



# Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 03:59 am BST

PDB ID : 2I2X  
Title : Crystal structure of methanol:cobalamin methyltransferase complex MtaBC from *Methanosarcina barkeri*  
Authors : Hagemeyer, C.H.; Kruer, M.; Thauer, R.K.; Warkentin, E.; Ermler, U.  
Deposited on : 2006-08-17  
Resolution : 2.50 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

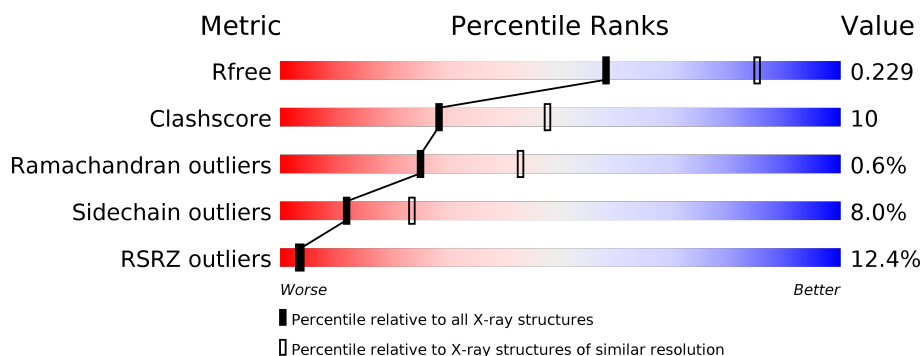
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.











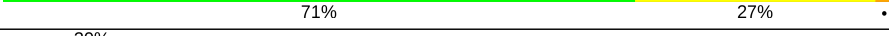

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	461	
1	C	461	
1	E	461	
1	G	461	
1	I	461	
1	K	461	

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Mol	Chain	Length	Quality of chain
1	M	461	 83% 13% .
1	O	461	 81% 16% .
2	B	258	 22% 66% 29% . .
2	D	258	 28% 69% 29% .
2	F	258	 34% 72% 25% . .
2	H	258	 45% 71% 26% .
2	J	258	 22% 70% 27% . .
2	L	258	 38% 73% 23% .
2	N	258	 48% 71% 27% .
2	P	258	 20% 72% 23% .

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 45566 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 Methyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	459	Total	C	N	O	S	0	0	0
			3534	2216	589	695	34			
1	C	459	Total	C	N	O	S	0	0	0
			3534	2216	589	695	34			
1	E	459	Total	C	N	O	S	0	0	0
			3534	2216	589	695	34			
1	G	459	Total	C	N	O	S	0	0	0
			3534	2216	589	695	34			
1	I	459	Total	C	N	O	S	0	0	0
			3534	2216	589	695	34			
1	K	459	Total	C	N	O	S	0	0	0
			3534	2216	589	695	34			
1	M	459	Total	C	N	O	S	0	0	0
			3534	2216	589	695	34			
1	O	459	Total	C	N	O	S	0	0	0
			3534	2216	589	695	34			

- Molecule 2 is a protein called Methyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	258	Total	C	N	O	S	0	0	0
			1951	1238	311	389	13			
2	D	258	Total	C	N	O	S	0	0	0
			1951	1238	311	389	13			
2	F	258	Total	C	N	O	S	0	0	0
			1951	1238	311	389	13			
2	H	258	Total	C	N	O	S	0	0	0
			1951	1238	311	389	13			
2	J	258	Total	C	N	O	S	0	0	0
			1951	1238	311	389	13			
2	L	258	Total	C	N	O	S	0	0	0
			1951	1238	311	389	13			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	258	Total 1951	C 1238	N 311	O 389	S 13	0	0	0
2	P	258	Total 1951	C 1238	N 311	O 389	S 13	0	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total 1	Zn 1	0	0
3	K	1	Total 1	Zn 1	0	0
3	E	2	Total 2	Zn 2	0	0
3	I	2	Total 2	Zn 2	0	0
3	C	1	Total 1	Zn 1	0	0
3	A	2	Total 2	Zn 2	0	0
3	O	1	Total 1	Zn 1	0	0
3	M	2	Total 2	Zn 2	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

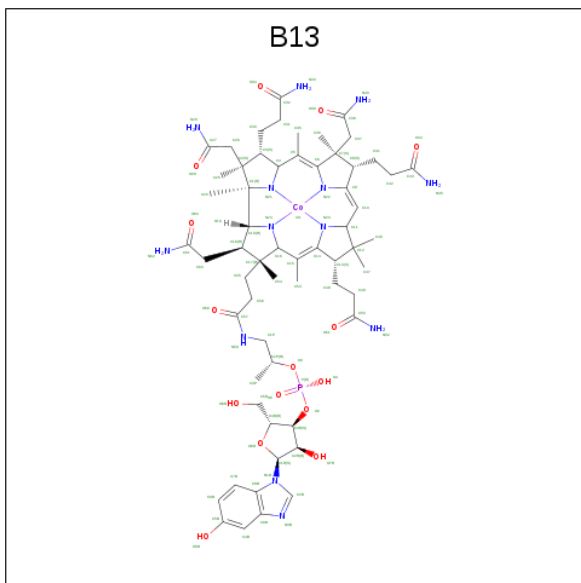
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total 1	K 1	0	0
4	K	1	Total 1	K 1	0	0
4	E	1	Total 1	K 1	0	0
4	I	1	Total 1	K 1	0	0
4	C	1	Total 1	K 1	0	0
4	A	1	Total 1	K 1	0	0
4	O	1	Total 1	K 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	M	1	Total K 1 1	0	0

- Molecule 5 is 5-HYDROXYBENZIMIDAZOLYLCOB(III)AMIDE (three-letter code: B13) (formula:  $C_{60}H_{88}CoN_{13}O_{15}P$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	B	1	Total	C	Co	N	O	P	0	0
			90	60	1	13	15	1		
5	D	1	Total	C	Co	N	O	P	0	0
			90	60	1	13	15	1		
5	F	1	Total	C	Co	N	O	P	0	0
			90	60	1	13	15	1		
5	H	1	Total	C	Co	N	O	P	0	0
			90	60	1	13	15	1		
5	J	1	Total	C	Co	N	O	P	0	0
			90	60	1	13	15	1		
5	L	1	Total	C	Co	N	O	P	0	0
			90	60	1	13	15	1		
5	N	1	Total	C	Co	N	O	P	0	0
			90	60	1	13	15	1		
5	P	1	Total	C	Co	N	O	P	0	0
			90	60	1	13	15	1		

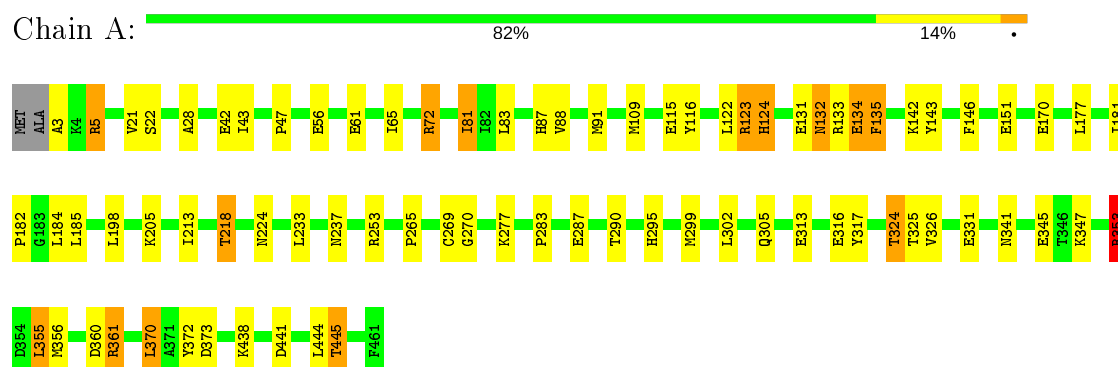
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	162	Total 162	O 162	0	0
6	B	36	Total 36	O 36	0	0
6	C	183	Total 183	O 183	0	0
6	D	27	Total 27	O 27	0	0
6	E	20	Total 20	O 20	0	0
6	F	6	Total 6	O 6	0	0
6	G	47	Total 47	O 47	0	0
6	H	1	Total 1	O 1	0	0
6	I	93	Total 93	O 93	0	0
6	J	15	Total 15	O 15	0	0
6	K	99	Total 99	O 99	0	0
6	L	18	Total 18	O 18	0	0
6	M	95	Total 95	O 95	0	0
6	N	18	Total 18	O 18	0	0
6	O	111	Total 111	O 111	0	0
6	P	15	Total 15	O 15	0	0

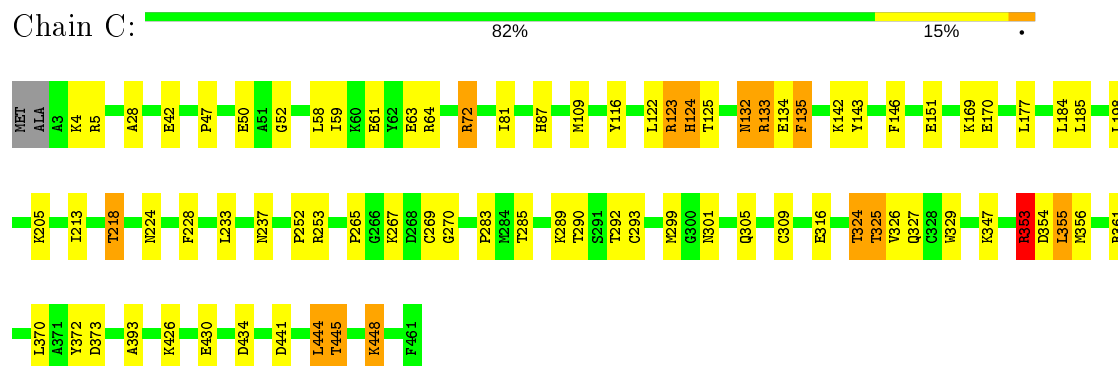
### 3 Residue-property plots [i](#)

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

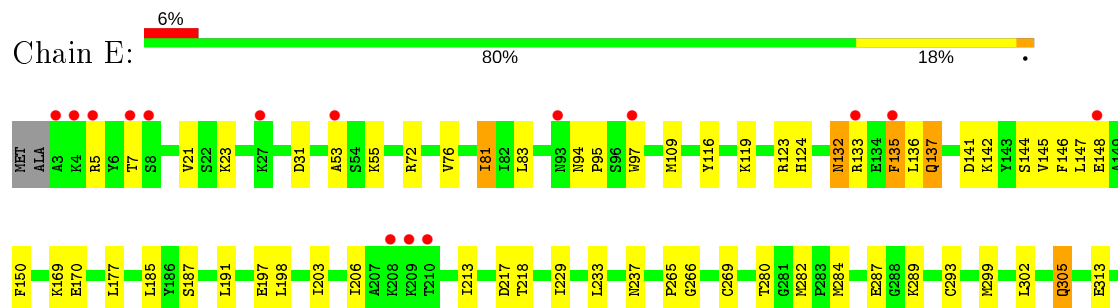
#### • Molecule 1: Methyltransferase 1



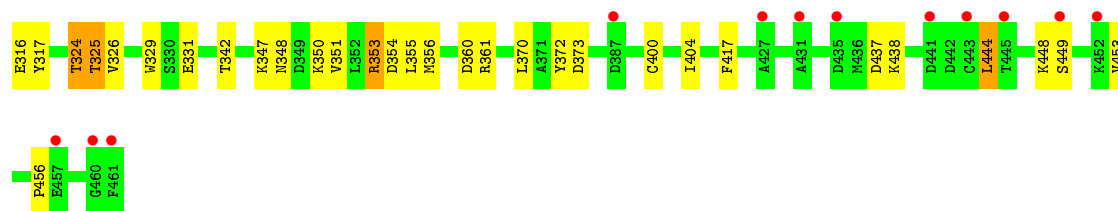
#### • Molecule 1: Methyltransferase 1



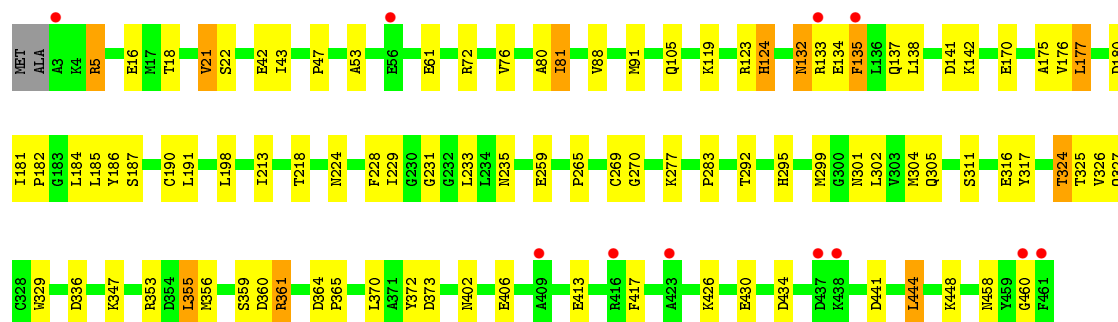
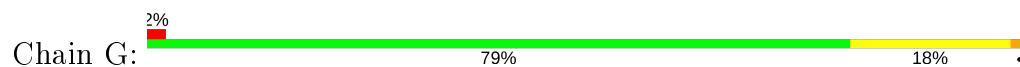
#### • Molecule 1: Methyltransferase 1



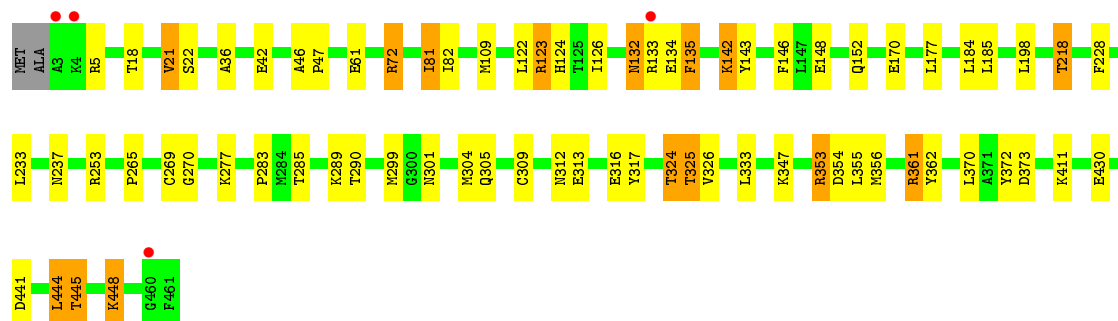
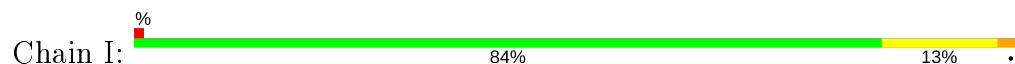




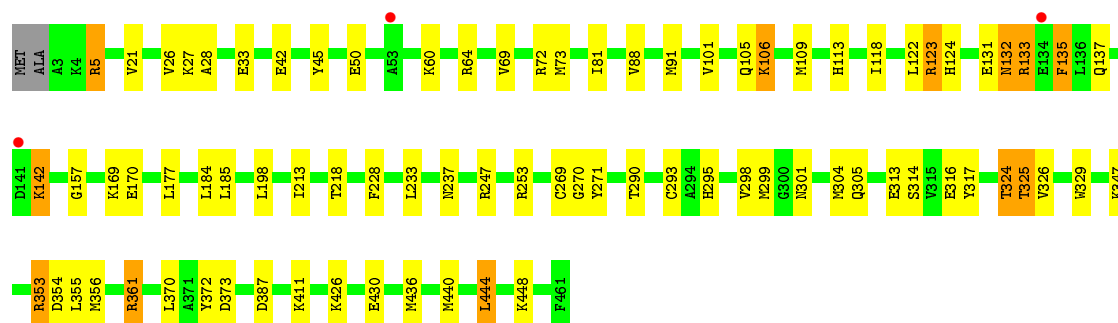
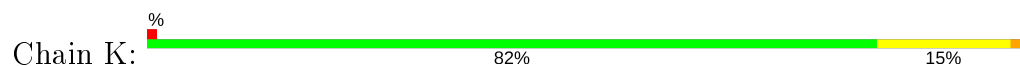
• Molecule 1: Methyltransferase 1




• Molecule 1: Methyltransferase 1

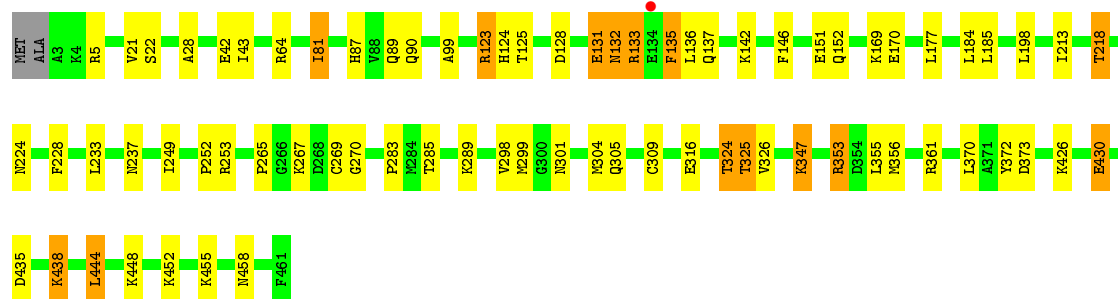


• Molecule 1: Methyltransferase 1




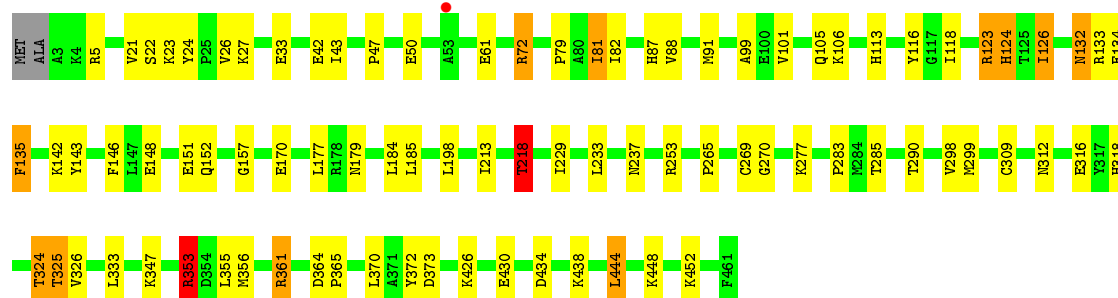
• Molecule 1: Methyltransferase 1

Chain M: 



