Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:50 AM UTC

PDB ID	:	9MR9 / pdb_00009mr9
Title	:	Crystal structure of AU-15330 in complex with the bromodomain of human BRM (SMARCA2) and pVHL:ElonginC:ElonginB
Authors	:	Wang, M.; Xu, C.
Deposited on	:	2025-01-07
Resolution	:	3.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

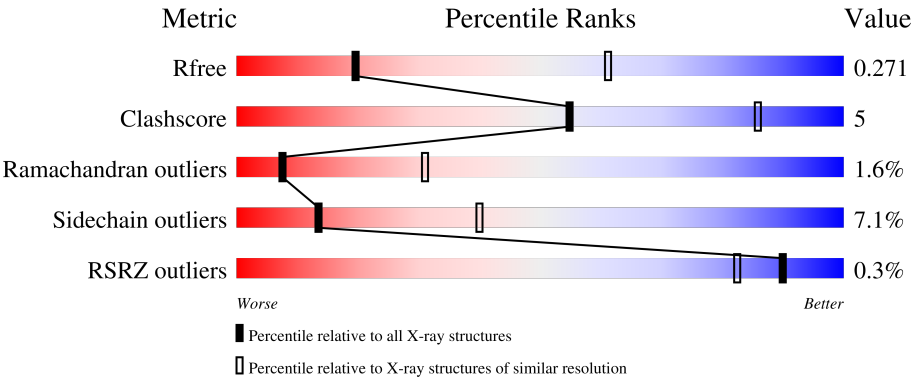
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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 <=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	122	71% 20% • •
1	E	122	72% 22% • 5%
1	I	122	71% 22% • 5%
1	M	122	74% 18% • 5%
1	Q	122	70% 25% • •

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Mol	Chain	Length	Quality of chain
1	U	122	2% 52% 34% 8%
1	Y	122	75% 20%
1	c	122	65% 26% 5%
2	B	161	78% 16% 6%
2	F	161	74% 18% 6%
2	J	161	74% 21%
2	N	161	82% 12%
2	R	161	75% 17% 6%
2	V	161	75% 18% 6%
2	Z	161	75% 17% 6%
2	d	161	72% 20% 6%
3	C	96	77% 20%
3	G	96	84% 16%
3	K	96	80% 18%
3	O	96	85% 14%
3	S	96	83% 12%
3	W	96	80% 18%
3	a	96	80% 19%
3	e	96	89% 10%
4	D	104	82% 17%
4	H	104	81% 14%
4	L	104	86% 13%
4	P	104	87% 13%
4	T	104	89% 10%
4	X	104	87% 13%

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Mol	Chain	Length	Quality of chain
4	b	104	2% 95% 5%
4	f	104	2% 91% 8%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 31004 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 Isoform Short of Probable global transcription activator SNF2L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	117	Total	C	N	O	S	0	0	0
			962	612	169	178	3			
1	E	116	Total	C	N	O	S	0	0	0
			953	606	167	177	3			
1	I	116	Total	C	N	O	S	0	0	0
			953	606	167	177	3			
1	M	116	Total	C	N	O	S	0	0	0
			953	606	167	177	3			
1	Q	118	Total	C	N	O	S	0	0	0
			971	616	169	183	3			
1	U	117	Total	C	N	O	S	0	0	0
			962	611	168	180	3			
1	Y	118	Total	C	N	O	S	0	1	0
			981	622	172	184	3			
1	c	118	Total	C	N	O	S	0	0	0
			971	616	169	183	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1372	SER	-	expression tag	UNP P51531
E	1372	SER	-	expression tag	UNP P51531
I	1372	SER	-	expression tag	UNP P51531
M	1372	SER	-	expression tag	UNP P51531
Q	1372	SER	-	expression tag	UNP P51531
U	1372	SER	-	expression tag	UNP P51531
Y	1372	SER	-	expression tag	UNP P51531
c	1372	SER	-	expression tag	UNP P51531

- Molecule 2 is a protein called von Hippel-Lindau disease tumor suppressor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	151	Total	C	N	O	S	0	0	0
			1243	787	233	221	2			
2	F	152	Total	C	N	O	S	0	0	0
			1246	789	233	222	2			
2	J	156	Total	C	N	O	S	0	1	0
			1279	808	240	229	2			
2	N	156	Total	C	N	O	S	0	1	0
			1290	814	245	229	2			
2	R	152	Total	C	N	O	S	0	0	0
			1250	792	234	222	2			
2	V	152	Total	C	N	O	S	0	0	0
			1250	792	234	222	2			
2	Z	152	Total	C	N	O	S	0	0	0
			1250	792	234	222	2			
2	d	152	Total	C	N	O	S	0	1	0
			1257	797	236	222	2			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	53	GLY	-	expression tag	UNP P40337
F	53	GLY	-	expression tag	UNP P40337
J	53	GLY	-	expression tag	UNP P40337
N	53	GLY	-	expression tag	UNP P40337
R	53	GLY	-	expression tag	UNP P40337
V	53	GLY	-	expression tag	UNP P40337
Z	53	GLY	-	expression tag	UNP P40337
d	53	GLY	-	expression tag	UNP P40337

- Molecule 3 is a protein called Elongin-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	96	Total	C	N	O	S	0	0	0
			760	487	122	145	6			
3	G	96	Total	C	N	O	S	0	0	0
			760	487	122	145	6			
3	K	96	Total	C	N	O	S	0	0	0
			760	487	122	145	6			
3	O	96	Total	C	N	O	S	0	0	0
			760	487	122	145	6			
3	S	96	Total	C	N	O	S	0	0	0
			760	487	122	145	6			
3	W	96	Total	C	N	O	S	0	0	0
			760	487	122	145	6			

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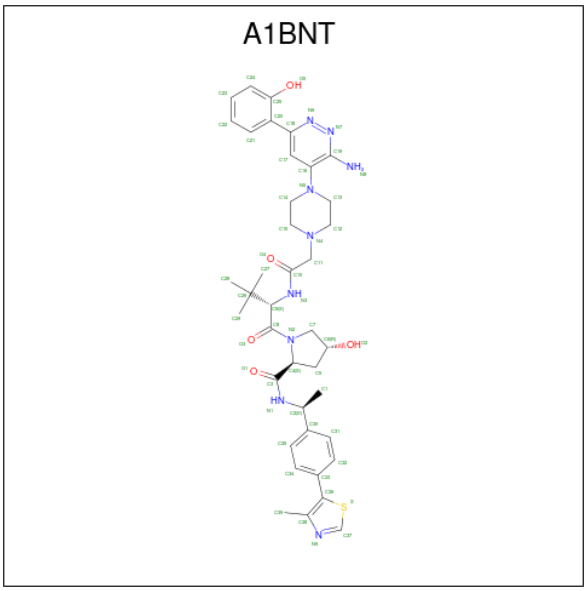
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	a	96	Total	C	N	O	S	0	0	0
			760	487	122	145	6			
3	e	96	Total	C	N	O	S	0	0	0
			760	487	122	145	6			

- Molecule 4 is a protein called Elongin-B.

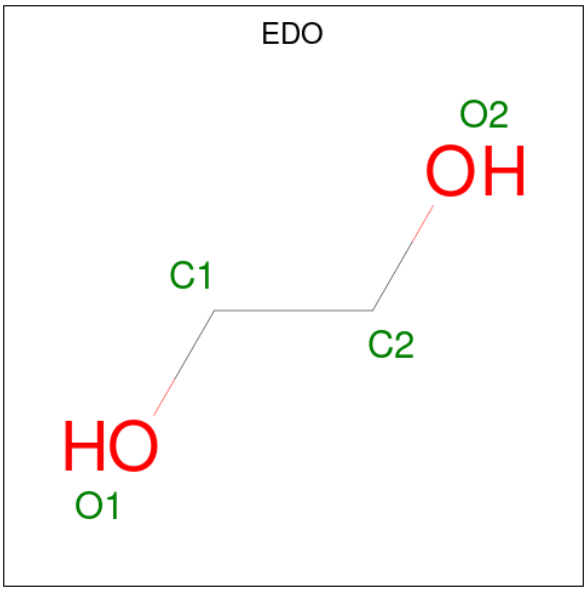
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	104	Total	C	N	O	S	0	0	0
			823	520	138	160	5			
4	H	104	Total	C	N	O	S	0	0	0
			823	520	138	160	5			
4	L	104	Total	C	N	O	S	0	0	0
			823	520	138	160	5			
4	P	104	Total	C	N	O	S	0	0	0
			823	520	138	160	5			
4	T	104	Total	C	N	O	S	0	0	0
			823	520	138	160	5			
4	X	104	Total	C	N	O	S	0	0	0
			823	520	138	160	5			
4	b	104	Total	C	N	O	S	0	0	0
			823	520	138	160	5			
4	f	104	Total	C	N	O	S	0	0	0
			823	520	138	160	5			

- Molecule 5 is N-({4-[(6M)-3-amino-6-(2-hydroxyphenyl)pyridazin-4-yl]piperazin-1-yl}acetyl)-3-methyl-L-valyl-(4R)-4-hydroxy-N-{(1S)-1-[4-(4-methyl-1,3-thiazol-5-yl)phenyl]ethyl}-L-prolinamide (CCD ID: A1BNT) (formula: $C_{39}H_{49}N_9O_5S$) (labeled as "Ligand of Interest" by depositor).



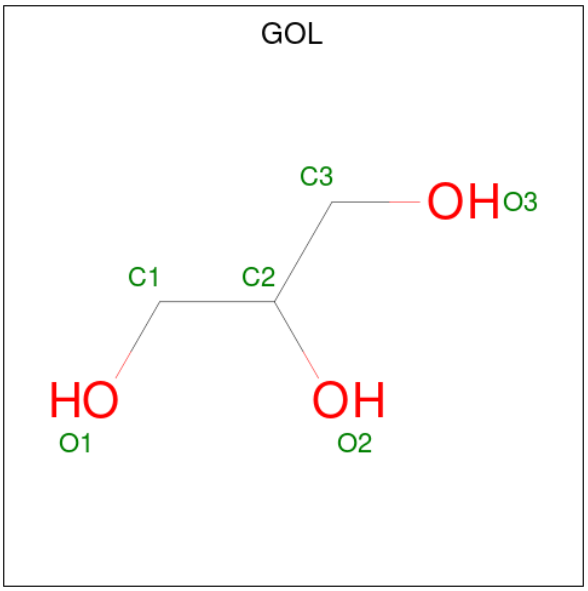
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	S	0	0
			54	39	9	5	1		
5	F	1	Total	C	N	O	S	0	0
			54	39	9	5	1		
5	J	1	Total	C	N	O	S	0	0
			54	39	9	5	1		
5	N	1	Total	C	N	O	S	0	0
			54	39	9	5	1		
5	Q	1	Total	C	N	O	S	0	0
			54	39	9	5	1		
5	V	1	Total	C	N	O	S	0	0
			54	39	9	5	1		
5	Z	1	Total	C	N	O	S	0	0
			54	39	9	5	1		
5	d	1	Total	C	N	O	S	0	0
			54	39	9	5	1		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		
6	F	1	Total	C	O	0	0
			4	2	2		
6	J	1	Total	C	O	0	0
			4	2	2		
6	R	1	Total	C	O	0	0
			4	2	2		
6	c	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	J	1	Total C O 6 3 3	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	6	Total O 6 6	0	0
8	B	7	Total O 7 7	0	0
8	C	5	Total O 5 5	0	0
8	D	2	Total O 2 2	0	0
8	E	6	Total O 6 6	0	0
8	F	4	Total O 4 4	0	0
8	G	3	Total O 3 3	0	0
8	H	2	Total O 2 2	0	0
8	I	6	Total O 6 6	0	0
8	J	2	Total O 2 2	0	0
8	K	4	Total O 4 4	0	0

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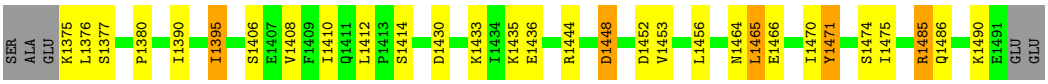
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	L	1	Total O 1 1	0	0
8	M	6	Total O 6 6	0	0
8	N	10	Total O 10 10	0	0
8	O	3	Total O 3 3	0	0
8	P	3	Total O 3 3	0	0
8	Q	1	Total O 1 1	0	0
8	R	2	Total O 2 2	0	0
8	S	1	Total O 1 1	0	0
8	T	2	Total O 2 2	0	0
8	U	1	Total O 1 1	0	0
8	V	4	Total O 4 4	0	0
8	W	2	Total O 2 2	0	0
8	X	2	Total O 2 2	0	0
8	Z	4	Total O 4 4	0	0
8	a	2	Total O 2 2	0	0
8	b	2	Total O 2 2	0	0
8	c	3	Total O 3 3	0	0
8	d	1	Total O 1 1	0	0
8	e	6	Total O 6 6	0	0
8	f	4	Total O 4 4	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: Isoform Short of Probable global transcription activator SNF2L2

Chain A:



• Molecule 1: Isoform Short of Probable global transcription activator SNF2L2

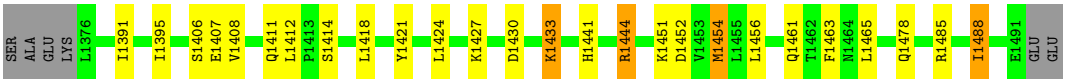
Chain E:

• Molecule 1: Isoform Short of Probable global transcription activator SNF2L2

Chain I:

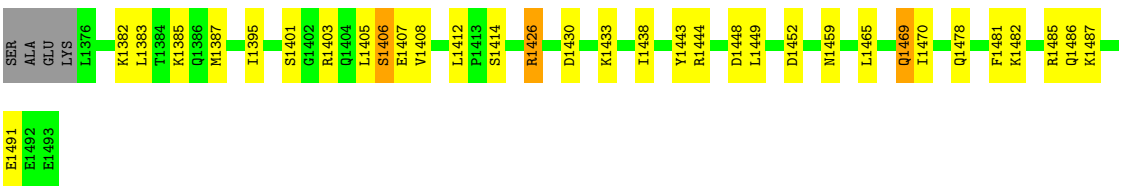
• Molecule 1: Isoform Short of Probable global transcription activator SNF2L2

Chain M:



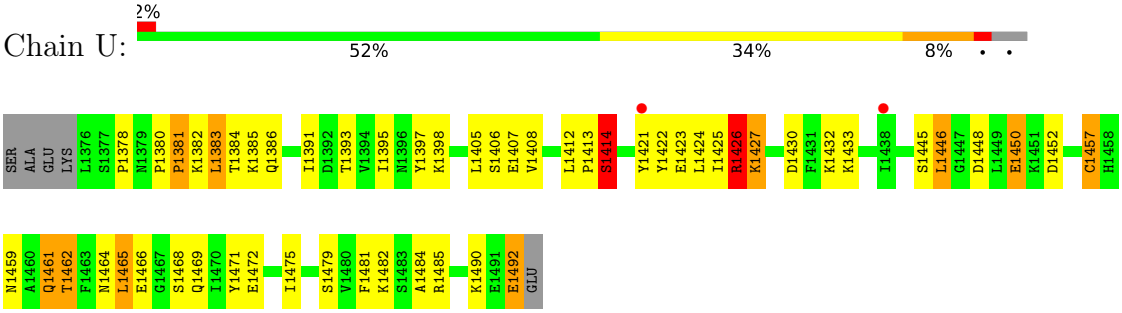
• Molecule 1: Isoform Short of Probable global transcription activator SNF2L2

Chain Q:



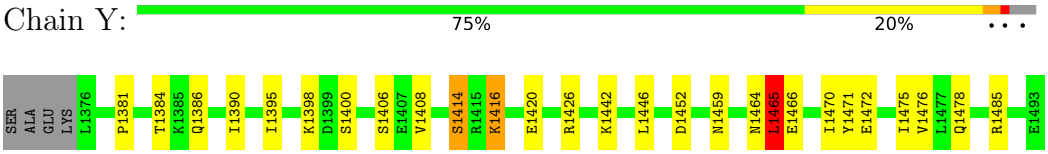
• Molecule 1: Isoform Short of Probable global transcription activator SNF2L2

Chain U:



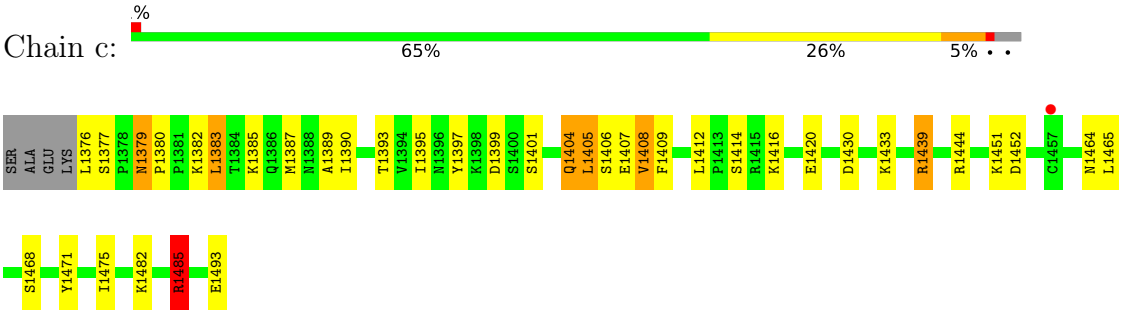
• Molecule 1: Isoform Short of Probable global transcription activator SNF2L2

Chain Y:



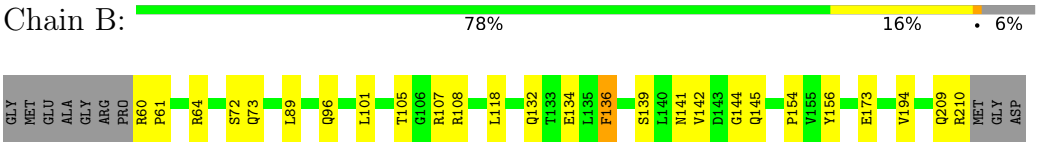
• Molecule 1: Isoform Short of Probable global transcription activator SNF2L2

Chain c:



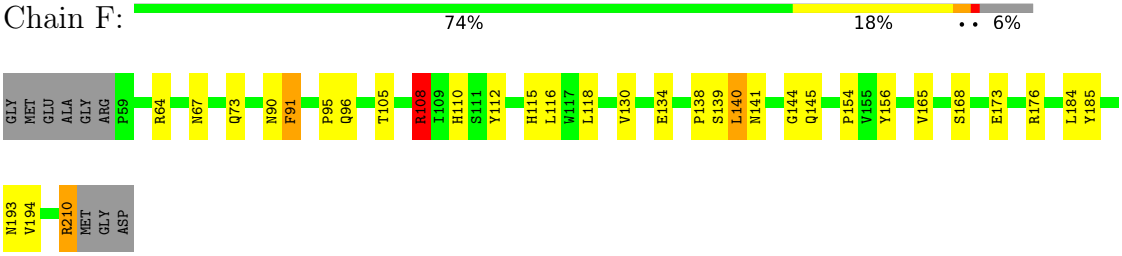
• Molecule 2: von Hippel-Lindau disease tumor suppressor

Chain B:



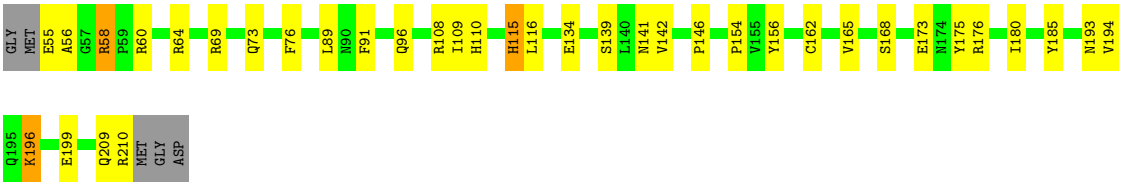
• Molecule 2: von Hippel-Lindau disease tumor suppressor

