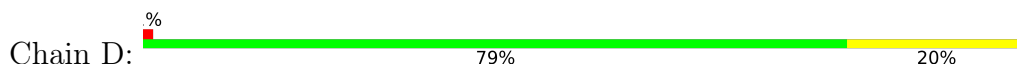
- Molecule 1: Acetypolyamine amidohydrolase

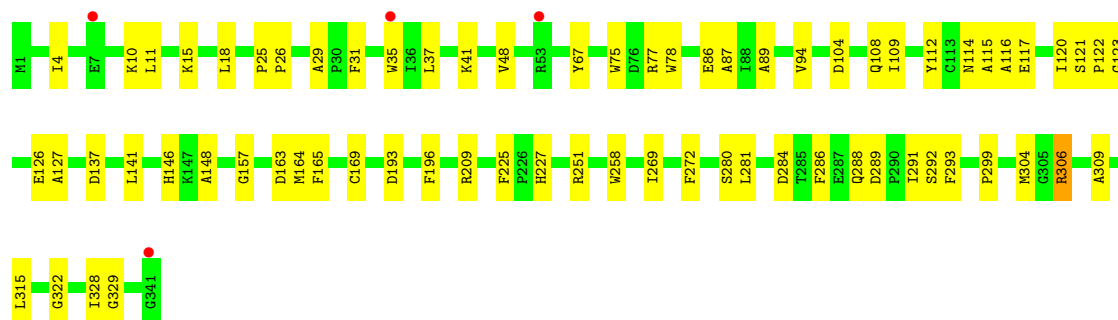


- Molecule 1: Acetypolyamine amidohydrolase

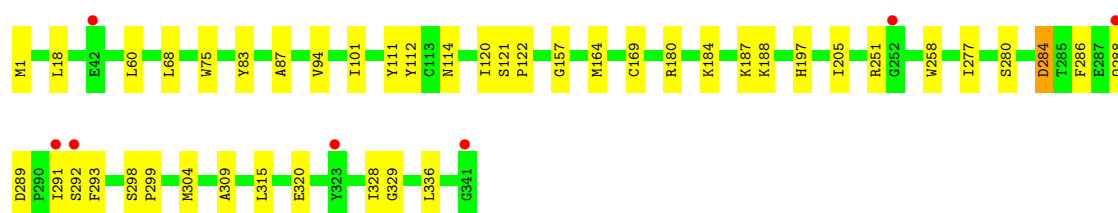
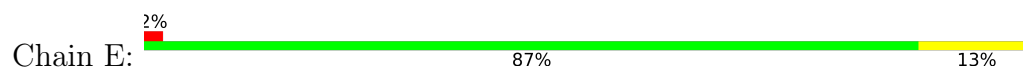


- Molecule 1: Acetypolyamine amidohydrolase

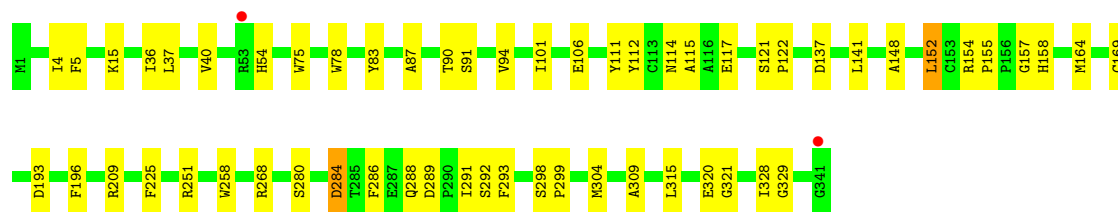
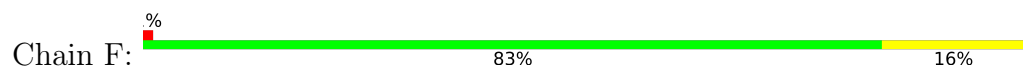




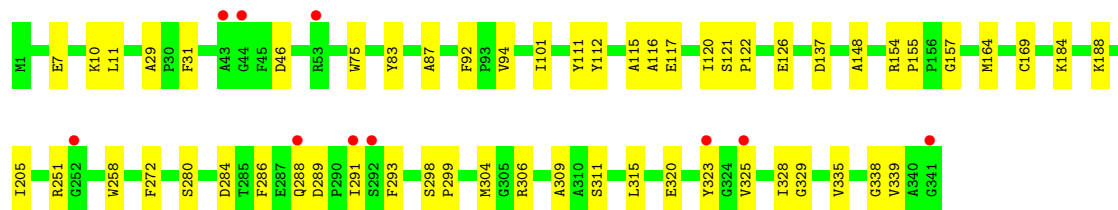
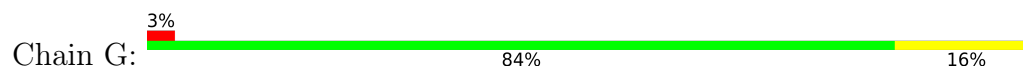
• Molecule 1: Acetylpolysamine amidohydrolase



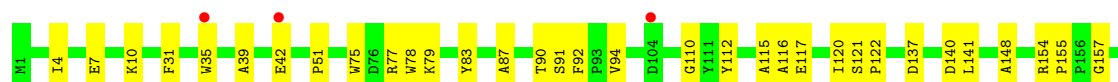
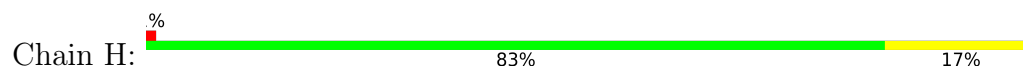
• Molecule 1: Acetylpolysamine amidohydrolase



• Molecule 1: Acetylpolysamine amidohydrolase

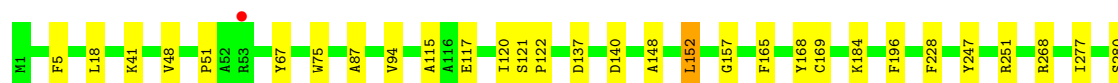
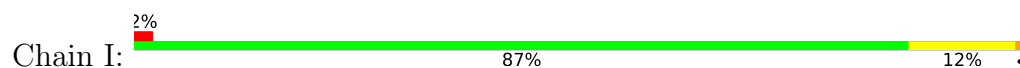


• Molecule 1: Acetylpolysamine amidohydrolase

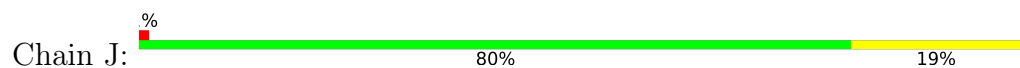




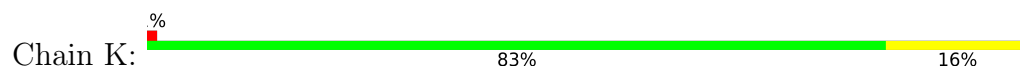
• Molecule 1: Acetypolyamine amidohydrolase



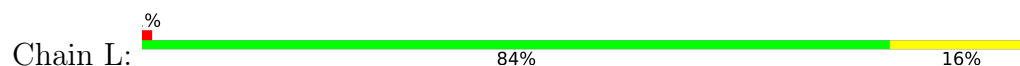
• Molecule 1: Acetypolyamine amidohydrolase



• Molecule 1: Acetypolyamine amidohydrolase



• Molecule 1: Acetypolyamine amidohydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	118.66Å 119.73Å 119.53Å 98.09° 95.15° 115.33°	Depositor
Resolution (Å)	50.00 – 2.25 50.00 – 2.25	Depositor EDS
% Data completeness (in resolution range)	94.1 (50.00-2.25) 94.0 (50.00-2.25)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.46 (at 2.25Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.171 , 0.202 0.172 , 0.202	Depositor DCC
R_{free} test set	13416 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	19.6	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 46.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.004 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	33797	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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: DMS, NA, K, B3N, ZN

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	0.44	0/2636	0.88	2/3582 (0.1%)
1	B	0.42	0/2636	0.85	2/3582 (0.1%)
1	C	0.43	0/2636	0.87	3/3582 (0.1%)
1	D	0.43	0/2636	0.87	3/3582 (0.1%)
1	E	0.41	0/2636	0.86	1/3582 (0.0%)
1	F	0.41	0/2636	0.86	3/3582 (0.1%)
1	G	0.42	0/2636	0.85	1/3582 (0.0%)
1	H	0.42	0/2636	0.87	1/3582 (0.0%)
1	I	0.41	0/2636	0.87	2/3582 (0.1%)
1	J	0.40	0/2631	0.85	2/3577 (0.1%)
1	K	0.43	0/2636	0.88	3/3582 (0.1%)
1	L	0.42	0/2636	0.86	0/3582
All	All	0.42	0/31627	0.86	23/42979 (0.1%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	205	ILE	N-CA-C	6.06	116.80	110.62
1	E	205	ILE	N-CA-C	5.71	116.44	110.62
1	C	217	LEU	N-CA-C	-5.61	100.56	109.59
1	J	205	ILE	N-CA-C	5.48	116.21	110.62
1	J	228	PHE	N-CA-C	5.46	119.26	112.59
1	D	225	PHE	N-CA-C	-5.36	103.43	109.60
1	C	16	THR	N-CA-C	5.36	117.96	109.50
1	A	320	GLU	CB-CA-C	-5.32	108.77	116.54
1	B	205	ILE	N-CA-C	5.30	116.03	110.62
1	K	295	LYS	N-CA-C	5.30	116.80	109.54
1	F	225	PHE	N-CA-C	-5.30	102.48	109.84
1	F	321	GLY	N-CA-C	5.29	120.34	112.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	158	HIS	N-CA-C	5.25	119.18	112.87
1	H	295	LYS	N-CA-C	5.23	116.71	109.54
1	D	281	LEU	N-CA-C	5.19	117.21	108.96
1	I	295	LYS	N-CA-C	5.14	116.59	109.54
1	G	205	ILE	N-CA-C	5.13	115.34	110.42
1	A	16	THR	N-CA-C	5.11	117.57	109.50
1	I	228	PHE	N-CA-C	5.07	118.77	112.59
1	K	228	PHE	N-CA-C	5.04	118.96	112.41
1	C	205	ILE	N-CA-C	5.03	115.75	110.62
1	B	320	GLU	CB-CA-C	-5.01	109.22	116.54
1	D	116	ALA	N-CA-C	5.00	119.15	113.19