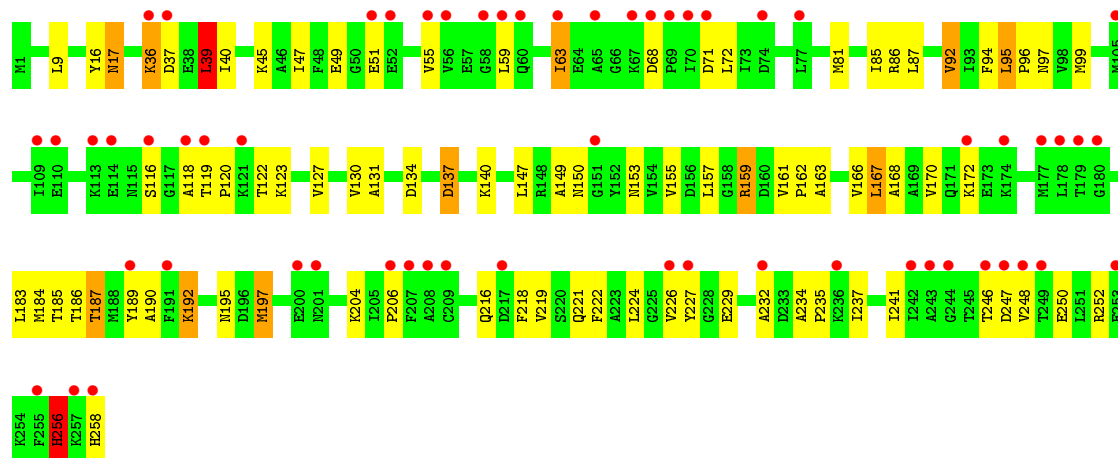
• Molecule 1: Methyltransferase 1

Chain O: 



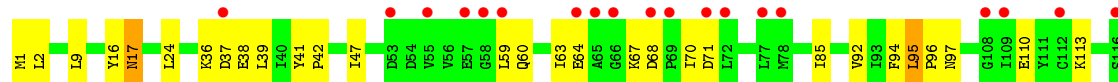
• Molecule 2: Methyltransferase 1

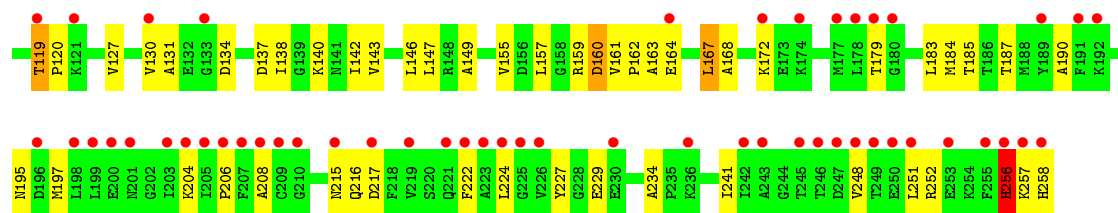
Chain B: 



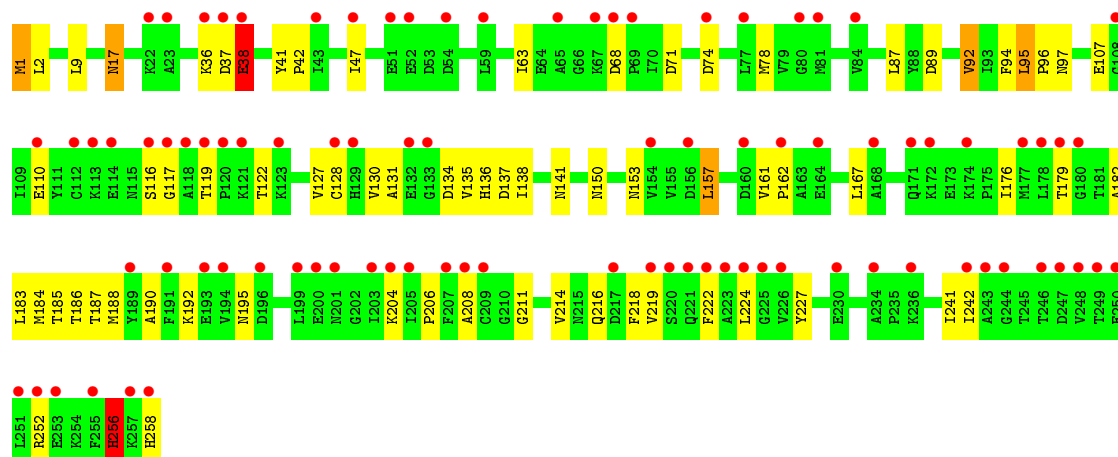
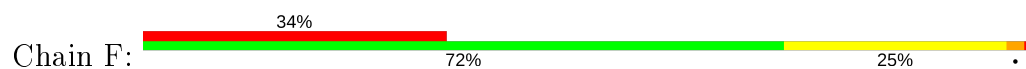
• Molecule 2: Methyltransferase 1

Chain D: 

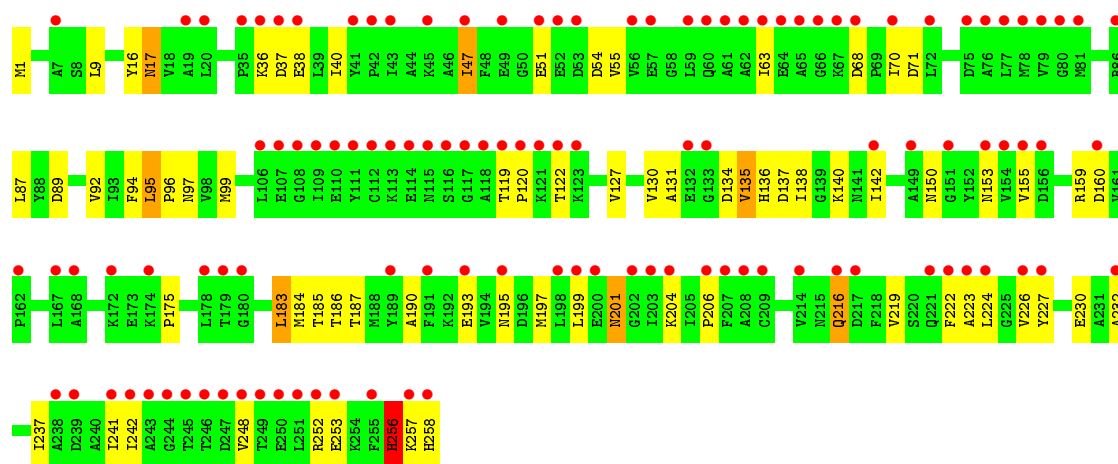




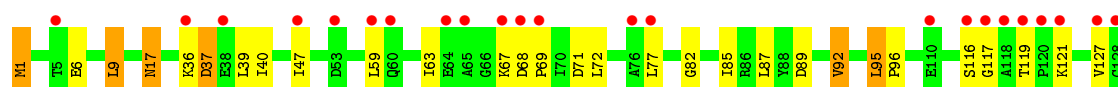
• Molecule 2: Methyltransferase 1

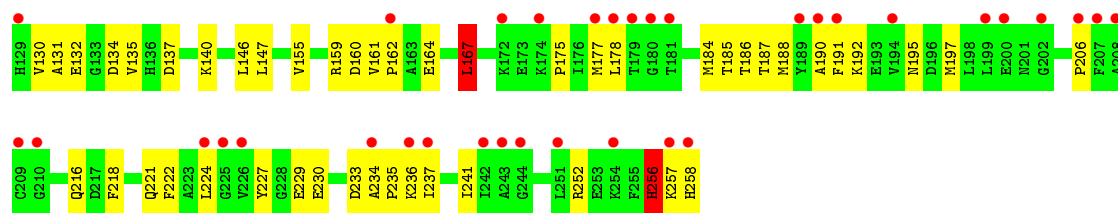


• Molecule 2: Methyltransferase 1

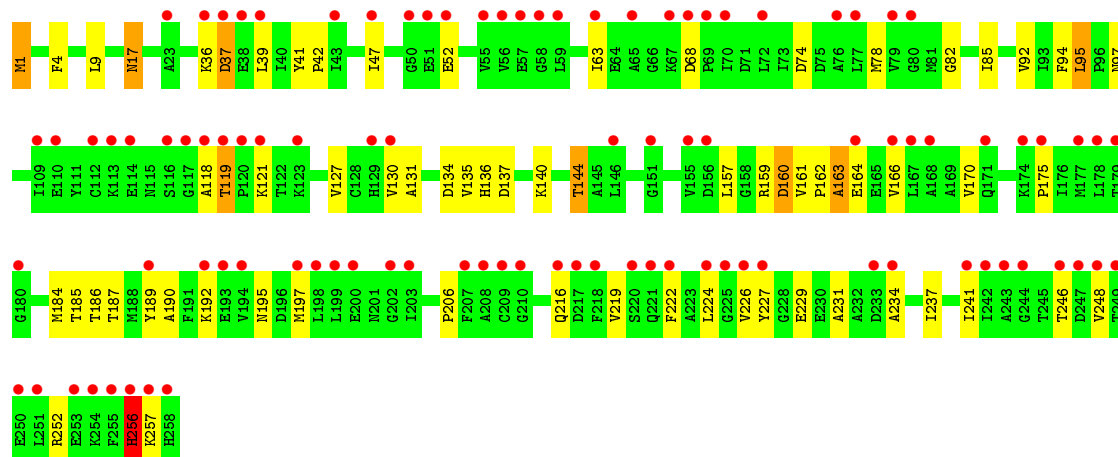
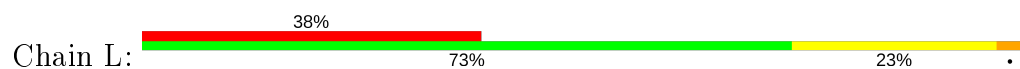


• Molecule 2: Methyltransferase 1

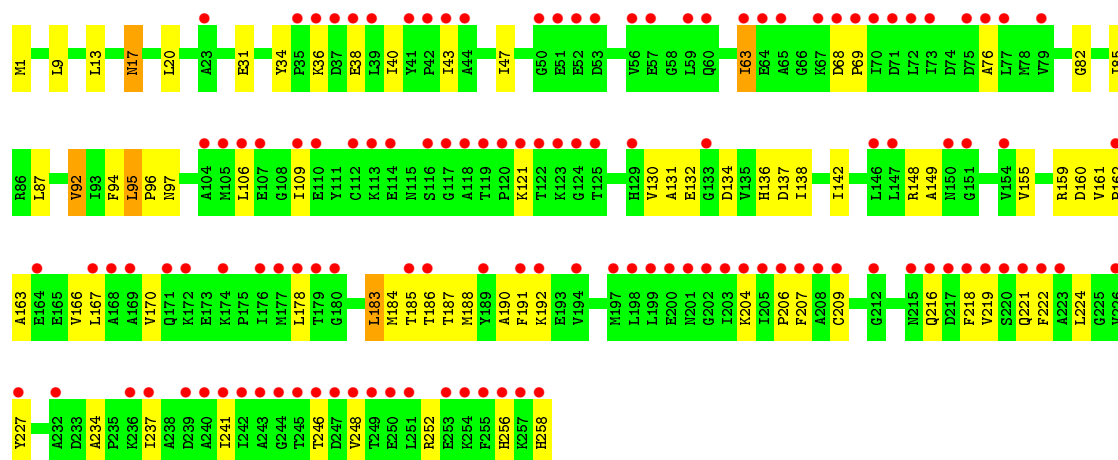
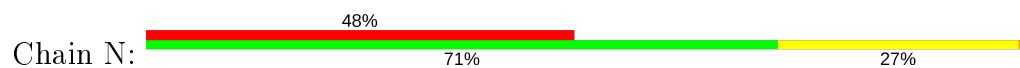




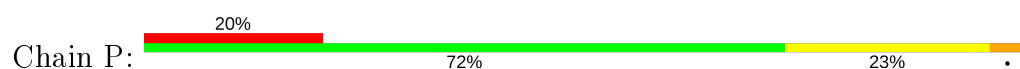
• Molecule 2: Methyltransferase 1

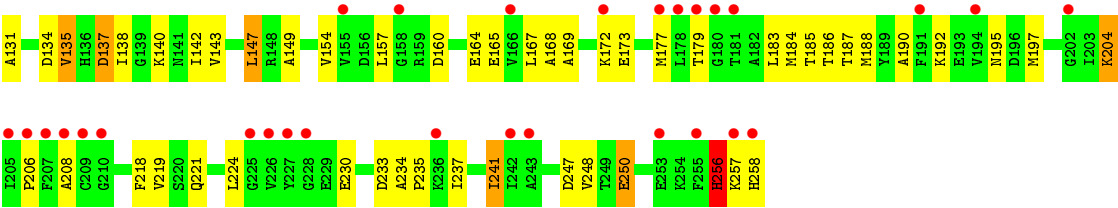


• Molecule 2: Methyltransferase 1



• Molecule 2: Methyltransferase 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.75Å 172.85Å 190.54Å 90.00° 98.86° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 20.02 – 2.51	Depositor EDS
% Data completeness (in resolution range)	98.5 (20.00-2.50) 98.5 (20.02-2.51)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.47 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.182 , 0.231 0.182 , 0.229	Depositor DCC
$R_{free}$ test set	10921 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.3	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 52.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	45566	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.35% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, K, B13

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	0.72	1/3595 (0.0%)	0.78	5/4852 (0.1%)
1	C	0.70	0/3595	0.78	5/4852 (0.1%)
1	E	0.51	0/3595	0.62	0/4852
1	G	0.54	0/3595	0.64	1/4852 (0.0%)
1	I	0.60	0/3595	0.70	3/4852 (0.1%)
1	K	0.60	0/3595	0.68	2/4852 (0.0%)
1	M	0.60	0/3595	0.69	2/4852 (0.0%)
1	O	0.62	0/3595	0.72	6/4852 (0.1%)
2	B	0.48	0/1980	0.66	1/2682 (0.0%)
2	D	0.47	0/1980	0.65	0/2682
2	F	0.46	0/1980	0.59	0/2682
2	H	0.45	0/1980	0.59	0/2682
2	J	0.47	0/1980	0.63	1/2682 (0.0%)
2	L	0.46	0/1980	0.60	0/2682
2	N	0.48	0/1980	0.61	0/2682
2	P	0.48	0/1980	0.65	0/2682
All	All	0.57	1/44600 (0.0%)	0.68	26/60272 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	56	GLU	CG-CD	5.18	1.59	1.51

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	361	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	A	361	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	C	353	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	M	123	ARG	NE-CZ-NH2	-7.65	116.48	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	361	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	A	218	THR	CB-CA-C	-6.62	93.72	111.60
1	O	218	THR	CB-CA-C	-6.48	94.09	111.60
1	O	123	ARG	NE-CZ-NH2	-6.35	117.13	120.30
1	C	123	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	M	123	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	O	361	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	A	353	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	C	218	THR	CB-CA-C	-5.70	96.20	111.60
1	I	218	THR	CB-CA-C	-5.60	96.49	111.60
1	O	353	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	K	361	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	I	123	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	C	123	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	A	123	ARG	NE-CZ-NH2	-5.29	117.65	120.30
2	B	39	LEU	CA-CB-CG	5.23	127.32	115.30
1	K	123	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	O	123	ARG	NE-CZ-NH1	5.15	122.88	120.30
2	J	167	LEU	CA-CB-CG	5.11	127.04	115.30
1	G	361	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	C	353	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	A	355	LEU	CA-CB-CG	5.02	126.85	115.30

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	3534	0	3462	49	0
1	C	3534	0	3462	56	0
1	E	3534	0	3462	54	0
1	G	3534	0	3462	63	0
1	I	3534	0	3462	51	0
1	K	3534	0	3462	61	0
1	M	3534	0	3462	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	3534	0	3462	57	0
2	B	1951	0	1952	64	0
2	D	1951	0	1952	55	0
2	F	1951	0	1952	54	0
2	H	1951	0	1952	52	0
2	J	1951	0	1952	53	0
2	L	1951	0	1952	49	0
2	N	1951	0	1952	50	0
2	P	1951	0	1952	47	0
3	A	2	0	0	0	0
3	C	1	0	0	0	0
3	E	2	0	0	0	0
3	G	1	0	0	0	0
3	I	2	0	0	0	0
3	K	1	0	0	0	0
3	M	2	0	0	0	0
3	O	1	0	0	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
4	K	1	0	0	0	0
4	M	1	0	0	0	0
4	O	1	0	0	0	0
5	B	90	0	81	9	0
5	D	90	0	81	13	0
5	F	90	0	81	7	0
5	H	90	0	81	10	0
5	J	90	0	81	13	0
5	L	90	0	81	10	0
5	N	90	0	81	11	0
5	P	90	0	81	9	0
6	A	162	0	0	4	0
6	B	36	0	0	1	0
6	C	183	0	0	3	0
6	D	27	0	0	0	0
6	E	20	0	0	0	0
6	F	6	0	0	0	0
6	G	47	0	0	3	0
6	H	1	0	0	0	0
6	I	93	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	J	15	0	0	0	0
6	K	99	0	0	4	0
6	L	18	0	0	1	0
6	M	95	0	0	4	0
6	N	18	0	0	0	0
6	O	111	0	0	4	0
6	P	15	0	0	0	0
All	All	45566	0	43960	865	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 10.