Chain F:



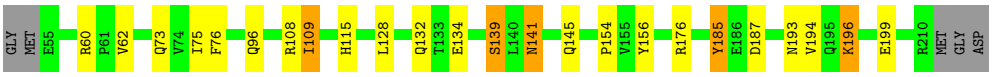
• Molecule 2: von Hippel-Lindau disease tumor suppressor

Chain J:



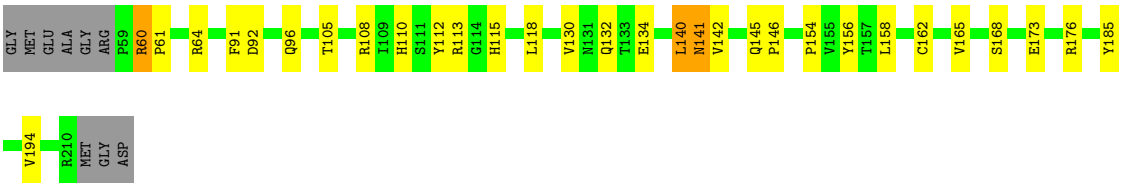
• Molecule 2: von Hippel-Lindau disease tumor suppressor

Chain N:



• Molecule 2: von Hippel-Lindau disease tumor suppressor

Chain R:

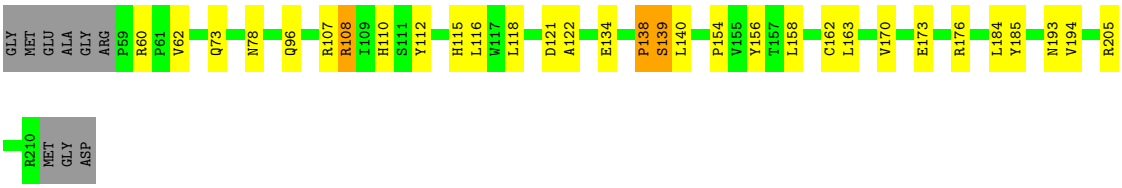


• Molecule 2: von Hippel-Lindau disease tumor suppressor

Chain V:

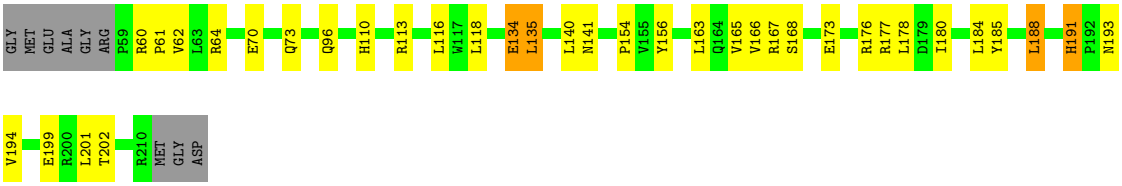
• Molecule 2: von Hippel-Lindau disease tumor suppressor

Chain Z:



• Molecule 2: von Hippel-Lindau disease tumor suppressor

Chain d:

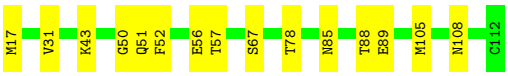


• Molecule 3: Elongin-C

Chain C:

• Molecule 3: Elongin-C

Chain G:



• Molecule 3: Elongin-C

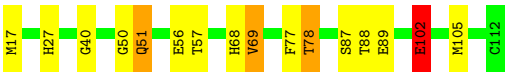
Chain K:

• Molecule 3: Elongin-C

Chain O:

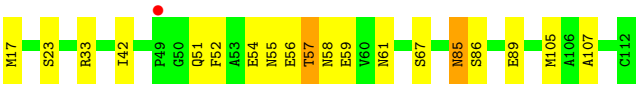
• Molecule 3: Elongin-C

Chain S:



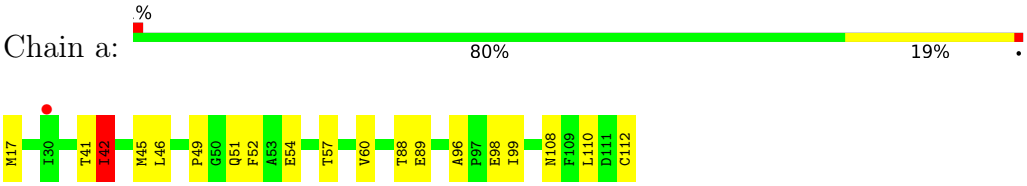
• Molecule 3: Elongin-C

Chain W:



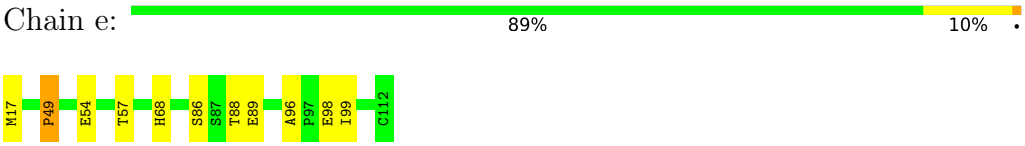
• Molecule 3: Elongin-C

Chain a:



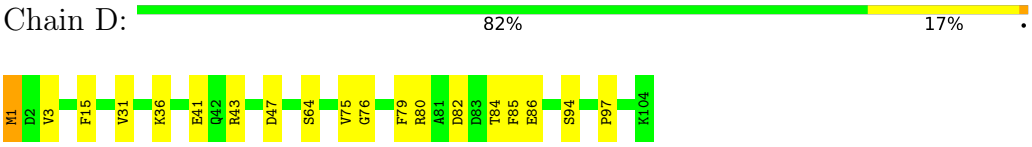
• Molecule 3: Elongin-C

Chain e:



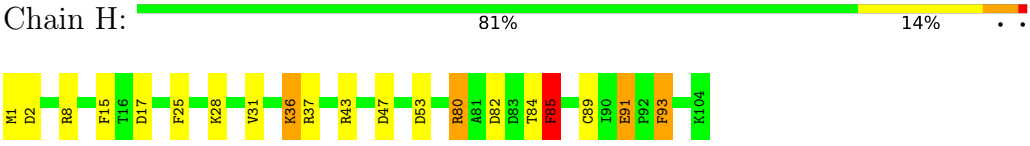
• Molecule 4: Elongin-B

Chain D:



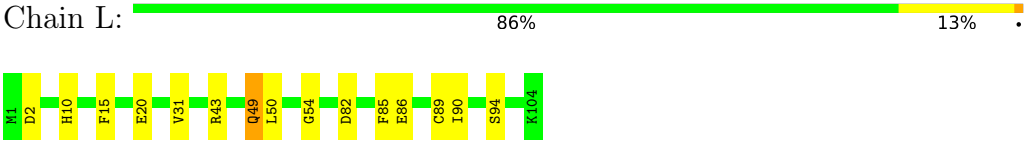
• Molecule 4: Elongin-B

Chain H:



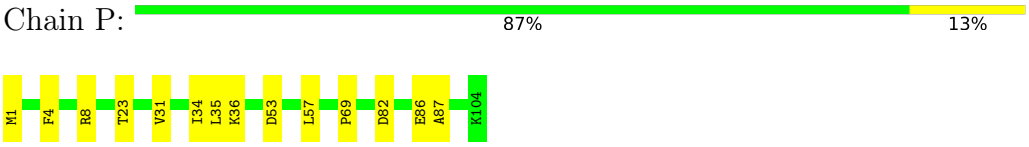
• Molecule 4: Elongin-B

Chain L:



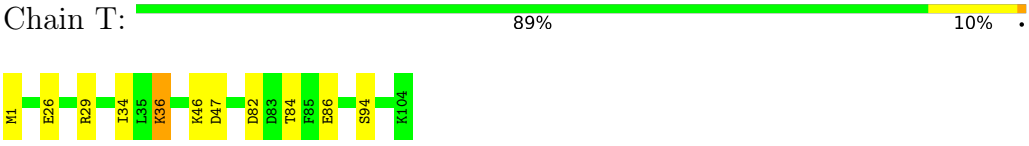
• Molecule 4: Elongin-B

Chain P:



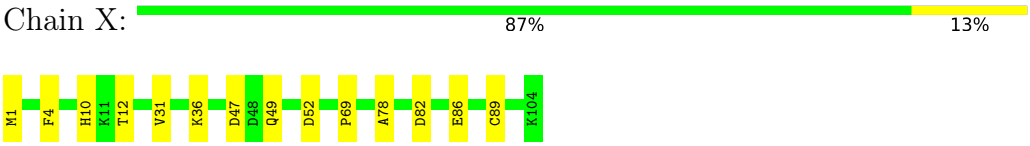
• Molecule 4: Elongin-B

Chain T:



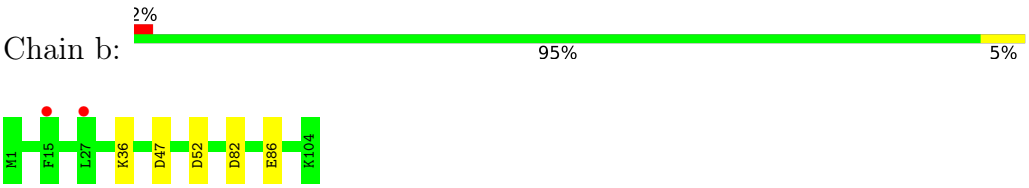
• Molecule 4: Elongin-B

Chain X:



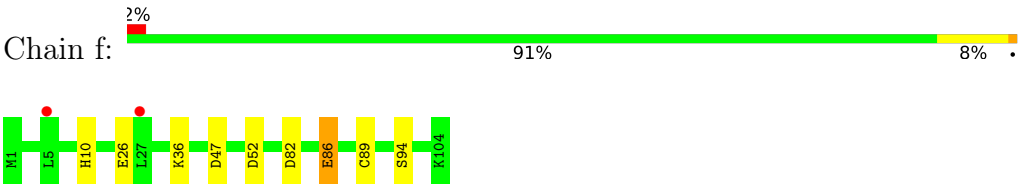
• Molecule 4: Elongin-B

Chain b:



• Molecule 4: Elongin-B

Chain f:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	56.95Å 298.50Å 142.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.87 – 3.30 29.87 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.9 (29.87-3.30) 98.9 (29.87-3.30)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.58 (at 3.31Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.219 , 0.275 0.219 , 0.271	Depositor DCC
R_{free} test set	3501 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	72.7	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 54.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.077 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	31004	wwPDB-VP
Average B, all atoms (Å^2)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.93% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, A1BNT, EDO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.19	5/978 (0.5%)	1.53	2/1312 (0.2%)
1	E	1.13	2/969 (0.2%)	1.54	5/1301 (0.4%)
1	I	1.16	2/969 (0.2%)	1.54	5/1301 (0.4%)
1	M	1.08	1/969 (0.1%)	1.62	6/1301 (0.5%)
1	Q	1.14	2/987 (0.2%)	1.64	5/1325 (0.4%)
1	U	1.21	2/978 (0.2%)	1.72	8/1313 (0.6%)
1	Y	1.12	1/998 (0.1%)	1.62	12/1340 (0.9%)
1	c	1.00	0/987	1.59	2/1325 (0.2%)
2	B	1.07	1/1275 (0.1%)	1.42	1/1738 (0.1%)
2	F	1.09	4/1279 (0.3%)	1.39	2/1745 (0.1%)
2	J	1.07	4/1313 (0.3%)	1.43	5/1792 (0.3%)
2	N	1.08	5/1323 (0.4%)	1.40	3/1802 (0.2%)
2	R	1.07	2/1283 (0.2%)	1.39	1/1749 (0.1%)
2	V	1.13	3/1283 (0.2%)	1.45	8/1749 (0.5%)
2	Z	1.13	5/1283 (0.4%)	1.44	5/1749 (0.3%)
2	d	0.97	0/1294	1.37	0/1764
3	C	1.22	3/777 (0.4%)	1.49	2/1050 (0.2%)
3	G	1.23	1/777 (0.1%)	1.46	3/1050 (0.3%)
3	K	1.22	4/777 (0.5%)	1.48	3/1050 (0.3%)
3	O	1.14	1/777 (0.1%)	1.48	2/1050 (0.2%)
3	S	1.19	5/777 (0.6%)	1.46	2/1050 (0.2%)
3	W	1.17	3/777 (0.4%)	1.57	6/1050 (0.6%)
3	a	1.09	1/777 (0.1%)	1.47	1/1050 (0.1%)
3	e	1.07	0/777	1.44	0/1050
4	D	1.11	2/839 (0.2%)	1.47	5/1132 (0.4%)
4	H	1.13	2/839 (0.2%)	1.49	4/1132 (0.4%)
4	L	1.08	1/839 (0.1%)	1.45	4/1132 (0.4%)
4	P	1.16	4/839 (0.5%)	1.44	3/1132 (0.3%)
4	T	1.11	0/839	1.46	3/1132 (0.3%)
4	X	1.17	1/839 (0.1%)	1.45	2/1132 (0.2%)
4	b	0.96	0/839	1.33	0/1132
4	f	0.97	0/839	1.34	0/1132

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
All	All	1.11	67/31096 (0.2%)	1.48	110/42062 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	F	0	1
2	Z	0	1
3	G	0	1
4	D	0	1
4	P	0	1
All	All	0	5

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	196	LYS	C-O	7.68	1.32	1.24
3	S	78	THR	C-O	7.40	1.32	1.24
3	W	61	ASN	C-O	7.39	1.32	1.24
4	X	78	ALA	C-O	7.10	1.31	1.23
1	E	1472	GLU	C-O	6.72	1.31	1.24
2	Z	116	LEU	C-O	6.62	1.32	1.24
2	R	158	LEU	C-O	-6.56	1.16	1.24
3	W	42	ILE	C-O	6.52	1.31	1.24
1	A	1453	VAL	C-O	-6.46	1.16	1.24
3	G	105	MET	C-O	6.46	1.31	1.24
3	K	81	VAL	C-O	6.40	1.31	1.24
1	A	1470	ILE	C-O	6.29	1.31	1.24
3	K	78	THR	C-O	6.11	1.31	1.24
2	Z	162	CYS	C-O	6.11	1.31	1.24
1	I	1442	LYS	C-O	6.10	1.31	1.24
2	Z	121	ASP	C-O	6.00	1.31	1.24
1	A	1471	TYR	C-O	-6.00	1.17	1.24
1	A	1474	SER	C-O	5.99	1.31	1.24
4	P	57	LEU	C-O	5.98	1.31	1.24
3	S	105	MET	C-O	5.96	1.31	1.24
2	N	185	TYR	C-O	5.95	1.31	1.24
3	a	42	ILE	C-O	5.95	1.31	1.24
1	M	1411	GLN	C-O	5.78	1.30	1.24
2	N	109	ILE	C-O	5.61	1.29	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	162	CYS	C-O	5.59	1.30	1.24
4	P	8	ARG	C-O	-5.57	1.17	1.24
1	U	1457	CYS	C-O	5.53	1.30	1.24
4	D	3	VAL	C-O	-5.50	1.18	1.24
2	N	196	LYS	C-O	5.49	1.30	1.24
3	O	81	VAL	C-O	5.45	1.30	1.24
2	V	130	VAL	C-O	5.43	1.29	1.24
2	F	90	ASN	C-O	5.39	1.30	1.23
4	P	34	ILE	C-O	5.39	1.29	1.23
2	F	95	PRO	C-O	-5.36	1.17	1.23
3	C	78	THR	C-O	5.34	1.30	1.24
3	C	105	MET	C-O	5.34	1.30	1.24
2	J	89	LEU	C-O	5.34	1.30	1.24
2	R	162	CYS	C-O	5.34	1.30	1.24
2	Z	62	VAL	C-O	5.30	1.29	1.24
4	H	8	ARG	C-O	5.29	1.29	1.24
1	Q	1448	ASP	C-O	5.27	1.30	1.24
2	F	116	LEU	C-O	5.22	1.30	1.24
2	B	136	PHE	C-O	5.21	1.30	1.24
3	K	38	THR	C-O	5.21	1.30	1.24
3	S	77	PHE	C-O	5.20	1.30	1.24
4	P	23	THR	N-CA	5.19	1.51	1.45
3	C	95	ILE	C-O	5.18	1.29	1.24
3	S	69	VAL	C-O	5.18	1.29	1.24
4	D	97	PRO	C-O	-5.17	1.17	1.23
2	J	116	LEU	C-O	5.17	1.30	1.24
3	W	105	MET	C-O	5.16	1.30	1.24
4	H	2	ASP	C-O	-5.15	1.17	1.23
2	N	62	VAL	C-O	5.14	1.29	1.24
1	A	1410	ILE	C-O	5.13	1.29	1.24
1	U	1448	ASP	C-O	5.13	1.30	1.24
2	F	108	ARG	C-O	-5.12	1.17	1.23
2	Z	107	ARG	C-O	5.08	1.29	1.23
2	V	198	LEU	C-O	5.07	1.29	1.24
1	Y	1459	ASN	C-O	5.07	1.29	1.24
1	E	1383	LEU	C-O	5.06	1.29	1.24
4	L	90	ILE	C-O	5.06	1.29	1.24
1	I	1391	ILE	C-O	5.04	1.30	1.24
1	Q	1481	PHE	C-O	5.04	1.29	1.24
2	N	187	ASP	C-O	5.02	1.29	1.24
3	S	27	HIS	C-O	-5.01	1.18	1.23
2	V	108	ARG	C-O	5.00	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	100	ALA	C-O	5.00	1.29	1.24