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	2568	0	2490	35	0
1	B	2568	0	2491	31	0
1	C	2568	0	2490	32	0
1	D	2568	0	2490	44	0
1	E	2568	0	2490	31	0
1	F	2568	0	2490	36	0
1	G	2568	0	2491	30	0
1	H	2568	0	2490	36	0
1	I	2568	0	2491	25	0
1	J	2563	0	2488	38	0
1	K	2568	0	2491	35	0
1	L	2568	0	2490	34	0
2	A	40	0	60	0	0
2	B	36	0	54	3	0
2	C	24	0	36	3	0
2	D	44	0	66	1	0
2	E	40	0	60	2	0
2	F	44	0	66	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	40	0	60	2	0
2	H	32	0	48	0	0
2	I	32	0	48	0	0
2	J	28	0	42	2	0
2	K	40	0	60	1	0
2	L	32	0	48	1	0
3	A	22	0	24	0	0
3	B	22	0	24	0	0
3	C	22	0	24	0	0
3	D	22	0	24	0	0
3	E	22	0	24	0	0
3	F	22	0	24	0	0
3	G	22	0	24	0	0
3	H	22	0	24	1	0
3	I	22	0	24	0	0
3	J	22	0	24	1	0
3	K	22	0	24	1	0
3	L	22	0	24	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
4	G	2	0	0	0	0
4	H	2	0	0	0	0
4	I	1	0	0	0	0
4	J	2	0	0	0	0
4	K	2	0	0	0	0
4	L	2	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
5	L	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
6	I	1	0	0	0	0
6	J	1	0	0	0	0
6	K	1	0	0	0	0
6	L	1	0	0	0	0
7	A	184	0	0	1	0
7	B	165	0	0	2	0
7	C	192	0	0	3	0
7	D	187	0	0	5	0
7	E	181	0	0	1	0
7	F	196	0	0	2	0
7	G	184	0	0	2	0
7	H	183	0	0	1	0
7	I	204	0	0	0	0
7	J	174	0	0	1	0
7	K	211	0	0	1	0
7	L	182	0	0	1	0
All	All	33797	0	30818	404	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 (404) 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:E:289:ASP:OD1	1:E:291:ILE:HG13	1.84	0.78
1:E:284:ASP:HB2	1:E:291:ILE:HD11	1.70	0.73
1:G:289:ASP:OD1	1:G:291:ILE:HG12	1.89	0.72
1:C:284:ASP:HB3	1:C:322:GLY:HA2	1.71	0.72
2:G:417:DMS:H21	7:G:2267:HOH:O	1.88	0.72
1:E:18:LEU:HD23	1:H:90:THR:HG22	1.74	0.69
1:L:157:GLY:HA2	1:L:169:CYS:HB3	1.73	0.69
1:E:291:ILE:HD12	1:E:291:ILE:C	2.18	0.68
1:C:251:ARG:HG3	7:C:2114:HOH:O	1.94	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:289:ASP:OD1	1:J:291:ILE:HG12	1.94	0.67
1:D:114:ASN:HD22	1:D:164:MET:HG3	1.60	0.67
1:F:157:GLY:HA2	1:F:169:CYS:HB3	1.77	0.66
1:K:157:GLY:HA2	1:K:169:CYS:HB3	1.76	0.66
1:K:284:ASP:HB3	1:K:322:GLY:HA2	1.78	0.66
1:K:7:GLU:O	1:K:10:LYS:HG2	1.95	0.66
1:B:157:GLY:HA2	1:B:169:CYS:HB3	1.78	0.65
1:D:157:GLY:HA2	1:D:169:CYS:HB3	1.77	0.65
1:G:306:ARG:HD2	1:G:338:GLY:O	1.96	0.65
1:H:51:PRO:HA	1:H:137:ASP:OD2	1.97	0.64
1:A:35:TRP:HA	1:A:35:TRP:CE3	2.33	0.64
1:L:284:ASP:HB3	1:L:322:GLY:HA2	1.79	0.64
1:C:157:GLY:HA2	1:C:169:CYS:HB3	1.79	0.64
1:K:75:TRP:CE2	1:K:122:PRO:HG3	2.33	0.64
1:C:306:ARG:HG2	1:C:338:GLY:O	1.98	0.63
1:C:4:ILE:N	1:C:4:ILE:HD12	2.13	0.63
1:G:157:GLY:HA2	1:G:169:CYS:HB3	1.81	0.63
1:I:157:GLY:HA2	1:I:169:CYS:HB3	1.81	0.63
1:F:289:ASP:OD1	1:F:291:ILE:HG12	1.99	0.63
1:H:75:TRP:CE2	1:H:122:PRO:HG3	2.34	0.62
1:A:251:ARG:HG3	7:A:1782:HOH:O	1.99	0.62
1:H:284:ASP:HB3	1:H:322:GLY:HA2	1.80	0.62
1:J:157:GLY:HA2	1:J:169:CYS:HB3	1.81	0.62
1:D:289:ASP:OD1	1:D:291:ILE:HG12	2.01	0.61
1:C:37:LEU:HG	1:C:41:LYS:HE3	1.82	0.61
1:D:37:LEU:HG	1:D:41:LYS:HE3	1.81	0.61
1:E:180:ARG:O	1:E:184:LYS:HG2	2.01	0.60
1:D:41:LYS:HE2	1:D:48:VAL:HG21	1.83	0.60
1:A:35:TRP:HA	1:A:35:TRP:HE3	1.67	0.60
1:A:289:ASP:OD1	1:A:291:ILE:HG12	2.01	0.60
1:F:268:ARG:HD3	7:F:1554:HOH:O	2.01	0.60
1:H:157:GLY:HA2	1:H:169:CYS:HB3	1.84	0.59
1:H:35:TRP:HA	1:H:35:TRP:CE3	2.36	0.59
1:A:75:TRP:CE2	1:A:122:PRO:HG3	2.37	0.59
1:B:4:ILE:HD11	1:B:141:LEU:HD11	1.83	0.59
1:D:286:PHE:CE2	1:D:288:GLN:HB2	2.37	0.59
1:J:251:ARG:HA	1:J:293:PHE:CD2	2.38	0.59
1:D:75:TRP:CE2	1:D:122:PRO:HG3	2.37	0.59
1:A:157:GLY:HA2	1:A:169:CYS:HB3	1.84	0.58
1:L:115:ALA:HB1	1:L:117:GLU:OE1	2.03	0.58
1:H:115:ALA:HB1	1:H:117:GLU:OE1	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:140:ASP:OD1	1:J:184:LYS:HE3	2.04	0.58
1:G:87:ALA:HB3	1:G:120:ILE:HB	1.86	0.58
1:F:75:TRP:CE2	1:F:122:PRO:HG3	2.39	0.58
1:H:251:ARG:HA	1:H:293:PHE:CD2	2.39	0.57
1:J:75:TRP:CE2	1:J:122:PRO:HG3	2.39	0.57
1:E:251:ARG:HA	1:E:293:PHE:CD2	2.39	0.57
1:F:280:SER:HB3	1:F:320:GLU:HG3	1.85	0.57
1:F:286:PHE:CE2	1:F:288:GLN:HB2	2.39	0.57
1:J:51:PRO:HA	1:J:137:ASP:OD1	2.04	0.57
1:C:286:PHE:CE2	1:C:288:GLN:HB2	2.40	0.57
1:I:309:ALA:HA	1:I:315:LEU:HD11	1.87	0.57
1:K:84:LYS:HB2	1:K:84:LYS:NZ	2.20	0.57
1:I:87:ALA:HB3	1:I:120:ILE:HB	1.86	0.57
1:A:90:THR:HG22	1:I:18:LEU:HD23	1.87	0.56
1:B:328:ILE:HG23	1:B:329:GLY:N	2.21	0.56
1:G:7:GLU:O	1:G:10:LYS:HG2	2.05	0.56
1:G:75:TRP:CE2	1:G:122:PRO:HG3	2.41	0.56
1:J:309:ALA:HA	1:J:315:LEU:HD11	1.87	0.56
1:B:289:ASP:OD1	1:B:291:ILE:HG12	2.05	0.56
1:A:328:ILE:HG23	1:A:329:GLY:N	2.20	0.56
1:K:51:PRO:HA	1:K:137:ASP:OD1	2.06	0.56
1:A:258:TRP:CH2	1:A:304:MET:HE2	2.41	0.55
1:A:309:ALA:HA	1:A:315:LEU:HD11	1.88	0.55
1:B:87:ALA:HB3	1:B:120:ILE:HB	1.87	0.55
1:E:157:GLY:HA2	1:E:169:CYS:HB3	1.88	0.55
1:H:35:TRP:HA	1:H:35:TRP:HE3	1.70	0.55
1:I:75:TRP:CE2	1:I:122:PRO:HG3	2.41	0.55
1:K:84:LYS:HB2	1:K:84:LYS:HZ2	1.71	0.55
1:A:75:TRP:NE1	1:A:122:PRO:HG3	2.21	0.55
1:D:104:ASP:O	1:D:108:GLN:HG3	2.06	0.55
1:H:7:GLU:O	1:H:10:LYS:HG2	2.06	0.55
1:B:280:SER:HB3	1:B:320:GLU:HG3	1.88	0.55
1:C:328:ILE:HG23	1:C:329:GLY:N	2.22	0.55
1:F:121:SER:HB2	1:F:122:PRO:CD	2.37	0.55
1:J:286:PHE:CE2	1:J:288:GLN:HB2	2.42	0.55
1:F:15:LYS:HE2	1:F:15:LYS:HA	1.88	0.54
1:L:251:ARG:HA	1:L:293:PHE:CD2	2.42	0.54
1:B:75:TRP:CE2	1:B:122:PRO:HG3	2.43	0.54
1:L:75:TRP:CE2	1:L:122:PRO:HG3	2.41	0.54
1:L:75:TRP:NE1	1:L:122:PRO:HG3	2.23	0.54
1:L:258:TRP:CH2	1:L:304:MET:HE2	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:29:ALA:HB3	1:J:31:PHE:CE1	2.43	0.54
1:D:87:ALA:HB3	1:D:120:ILE:HB	1.90	0.54
1:G:251:ARG:HA	1:G:293:PHE:CD2	2.43	0.54
1:B:298:SER:HB2	1:B:299:PRO:HD3	1.90	0.54
1:H:289:ASP:OD1	1:H:291:ILE:HG12	2.07	0.54
1:C:2:ARG:HD2	1:C:141:LEU:HD11	1.90	0.53
1:K:298:SER:HB2	1:K:299:PRO:HD3	1.90	0.53
1:E:87:ALA:HB3	1:E:120:ILE:HB	1.91	0.53
1:E:284:ASP:CB	1:E:291:ILE:HD11	2.38	0.53
1:J:5:PHE:CD1	1:J:152:LEU:HD13	2.42	0.53
1:B:286:PHE:CE2	1:B:288:GLN:HB2	2.43	0.53
1:A:87:ALA:HB3	1:A:120:ILE:HB	1.91	0.53
1:L:35:TRP:CZ3	1:L:326:PRO:HA	2.44	0.53
1:C:280:SER:HB3	1:C:320:GLU:HG3	1.90	0.53
1:I:284:ASP:HB3	1:I:322:GLY:HA2	1.91	0.52
1:K:286:PHE:CE2	1:K:288:GLN:HB2	2.45	0.52
1:F:121:SER:HB2	1:F:122:PRO:HD2	1.92	0.52
1:G:101:ILE:HG12	1:G:111:TYR:CZ	2.45	0.52
1:K:289:ASP:OD1	1:K:291:ILE:HG12	2.09	0.52
1:B:309:ALA:HA	1:B:315:LEU:HD11	1.90	0.52
1:E:291:ILE:HD12	1:E:292:SER:N	2.25	0.52
1:J:115:ALA:HB1	1:J:117:GLU:OE1	2.08	0.52
1:B:148:ALA:HA	1:B:315:LEU:O	2.09	0.52
1:D:18:LEU:HD23	1:J:90:THR:HG22	1.90	0.52
1:J:91:SER:O	1:J:110:GLY:HA3	2.10	0.52
1:D:146:HIS:HD2	7:D:435:HOH:O	1.93	0.52
1:J:148:ALA:HA	1:J:315:LEU:O	2.10	0.52
1:E:101:ILE:HG12	1:E:111:TYR:CZ	2.44	0.52
1:G:258:TRP:CH2	1:G:304:MET:HE2	2.45	0.52
1:K:258:TRP:CZ3	1:K:304:MET:HE2	2.44	0.52
1:A:15:LYS:HE2	1:A:15:LYS:HA	1.91	0.51
1:J:4:ILE:HG22	1:J:51:PRO:HG3	1.92	0.51
1:H:258:TRP:CH2	1:H:304:MET:HE2	2.45	0.51
1:I:196:PHE:CG	1:I:292:SER:HB2	2.46	0.51
1:K:225:PHE:CD2	3:K:401:B3N:H81	2.45	0.51
1:K:280:SER:HB3	1:K:320:GLU:HG3	1.92	0.51
1:I:51:PRO:HA	1:I:137:ASP:OD2	2.10	0.51
1:C:298:SER:HB2	1:C:299:PRO:HD3	1.92	0.51
1:L:112:TYR:O	1:L:164:MET:HA	2.11	0.51
1:E:251:ARG:HG3	7:E:1995:HOH:O	2.10	0.50
1:A:92:PHE:HZ	1:A:116:ALA:HB2	1.77	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:3:VAL:HB	1:L:48:VAL:HG22	1.93	0.50
1:G:83:TYR:CZ	2:G:342:DMS:H23	2.47	0.50
1:F:298:SER:HB2	1:F:299:PRO:HD3	1.93	0.50
1:F:209:ARG:HD2	7:F:1274:HOH:O	2.11	0.50
1:I:115:ALA:HB1	1:I:117:GLU:OE1	2.11	0.50
1:A:121:SER:HB2	1:A:122:PRO:CD	2.42	0.50
1:B:251:ARG:HA	1:B:293:PHE:CD2	2.46	0.50
1:L:87:ALA:HB3	1:L:120:ILE:HB	1.93	0.50
1:B:78:TRP:CE2	1:B:87:ALA:HA	2.47	0.50
1:D:15:LYS:HG2	1:D:86:GLU:OE2	2.11	0.50
1:G:298:SER:HB2	1:G:299:PRO:HD3	1.94	0.50
1:A:148:ALA:HA	1:A:315:LEU:O	2.11	0.49
1:C:75:TRP:CE2	1:C:122:PRO:HG3	2.47	0.49
1:G:280:SER:HB3	1:G:320:GLU:HG3	1.94	0.49
1:F:148:ALA:HA	1:F:315:LEU:O	2.12	0.49
1:F:251:ARG:HA	1:F:293:PHE:CD2	2.47	0.49
1:J:4:ILE:HD11	1:J:141:LEU:HD11	1.94	0.49
1:L:286:PHE:CE2	1:L:288:GLN:HB2	2.48	0.49
1:D:35:TRP:HA	1:D:35:TRP:CE3	2.47	0.49
1:F:115:ALA:HB1	1:F:117:GLU:OE1	2.12	0.49
1:I:251:ARG:HA	1:I:293:PHE:CD2	2.47	0.49
1:A:115:ALA:HB1	1:A:117:GLU:OE1	2.13	0.49
1:E:83:TYR:CZ	2:E:342:DMS:H23	2.48	0.49
1:F:75:TRP:NE1	1:F:122:PRO:HG3	2.27	0.49
1:H:290:PRO:HB2	3:H:407:B3N:H212	1.94	0.49
1:I:5:PHE:CD1	1:I:152:LEU:HD13	2.48	0.49
1:L:92:PHE:HZ	1:L:116:ALA:HB2	1.77	0.49
1:D:309:ALA:HA	1:D:315:LEU:HD11	1.94	0.49
1:J:277:ILE:HB	1:J:315:LEU:HD23	1.94	0.49
1:B:18:LEU:HD23	1:F:90:THR:HG22	1.95	0.48
1:B:258:TRP:CH2	1:B:304:MET:HE2	2.48	0.48
1:E:121:SER:HB2	1:E:122:PRO:CD	2.43	0.48
1:F:258:TRP:CH2	1:F:304:MET:HE2	2.48	0.48
1:K:251:ARG:HA	1:K:293:PHE:CD2	2.48	0.48
1:B:29:ALA:HB3	1:B:31:PHE:CE1	2.49	0.48
1:C:92:PHE:HZ	1:C:116:ALA:HB2	1.78	0.48
1:J:126:GLU:CD	1:J:126:GLU:H	2.21	0.48
1:J:258:TRP:CH2	1:J:304:MET:HE2	2.48	0.48
1:F:309:ALA:HA	1:F:315:LEU:HD11	1.96	0.48
1:G:251:ARG:HG3	7:G:2031:HOH:O	2.13	0.48
1:H:78:TRP:CE2	1:H:87:ALA:HA	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:154:ARG:HA	1:L:155:PRO:C	2.38	0.48
1:H:91:SER:O	1:H:110:GLY:HA3	2.13	0.48
2:C:405:DMS:H11	7:C:1167:HOH:O	2.13	0.48
1:E:291:ILE:C	1:E:291:ILE:CD1	2.86	0.48
1:J:87:ALA:HB3	1:J:120:ILE:HB	1.95	0.48
1:G:335:VAL:O	1:G:339:VAL:HG23	2.13	0.48
1:H:298:SER:HB2	1:H:299:PRO:HD3	1.95	0.48
1:E:75:TRP:CE2	1:E:122:PRO:HG3	2.49	0.48
1:I:121:SER:HB2	1:I:122:PRO:CD	2.44	0.48
1:B:115:ALA:HB1	1:B:117:GLU:OE1	2.13	0.47
1:H:286:PHE:CE2	1:H:288:GLN:HB2	2.48	0.47
1:F:196:PHE:CD1	1:F:292:SER:HB2	2.49	0.47
1:K:148:ALA:HA	1:K:315:LEU:O	2.14	0.47
1:L:196:PHE:CD1	1:L:292:SER:HB2	2.49	0.47
1:D:251:ARG:HA	1:D:293:PHE:CD2	2.49	0.47
1:K:91:SER:O	1:K:110:GLY:HA3	2.14	0.47
1:H:112:TYR:O	1:H:164:MET:HA	2.15	0.47
1:I:148:ALA:HA	1:I:315:LEU:O	2.14	0.47
1:K:213:PHE:HB2	1:K:272:PHE:CD2	2.49	0.47
1:K:121:SER:HB2	1:K:122:PRO:CD	2.45	0.47
1:A:91:SER:O	1:A:110:GLY:HA3	2.15	0.47
1:I:121:SER:HB2	1:I:122:PRO:HD2	1.97	0.47
1:C:112:TYR:O	1:C:164:MET:HA	2.15	0.47
1:F:114:ASN:HD22	1:F:164:MET:HG3	1.80	0.47
1:D:4:ILE:HD11	1:D:141:LEU:HD11	1.97	0.46
1:E:280:SER:HB3	1:E:320:GLU:HG3	1.97	0.46
1:H:196:PHE:CD1	1:H:292:SER:HB2	2.50	0.46
1:I:298:SER:HB2	1:I:299:PRO:HD3	1.97	0.46
1:J:112:TYR:O	1:J:164:MET:HA	2.15	0.46
1:C:289:ASP:OD1	1:C:291:ILE:HG12	2.15	0.46
1:F:101:ILE:HG12	1:F:111:TYR:CZ	2.50	0.46
1:F:196:PHE:CG	1:F:292:SER:HB2	2.51	0.46
1:H:75:TRP:NE1	1:H:122:PRO:HG3	2.31	0.46
1:C:146:HIS:HD2	7:C:452:HOH:O	1.98	0.46
1:F:78:TRP:CE2	1:F:87:ALA:HA	2.51	0.46
1:H:39:ALA:HA	1:H:42:GLU:HG2	1.98	0.46
1:E:309:ALA:HA	1:E:315:LEU:HD11	1.97	0.46
1:A:251:ARG:HA	1:A:293:PHE:CD2	2.50	0.46
1:C:78:TRP:CE2	1:C:87:ALA:HA	2.51	0.46
1:A:280:SER:HB3	1:A:320:GLU:HG3	1.98	0.46
1:F:284:ASP:O	1:F:292:SER:HB3	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:115:ALA:HB1	1:G:117:GLU:OE1	2.16	0.46
1:G:188:LYS:HD2	1:G:272:PHE:CZ	2.51	0.46
1:L:298:SER:HB2	1:L:299:PRO:HD3	1.98	0.46
1:E:121:SER:HB2	1:E:122:PRO:HD2	1.97	0.46
1:H:87:ALA:HB3	1:H:120:ILE:HB	1.99	0.45
1:J:328:ILE:HG23	1:J:329:GLY:N	2.31	0.45
1:E:114:ASN:HD22	1:E:164:MET:HG3	1.82	0.45
1:G:121:SER:HB2	1:G:122:PRO:CD	2.47	0.45
1:G:328:ILE:HG23	1:G:329:GLY:N	2.31	0.45
1:I:289:ASP:OD1	1:I:291:ILE:HG12	2.16	0.45
1:C:258:TRP:CH2	1:C:304:MET:HE2	2.50	0.45
1:E:187:LYS:C	1:E:188:LYS:HG2	2.41	0.45
1:E:197:HIS:HE1	1:E:291:ILE:HD13	1.81	0.45
1:I:140:ASP:OD1	1:I:184:LYS:HE3	2.16	0.45
1:I:325:VAL:HB	1:I:327:GLU:OE2	2.16	0.45
1:K:196:PHE:CG	1:K:292:SER:HB2	2.50	0.45
1:K:328:ILE:HG23	1:K:329:GLY:N	2.31	0.45
1:D:115:ALA:HB1	1:D:117:GLU:OE1	2.16	0.45
1:F:154:ARG:HA	1:F:155:PRO:C	2.42	0.45
1:G:286:PHE:CE2	1:G:288:GLN:HB2	2.52	0.45
1:L:121:SER:HB2	1:L:122:PRO:CD	2.47	0.45
1:L:283:VAL:HG21	1:L:328:ILE:HG13	1.98	0.45
1:K:258:TRP:CH2	1:K:304:MET:HE2	2.51	0.45
1:A:298:SER:HB2	1:A:299:PRO:HD3	1.97	0.45
1:D:328:ILE:HG23	1:D:329:GLY:N	2.31	0.45
2:D:343:DMS:H13	1:J:234:GLU:HG2	1.99	0.45
1:G:29:ALA:HB3	1:G:31:PHE:CE1	2.52	0.45
1:L:92:PHE:CZ	1:L:116:ALA:HB2	2.52	0.45
1:B:196:PHE:CG	1:B:292:SER:HB2	2.51	0.45
1:D:193:ASP:HA	1:D:280:SER:HB2	1.99	0.45
1:B:251:ARG:HG3	7:B:1754:HOH:O	2.16	0.45
1:E:1:MET:SD	1:E:336:LEU:HD22	2.57	0.45
1:E:112:TYR:O	1:E:164:MET:HA	2.16	0.45
1:K:154:ARG:HA	1:K:155:PRO:C	2.41	0.45
1:L:328:ILE:HG23	1:L:329:GLY:N	2.32	0.45
1:A:187:LYS:C	1:A:188:LYS:HG2	2.41	0.45
1:K:87:ALA:HB3	1:K:120:ILE:HB	1.98	0.45
1:L:67:TYR:OH	1:L:165:PHE:HB3	2.17	0.45
1:A:121:SER:HB2	1:A:122:PRO:HD2	1.99	0.44
1:C:104:ASP:O	1:C:108:GLN:HG3	2.17	0.44
1:J:83:TYR:CZ	2:J:403:DMS:H23	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:GLU:H	1:A:126:GLU:CD	2.25	0.44
1:C:88:ILE:HG12	1:C:119:ALA:HB2	1.99	0.44
1:C:121:SER:HB2	1:C:122:PRO:CD	2.47	0.44
1:G:323:TYR:HD2	1:G:325:VAL:HG13	1.82	0.44
1:L:289:ASP:OD1	1:L:291:ILE:HG12	2.18	0.44
1:B:104:ASP:O	1:B:108:GLN:HG3	2.17	0.44
1:D:121:SER:HB2	1:D:122:PRO:HD2	1.99	0.44
1:H:280:SER:HB3	1:H:320:GLU:HG3	1.99	0.44
1:A:89:ALA:HB2	1:A:109:ILE:HG12	1.98	0.44
1:A:328:ILE:HG23	1:A:329:GLY:H	1.81	0.44
1:D:77:ARG:HD3	7:D:838:HOH:O	2.17	0.44
1:G:309:ALA:C	1:G:311:SER:H	2.25	0.44
1:K:101:ILE:HG12	1:K:111:TYR:CZ	2.52	0.44
1:L:309:ALA:HA	1:L:315:LEU:HD11	1.98	0.44
2:B:403:DMS:H23	1:F:83:TYR:CZ	2.52	0.44
1:C:121:SER:HB2	1:C:122:PRO:HD2	1.99	0.44
1:D:11:LEU:HB2	1:D:127:ALA:HB2	1.99	0.44
1:H:121:SER:HB2	1:H:122:PRO:CD	2.47	0.44
1:J:129:LEU:HD13	2:J:423:DMS:H21	2.00	0.44
1:D:306:ARG:HD2	1:G:299:PRO:HB2	1.98	0.44
1:K:309:ALA:HA	1:K:315:LEU:HD11	1.98	0.44
1:H:148:ALA:HA	1:H:315:LEU:O	2.18	0.44
1:L:258:TRP:CZ3	1:L:304:MET:HE2	2.52	0.44
1:B:91:SER:O	1:B:110:GLY:HA3	2.17	0.44
1:C:87:ALA:HB3	1:C:120:ILE:HB	1.99	0.44
1:C:198:HIS:CE1	1:C:200:ASN:HA	2.51	0.44
1:E:328:ILE:HG23	1:E:329:GLY:N	2.33	0.44
1:L:91:SER:O	1:L:110:GLY:HA3	2.18	0.44
1:D:89:ALA:HB2	1:D:109:ILE:HG12	1.98	0.43
1:E:258:TRP:CH2	1:E:304:MET:HE2	2.53	0.43
1:I:280:SER:HB3	1:I:320:GLU:HG3	2.00	0.43
1:F:284:ASP:HB3	1:F:291:ILE:HD11	1.99	0.43
1:H:31:PHE:HD2	1:H:35:TRP:CD1	2.37	0.43
1:K:78:TRP:CE2	1:K:87:ALA:HA	2.53	0.43
1:B:253:THR:HG23	1:B:257:VAL:HB	2.00	0.43
1:C:10:LYS:NZ	1:C:10:LYS:HB3	2.32	0.43
1:D:78:TRP:CE2	1:D:87:ALA:HA	2.53	0.43
1:K:29:ALA:HB3	1:K:31:PHE:CD1	2.52	0.43
1:J:101:ILE:HG12	1:J:111:TYR:CZ	2.52	0.43
1:C:60:LEU:HD23	1:C:68:LEU:HD12	2.00	0.43
1:C:251:ARG:HA	1:C:293:PHE:CD2	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:112:TYR:O	1:K:164:MET:HA	2.18	0.43
1:L:117:GLU:HG3	3:L:407:B3N:H92	2.01	0.43
1:C:309:ALA:HA	1:C:315:LEU:HD11	2.00	0.43
1:E:298:SER:HB2	1:E:299:PRO:HD3	2.01	0.43
1:H:154:ARG:HA	1:H:155:PRO:C	2.43	0.43
1:J:105:ILE:HG23	1:J:106:GLU:N	2.33	0.43
1:J:168:TYR:CE2	3:J:407:B3N:H71	2.52	0.43
1:B:83:TYR:CZ	2:B:342:DMS:H23	2.54	0.43
1:C:53:ARG:HG3	2:C:423:DMS:H23	2.00	0.43
1:D:258:TRP:CH2	1:D:304:MET:HE2	2.54	0.43
1:D:269:ILE:O	1:D:272:PHE:HB3	2.18	0.43
1:D:299:PRO:HB2	1:G:306:ARG:HD3	2.00	0.43
1:E:197:HIS:CE1	1:E:291:ILE:HD13	2.54	0.43
1:F:112:TYR:O	1:F:164:MET:HA	2.18	0.43
1:J:196:PHE:CD1	1:J:292:SER:HB2	2.54	0.43
1:J:335:VAL:O	1:J:339:VAL:HG23	2.18	0.43
1:I:277:ILE:HB	1:I:315:LEU:CD2	2.49	0.43
1:J:121:SER:HB2	1:J:122:PRO:CD	2.49	0.43
1:K:75:TRP:CZ2	1:K:122:PRO:HG3	2.54	0.43
1:L:34:GLU:HG3	1:L:35:TRP:HD1	1.83	0.43
1:D:163:ASP:OD1	1:D:164:MET:HE2	2.17	0.43
1:D:284:ASP:HB3	1:D:322:GLY:HA2	2.01	0.43
1:G:154:ARG:HA	1:G:155:PRO:C	2.42	0.43
2:B:417:DMS:H23	1:L:69:ASN:HB2	2.01	0.42
1:A:286:PHE:CE2	1:A:288:GLN:HB2	2.54	0.42
1:B:123:GLY:HA2	1:B:126:GLU:OE1	2.19	0.42
1:F:328:ILE:HG23	1:F:329:GLY:N	2.34	0.42
1:K:277:ILE:HB	1:K:315:LEU:HD23	2.00	0.42
1:L:78:TRP:CE2	1:L:87:ALA:HA	2.55	0.42
1:D:227:HIS:ND1	7:D:812:HOH:O	2.27	0.42
1:F:193:ASP:HA	1:F:280:SER:HB2	2.00	0.42
1:H:140:ASP:OD1	1:H:184:LYS:HE3	2.20	0.42
1:D:75:TRP:HZ3	1:D:86:GLU:HA	1.84	0.42
1:D:121:SER:HB2	1:D:122:PRO:CD	2.49	0.42
1:D:196:PHE:CD1	1:D:292:SER:HB2	2.54	0.42
1:K:115:ALA:HB1	1:K:117:GLU:OE1	2.18	0.42
1:L:31:PHE:O	1:L:34:GLU:HG2	2.20	0.42
1:L:77:ARG:HD3	7:L:416:HOH:O	2.18	0.42
1:G:11:LEU:HD13	1:G:126:GLU:HB3	2.02	0.42
1:J:227:HIS:ND1	7:J:818:HOH:O	2.36	0.42
1:C:92:PHE:CZ	1:C:116:ALA:HB2	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:60:LEU:HD23	1:E:68:LEU:HD12	2.01	0.42
1:F:37:LEU:O	1:F:40:VAL:HG22	2.20	0.42
1:I:41:LYS:HE3	1:I:48:VAL:HG21	2.02	0.42
1:I:196:PHE:CD2	1:I:292:SER:HB2	2.54	0.42
1:K:277:ILE:HB	1:K:315:LEU:CD2	2.50	0.42
1:C:70:PHE:CZ	1:C:109:ILE:HA	2.54	0.42
1:G:112:TYR:O	1:G:164:MET:HA	2.19	0.42
1:J:277:ILE:HB	1:J:315:LEU:CD2	2.50	0.42
1:K:83:TYR:CZ	2:K:403:DMS:H23	2.55	0.42
1:A:92:PHE:CZ	1:A:116:ALA:HB2	2.54	0.42
1:H:77:ARG:HD3	7:H:364:HOH:O	2.19	0.42
1:A:252:GLY:O	1:A:295:LYS:HE2	2.20	0.42
1:G:92:PHE:HZ	1:G:116:ALA:HB2	1.84	0.42
1:G:148:ALA:HA	1:G:315:LEU:O	2.20	0.42
1:H:4:ILE:HD11	1:H:141:LEU:HD11	2.02	0.42
1:I:277:ILE:HB	1:I:315:LEU:HD23	2.01	0.42
1:L:191:ILE:HG12	1:L:278:VAL:HB	2.02	0.42
1:D:67:TYR:OH	1:D:165:PHE:HB3	2.19	0.41
1:F:4:ILE:HD11	1:F:141:LEU:HD11	2.02	0.41
1:J:301:TYR:O	1:J:335:VAL:HA	2.20	0.41
1:B:209:ARG:HD2	7:B:1593:HOH:O	2.19	0.41
2:E:403:DMS:H23	1:H:83:TYR:CZ	2.55	0.41
1:F:36:ILE:O	1:F:40:VAL:HG13	2.20	0.41
1:H:277:ILE:HB	1:H:315:LEU:HD23	2.01	0.41
1:A:154:ARG:HA	1:A:155:PRO:C	2.45	0.41
1:D:15:LYS:HG2	1:D:86:GLU:CD	2.45	0.41
1:D:209:ARG:HD2	7:D:1245:HOH:O	2.20	0.41
1:E:277:ILE:HB	1:E:315:LEU:CD2	2.50	0.41
1:B:112:TYR:O	1:B:164:MET:HA	2.20	0.41
1:F:54:HIS:NE2	1:F:137:ASP:OD1	2.47	0.41
1:G:121:SER:HB2	1:G:122:PRO:HD2	2.01	0.41
1:H:258:TRP:CZ3	1:H:304:MET:HE2	2.56	0.41
1:K:309:ALA:C	1:K:311:SER:H	2.28	0.41
1:C:91:SER:O	1:C:110:GLY:HA3	2.20	0.41
1:D:25:PRO:HA	1:D:26:PRO:HD3	1.96	0.41
1:I:67:TYR:OH	1:I:165:PHE:HB3	2.21	0.41
1:A:6:SER:HB2	1:A:51:PRO:HG3	2.02	0.41
1:A:193:ASP:HA	1:A:280:SER:HB2	2.02	0.41
1:H:92:PHE:HZ	1:H:116:ALA:HB2	1.86	0.41
1:J:302:ILE:HG22	1:J:306:ARG:NH2	2.35	0.41
1:B:7:GLU:O	1:B:10:LYS:HG2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:89:ALA:HB2	1:J:109:ILE:HG12	2.02	0.41
1:A:200:ASN:HB2	1:A:229:LEU:HD23	2.02	0.41
1:B:328:ILE:CG2	1:B:329:GLY:N	2.83	0.41
1:D:29:ALA:HB3	1:D:31:PHE:CE1	2.56	0.41
1:D:112:TYR:O	1:D:164:MET:HA	2.21	0.41
1:E:286:PHE:CE2	1:E:288:GLN:HB2	2.56	0.41
1:J:1:MET:SD	1:J:336:LEU:HD22	2.61	0.41
1:J:25:PRO:HA	1:J:26:PRO:HD3	1.94	0.41
1:L:126:GLU:H	1:L:126:GLU:CD	2.29	0.41
1:B:177:ALA:HB1	1:B:316:LEU:CD2	2.50	0.41
1:H:298:SER:N	1:H:299:PRO:CD	2.84	0.41
1:B:88:ILE:HG12	1:B:119:ALA:HB2	2.03	0.40
2:C:421:DMS:H11	7:K:580:HOH:O	2.20	0.40
1:D:37:LEU:O	1:D:41:LYS:HG3	2.21	0.40
1:D:148:ALA:HA	1:D:315:LEU:O	2.20	0.40
1:H:256:SER:O	1:H:260:GLU:HG3	2.21	0.40
1:A:25:PRO:HA	1:A:26:PRO:HD3	2.00	0.40
1:D:123:GLY:HA2	1:D:126:GLU:OE1	2.20	0.40
1:K:298:SER:N	1:K:299:PRO:CD	2.84	0.40
1:B:11:LEU:HB2	1:B:127:ALA:HB2	2.03	0.40
1:D:251:ARG:HG3	7:D:2143:HOH:O	2.22	0.40
1:F:5:PHE:CD1	1:F:152:LEU:HD13	2.57	0.40
1:F:106:GLU:CD	1:F:106:GLU:H	2.29	0.40
1:L:142:ILE:HG22	2:L:415:DMS:H13	2.03	0.40
1:A:140:ASP:OD1	1:A:184:LYS:HE3	2.21	0.40
1:I:247:TYR:OH	1:I:268:ARG:HD2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	339/341 (99%)	328 (97%)	10 (3%)	1 (0%)	36	40
1	B	339/341 (99%)	325 (96%)	13 (4%)	1 (0%)	36	40
1	C	339/341 (99%)	328 (97%)	10 (3%)	1 (0%)	36	40
1	D	339/341 (99%)	326 (96%)	12 (4%)	1 (0%)	36	40
1	E	339/341 (99%)	326 (96%)	12 (4%)	1 (0%)	36	40
1	F	339/341 (99%)	326 (96%)	12 (4%)	1 (0%)	36	40
1	G	339/341 (99%)	325 (96%)	13 (4%)	1 (0%)	36	40
1	H	339/341 (99%)	323 (95%)	15 (4%)	1 (0%)	36	40
1	I	339/341 (99%)	323 (95%)	15 (4%)	1 (0%)	36	40
1	J	338/341 (99%)	323 (96%)	14 (4%)	1 (0%)	36	40
1	K	339/341 (99%)	325 (96%)	13 (4%)	1 (0%)	36	40
1	L	339/341 (99%)	326 (96%)	12 (4%)	1 (0%)	36	40
All	All	4067/4092 (99%)	3904 (96%)	151 (4%)	12 (0%)	36	40