All (865) 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:P:233:ASP:O	2:P:237:ILE:HG22	1.56	1.05
1:M:353:ARG:HA	1:M:356:MET:CE	1.92	0.99
1:K:353:ARG:HA	1:K:356:MET:CE	1.95	0.97
2:L:134:ASP:HB2	2:L:187:THR:HG21	1.46	0.94
2:B:17:ASN:HD22	2:B:17:ASN:H	1.14	0.91
2:F:134:ASP:HB2	2:F:187:THR:HG21	1.54	0.90
2:H:219:VAL:HG21	2:H:227:TYR:HB2	1.54	0.89
2:F:37:ASP:O	2:F:38:GLU:HB3	1.73	0.88
2:F:68:ASP:HB3	2:F:71:ASP:HB2	1.54	0.88
2:L:184:MET:HG2	5:L:500:B13:H302	1.55	0.87
1:A:72:ARG:NH2	6:A:681:HOH:O	2.09	0.85
2:F:184:MET:HG2	5:F:500:B13:H302	1.58	0.85
2:L:219:VAL:HG21	2:L:227:TYR:HB2	1.57	0.85
1:O:218:THR:HG21	1:O:269:CYS:SG	2.17	0.85
1:E:354:ASP:OD2	2:F:1:MET:HA	1.77	0.85
1:O:316:GLU:O	1:O:325:THR:HG21	1.77	0.84
2:J:17:ASN:HD22	2:J:17:ASN:H	1.24	0.84
2:B:167:LEU:HB2	2:B:197:MET:HE1	1.58	0.84
2:H:134:ASP:HB2	2:H:187:THR:HG21	1.58	0.84
2:P:177:MET:HE1	2:P:237:ILE:HG13	1.59	0.82
2:B:226:VAL:HG11	2:B:237:ILE:HD11	1.59	0.82
1:G:218:THR:HG21	1:G:269:CYS:SG	2.18	0.82
2:D:17:ASN:H	2:D:17:ASN:HD22	1.26	0.81
1:O:229:ILE:HD11	2:P:138:ILE:HD13	1.63	0.80
5:D:500:B13:H363	5:D:500:B13:H401	1.45	0.80
2:L:137:ASP:HB2	5:L:500:B13:H522	1.47	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:GLN:HA	1:A:356:MET:CE	2.12	0.79
2:N:134:ASP:HB2	2:N:187:THR:HG21	1.65	0.79
1:I:218:THR:HG21	1:I:269:CYS:SG	2.24	0.77
1:C:316:GLU:O	1:C:325:THR:HG21	1.85	0.77
1:A:316:GLU:O	1:A:325:THR:HG21	1.84	0.77
1:A:353:ARG:HA	1:A:356:MET:HE2	1.65	0.77
1:G:353:ARG:HA	1:G:356:MET:CE	2.16	0.76
1:E:316:GLU:O	1:E:325:THR:HG21	1.85	0.76
1:A:305:GLN:HA	1:A:356:MET:HE3	1.68	0.76
1:M:218:THR:HG21	1:M:269:CYS:SG	2.24	0.76
1:O:353:ARG:HA	1:O:356:MET:CE	2.14	0.76
2:N:137:ASP:HB2	5:N:500:B13:H522	1.50	0.76
1:E:280:THR:HB	1:E:282:MET:HG3	1.69	0.75
2:B:85:ILE:HD11	2:B:149:ALA:HB1	1.67	0.75
1:E:218:THR:HG21	1:E:269:CYS:SG	2.26	0.75
1:C:324:THR:HG22	1:C:327:GLN:HG3	1.68	0.74
2:P:195:ASN:HD21	2:P:224:LEU:H	1.35	0.74
1:G:353:ARG:HD3	1:G:372:TYR:CE1	2.22	0.74
2:J:68:ASP:HB3	2:J:71:ASP:HB2	1.68	0.73
1:C:324:THR:CG2	1:C:326:VAL:HG22	2.18	0.73
1:M:353:ARG:HA	1:M:356:MET:HE1	1.71	0.73
1:C:218:THR:HG21	1:C:269:CYS:SG	2.29	0.73
2:B:17:ASN:H	2:B:17:ASN:ND2	1.86	0.73
1:E:444:LEU:O	1:E:448:LYS:HB2	1.89	0.73
1:K:218:THR:HG21	1:K:269:CYS:SG	2.29	0.73
2:B:216:GLN:HE21	2:B:258:HIS:HD2	1.34	0.73
2:H:137:ASP:HB2	5:H:500:B13:H522	1.53	0.72
1:K:316:GLU:O	1:K:325:THR:HG21	1.88	0.72
2:N:191:PHE:HE2	2:N:209:CYS:HB3	1.52	0.72
2:L:131:ALA:HB1	2:L:190:ALA:HB3	1.71	0.72
1:K:72:ARG:NH2	6:K:587:HOH:O	2.22	0.72
2:F:185:THR:HG23	5:F:500:B13:H332	1.55	0.71
2:H:17:ASN:H	2:H:17:ASN:HD22	1.39	0.71
1:K:317:TYR:HE1	1:K:324:THR:HG21	1.56	0.71
2:P:94:PHE:H	2:P:97:ASN:HD22	1.37	0.71
1:A:218:THR:HG21	1:A:269:CYS:SG	2.31	0.70
2:H:219:VAL:CG2	2:H:227:TYR:HB2	2.22	0.70
1:I:361:ARG:NH2	1:I:373:ASP:OD1	2.24	0.70
1:I:353:ARG:HA	1:I:356:MET:HE2	1.73	0.70
1:M:316:GLU:O	1:M:325:THR:HG21	1.90	0.70
2:D:85:ILE:HD11	2:D:149:ALA:O	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:219:VAL:HG21	2:N:227:TYR:HB2	1.73	0.70
2:D:137:ASP:HB2	5:D:500:B13:H522	1.57	0.69
2:P:68:ASP:HB3	2:P:71:ASP:HB2	1.72	0.69
1:K:353:ARG:HA	1:K:356:MET:HE1	1.75	0.69
2:N:17:ASN:H	2:N:17:ASN:HD22	1.38	0.69
1:G:316:GLU:O	1:G:325:THR:HG21	1.91	0.69
1:K:28:ALA:HB2	1:K:213:ILE:HD12	1.74	0.69
2:F:219:VAL:HG21	2:F:227:TYR:HB2	1.74	0.69
2:H:94:PHE:H	2:H:97:ASN:HD22	1.41	0.69
2:B:134:ASP:OD2	2:B:187:THR:HG21	1.92	0.69
2:J:184:MET:HG2	5:J:500:B13:H302	1.73	0.69
2:B:130:VAL:HG23	2:B:140:LYS:HD3	1.74	0.69
2:P:17:ASN:H	2:P:17:ASN:HD22	1.39	0.69
2:P:134:ASP:HB2	2:P:187:THR:HG21	1.74	0.69
1:I:316:GLU:O	1:I:325:THR:HG21	1.91	0.69
5:P:500:B13:H601	5:P:500:B13:H262	1.75	0.68
1:C:28:ALA:HB2	1:C:213:ILE:HD13	1.76	0.68
1:I:354:ASP:OD2	2:J:1:MET:HA	1.94	0.68
2:B:185:THR:H	5:B:500:B13:H332	1.40	0.68
1:K:26:VAL:CG1	1:K:213:ILE:HD13	2.23	0.68
2:H:195:ASN:ND2	2:H:224:LEU:HB2	2.09	0.68
2:P:206:PRO:HG2	2:P:241:ILE:HD12	1.76	0.68
1:G:16:GLU:OE2	1:M:347:LYS:NZ	2.25	0.68
2:J:131:ALA:HB1	2:J:190:ALA:HB3	1.75	0.68
1:K:305:GLN:HA	1:K:356:MET:HE3	1.76	0.67
5:L:500:B13:H262	5:L:500:B13:H601	1.76	0.67
2:B:216:GLN:HE22	2:B:258:HIS:H	1.41	0.67
1:M:361:ARG:NH2	1:M:373:ASP:OD1	2.27	0.67
2:J:192:LYS:HG2	2:J:222:PHE:CE2	2.29	0.67
2:B:168:ALA:O	2:B:172:LYS:HG2	1.94	0.67
2:F:131:ALA:HB1	2:F:190:ALA:HB3	1.76	0.67
2:D:41:TYR:HB3	2:D:42:PRO:HD3	1.76	0.67
1:G:301:ASN:HD22	1:G:304:MET:CE	2.07	0.67
2:F:17:ASN:H	2:F:17:ASN:HD22	1.41	0.66
1:O:132:ASN:HD22	1:O:134:GLU:H	1.43	0.66
1:G:426:LYS:O	1:G:430:GLU:HG3	1.95	0.66
1:I:353:ARG:HD3	1:I:372:TYR:CE1	2.30	0.66
2:P:37:ASP:O	2:P:39:LEU:N	2.25	0.66
5:F:500:B13:H601	5:F:500:B13:H252	1.76	0.66
5:H:500:B13:H252	5:H:500:B13:H601	1.75	0.66
5:B:500:B13:H361	5:B:500:B13:H351	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:134:ASP:HB2	2:D:187:THR:HG21	1.77	0.66
1:C:132:ASN:ND2	1:C:135:PHE:H	1.94	0.66
1:I:317:TYR:HE1	1:I:324:THR:HG21	1.59	0.66
1:M:123:ARG:NH2	1:M:265:PRO:O	2.28	0.66
1:G:301:ASN:HD22	1:G:304:MET:HE2	1.60	0.65
1:I:361:ARG:HH22	1:I:373:ASP:CG	2.00	0.65
1:G:417:PHE:HZ	2:H:97:ASN:HD21	1.43	0.65
2:B:192:LYS:HG2	2:B:222:PHE:HE2	1.62	0.65
1:O:43:ILE:HG22	1:O:81:ILE:HD11	1.79	0.65
2:B:206:PRO:HG2	2:B:241:ILE:HD12	1.79	0.65
1:M:353:ARG:HD3	1:M:372:TYR:CE1	2.31	0.65
2:B:166:VAL:O	2:B:170:VAL:HG23	1.97	0.65
1:G:5:ARG:HA	1:G:259:GLU:HG2	1.80	0.64
2:F:195:ASN:HD21	2:F:224:LEU:H	1.43	0.64
2:N:184:MET:HG2	5:N:500:B13:H302	1.78	0.64
2:D:185:THR:H	5:D:500:B13:H332	1.46	0.64
1:I:305:GLN:HA	1:I:356:MET:CE	2.28	0.64
2:P:85:ILE:HD11	2:P:149:ALA:HB1	1.79	0.64
1:A:5:ARG:HD2	6:A:657:HOH:O	1.97	0.64
6:G:530:HOH:O	2:H:1:MET:HB3	1.97	0.64
1:M:353:ARG:HA	1:M:356:MET:HE2	1.79	0.64
1:C:353:ARG:HA	1:C:356:MET:HE2	1.78	0.64
2:J:17:ASN:N	2:J:17:ASN:HD22	1.94	0.64
2:J:87:LEU:HB3	2:J:92:VAL:HG22	1.79	0.63
2:D:216:GLN:HE21	2:D:258:HIS:HD2	1.46	0.63
1:G:302:LEU:HB2	1:G:360:ASP:HB2	1.81	0.63
5:J:500:B13:H351	5:J:500:B13:H361	1.80	0.63
2:F:17:ASN:HD22	2:F:17:ASN:N	1.96	0.63
2:F:216:GLN:HE22	2:F:258:HIS:H	1.45	0.63
1:G:132:ASN:C	1:G:132:ASN:HD22	2.01	0.63
2:B:137:ASP:HB2	5:B:500:B13:H522	1.64	0.63
5:D:500:B13:H363	5:D:500:B13:N40	2.14	0.63
2:B:216:GLN:HE21	2:B:258:HIS:CD2	2.16	0.62
1:G:361:ARG:HH22	1:G:373:ASP:CG	2.03	0.62
2:N:185:THR:HG23	5:N:500:B13:H332	1.64	0.62
1:C:353:ARG:HA	1:C:356:MET:CE	2.29	0.62
2:D:222:PHE:O	2:D:252:ARG:NH2	2.32	0.62
6:M:611:HOH:O	2:N:138:ILE:HG12	1.99	0.62
2:P:247:ASP:HB3	2:P:250:GLU:HB2	1.81	0.62
2:D:131:ALA:HB1	2:D:190:ALA:HB3	1.81	0.62
2:P:168:ALA:O	2:P:172:LYS:HG2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:192:LYS:HG2	2:B:222:PHE:CE2	2.34	0.61
2:B:195:ASN:HD21	2:B:224:LEU:H	1.47	0.61
2:D:168:ALA:O	2:D:172:LYS:HG2	2.00	0.61
2:D:215:ASN:HD22	2:D:217:ASP:H	1.48	0.61
2:P:185:THR:HG23	5:P:500:B13:H332	1.65	0.61
1:K:133:ARG:HD2	2:L:160:ASP:HB3	1.80	0.61
1:C:42:GLU:OE2	1:C:123:ARG:HD2	2.00	0.61
1:O:72:ARG:NH2	6:O:616:HOH:O	2.33	0.61
1:G:460:GLY:HA2	6:G:554:HOH:O	2.00	0.61
2:P:177:MET:CE	2:P:237:ILE:HG13	2.30	0.61
1:E:305:GLN:HA	1:E:356:MET:HE3	1.82	0.61
2:J:195:ASN:HD21	2:J:224:LEU:H	1.47	0.61
1:M:305:GLN:HA	1:M:356:MET:HE3	1.82	0.61
1:M:426:LYS:HE3	1:M:430:GLU:OE2	2.00	0.61
1:O:132:ASN:ND2	1:O:134:GLU:H	1.98	0.61
2:P:131:ALA:HB1	2:P:190:ALA:HB3	1.81	0.61
1:C:426:LYS:O	1:C:430:GLU:HG3	2.01	0.61
2:N:94:PHE:H	2:N:97:ASN:HD22	1.49	0.61
5:D:500:B13:H361	5:D:500:B13:H351	1.83	0.61
2:F:94:PHE:H	2:F:97:ASN:HD22	1.48	0.60
2:H:135:VAL:HG22	2:H:159:ARG:HE	1.66	0.60
2:L:82:GLY:HA2	2:L:85:ILE:HD12	1.81	0.60
2:N:94:PHE:H	2:N:97:ASN:ND2	1.98	0.60
2:N:166:VAL:O	2:N:170:VAL:HG23	2.01	0.60
1:C:289:LYS:HD3	1:C:301:ASN:ND2	2.16	0.60
1:E:237:ASN:HA	2:F:95:LEU:HB2	1.83	0.60
1:C:4:LYS:HG2	6:O:629:HOH:O	2.02	0.60
1:O:132:ASN:ND2	1:O:135:PHE:H	1.98	0.60
2:F:252:ARG:O	2:F:256:HIS:HB2	2.00	0.60
1:M:133:ARG:HH11	1:M:133:ARG:CG	2.14	0.60
1:G:224:ASN:O	1:G:228:PHE:HD2	1.84	0.60
2:J:37:ASP:HB3	2:J:40:ILE:HB	1.84	0.60
2:L:224:LEU:HA	2:L:248:VAL:HG21	1.83	0.59
1:A:42:GLU:OE2	1:A:123:ARG:HD2	2.03	0.59
2:F:179:THR:HG22	2:F:208:ALA:HB3	1.85	0.59
1:I:312:ASN:HB3	1:I:333:LEU:HD11	1.85	0.59
2:L:222:PHE:O	2:L:252:ARG:NH2	2.36	0.59
1:C:324:THR:HG23	1:C:326:VAL:HG22	1.85	0.59
2:N:224:LEU:HA	2:N:248:VAL:HG21	1.83	0.59
2:N:40:ILE:HA	2:N:43:ILE:HD12	1.85	0.59
5:H:500:B13:O58	5:H:500:B13:H532	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:219:VAL:CG2	2:N:227:TYR:HB2	2.33	0.59
2:B:206:PRO:HG2	2:B:241:ILE:CD1	2.33	0.58
2:J:216:GLN:HE21	2:J:258:HIS:HD2	1.49	0.58
1:K:317:TYR:CE1	1:K:324:THR:HG21	2.35	0.58
2:P:184:MET:HG2	5:P:500:B13:H302	1.85	0.58
1:E:444:LEU:CD2	1:E:448:LYS:HD2	2.32	0.58
2:J:185:THR:HG23	5:J:500:B13:H332	1.68	0.58
2:N:137:ASP:HB2	5:N:500:B13:N52	2.18	0.58
2:B:94:PHE:H	2:B:97:ASN:HD22	1.51	0.58
2:L:17:ASN:HD22	2:L:17:ASN:H	1.52	0.58
1:M:42:GLU:OE2	1:M:123:ARG:HD2	2.03	0.58
2:D:94:PHE:H	2:D:97:ASN:HD22	1.51	0.58
2:H:130:VAL:HG23	2:H:140:LYS:HD3	1.86	0.58
1:K:293:CYS:HB3	1:K:329:TRP:CZ2	2.39	0.58
1:E:132:ASN:ND2	1:E:135:PHE:H	2.02	0.58
1:G:18:THR:HG23	1:G:21:VAL:HG13	1.86	0.58
1:I:444:LEU:HD22	1:I:448:LYS:HD2	1.85	0.58
2:J:185:THR:H	5:J:500:B13:H332	1.50	0.58
2:B:189:TYR:O	2:B:192:LYS:HB2	2.04	0.58
2:P:234:ALA:HB3	2:P:235:PRO:HD3	1.85	0.58
2:B:184:MET:HG2	5:B:500:B13:H302	1.84	0.57
1:E:373:ASP:HB3	2:F:1:MET:HE3	1.86	0.57
1:I:305:GLN:HA	1:I:356:MET:HE3	1.84	0.57
1:I:444:LEU:O	1:I:448:LYS:HB2	2.04	0.57
1:G:353:ARG:HA	1:G:356:MET:HE3	1.84	0.57
2:H:37:ASP:O	2:H:38:GLU:HB3	2.04	0.57
2:B:36:LYS:H	2:B:36:LYS:HD3	1.69	0.57
2:H:185:THR:HG23	5:H:500:B13:H332	1.68	0.57
1:E:444:LEU:HD22	1:E:448:LYS:HD2	1.85	0.57
2:H:199:LEU:C	2:H:201:ASN:H	2.07	0.57
2:H:17:ASN:N	2:H:17:ASN:HD22	2.03	0.57
2:J:216:GLN:HE21	2:J:258:HIS:CD2	2.21	0.57
1:K:132:ASN:C	1:K:132:ASN:HD22	2.07	0.57
1:O:42:GLU:OE2	1:O:123:ARG:HD2	2.04	0.57
2:P:138:ILE:O	2:P:142:ILE:HG13	2.04	0.57
2:P:185:THR:H	5:P:500:B13:H332	1.51	0.57
1:G:231:GLY:HA3	1:G:235:ASN:ND2	2.20	0.57
2:L:130:VAL:HG12	2:L:134:ASP:HB3	1.87	0.57
5:N:500:B13:H262	5:N:500:B13:H601	1.87	0.57
2:B:195:ASN:ND2	2:B:224:LEU:H	2.03	0.57
2:H:197:MET:HG2	2:H:197:MET:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:184:MET:HG2	5:H:500:B13:H302	1.86	0.57
2:L:127:VAL:HG23	2:L:175:PRO:HG3	1.85	0.57
1:K:169:LYS:HD2	5:L:500:B13:H473	1.87	0.57
2:B:94:PHE:H	2:B:97:ASN:ND2	2.03	0.56
1:M:444:LEU:O	1:M:448:LYS:HB2	2.05	0.56
1:C:305:GLN:HA	1:C:356:MET:CE	2.35	0.56
2:D:17:ASN:HD22	2:D:17:ASN:N	2.02	0.56
5:D:500:B13:H601	5:D:500:B13:H262	1.87	0.56
2:N:252:ARG:O	2:N:256:HIS:HB2	2.05	0.56
2:B:226:VAL:HG11	2:B:237:ILE:CD1	2.31	0.56
2:D:37:ASP:O	2:D:39:LEU:N	2.29	0.56
1:G:123:ARG:NH2	1:G:265:PRO:O	2.39	0.56
2:P:188:MET:HB3	2:P:218:PHE:CZ	2.41	0.56
1:E:448:LYS:HE3	1:E:456:PRO:HG2	1.86	0.56
1:A:132:ASN:ND2	1:A:135:PHE:H	2.03	0.56
1:A:265:PRO:HA	1:A:283:PRO:O	2.06	0.56
1:E:229:ILE:HD11	2:F:138:ILE:HD13	1.88	0.56
1:K:132:ASN:ND2	1:K:135:PHE:H	2.03	0.56
1:E:353:ARG:HD3	1:E:372:TYR:CE1	2.40	0.56
2:N:131:ALA:HB1	2:N:190:ALA:HB3	1.86	0.56
1:O:444:LEU:O	1:O:448:LYS:HB2	2.06	0.56
2:B:45:LYS:HE3	2:B:49:GLU:OE2	2.05	0.56
1:C:293:CYS:HB3	1:C:329:TRP:CZ2	2.40	0.56
1:K:354:ASP:OD2	2:L:1:MET:HA	2.06	0.56
1:M:87:HIS:NE2	1:M:124:HIS:HD2	2.04	0.56
2:N:216:GLN:HE22	2:N:258:HIS:H	1.54	0.56
5:F:500:B13:H351	5:F:500:B13:H361	1.88	0.55
2:J:37:ASP:O	2:J:39:LEU:N	2.30	0.55
1:K:5:ARG:NH2	6:K:611:HOH:O	2.30	0.55
2:B:68:ASP:HB3	2:B:71:ASP:HB2	1.88	0.55
2:F:137:ASP:HB3	2:F:141:ASN:ND2	2.21	0.55
1:G:444:LEU:O	1:G:448:LYS:HB2	2.06	0.55
2:D:138:ILE:HG13	5:D:500:B13:O51	2.06	0.55
1:O:312:ASN:HB3	1:O:333:LEU:HD11	1.88	0.55
1:I:123:ARG:NH2	1:I:265:PRO:O	2.40	0.55
2:J:218:PHE:O	2:J:221:GLN:HG2	2.07	0.55
1:A:47:PRO:HB3	1:A:61:GLU:HG2	1.88	0.55
2:F:176:ILE:HD13	2:F:242:ILE:HD11	1.87	0.55
6:I:562:HOH:O	2:J:96:PRO:HG2	2.07	0.55
2:P:130:VAL:HG23	2:P:140:LYS:HD3	1.88	0.55
5:B:500:B13:H262	5:B:500:B13:H601	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:59:LEU:HD11	2:J:77:LEU:HD21	1.88	0.55
2:N:106:LEU:HD11	2:N:148:ARG:HD3	1.88	0.55
2:H:222:PHE:O	2:H:252:ARG:NH2	2.39	0.55
1:O:132:ASN:C	1:O:132:ASN:HD22	2.10	0.55
1:O:99:ALA:HB2	1:O:152:GLN:HB3	1.89	0.54
1:O:265:PRO:HA	1:O:283:PRO:O	2.07	0.54
2:H:131:ALA:HB1	2:H:190:ALA:HB3	1.89	0.54
2:H:136:HIS:HB3	2:H:183:LEU:HD13	1.89	0.54
2:H:87:LEU:HD22	2:H:92:VAL:HG21	1.89	0.54
1:C:72:ARG:NH2	6:C:515:HOH:O	2.39	0.54
1:E:342:THR:HG22	1:G:355:LEU:HD12	1.90	0.54
2:H:195:ASN:HD21	2:H:224:LEU:H	1.54	0.54
2:D:127:VAL:HG13	2:D:157:LEU:HD23	1.89	0.54
1:G:132:ASN:ND2	1:G:134:GLU:H	2.04	0.54
1:A:353:ARG:HA	1:A:356:MET:CE	2.36	0.54
2:B:127:VAL:HG13	2:B:157:LEU:HD23	1.89	0.54
2:P:164:GLU:HA	2:P:197:MET:HE1	1.89	0.54
1:G:187:SER:HA	1:G:191:LEU:HD12	1.89	0.54
2:H:51:GLU:O	2:H:55:VAL:HG23	2.08	0.54
1:I:441:ASP:O	1:I:445:THR:HG23	2.07	0.54
1:K:69:VAL:O	1:K:73:MET:HG2	2.08	0.54
1:M:224:ASN:ND2	1:M:269:CYS:HB2	2.22	0.54