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Q	1459	ASN	CB-CA-C	10.05	129.22	110.63
1	c	1379	ASN	CA-CB-CG	8.50	121.10	112.60
1	U	1422	TYR	CA-C-O	-7.73	112.35	120.55
1	c	1485	ARG	CG-CD-NE	7.68	128.89	112.00
3	a	49	PRO	CB-CA-C	-7.12	102.27	111.46
1	M	1433	LYS	O-C-N	6.84	129.37	122.12
2	J	115	HIS	CA-C-O	-6.81	114.14	121.56
2	J	180	ILE	CA-C-N	6.79	129.59	120.50
2	J	180	ILE	C-N-CA	6.79	129.59	120.50
1	U	1433	LYS	CA-C-O	-6.64	112.33	119.97
4	H	93	PHE	CA-CB-CG	6.57	120.37	113.80
2	V	110	HIS	CB-CA-C	6.57	120.83	110.19
3	K	61	ASN	CA-C-O	-6.35	113.98	120.71
1	E	1399	ASP	CA-C-N	6.34	128.77	120.28
1	E	1399	ASP	C-N-CA	6.34	128.77	120.28
3	C	88	THR	CB-CA-C	6.24	117.47	109.80
1	U	1462	THR	CA-C-O	-6.16	114.35	120.82
1	Y	1478	GLN	CA-C-O	-6.16	114.30	121.07
2	N	128	LEU	CA-C-O	-6.15	114.45	121.58
1	M	1433	LYS	CA-C-O	-6.02	114.17	120.55
1	M	1461	GLN	CA-C-N	5.97	128.28	120.28
1	M	1461	GLN	C-N-CA	5.97	128.28	120.28
2	B	89	LEU	CA-C-O	-5.96	114.20	120.58
1	U	1462	THR	N-CA-C	5.95	117.43	111.07
3	O	30	ILE	CA-C-O	-5.91	113.89	120.74
4	L	31	VAL	O-C-N	5.84	127.77	121.87
4	P	53	ASP	CA-C-N	5.78	126.36	120.00
4	P	53	ASP	C-N-CA	5.78	126.36	120.00
2	V	195	GLN	CA-C-N	5.77	128.01	120.28
2	V	195	GLN	C-N-CA	5.77	128.01	120.28
1	Y	1381	PRO	CA-C-N	5.76	128.27	120.38
1	Y	1381	PRO	C-N-CA	5.76	128.27	120.38
4	T	34	ILE	CA-C-O	-5.75	113.59	120.78
2	F	210	ARG	CA-C-O	-5.64	111.21	120.80
4	D	76	GLY	CA-C-O	-5.63	116.51	121.58
2	J	175	TYR	O-C-N	5.63	128.62	122.20
1	Y	1420	GLU	CA-C-N	5.62	127.75	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Y	1420	GLU	C-N-CA	5.62	127.75	120.44
2	V	128	LEU	CA-C-O	-5.62	115.06	121.58
4	H	31	VAL	O-C-N	5.62	127.32	121.87
3	W	23	SER	CA-C-N	5.59	128.03	120.38
3	W	23	SER	C-N-CA	5.59	128.03	120.38
1	M	1441	HIS	CA-C-O	-5.58	113.70	120.12
3	C	62	PHE	CB-CA-C	5.54	118.79	109.48
1	E	1438	ILE	CA-C-N	5.54	128.26	120.28
1	E	1438	ILE	C-N-CA	5.54	128.26	120.28
4	P	31	VAL	O-C-N	5.53	127.45	121.87
2	R	146	PRO	CB-CA-C	-5.53	103.74	110.98
1	I	1439	ARG	CA-C-O	-5.49	115.03	120.90
2	V	64	ARG	CA-C-O	-5.47	114.86	120.99
3	W	67	SER	O-C-N	5.46	127.69	122.07
4	D	41	GLU	CA-C-O	-5.44	112.99	119.35
1	Q	1438	ILE	O-C-N	5.44	127.43	121.83
1	Y	1466	GLU	CA-C-O	-5.44	115.79	121.55
1	U	1393	THR	CA-C-O	-5.43	114.67	120.42
2	Z	163	LEU	CA-C-O	-5.43	115.09	120.90
4	D	31	VAL	CA-C-O	-5.41	115.12	120.85
3	K	44	ALA	CA-C-O	-5.39	114.71	120.42
1	Y	1476	VAL	O-C-N	5.36	127.16	121.91
3	O	19	VAL	CA-C-O	-5.35	116.00	121.67
1	Y	1476	VAL	CA-C-O	-5.34	115.51	121.17
2	J	175	TYR	CA-C-O	-5.33	114.23	120.20
2	V	111	SER	CA-C-O	-5.32	114.15	121.98
1	A	1390	ILE	O-C-N	5.32	127.26	121.94
3	G	43	LYS	CA-C-N	5.32	127.84	120.29
3	G	43	LYS	C-N-CA	5.32	127.84	120.29
4	L	54	GLY	CA-C-O	-5.31	114.41	120.09
2	N	141	ASN	CB-CA-C	-5.29	100.94	109.72
4	H	85	PHE	CA-CB-CG	5.28	119.08	113.80
1	A	1395	ILE	O-C-N	5.28	127.06	121.89
4	X	52	ASP	CA-CB-CG	5.27	117.87	112.60
1	E	1447	GLY	CA-C-O	-5.27	115.64	120.80
2	Z	122	ALA	CA-C-N	5.26	125.68	119.94
2	Z	122	ALA	C-N-CA	5.26	125.68	119.94
4	H	91	GLU	CB-CG-CD	5.25	121.53	112.60
3	K	19	VAL	CA-C-O	-5.25	116.10	121.67
1	U	1421	TYR	CA-C-N	5.24	127.30	120.28
1	U	1421	TYR	C-N-CA	5.24	127.30	120.28
4	L	20	GLU	CA-C-N	5.23	128.26	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	L	20	GLU	C-N-CA	5.23	128.26	120.31
1	Q	1426	ARG	N-CA-C	-5.22	106.76	113.23
1	M	1444	ARG	CB-CG-CD	5.22	123.30	111.30
3	S	102	GLU	O-C-N	5.21	127.64	122.12
3	S	40	GLY	O-C-N	5.18	127.17	122.19
1	I	1421	TYR	CA-C-N	5.17	127.64	120.29
1	I	1421	TYR	C-N-CA	5.17	127.64	120.29
1	Y	1400	SER	CA-C-O	-5.17	115.37	120.90
2	Z	170	VAL	N-CA-C	-5.16	104.43	110.05
2	V	64	ARG	CB-CG-CD	5.16	123.16	111.30
2	V	110	HIS	CA-CB-CG	5.14	118.94	113.80
2	F	67	ASN	CA-C-O	-5.13	116.21	122.41
4	T	46	LYS	CA-C-N	5.12	131.32	121.54
4	T	46	LYS	C-N-CA	5.12	131.32	121.54
3	W	33	ARG	CA-C-N	5.12	127.39	120.38
3	W	33	ARG	C-N-CA	5.12	127.39	120.38
1	I	1416	LYS	CA-C-N	5.12	127.09	120.44
1	I	1416	LYS	C-N-CA	5.12	127.09	120.44
4	D	75	VAL	CA-C-N	5.10	125.52	120.31
4	D	75	VAL	C-N-CA	5.10	125.52	120.31
1	Y	1384	THR	CA-C-N	5.09	127.06	120.44
1	Y	1384	THR	C-N-CA	5.09	127.06	120.44
3	W	107	ALA	O-C-N	5.08	127.37	122.09
3	G	78	THR	O-C-N	5.07	127.51	122.08
1	U	1464	ASN	N-CA-C	-5.05	106.71	112.92
2	Z	78	ASN	CA-C-O	-5.03	115.78	121.66
1	Q	1478	GLN	CA-C-N	5.03	127.01	120.28
1	Q	1478	GLN	C-N-CA	5.03	127.01	120.28
2	N	75	ILE	CA-C-O	-5.02	114.79	120.66
4	X	31	VAL	O-C-N	5.00	126.93	121.87
1	Y	1390	ILE	CA-C-O	-5.00	115.85	121.05

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	79	PHE	Peptide
2	F	91	PHE	Mainchain
3	G	50	GLY	Peptide
4	P	35	LEU	Mainchain
2	Z	138	PRO	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	962	0	998	21	1
1	E	953	0	985	10	0
1	I	953	0	985	25	0
1	M	953	0	985	7	0
1	Q	971	0	997	12	0
1	U	962	0	991	36	0
1	Y	981	0	1003	10	1
1	c	971	0	997	21	1
2	B	1243	0	1245	15	0
2	F	1246	0	1242	14	0
2	J	1279	0	1263	17	0
2	N	1290	0	1291	11	0
2	R	1250	0	1253	19	0
2	V	1250	0	1253	10	0
2	Z	1250	0	1253	10	0
2	d	1257	0	1260	25	1
3	C	760	0	749	7	1
3	G	760	0	749	6	0
3	K	760	0	749	5	0
3	O	760	0	749	3	0
3	S	760	0	749	6	0
3	W	760	0	749	4	0
3	a	760	0	749	12	0
3	e	760	0	749	3	0
4	D	823	0	824	5	0
4	H	823	0	824	6	0
4	L	823	0	824	5	0
4	P	823	0	824	2	0
4	T	823	0	824	2	0
4	X	823	0	824	2	0
4	b	823	0	824	0	0
4	f	823	0	824	3	1
5	B	54	0	0	0	0
5	F	54	0	0	2	0
5	J	54	0	0	4	0
5	N	54	0	0	3	0
5	Q	54	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	V	54	0	0	2	0
5	Z	54	0	0	2	0
5	d	54	0	0	1	0
6	B	4	0	6	0	0
6	F	8	0	12	0	0
6	J	4	0	6	0	0
6	R	4	0	6	1	0
6	c	4	0	6	0	0
7	J	6	0	8	0	0
8	A	6	0	0	1	0
8	B	7	0	0	0	0
8	C	5	0	0	0	0
8	D	2	0	0	0	0
8	E	6	0	0	0	0
8	F	4	0	0	0	0
8	G	3	0	0	0	0
8	H	2	0	0	0	0
8	I	6	0	0	0	0
8	J	2	0	0	0	0
8	K	4	0	0	0	0
8	L	1	0	0	0	0
8	M	6	0	0	0	0
8	N	10	0	0	0	0
8	O	3	0	0	0	0
8	P	3	0	0	0	0
8	Q	1	0	0	0	0
8	R	2	0	0	0	0
8	S	1	0	0	0	0
8	T	2	0	0	0	0
8	U	1	0	0	0	0
8	V	4	0	0	0	0
8	W	2	0	0	0	0
8	X	2	0	0	0	0
8	Z	4	0	0	0	0
8	a	2	0	0	0	0
8	b	2	0	0	0	0
8	c	3	0	0	1	0
8	d	1	0	0	0	0
8	e	6	0	0	0	0
8	f	4	0	0	1	0
All	All	31004	0	30629	298	3