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	VAL
1	C	94	VAL
1	E	94	VAL
1	F	94	VAL
1	G	94	VAL
1	J	94	VAL
1	K	94	VAL
1	L	94	VAL
1	B	94	VAL
1	D	94	VAL
1	H	94	VAL
1	I	94	VAL

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	253/253 (100%)	252 (100%)	1 (0%)	84	89
1	B	253/253 (100%)	251 (99%)	2 (1%)	73	80
1	C	253/253 (100%)	250 (99%)	3 (1%)	63	74
1	D	253/253 (100%)	250 (99%)	3 (1%)	63	74
1	E	253/253 (100%)	252 (100%)	1 (0%)	84	89
1	F	253/253 (100%)	250 (99%)	3 (1%)	63	74
1	G	253/253 (100%)	249 (98%)	4 (2%)	55	66
1	H	253/253 (100%)	252 (100%)	1 (0%)	84	89
1	I	253/253 (100%)	250 (99%)	3 (1%)	63	74
1	J	253/253 (100%)	249 (98%)	4 (2%)	55	66
1	K	253/253 (100%)	251 (99%)	2 (1%)	73	80
1	L	253/253 (100%)	252 (100%)	1 (0%)	84	89
All	All	3036/3036 (100%)	3008 (99%)	28 (1%)	70	79