1:O:143:TYR:O	1:O:146:PHE:HB3	2.07	0.54
1:O:353:ARG:HD3	1:O:372:TYR:CE1	2.43	0.54
1:M:224:ASN:HD21	1:M:269:CYS:HB2	1.73	0.54
1:C:265:PRO:HA	1:C:283:PRO:O	2.07	0.54
1:K:444:LEU:O	1:K:448:LYS:HB2	2.08	0.54
1:M:43:ILE:HG22	1:M:81:ILE:HD11	1.90	0.54
1:E:354:ASP:HB3	2:F:2:LEU:HD12	1.90	0.53
2:L:134:ASP:OD1	2:L:136:HIS:ND1	2.32	0.53
2:L:166:VAL:O	2:L:170:VAL:HG23	2.08	0.53
1:O:132:ASN:HD22	1:O:134:GLU:N	2.05	0.53
2:P:218:PHE:O	2:P:221:GLN:HG2	2.08	0.53
2:F:192:LYS:HG2	2:F:222:PHE:CE2	2.42	0.53
2:D:179:THR:HG22	2:D:208:ALA:HB3	1.90	0.53
2:D:216:GLN:HE21	2:D:258:HIS:CD2	2.26	0.53
1:O:353:ARG:HA	1:O:356:MET:HE3	1.88	0.53
1:K:132:ASN:HD21	1:K:135:PHE:H	1.56	0.53
1:O:361:ARG:HH22	1:O:373:ASP:CG	2.11	0.53
2:P:195:ASN:ND2	2:P:224:LEU:H	2.06	0.53
1:M:131:GLU:HB2	1:M:136:LEU:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:LEU:HB2	1:A:360:ASP:HB2	1.91	0.53
2:D:206:PRO:HG2	2:D:241:ILE:HD12	1.91	0.53
1:K:109:MET:HE1	1:K:122:LEU:HD13	1.91	0.53
1:G:132:ASN:HD21	1:G:134:GLU:HG2	1.74	0.53
1:M:89:GLN:NE2	1:M:90:GLN:HB3	2.24	0.53
2:D:17:ASN:ND2	2:D:17:ASN:H	2.03	0.52
2:L:219:VAL:CG2	2:L:227:TYR:HB2	2.35	0.52
2:F:135:VAL:CG1	2:F:135:VAL:O	2.57	0.52
2:H:230:GLU:HG3	2:H:232:ALA:H	1.74	0.52
2:H:206:PRO:HG2	2:H:241:ILE:HD12	1.90	0.52
5:J:500:B13:H401	5:J:500:B13:H363	1.73	0.52
1:A:3:ALA:HB2	6:A:675:HOH:O	2.09	0.52
2:B:167:LEU:HB2	2:B:197:MET:CE	2.36	0.52
1:E:331:GLU:HB3	1:G:292:THR:HG21	1.90	0.52
1:M:353:ARG:CA	1:M:356:MET:HE1	2.39	0.52
1:M:435:ASP:OD2	1:M:438:LYS:HB2	2.09	0.52
1:K:290:THR:O	1:K:290:THR:HG22	2.10	0.52
1:O:218:THR:HG23	1:O:270:GLY:N	2.25	0.52
2:D:215:ASN:ND2	2:D:217:ASP:H	2.08	0.52
2:H:136:HIS:CB	2:H:183:LEU:HD13	2.40	0.52
1:M:64:ARG:NE	6:M:565:HOH:O	2.42	0.52
2:N:216:GLN:HE21	2:N:258:HIS:HD2	1.55	0.52
1:I:218:THR:HG23	1:I:270:GLY:CA	2.39	0.52
2:N:191:PHE:CE2	2:N:209:CYS:HB3	2.40	0.52
1:O:132:ASN:HD21	1:O:135:PHE:H	1.58	0.52
1:E:324:THR:CG2	1:E:326:VAL:HG22	2.40	0.52
1:G:229:ILE:HD11	2:H:138:ILE:HD13	1.90	0.52
1:M:99:ALA:HB2	1:M:152:GLN:HB3	1.92	0.52
1:M:169:LYS:HD2	5:N:500:B13:H473	1.92	0.52
2:F:128:CYS:O	2:F:157:LEU:HB2	2.10	0.51
2:F:227:TYR:H	2:F:256:HIS:HE1	1.58	0.51
1:K:353:ARG:HA	1:K:356:MET:HE2	1.83	0.51
1:C:133:ARG:HD2	2:D:160:ASP:HB3	1.91	0.51
1:C:305:GLN:HA	1:C:356:MET:HE3	1.91	0.51
2:H:122:THR:HG21	2:H:153:ASN:HB2	1.92	0.51
1:G:364:ASP:CG	1:G:365:PRO:HD2	2.31	0.51
2:B:184:MET:HB2	2:B:187:THR:HB	1.92	0.51
2:F:184:MET:HE1	5:F:500:B13:H353	1.92	0.51
2:H:95:LEU:HB3	2:H:96:PRO:HD3	1.93	0.51
1:I:218:THR:HG23	1:I:270:GLY:N	2.26	0.51
2:J:37:ASP:C	2:J:39:LEU:H	2.14	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:132:ASN:HD21	1:M:135:PHE:H	1.59	0.51
1:O:23:LYS:HD3	1:O:24:TYR:CZ	2.46	0.51
1:A:109:MET:HE3	1:A:122:LEU:HD13	1.91	0.51
5:B:500:B13:H252	5:B:500:B13:C61	2.41	0.51
2:J:167:LEU:HG	2:J:197:MET:HG2	1.91	0.51
1:K:27:LYS:HG2	1:K:33:GLU:HG2	1.92	0.51
1:O:87:HIS:NE2	1:O:124:HIS:HD2	2.08	0.51
1:E:280:THR:HB	1:E:282:MET:CG	2.41	0.51
1:C:125:THR:HG21	1:C:267:LYS:HE2	1.93	0.51
1:I:132:ASN:C	1:I:132:ASN:HD22	2.14	0.51
1:O:353:ARG:HA	1:O:356:MET:HE2	1.92	0.51
1:A:109:MET:CE	1:A:122:LEU:HD13	2.41	0.51
1:A:143:TYR:O	1:A:146:PHE:HB3	2.11	0.51
1:I:109:MET:HE3	1:I:122:LEU:HD22	1.93	0.50
1:K:237:ASN:HA	2:L:95:LEU:HB2	1.92	0.50
2:L:159:ARG:O	2:L:161:VAL:N	2.44	0.50
1:K:50:GLU:CD	1:K:50:GLU:H	2.14	0.50
1:M:137:GLN:HG2	6:M:612:HOH:O	2.11	0.50
1:I:237:ASN:HA	2:J:95:LEU:HB2	1.93	0.50
2:P:179:THR:HG22	2:P:208:ALA:HB3	1.93	0.50
1:A:353:ARG:HD3	1:A:372:TYR:CE1	2.46	0.50
1:E:293:CYS:HB3	1:E:329:TRP:CE2	2.47	0.50
1:E:31:ASP:O	1:E:119:LYS:HG2	2.10	0.50
2:F:94:PHE:H	2:F:97:ASN:ND2	2.09	0.50
2:L:135:VAL:HG22	2:L:159:ARG:HE	1.77	0.50
2:N:206:PRO:HG2	2:N:241:ILE:HD12	1.92	0.50
1:A:324:THR:CG2	1:A:326:VAL:HG22	2.42	0.50
2:B:162:PRO:O	2:B:163:ALA:HB3	2.12	0.50
1:E:293:CYS:HB3	1:E:329:TRP:CZ2	2.46	0.50
2:F:122:THR:HG21	2:F:153:ASN:HB2	1.94	0.50
2:P:167:LEU:HB2	2:P:197:MET:HE1	1.93	0.50
2:P:167:LEU:HB2	2:P:197:MET:CE	2.41	0.50
2:D:184:MET:HG2	5:D:500:B13:H302	1.94	0.50
2:L:195:ASN:HD21	2:L:224:LEU:H	1.60	0.50
2:L:41:TYR:HB3	2:L:42:PRO:HD3	1.92	0.50
2:B:234:ALA:HB3	2:B:235:PRO:HD3	1.93	0.50
2:F:195:ASN:ND2	2:F:224:LEU:HB2	2.27	0.50
1:A:305:GLN:HA	1:A:356:MET:HE1	1.91	0.50
1:C:28:ALA:HB2	1:C:213:ILE:CD1	2.41	0.50
1:C:59:ILE:O	1:C:63:GLU:HG3	2.12	0.50
2:P:230:GLU:O	2:P:233:ASP:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:400:CYS:O	1:E:404:ILE:HG12	2.12	0.49
1:I:18:THR:CG2	1:I:21:VAL:HG13	2.42	0.49
1:K:353:ARG:HD3	1:K:372:TYR:CE1	2.47	0.49
1:C:361:ARG:HH22	1:C:373:ASP:CG	2.15	0.49
2:J:134:ASP:OD2	2:J:187:THR:HG21	2.11	0.49
2:J:195:ASN:ND2	2:J:224:LEU:HB2	2.27	0.49
1:K:361:ARG:HH22	1:K:373:ASP:CG	2.15	0.49
2:F:135:VAL:HG12	2:F:135:VAL:O	2.12	0.49
1:G:132:ASN:ND2	1:G:134:GLU:HG2	2.28	0.49
1:K:361:ARG:NH2	1:K:373:ASP:OD1	2.45	0.49
2:H:223:ALA:O	2:H:248:VAL:HG11	2.13	0.49
1:M:353:ARG:CA	1:M:356:MET:CE	2.80	0.49
2:P:31:GLU:HA	2:P:34:TYR:CD1	2.48	0.49
1:O:133:ARG:NH2	2:P:165:GLU:OE2	2.46	0.49
2:F:127:VAL:HG13	2:F:157:LEU:HD23	1.93	0.49
2:N:138:ILE:HG13	5:N:500:B13:C50	2.43	0.49
1:O:132:ASN:HD21	1:O:134:GLU:HG2	1.76	0.49
2:N:31:GLU:HA	2:N:34:TYR:CD1	2.48	0.49
1:A:317:TYR:HA	1:A:325:THR:HG21	1.93	0.49
2:F:116:SER:OG	2:F:117:GLY:N	2.44	0.49
2:B:252:ARG:HG2	2:B:256:HIS:CE1	2.48	0.49
2:D:185:THR:HG23	5:D:500:B13:H332	1.78	0.49
1:K:42:GLU:OE2	1:K:123:ARG:HD2	2.12	0.49
1:M:218:THR:HG23	1:M:270:GLY:N	2.27	0.49
1:O:113:HIS:HD2	1:O:118:ILE:O	1.96	0.49
2:B:17:ASN:HD22	2:B:17:ASN:N	1.95	0.49
2:H:195:ASN:HD22	2:H:224:LEU:HB2	1.78	0.49
1:I:148:GLU:O	1:I:152:GLN:HG2	2.11	0.49
1:I:317:TYR:CE1	1:I:324:THR:HG21	2.44	0.49
1:E:317:TYR:HA	1:E:325:THR:CG2	2.43	0.48
1:K:60:LYS:HE3	1:K:64:ARG:HE	1.78	0.48
1:M:265:PRO:HA	1:M:283:PRO:O	2.12	0.48
1:I:81:ILE:HD13	1:I:82:ILE:O	2.13	0.48
1:G:133:ARG:HD2	2:H:160:ASP:HB3	1.95	0.48
1:E:136:LEU:HD21	1:E:169:LYS:HE3	1.96	0.48
2:F:37:ASP:O	2:F:38:GLU:CB	2.54	0.48
5:H:500:B13:H363	5:H:500:B13:H401	1.79	0.48
1:M:237:ASN:HA	2:N:95:LEU:HB2	1.95	0.48
2:B:232:ALA:O	2:B:235:PRO:HD2	2.14	0.48
1:C:52:GLY:HA2	1:C:58:LEU:HD13	1.96	0.48
2:D:167:LEU:HB2	2:D:197:MET:HE3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:ILE:HB	1:A:182:PRO:HD3	1.95	0.48
6:C:686:HOH:O	2:D:138:ILE:HG12	2.13	0.48
1:G:132:ASN:HD21	1:G:135:PHE:H	1.61	0.48
2:J:137:ASP:HB2	5:J:500:B13:H522	1.78	0.48
1:K:317:TYR:HA	1:K:325:THR:CG2	2.44	0.48
1:M:347:LYS:HE3	6:M:616:HOH:O	2.13	0.48
1:E:354:ASP:CB	2:F:2:LEU:HD12	2.44	0.48
1:G:22:SER:HB3	1:G:277:LYS:HE3	1.96	0.48
1:G:47:PRO:HB3	1:G:61:GLU:HG2	1.95	0.48
1:K:387:ASP:HB2	6:K:614:HOH:O	2.13	0.48
2:L:144:THR:HG22	6:L:518:HOH:O	2.13	0.48
5:D:500:B13:H19	5:D:500:B13:H262	1.61	0.48
1:E:350:LYS:HG2	1:E:353:ARG:NH2	2.29	0.48
1:E:305:GLN:HA	1:E:356:MET:CE	2.44	0.48
1:E:289:LYS:NZ	1:G:336:ASP:OD1	2.47	0.48
1:I:265:PRO:HA	1:I:283:PRO:O	2.14	0.48
1:I:36:ALA:HA	6:I:568:HOH:O	2.14	0.48
1:E:31:ASP:OD1	1:K:27:LYS:NZ	2.32	0.47
2:F:130:VAL:HG12	2:F:134:ASP:HB3	1.96	0.47
1:G:324:THR:HG22	1:G:327:GLN:HG3	1.96	0.47
1:K:26:VAL:HG12	1:K:213:ILE:HD13	1.95	0.47
1:M:361:ARG:HH22	1:M:373:ASP:CG	2.16	0.47
1:O:324:THR:CG2	1:O:326:VAL:HG22	2.44	0.47
2:P:195:ASN:ND2	2:P:224:LEU:HB2	2.29	0.47
1:A:324:THR:HG23	1:A:326:VAL:HG22	1.96	0.47
1:A:331:GLU:HG2	1:C:292:THR:HG21	1.96	0.47
1:C:132:ASN:C	1:C:132:ASN:HD22	2.18	0.47
2:N:20:LEU:HD11	1:O:116:TYR:CE1	2.49	0.47
1:A:317:TYR:HA	1:A:325:THR:CG2	2.44	0.47
2:D:167:LEU:HB2	2:D:197:MET:CE	2.44	0.47
2:J:177:MET:HG2	2:J:178:LEU:N	2.29	0.47
2:N:85:ILE:HD11	2:N:149:ALA:O	2.15	0.47
1:E:361:ARG:NH2	1:E:373:ASP:OD1	2.47	0.47
1:I:301:ASN:HD22	1:I:304:MET:CE	2.27	0.47
2:J:127:VAL:HG23	2:J:175:PRO:HG3	1.96	0.47
2:L:189:TYR:HD2	2:L:192:LYS:HG3	1.79	0.47
1:K:88:VAL:HG22	1:K:91:MET:SD	2.54	0.47
2:L:52:GLU:CD	2:L:52:GLU:H	2.17	0.47
1:A:224:ASN:ND2	1:A:269:CYS:HB2	2.30	0.47
2:H:127:VAL:HG22	2:H:155:VAL:CG1	2.45	0.47
1:I:42:GLU:OE2	1:I:123:ARG:HD2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:317:TYR:CE1	1:K:324:THR:CG2	2.97	0.47
2:L:189:TYR:O	2:L:192:LYS:HB2	2.15	0.47
2:L:37:ASP:O	2:L:39:LEU:N	2.43	0.47
1:E:83:LEU:HD13	1:E:109:MET:CE	2.45	0.47
2:H:138:ILE:O	2:H:142:ILE:HG13	2.14	0.47
2:L:227:TYR:CZ	2:L:229:GLU:HB3	2.49	0.47
1:M:455:LYS:HB2	1:M:458:ASN:ND2	2.29	0.47
1:O:50:GLU:CD	1:O:50:GLU:H	2.18	0.47
1:A:28:ALA:HB2	1:A:213:ILE:HD13	1.97	0.47
1:C:218:THR:HG23	1:C:270:GLY:CA	2.45	0.47
2:F:95:LEU:HB3	2:F:96:PRO:HD3	1.97	0.47
2:J:17:ASN:H	2:J:17:ASN:ND2	2.00	0.47
1:I:228:PHE:CE2	5:J:500:B13:H543	2.49	0.47
1:K:411:LYS:HE3	2:L:4:PHE:O	2.14	0.47
1:M:128:ASP:HA	1:M:146:PHE:CE1	2.50	0.47
1:O:133:ARG:HD2	2:P:160:ASP:HB3	1.97	0.47
1:A:65:ILE:HG23	1:A:326:VAL:HG11	1.97	0.47
1:E:203:ILE:O	1:E:206:ILE:HB	2.15	0.47
1:G:175:ALA:HB1	1:G:180:ASP:HB3	1.96	0.47
1:M:125:THR:HG21	1:M:267:LYS:HE2	1.96	0.47
1:O:356:MET:HE3	1:O:356:MET:HB2	1.60	0.47
1:G:224:ASN:HD21	1:G:269:CYS:HB2	1.79	0.47
2:H:185:THR:H	5:H:500:B13:H332	1.62	0.47
2:N:17:ASN:H	2:N:17:ASN:ND2	2.11	0.47
2:B:116:SER:C	2:B:118:ALA:H	2.18	0.47
1:K:313:GLU:O	1:K:314:SER:HB2	2.15	0.47
1:C:169:LYS:HD2	5:D:500:B13:H473	1.96	0.46
2:D:68:ASP:HB3	2:D:71:ASP:HB2	1.96	0.46
1:C:123:ARG:NH2	1:C:265:PRO:O	2.47	0.46
2:H:135:VAL:O	2:H:135:VAL:CG1	2.62	0.46
1:M:28:ALA:HB2	1:M:213:ILE:HD13	1.97	0.46
2:F:216:GLN:NE2	2:F:258:HIS:H	2.13	0.46
2:H:127:VAL:HG23	2:H:175:PRO:HG3	1.96	0.46
2:H:37:ASP:HB3	2:H:40:ILE:HB	1.98	0.46
1:I:324:THR:CG2	1:I:326:VAL:HG22	2.45	0.46
2:J:137:ASP:OD2	2:J:159:ARG:HD2	2.16	0.46
1:K:353:ARG:CA	1:K:356:MET:HE1	2.45	0.46
2:N:222:PHE:O	2:N:252:ARG:NH2	2.47	0.46
1:A:88:VAL:HG22	1:A:91:MET:SD	2.56	0.46
2:B:122:THR:HG21	2:B:153:ASN:HB2	1.98	0.46
2:B:219:VAL:HG21	2:B:227:TYR:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:157:LEU:HD12	2:F:161:VAL:HG11	1.97	0.46
1:G:176:VAL:HG13	1:G:177:LEU:HD13	1.97	0.46
1:G:80:ALA:HA	1:G:119:LYS:O	2.16	0.46
1:I:353:ARG:HD3	1:I:372:TYR:CZ	2.50	0.46
2:P:94:PHE:H	2:P:97:ASN:ND2	2.07	0.46
1:C:132:ASN:HD21	1:C:135:PHE:H	1.60	0.46
1:G:181:ILE:HB	1:G:182:PRO:HD3	1.98	0.46
1:K:293:CYS:HB3	1:K:329:TRP:CE2	2.49	0.46
1:E:132:ASN:HD22	1:E:132:ASN:C	2.19	0.46
1:E:147:LEU:HD22	1:E:206:ILE:HD11	1.97	0.46
1:K:317:TYR:HA	1:K:325:THR:HG21	1.98	0.46
1:O:79:PRO:HD2	6:O:595:HOH:O	2.16	0.46
2:D:159:ARG:O	2:D:161:VAL:HG23	2.15	0.46
2:J:116:SER:OG	2:J:117:GLY:N	2.49	0.46
2:L:192:LYS:HG2	2:L:222:PHE:HE2	1.80	0.46
2:L:206:PRO:HG2	2:L:241:ILE:HD12	1.96	0.46
2:H:135:VAL:O	2:H:135:VAL:HG13	2.15	0.46
5:N:500:B13:H262	5:N:500:B13:H19	1.69	0.46
2:B:185:THR:HG23	5:B:500:B13:H332	1.80	0.46
2:D:162:PRO:O	2:D:164:GLU:N	2.49	0.46
2:F:185:THR:HA	2:F:188:MET:HG3	1.98	0.46
1:M:133:ARG:HH11	1:M:133:ARG:HG2	1.80	0.46
1:O:237:ASN:HA	2:P:95:LEU:HB2	1.97	0.46
1:A:290:THR:HG22	1:A:290:THR:O	2.16	0.46
2:B:16:TYR:CD1	1:C:116:TYR:HB3	2.50	0.46
1:C:353:ARG:HD3	1:C:372:TYR:CE1	2.51	0.46
2:F:184:MET:HB3	2:F:186:THR:HG22	1.98	0.46
2:F:184:MET:HG2	5:F:500:B13:C30	2.38	0.46
5:H:500:B13:H411	5:H:500:B13:H362	1.75	0.46
1:K:301:ASN:HD22	1:K:304:MET:HE2	1.81	0.46
2:P:17:ASN:N	2:P:17:ASN:HD22	2.10	0.46
6:A:673:HOH:O	1:C:289:LYS:HE3	2.16	0.45
1:K:426:LYS:O	1:K:430:GLU:HG2	2.16	0.45
2:B:81:MET:O	2:B:85:ILE:HD12	2.16	0.45
1:I:142:LYS:HB2	6:I:540:HOH:O	2.16	0.45
2:J:206:PRO:HG2	2:J:241:ILE:HD12	1.98	0.45
2:L:118:ALA:O	2:L:119:THR:HB	2.16	0.45
1:O:325:THR:CG2	1:O:326:VAL:N	2.79	0.45
2:D:59:LEU:O	2:D:63:ILE:HG12	2.17	0.45
2:H:252:ARG:O	2:H:256:HIS:HB2	2.17	0.45
2:N:219:VAL:HG21	2:N:227:TYR:CB	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:HIS:HD2	6:B:534:HOH:O	1.99	0.45
1:G:186:TYR:O	1:G:190:CYS:HB2	2.16	0.45
1:I:143:TYR:O	1:I:146:PHE:HB3	2.16	0.45
1:I:290:THR:O	1:I:290:THR:HG22	2.16	0.45
2:J:135:VAL:O	2:J:135:VAL:CG1	2.64	0.45
2:P:137:ASP:HB2	5:P:500:B13:H522	1.81	0.45
2:B:161:VAL:HA	2:B:162:PRO:HD3	1.64	0.45
1:C:444:LEU:O	1:C:448:LYS:HB2	2.17	0.45
2:H:70:ILE:HD11	2:H:120:PRO:HA	1.98	0.45
1:A:116:TYR:HB3	2:D:16:TYR:CD1	2.52	0.45
1:G:292:THR:HA	1:G:295:HIS:O	2.17	0.45
5:J:500:B13:H19	5:J:500:B13:H262	1.66	0.45
1:K:356:MET:HE2	1:K:356:MET:HB2	1.56	0.45
2:L:161:VAL:HA	2:L:162:PRO:HD3	1.78	0.45
2:N:163:ALA:O	2:N:166:VAL:HB	2.16	0.45
1:G:361:ARG:NH2	1:G:373:ASP:OD1	2.49	0.45
1:I:411:LYS:HD3	2:J:6:GLU:HG2	1.98	0.45
2:J:59:LEU:O	2:J:63:ILE:HG12	2.16	0.45
1:K:137:GLN:NE2	1:K:142:LYS:HE2	2.31	0.45
2:F:136:HIS:CB	2:F:183:LEU:HD13	2.46	0.45
2:H:47:ILE:HD12	2:H:55:VAL:HG22	1.98	0.45
2:N:192:LYS:HG2	2:N:222:PHE:HE2	1.81	0.45
1:A:341:ASN:O	1:A:345:GLU:HG2	2.17	0.45
1:C:224:ASN:O	1:C:228:PHE:CD2	2.70	0.45
2:D:252:ARG:O	2:D:256:HIS:HB2	2.17	0.45
1:E:55:LYS:HG3	1:E:97:TRP:CD2	2.52	0.45
1:G:105:GLN:NE2	1:G:124:HIS:HE1	2.15	0.45
1:G:42:GLU:OE2	1:G:123:ARG:HD2	2.17	0.45
1:G:224:ASN:ND2	1:G:269:CYS:HB2	2.32	0.45
5:L:500:B13:H252	5:L:500:B13:C61	2.47	0.45
1:M:324:THR:CG2	1:M:326:VAL:HG22	2.47	0.45