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 (298) 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)
2:d:163:LEU:HD22	2:d:188:LEU:CD2	2.04	0.88
3:a:46:LEU:HD22	3:a:57:THR:HG22	1.58	0.85
2:d:180:ILE:HD11	2:d:185:TYR:CD1	2.14	0.83
2:d:180:ILE:HD11	2:d:185:TYR:CE1	2.14	0.82
1:A:1380:PRO:HG3	1:I:1475:ILE:CD1	2.10	0.82
1:Q:1469:GLN:HE21	1:Q:1469:GLN:HA	1.49	0.77
1:c:1485:ARG:HG2	1:c:1485:ARG:HH11	1.49	0.77
2:d:116:LEU:HD11	2:d:135:LEU:CD1	2.17	0.75
1:c:1464:ASN:ND2	5:d:301:A1BNT:N7	2.34	0.74
1:A:1380:PRO:CG	1:I:1475:ILE:HD12	2.18	0.73
1:c:1389:ALA:O	1:c:1393:THR:HG23	1.89	0.73
1:A:1380:PRO:HG3	1:I:1475:ILE:HD12	1.72	0.72
2:V:73:GLN:H	2:V:141:ASN:HD21	1.35	0.71
1:A:1395:ILE:O	1:A:1406:SER:OG	2.09	0.70
1:U:1395:ILE:O	1:U:1406:SER:OG	2.10	0.70
2:R:140:LEU:H	2:R:140:LEU:HD22	1.55	0.70
2:d:61:PRO:O	2:d:64:ARG:NH1	2.25	0.70
1:c:1390:ILE:O	1:c:1393:THR:OG1	2.11	0.69
2:d:116:LEU:HD11	2:d:135:LEU:HD13	1.73	0.69
2:N:73:GLN:H	2:N:141:ASN:HD21	1.42	0.67
2:d:73:GLN:H	2:d:141:ASN:HD21	1.40	0.67
1:E:1395:ILE:O	1:E:1406:SER:OG	2.12	0.67
2:d:163:LEU:CD2	2:d:188:LEU:CD2	2.71	0.67
1:M:1395:ILE:O	1:M:1406:SER:OG	2.14	0.66
1:U:1380:PRO:HB2	1:U:1381:PRO:CD	2.25	0.66
2:J:73:GLN:H	2:J:141:ASN:HD21	1.43	0.65
2:F:115:HIS:ND1	5:F:301:A1BNT:O2	2.30	0.64
1:U:1457:CYS:O	1:U:1461:GLN:N	2.27	0.64
3:C:63:ARG:HE	3:C:64:GLU:HG2	1.64	0.63
1:c:1395:ILE:O	1:c:1406:SER:OG	2.13	0.63
1:A:1444:ARG:CD	1:I:1454:MET:HE3	2.28	0.63
1:I:1395:ILE:O	1:I:1406:SER:OG	2.15	0.63
2:R:92:ASP:O	1:Y:1416:LYS:NZ	2.31	0.63
1:Q:1383:LEU:HD21	1:Q:1444:ARG:O	1.98	0.63
1:U:1380:PRO:HB2	1:U:1381:PRO:HD2	1.80	0.62
4:f:86:GLU:OE2	8:f:201:HOH:O	2.16	0.62
1:Y:1395:ILE:O	1:Y:1406:SER:OG	2.15	0.62
2:d:73:GLN:HE22	2:d:110[B]:HIS:CD2	2.17	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:d:163:LEU:HD22	2:d:188:LEU:HD23	1.81	0.62
2:R:140:LEU:HD22	2:R:140:LEU:N	2.15	0.61
2:d:163:LEU:HD22	2:d:188:LEU:HD22	1.82	0.61
2:Z:110:HIS:HE1	2:Z:112:TYR:OH	1.83	0.61
3:K:68:HIS:HB3	4:L:94:SER:O	2.01	0.60
3:G:31:VAL:HG12	4:H:15:PHE:HB2	1.83	0.60
1:I:1418:LEU:HD13	2:J:69:ARG:HH12	1.67	0.60
1:c:1404:GLN:O	1:c:1404:GLN:HG3	2.00	0.60
2:d:180:ILE:CD1	2:d:185:TYR:CE1	2.85	0.60
2:Z:158:LEU:N	3:a:112:CYS:OXT	2.35	0.60
1:E:1466:GLU:HG3	1:Y:1446:LEU:HD12	1.84	0.59
4:D:1:MET:SD	4:D:64:SER:OG	2.59	0.59
1:U:1445:SER:O	1:U:1446:LEU:HB2	2.01	0.59
1:I:1408:VAL:HB	2:J:110[A]:HIS:CD2	2.37	0.59
1:Q:1407:GLU:CD	2:R:110:HIS:HB2	2.28	0.59
2:B:72:SER:HA	2:B:141:ASN:ND2	2.17	0.58
1:U:1382:LYS:O	1:U:1385:LYS:N	2.36	0.58
2:F:73:GLN:H	2:F:141:ASN:HD21	1.51	0.58
2:B:60:ARG:HB3	2:B:61:PRO:HD3	1.85	0.58
2:d:62:VAL:CG2	2:d:202:THR:HG23	2.35	0.57
3:G:67:SER:OG	4:H:93:PHE:HB3	2.05	0.57
1:U:1481:PHE:O	1:U:1484:ALA:HB3	2.04	0.57
1:A:1444:ARG:HG3	1:I:1454:MET:CE	2.34	0.57
4:D:80:ARG:HA	4:D:84:THR:O	2.04	0.57
2:R:141:ASN:H	6:R:301:EDO:H12	1.69	0.57
1:U:1424:LEU:O	1:U:1426:ARG:NH1	2.37	0.57
1:Y:1414:SER:OG	1:Y:1416:LYS:HG2	2.04	0.57
1:I:1407:GLU:OE1	2:J:110[B]:HIS:CD2	2.58	0.56
2:d:180:ILE:HD13	2:d:184:LEU:HB2	1.88	0.56
2:d:135:LEU:HD21	2:d:201:LEU:CD1	2.35	0.56
3:C:31:VAL:HG12	4:D:15:PHE:HB2	1.88	0.56
2:d:116:LEU:HD11	2:d:135:LEU:HD12	1.87	0.56
1:A:1395:ILE:CD1	1:A:1435:LYS:HE2	2.36	0.56
1:U:1450:GLU:HG2	1:U:1481:PHE:HE2	1.72	0.55
1:U:1425:ILE:CD1	1:U:1462:THR:HB	2.37	0.55
5:Q:1501:A1BNT:N8	5:Q:1501:A1BNT:C14	2.69	0.55
1:U:1413:PRO:HB3	5:V:301:A1BNT:C29	2.36	0.55
1:U:1450:GLU:HG3	1:U:1485:ARG:NH1	2.22	0.55
2:B:73:GLN:H	2:B:141:ASN:HD21	1.54	0.55
3:e:68:HIS:HB3	4:f:94:SER:O	2.07	0.55
2:J:76:PHE:CZ	2:J:109:ILE:HD11	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:1461:GLN:HG3	1:U:1471:TYR:CE2	2.42	0.55
1:U:1425:ILE:HD11	1:U:1462:THR:HB	1.87	0.54
3:a:42:ILE:HD11	3:a:110:LEU:CD2	2.38	0.54
1:U:1425:ILE:HG22	1:U:1425:ILE:O	2.08	0.54
3:W:51:GLN:HB3	3:W:57:THR:HG23	1.89	0.54
1:c:1383:LEU:HD12	1:c:1387:MET:HE3	1.89	0.54
2:B:60:ARG:CB	2:B:61:PRO:CD	2.85	0.54
2:R:60:ARG:N	2:R:61:PRO:HD2	2.22	0.54
1:Q:1387:MET:HE1	1:Q:1443:TYR:HB2	1.88	0.54
1:U:1413:PRO:O	1:U:1414:SER:O	2.26	0.54
2:V:132:GLN:NE2	3:W:85:ASN:O	2.41	0.54
1:A:1444:ARG:CG	1:I:1454:MET:HE3	2.37	0.54
1:c:1379:ASN:HB2	1:c:1380:PRO:HD2	1.89	0.54
2:d:62:VAL:HG21	2:d:202:THR:HG23	1.90	0.53
1:c:1485:ARG:NE	8:c:1601:HOH:O	2.25	0.53
2:N:76:PHE:CZ	2:N:109:ILE:HD11	2.43	0.53
2:B:60:ARG:CB	2:B:61:PRO:HD3	2.38	0.53
3:a:42:ILE:CD1	3:a:42:ILE:N	2.72	0.53
3:a:46:LEU:HD22	3:a:57:THR:CG2	2.35	0.53
2:J:115:HIS:ND1	5:J:301:A1BNT:O2	2.40	0.53
1:A:1444:ARG:HD2	1:I:1454:MET:HE3	1.90	0.53
1:U:1397:TYR:CE1	1:U:1405:LEU:HD12	2.44	0.53
1:U:1427:LYS:O	1:U:1459:ASN:ND2	2.42	0.53
2:R:142:VAL:HG23	2:R:145:GLN:HE21	1.72	0.52
1:c:1408:VAL:HG13	1:c:1409:PHE:CD1	2.44	0.52
2:d:70:GLU:OE2	2:d:113:ARG:HD3	2.10	0.52
1:c:1399:ASP:HB3	1:c:1405:LEU:HD22	1.91	0.52
1:I:1407:GLU:OE1	2:J:110[B]:HIS:HD2	1.92	0.52
2:R:60:ARG:H	2:R:61:PRO:HD2	1.75	0.51
1:M:1418:LEU:HD22	5:N:301:A1BNT:C14	2.40	0.51
1:c:1379:ASN:HB2	1:c:1380:PRO:CD	2.40	0.51
1:U:1450:GLU:HG2	1:U:1481:PHE:CE2	2.45	0.51
1:U:1425:ILE:C	1:U:1427:LYS:H	2.18	0.51
1:M:1424:LEU:HD23	1:M:1463:PHE:HD1	1.76	0.51
3:S:50:GLY:HA2	3:S:57:THR:OG1	2.11	0.50
1:A:1448:ASP:OD2	1:I:1482:LYS:HE3	2.11	0.50
1:E:1466:GLU:CG	1:Y:1446:LEU:HD12	2.41	0.50
1:c:1408:VAL:HG13	1:c:1409:PHE:CE1	2.45	0.50
1:I:1471:TYR:O	1:I:1475:ILE:HG12	2.12	0.50
4:D:43:ARG:HH12	4:D:85:PHE:HA	1.76	0.50
1:Y:1464:ASN:OD1	1:Y:1470:ILE:HB	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:1383:LEU:HD22	1:U:1383:LEU:O	2.12	0.50
4:H:37:ARG:NH1	4:H:80:ARG:O	2.45	0.49
2:V:62:VAL:CG1	2:V:202:THR:HG23	2.42	0.49
1:A:1380:PRO:CG	1:I:1475:ILE:CD1	2.83	0.49
2:J:154:PRO:HG2	2:J:156:TYR:CE1	2.48	0.49
3:K:17:MET:HE1	3:K:33:ARG:NH1	2.27	0.49
2:N:76:PHE:CE2	2:N:109:ILE:HD13	2.48	0.49
1:A:1380:PRO:HG2	1:I:1475:ILE:HD12	1.95	0.49
2:N:115:HIS:ND1	5:N:301:A1BNT:O2	2.41	0.49
5:Z:301:A1BNT:O5	5:Z:301:A1BNT:N6	2.42	0.49
5:Q:1501:A1BNT:N6	5:Q:1501:A1BNT:O5	2.46	0.49
1:U:1423:GLU:O	1:U:1426:ARG:HD3	2.12	0.49
3:C:83:TYR:HB3	3:C:90:ILE:HD13	1.95	0.48
3:K:48:GLY:O	3:K:55:ASN:O	2.31	0.48
1:U:1465:LEU:O	1:U:1471:TYR:CE2	2.65	0.48
2:R:132:GLN:NE2	3:S:87:SER:OG	2.45	0.48
1:c:1404:GLN:HE21	1:c:1407:GLU:N	2.11	0.48
2:B:73:GLN:OE1	2:B:108:ARG:NH2	2.47	0.48
5:J:301:A1BNT:O5	5:J:301:A1BNT:N6	2.46	0.48
1:A:1444:ARG:HG3	1:I:1454:MET:HE2	1.94	0.48
1:Q:1469:GLN:HA	1:Q:1469:GLN:NE2	2.24	0.48
2:V:60:ARG:H	2:V:61:PRO:HD2	1.78	0.48
2:Z:115:HIS:ND1	5:Z:301:A1BNT:O2	2.38	0.48
1:I:1397:TYR:C	1:I:1397:TYR:CD1	2.91	0.48
1:c:1383:LEU:CD1	1:c:1387:MET:HE3	2.43	0.48
1:A:1380:PRO:HB3	1:I:1471:TYR:OH	2.14	0.48
2:F:73:GLN:OE1	2:F:108:ARG:NH2	2.47	0.48
1:A:1444:ARG:CG	1:I:1454:MET:CE	2.92	0.48
2:Z:73:GLN:OE1	2:Z:108:ARG:NH2	2.47	0.48
2:F:110:HIS:HE1	2:F:112:TYR:CZ	2.32	0.47
4:P:4:PHE:CE2	4:P:69:PRO:HG3	2.49	0.47
1:U:1380:PRO:CB	1:U:1381:PRO:CD	2.92	0.47
3:a:42:ILE:N	3:a:42:ILE:HD13	2.30	0.47
4:H:25:PHE:HB2	4:H:53:ASP:HB3	1.95	0.47
1:U:1397:TYR:HE1	1:U:1405:LEU:HD12	1.79	0.47
2:J:76:PHE:CE2	2:J:109:ILE:HD13	2.49	0.47
1:M:1421:TYR:HD1	1:M:1463:PHE:CD2	2.33	0.47
2:V:59:PRO:HD3	2:V:92:ASP:OD1	2.15	0.47
1:I:1412:LEU:HG	1:I:1430:ASP:HB3	1.96	0.47
3:S:69:VAL:HG21	3:S:102:GLU:HB3	1.95	0.47
1:c:1404:GLN:NE2	1:c:1406:SER:OG	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:1387:MET:HG2	1:Q:1449:LEU:HD22	1.95	0.47
2:R:60:ARG:N	2:R:61:PRO:CD	2.77	0.47
1:U:1445:SER:O	1:U:1446:LEU:CB	2.63	0.47
2:F:144:GLY:O	2:F:145:GLN:C	2.58	0.47
1:A:1485:ARG:NH1	8:A:1501:HOH:O	2.48	0.46
2:F:154:PRO:HG2	2:F:156:TYR:CE1	2.50	0.46
2:R:64:ARG:HD2	2:R:91:PHE:O	2.14	0.46
2:N:154:PRO:HG2	2:N:156:TYR:CE1	2.50	0.46
1:U:1471:TYR:CE1	1:U:1475:ILE:HD11	2.50	0.46
5:V:301:A1BNT:N6	5:V:301:A1BNT:O5	2.46	0.46
2:B:72:SER:HA	2:B:141:ASN:HD21	1.77	0.46
2:Z:110:HIS:CE1	2:Z:112:TYR:CZ	3.04	0.46
2:F:184:LEU:HD21	3:G:108:ASN:ND2	2.31	0.46
3:a:41:THR:O	3:a:45:MET:N	2.48	0.46
2:V:154:PRO:HG2	2:V:156:TYR:CE1	2.51	0.46
2:Z:154:PRO:HG2	2:Z:156:TYR:CE1	2.51	0.45
2:J:176:ARG:HA	2:J:185:TYR:CE1	2.51	0.45
5:N:301:A1BNT:N6	5:N:301:A1BNT:O5	2.48	0.45
2:d:154:PRO:HG2	2:d:156:TYR:CE1	2.52	0.45
2:B:209:GLN:O	2:B:210:ARG:C	2.59	0.45
2:J:64:ARG:HD2	2:J:91:PHE:O	2.17	0.45
2:B:139:SER:HB2	2:N:139:SER:OG	2.16	0.45
3:a:45:MET:HE1	3:a:60:VAL:HG13	1.98	0.45
2:B:101:LEU:HD23	2:B:107:ARG:NH2	2.31	0.45
1:E:1465:LEU:HD13	1:Y:1386:GLN:CD	2.42	0.45
1:Q:1401:SER:O	2:R:108:ARG:NH1	2.49	0.45
2:Z:176:ARG:HA	2:Z:185:TYR:CE1	2.52	0.45
2:B:154:PRO:HG2	2:B:156:TYR:CE1	2.51	0.45
2:V:73:GLN:NE2	2:V:110:HIS:HB2	2.31	0.45
2:d:134:GLU:C	2:d:135:LEU:HD23	2.41	0.45
1:I:1464:ASN:ND2	5:J:301:A1BNT:N7	2.51	0.45
1:Q:1395:ILE:O	1:Q:1406:SER:OG	2.31	0.45
2:V:62:VAL:HG22	2:V:63:LEU:H	1.82	0.45
1:Y:1414:SER:OG	1:Y:1416:LYS:CG	2.64	0.45
1:Q:1403:ARG:NH2	1:Q:1405:LEU:HD23	2.32	0.45
1:U:1465:LEU:HG	1:U:1466:GLU:N	2.32	0.45
1:Y:1464:ASN:O	1:Y:1465:LEU:HG	2.17	0.45
3:C:96:ALA:O	3:C:99:ILE:HG22	2.17	0.44
2:N:196:LYS:O	2:N:199:GLU:HB2	2.16	0.44
1:c:1439:ARG:HD2	1:c:1439:ARG:HA	1.71	0.44
2:d:176:ARG:HA	2:d:185:TYR:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1471:TYR:CE1	1:I:1475:ILE:HD11	2.53	0.44
2:R:110:HIS:HE1	2:R:112:TYR:CZ	2.35	0.44
1:E:1418:LEU:HD12	1:E:1420:GLU:OE2	2.18	0.44
1:c:1397:TYR:CE2	1:c:1405:LEU:HD21	2.52	0.44
1:E:1464:ASN:OD1	1:E:1470:ILE:HB	2.16	0.44
2:J:58:ARG:CG	2:J:58:ARG:HH21	2.30	0.44
2:R:154:PRO:HG2	2:R:156:TYR:CE1	2.53	0.44
1:U:1386:GLN:NE2	1:U:1492:GLU:OE2	2.51	0.44
1:U:1407:GLU:CD	2:V:110:HIS:HB3	2.43	0.44
2:B:61:PRO:O	2:B:64:ARG:HD3	2.17	0.44
2:N:132:GLN:NE2	3:O:85:ASN:O	2.51	0.44
1:U:1450:GLU:HA	1:U:1481:PHE:CE2	2.53	0.44
3:G:85:ASN:ND2	1:I:1402:GLY:HA2	2.33	0.44
2:J:209:GLN:O	2:J:210:ARG:C	2.60	0.44
2:Z:184:LEU:HD21	3:a:108:ASN:ND2	2.33	0.44
3:e:96:ALA:O	3:e:99:ILE:HG22	2.18	0.44
2:F:165:VAL:O	2:F:168:SER:OG	2.34	0.43
4:L:49:GLN:NE2	4:L:50:LEU:O	2.52	0.43
3:K:31:VAL:HG12	4:L:15:PHE:HB2	1.98	0.43
1:c:1471:TYR:CE1	1:c:1475:ILE:HD11	2.53	0.43
1:E:1412:LEU:HG	1:E:1430:ASP:HB3	2.00	0.43
2:J:196:LYS:O	2:J:199:GLU:HB2	2.18	0.43
2:R:60:ARG:H	2:R:61:PRO:CD	2.30	0.43
2:d:180:ILE:HD12	2:d:180:ILE:C	2.43	0.43
3:C:68:HIS:HB3	4:D:94:SER:O	2.19	0.43
1:E:1464:ASN:O	1:E:1465:LEU:HG	2.18	0.43
1:U:1405:LEU:HD23	1:U:1405:LEU:HA	1.88	0.43
1:U:1397:TYR:CD1	1:U:1397:TYR:C	2.97	0.43
2:d:166:VAL:CG1	2:d:188:LEU:HD11	2.49	0.43
1:A:1471:TYR:CE1	1:A:1475:ILE:HD11	2.54	0.43
3:S:56:GLU:O	3:S:56:GLU:HG3	2.18	0.43
3:S:68:HIS:HB3	4:T:94:SER:O	2.19	0.43
2:Z:110:HIS:HE1	2:Z:112:TYR:CZ	2.35	0.43
1:c:1405:LEU:H	1:c:1405:LEU:HD23	1.82	0.43
2:B:132:GLN:NE2	3:C:86:SER:C	2.77	0.43
2:J:76:PHE:CZ	2:J:109:ILE:CD1	3.02	0.43
1:A:1464:ASN:O	1:A:1465:LEU:HG	2.19	0.42
2:N:76:PHE:CZ	2:N:109:ILE:CD1	3.02	0.42
2:V:76:PHE:O	2:V:106:GLY:HA2	2.19	0.42
4:H:80:ARG:NH1	4:H:85:PHE:HB3	2.34	0.42
2:N:176:ARG:HA	2:N:185:TYR:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:138:PRO:C	2:Z:139:SER:O	2.62	0.42
5:F:301:A1BNT:N6	5:F:301:A1BNT:O5	2.52	0.42
4:L:10:HIS:CD2	4:L:89:CYS:HB3	2.54	0.42
1:Q:1382:LYS:HA	1:Q:1385:LYS:HE3	2.01	0.42
1:E:1456:LEU:C	1:E:1456:LEU:HD23	2.44	0.42
3:G:51:GLN:HB2	3:G:56:GLU:O	2.20	0.42
2:B:144:GLY:O	2:B:145:GLN:C	2.63	0.42
2:F:184:LEU:HD21	3:G:108:ASN:HD22	1.84	0.42
1:U:1380:PRO:HG2	1:U:1383:LEU:HB3	2.02	0.42
1:Y:1471:TYR:CE1	1:Y:1475:ILE:HD11	2.54	0.42
1:A:1412:LEU:HG	1:A:1430:ASP:HB3	2.00	0.42
3:K:96:ALA:O	3:K:99:ILE:HG22	2.20	0.42
2:B:136:PHE:HA	2:N:145:GLN:OE1	2.20	0.42
3:C:33:ARG:NH2	3:C:56:GLU:HB2	2.35	0.42
1:I:1418:LEU:HD22	5:J:301:A1BNT:C14	2.48	0.42
1:M:1454:MET:HE3	1:M:1478:GLN:HG2	2.00	0.42
5:Q:1501:A1BNT:O2	2:R:115:HIS:ND1	2.47	0.42
3:S:51:GLN:HE21	3:S:51:GLN:HB3	1.73	0.42
3:a:96:ALA:O	3:a:99:ILE:HG22	2.20	0.42
2:F:176:ARG:HA	2:F:185:TYR:CE1	2.55	0.41
2:J:108:ARG:NH1	2:J:146:PRO:HG3	2.34	0.41
3:W:54:GLU:HG3	3:W:56:GLU:HG2	2.01	0.41
4:P:86:GLU:HG3	4:P:87:ALA:O	2.20	0.41
4:L:43:ARG:HH12	4:L:85:PHE:HA	1.84	0.41
3:O:96:ALA:O	3:O:99:ILE:HG22	2.19	0.41
4:X:10:HIS:CD2	4:X:89:CYS:HB3	2.55	0.41
1:E:1471:TYR:CE1	1:E:1475:ILE:HD11	2.55	0.41
1:U:1425:ILE:C	1:U:1427:LYS:N	2.77	0.41
3:e:49:PRO:O	3:e:57:THR:OG1	2.34	0.41
2:d:167:ARG:HD3	2:d:191:HIS:CD2	2.56	0.41
2:R:165:VAL:O	2:R:168:SER:OG	2.31	0.41
4:T:26:GLU:O	4:T:29:ARG:HB2	2.21	0.41
2:F:64:ARG:HD2	2:F:91:PHE:O	2.21	0.41
3:W:51:GLN:NE2	3:W:58:ASN:OD1	2.53	0.41
1:U:1412:LEU:HG	1:U:1430:ASP:HB3	2.01	0.41
2:J:165:VAL:O	2:J:168:SER:OG	2.33	0.41
1:Q:1487:LYS:O	1:Q:1491:GLU:HB2	2.21	0.41
2:R:176:ARG:HA	2:R:185:TYR:CE1	2.55	0.41
4:H:28:LYS:NZ	4:H:53:ASP:OD1	2.52	0.40
3:a:51:GLN:HG3	3:a:57:THR:HB	2.02	0.40
1:c:1412:LEU:HG	1:c:1430:ASP:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:115:HIS:O	2:F:138:PRO:HD2	2.21	0.40
2:F:140:LEU:N	2:F:140:LEU:HD22	2.36	0.40
1:A:1376:LEU:HD12	1:A:1376:LEU:HA	1.92	0.40
1:M:1456:LEU:C	1:M:1456:LEU:HD23	2.46	0.40
3:O:22:ILE:HA	3:O:27:HIS:O	2.22	0.40
1:Q:1412:LEU:HG	1:Q:1430:ASP:HB3	2.03	0.40
2:R:130:VAL:O	2:R:130:VAL:HG13	2.22	0.40
4:X:4:PHE:CE2	4:X:69:PRO:HG3	2.57	0.40
3:a:42:ILE:HD11	3:a:110:LEU:HD22	2.04	0.40
4:f:10:HIS:CD2	4:f:89:CYS:HB3	2.56	0.40
1:A:1456:LEU:HD23	1:A:1456:LEU:C	2.47	0.40
2:F:130:VAL:HG13	2:F:130:VAL:O	2.22	0.40
1:M:1412:LEU:HG	1:M:1430:ASP:HB3	2.04	0.40
2:d:165:VAL:O	2:d:168:SER:OG	2.33	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:d:177:ARG:NE	4:f:26:GLU:OE2[1_455]	1.97	0.23
1:A:1466:GLU:OE1	1:c:1485:ARG:NH2[2_556]	2.19	0.01
3:C:28:GLU:OE2	1:Y:1426:ARG:NH1[1_554]	2.19	0.01

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	115/122 (94%)	109 (95%)	5 (4%)	1 (1%)	14 43
1	E	114/122 (93%)	105 (92%)	9 (8%)	0	100 100
1	I	114/122 (93%)	111 (97%)	3 (3%)	0	100 100
1	M	114/122 (93%)	110 (96%)	3 (3%)	1 (1%)	14 43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	116/122 (95%)	110 (95%)	6 (5%)	0	100	100
1	U	115/122 (94%)	95 (83%)	14 (12%)	6 (5%)	1	11
1	Y	117/122 (96%)	110 (94%)	6 (5%)	1 (1%)	14	43
1	c	116/122 (95%)	111 (96%)	4 (3%)	1 (1%)	14	43
2	B	149/161 (92%)	138 (93%)	10 (7%)	1 (1%)	18	49
2	F	150/161 (93%)	138 (92%)	11 (7%)	1 (1%)	18	49
2	J	155/161 (96%)	143 (92%)	9 (6%)	3 (2%)	6	28
2	N	155/161 (96%)	142 (92%)	12 (8%)	1 (1%)	21	52
2	R	150/161 (93%)	139 (93%)	11 (7%)	0	100	100
2	V	150/161 (93%)	135 (90%)	13 (9%)	2 (1%)	9	35
2	Z	150/161 (93%)	142 (95%)	7 (5%)	1 (1%)	18	49
2	d	151/161 (94%)	142 (94%)	9 (6%)	0	100	100
3	C	94/96 (98%)	87 (93%)	5 (5%)	2 (2%)	5	26
3	G	94/96 (98%)	84 (89%)	7 (7%)	3 (3%)	3	19
3	K	94/96 (98%)	85 (90%)	6 (6%)	3 (3%)	3	19
3	O	94/96 (98%)	86 (92%)	4 (4%)	4 (4%)	2	14
3	S	94/96 (98%)	81 (86%)	11 (12%)	2 (2%)	5	26
3	W	94/96 (98%)	86 (92%)	6 (6%)	2 (2%)	5	26
3	a	94/96 (98%)	87 (93%)	4 (4%)	3 (3%)	3	19
3	e	94/96 (98%)	84 (89%)	7 (7%)	3 (3%)	3	19
4	D	102/104 (98%)	92 (90%)	8 (8%)	2 (2%)	6	27
4	H	102/104 (98%)	92 (90%)	6 (6%)	4 (4%)	2	16
4	L	102/104 (98%)	94 (92%)	7 (7%)	1 (1%)	12	40
4	P	102/104 (98%)	95 (93%)	6 (6%)	1 (1%)	12	40
4	T	102/104 (98%)	92 (90%)	7 (7%)	3 (3%)	3	21
4	X	102/104 (98%)	95 (93%)	5 (5%)	2 (2%)	6	27
4	b	102/104 (98%)	95 (93%)	5 (5%)	2 (2%)	6	27
4	f	102/104 (98%)	95 (93%)	5 (5%)	2 (2%)	6	27
All	All	3699/3864 (96%)	3410 (92%)	231 (6%)	58 (2%)	7	31

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	51	GLN
2	J	139	SER
1	U	1414	SER
2	Z	139	SER
1	A	1490	LYS
2	F	139	SER
3	K	52	PHE
3	O	52	PHE
4	T	47	ASP
1	U	1381	PRO
1	U	1446	LEU
2	V	60	ARG
2	V	139	SER
4	X	47	ASP
3	a	54	GLU
1	c	1401	SER
3	e	49	PRO
2	B	142	VAL
3	C	52	PHE
4	D	82	ASP
3	G	88	THR
3	G	89	GLU
4	H	47	ASP
4	H	82	ASP
4	H	89	CYS
3	K	88	THR
3	K	89	GLU
4	L	82	ASP
3	O	85	ASN
3	O	88	THR
3	O	89	GLU
4	P	82	ASP
3	S	88	THR
3	S	89	GLU
4	T	82	ASP
1	U	1378	PRO
3	W	52	PHE
4	X	82	ASP
3	a	88	THR
3	a	89	GLU
3	e	88	THR
4	f	82	ASP
4	D	47	ASP