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LYS
1	B	137	ASP
1	B	284	ASP
1	C	4	ILE
1	C	10	LYS
1	C	117	GLU
1	D	10	LYS
1	D	137	ASP
1	D	306	ARG
1	E	284	ASP
1	F	91	SER
1	F	152	LEU
1	F	284	ASP
1	G	46	ASP
1	G	137	ASP
1	G	184	LYS
1	G	284	ASP
1	H	79	LYS
1	I	152	LEU
1	I	168	TYR
1	I	292	SER
1	J	10	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	18	LEU
1	J	91	SER
1	J	117	GLU
1	K	46	ASP
1	K	117	GLU
1	L	327	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	246	ASN
1	B	69	ASN
1	C	146	HIS
1	C	227	HIS
1	C	334	ASN
1	D	114	ASN
1	D	146	HIS
1	D	288	GLN
1	E	146	HIS
1	F	198	HIS
1	F	246	ASN
1	F	334	ASN
1	G	146	HIS
1	G	227	HIS
1	G	334	ASN
1	I	146	HIS
1	J	69	ASN
1	J	227	HIS
1	L	13	ASN
1	L	331	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 167 ligands modelled in this entry, 47 are monoatomic - leaving 120 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	DMS	F	405	-	3,3,3	0.91	0	3,3,3	1.01	0
2	DMS	D	423	-	3,3,3	0.92	0	3,3,3	1.04	0
2	DMS	K	413	-	3,3,3	0.95	0	3,3,3	1.05	0
2	DMS	E	421	-	3,3,3	0.89	0	3,3,3	1.03	0
2	DMS	D	342	-	3,3,3	0.92	0	3,3,3	1.02	0
2	DMS	F	411	-	3,3,3	0.88	0	3,3,3	1.03	0
3	B3N	G	401	6	22,22,22	2.28	9 (40%)	26,27,27	0.81	0
2	DMS	C	421	-	3,3,3	0.90	0	3,3,3	1.06	0
2	DMS	D	417	-	3,3,3	0.92	0	3,3,3	1.06	0
2	DMS	K	342	-	3,3,3	0.89	0	3,3,3	1.04	0
2	DMS	L	413	-	3,3,3	0.89	0	3,3,3	1.03	0
2	DMS	E	405	-	3,3,3	0.89	0	3,3,3	1.00	0
2	DMS	G	343	-	3,3,3	0.90	0	3,3,3	1.00	0
2	DMS	I	405	-	3,3,3	0.90	0	3,3,3	1.03	0
2	DMS	B	423	-	3,3,3	0.91	0	3,3,3	1.03	0
2	DMS	K	417	-	3,3,3	0.89	0	3,3,3	1.04	0
2	DMS	A	421	-	3,3,3	0.91	0	3,3,3	1.05	0
2	DMS	E	423	-	3,3,3	0.90	0	3,3,3	1.04	0
2	DMS	E	413	-	3,3,3	0.90	0	3,3,3	1.06	0
2	DMS	J	423	-	3,3,3	0.91	0	3,3,3	1.04	0
3	B3N	A	401	6	22,22,22	2.22	8 (36%)	26,27,27	0.80	0
3	B3N	F	407	6	22,22,22	2.12	7 (31%)	26,27,27	0.77	0
2	DMS	B	403	-	3,3,3	0.85	0	3,3,3	1.02	0
2	DMS	G	423	-	3,3,3	0.93	0	3,3,3	1.04	0
3	B3N	D	407	6	22,22,22	2.22	8 (36%)	26,27,27	0.80	0
2	DMS	A	415	-	3,3,3	0.91	0	3,3,3	1.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DMS	I	421	-	3,3,3	0.92	0	3,3,3	1.07	0
2	DMS	H	411	-	3,3,3	0.93	0	3,3,3	1.04	0
2	DMS	K	419	-	3,3,3	0.94	0	3,3,3	1.02	0
2	DMS	D	405	-	3,3,3	0.85	0	3,3,3	1.01	0
2	DMS	K	423	-	3,3,3	0.91	0	3,3,3	1.03	0
2	DMS	G	415	-	3,3,3	0.92	0	3,3,3	1.05	0
2	DMS	A	413	-	3,3,3	0.88	0	3,3,3	1.04	0
2	DMS	B	411	-	3,3,3	0.92	0	3,3,3	1.04	0
2	DMS	A	342	-	3,3,3	0.92	0	3,3,3	1.03	0
2	DMS	C	419	-	3,3,3	0.91	0	3,3,3	1.04	0
2	DMS	H	423	-	3,3,3	0.93	0	3,3,3	1.03	0
2	DMS	I	423	-	3,3,3	0.92	0	3,3,3	1.04	0
3	B3N	C	401	6	22,22,22	2.17	8 (36%)	26,27,27	0.96	1 (3%)
2	DMS	E	419	-	3,3,3	0.92	0	3,3,3	1.04	0
2	DMS	A	417	-	3,3,3	0.89	0	3,3,3	1.05	0
2	DMS	F	343	-	3,3,3	0.89	0	3,3,3	1.05	0
2	DMS	E	415	-	3,3,3	0.92	0	3,3,3	1.05	0
2	DMS	H	415	-	3,3,3	0.92	0	3,3,3	1.04	0
3	B3N	H	407	6	22,22,22	2.35	9 (40%)	26,27,27	0.89	1 (3%)
2	DMS	F	413	-	3,3,3	0.89	0	3,3,3	1.04	0
2	DMS	F	415	-	3,3,3	0.93	0	3,3,3	1.05	0
2	DMS	G	405	-	3,3,3	0.88	0	3,3,3	1.02	0
2	DMS	H	417	-	3,3,3	0.89	0	3,3,3	1.05	0
2	DMS	H	405	-	3,3,3	0.90	0	3,3,3	1.01	0
2	DMS	H	421	-	3,3,3	0.94	0	3,3,3	1.05	0
3	B3N	E	401	6	22,22,22	2.32	9 (40%)	26,27,27	0.78	0
2	DMS	B	415	-	3,3,3	0.94	0	3,3,3	1.03	0
2	DMS	B	342	-	3,3,3	0.89	0	3,3,3	1.04	0
2	DMS	D	419	-	3,3,3	0.89	0	3,3,3	1.06	0
2	DMS	J	419	-	3,3,3	0.91	0	3,3,3	1.05	0
3	B3N	B	407	6	22,22,22	2.28	9 (40%)	26,27,27	0.77	0
2	DMS	I	419	-	3,3,3	0.91	0	3,3,3	1.04	0
2	DMS	A	419	-	3,3,3	0.90	0	3,3,3	1.04	0
2	DMS	F	423	-	3,3,3	0.91	0	3,3,3	1.03	0
2	DMS	G	419	-	3,3,3	0.90	0	3,3,3	1.04	0
2	DMS	D	343	-	3,3,3	0.92	0	3,3,3	1.06	0
2	DMS	C	423	-	3,3,3	0.90	0	3,3,3	1.03	0
2	DMS	C	411	-	3,3,3	0.91	0	3,3,3	1.03	0
2	DMS	A	411	-	3,3,3	0.91	0	3,3,3	1.01	0
2	DMS	D	421	-	3,3,3	0.91	0	3,3,3	1.05	0
2	DMS	L	415	-	3,3,3	0.92	0	3,3,3	1.05	0
2	DMS	K	403	-	3,3,3	0.90	0	3,3,3	1.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DMS	A	423	-	3,3,3	0.91	0	3,3,3	1.02	0
2	DMS	A	405	-	3,3,3	0.87	0	3,3,3	1.01	0
2	DMS	C	415	-	3,3,3	0.92	0	3,3,3	1.03	0
2	DMS	F	421	-	3,3,3	0.91	0	3,3,3	1.05	0
2	DMS	L	417	-	3,3,3	0.88	0	3,3,3	1.05	0
2	DMS	H	413	-	3,3,3	0.90	0	3,3,3	1.03	0
2	DMS	D	411	-	3,3,3	0.94	0	3,3,3	1.03	0
2	DMS	F	419	-	3,3,3	0.90	0	3,3,3	1.04	0
2	DMS	D	403	-	3,3,3	0.93	0	3,3,3	1.05	0
2	DMS	G	417	-	3,3,3	0.93	0	3,3,3	1.01	0
2	DMS	L	421	-	3,3,3	0.90	0	3,3,3	1.04	0
2	DMS	L	405	-	3,3,3	0.92	0	3,3,3	1.02	0
2	DMS	L	342	-	3,3,3	0.92	0	3,3,3	1.07	0
2	DMS	K	411	-	3,3,3	0.92	0	3,3,3	1.03	0
2	DMS	B	405	-	3,3,3	0.90	0	3,3,3	1.00	0
2	DMS	B	413	-	3,3,3	0.92	0	3,3,3	1.05	0
2	DMS	E	411	-	3,3,3	0.93	0	3,3,3	1.03	0
2	DMS	K	405	-	3,3,3	0.90	0	3,3,3	1.03	0
2	DMS	E	417	-	3,3,3	0.91	0	3,3,3	1.05	0
2	DMS	F	342	-	3,3,3	0.95	0	3,3,3	1.04	0
2	DMS	I	417	-	3,3,3	0.92	0	3,3,3	1.05	0
2	DMS	B	417	-	3,3,3	0.91	0	3,3,3	1.04	0
2	DMS	F	417	-	3,3,3	0.89	0	3,3,3	1.05	0
2	DMS	G	413	-	3,3,3	0.90	0	3,3,3	1.04	0
2	DMS	I	411	-	3,3,3	0.93	0	3,3,3	1.04	0
2	DMS	I	415	-	3,3,3	0.93	0	3,3,3	1.07	0
2	DMS	J	403	-	3,3,3	0.89	0	3,3,3	1.04	0
2	DMS	H	419	-	3,3,3	0.91	0	3,3,3	1.03	0
2	DMS	K	415	-	3,3,3	0.92	0	3,3,3	1.05	0
2	DMS	G	403	-	3,3,3	0.88	0	3,3,3	1.03	0
2	DMS	L	423	-	3,3,3	0.91	0	3,3,3	1.05	0
3	B3N	L	407	6	22,22,22	2.21	8 (36%)	26,27,27	0.78	0
2	DMS	A	403	-	3,3,3	0.86	0	3,3,3	1.08	0
2	DMS	I	413	-	3,3,3	0.92	0	3,3,3	1.00	0
2	DMS	B	419	-	3,3,3	0.90	0	3,3,3	1.06	0
2	DMS	F	344	-	3,3,3	0.91	0	3,3,3	1.03	0
2	DMS	J	413	-	3,3,3	0.90	0	3,3,3	1.05	0
2	DMS	J	415	-	3,3,3	0.90	0	3,3,3	1.07	0
3	B3N	K	401	6	22,22,22	2.36	8 (36%)	26,27,27	0.91	1 (3%)
3	B3N	I	401	6	22,22,22	2.25	8 (36%)	26,27,27	0.81	0
2	DMS	C	405	-	3,3,3	0.95	0	3,3,3	1.00	0
2	DMS	D	415	-	3,3,3	0.93	0	3,3,3	1.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DMS	G	342	-	3,3,3	0.90	0	3,3,3	1.04	0
2	DMS	E	342	-	3,3,3	0.86	0	3,3,3	1.04	0
2	DMS	J	417	-	3,3,3	0.91	0	3,3,3	1.04	0
3	B3N	J	407	6	22,22,22	2.34	8 (36%)	26,27,27	1.02	1 (3%)
2	DMS	E	403	-	3,3,3	0.88	0	3,3,3	1.04	0
2	DMS	J	405	-	3,3,3	0.92	0	3,3,3	1.02	0
2	DMS	D	413	-	3,3,3	0.91	0	3,3,3	1.05	0
2	DMS	L	419	-	3,3,3	0.90	0	3,3,3	1.04	0
2	DMS	G	411	-	3,3,3	0.92	0	3,3,3	1.02	0
2	DMS	K	421	-	3,3,3	0.92	0	3,3,3	1.05	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	B3N	L	407	6	-	6/20/20/20	0/1/1/1
3	B3N	B	407	6	-	6/20/20/20	0/1/1/1
3	B3N	F	407	6	-	5/20/20/20	0/1/1/1
3	B3N	J	407	6	-	5/20/20/20	0/1/1/1
3	B3N	D	407	6	-	6/20/20/20	0/1/1/1
3	B3N	K	401	6	-	3/20/20/20	0/1/1/1
3	B3N	I	401	6	-	6/20/20/20	0/1/1/1
3	B3N	C	401	6	-	3/20/20/20	0/1/1/1
3	B3N	G	401	6	-	6/20/20/20	0/1/1/1
3	B3N	H	407	6	-	6/20/20/20	0/1/1/1
3	B3N	A	401	6	-	6/20/20/20	0/1/1/1
3	B3N	E	401	6	-	6/20/20/20	0/1/1/1

All (99) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	407	B3N	O4-N3	-6.78	1.23	1.40
3	C	401	B3N	O4-N3	-6.77	1.23	1.40
3	L	407	B3N	O4-N3	-6.77	1.23	1.40
3	A	401	B3N	O4-N3	-6.77	1.23	1.40
3	B	407	B3N	O4-N3	-6.77	1.23	1.40
3	H	407	B3N	O4-N3	-6.77	1.23	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	407	B3N	O4-N3	-6.77	1.23	1.40
3	G	401	B3N	O4-N3	-6.76	1.23	1.40
3	I	401	B3N	O4-N3	-6.76	1.23	1.40
3	E	401	B3N	O4-N3	-6.75	1.23	1.40
3	K	401	B3N	O4-N3	-6.75	1.23	1.40
3	J	407	B3N	O4-N3	-6.75	1.23	1.40
3	K	401	B3N	C17-N20	3.59	1.45	1.37
3	C	401	B3N	C17-N20	3.54	1.45	1.37
3	E	401	B3N	C17-N20	3.52	1.45	1.37
3	J	407	B3N	C17-N20	3.51	1.45	1.37
3	K	401	B3N	C19-C14	3.49	1.44	1.39
3	J	407	B3N	C19-C14	3.46	1.44	1.39
3	A	401	B3N	C17-N20	3.42	1.45	1.37
3	K	401	B3N	C18-C17	3.40	1.45	1.39
3	K	401	B3N	C19-C18	3.36	1.44	1.38
3	B	407	B3N	C17-N20	3.35	1.45	1.37
3	G	401	B3N	C17-N20	3.31	1.45	1.37
3	H	407	B3N	C18-C17	3.31	1.45	1.39
3	I	401	B3N	C17-N20	3.25	1.45	1.37
3	H	407	B3N	C19-C18	3.20	1.44	1.38
3	L	407	B3N	C17-N20	3.19	1.44	1.37
3	H	407	B3N	C16-C17	3.18	1.45	1.39
3	H	407	B3N	C19-C14	3.17	1.44	1.39
3	H	407	B3N	C17-N20	3.17	1.44	1.37
3	I	401	B3N	C18-C17	3.17	1.45	1.39
3	D	407	B3N	C17-N20	3.14	1.44	1.37
3	I	401	B3N	C19-C14	3.14	1.44	1.39
3	B	407	B3N	C19-C14	3.14	1.44	1.39
3	B	407	B3N	C16-C15	3.12	1.43	1.38
3	E	401	B3N	C16-C15	3.09	1.43	1.38
3	F	407	B3N	C17-N20	3.08	1.44	1.37
3	H	407	B3N	C16-C15	3.08	1.43	1.38
3	E	401	B3N	C19-C18	3.07	1.43	1.38
3	E	401	B3N	C19-C14	3.05	1.44	1.39
3	L	407	B3N	C19-C14	3.05	1.44	1.39
3	J	407	B3N	C18-C17	3.04	1.45	1.39
3	J	407	B3N	C19-C18	3.03	1.43	1.38
3	A	401	B3N	C19-C14	3.00	1.44	1.39
3	G	401	B3N	C18-C17	2.99	1.44	1.39
3	E	401	B3N	C18-C17	2.99	1.44	1.39
3	G	401	B3N	C19-C18	2.99	1.43	1.38
3	G	401	B3N	C19-C14	2.97	1.43	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	401	B3N	C16-C15	2.96	1.43	1.38
3	I	401	B3N	C19-C18	2.96	1.43	1.38
3	K	401	B3N	C16-C17	2.95	1.44	1.39
3	D	407	B3N	C19-C14	2.95	1.43	1.39
3	L	407	B3N	C18-C17	2.93	1.44	1.39
3	J	407	B3N	C16-C15	2.92	1.43	1.38
3	L	407	B3N	C19-C18	2.91	1.43	1.38
3	D	407	B3N	C18-C17	2.91	1.44	1.39
3	B	407	B3N	C18-C17	2.87	1.44	1.39
3	D	407	B3N	C16-C15	2.85	1.43	1.38
3	C	401	B3N	C19-C14	2.85	1.43	1.39
3	G	401	B3N	C16-C15	2.83	1.43	1.38
3	B	407	B3N	C19-C18	2.82	1.43	1.38
3	J	407	B3N	C16-C17	2.81	1.44	1.39
3	F	407	B3N	C19-C14	2.81	1.43	1.39
3	D	407	B3N	C16-C17	2.80	1.44	1.39
3	B	407	B3N	C16-C17	2.79	1.44	1.39
3	G	401	B3N	C16-C17	2.77	1.44	1.39
3	A	401	B3N	C16-C17	2.74	1.44	1.39
3	F	407	B3N	C18-C17	2.73	1.44	1.39
3	I	401	B3N	C16-C15	2.72	1.43	1.38
3	A	401	B3N	C16-C15	2.71	1.43	1.38
3	C	401	B3N	C19-C18	2.71	1.43	1.38
3	D	407	B3N	C19-C18	2.71	1.43	1.38
3	A	401	B3N	C19-C18	2.69	1.43	1.38
3	L	407	B3N	C16-C17	2.69	1.44	1.39
3	K	401	B3N	C15-C14	2.69	1.43	1.39
3	E	401	B3N	C16-C17	2.68	1.44	1.39
3	A	401	B3N	C18-C17	2.68	1.44	1.39
3	I	401	B3N	C16-C17	2.63	1.44	1.39
3	L	407	B3N	C16-C15	2.62	1.43	1.38
3	C	401	B3N	C16-C17	2.62	1.44	1.39
3	F	407	B3N	C16-C17	2.60	1.44	1.39
3	D	407	B3N	C15-C14	2.59	1.43	1.39
3	E	401	B3N	C1-N3	2.58	1.35	1.32
3	J	407	B3N	C15-C14	2.57	1.43	1.39
3	H	407	B3N	C15-C14	2.56	1.43	1.39
3	F	407	B3N	C16-C15	2.54	1.42	1.38
3	C	401	B3N	C16-C15	2.50	1.42	1.38
3	G	401	B3N	C15-C14	2.49	1.43	1.39
3	C	401	B3N	C18-C17	2.43	1.43	1.39
3	E	401	B3N	C15-C14	2.37	1.43	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	401	B3N	C15-C14	2.33	1.42	1.39
3	G	401	B3N	C1-N3	2.31	1.34	1.32
3	B	407	B3N	C15-C14	2.30	1.42	1.39
3	A	401	B3N	C15-C14	2.30	1.42	1.39
3	F	407	B3N	C19-C18	2.27	1.42	1.38
3	B	407	B3N	C1-N3	2.18	1.34	1.32
3	H	407	B3N	C1-N3	2.14	1.34	1.32
3	L	407	B3N	C15-C14	2.11	1.42	1.39
3	C	401	B3N	C15-C14	2.06	1.42	1.39