1:O:318:HIS:O	1:O:325:THR:HB	2.17	0.45
1:O:87:HIS:NE2	1:O:124:HIS:CD2	2.85	0.45
1:A:356:MET:HB2	1:A:356:MET:HE3	1.80	0.44
1:C:237:ASN:HA	2:D:95:LEU:HB2	1.99	0.44
2:F:222:PHE:O	2:F:252:ARG:NH2	2.50	0.44
1:I:126:ILE:N	1:I:126:ILE:HD12	2.32	0.44
2:D:248:VAL:HA	2:D:251:LEU:HD12	1.98	0.44
1:I:325:THR:CG2	1:I:326:VAL:N	2.81	0.44
2:L:130:VAL:CG1	2:L:134:ASP:HB3	2.46	0.44
2:N:130:VAL:CG1	2:N:134:ASP:HB3	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:289:LYS:NZ	1:I:301:ASN:HD21	2.15	0.44
2:J:63:ILE:HG23	2:J:72:LEU:HD12	1.99	0.44
1:M:224:ASN:O	1:M:228:PHE:HD2	2.01	0.44
2:D:227:TYR:CE2	2:D:229:GLU:HB3	2.52	0.44
1:G:325:THR:O	1:G:329:TRP:HD1	2.01	0.44
2:H:95:LEU:HD22	2:H:99:MET:HG2	2.00	0.44
5:J:500:B13:H362	5:J:500:B13:H411	1.81	0.44
1:O:81:ILE:HD13	1:O:82:ILE:N	2.33	0.44
1:C:87:HIS:NE2	1:C:124:HIS:HD2	2.14	0.44
1:E:302:LEU:HB2	1:E:360:ASP:HB2	1.98	0.44
2:L:130:VAL:HG23	2:L:140:LYS:HD3	1.99	0.44
2:L:234:ALA:O	2:L:237:ILE:HG22	2.18	0.44
1:M:133:ARG:CG	1:M:133:ARG:NH1	2.80	0.44
2:P:204:LYS:HZ1	2:P:248:VAL:H	1.66	0.44
1:A:317:TYR:HE1	1:A:324:THR:HG21	1.82	0.44
2:B:59:LEU:HD23	2:B:72:LEU:HD13	2.00	0.44
1:K:228:PHE:HE1	1:K:295:HIS:HB2	1.82	0.44
2:N:162:PRO:O	2:N:163:ALA:HB3	2.18	0.44
2:P:82:GLY:HA2	2:P:85:ILE:HD12	2.00	0.44
1:A:132:ASN:HD22	1:A:134:GLU:H	1.66	0.44
1:C:218:THR:HG23	1:C:270:GLY:N	2.33	0.44
1:C:441:ASP:O	1:C:445:THR:HG23	2.18	0.44
1:M:132:ASN:ND2	1:M:135:PHE:H	2.14	0.44
2:N:13:LEU:C	2:N:13:LEU:HD12	2.38	0.44
2:N:218:PHE:O	2:N:221:GLN:HG2	2.18	0.44
5:P:500:B13:H363	5:P:500:B13:H401	1.83	0.44
1:C:356:MET:HE3	1:C:356:MET:HB2	1.82	0.44
1:C:237:ASN:O	2:D:96:PRO:HD3	2.18	0.44
2:F:188:MET:HB3	2:F:218:PHE:CZ	2.52	0.44
1:G:18:THR:CG2	1:G:21:VAL:HG13	2.47	0.44
1:M:64:ARG:CZ	2:P:258:HIS:OXT	2.66	0.44
1:G:138:LEU:HD12	1:G:458:ASN:HB3	1.98	0.44
2:H:216:GLN:NE2	2:H:258:HIS:H	2.15	0.44
2:J:130:VAL:HG23	2:J:140:LYS:HD3	2.00	0.44
1:K:105:GLN:O	1:K:109:MET:HG3	2.18	0.44
2:B:51:GLU:O	2:B:55:VAL:HG23	2.18	0.43
1:G:324:THR:CG2	1:G:326:VAL:HG22	2.48	0.43
1:G:325:THR:HG23	1:G:326:VAL:N	2.32	0.43
2:J:227:TYR:H	2:J:256:HIS:HE1	1.66	0.43
2:L:219:VAL:HG21	2:L:227:TYR:CB	2.38	0.43
1:M:356:MET:HE2	1:M:356:MET:HB2	1.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:138:ILE:O	2:N:142:ILE:HG13	2.18	0.43
1:C:293:CYS:HB3	1:C:329:TRP:CE2	2.53	0.43
1:C:355:LEU:HD13	2:D:2:LEU:CD1	2.48	0.43
1:M:301:ASN:HD22	1:M:304:MET:HE2	1.83	0.43
2:B:131:ALA:HB1	2:B:190:ALA:HB3	1.99	0.43
1:C:373:ASP:N	1:C:373:ASP:OD1	2.50	0.43
1:C:47:PRO:HB3	1:C:61:GLU:HG2	2.00	0.43
2:D:159:ARG:O	2:D:161:VAL:N	2.51	0.43
1:I:72:ARG:NH2	6:K:520:HOH:O	2.51	0.43
2:L:94:PHE:H	2:L:97:ASN:HD22	1.66	0.43
2:N:95:LEU:HB3	2:N:96:PRO:HD3	1.99	0.43
2:B:17:ASN:ND2	2:B:17:ASN:N	2.57	0.43
1:E:145:VAL:HA	1:E:148:GLU:OE1	2.18	0.43
2:H:68:ASP:HB3	2:H:71:ASP:HB2	2.00	0.43
2:J:130:VAL:HG12	2:J:134:ASP:HB3	1.99	0.43
1:K:113:HIS:HD2	1:K:118:ILE:O	2.02	0.43
5:N:500:B13:H252	5:N:500:B13:C61	2.48	0.43
1:A:43:ILE:HG22	1:A:81:ILE:HD11	2.01	0.43
1:A:237:ASN:O	2:B:96:PRO:HD3	2.18	0.43
2:B:95:LEU:HD22	2:B:99:MET:HG2	2.01	0.43
2:D:127:VAL:HG22	2:D:155:VAL:HG13	2.00	0.43
2:L:163:ALA:HB1	2:L:197:MET:HE1	2.01	0.43
1:O:27:LYS:HE3	1:O:33:GLU:OE2	2.19	0.43
2:B:37:ASP:HB3	2:B:40:ILE:HB	2.01	0.43
2:D:95:LEU:HB3	2:D:96:PRO:HD3	2.01	0.43
1:G:132:ASN:ND2	1:G:135:PHE:H	2.15	0.43
2:N:87:LEU:HD22	2:N:92:VAL:HG21	2.01	0.43
2:F:87:LEU:HB3	2:F:92:VAL:HG22	1.99	0.43
2:H:216:GLN:HE21	2:H:258:HIS:HB2	1.83	0.43
2:J:127:VAL:HG22	2:J:155:VAL:CG1	2.49	0.43
1:K:218:THR:HG23	1:K:270:GLY:N	2.33	0.43
1:O:106:LYS:NZ	1:O:157:GLY:O	2.51	0.43
2:J:82:GLY:HA2	2:J:85:ILE:HD12	2.01	0.43
2:B:229:GLU:O	5:B:500:B13:H2R	2.19	0.43
1:E:361:ARG:HH22	1:E:373:ASP:CG	2.22	0.43
1:K:45:TYR:HB3	1:K:326:VAL:CG1	2.49	0.43
1:A:361:ARG:NH2	1:A:373:ASP:OD1	2.51	0.43
1:E:132:ASN:HD21	1:E:135:PHE:H	1.65	0.43
5:H:500:B13:H19	5:H:500:B13:H262	1.85	0.43
5:J:500:B13:H472	5:J:500:B13:H481	1.96	0.43
2:L:206:PRO:HG2	2:L:241:ILE:CD1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:82:GLY:HA2	2:N:85:ILE:HD12	2.00	0.43
1:O:105:GLN:NE2	1:O:124:HIS:HE1	2.17	0.43
1:O:26:VAL:CG1	1:O:213:ILE:HD13	2.49	0.43
1:A:287:GLU:OE1	1:A:313:GLU:OE2	2.36	0.42
5:D:500:B13:H411	5:D:500:B13:H362	1.73	0.42
1:G:402:ASN:O	1:G:406:GLU:HG3	2.18	0.42
2:J:17:ASN:N	2:J:17:ASN:ND2	2.62	0.42
1:O:364:ASP:CG	1:O:365:PRO:HD2	2.38	0.42
2:B:224:LEU:HA	2:B:248:VAL:HG21	2.00	0.42
1:E:317:TYR:HA	1:E:325:THR:HG22	2.01	0.42
2:H:242:ILE:HG22	2:H:242:ILE:O	2.19	0.42
1:I:285:THR:OG1	1:I:309:CYS:HB2	2.19	0.42
2:J:161:VAL:HA	2:J:162:PRO:HD3	1.95	0.42
2:J:233:ASP:O	2:J:237:ILE:HG22	2.19	0.42
1:A:370:LEU:HD12	1:A:370:LEU:HA	1.93	0.42
2:D:95:LEU:HD11	2:D:142:ILE:HG12	2.01	0.42
1:E:417:PHE:HZ	2:F:97:ASN:HD21	1.67	0.42
1:G:305:GLN:HA	1:G:356:MET:HE1	2.02	0.42
1:G:43:ILE:HG22	1:G:81:ILE:HD11	2.01	0.42
2:H:224:LEU:HA	2:H:248:VAL:HG21	2.01	0.42
1:I:81:ILE:HD13	1:I:82:ILE:N	2.34	0.42
2:B:63:ILE:H	2:B:63:ILE:HG12	1.73	0.42
1:C:64:ARG:HD2	6:C:533:HOH:O	2.19	0.42
1:K:324:THR:CG2	1:K:326:VAL:HG22	2.49	0.42
1:O:47:PRO:HB3	1:O:61:GLU:HG2	2.01	0.42
1:A:441:ASP:O	1:A:445:THR:HG23	2.19	0.42
2:B:130:VAL:HG12	2:B:134:ASP:HB3	2.01	0.42
1:C:224:ASN:HB3	1:C:228:PHE:HE2	1.85	0.42
2:D:161:VAL:HA	2:D:162:PRO:HD3	1.70	0.42
1:G:119:LYS:HE3	6:G:561:HOH:O	2.18	0.42
2:H:256:HIS:HB3	2:H:257:LYS:H	1.59	0.42
2:J:188:MET:O	2:J:191:PHE:HB2	2.18	0.42
2:J:67:LYS:HB3	2:J:68:ASP:H	1.65	0.42
1:K:436:MET:O	1:K:440:MET:HG2	2.19	0.42
5:N:500:B13:H401	5:N:500:B13:H8	1.84	0.42
1:O:426:LYS:O	1:O:430:GLU:HG3	2.19	0.42
2:D:256:HIS:HB3	2:D:257:LYS:H	1.57	0.42
2:F:161:VAL:HA	2:F:162:PRO:HD3	1.73	0.42
1:G:76:VAL:O	1:G:76:VAL:HG12	2.19	0.42
1:G:88:VAL:HG22	1:G:91:MET:SD	2.59	0.42
1:I:18:THR:HG23	1:I:21:VAL:HG13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:218:THR:HG23	1:K:270:GLY:CA	2.50	0.42
1:M:128:ASP:HA	1:M:146:PHE:HE1	1.84	0.42
2:B:37:ASP:O	2:B:39:LEU:N	2.49	0.42
2:B:59:LEU:O	2:B:63:ILE:HG12	2.19	0.42
2:F:136:HIS:HB2	2:F:183:LEU:HD13	2.02	0.42
1:K:106:LYS:NZ	1:K:157:GLY:O	2.53	0.42
2:L:192:LYS:HG2	2:L:222:PHE:CE2	2.54	0.42
5:L:500:B13:H351	5:L:500:B13:H361	2.01	0.42
1:M:353:ARG:HD3	1:M:372:TYR:CZ	2.55	0.42
2:N:132:GLU:HB3	2:N:161:VAL:O	2.20	0.42
1:O:22:SER:HB3	1:O:277:LYS:HE3	2.02	0.42
1:A:132:ASN:C	1:A:132:ASN:HD22	2.23	0.42
1:A:22:SER:HB3	1:A:277:LYS:HE3	2.02	0.42
1:I:132:ASN:HD21	1:I:135:PHE:H	1.66	0.42
1:K:101:VAL:O	1:K:105:GLN:HG3	2.20	0.42
1:M:249:ILE:O	1:M:252:PRO:HD2	2.19	0.42
2:D:67:LYS:HB3	2:D:68:ASP:H	1.56	0.42
5:F:500:B13:H362	5:F:500:B13:H411	1.67	0.42
2:L:17:ASN:HD22	2:L:17:ASN:N	2.15	0.42
1:M:289:LYS:NZ	1:M:301:ASN:HD21	2.18	0.42
2:N:234:ALA:O	2:N:237:ILE:HG22	2.20	0.42
1:O:126:ILE:N	1:O:126:ILE:HD12	2.34	0.42
1:O:285:THR:OG1	1:O:309:CYS:HB2	2.20	0.42
2:D:110:GLU:HA	2:D:113:LYS:HB2	2.02	0.42
2:D:134:ASP:OD2	2:D:187:THR:HG21	2.20	0.42
1:E:187:SER:HA	1:E:191:LEU:HD12	2.01	0.42
1:E:203:ILE:HA	1:E:206:ILE:HD12	2.02	0.42
2:F:41:TYR:HB3	2:F:42:PRO:HD3	2.02	0.42
1:G:132:ASN:OD1	1:G:137:GLN:NE2	2.51	0.42
1:G:218:THR:HG23	1:G:270:GLY:N	2.35	0.42
2:L:135:VAL:HG13	2:L:135:VAL:O	2.19	0.42
2:N:130:VAL:HG12	2:N:134:ASP:HB3	2.02	0.42
2:N:43:ILE:HG21	2:N:76:ALA:HB1	2.01	0.42
1:E:132:ASN:OD1	1:E:137:GLN:NE2	2.53	0.41
2:D:130:VAL:HG23	2:D:140:LYS:HD3	2.02	0.41
2:N:161:VAL:HA	2:N:162:PRO:HD3	1.78	0.41
1:O:452:LYS:HA	1:O:452:LYS:HD3	1.95	0.41
1:A:87:HIS:NE2	1:A:124:HIS:CD2	2.89	0.41
2:F:216:GLN:HE21	2:F:258:HIS:HD2	1.68	0.41
2:J:135:VAL:HB	5:J:500:B13:H421	2.02	0.41
2:J:159:ARG:O	2:J:161:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:234:ALA:HB3	2:J:235:PRO:HD3	2.01	0.41
5:J:500:B13:N40	5:J:500:B13:H363	2.35	0.41
5:B:500:B13:H411	5:B:500:B13:H362	1.80	0.41
2:D:195:ASN:HD22	2:D:224:LEU:HB2	1.86	0.41
2:D:70:ILE:HD11	2:D:120:PRO:HG3	2.01	0.41
1:E:266:GLY:HA3	1:E:284:MET:SD	2.60	0.41
1:G:356:MET:HB2	1:G:356:MET:HE3	1.83	0.41
1:K:106:LYS:HD3	1:K:106:LYS:HA	1.76	0.41
2:L:226:VAL:HG11	2:L:237:ILE:HD11	2.02	0.41
2:L:74:ASP:HA	2:L:78:MET:HB2	2.02	0.41
2:N:178:LEU:O	2:N:207:PHE:HA	2.21	0.41
2:P:147:LEU:HB3	2:P:154:VAL:HG21	2.01	0.41
2:B:216:GLN:NE2	2:B:258:HIS:H	2.15	0.41
2:B:95:LEU:HB3	2:B:96:PRO:HD3	2.03	0.41
1:C:143:TYR:O	1:C:146:PHE:HB3	2.21	0.41
1:C:354:ASP:OD2	2:D:1:MET:HA	2.20	0.41
1:E:287:GLU:OE1	1:E:313:GLU:OE2	2.38	0.41
1:I:317:TYR:HE1	1:I:324:THR:CG2	2.30	0.41
2:L:185:THR:HG23	5:L:500:B13:H332	1.86	0.41
1:M:452:LYS:HD3	1:M:452:LYS:HA	1.78	0.41
5:P:500:B13:H411	5:P:500:B13:H362	1.74	0.41
2:B:195:ASN:HD22	2:B:224:LEU:HB2	1.84	0.41
1:E:146:PHE:CZ	1:E:150:PHE:HE2	2.39	0.41
2:F:74:ASP:HA	2:F:78:MET:HB2	2.03	0.41
1:I:22:SER:HB3	1:I:277:LYS:HE3	2.02	0.41
2:L:256:HIS:HB3	2:L:257:LYS:H	1.57	0.41
2:N:159:ARG:O	2:N:161:VAL:N	2.52	0.41
1:C:109:MET:HE1	1:C:122:LEU:HD13	2.01	0.41
2:D:60:GLN:O	2:D:64:GLU:HG3	2.21	0.41
2:F:214:VAL:HG12	2:F:227:TYR:CE1	2.55	0.41
5:H:500:B13:H472	5:H:500:B13:H481	1.88	0.41
2:J:252:ARG:O	2:J:256:HIS:HB2	2.21	0.41
2:N:136:HIS:CB	2:N:183:LEU:HD13	2.51	0.41
1:O:126:ILE:N	1:O:126:ILE:CD1	2.84	0.41
1:A:131:GLU:OE2	2:B:159:ARG:NH2	2.52	0.41
1:A:218:THR:HG23	1:A:270:GLY:CA	2.50	0.41
2:B:87:LEU:HB3	2:B:92:VAL:HG22	2.03	0.41
1:C:290:THR:HG22	1:C:290:THR:O	2.21	0.41
1:I:301:ASN:HD22	1:I:304:MET:HE2	1.85	0.41
5:L:500:B13:H262	5:L:500:B13:H19	1.83	0.41
5:L:500:B13:H18	5:L:500:B13:H621	1.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:135:VAL:HB	5:P:500:B13:C43	2.50	0.41
1:A:123:ARG:NH2	1:A:265:PRO:O	2.53	0.41
1:I:47:PRO:HB3	1:I:61:GLU:HG2	2.02	0.41
2:J:159:ARG:HB3	2:J:160:ASP:H	1.63	0.41
2:L:135:VAL:O	2:L:135:VAL:CG1	2.68	0.41
1:M:87:HIS:NE2	1:M:124:HIS:CD2	2.87	0.41
1:O:132:ASN:ND2	1:O:134:GLU:HG2	2.36	0.41
2:P:143:VAL:HG21	5:P:500:B13:C9B	2.50	0.41
2:P:169:ALA:O	2:P:173:GLU:HG2	2.21	0.41
2:P:256:HIS:HB3	2:P:257:LYS:H	1.76	0.41
2:P:95:LEU:HB3	2:P:96:PRO:HD3	2.02	0.41
1:E:116:TYR:HB3	2:H:16:TYR:CD1	2.55	0.41
2:H:193:GLU:O	2:H:197:MET:HB3	2.20	0.41
1:I:317:TYR:CE1	1:I:324:THR:CG2	3.04	0.41
1:K:247:ARG:CZ	1:K:271:TYR:HB2	2.50	0.41
1:O:101:VAL:O	1:O:105:GLN:HG3	2.21	0.41
2:P:37:ASP:O	2:P:37:ASP:OD2	2.39	0.41
1:A:83:LEU:HB2	1:A:109:MET:HE1	2.03	0.41
2:B:159:ARG:O	2:B:161:VAL:HG23	2.21	0.41
2:B:247:ASP:HB3	2:B:250:GLU:HB2	2.01	0.41
1:C:305:GLN:HA	1:C:356:MET:HE1	2.03	0.41
1:C:50:GLU:H	1:C:50:GLU:CD	2.24	0.41
2:D:119:THR:HA	2:D:120:PRO:HD3	1.90	0.41
2:F:182:ALA:O	2:F:211:GLY:HA3	2.21	0.41
1:G:317:TYR:HA	1:G:325:THR:CG2	2.50	0.41
1:O:132:ASN:C	1:O:132:ASN:ND2	2.75	0.41
1:E:94:ASN:HB2	1:E:97:TRP:CD1	2.56	0.40
2:J:132:GLU:HB3	2:J:161:VAL:O	2.21	0.40
1:M:325:THR:CG2	1:M:326:VAL:N	2.83	0.40
2:N:63:ILE:H	2:N:63:ILE:HG12	1.74	0.40
1:O:88:VAL:HG22	1:O:91:MET:SD	2.62	0.40
2:B:218:PHE:O	2:B:221:GLN:HG2	2.21	0.40
1:C:224:ASN:HB3	1:C:228:PHE:CE2	2.56	0.40
1:E:76:VAL:O	1:E:76:VAL:HG12	2.22	0.40
2:F:206:PRO:HG2	2:F:241:ILE:CD1	2.51	0.40
1:K:325:THR:CG2	1:K:326:VAL:N	2.85	0.40
1:K:131:GLU:OE2	2:L:159:ARG:NH2	2.54	0.40
2:L:231:ALA:HB2	5:L:500:B13:O6R	2.21	0.40
5:N:500:B13:H362	5:N:500:B13:H411	1.79	0.40
1:G:132:ASN:HD22	1:G:134:GLU:H	1.67	0.40
1:I:46:ALA:HA	1:I:47:PRO:HD3	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:285:THR:OG1	1:M:309:CYS:HB2	2.22	0.40
1:O:290:THR:O	1:O:290:THR:HG22	2.22	0.40
2:D:143:VAL:HG13	2:D:234:ALA:CB	2.52	0.40
1:E:94:ASN:O	1:E:95:PRO:C	2.59	0.40
1:G:265:PRO:HA	1:G:283:PRO:O	2.21	0.40
2:H:226:VAL:HG11	2:H:237:ILE:HG12	2.04	0.40
1:I:228:PHE:CE2	5:J:500:B13:C54	3.05	0.40
2:J:134:ASP:HB2	2:J:187:THR:HG21	2.03	0.40
2:J:229:GLU:HG3	2:J:230:GLU:H	1.86	0.40
1:O:179:ASN:HA	6:O:526:HOH:O	2.20	0.40
1:C:252:PRO:HG3	1:C:393:ALA:HA	2.04	0.40
1:C:285:THR:OG1	1:C:309:CYS:HB2	2.20	0.40
2:D:138:ILE:HG13	5:D:500:B13:C50	2.52	0.40
1:E:123:ARG:NH2	1:E:265:PRO:O	2.54	0.40
1:E:348:ASN:O	1:E:351:VAL:HG12	2.20	0.40
1:I:362:TYR:HB2	2:J:9:LEU:HD21	2.03	0.40
1:K:353:ARG:CA	1:K:356:MET:CE	2.83	0.40
1:M:132:ASN:C	1:M:132:ASN:HD22	2.24	0.40
2:N:87:LEU:HD22	2:N:92:VAL:CG2	2.52	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	457/461 (99%)	442 (97%)	15 (3%)	0	100	100
1	C	457/461 (99%)	440 (96%)	17 (4%)	0	100	100
1	E	457/461 (99%)	433 (95%)	21 (5%)	3 (1%)	22	39
1	G	457/461 (99%)	434 (95%)	22 (5%)	1 (0%)	47	68
1	I	457/461 (99%)	439 (96%)	17 (4%)	1 (0%)	47	68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	457/461 (99%)	439 (96%)	18 (4%)	0	100	100
1	M	457/461 (99%)	439 (96%)	18 (4%)	0	100	100
1	O	457/461 (99%)	439 (96%)	18 (4%)	0	100	100
2	B	256/258 (99%)	239 (93%)	13 (5%)	4 (2%)	9	17
2	D	256/258 (99%)	224 (88%)	28 (11%)	4 (2%)	9	17
2	F	256/258 (99%)	227 (89%)	26 (10%)	3 (1%)	13	24
2	H	256/258 (99%)	235 (92%)	18 (7%)	3 (1%)	13	24
2	J	256/258 (99%)	237 (93%)	14 (6%)	5 (2%)	7	12
2	L	256/258 (99%)	235 (92%)	15 (6%)	6 (2%)	6	10
2	N	256/258 (99%)	229 (90%)	23 (9%)	4 (2%)	9	17
2	P	256/258 (99%)	240 (94%)	13 (5%)	3 (1%)	13	24
All	All	5704/5752 (99%)	5371 (94%)	296 (5%)	37 (1%)	25	43