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Mol	Chain	Res	Type
3	G	52	PHE
4	H	36	LYS
4	T	36	LYS
1	U	1426	ARG
1	Y	1465	LEU
4	b	82	ASP
3	e	89	GLU
2	J	56	ALA
2	J	142	VAL
2	N	139	SER
1	U	1465	LEU
4	b	47	ASP
4	f	47	ASP
3	W	85	ASN
1	M	1488	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	110/114 (96%)	99 (90%)	11 (10%)	7 27
1	E	109/114 (96%)	98 (90%)	11 (10%)	7 26
1	I	109/114 (96%)	97 (89%)	12 (11%)	6 23
1	M	109/114 (96%)	96 (88%)	13 (12%)	5 20
1	Q	111/114 (97%)	99 (89%)	12 (11%)	6 23
1	U	110/114 (96%)	91 (83%)	19 (17%)	2 9
1	Y	112/114 (98%)	103 (92%)	9 (8%)	11 36
1	c	111/114 (97%)	90 (81%)	21 (19%)	1 7
2	B	141/147 (96%)	135 (96%)	6 (4%)	26 54
2	F	141/147 (96%)	131 (93%)	10 (7%)	13 40
2	J	143/147 (97%)	135 (94%)	8 (6%)	19 47
2	N	145/147 (99%)	139 (96%)	6 (4%)	27 55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	R	142/147 (97%)	132 (93%)	10 (7%)	14	41
2	V	142/147 (97%)	131 (92%)	11 (8%)	12	37
2	Z	142/147 (97%)	132 (93%)	10 (7%)	14	41
2	d	143/147 (97%)	130 (91%)	13 (9%)	9	31
3	C	85/85 (100%)	79 (93%)	6 (7%)	13	40
3	G	85/85 (100%)	83 (98%)	2 (2%)	43	65
3	K	85/85 (100%)	82 (96%)	3 (4%)	32	58
3	O	85/85 (100%)	82 (96%)	3 (4%)	32	58
3	S	85/85 (100%)	81 (95%)	4 (5%)	23	52
3	W	85/85 (100%)	79 (93%)	6 (7%)	13	40
3	a	85/85 (100%)	81 (95%)	4 (5%)	23	52
3	e	85/85 (100%)	81 (95%)	4 (5%)	23	52
4	D	92/92 (100%)	89 (97%)	3 (3%)	33	59
4	H	92/92 (100%)	84 (91%)	8 (9%)	9	32
4	L	92/92 (100%)	89 (97%)	3 (3%)	33	59
4	P	92/92 (100%)	90 (98%)	2 (2%)	45	66
4	T	92/92 (100%)	88 (96%)	4 (4%)	26	54
4	X	92/92 (100%)	87 (95%)	5 (5%)	20	49
4	b	92/92 (100%)	89 (97%)	3 (3%)	33	59
4	f	92/92 (100%)	89 (97%)	3 (3%)	33	59
All	All	3436/3504 (98%)	3191 (93%)	245 (7%)	13	40

All (245) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1375	LYS
1	A	1377	SER
1	A	1408	VAL
1	A	1414	SER
1	A	1433	LYS
1	A	1436	GLU
1	A	1448	ASP
1	A	1452	ASP
1	A	1465	LEU
1	A	1485	ARG

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Mol	Chain	Res	Type
1	A	1486	GLN
2	B	96	GLN
2	B	105	THR
2	B	118	LEU
2	B	134	GLU
2	B	173	GLU
2	B	194	VAL
3	C	17	MET
3	C	57	THR
3	C	63	ARG
3	C	88	THR
3	C	90	ILE
3	C	98	GLU
4	D	1	MET
4	D	36	LYS
4	D	86	GLU
1	E	1376	LEU
1	E	1408	VAL
1	E	1414	SER
1	E	1432	LYS
1	E	1433	LYS
1	E	1435	LYS
1	E	1448	ASP
1	E	1452	ASP
1	E	1462	THR
1	E	1465	LEU
1	E	1485	ARG
2	F	96	GLN
2	F	105	THR
2	F	108	ARG
2	F	118	LEU
2	F	134	GLU
2	F	140	LEU
2	F	173	GLU
2	F	193	ASN
2	F	194	VAL
2	F	210	ARG
3	G	17	MET
3	G	57	THR
4	H	1	MET
4	H	17	ASP
4	H	36	LYS

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Mol	Chain	Res	Type
4	H	43	ARG
4	H	80	ARG
4	H	84	THR
4	H	85	PHE
4	H	91	GLU
1	I	1376	LEU
1	I	1384	THR
1	I	1385	LYS
1	I	1391	ILE
1	I	1408	VAL
1	I	1414	SER
1	I	1433	LYS
1	I	1452	ASP
1	I	1458	HIS
1	I	1465	LEU
1	I	1485	ARG
1	I	1486	GLN
2	J	55	GLU
2	J	58	ARG
2	J	60	ARG
2	J	96	GLN
2	J	134	GLU
2	J	173	GLU
2	J	193	ASN
2	J	194	VAL
3	K	17	MET
3	K	52	PHE
3	K	98	GLU
4	L	2	ASP
4	L	49	GLN
4	L	86	GLU
1	M	1391	ILE
1	M	1407	GLU
1	M	1408	VAL
1	M	1414	SER
1	M	1427	LYS
1	M	1433	LYS
1	M	1444	ARG
1	M	1451	LYS
1	M	1452	ASP
1	M	1454	MET
1	M	1465	LEU

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Mol	Chain	Res	Type
1	M	1485	ARG
1	M	1488	ILE
2	N	60	ARG
2	N	96	GLN
2	N	108	ARG
2	N	134	GLU
2	N	193	ASN
2	N	194	VAL
3	O	17	MET
3	O	86	SER
3	O	98	GLU
4	P	1	MET
4	P	36	LYS
1	Q	1406	SER
1	Q	1408	VAL
1	Q	1414	SER
1	Q	1426	ARG
1	Q	1433	LYS
1	Q	1452	ASP
1	Q	1465	LEU
1	Q	1469	GLN
1	Q	1470	ILE
1	Q	1482	LYS
1	Q	1485	ARG
1	Q	1486	GLN
2	R	60	ARG
2	R	96	GLN
2	R	105	THR
2	R	113	ARG
2	R	118	LEU
2	R	134	GLU
2	R	140	LEU
2	R	141	ASN
2	R	173	GLU
2	R	194	VAL
3	S	17	MET
3	S	51	GLN
3	S	78	THR
3	S	102	GLU
4	T	1	MET
4	T	36	LYS
4	T	84	THR

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Mol	Chain	Res	Type
4	T	86	GLU
1	U	1383	LEU
1	U	1384	THR
1	U	1391	ILE
1	U	1398	LYS
1	U	1408	VAL
1	U	1414	SER
1	U	1426	ARG
1	U	1427	LYS
1	U	1432	LYS
1	U	1450	GLU
1	U	1452	ASP
1	U	1461	GLN
1	U	1468	SER
1	U	1469	GLN
1	U	1472	GLU
1	U	1479	SER
1	U	1482	LYS
1	U	1490	LYS
1	U	1492	GLU
2	V	64	ARG
2	V	96	GLN
2	V	110	HIS
2	V	118	LEU
2	V	134	GLU
2	V	137	VAL
2	V	140	LEU
2	V	173	GLU
2	V	182	ARG
2	V	194	VAL
2	V	205	ARG
3	W	17	MET
3	W	55	ASN
3	W	57	THR
3	W	59	GLU
3	W	86	SER
3	W	89	GLU
4	X	1	MET
4	X	12	THR
4	X	36	LYS
4	X	49	GLN
4	X	86	GLU

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Mol	Chain	Res	Type
1	Y	1398	LYS
1	Y	1408	VAL
1	Y	1414	SER
1	Y	1416	LYS
1	Y	1442	LYS
1	Y	1452	ASP
1	Y	1465	LEU
1	Y	1472	GLU
1	Y	1485	ARG
2	Z	60	ARG
2	Z	96	GLN
2	Z	108	ARG
2	Z	118	LEU
2	Z	134	GLU
2	Z	140	LEU
2	Z	173	GLU
2	Z	193	ASN
2	Z	194	VAL
2	Z	205	ARG
3	a	17	MET
3	a	42	ILE
3	a	52	PHE
3	a	98	GLU
4	b	36	LYS
4	b	52	ASP
4	b	86	GLU
1	c	1376	LEU
1	c	1377	SER
1	c	1382	LYS
1	c	1383	LEU
1	c	1385	LYS
1	c	1404	GLN
1	c	1405	LEU
1	c	1408	VAL
1	c	1414	SER
1	c	1416	LYS
1	c	1420	GLU
1	c	1433	LYS
1	c	1439	ARG
1	c	1444	ARG
1	c	1451	LYS
1	c	1452	ASP

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Mol	Chain	Res	Type
1	c	1465	LEU
1	c	1468	SER
1	c	1482	LYS
1	c	1485	ARG
1	c	1493	GLU
2	d	60	ARG
2	d	96	GLN
2	d	118	LEU
2	d	134	GLU
2	d	135	LEU
2	d	140	LEU
2	d	173	GLU
2	d	178	LEU
2	d	188	LEU
2	d	191	HIS
2	d	193	ASN
2	d	194	VAL
2	d	199	GLU
3	e	17	MET
3	e	54	GLU
3	e	86	SER
3	e	98	GLU
4	f	36	LYS
4	f	52	ASP
4	f	86	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1461	GLN
2	B	125	HIS
2	B	141	ASN
3	C	61	ASN
4	D	10	HIS
1	E	1404	GLN
2	F	110	HIS
2	F	141	ASN
3	G	51	GLN
3	G	61	ASN
3	G	85	ASN
3	G	108	ASN
1	I	1464	ASN

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Mol	Chain	Res	Type
2	J	141	ASN
2	J	174	ASN
3	K	61	ASN
4	L	10	HIS
1	M	1441	HIS
1	M	1461	GLN
1	M	1464	ASN
1	M	1478	GLN
2	N	132	GLN
2	N	141	ASN
2	N	174	ASN
3	O	55	ASN
3	O	61	ASN
4	P	10	HIS
1	Q	1441	HIS
1	Q	1461	GLN
1	Q	1469	GLN
2	R	110	HIS
2	R	132	GLN
2	R	145	GLN
2	R	174	ASN
3	S	51	GLN
3	S	55	ASN
3	S	61	ASN
4	T	10	HIS
1	U	1386	GLN
1	U	1464	ASN
1	U	1469	GLN
2	V	132	GLN
2	V	141	ASN
2	V	174	ASN
3	W	51	GLN
3	W	55	ASN
3	W	61	ASN
4	X	10	HIS
1	Y	1461	GLN
2	Z	110	HIS
2	Z	132	GLN
2	Z	141	ASN
2	Z	174	ASN
3	a	51	GLN
3	a	61	ASN

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Mol	Chain	Res	Type
3	a	108	ASN
4	b	10	HIS
1	c	1379	ASN
1	c	1404	GLN
1	c	1441	HIS
1	c	1461	GLN
1	c	1464	ASN
2	d	73	GLN
2	d	141	ASN
2	d	174	ASN
3	e	51	GLN
3	e	61	ASN
3	e	108	ASN
4	f	10	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

15 ligands are modelled in this entry.

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	$\#\|Z\|>2$
5	A1BNT	J	301	-	58,59,59	1.06	5 (8%)	82,86,86	1.75	16 (19%)
5	A1BNT	B	301	-	58,59,59	1.13	5 (8%)	82,86,86	1.67	19 (23%)
6	EDO	B	302	-	3,3,3	0.14	0	2,2,2	0.18	0
6	EDO	F	302	-	3,3,3	0.09	0	2,2,2	0.22	0
5	A1BNT	V	301	-	58,59,59	0.98	3 (5%)	82,86,86	1.81	14 (17%)
5	A1BNT	N	301	-	58,59,59	1.15	6 (10%)	82,86,86	1.76	13 (15%)
7	GOL	J	302	-	5,5,5	0.14	0	5,5,5	0.32	0
6	EDO	R	301	-	3,3,3	0.10	0	2,2,2	0.24	0
5	A1BNT	Z	301	-	58,59,59	1.07	5 (8%)	82,86,86	1.70	16 (19%)
5	A1BNT	Q	1501	-	58,59,59	1.11	4 (6%)	82,86,86	1.72	18 (21%)
6	EDO	c	1501	-	3,3,3	0.07	0	2,2,2	0.12	0
6	EDO	J	303	-	3,3,3	0.01	0	2,2,2	0.04	0
5	A1BNT	d	301	-	58,59,59	1.00	4 (6%)	82,86,86	1.93	15 (18%)
6	EDO	F	303	-	3,3,3	0.13	0	2,2,2	0.07	0
5	A1BNT	F	301	-	58,59,59	1.10	4 (6%)	82,86,86	1.81	19 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	A1BNT	J	301	-	-	0/46/68/68	0/6/6/6
5	A1BNT	B	301	-	-	3/46/68/68	0/6/6/6
6	EDO	B	302	-	-	1/1/1/1	-
6	EDO	F	302	-	-	0/1/1/1	-
5	A1BNT	V	301	-	-	9/46/68/68	0/6/6/6
5	A1BNT	N	301	-	-	2/46/68/68	0/6/6/6
7	GOL	J	302	-	-	2/4/4/4	-
6	EDO	R	301	-	-	0/1/1/1	-
5	A1BNT	Z	301	-	-	0/46/68/68	0/6/6/6
5	A1BNT	Q	1501	-	-	6/46/68/68	0/6/6/6
6	EDO	c	1501	-	-	1/1/1/1	-
6	EDO	J	303	-	-	0/1/1/1	-
5	A1BNT	d	301	-	-	11/46/68/68	0/6/6/6
6	EDO	F	303	-	-	1/1/1/1	-
5	A1BNT	F	301	-	-	3/46/68/68	0/6/6/6

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Q	1501	A1BNT	C38-N9	-5.39	1.30	1.38
5	F	301	A1BNT	C38-N9	-4.80	1.31	1.38
5	B	301	A1BNT	C38-N9	-4.75	1.31	1.38
5	Z	301	A1BNT	C38-N9	-4.62	1.31	1.38
5	N	301	A1BNT	C38-N9	-4.37	1.32	1.38
5	V	301	A1BNT	C38-N9	-4.27	1.32	1.38
5	d	301	A1BNT	C38-N9	-4.07	1.32	1.38
5	N	301	A1BNT	C26-C9	-3.66	1.50	1.55
5	J	301	A1BNT	C38-N9	-3.47	1.33	1.38
5	J	301	A1BNT	C19-N7	-2.82	1.29	1.34
5	J	301	A1BNT	N7-N6	-2.80	1.27	1.34
5	Z	301	A1BNT	C7-C6	2.78	1.56	1.52
5	F	301	A1BNT	N7-N6	-2.63	1.27	1.34
5	B	301	A1BNT	C7-C6	2.49	1.55	1.52
5	N	301	A1BNT	C9-C8	-2.47	1.50	1.53
5	B	301	A1BNT	C9-C8	-2.45	1.50	1.53
5	Z	301	A1BNT	C9-C8	-2.44	1.50	1.53
5	F	301	A1BNT	C19-N7	-2.39	1.30	1.34
5	d	301	A1BNT	C7-C6	2.39	1.55	1.52
5	Z	301	A1BNT	N7-N6	-2.30	1.28	1.34
5	B	301	A1BNT	C26-C9	-2.27	1.52	1.55
5	F	301	A1BNT	C4-C3	-2.23	1.47	1.52
5	Q	1501	A1BNT	N7-N6	-2.23	1.28	1.34
5	J	301	A1BNT	C26-C9	-2.19	1.52	1.55
5	V	301	A1BNT	C19-N8	2.17	1.39	1.34
5	d	301	A1BNT	C19-N8	2.17	1.39	1.34
5	d	301	A1BNT	N7-N6	-2.14	1.28	1.34
5	Z	301	A1BNT	C26-C9	-2.14	1.52	1.55
5	B	301	A1BNT	N7-N6	-2.11	1.28	1.34
5	N	301	A1BNT	N7-N6	-2.10	1.29	1.34
5	Q	1501	A1BNT	C19-N8	2.05	1.39	1.34
5	J	301	A1BNT	C16-C19	-2.04	1.39	1.41
5	N	301	A1BNT	C19-N8	2.03	1.39	1.34
5	N	301	A1BNT	C5-C6	2.03	1.56	1.52
5	Q	1501	A1BNT	C7-C6	2.02	1.55	1.52
5	V	301	A1BNT	C5-C6	2.02	1.56	1.52