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	407	B3N	C6-C5-C1	-3.55	103.34	113.19
3	C	401	B3N	C6-C5-C1	-3.02	104.81	113.19
3	H	407	B3N	O2-C1-N3	-2.44	120.28	123.27
3	K	401	B3N	C10-N12-C13	2.07	126.78	122.11

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	B3N	N3-C1-C5-C6
3	B	407	B3N	N3-C1-C5-C6
3	A	401	B3N	C1-C5-C6-C7
3	E	401	B3N	C1-C5-C6-C7
3	F	407	B3N	C1-C5-C6-C7
3	H	407	B3N	C1-C5-C6-C7
3	I	401	B3N	C1-C5-C6-C7
3	B	407	B3N	C1-C5-C6-C7
3	D	407	B3N	C1-C5-C6-C7
3	G	401	B3N	C1-C5-C6-C7
3	L	407	B3N	C1-C5-C6-C7
3	K	401	B3N	C1-C5-C6-C7
3	C	401	B3N	N12-C10-C9-C8
3	D	407	B3N	N12-C10-C9-C8
3	H	407	B3N	N12-C10-C9-C8
3	L	407	B3N	N12-C10-C9-C8
3	A	401	B3N	N12-C10-C9-C8
3	I	401	B3N	N12-C10-C9-C8
3	E	401	B3N	N12-C10-C9-C8
3	G	401	B3N	N12-C10-C9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	407	B3N	N3-C1-C5-C6
3	E	401	B3N	N3-C1-C5-C6
3	F	407	B3N	N3-C1-C5-C6
3	G	401	B3N	N3-C1-C5-C6
3	H	407	B3N	N3-C1-C5-C6
3	I	401	B3N	N3-C1-C5-C6
3	L	407	B3N	N3-C1-C5-C6
3	B	407	B3N	N12-C10-C9-C8
3	J	407	B3N	C5-C6-C7-C8
3	B	407	B3N	C7-C8-C9-C10
3	E	401	B3N	C6-C7-C8-C9
3	F	407	B3N	C6-C7-C8-C9
3	F	407	B3N	C7-C8-C9-C10
3	K	401	B3N	C6-C7-C8-C9
3	E	401	B3N	C7-C8-C9-C10
3	G	401	B3N	C7-C8-C9-C10
3	C	401	B3N	C6-C7-C8-C9
3	A	401	B3N	C7-C8-C9-C10
3	L	407	B3N	C7-C8-C9-C10
3	I	401	B3N	C7-C8-C9-C10
3	J	407	B3N	N12-C10-C9-C8
3	D	407	B3N	C7-C8-C9-C10
3	H	407	B3N	C7-C8-C9-C10
3	I	401	B3N	O2-C1-C5-C6
3	L	407	B3N	O2-C1-C5-C6
3	J	407	B3N	C6-C7-C8-C9
3	B	407	B3N	C6-C7-C8-C9
3	D	407	B3N	O2-C1-C5-C6
3	H	407	B3N	O2-C1-C5-C6
3	A	401	B3N	C6-C7-C8-C9
3	E	401	B3N	O2-C1-C5-C6
3	G	401	B3N	O2-C1-C5-C6
3	G	401	B3N	C6-C7-C8-C9
3	C	401	B3N	C7-C8-C9-C10
3	A	401	B3N	O2-C1-C5-C6
3	B	407	B3N	O2-C1-C5-C6
3	F	407	B3N	O2-C1-C5-C6
3	I	401	B3N	C6-C7-C8-C9
3	L	407	B3N	C6-C7-C8-C9
3	H	407	B3N	C6-C7-C8-C9
3	J	407	B3N	N3-C1-C5-C6
3	D	407	B3N	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	K	401	B3N	N12-C10-C9-C8
3	J	407	B3N	O2-C1-C5-C6

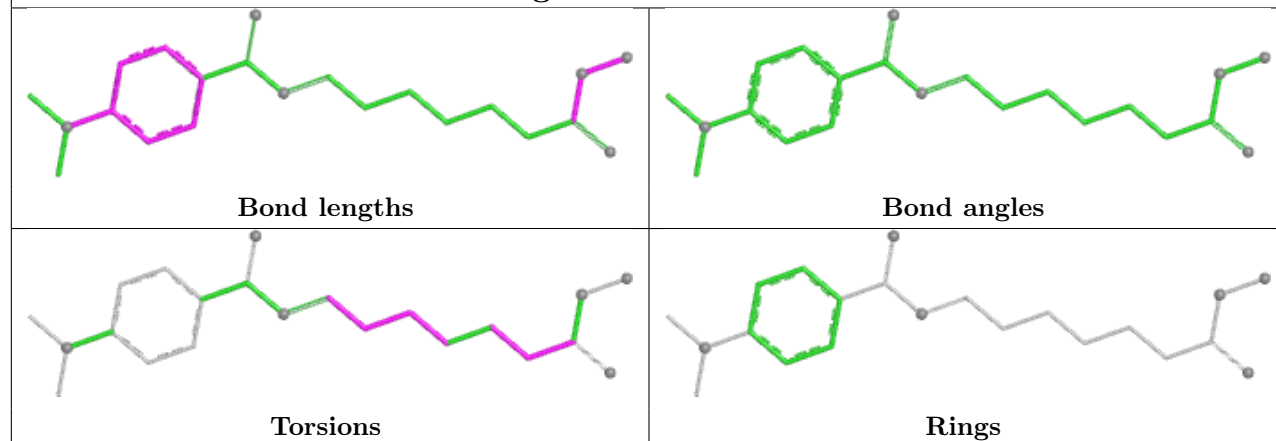
There are no ring outliers.

19 monomers are involved in 19 short contacts:

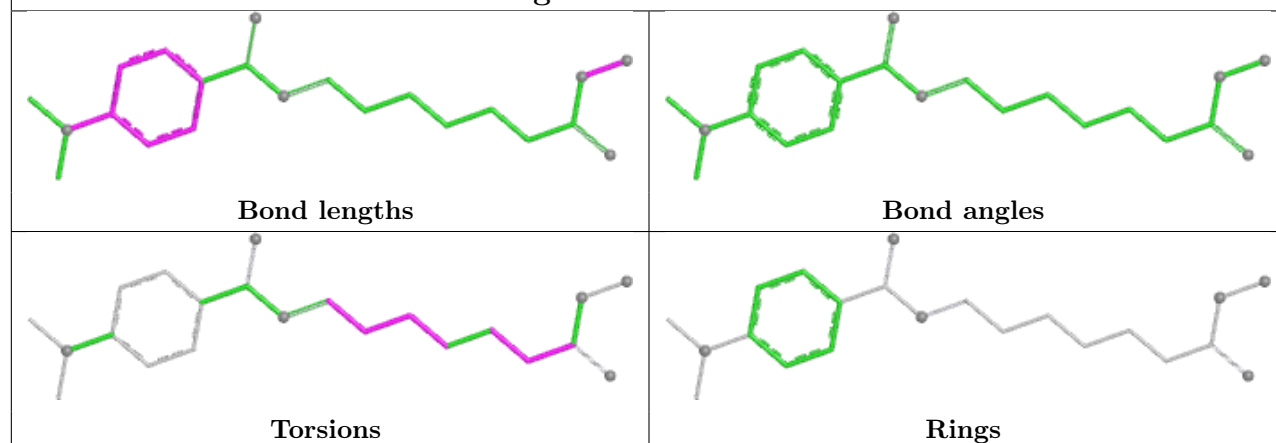
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	421	DMS	1	0
2	J	423	DMS	1	0
2	B	403	DMS	1	0
3	H	407	B3N	1	0
2	B	342	DMS	1	0
2	D	343	DMS	1	0
2	C	423	DMS	1	0
2	L	415	DMS	1	0
2	K	403	DMS	1	0
2	G	417	DMS	1	0
2	B	417	DMS	1	0
2	J	403	DMS	1	0
3	L	407	B3N	1	0
3	K	401	B3N	1	0
2	C	405	DMS	1	0
2	G	342	DMS	1	0
2	E	342	DMS	1	0
3	J	407	B3N	1	0
2	E	403	DMS	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.