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	256	HIS
2	F	256	HIS
2	H	256	HIS
2	L	37	ASP
2	L	256	HIS
2	B	256	HIS
2	D	163	ALA
1	E	53	ALA
1	E	305	GLN
2	F	38	GLU
1	G	53	ALA
2	J	256	HIS
2	J	257	LYS
2	D	119	THR
2	D	160	ASP
2	H	119	THR
2	J	119	THR
2	L	119	THR
2	F	119	THR
2	J	37	ASP
2	L	160	ASP
2	L	163	ALA

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Mol	Chain	Res	Type
2	N	69	PRO
2	P	38	GLU
2	P	119	THR
2	P	256	HIS
2	B	119	THR
2	H	201	ASN
2	J	69	PRO
2	L	68	ASP
2	N	68	ASP
2	N	186	THR
2	B	159	ARG
2	B	192	LYS
1	I	313	GLU
2	N	160	ASP
1	E	81	ILE

### 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	373/374 (100%)	344 (92%)	29 (8%)	12	24
1	C	373/374 (100%)	344 (92%)	29 (8%)	12	24
1	E	373/374 (100%)	339 (91%)	34 (9%)	9	18
1	G	373/374 (100%)	346 (93%)	27 (7%)	14	28
1	I	373/374 (100%)	345 (92%)	28 (8%)	13	26
1	K	373/374 (100%)	348 (93%)	25 (7%)	16	31
1	M	373/374 (100%)	344 (92%)	29 (8%)	12	24
1	O	373/374 (100%)	343 (92%)	30 (8%)	12	23
2	B	206/206 (100%)	183 (89%)	23 (11%)	6	11
2	D	206/206 (100%)	192 (93%)	14 (7%)	16	30
2	F	206/206 (100%)	189 (92%)	17 (8%)	11	22
2	H	206/206 (100%)	190 (92%)	16 (8%)	12	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	J	206/206 (100%)	190 (92%)	16 (8%)	12	24
2	L	206/206 (100%)	190 (92%)	16 (8%)	12	24
2	N	206/206 (100%)	189 (92%)	17 (8%)	11	22
2	P	206/206 (100%)	184 (89%)	22 (11%)	6	13
All	All	4632/4640 (100%)	4260 (92%)	372 (8%)	12	23

All (372) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ARG
1	A	21	VAL
1	A	72	ARG
1	A	81	ILE
1	A	115	GLU
1	A	124	HIS
1	A	132	ASN
1	A	133	ARG
1	A	134	GLU
1	A	135	PHE
1	A	142	LYS
1	A	151	GLU
1	A	170	GLU
1	A	177	LEU
1	A	184	LEU
1	A	185	LEU
1	A	198	LEU
1	A	205	LYS
1	A	233	LEU
1	A	253	ARG
1	A	299	MET
1	A	324	THR
1	A	347	LYS
1	A	353	ARG
1	A	355	LEU
1	A	370	LEU
1	A	438	LYS
1	A	444	LEU
1	A	445	THR
2	B	9	LEU
2	B	17	ASN
2	B	36	LYS

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Mol	Chain	Res	Type
2	B	39	LEU
2	B	47	ILE
2	B	63	ILE
2	B	86	ARG
2	B	92	VAL
2	B	95	LEU
2	B	120	PRO
2	B	123	LYS
2	B	137	ASP
2	B	147	LEU
2	B	150	ASN
2	B	155	VAL
2	B	167	LEU
2	B	183	LEU
2	B	186	THR
2	B	187	THR
2	B	197	MET
2	B	204	LYS
2	B	246	THR
2	B	256	HIS
1	C	5	ARG
1	C	72	ARG
1	C	81	ILE
1	C	124	HIS
1	C	132	ASN
1	C	133	ARG
1	C	134	GLU
1	C	135	PHE
1	C	142	LYS
1	C	151	GLU
1	C	170	GLU
1	C	177	LEU
1	C	184	LEU
1	C	185	LEU
1	C	198	LEU
1	C	205	LYS
1	C	233	LEU
1	C	253	ARG
1	C	299	MET
1	C	324	THR
1	C	325	THR
1	C	347	LYS