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	N	301	A1BNT	S-C37-N9	-7.07	110.00	116.08
5	F	301	A1BNT	S-C37-N9	-6.67	110.35	116.08
5	d	301	A1BNT	C6-C7-N2	6.48	109.25	103.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	d	301	A1BNT	S-C37-N9	-6.47	110.52	116.08
5	d	301	A1BNT	C37-N9-C38	6.31	117.81	110.71
5	V	301	A1BNT	S-C37-N9	-6.31	110.66	116.08
5	J	301	A1BNT	S-C37-N9	-6.23	110.72	116.08
5	Q	1501	A1BNT	S-C37-N9	-5.98	110.94	116.08
5	V	301	A1BNT	C37-N9-C38	5.78	117.21	110.71
5	Q	1501	A1BNT	C37-N9-C38	5.70	117.12	110.71
5	Z	301	A1BNT	S-C37-N9	-5.66	111.21	116.08
5	N	301	A1BNT	C37-N9-C38	5.65	117.06	110.71
5	N	301	A1BNT	C8-C9-N3	-5.60	100.60	107.40
5	B	301	A1BNT	S-C37-N9	-5.51	111.34	116.08
5	Z	301	A1BNT	C37-N9-C38	5.13	116.47	110.71
5	d	301	A1BNT	C17-C18-N6	-5.09	117.80	121.61
5	F	301	A1BNT	C37-N9-C38	5.06	116.39	110.71
5	J	301	A1BNT	C37-N9-C38	4.97	116.30	110.71
5	d	301	A1BNT	C5-C4-N2	4.77	108.85	103.17
5	B	301	A1BNT	C37-N9-C38	4.68	115.97	110.71
5	V	301	A1BNT	C17-C18-N6	-4.66	118.12	121.61
5	Q	1501	A1BNT	C11-N4-C12	4.64	118.37	111.14
5	F	301	A1BNT	C32-C33-C36	-4.48	113.72	120.84
5	V	301	A1BNT	C14-N5-C13	4.48	121.64	111.57
5	B	301	A1BNT	C5-C4-N2	4.42	108.43	103.17
5	Z	301	A1BNT	C5-C4-N2	4.40	108.41	103.17
5	J	301	A1BNT	C5-C4-N2	4.31	108.30	103.17
5	Z	301	A1BNT	C9-C8-N2	4.23	123.51	118.46
5	V	301	A1BNT	C11-N4-C15	4.07	117.47	111.14
5	F	301	A1BNT	C5-C4-N2	3.94	107.86	103.17
5	B	301	A1BNT	C17-C18-N6	-3.92	118.68	121.61
5	Z	301	A1BNT	C6-C7-N2	3.84	106.70	103.00
5	B	301	A1BNT	C6-C7-N2	3.80	106.66	103.00
5	J	301	A1BNT	C7-N2-C4	-3.75	106.86	111.83
5	V	301	A1BNT	C38-C36-S	-3.75	107.34	109.64
5	F	301	A1BNT	C34-C33-C36	3.71	126.74	120.84
5	Q	1501	A1BNT	C5-C4-N2	3.53	107.38	103.17
5	F	301	A1BNT	C17-C18-N6	-3.46	119.02	121.61
5	d	301	A1BNT	C8-C9-N3	3.42	111.55	107.40
5	J	301	A1BNT	C17-C18-N6	-3.39	119.07	121.61
5	N	301	A1BNT	C37-S-C36	3.33	90.71	88.96
5	J	301	A1BNT	C38-C36-S	-3.30	107.62	109.64
5	Z	301	A1BNT	C1-C2-C30	-3.28	104.51	112.22
5	N	301	A1BNT	C5-C4-N2	3.27	107.07	103.17
5	Q	1501	A1BNT	C32-C33-C36	-3.24	115.69	120.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	d	301	A1BNT	C14-N5-C16	-3.20	108.59	116.19
5	N	301	A1BNT	C17-C18-N6	-3.16	119.25	121.61
5	F	301	A1BNT	C1-C2-N1	-3.14	103.26	109.00
5	B	301	A1BNT	C32-C33-C36	-3.04	116.00	120.84
5	F	301	A1BNT	C7-N2-C4	-3.00	107.86	111.83
5	d	301	A1BNT	C33-C36-S	2.97	124.30	118.77
5	d	301	A1BNT	C33-C36-C38	-2.95	126.81	130.81
5	J	301	A1BNT	C33-C36-S	2.90	124.17	118.77
5	J	301	A1BNT	C37-S-C36	2.89	90.48	88.96
5	d	301	A1BNT	C6-C5-C4	2.88	107.12	103.75
5	Z	301	A1BNT	C32-C33-C36	-2.86	116.30	120.84
5	V	301	A1BNT	C37-S-C36	2.84	90.45	88.96
5	N	301	A1BNT	C38-C36-S	-2.82	107.91	109.64
5	N	301	A1BNT	C28-C26-C9	-2.81	103.97	109.71
5	Q	1501	A1BNT	C17-C18-N6	-2.80	119.51	121.61
5	J	301	A1BNT	C32-C33-C36	-2.79	116.41	120.84
5	Q	1501	A1BNT	C11-N4-C15	-2.75	106.88	111.14
5	B	301	A1BNT	C8-C9-N3	-2.74	104.07	107.40
5	N	301	A1BNT	C32-C33-C36	-2.72	116.52	120.84
5	F	301	A1BNT	C18-N6-N7	2.70	123.99	119.93
5	J	301	A1BNT	C5-C6-C7	-2.65	100.22	103.18
5	J	301	A1BNT	O4-C10-C11	-2.65	116.38	121.02
5	Q	1501	A1BNT	C1-C2-C30	-2.65	106.00	112.22
5	Z	301	A1BNT	C26-C9-C8	-2.65	109.70	113.23
5	V	301	A1BNT	C5-C4-N2	2.63	106.30	103.17
5	B	301	A1BNT	C20-C18-N6	2.61	119.65	115.90
5	F	301	A1BNT	C5-C6-C7	-2.58	100.30	103.18
5	J	301	A1BNT	C12-C13-N5	-2.56	105.39	110.78
5	Q	1501	A1BNT	C17-C16-N5	-2.56	118.86	122.59
5	F	301	A1BNT	C38-C36-S	-2.55	108.07	109.64
5	B	301	A1BNT	C12-C13-N5	-2.55	105.42	110.78
5	V	301	A1BNT	C27-C26-C9	2.54	114.92	109.71
5	B	301	A1BNT	C35-C34-C33	-2.52	118.11	120.80
5	F	301	A1BNT	C26-C9-C8	-2.52	109.87	113.23
5	Z	301	A1BNT	C17-C18-N6	-2.51	119.73	121.61
5	N	301	A1BNT	C13-C12-N4	-2.51	105.59	110.65
5	B	301	A1BNT	C26-C9-N3	-2.48	108.07	111.94
5	d	301	A1BNT	C26-C9-C8	-2.48	109.93	113.23
5	B	301	A1BNT	C9-C8-N2	2.47	121.41	118.46
5	F	301	A1BNT	C12-C13-N5	-2.47	105.59	110.78
5	d	301	A1BNT	C27-C26-C9	2.47	114.76	109.71
5	Q	1501	A1BNT	C8-C9-N3	-2.46	104.41	107.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	V	301	A1BNT	C18-N6-N7	2.46	123.63	119.93
5	J	301	A1BNT	C34-C33-C36	2.45	124.74	120.84
5	Z	301	A1BNT	C33-C36-S	2.45	123.32	118.77
5	V	301	A1BNT	C7-N2-C4	-2.44	108.60	111.83
5	Q	1501	A1BNT	C9-C8-N2	2.44	121.37	118.46
5	F	301	A1BNT	C11-C10-N3	2.42	121.66	115.70
5	F	301	A1BNT	O4-C10-C11	-2.41	116.80	121.02
5	Z	301	A1BNT	C8-C9-N3	-2.38	104.52	107.40
5	J	301	A1BNT	C18-N6-N7	2.35	123.47	119.93
5	Q	1501	A1BNT	C2-N1-C3	2.33	126.14	122.91
5	J	301	A1BNT	C6-C7-N2	2.33	105.25	103.00
5	B	301	A1BNT	C18-N6-N7	2.33	123.43	119.93
5	Z	301	A1BNT	C12-C13-N5	-2.29	105.97	110.78
5	d	301	A1BNT	O4-C10-C11	-2.28	117.02	121.02
5	N	301	A1BNT	C15-C14-N5	-2.26	106.03	110.78
5	V	301	A1BNT	C33-C36-S	2.24	122.94	118.77
5	Q	1501	A1BNT	O3-C8-N2	-2.23	117.37	121.38
5	B	301	A1BNT	O3-C8-N2	-2.21	117.41	121.38
5	J	301	A1BNT	C28-C26-C9	-2.18	105.25	109.71
5	N	301	A1BNT	C12-C13-N5	-2.18	106.20	110.78
5	V	301	A1BNT	C10-C11-N4	-2.17	108.36	113.41
5	d	301	A1BNT	C13-C12-N4	2.17	115.02	110.65
5	F	301	A1BNT	C6-C7-N2	2.15	105.07	103.00
5	Z	301	A1BNT	C29-C26-C9	2.14	114.10	109.71
5	B	301	A1BNT	C15-C14-N5	-2.14	106.28	110.78
5	B	301	A1BNT	C5-C4-C3	-2.14	107.27	111.36
5	Q	1501	A1BNT	C17-C16-C19	-2.13	115.54	119.06
5	F	301	A1BNT	C14-C15-N4	-2.13	106.36	110.65
5	B	301	A1BNT	C34-C33-C36	2.12	124.22	120.84
5	d	301	A1BNT	C36-C38-N9	-2.10	112.97	114.99
5	Q	1501	A1BNT	O4-C10-C11	-2.09	117.35	121.02
5	B	301	A1BNT	C33-C36-S	2.08	122.64	118.77
5	Z	301	A1BNT	C38-C36-S	-2.08	108.37	109.64
5	F	301	A1BNT	C35-C34-C33	-2.08	118.58	120.80
5	B	301	A1BNT	C1-C2-C30	-2.07	107.35	112.22
5	Q	1501	A1BNT	C29-C26-C9	2.06	113.93	109.71
5	Q	1501	A1BNT	C20-C18-N6	2.06	118.86	115.90
5	Z	301	A1BNT	C34-C33-C36	2.05	124.10	120.84
5	Z	301	A1BNT	O4-C10-C11	-2.05	117.43	121.02
5	F	301	A1BNT	C6-C5-C4	-2.02	101.39	103.75
5	V	301	A1BNT	C1-C2-C30	-2.02	107.48	112.22
5	N	301	A1BNT	O4-C10-N3	-2.01	119.56	122.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	Q	1501	A1BNT	C10-C11-N4	2.00	118.07	113.41

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	Q	1501	A1BNT	C10-C11-N4-C12
5	V	301	A1BNT	C28-C26-C9-N3
5	V	301	A1BNT	C28-C26-C9-C8
5	V	301	A1BNT	C27-C26-C9-N3
5	V	301	A1BNT	C27-C26-C9-C8
5	V	301	A1BNT	C29-C26-C9-N3
5	V	301	A1BNT	C29-C26-C9-C8
5	d	301	A1BNT	C28-C26-C9-N3
5	d	301	A1BNT	C28-C26-C9-C8
5	d	301	A1BNT	C27-C26-C9-N3
5	d	301	A1BNT	C27-C26-C9-C8
5	d	301	A1BNT	C29-C26-C9-N3
5	d	301	A1BNT	C29-C26-C9-C8
7	J	302	GOL	O1-C1-C2-O2
7	J	302	GOL	O1-C1-C2-C3
5	Q	1501	A1BNT	C17-C16-N5-C14
5	Q	1501	A1BNT	C19-C16-N5-C14
5	B	301	A1BNT	C29-C26-C9-N3
5	N	301	A1BNT	C29-C26-C9-N3
5	d	301	A1BNT	C17-C16-N5-C14
5	d	301	A1BNT	C17-C16-N5-C13
5	Q	1501	A1BNT	N3-C10-C11-N4
5	Q	1501	A1BNT	O4-C10-C11-N4
5	V	301	A1BNT	C17-C16-N5-C13
5	B	301	A1BNT	C27-C26-C9-N3
6	F	303	EDO	O1-C1-C2-O2
5	Q	1501	A1BNT	C17-C16-N5-C13
5	B	301	A1BNT	C28-C26-C9-N3
5	N	301	A1BNT	C28-C26-C9-N3
5	F	301	A1BNT	N1-C2-C30-C35
5	V	301	A1BNT	N1-C2-C30-C31
5	d	301	A1BNT	C19-C16-N5-C14
5	V	301	A1BNT	N1-C2-C30-C35
5	F	301	A1BNT	N1-C2-C30-C31
5	F	301	A1BNT	C17-C16-N5-C13
6	B	302	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
6	c	1501	EDO	O1-C1-C2-O2
5	d	301	A1BNT	C19-C16-N5-C13
5	d	301	A1BNT	C10-C11-N4-C12

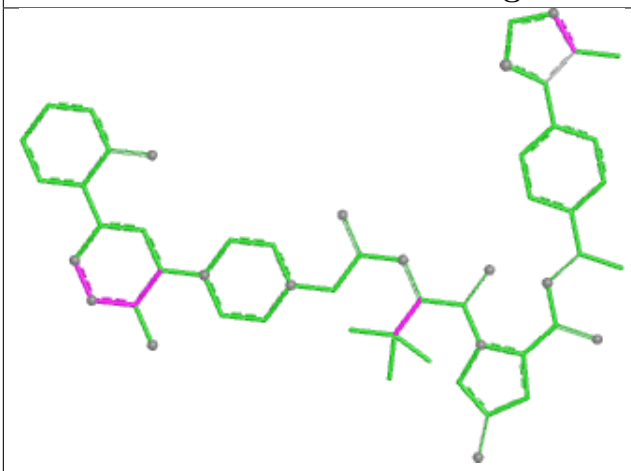
There are no ring outliers.

8 monomers are involved in 18 short contacts:

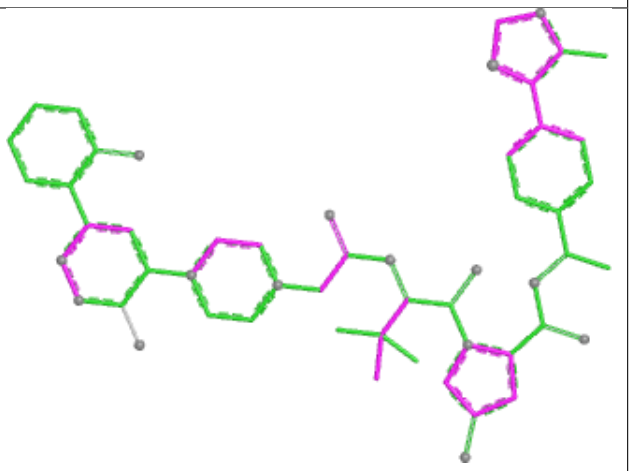
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	301	A1BNT	4	0
5	V	301	A1BNT	2	0
5	N	301	A1BNT	3	0
6	R	301	EDO	1	0
5	Z	301	A1BNT	2	0
5	Q	1501	A1BNT	3	0
5	d	301	A1BNT	1	0
5	F	301	A1BNT	2	0

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

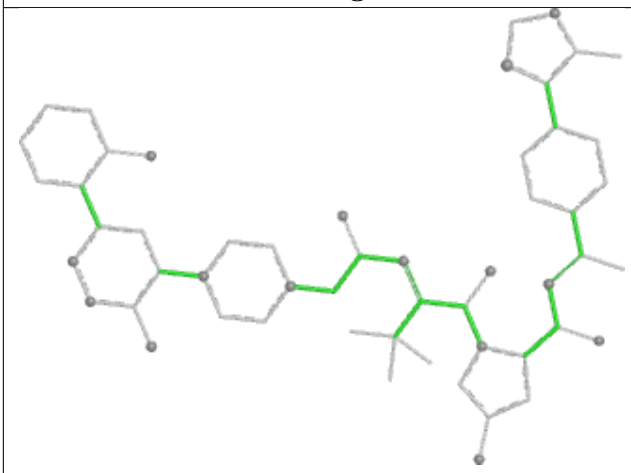
Ligand A1BNT J 301



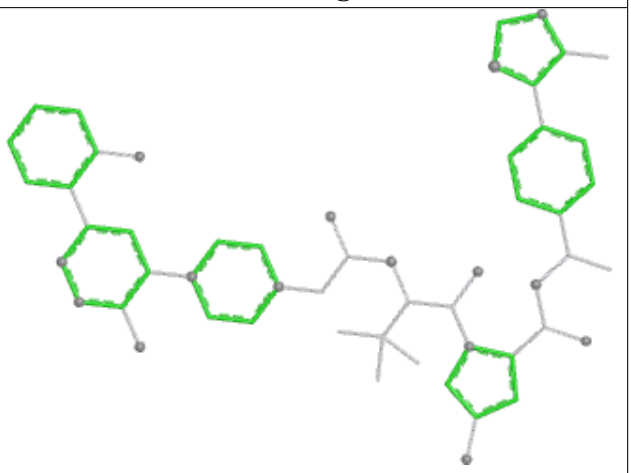
Bond lengths



Bond angles

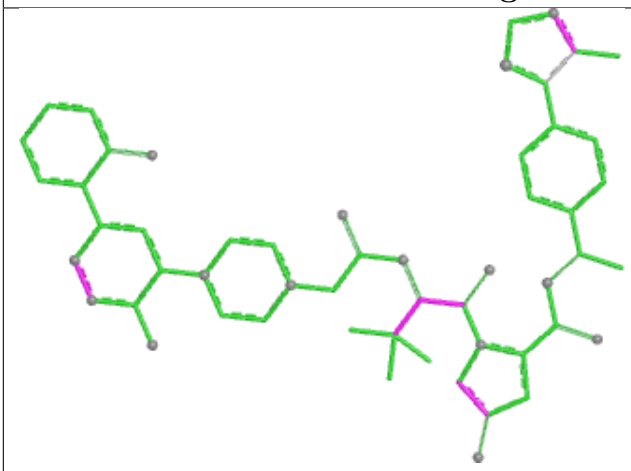


Torsions

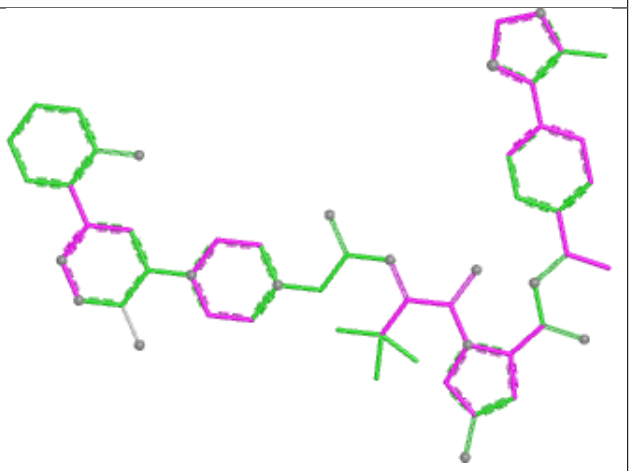


Rings

Ligand A1BNT B 301



Bond lengths



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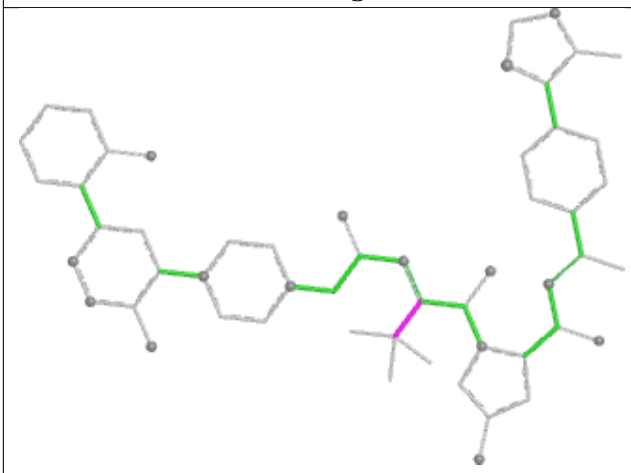
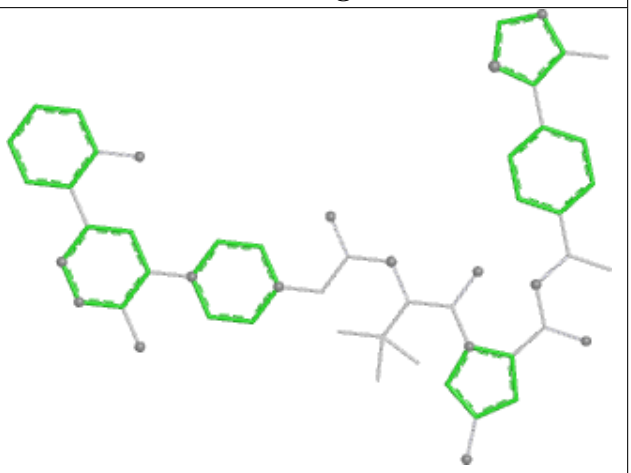
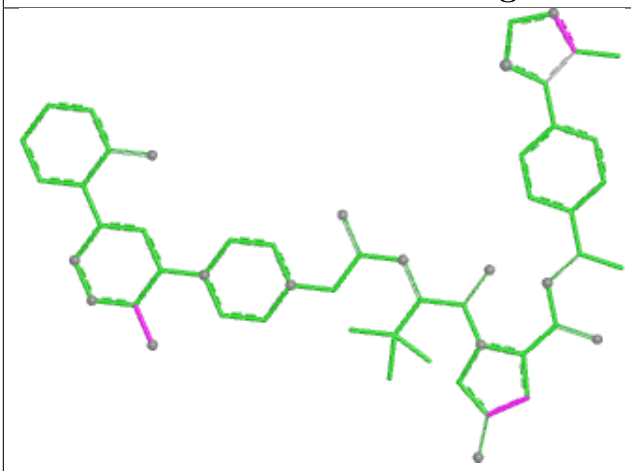