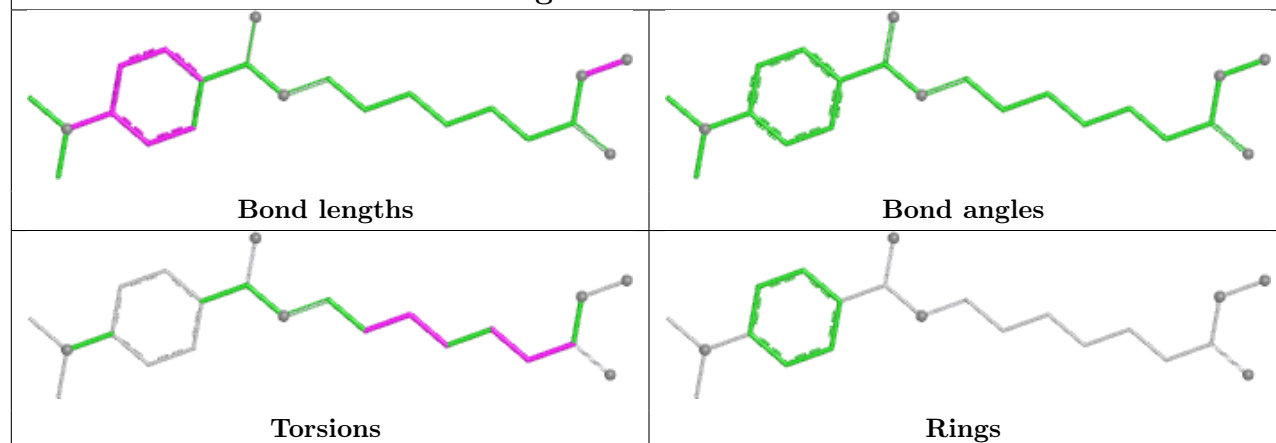
Ligand B3N G 401



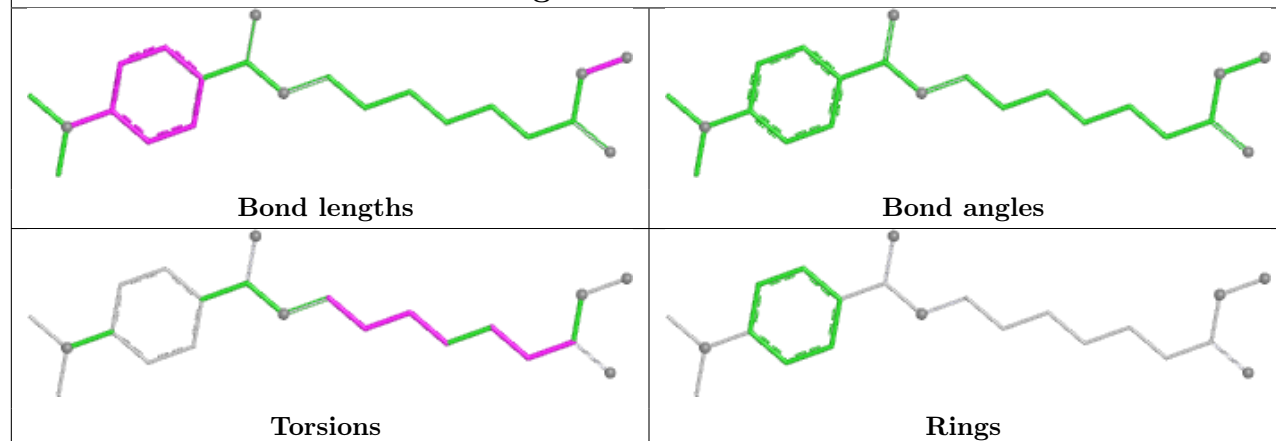
Ligand B3N A 401



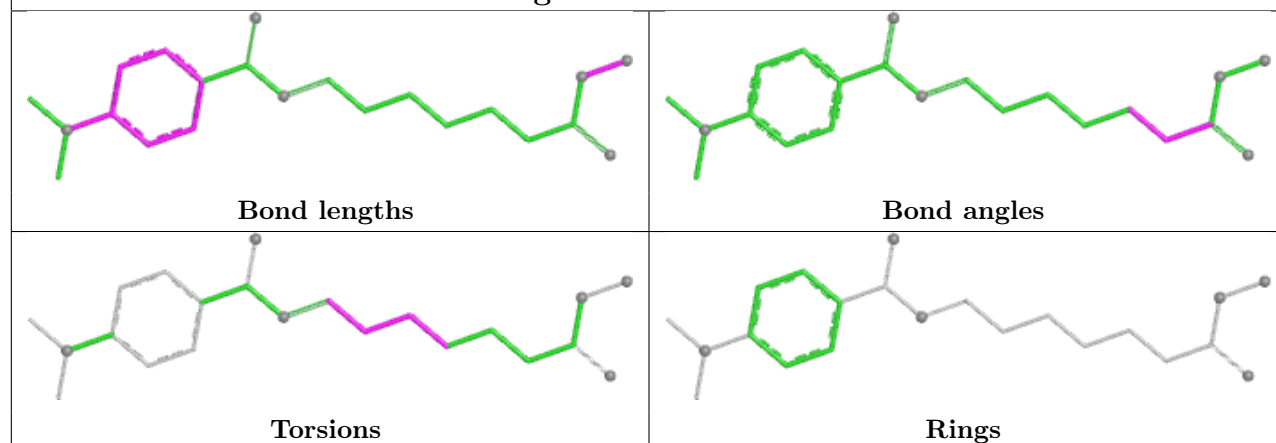
Ligand B3N F 407



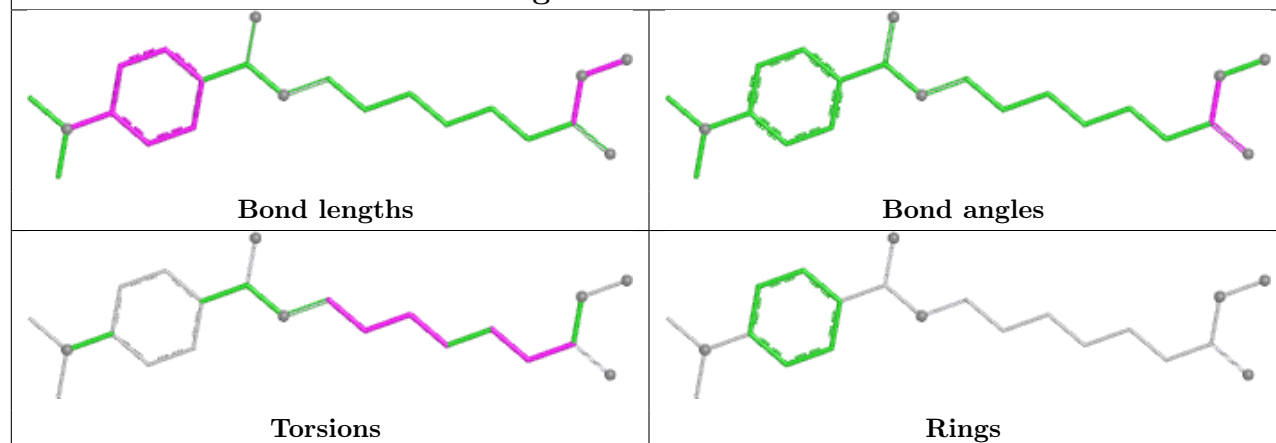
Ligand B3N D 407



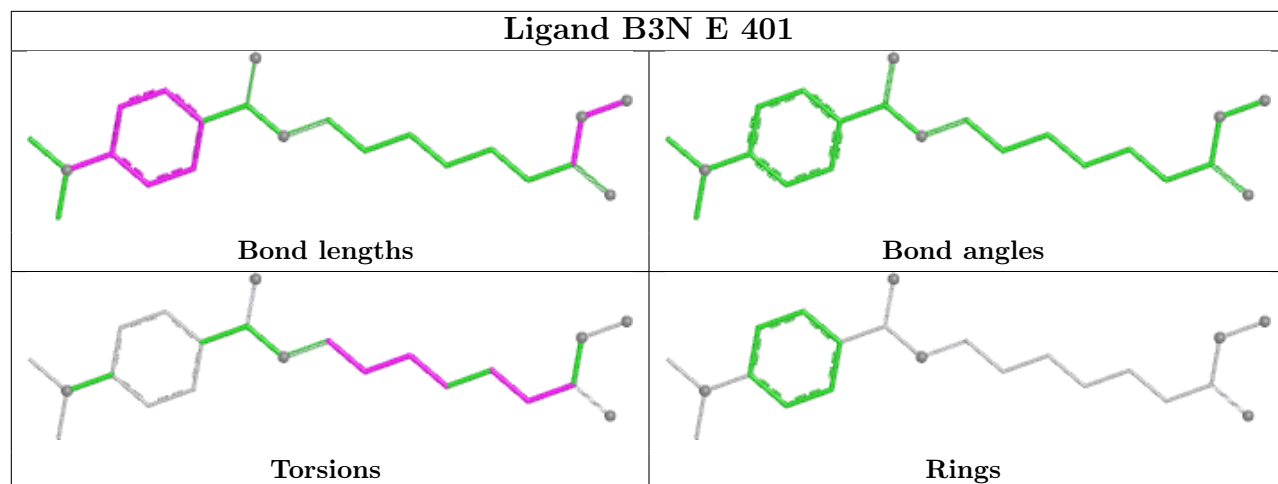
Ligand B3N C 401



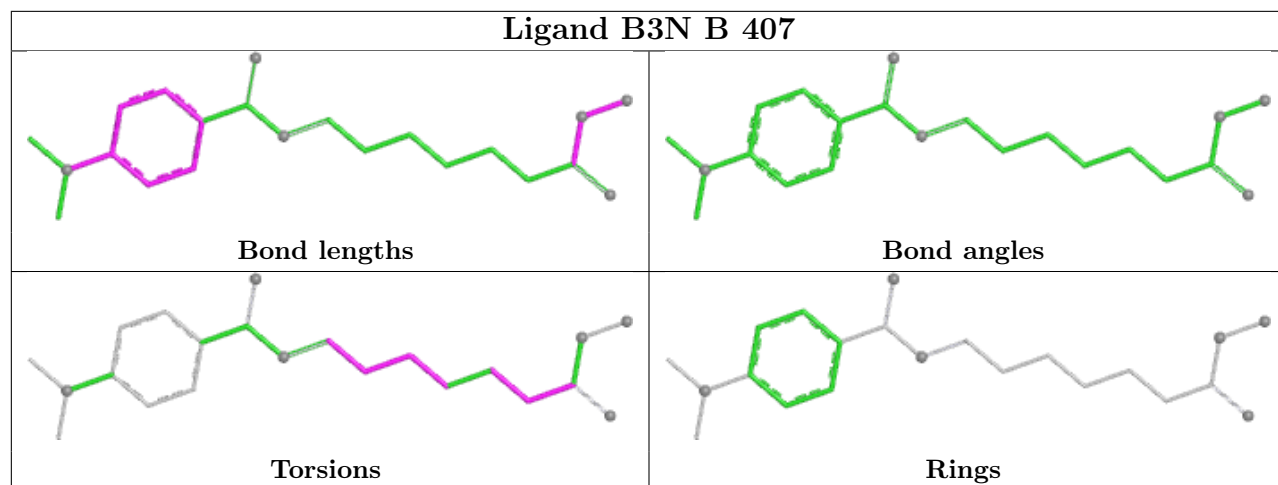
Ligand B3N H 407



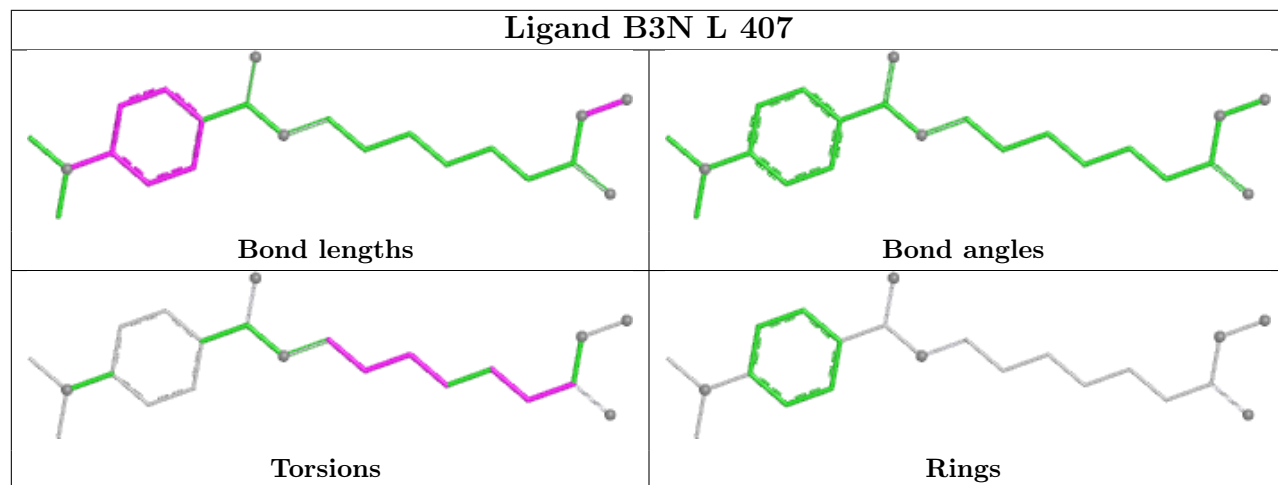
Ligand B3N E 401

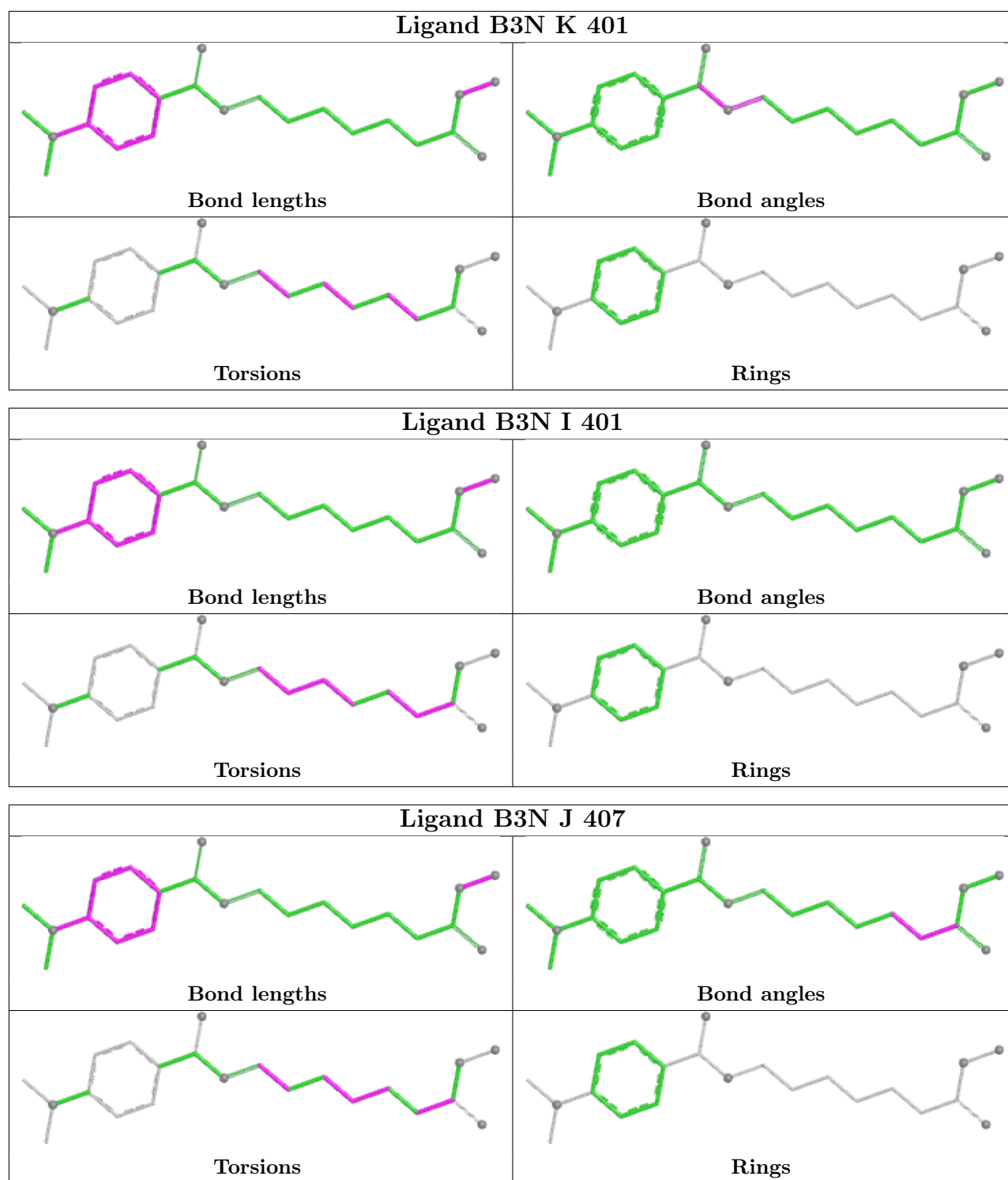


Ligand B3N B 407



Ligand B3N L 407





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	341/341 (100%)	-0.30	3 (0%) 81 82	10, 19, 31, 48	0
1	B	341/341 (100%)	-0.08	7 (2%) 63 64	12, 23, 37, 53	0
1	C	341/341 (100%)	-0.29	3 (0%) 81 82	10, 20, 32, 49	0
1	D	341/341 (100%)	-0.30	4 (1%) 76 77	11, 21, 31, 48	0
1	E	341/341 (100%)	-0.16	7 (2%) 63 64	11, 23, 37, 50	0
1	F	341/341 (100%)	-0.37	2 (0%) 85 86	11, 20, 31, 46	0
1	G	341/341 (100%)	-0.13	10 (2%) 53 54	12, 23, 38, 50	0
1	H	341/341 (100%)	-0.26	4 (1%) 76 77	10, 22, 33, 47	0
1	I	341/341 (100%)	-0.28	6 (1%) 67 68	10, 20, 33, 48	0
1	J	340/341 (99%)	-0.17	3 (0%) 81 82	12, 23, 39, 53	0
1	K	341/341 (100%)	-0.29	4 (1%) 76 77	10, 20, 32, 48	0
1	L	341/341 (100%)	-0.25	3 (0%) 81 82	12, 21, 33, 46	0
All	All	4091/4092 (99%)	-0.24	56 (1%) 73 74	10, 21, 35, 53	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	323	TYR	5.2
1	H	35	TRP	5.1
1	B	323	TYR	5.0
1	K	323	TYR	4.7
1	A	35	TRP	4.1
1	D	35	TRP	3.8
1	I	324	GLY	3.7
1	F	341	GLY	3.5
1	L	35	TRP	3.3
1	E	341	GLY	3.1
1	B	325	VAL	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	K	324	GLY	3.0
1	L	341	GLY	2.9
1	J	323	TYR	2.9
1	B	341	GLY	2.8
1	I	341	GLY	2.8
1	I	325	VAL	2.7
1	C	341	GLY	2.7
1	H	341	GLY	2.7
1	G	292	SER	2.7
1	K	53	ARG	2.6
1	B	53	ARG	2.6
1	D	341	GLY	2.6
1	E	42	GLU	2.6
1	G	323	TYR	2.6
1	C	53	ARG	2.5
1	D	53	ARG	2.5
1	G	325	VAL	2.5
1	D	7	GLU	2.5
1	E	323	TYR	2.5
1	G	53	ARG	2.5
1	G	341	GLY	2.5
1	H	42	GLU	2.4
1	B	292	SER	2.4
1	E	292	SER	2.4
1	G	43	ALA	2.4
1	A	53	ARG	2.4
1	B	252	GLY	2.3
1	K	325	VAL	2.3
1	C	324	GLY	2.3
1	I	53	ARG	2.3
1	G	291	ILE	2.3
1	J	340	ALA	2.3
1	B	42	GLU	2.3
1	G	252	GLY	2.2
1	G	288	GLN	2.2
1	E	291	ILE	2.2
1	H	104	ASP	2.1
1	E	288	GLN	2.1
1	G	44	GLY	2.1
1	I	291	ILE	2.1
1	L	34	GLU	2.1
1	A	288	GLN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	252	GLY	2.1
1	F	53	ARG	2.1
1	J	53	ARG	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	DMS	J	415	4/4	0.79	0.29	58,58,60,60	0
2	DMS	E	417	4/4	0.80	0.28	63,64,64,65	0
2	DMS	H	423	4/4	0.80	0.28	70,71,71,72	0
2	DMS	B	423	4/4	0.80	0.31	76,77,77,78	0
2	DMS	F	419	4/4	0.82	0.25	65,65,66,66	0
2	DMS	I	417	4/4	0.82	0.26	66,66,67,67	0
2	DMS	F	423	4/4	0.82	0.28	72,73,73,73	0
2	DMS	D	417	4/4	0.83	0.28	63,65,65,65	0
2	DMS	K	419	4/4	0.83	0.27	72,72,73,73	0
3	B3N	K	401	22/22	0.83	0.20	29,43,46,59	0
2	DMS	L	423	4/4	0.84	0.26	72,73,73,73	0
2	DMS	I	415	4/4	0.84	0.28	61,61,62,62	0
2	DMS	C	423	4/4	0.85	0.27	72,73,73,73	0
2	DMS	J	417	4/4	0.85	0.23	65,65,65,66	0
2	DMS	B	413	4/4	0.85	0.25	65,65,66,67	0
2	DMS	L	417	4/4	0.85	0.23	76,76,76,76	0
2	DMS	B	417	4/4	0.85	0.23	70,70,71,71	0
2	DMS	A	423	4/4	0.85	0.25	67,68,68,69	0
2	DMS	F	415	4/4	0.86	0.24	59,60,61,61	0
3	B3N	I	401	22/22	0.86	0.18	29,48,52,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	B3N	J	407	22/22	0.86	0.17	29,47,49,49	0
2	DMS	D	423	4/4	0.86	0.25	70,71,71,71	0
4	K	J	345	1/1	0.86	0.15	48,48,48,48	1
2	DMS	J	419	4/4	0.87	0.22	66,67,68,68	0
2	DMS	K	417	4/4	0.87	0.26	66,66,66,66	0
2	DMS	G	417	4/4	0.87	0.24	66,67,67,68	0
2	DMS	H	415	4/4	0.87	0.24	60,61,61,62	0
2	DMS	E	423	4/4	0.87	0.24	69,69,69,70	0
2	DMS	E	421	4/4	0.87	0.24	67,67,68,69	0
2	DMS	B	415	4/4	0.87	0.28	70,72,72,72	0
2	DMS	C	421	4/4	0.87	0.22	59,60,60,60	0
4	K	G	347	1/1	0.87	0.19	47,47,47,47	1
2	DMS	D	415	4/4	0.87	0.25	65,66,66,66	0
2	DMS	L	342	4/4	0.88	0.21	57,58,59,59	0
2	DMS	D	421	4/4	0.88	0.20	58,58,58,59	0
2	DMS	C	415	4/4	0.88	0.26	64,65,65,65	0
2	DMS	E	415	4/4	0.88	0.26	69,70,71,71	0
2	DMS	F	421	4/4	0.88	0.22	60,60,61,61	0
4	K	A	346	1/1	0.88	0.12	39,39,39,39	1
2	DMS	G	419	4/4	0.88	0.22	69,70,70,71	0
2	DMS	L	419	4/4	0.88	0.23	69,69,69,69	0
4	K	K	346	1/1	0.88	0.11	40,40,40,40	1
3	B3N	E	401	22/22	0.89	0.15	29,43,49,49	0
2	DMS	H	417	4/4	0.89	0.22	67,67,67,67	0
2	DMS	L	421	4/4	0.89	0.21	61,61,62,62	0
2	DMS	F	343	4/4	0.89	0.21	58,58,58,59	0
2	DMS	B	419	4/4	0.89	0.19	66,66,66,67	0
4	K	F	348	1/1	0.89	0.10	41,41,41,41	1
2	DMS	K	415	4/4	0.89	0.23	59,60,60,60	0
2	DMS	D	343	4/4	0.89	0.22	62,63,64,64	0
3	B3N	B	407	22/22	0.89	0.15	29,45,46,47	0
2	DMS	I	419	4/4	0.90	0.21	63,63,63,64	0
2	DMS	I	423	4/4	0.90	0.19	60,61,61,61	0
2	DMS	A	419	4/4	0.90	0.20	61,61,62,62	0
2	DMS	A	415	4/4	0.90	0.24	62,63,63,63	0
2	DMS	G	423	4/4	0.90	0.21	69,69,69,70	0
3	B3N	F	407	22/22	0.90	0.13	29,36,38,39	0
3	B3N	G	401	22/22	0.90	0.14	29,42,43,45	0
3	B3N	H	407	22/22	0.90	0.14	29,36,38,38	0
2	DMS	J	423	4/4	0.90	0.22	68,68,68,69	0
2	DMS	K	421	4/4	0.90	0.18	57,58,59,59	0