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Mol	Chain	Res	Type
1	C	353	ARG
1	C	355	LEU
1	C	370	LEU
1	C	434	ASP
1	C	444	LEU
1	C	445	THR
1	C	448	LYS
2	D	9	LEU
2	D	17	ASN
2	D	24	LEU
2	D	36	LYS
2	D	38	GLU
2	D	47	ILE
2	D	92	VAL
2	D	95	LEU
2	D	146	LEU
2	D	147	LEU
2	D	167	LEU
2	D	183	LEU
2	D	204	LYS
2	D	256	HIS
1	E	5	ARG
1	E	7	THR
1	E	21	VAL
1	E	23	LYS
1	E	72	ARG
1	E	81	ILE
1	E	124	HIS
1	E	132	ASN
1	E	133	ARG
1	E	135	PHE
1	E	137	GLN
1	E	141	ASP
1	E	142	LYS
1	E	144	SER
1	E	170	GLU
1	E	177	LEU
1	E	185	LEU
1	E	197	GLU
1	E	198	LEU
1	E	213	ILE
1	E	217	ASP

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Mol	Chain	Res	Type
1	E	233	LEU
1	E	299	MET
1	E	324	THR
1	E	325	THR
1	E	347	LYS
1	E	353	ARG
1	E	355	LEU
1	E	370	LEU
1	E	437	ASP
1	E	438	LYS
1	E	444	LEU
1	E	449	SER
1	E	453	VAL
2	F	1	MET
2	F	9	LEU
2	F	17	ASN
2	F	36	LYS
2	F	38	GLU
2	F	47	ILE
2	F	63	ILE
2	F	89	ASP
2	F	92	VAL
2	F	95	LEU
2	F	107	GLU
2	F	110	GLU
2	F	150	ASN
2	F	157	LEU
2	F	167	LEU
2	F	204	LYS
2	F	256	HIS
1	G	5	ARG
1	G	21	VAL
1	G	72	ARG
1	G	81	ILE
1	G	124	HIS
1	G	132	ASN
1	G	135	PHE
1	G	141	ASP
1	G	142	LYS
1	G	170	GLU
1	G	177	LEU
1	G	184	LEU

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Mol	Chain	Res	Type
1	G	185	LEU
1	G	198	LEU
1	G	213	ILE
1	G	233	LEU
1	G	299	MET
1	G	311	SER
1	G	324	THR
1	G	347	LYS
1	G	355	LEU
1	G	359	SER
1	G	370	LEU
1	G	413	GLU
1	G	434	ASP
1	G	441	ASP
1	G	444	LEU
2	H	9	LEU
2	H	17	ASN
2	H	36	LYS
2	H	47	ILE
2	H	54	ASP
2	H	63	ILE
2	H	89	ASP
2	H	95	LEU
2	H	135	VAL
2	H	150	ASN
2	H	183	LEU
2	H	186	THR
2	H	204	LYS
2	H	216	GLN
2	H	253	GLU
2	H	256	HIS
1	I	5	ARG
1	I	21	VAL
1	I	72	ARG
1	I	81	ILE
1	I	124	HIS
1	I	132	ASN
1	I	133	ARG
1	I	134	GLU
1	I	135	PHE
1	I	142	LYS
1	I	170	GLU

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Mol	Chain	Res	Type
1	I	177	LEU
1	I	184	LEU
1	I	185	LEU
1	I	198	LEU
1	I	233	LEU
1	I	253	ARG
1	I	299	MET
1	I	324	THR
1	I	325	THR
1	I	347	LYS
1	I	353	ARG
1	I	355	LEU
1	I	370	LEU
1	I	430	GLU
1	I	444	LEU
1	I	445	THR
1	I	448	LYS
2	J	1	MET
2	J	9	LEU
2	J	17	ASN
2	J	36	LYS
2	J	47	ILE
2	J	89	ASP
2	J	92	VAL
2	J	95	LEU
2	J	121	LYS
2	J	146	LEU
2	J	147	LEU
2	J	164	GLU
2	J	167	LEU
2	J	186	THR
2	J	236	LYS
2	J	256	HIS
1	K	5	ARG
1	K	21	VAL
1	K	81	ILE
1	K	106	LYS
1	K	124	HIS
1	K	132	ASN
1	K	133	ARG
1	K	135	PHE
1	K	142	LYS

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Mol	Chain	Res	Type
1	K	170	GLU
1	K	177	LEU
1	K	184	LEU
1	K	185	LEU
1	K	198	LEU
1	K	233	LEU
1	K	253	ARG
1	K	298	VAL
1	K	299	MET
1	K	324	THR
1	K	325	THR
1	K	347	LYS
1	K	353	ARG
1	K	355	LEU
1	K	370	LEU
1	K	444	LEU
2	L	1	MET
2	L	9	LEU
2	L	17	ASN
2	L	36	LYS
2	L	47	ILE
2	L	63	ILE
2	L	92	VAL
2	L	95	LEU
2	L	121	LYS
2	L	144	THR
2	L	157	LEU
2	L	164	GLU
2	L	186	THR
2	L	216	GLN
2	L	246	THR
2	L	256	HIS
1	M	5	ARG
1	M	21	VAL
1	M	22	SER
1	M	81	ILE
1	M	131	GLU
1	M	132	ASN
1	M	133	ARG
1	M	135	PHE
1	M	142	LYS
1	M	151	GLU

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Mol	Chain	Res	Type
1	M	170	GLU
1	M	177	LEU
1	M	184	LEU
1	M	185	LEU
1	M	198	LEU
1	M	218	THR
1	M	233	LEU
1	M	253	ARG
1	M	298	VAL
1	M	299	MET
1	M	324	THR
1	M	325	THR
1	M	347	LYS
1	M	353	ARG
1	M	355	LEU
1	M	370	LEU
1	M	430	GLU
1	M	438	LYS
1	M	444	LEU
2	N	1	MET
2	N	9	LEU
2	N	17	ASN
2	N	36	LYS
2	N	38	GLU
2	N	47	ILE
2	N	63	ILE
2	N	92	VAL
2	N	95	LEU
2	N	109	ILE
2	N	121	LYS
2	N	155	VAL
2	N	167	LEU
2	N	183	LEU
2	N	188	MET
2	N	204	LYS
2	N	246	THR
1	O	5	ARG
1	O	21	VAL
1	O	72	ARG
1	O	81	ILE
1	O	124	HIS
1	O	126	ILE

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Mol	Chain	Res	Type
1	O	132	ASN
1	O	135	PHE
1	O	142	LYS
1	O	148	GLU
1	O	151	GLU
1	O	170	GLU
1	O	177	LEU
1	O	184	LEU
1	O	185	LEU
1	O	198	LEU
1	O	218	THR
1	O	233	LEU
1	O	253	ARG
1	O	298	VAL
1	O	299	MET
1	O	324	THR
1	O	325	THR
1	O	347	LYS
1	O	353	ARG
1	O	355	LEU
1	O	370	LEU
1	O	434	ASP
1	O	438	LYS
1	O	444	LEU
2	P	1	MET
2	P	9	LEU
2	P	17	ASN
2	P	36	LYS
2	P	39	LEU
2	P	47	ILE
2	P	63	ILE
2	P	71	ASP
2	P	95	LEU
2	P	119	THR
2	P	135	VAL
2	P	137	ASP
2	P	147	LEU
2	P	157	LEU
2	P	183	LEU
2	P	186	THR
2	P	192	LYS
2	P	204	LYS

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Mol	Chain	Res	Type
2	P	219	VAL
2	P	241	ILE
2	P	250	GLU
2	P	256	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (112) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	GLN
1	A	124	HIS
1	A	132	ASN
1	A	137	GLN
1	A	156	ASN
1	A	222	GLN
1	A	295	HIS
1	A	301	ASN
2	B	17	ASN
2	B	60	GLN
2	B	97	ASN
2	B	195	ASN
2	B	201	ASN
2	B	216	GLN
2	B	258	HIS
1	C	105	GLN
1	C	113	HIS
1	C	124	HIS
1	C	132	ASN
1	C	222	GLN
1	C	301	ASN
2	D	17	ASN
2	D	97	ASN
2	D	195	ASN
2	D	215	ASN
2	D	216	GLN
2	D	258	HIS
1	E	105	GLN
1	E	124	HIS
1	E	132	ASN
1	E	137	GLN
1	E	301	ASN
2	F	17	ASN
2	F	97	ASN

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Mol	Chain	Res	Type
2	F	195	ASN
2	F	215	ASN
2	F	216	GLN
2	F	256	HIS
1	G	89	GLN
1	G	105	GLN
1	G	113	HIS
1	G	124	HIS
1	G	132	ASN
1	G	137	GLN
1	G	222	GLN
1	G	235	ASN
1	G	295	HIS
1	G	301	ASN
2	H	17	ASN
2	H	97	ASN
2	H	195	ASN
2	H	201	ASN
2	H	216	GLN
2	H	256	HIS
1	I	105	GLN
1	I	113	HIS
1	I	124	HIS
1	I	132	ASN
1	I	137	GLN
1	I	222	GLN
1	I	295	HIS
1	I	301	ASN
2	J	17	ASN
2	J	97	ASN
2	J	195	ASN
2	J	256	HIS
2	J	258	HIS
1	K	105	GLN
1	K	113	HIS
1	K	124	HIS
1	K	132	ASN
1	K	137	GLN
1	K	156	ASN
1	K	222	GLN
1	K	295	HIS
1	K	301	ASN

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Mol	Chain	Res	Type
1	K	348	ASN
2	L	17	ASN
2	L	97	ASN
2	L	195	ASN
2	L	215	ASN
2	L	216	GLN
2	L	256	HIS
1	M	89	GLN
1	M	93	ASN
1	M	105	GLN
1	M	113	HIS
1	M	124	HIS
1	M	132	ASN
1	M	222	GLN
1	M	295	HIS
1	M	301	ASN
2	N	17	ASN
2	N	60	GLN
2	N	97	ASN
2	N	195	ASN
2	N	215	ASN
2	N	216	GLN
1	O	105	GLN
1	O	113	HIS
1	O	124	HIS
1	O	132	ASN
1	O	137	GLN
1	O	156	ASN
1	O	301	ASN
1	O	348	ASN
2	P	17	ASN
2	P	60	GLN
2	P	97	ASN
2	P	195	ASN
2	P	216	GLN
2	P	258	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 28 ligands modelled in this entry, 20 are monoatomic - leaving 8 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	$\# Z  > 2$
5	B13	F	500	2	78,100,100	2.10	17 (21%)	100,164,164	1.87	24 (24%)
5	B13	B	500	2	78,100,100	2.08	17 (21%)	100,164,164	1.78	18 (18%)
5	B13	H	500	2	78,100,100	2.13	17 (21%)	100,164,164	1.86	19 (19%)
5	B13	N	500	2	78,100,100	2.11	17 (21%)	100,164,164	1.84	22 (22%)
5	B13	D	500	2	78,100,100	2.14	20 (25%)	100,164,164	1.86	24 (24%)
5	B13	J	500	2,6	78,100,100	2.08	16 (20%)	100,164,164	1.78	18 (18%)
5	B13	P	500	2	78,100,100	2.04	16 (20%)	100,164,164	1.96	24 (24%)
5	B13	L	500	2,6	78,100,100	2.11	18 (23%)	100,164,164	1.78	22 (22%)

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	B13	F	500	2	-	17/52/223/223	0/3/11/11
5	B13	B	500	2	-	16/52/223/223	0/3/11/11
5	B13	H	500	2	-	19/52/223/223	0/3/11/11
5	B13	N	500	2	-	22/52/223/223	0/3/11/11

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	B13	D	500	2	-	18/52/223/223	0/3/11/11
5	B13	J	500	2,6	-	20/52/223/223	0/3/11/11
5	B13	P	500	2	-	18/52/223/223	0/3/11/11
5	B13	L	500	2,6	-	19/52/223/223	0/3/11/11

All (138) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	500	B13	C5R-C4R	-8.92	1.21	1.51
5	D	500	B13	C5R-C4R	-8.89	1.22	1.51
5	P	500	B13	C5R-C4R	-8.78	1.22	1.51
5	J	500	B13	C5R-C4R	-8.78	1.22	1.51
5	L	500	B13	C5R-C4R	-8.77	1.22	1.51
5	H	500	B13	C5R-C4R	-8.69	1.22	1.51
5	F	500	B13	C5R-C4R	-8.68	1.22	1.51
5	N	500	B13	C5R-C4R	-8.64	1.22	1.51
5	D	500	B13	C6-N22	6.65	1.43	1.35
5	N	500	B13	C6-N22	6.59	1.43	1.35
5	H	500	B13	C6-N22	6.40	1.43	1.35
5	L	500	B13	C6-N22	6.22	1.43	1.35
5	B	500	B13	O5B-C5B	6.21	1.51	1.37
5	F	500	B13	C6-N22	6.18	1.43	1.35
5	J	500	B13	C6-N22	6.07	1.42	1.35
5	L	500	B13	O5B-C5B	6.07	1.51	1.37
5	H	500	B13	O5B-C5B	6.06	1.51	1.37
5	N	500	B13	O5B-C5B	5.99	1.51	1.37
5	F	500	B13	O5B-C5B	5.95	1.50	1.37
5	P	500	B13	C6-N22	5.87	1.42	1.35
5	D	500	B13	O5B-C5B	5.77	1.50	1.37
5	J	500	B13	C11-C10	-5.65	1.36	1.50
5	B	500	B13	C11-C10	-5.65	1.36	1.50
5	H	500	B13	C11-C10	-5.62	1.37	1.50
5	F	500	B13	C11-C10	-5.53	1.37	1.50
5	J	500	B13	O5B-C5B	5.49	1.49	1.37
5	P	500	B13	O5B-C5B	5.41	1.49	1.37
5	B	500	B13	C6-N22	5.35	1.41	1.35
5	L	500	B13	C11-C10	-5.34	1.37	1.50
5	D	500	B13	C11-C10	-5.31	1.37	1.50
5	P	500	B13	C11-C10	-5.31	1.37	1.50
5	N	500	B13	C11-C10	-5.25	1.37	1.50
5	H	500	B13	C6B-C5B	4.23	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	N	500	B13	C6B-C5B	3.96	1.46	1.38
5	D	500	B13	C6B-C5B	3.94	1.46	1.38
5	D	500	B13	C35-C5	3.92	1.56	1.50
5	L	500	B13	C6B-C5B	3.92	1.46	1.38
5	F	500	B13	C6B-C5B	3.91	1.46	1.38
5	L	500	B13	C35-C5	3.83	1.56	1.50
5	B	500	B13	C20-C1	3.76	1.61	1.52
5	J	500	B13	C6B-C5B	3.76	1.46	1.38
5	J	500	B13	C35-C5	3.73	1.56	1.50
5	B	500	B13	C6B-C5B	3.69	1.46	1.38
5	F	500	B13	C20-C1	3.68	1.61	1.52
5	J	500	B13	C20-C1	3.63	1.61	1.52
5	P	500	B13	C20-C1	3.61	1.61	1.52
5	B	500	B13	C35-C5	3.58	1.56	1.50
5	N	500	B13	C20-C1	3.58	1.61	1.52
5	J	500	B13	O8R-C5R	3.56	1.57	1.42
5	H	500	B13	C20-C1	3.54	1.61	1.52
5	H	500	B13	O8R-C5R	3.53	1.57	1.42
5	F	500	B13	O8R-C5R	3.48	1.57	1.42
5	L	500	B13	C20-C1	3.48	1.61	1.52
5	N	500	B13	O8R-C5R	3.48	1.57	1.42
5	N	500	B13	C35-C5	3.47	1.56	1.50
5	D	500	B13	O8R-C5R	3.43	1.56	1.42
5	L	500	B13	O8R-C5R	3.42	1.56	1.42
5	P	500	B13	C6B-C5B	3.42	1.45	1.38
5	F	500	B13	O6R-C1R	3.42	1.45	1.41
5	P	500	B13	O8R-C5R	3.42	1.56	1.42
5	B	500	B13	O8R-C5R	3.41	1.56	1.42
5	B	500	B13	C55-C17	3.39	1.60	1.55
5	H	500	B13	C35-C5	3.37	1.55	1.50
5	H	500	B13	C36-C7	3.35	1.60	1.54
5	D	500	B13	C25-C2	3.33	1.60	1.54
5	L	500	B13	O6R-C1R	3.29	1.45	1.41
5	P	500	B13	C35-C5	3.28	1.55	1.50
5	F	500	B13	C35-C5	3.27	1.55	1.50
5	H	500	B13	O6R-C1R	3.27	1.45	1.41
5	J	500	B13	C25-C2	3.16	1.60	1.54
5	L	500	B13	C55-C17	3.14	1.59	1.55
5	D	500	B13	C20-C1	3.14	1.60	1.52
5	F	500	B13	C36-C7	3.11	1.59	1.54
5	P	500	B13	C55-C17	3.11	1.59	1.55
5	N	500	B13	C36-C7	3.06	1.59	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	500	B13	C36-C7	3.06	1.59	1.54
5	N	500	B13	C55-C17	3.03	1.59	1.55
5	N	500	B13	O6R-C1R	3.00	1.45	1.41
5	H	500	B13	C55-C17	2.99	1.59	1.55
5	J	500	B13	C55-C17	2.92	1.59	1.55
5	J	500	B13	O6R-C1R	2.89	1.45	1.41
5	D	500	B13	C55-C17	2.86	1.59	1.55
5	F	500	B13	C7-C6	2.86	1.60	1.54
5	F	500	B13	C55-C17	2.84	1.59	1.55
5	P	500	B13	C25-C2	2.84	1.59	1.54
5	N	500	B13	C7-C6	2.83	1.60	1.54
5	B	500	B13	C25-C2	2.77	1.59	1.54
5	F	500	B13	C25-C2	2.77	1.59	1.54
5	D	500	B13	C36-C7	2.74	1.59	1.54
5	L	500	B13	C36-C7	2.73	1.59	1.54
5	P	500	B13	O6R-C1R	2.72	1.44	1.41
5	P	500	B13	C36-C7	2.69	1.59	1.54
5	D	500	B13	C2R-C3R	-2.63	1.47	1.52
5	N	500	B13	C25-C2	2.63	1.59	1.54
5	D	500	B13	C60-C61	-2.54	1.45	1.51
5	L	500	B13	C2R-C3R	-2.52	1.47	1.52
5	L	500	B13	C25-C2	2.49	1.59	1.54
5	B	500	B13	C36-C7	2.46	1.58	1.54
5	B	500	B13	O6R-C1R	2.45	1.44	1.41
5	H	500	B13	C25-C2	2.44	1.59	1.54
5	D	500	B13	C7-C6	2.40	1.59	1.54
5	D	500	B13	C4B-C5B	2.40	1.41	1.37
5	H	500	B13	C7-C6	2.39	1.59	1.54
5	L	500	B13	C7-C6	2.35	1.59	1.54
5	D	500	B13	O6R-C1R	2.32	1.44	1.41
5	B	500	B13	C30-C3	2.32	1.57	1.53
5	J	500	B13	C2R-C3R	-2.29	1.47	1.52
5	D	500	B13	C53-C15	2.27	1.54	1.50
5	F	500	B13	C4B-C5B	2.27	1.41	1.37
5	F	500	B13	C13-C14	2.26	1.56	1.52
5	L	500	B13	C13-C14	2.24	1.56	1.52
5	B	500	B13	C4B-C5B	2.22	1.41	1.37
5	H	500	B13	C2R-C3R	-2.21	1.48	1.52
5	N	500	B13	C2R-C3R	-2.21	1.48	1.52
5	N	500	B13	P-O4	-2.19	1.45	1.55
5	H	500	B13	P-O4	-2.18	1.45	1.55
5	D	500	B13	P-O4	-2.18	1.45	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	500	B13	C48-C13	2.17	1.59	1.54
5	L	500	B13	P-O4	-2.15	1.45	1.55
5	D	500	B13	C2-C1	2.15	1.60	1.54
5	P	500	B13	P-O4	-2.14	1.45	1.55
5	H	500	B13	C13-C14	2.11	1.56	1.52
5	J	500	B13	P-O4	-2.11	1.45	1.55
5	B	500	B13	P-O4	-2.10	1.45	1.55
5	L	500	B13	C2-C1	2.09	1.60	1.54
5	F	500	B13	P-O4	-2.08	1.45	1.55
5	B	500	B13	C2-C1	2.08	1.60	1.54
5	P	500	B13	C7-C6	2.07	1.59	1.54
5	J	500	B13	C30-C3	2.06	1.57	1.53
5	J	500	B13	C60-C61	-2.05	1.46	1.51
5	D	500	B13	O7R-C2R	-2.05	1.38	1.43
5	B	500	B13	C2R-C3R	-2.04	1.48	1.52
5	N	500	B13	C60-C61	-2.03	1.46	1.51
5	H	500	B13	C60-C61	-2.02	1.46	1.51
5	L	500	B13	C4B-C5B	2.02	1.41	1.37
5	P	500	B13	C2-C1	2.02	1.60	1.54
5	F	500	B13	C2R-C3R	-2.00	1.48	1.52
5	N	500	B13	C4B-C5B	2.00	1.41	1.37