Torsions

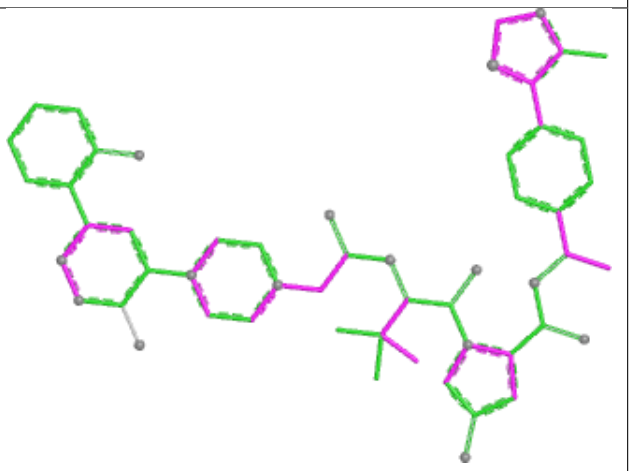


Rings

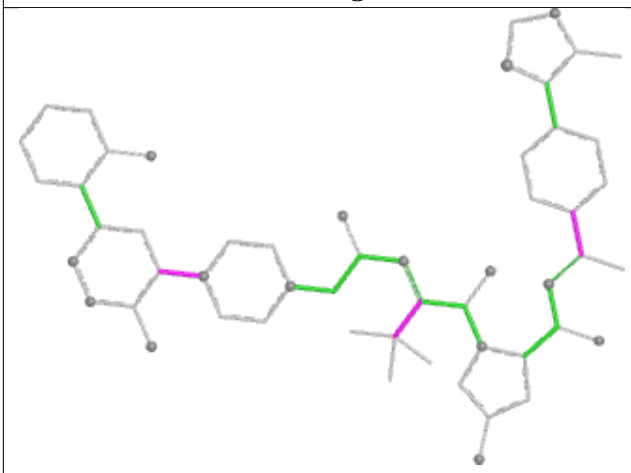
Ligand A1BNT V 301



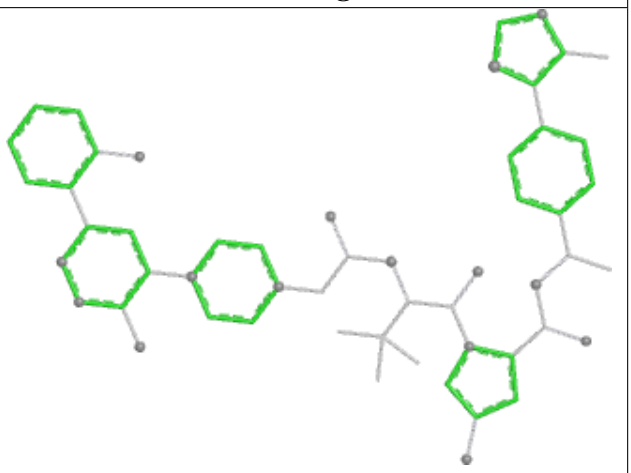
Bond lengths



Bond angles

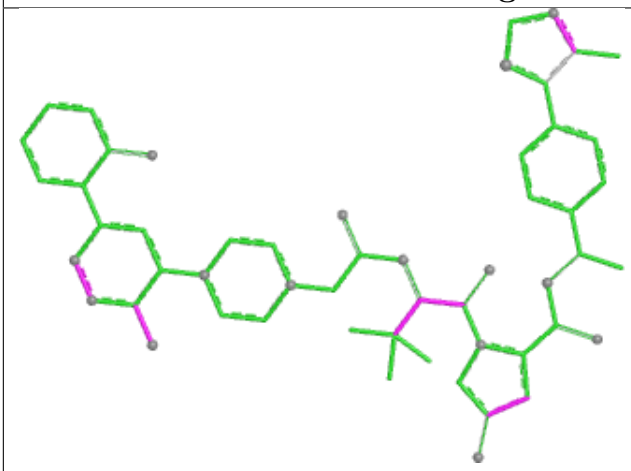


Torsions



Rings

Ligand A1BNT N 301



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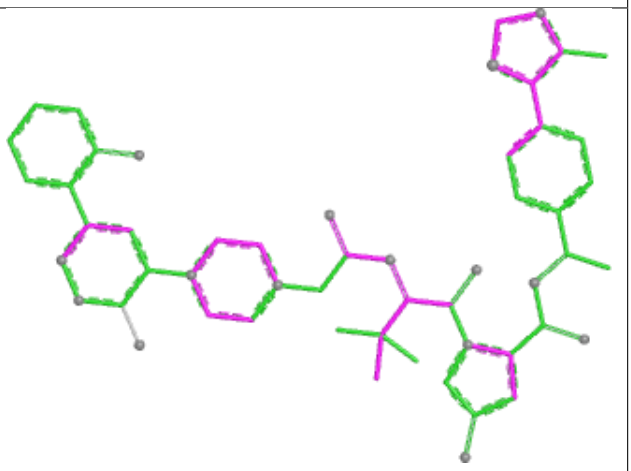
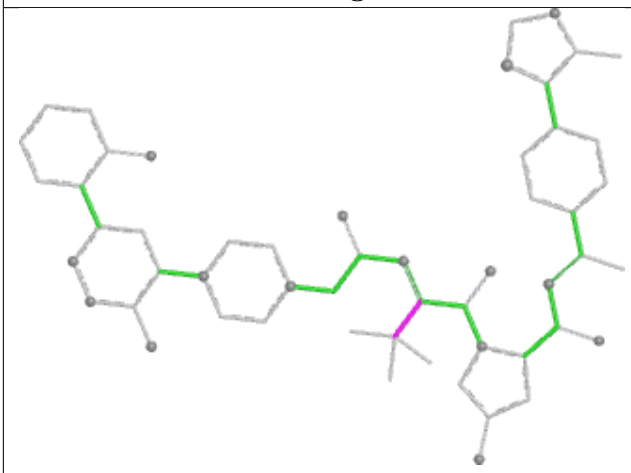
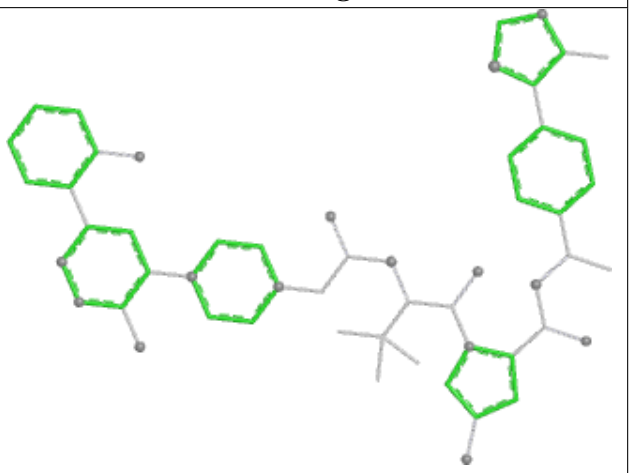


Bond angles

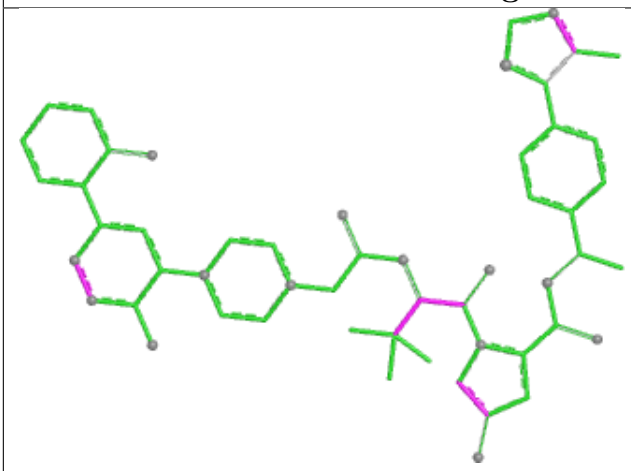


Torsions



Rings

Ligand A1BNT Z 301



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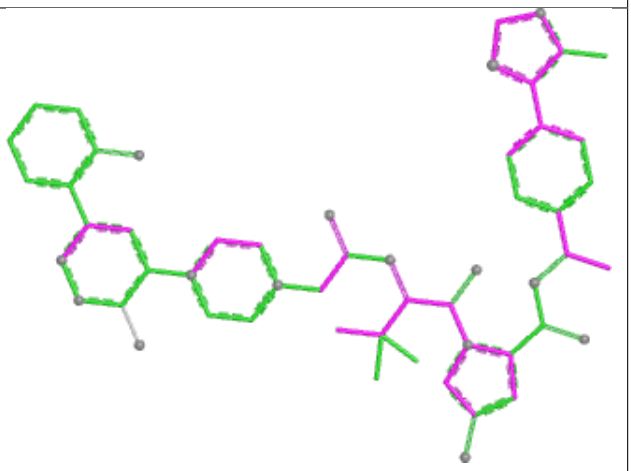
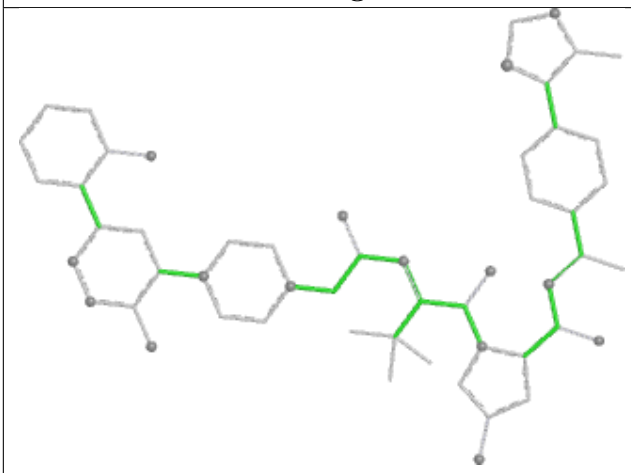
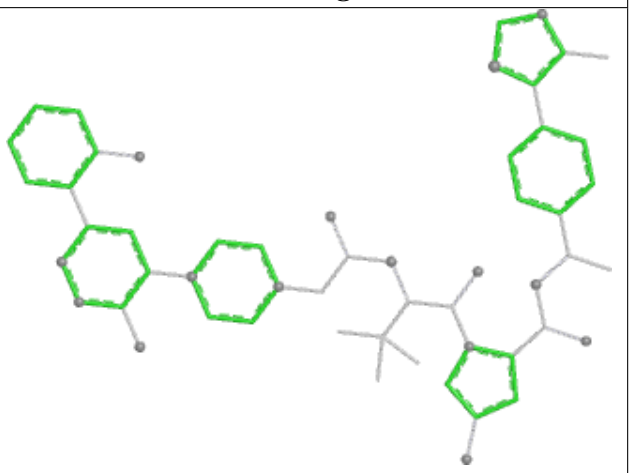


Bond angles

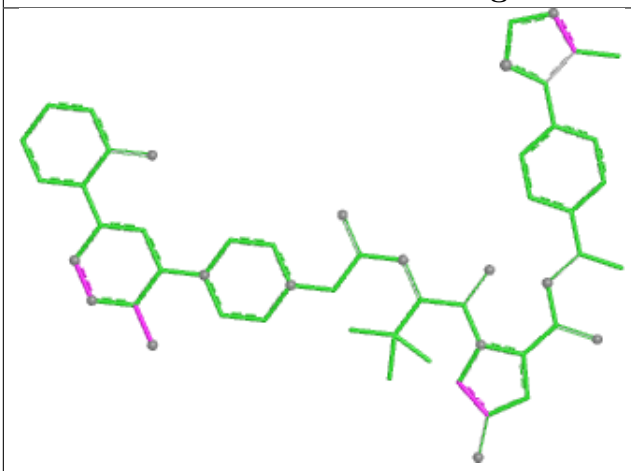


Torsions



Rings

Ligand A1BNT Q 1501



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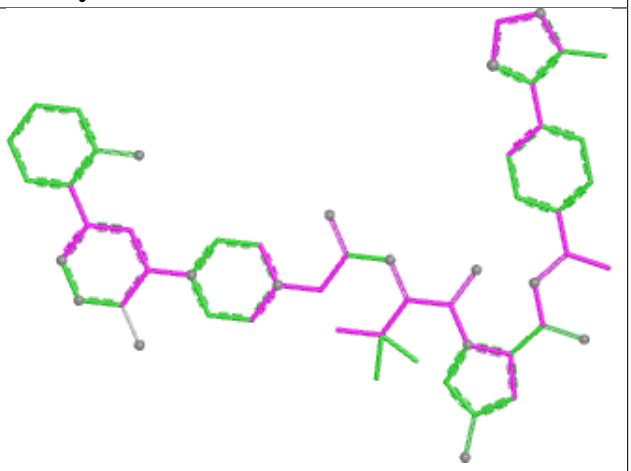
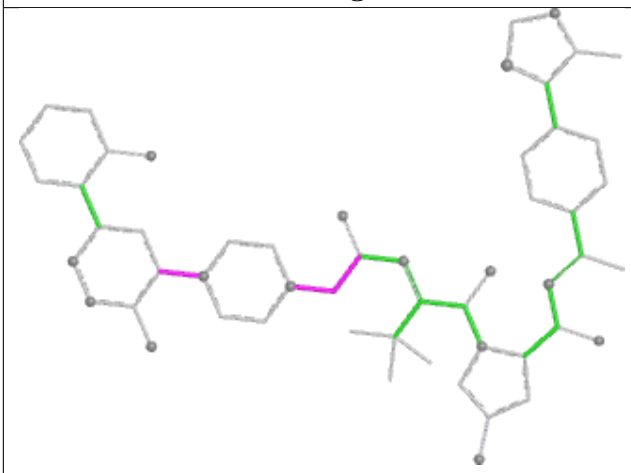


Bond angles



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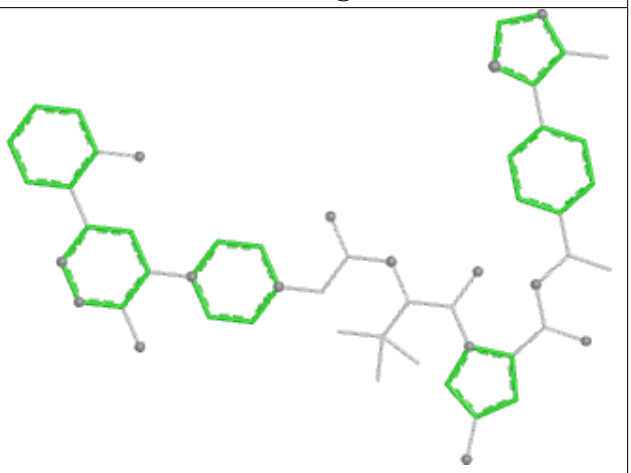
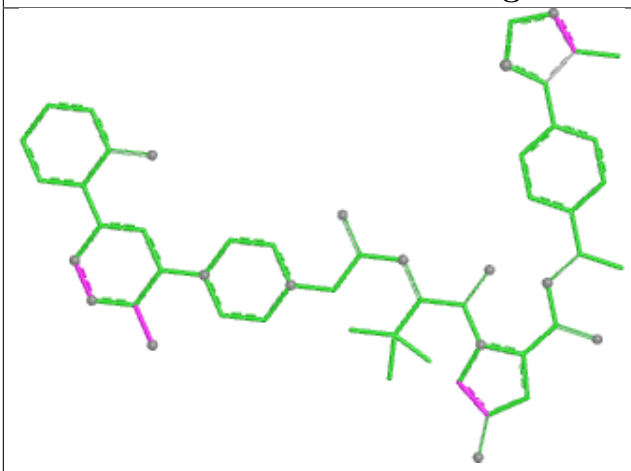


Rings

Ligand A1BNT d 301



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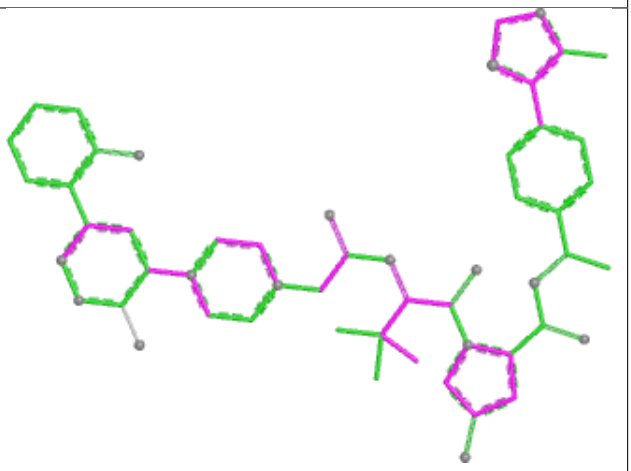
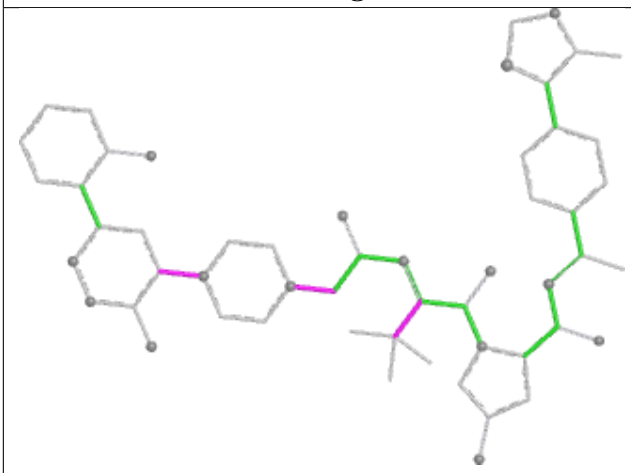
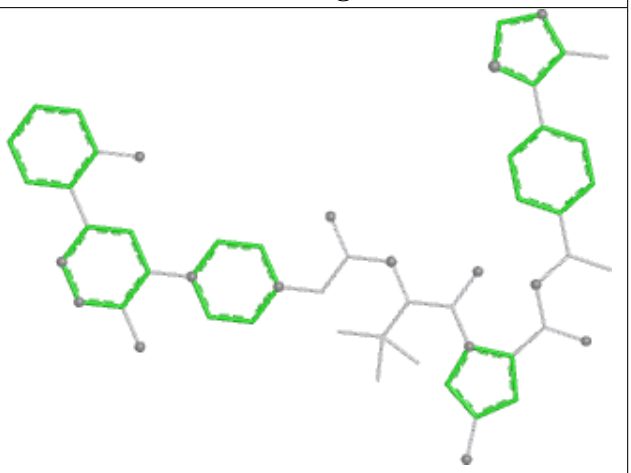