2	DMS	E	419	4/4	0.90	0.21	72,72,72,73	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	DMS	D	413	4/4	0.90	0.21	60,60,60,60	0
2	DMS	F	344	4/4	0.90	0.18	59,60,60,61	0
2	DMS	A	421	4/4	0.90	0.19	60,61,61,61	0
2	DMS	L	415	4/4	0.90	0.23	61,61,62,62	0
2	DMS	G	415	4/4	0.90	0.24	65,66,66,66	0
2	DMS	G	413	4/4	0.91	0.17	53,53,54,54	0
4	K	C	345	1/1	0.91	0.10	35,35,35,35	1
4	K	E	346	1/1	0.91	0.14	45,45,45,45	1
2	DMS	H	421	4/4	0.91	0.18	59,60,60,60	0
3	B3N	C	401	22/22	0.91	0.13	29,33,37,37	0
2	DMS	K	423	4/4	0.91	0.18	62,62,63,63	0
2	DMS	F	417	4/4	0.91	0.18	63,63,63,63	0
3	B3N	L	407	22/22	0.92	0.13	29,39,41,42	0
2	DMS	A	413	4/4	0.92	0.16	43,45,45,46	0
2	DMS	H	419	4/4	0.92	0.17	70,70,70,70	0
2	DMS	F	413	4/4	0.92	0.17	45,46,47,48	0
3	B3N	A	401	22/22	0.92	0.13	29,35,39,39	0
2	DMS	I	421	4/4	0.92	0.18	59,59,59,60	0
4	K	H	345	1/1	0.92	0.10	47,47,47,47	1
2	DMS	A	417	4/4	0.92	0.18	63,63,64,64	0
3	B3N	D	407	22/22	0.92	0.12	29,33,36,37	0
2	DMS	K	403	4/4	0.93	0.16	41,41,42,42	0
4	K	D	347	1/1	0.93	0.09	35,35,35,35	1
4	K	L	346	1/1	0.93	0.09	44,44,44,44	1
5	NA	I	343	1/1	0.93	0.04	20,20,20,20	0
2	DMS	B	411	4/4	0.94	0.12	40,40,40,41	0
2	DMS	G	411	4/4	0.94	0.12	33,34,34,35	0
2	DMS	D	403	4/4	0.94	0.15	46,47,47,49	0
2	DMS	F	342	4/4	0.94	0.13	42,43,44,45	0
2	DMS	D	419	4/4	0.94	0.16	67,67,68,68	0
2	DMS	E	411	4/4	0.94	0.15	43,44,44,44	0
2	DMS	K	413	4/4	0.94	0.13	40,42,42,43	0
2	DMS	E	413	4/4	0.94	0.15	46,47,48,48	0
2	DMS	G	342	4/4	0.94	0.15	52,52,52,52	0
2	DMS	C	419	4/4	0.94	0.16	61,62,62,63	0
4	K	B	346	1/1	0.95	0.15	42,42,42,42	1
2	DMS	E	403	4/4	0.95	0.13	46,47,47,47	0
2	DMS	L	405	4/4	0.95	0.13	45,46,46,46	0
2	DMS	A	411	4/4	0.95	0.12	38,38,38,41	0
2	DMS	A	403	4/4	0.95	0.13	42,43,43,44	0
2	DMS	B	403	4/4	0.95	0.15	48,49,50,50	0
2	DMS	D	342	4/4	0.95	0.12	36,36,36,37	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	DMS	G	343	4/4	0.95	0.12	42,42,43,43	0
2	DMS	G	403	4/4	0.95	0.14	54,55,55,55	0
2	DMS	F	411	4/4	0.95	0.12	41,41,42,42	0
5	NA	G	345	1/1	0.95	0.04	20,20,20,20	0
2	DMS	C	405	4/4	0.95	0.13	39,40,40,41	0
2	DMS	G	405	4/4	0.96	0.12	44,45,45,46	0
4	K	A	343	1/1	0.96	0.05	11,11,11,11	0
2	DMS	K	411	4/4	0.96	0.10	32,33,33,34	0
2	DMS	E	405	4/4	0.96	0.14	46,46,46,46	0
2	DMS	K	342	4/4	0.96	0.14	50,51,51,52	0
2	DMS	K	405	4/4	0.96	0.13	48,48,49,49	0
2	DMS	H	411	4/4	0.96	0.10	34,35,35,36	0
2	DMS	C	411	4/4	0.96	0.10	37,39,40,40	0
2	DMS	E	342	4/4	0.96	0.11	47,47,47,48	0
2	DMS	J	403	4/4	0.96	0.12	43,45,46,46	0
2	DMS	J	413	4/4	0.96	0.11	45,46,47,47	0
2	DMS	F	405	4/4	0.96	0.10	39,40,40,40	0
2	DMS	A	342	4/4	0.96	0.14	43,44,45,45	0
5	NA	E	344	1/1	0.96	0.03	20,20,20,20	0
5	NA	F	346	1/1	0.96	0.02	17,17,17,17	0
2	DMS	B	342	4/4	0.96	0.13	44,45,45,46	0
2	DMS	I	411	4/4	0.96	0.10	38,39,40,40	0
5	NA	K	344	1/1	0.96	0.04	17,17,17,17	0
2	DMS	H	413	4/4	0.97	0.10	43,43,45,45	0
2	DMS	B	405	4/4	0.97	0.12	43,44,44,45	0
5	NA	D	345	1/1	0.97	0.04	20,20,20,20	0
2	DMS	D	411	4/4	0.97	0.10	34,35,35,35	0
2	DMS	I	405	4/4	0.97	0.09	41,41,41,42	0
2	DMS	J	405	4/4	0.97	0.10	38,40,40,41	0
5	NA	H	343	1/1	0.97	0.03	20,20,20,20	0
2	DMS	I	413	4/4	0.97	0.10	38,39,39,40	0
2	DMS	H	405	4/4	0.97	0.10	43,44,44,44	0
6	ZN	G	346	1/1	0.97	0.06	29,29,29,29	0
4	K	F	345	1/1	0.98	0.03	14,14,14,14	0
2	DMS	L	413	4/4	0.98	0.09	42,42,42,43	0
2	DMS	A	405	4/4	0.98	0.09	37,37,38,38	0
5	NA	A	344	1/1	0.98	0.02	13,13,13,13	0
2	DMS	D	405	4/4	0.98	0.08	39,39,40,41	0
6	ZN	E	345	1/1	0.98	0.07	26,26,26,26	0
4	K	I	342	1/1	0.98	0.03	16,16,16,16	0
6	ZN	I	344	1/1	0.98	0.05	31,31,31,31	0
4	K	L	343	1/1	0.99	0.03	15,15,15,15	0

Continued on next page...

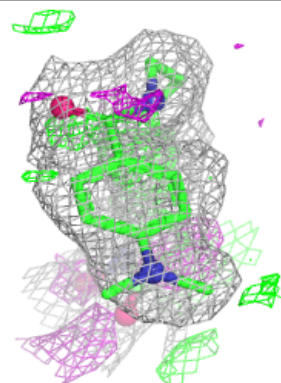
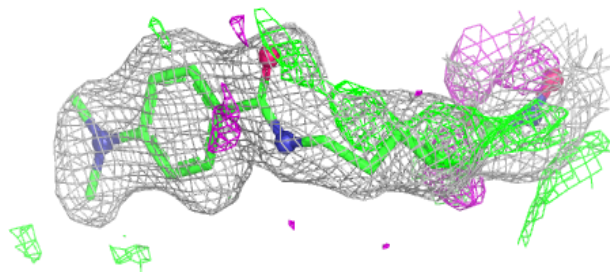
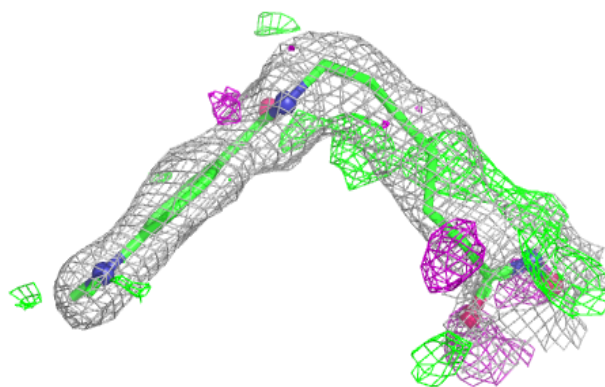
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	K	C	342	1/1	0.99	0.03	15,15,15,15	0
4	K	E	343	1/1	0.99	0.01	16,16,16,16	0
5	NA	J	343	1/1	0.99	0.04	13,13,13,13	0
5	NA	B	344	1/1	0.99	0.02	25,25,25,25	0
5	NA	L	344	1/1	0.99	0.01	20,20,20,20	0
6	ZN	B	345	1/1	0.99	0.05	29,29,29,29	0
4	K	D	344	1/1	0.99	0.03	16,16,16,16	0
4	K	K	343	1/1	0.99	0.04	13,13,13,13	0
4	K	H	342	1/1	0.99	0.03	15,15,15,15	0
6	ZN	J	344	1/1	0.99	0.04	30,30,30,30	0
6	ZN	K	345	1/1	0.99	0.05	31,31,31,31	0
6	ZN	C	344	1/1	1.00	0.02	22,22,22,22	0
6	ZN	D	346	1/1	1.00	0.01	22,22,22,22	0
4	K	B	343	1/1	1.00	0.01	19,19,19,19	0
6	ZN	F	347	1/1	1.00	0.04	21,21,21,21	0
5	NA	C	343	1/1	1.00	0.02	17,17,17,17	0
6	ZN	H	344	1/1	1.00	0.04	21,21,21,21	0
4	K	G	344	1/1	1.00	0.02	16,16,16,16	0
6	ZN	A	345	1/1	1.00	0.02	21,21,21,21	0
4	K	J	342	1/1	1.00	0.02	18,18,18,18	0
6	ZN	L	345	1/1	1.00	0.01	21,21,21,21	0

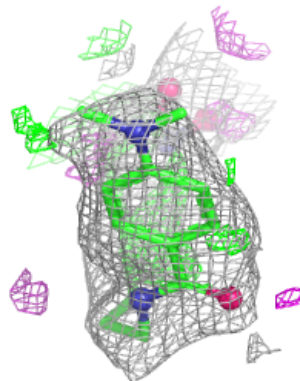
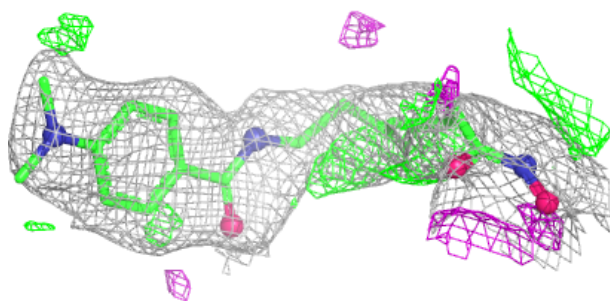
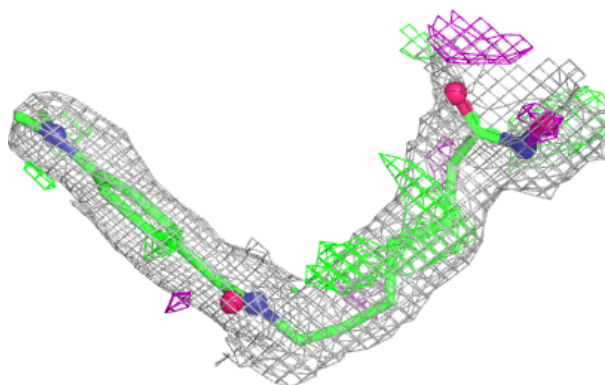
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around B3N K 401:

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

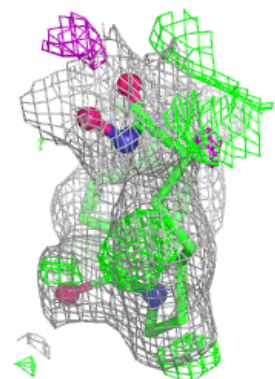
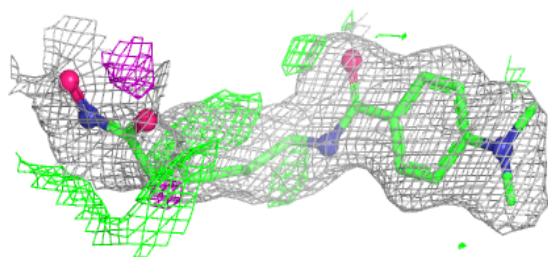
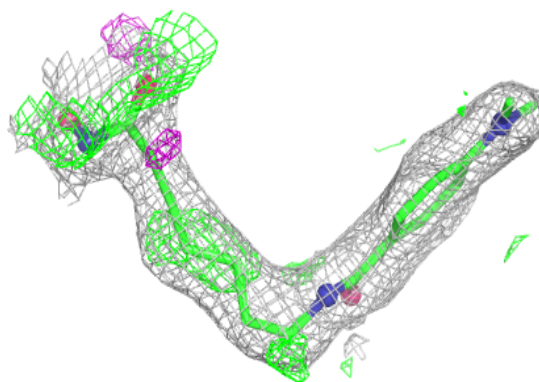
**Electron density around B3N I 401:**

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

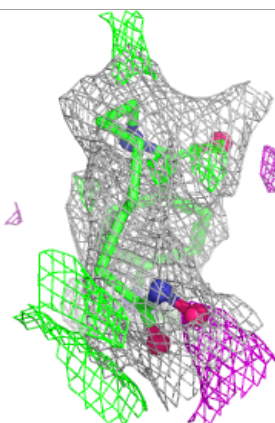
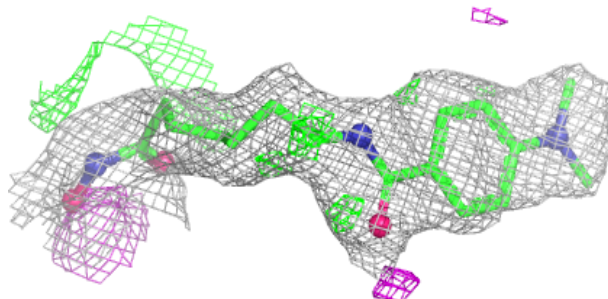
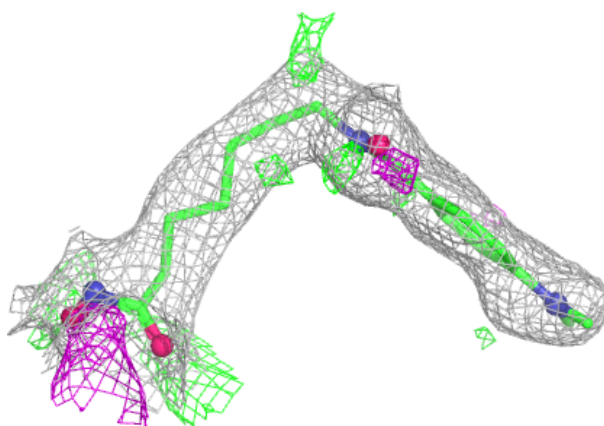


Electron density around B3N J 407:

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

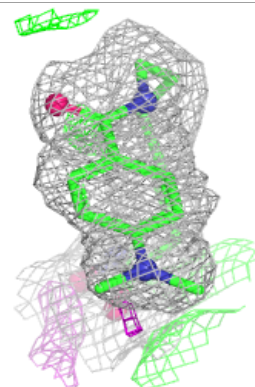
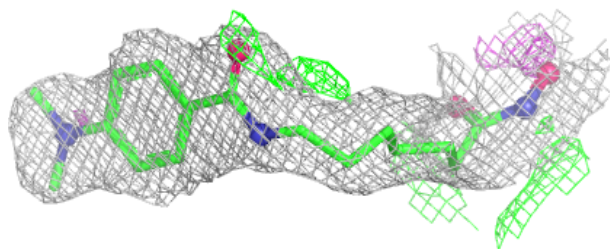
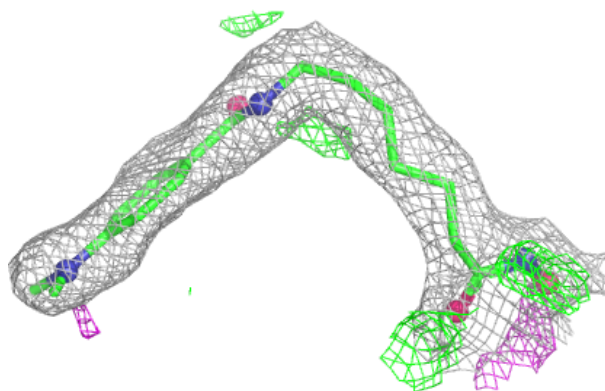
**Electron density around B3N E 401:**

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

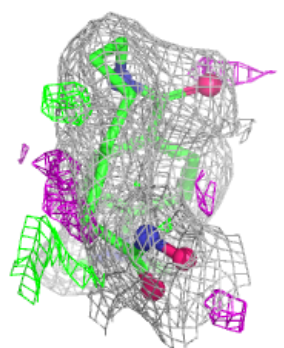
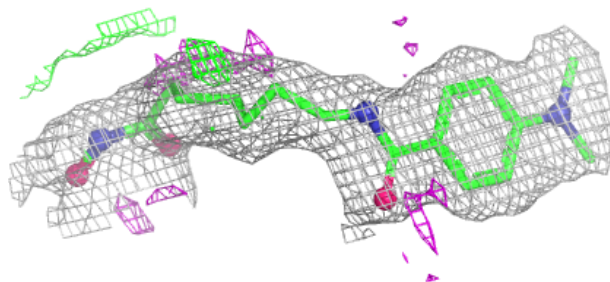
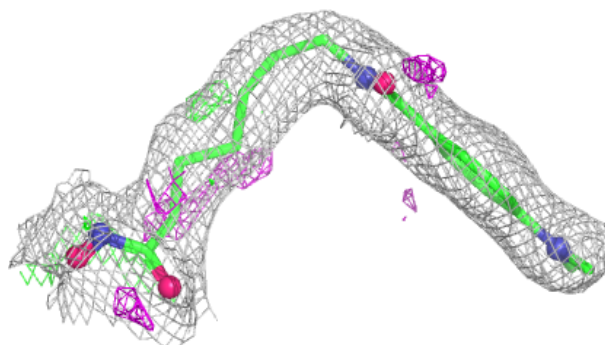


Electron density around B3N B 407:

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

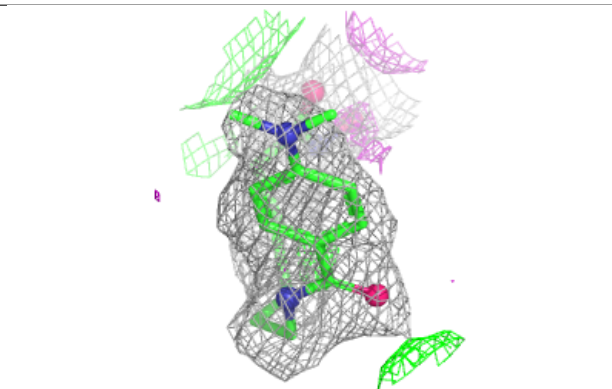
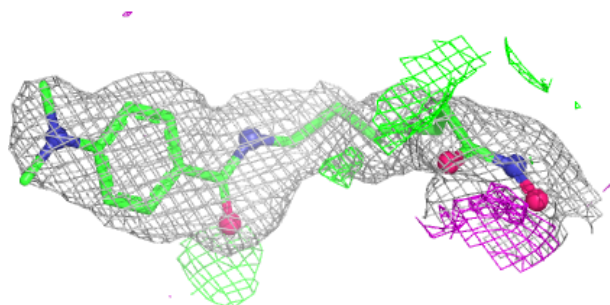
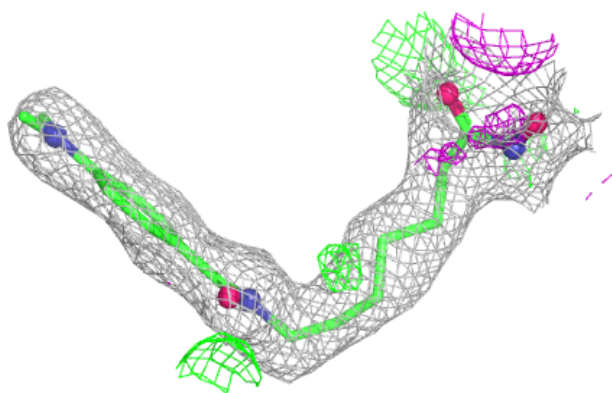
**Electron density around B3N F 407:**

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

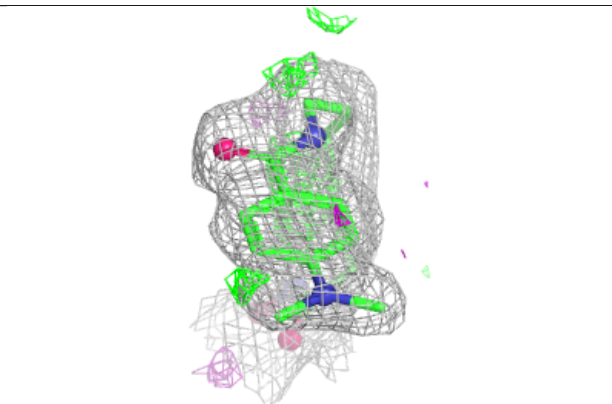
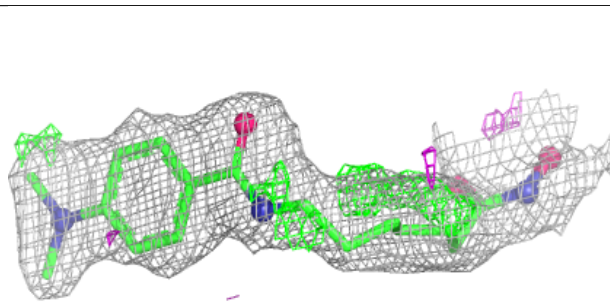
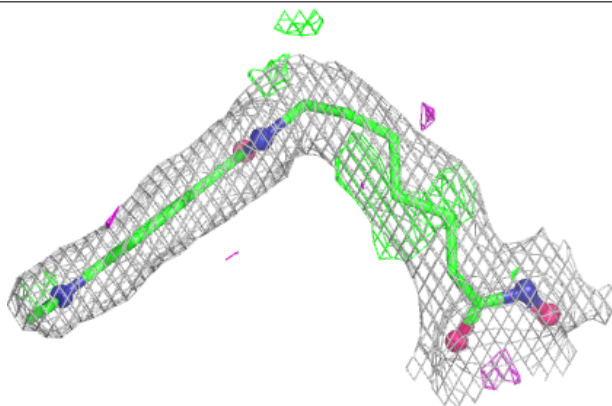


Electron density around B3N G 401:

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

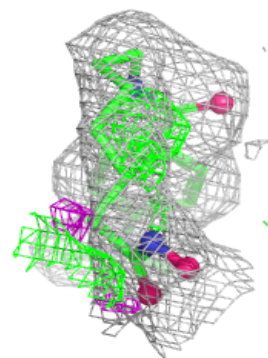
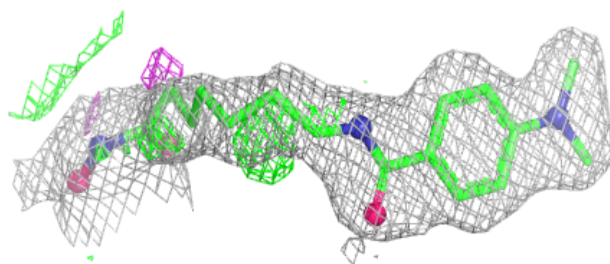
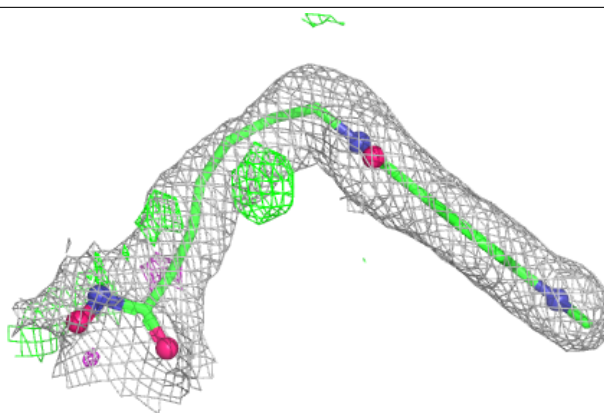
**Electron density around B3N H 407:**

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

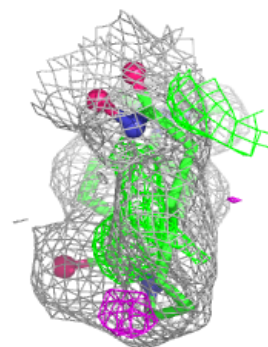
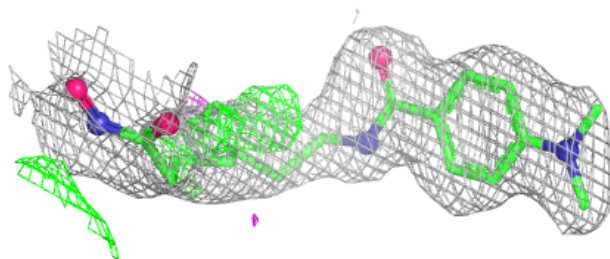
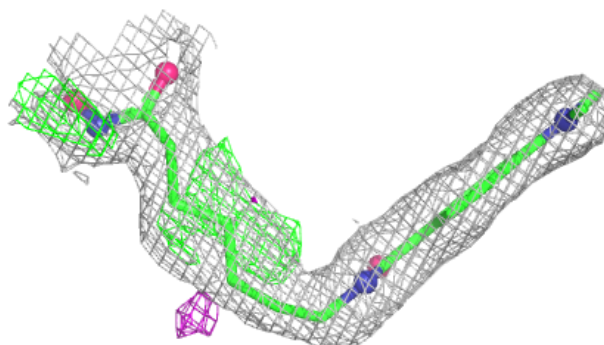


Electron density around B3N C 401:

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

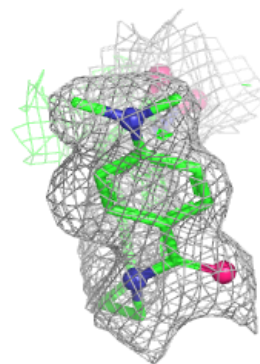
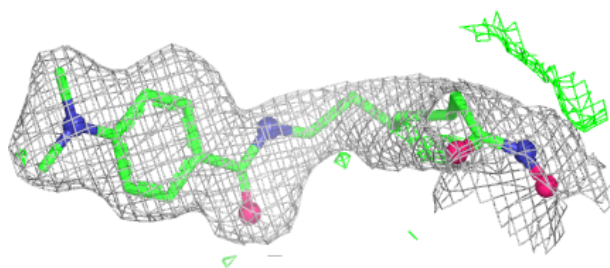
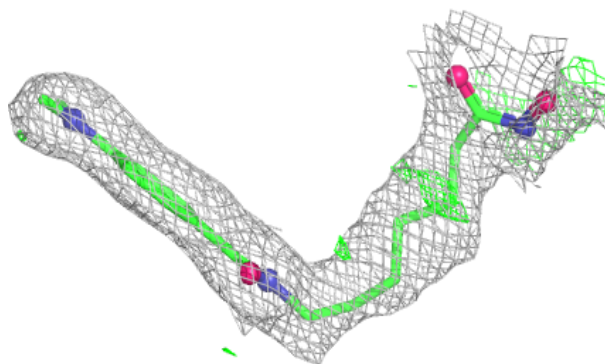
**Electron density around B3N L 407:**

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

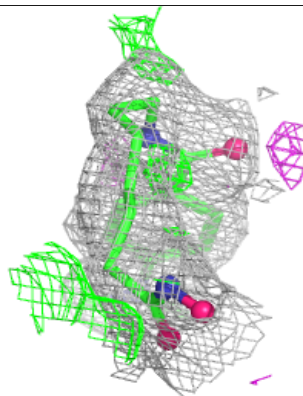
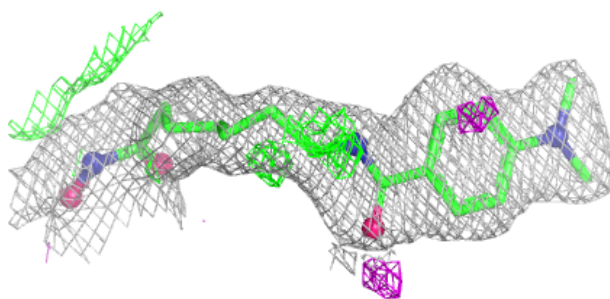
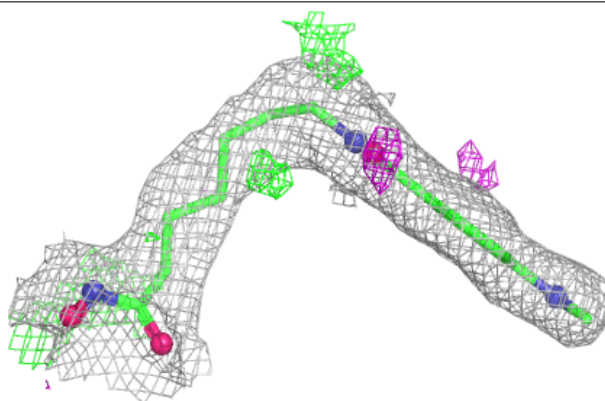


Electron density around B3N A 401:

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

**Electron density around B3N D 407:**

$2mF_o-DF_c$ (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.