Bond angles

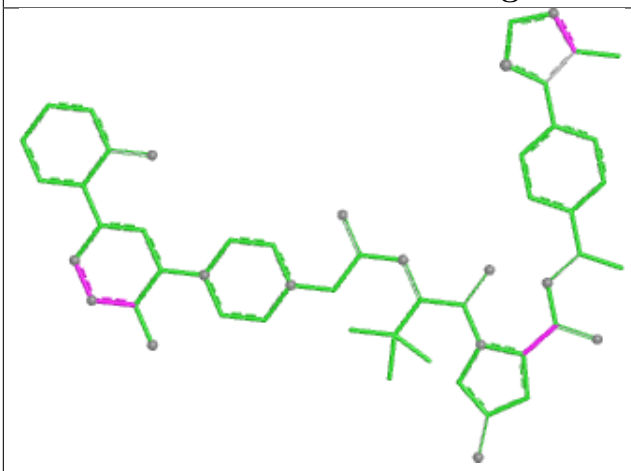


Torsions

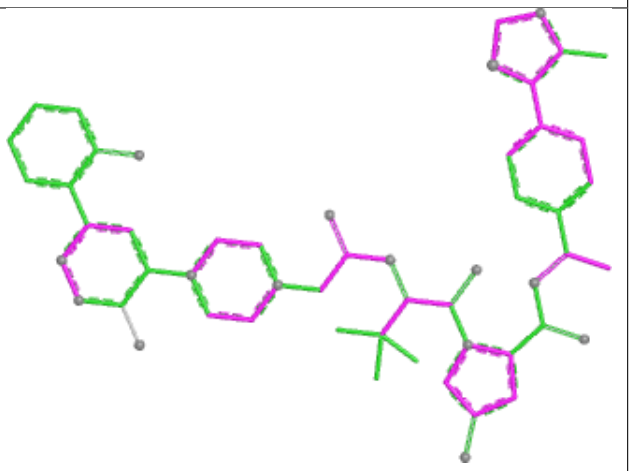


Rings

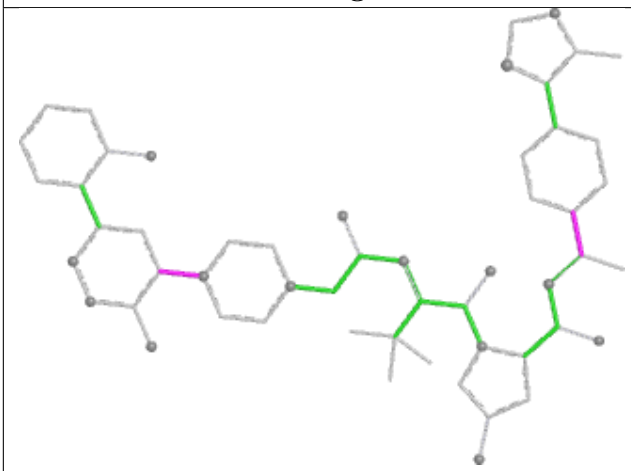
Ligand A1BNT F 301



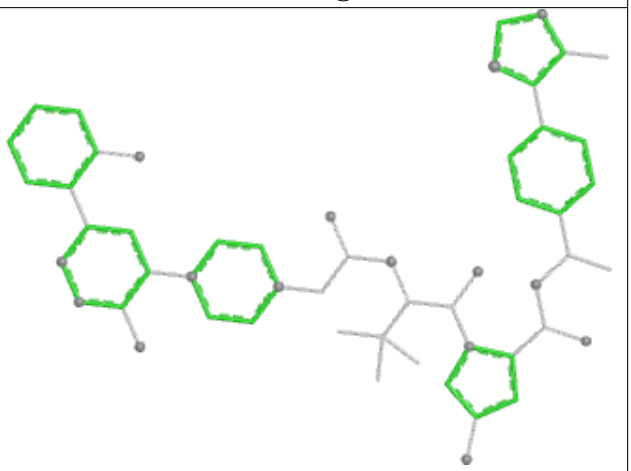
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

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, 95^{th} 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	117/122 (95%)	-0.49	0 100 100	38, 62, 93, 121	0
1	E	116/122 (95%)	-0.54	0 100 100	48, 65, 94, 120	0
1	I	116/122 (95%)	-0.46	0 100 100	48, 67, 103, 133	0
1	M	116/122 (95%)	-0.56	0 100 100	47, 69, 102, 128	0
1	Q	118/122 (96%)	-0.18	0 100 100	64, 99, 138, 159	0
1	U	117/122 (95%)	0.19	2 (1%) 69 50	94, 137, 168, 199	0
1	Y	118/122 (96%)	-0.53	0 100 100	29, 72, 97, 111	1 (0%)
1	c	118/122 (96%)	-0.18	1 (0%) 82 68	61, 89, 117, 127	0
2	B	151/161 (93%)	-0.53	0 100 100	31, 54, 121, 179	0
2	F	152/161 (94%)	-0.51	0 100 100	35, 56, 129, 200	0
2	J	156/161 (96%)	-0.57	0 100 100	22, 54, 111, 158	1 (0%)
2	N	156/161 (96%)	-0.55	0 100 100	23, 57, 118, 165	1 (0%)
2	R	152/161 (94%)	-0.50	0 100 100	50, 76, 130, 172	0
2	V	152/161 (94%)	-0.31	1 (0%) 84 70	64, 94, 136, 178	0
2	Z	152/161 (94%)	-0.36	0 100 100	46, 87, 153, 193	0
2	d	152/161 (94%)	-0.08	0 100 100	45, 105, 168, 188	1 (0%)
3	C	96/96 (100%)	-0.37	0 100 100	42, 61, 179, 214	0
3	G	96/96 (100%)	-0.36	0 100 100	44, 79, 170, 194	0
3	K	96/96 (100%)	-0.31	0 100 100	48, 83, 179, 218	0
3	O	96/96 (100%)	-0.24	0 100 100	52, 88, 191, 225	0
3	S	96/96 (100%)	-0.30	0 100 100	63, 96, 151, 190	0
3	W	96/96 (100%)	-0.18	1 (1%) 79 63	72, 100, 188, 234	0
3	a	96/96 (100%)	0.16	1 (1%) 79 63	87, 146, 189, 224	0
3	e	96/96 (100%)	0.29	0 100 100	124, 186, 238, 250	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
4	D	104/104 (100%)	-0.42	0	100	100	50, 76, 113, 163	0
4	H	104/104 (100%)	-0.25	0	100	100	57, 91, 129, 146	0
4	L	104/104 (100%)	-0.23	0	100	100	61, 95, 134, 226	0
4	P	104/104 (100%)	-0.28	0	100	100	64, 95, 139, 201	0
4	T	104/104 (100%)	-0.04	0	100	100	77, 122, 160, 180	0
4	X	104/104 (100%)	-0.09	0	100	100	73, 124, 166, 184	0
4	b	104/104 (100%)	0.14	2 (1%)	66	48	102, 167, 203, 218	0
4	f	104/104 (100%)	0.26	2 (1%)	66	48	136, 195, 256, 289	0
All	All	3759/3864 (97%)	-0.28	10 (0%)	90	82	22, 87, 184, 289	4 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	b	27	LEU	3.3
4	b	15	PHE	3.1
1	c	1457	CYS	2.8
4	f	5	LEU	2.6
4	f	27	LEU	2.5
1	U	1438	ILE	2.3
1	U	1421	TYR	2.3
2	V	149	ALA	2.1
3	W	49	PRO	2.1
3	a	30	ILE	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,

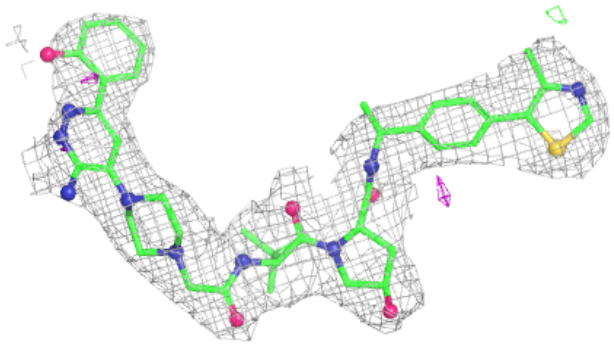
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

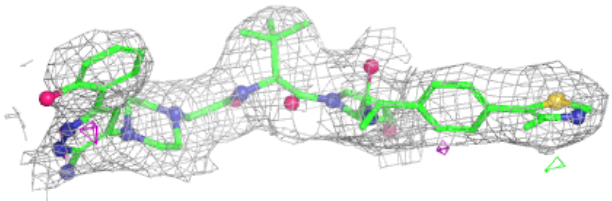
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	EDO	c	1501	4/4	0.78	0.10	79,86,90,92	0
6	EDO	R	301	4/4	0.81	0.13	64,69,72,72	0
6	EDO	F	303	4/4	0.85	0.12	62,64,64,65	0
6	EDO	B	302	4/4	0.89	0.12	68,74,76,76	0
6	EDO	F	302	4/4	0.90	0.17	62,66,68,69	0
6	EDO	J	303	4/4	0.91	0.07	69,71,73,79	0
5	A1BNT	d	301	54/54	0.91	0.10	65,74,91,95	0
5	A1BNT	V	301	54/54	0.91	0.10	66,84,109,113	0
7	GOL	J	302	6/6	0.92	0.10	73,79,82,82	0
5	A1BNT	Z	301	54/54	0.95	0.08	56,63,69,73	0
5	A1BNT	F	301	54/54	0.96	0.07	36,47,57,60	0
5	A1BNT	J	301	54/54	0.96	0.07	34,42,47,48	0
5	A1BNT	B	301	54/54	0.96	0.08	37,47,51,60	0
5	A1BNT	N	301	54/54	0.97	0.07	39,45,52,54	0
5	A1BNT	Q	1501	54/54	0.97	0.06	45,60,72,74	0

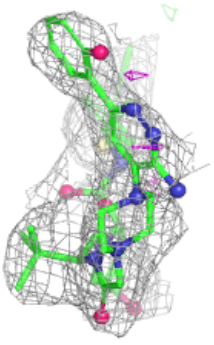
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1BNT d 301:

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

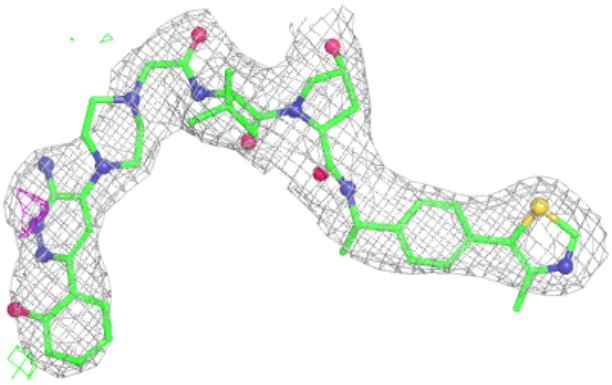


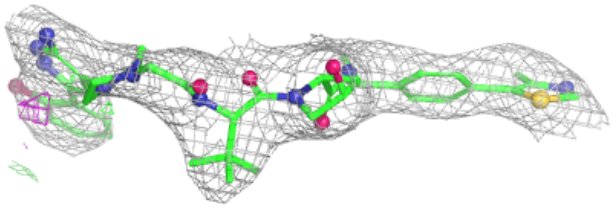


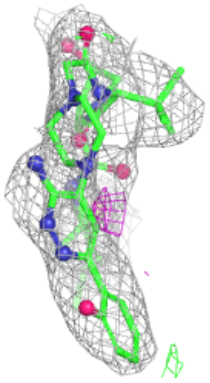


Electron density around A1BNT V 301:

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

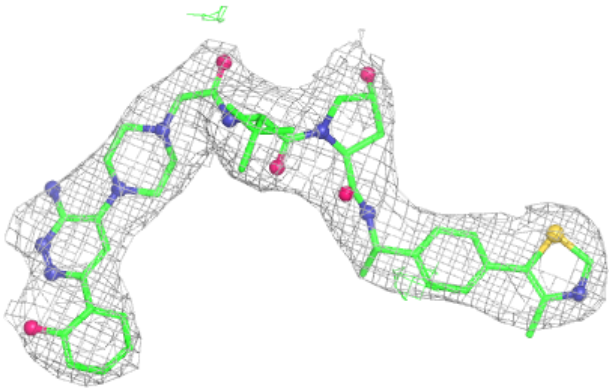


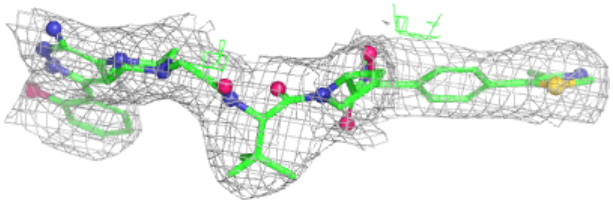


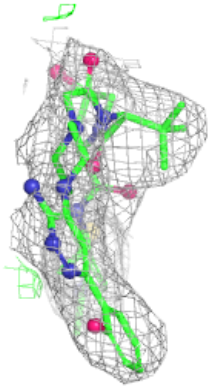


Electron density around A1BNT Z 301:

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

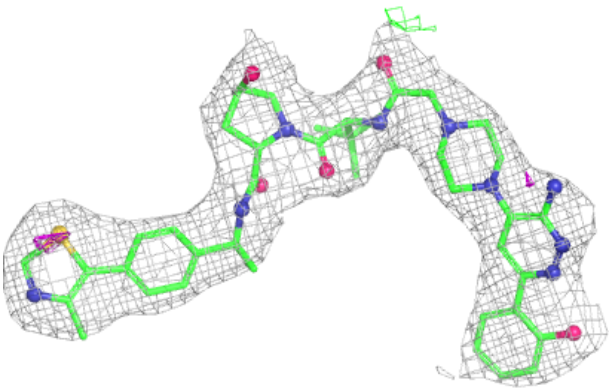


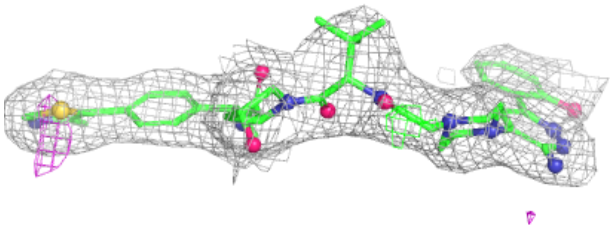


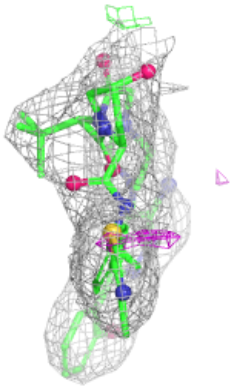


Electron density around A1BNT F 301:

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







Electron density around A1BNT J 301:

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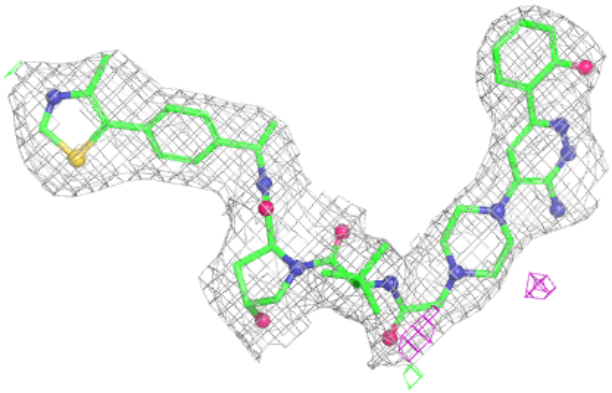
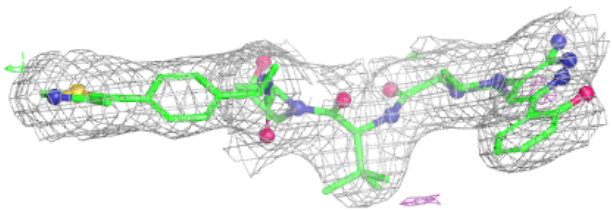
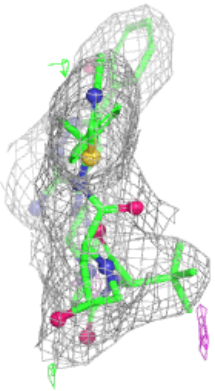
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

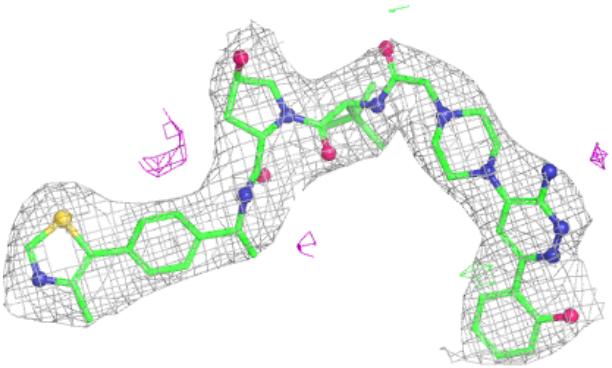


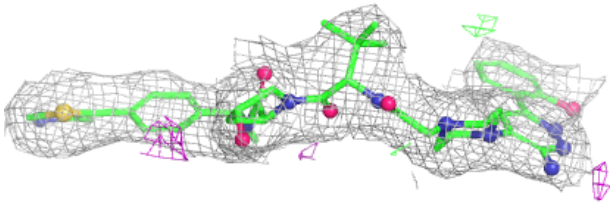


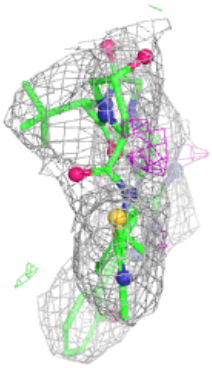


Electron density around A1BNT B 301:

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

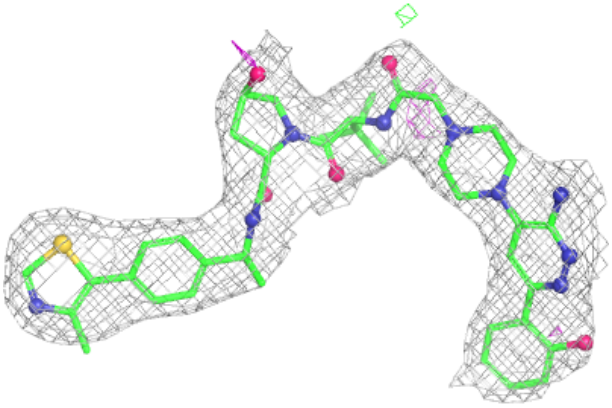


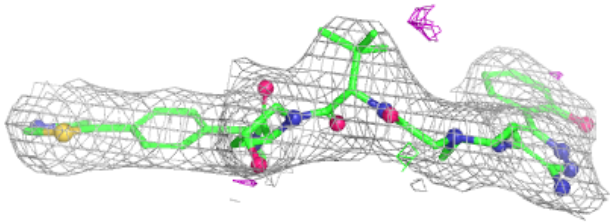


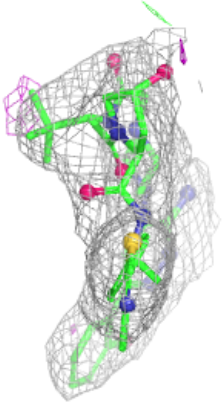


Electron density around A1BNT N 301:

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

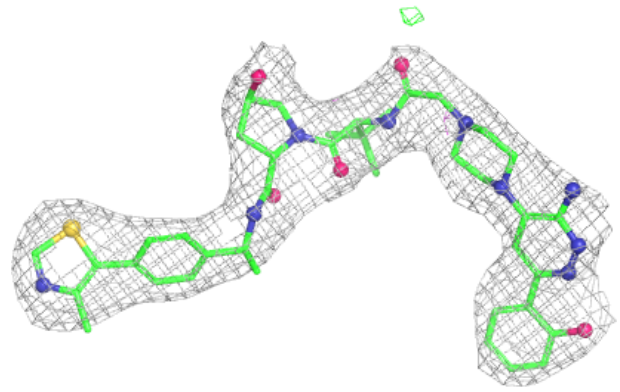


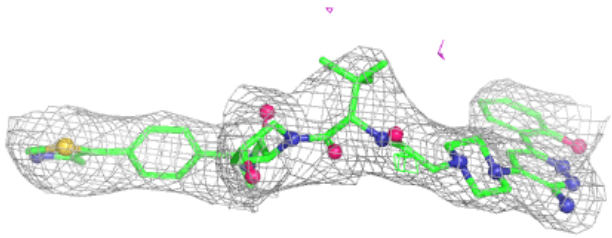


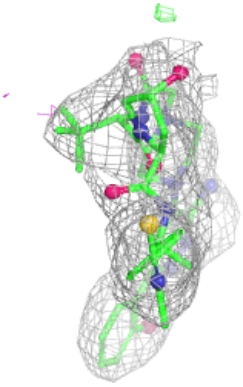


Electron density around A1BNT Q 1501:

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







6.5 Other polymers

There are no such residues in this entry.