All (171) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	500	B13	O6R-C4R-C5R	7.95	126.41	109.21
5	N	500	B13	O6R-C4R-C5R	7.94	126.38	109.21
5	B	500	B13	O6R-C4R-C5R	7.90	126.29	109.21
5	J	500	B13	O6R-C4R-C5R	7.57	125.58	109.21
5	P	500	B13	O6R-C4R-C5R	7.52	125.48	109.21
5	L	500	B13	O6R-C4R-C5R	7.47	125.36	109.21
5	D	500	B13	O6R-C4R-C5R	7.46	125.33	109.21
5	H	500	B13	O6R-C4R-C5R	7.20	124.78	109.21
5	H	500	B13	C5R-C4R-C3R	5.39	132.03	114.85
5	J	500	B13	C5R-C4R-C3R	5.31	131.76	114.85
5	P	500	B13	C5R-C4R-C3R	5.04	130.92	114.85
5	L	500	B13	C5R-C4R-C3R	5.04	130.92	114.85
5	F	500	B13	C5R-C4R-C3R	5.01	130.81	114.85
5	B	500	B13	O7R-C2R-C3R	4.84	124.90	111.17
5	H	500	B13	C60-C18-C17	4.76	122.74	114.44
5	D	500	B13	C5R-C4R-C3R	4.73	129.93	114.85
5	B	500	B13	C5R-C4R-C3R	4.73	129.92	114.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	500	B13	O7R-C2R-C3R	4.64	124.36	111.17
5	P	500	B13	O7R-C2R-C3R	4.62	124.30	111.17
5	N	500	B13	C5R-C4R-C3R	4.59	129.47	114.85
5	P	500	B13	C7B-C8B-N1B	-4.54	128.24	132.11
5	H	500	B13	O34-C32-C31	-4.52	107.80	121.07
5	H	500	B13	O7R-C2R-C3R	4.52	123.99	111.17
5	F	500	B13	O34-C32-C31	-4.34	108.33	121.07
5	N	500	B13	C53-C15-C14	-4.26	117.02	124.25
5	F	500	B13	O7R-C2R-C3R	4.21	123.12	111.17
5	P	500	B13	C7-C37-C38	4.20	126.89	114.25
5	J	500	B13	C18-C60-C61	4.19	124.44	113.97
5	D	500	B13	O34-C32-C31	-4.15	108.87	121.07
5	P	500	B13	C18-C60-C61	4.15	124.33	113.97
5	J	500	B13	O7R-C2R-C3R	4.15	122.94	111.17
5	B	500	B13	O34-C32-C31	-4.12	108.95	121.07
5	L	500	B13	O34-C32-C31	-4.11	108.98	121.07
5	L	500	B13	O7R-C2R-C3R	4.11	122.83	111.17
5	P	500	B13	O34-C32-C31	-4.07	109.11	121.07
5	H	500	B13	C53-C15-C14	-4.04	117.40	124.25
5	B	500	B13	C7B-C8B-N1B	-4.00	128.71	132.11
5	N	500	B13	O34-C32-C31	-3.98	109.38	121.07
5	H	500	B13	C7-C37-C38	3.97	126.19	114.25
5	F	500	B13	C7B-C8B-N1B	-3.91	128.78	132.11
5	D	500	B13	O7R-C2R-C3R	3.90	122.25	111.17
5	J	500	B13	C7-C37-C38	3.89	125.95	114.25
5	J	500	B13	O34-C32-C31	-3.87	109.69	121.07
5	H	500	B13	C54-C17-C55	-3.83	102.62	109.57
5	F	500	B13	C60-C18-C17	3.75	120.98	114.44
5	P	500	B13	C60-C18-C17	3.72	120.93	114.44
5	P	500	B13	C53-C15-C14	-3.71	117.95	124.25
5	F	500	B13	C53-C15-C14	-3.59	118.16	124.25
5	N	500	B13	C7-C37-C38	3.45	124.62	114.25
5	D	500	B13	C41-C42-C43	-3.43	100.96	112.59
5	J	500	B13	C53-C15-C14	-3.42	118.44	124.25
5	F	500	B13	C36-C7-C6	3.38	127.01	109.79
5	N	500	B13	C60-C18-C17	3.36	120.31	114.44
5	P	500	B13	C42-C41-C8	3.36	124.43	114.73
5	B	500	B13	C36-C7-C6	3.34	126.82	109.79
5	H	500	B13	O8R-C5R-C4R	3.31	122.64	111.29
5	H	500	B13	C18-C60-C61	3.31	122.22	113.97
5	N	500	B13	C36-C7-C6	3.30	126.64	109.79
5	F	500	B13	C18-C60-C61	3.29	122.17	113.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	500	B13	C18-C60-C61	3.29	122.17	113.97
5	L	500	B13	C53-C15-C14	-3.26	118.72	124.25
5	F	500	B13	O8R-C5R-C4R	3.24	122.41	111.29
5	D	500	B13	C41-C8-C7	-3.24	105.22	114.14
5	D	500	B13	C60-C18-C17	3.22	120.07	114.44
5	D	500	B13	C42-C41-C8	3.20	123.97	114.73
5	P	500	B13	C36-C7-C6	3.16	125.89	109.79
5	L	500	B13	C18-C60-C61	3.15	121.83	113.97
5	N	500	B13	O8R-C5R-C4R	3.15	122.10	111.29
5	J	500	B13	C7B-C8B-N1B	-3.11	129.46	132.11
5	L	500	B13	C60-C18-C17	3.10	119.84	114.44
5	D	500	B13	C7B-C8B-N1B	-3.08	129.48	132.11
5	B	500	B13	C17-C16-N24	3.06	112.58	109.20
5	H	500	B13	C42-C41-C8	3.05	123.53	114.73
5	P	500	B13	C6B-C7B-C8B	-3.05	115.02	119.70
5	H	500	B13	C36-C7-C6	3.03	125.26	109.79
5	L	500	B13	C7B-C8B-N1B	-3.01	129.55	132.11
5	D	500	B13	O2-C3R-C4R	-3.00	99.24	110.08
5	P	500	B13	C54-C17-C55	-3.00	104.13	109.57
5	N	500	B13	O2-C3R-C4R	-3.00	99.25	110.08
5	F	500	B13	C42-C41-C8	2.99	123.37	114.73
5	N	500	B13	C47-C12-C13	2.98	122.32	111.72
5	N	500	B13	C18-C60-C61	2.98	121.40	113.97
5	N	500	B13	C54-C17-C55	-2.97	104.17	109.57
5	L	500	B13	C36-C7-C6	2.97	124.94	109.79
5	N	500	B13	C36-C7-C37	-2.97	105.92	110.80
5	J	500	B13	C36-C7-C6	2.96	124.87	109.79
5	D	500	B13	C36-C7-C37	-2.95	105.94	110.80
5	D	500	B13	C36-C7-C6	2.95	124.83	109.79
5	D	500	B13	C7-C37-C38	2.92	123.02	114.25
5	L	500	B13	C36-C7-C37	-2.91	106.01	110.80
5	D	500	B13	C18-C60-C61	2.90	121.21	113.97
5	J	500	B13	C41-C42-C43	-2.85	102.91	112.59
5	L	500	B13	C42-C41-C8	2.85	122.95	114.73
5	L	500	B13	C31-C30-C3	-2.82	107.48	114.43
5	L	500	B13	C7-C37-C38	2.77	122.58	114.25
5	P	500	B13	C5B-C4B-C9B	-2.73	116.41	119.29
5	F	500	B13	C41-C8-C7	-2.70	106.70	114.14
5	F	500	B13	C36-C7-C37	-2.68	106.39	110.80
5	D	500	B13	C47-C12-C13	2.66	121.19	111.72
5	L	500	B13	C31-C32-N33	2.65	124.76	116.51
5	P	500	B13	C3P-C2P-C1P	-2.60	106.34	111.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	500	B13	O8R-C5R-C4R	2.60	120.20	111.29
5	B	500	B13	C12-C13-C14	2.59	105.61	100.79
5	J	500	B13	C3P-C2P-C1P	-2.59	106.37	111.39
5	B	500	B13	C6B-C7B-C8B	-2.58	115.74	119.70
5	L	500	B13	O2-C3R-C4R	-2.57	100.81	110.08
5	D	500	B13	C2P-C1P-N59	-2.56	109.16	112.93
5	N	500	B13	C42-C41-C8	2.55	122.08	114.73
5	L	500	B13	C47-C12-C13	2.55	120.77	111.72
5	P	500	B13	C31-C32-N33	2.53	124.37	116.51
5	D	500	B13	C4B-C9B-C8B	-2.51	118.53	121.10
5	D	500	B13	O8R-C5R-C4R	2.51	119.90	111.29
5	H	500	B13	O2-C3R-C4R	-2.51	101.01	110.08
5	N	500	B13	C7B-C8B-N1B	-2.50	129.97	132.11
5	L	500	B13	C6B-C7B-C8B	-2.50	115.86	119.70
5	B	500	B13	C36-C7-C37	-2.49	106.69	110.80
5	H	500	B13	C31-C32-N33	2.49	124.27	116.51
5	J	500	B13	O8R-C5R-C4R	2.47	119.77	111.29
5	D	500	B13	C31-C32-N33	2.45	124.14	116.51
5	B	500	B13	C60-C18-C17	2.44	118.70	114.44
5	F	500	B13	C7-C37-C38	2.44	121.58	114.25
5	F	500	B13	C3P-C2P-C1P	-2.42	106.69	111.39
5	F	500	B13	O2-C3R-C4R	-2.42	101.33	110.08
5	D	500	B13	O6R-C1R-C2R	2.40	110.43	106.93
5	J	500	B13	C47-C12-C13	2.40	120.24	111.72
5	F	500	B13	C25-C2-C3	2.38	116.42	111.80
5	J	500	B13	C6B-C7B-C8B	-2.36	116.08	119.70
5	P	500	B13	C37-C38-N40	2.35	123.95	116.52
5	H	500	B13	C37-C7-C8	-2.34	102.11	108.39
5	J	500	B13	C60-C18-C17	2.33	118.51	114.44
5	F	500	B13	C6B-C7B-C8B	-2.33	116.13	119.70
5	L	500	B13	C2-C26-C27	2.31	121.72	115.22
5	P	500	B13	O8R-C5R-C4R	2.31	119.21	111.29
5	H	500	B13	C6B-C7B-C8B	-2.31	116.16	119.70
5	F	500	B13	C31-C32-N33	2.30	123.67	116.51
5	L	500	B13	O6R-C1R-C2R	2.30	110.29	106.93
5	F	500	B13	C41-C42-C43	-2.30	104.80	112.59
5	N	500	B13	C31-C32-N33	2.28	123.62	116.51
5	P	500	B13	C1P-N59-C57	-2.28	117.73	122.69
5	H	500	B13	C47-C12-C13	2.27	119.80	111.72
5	J	500	B13	C5B-C4B-C9B	-2.27	116.89	119.29
5	B	500	B13	C31-C32-N33	2.26	123.55	116.51
5	F	500	B13	C31-C30-C3	-2.26	108.87	114.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	500	B13	C12-C13-C14	2.26	105.00	100.79
5	B	500	B13	C42-C41-C8	2.26	121.24	114.73
5	B	500	B13	C7-C37-C38	2.25	121.02	114.25
5	B	500	B13	C47-C12-C13	2.25	119.70	111.72
5	F	500	B13	C47-C12-C13	2.24	119.68	111.72
5	D	500	B13	C3P-C2P-C1P	-2.22	107.07	111.39
5	P	500	B13	C36-C7-C37	-2.22	107.14	110.80
5	N	500	B13	C47-C12-C46	-2.22	102.67	108.36
5	J	500	B13	C31-C32-N33	2.20	123.36	116.51
5	L	500	B13	C41-C42-C43	-2.18	105.18	112.59
5	N	500	B13	C6B-C7B-C8B	-2.17	116.37	119.70
5	J	500	B13	C42-C41-C8	2.17	120.98	114.73
5	P	500	B13	C25-C2-C3	2.14	115.95	111.80
5	P	500	B13	C7B-C8B-C9B	2.14	124.79	121.30
5	B	500	B13	O2-C3R-C4R	-2.13	102.39	110.08
5	L	500	B13	C11-N23-C14	-2.13	108.43	111.89
5	D	500	B13	C1P-N59-C57	-2.11	118.09	122.69
5	B	500	B13	C25-C2-C3	2.09	115.85	111.80
5	P	500	B13	C41-C8-C7	-2.07	108.44	114.14
5	H	500	B13	C7B-C8B-N1B	-2.07	130.35	132.11
5	N	500	B13	O6R-C1R-C2R	2.05	109.92	106.93
5	N	500	B13	C11-N23-C14	-2.05	108.56	111.89
5	D	500	B13	C7B-C8B-C9B	2.04	124.64	121.30
5	D	500	B13	P-O2-C3R	2.04	126.83	119.41
5	N	500	B13	C47-C12-C11	2.04	117.21	111.53
5	P	500	B13	C17-C16-N24	2.03	111.44	109.20
5	F	500	B13	C12-C13-C14	2.01	104.54	100.79
5	F	500	B13	O34-C32-N33	2.01	128.00	122.50

There are no chirality outliers.

All (149) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	P	500	B13	C3P-C2P-O3-P
5	P	500	B13	C1P-C2P-O3-P
5	P	500	B13	N59-C1P-C2P-O3
5	P	500	B13	N59-C1P-C2P-C3P
5	P	500	B13	C18-C60-C61-N62
5	P	500	B13	C18-C60-C61-O63
5	P	500	B13	C2-C3-C30-C31
5	P	500	B13	C7-C37-C38-O39
5	P	500	B13	C7-C37-C38-N40

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Mol	Chain	Res	Type	Atoms
5	F	500	B13	C1P-C2P-O3-P
5	F	500	B13	C18-C60-C61-N62
5	F	500	B13	C18-C60-C61-O63
5	F	500	B13	C2-C3-C30-C31
5	F	500	B13	C4-C3-C30-C31
5	F	500	B13	C38-C37-C7-C8
5	F	500	B13	C38-C37-C7-C6
5	F	500	B13	C38-C37-C7-C36
5	H	500	B13	N59-C1P-C2P-O3
5	H	500	B13	N59-C1P-C2P-C3P
5	H	500	B13	C18-C60-C61-N62
5	H	500	B13	C18-C60-C61-O63
5	H	500	B13	C2-C3-C30-C31
5	H	500	B13	C4-C3-C30-C31
5	H	500	B13	C14-C13-C48-C49
5	H	500	B13	C12-C13-C48-C49
5	H	500	B13	C38-C37-C7-C8
5	H	500	B13	C38-C37-C7-C6
5	H	500	B13	C38-C37-C7-C36
5	H	500	B13	C7-C37-C38-N40
5	N	500	B13	C3P-C2P-O3-P
5	N	500	B13	C1P-C2P-O3-P
5	N	500	B13	N59-C1P-C2P-C3P
5	N	500	B13	C18-C60-C61-N62
5	N	500	B13	C18-C60-C61-O63
5	N	500	B13	C3-C2-C26-C27
5	N	500	B13	C2-C3-C30-C31
5	N	500	B13	C4-C3-C30-C31
5	N	500	B13	C12-C13-C48-C49
5	N	500	B13	C7-C37-C38-N40
5	B	500	B13	C18-C60-C61-N62
5	B	500	B13	C18-C60-C61-O63
5	B	500	B13	C2-C3-C30-C31
5	B	500	B13	C4-C3-C30-C31
5	B	500	B13	C14-C13-C48-C49
5	B	500	B13	C12-C13-C48-C49
5	B	500	B13	C38-C37-C7-C36
5	B	500	B13	C7-C37-C38-O39
5	J	500	B13	N59-C1P-C2P-O3
5	J	500	B13	C18-C60-C61-N62
5	J	500	B13	C18-C60-C61-O63
5	J	500	B13	C2-C3-C30-C31

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Mol	Chain	Res	Type	Atoms
5	J	500	B13	C4-C3-C30-C31
5	J	500	B13	C14-C13-C48-C49
5	J	500	B13	C12-C13-C48-C49
5	J	500	B13	C38-C37-C7-C36
5	J	500	B13	C7-C37-C38-O39
5	L	500	B13	C2P-O3-P-O2
5	L	500	B13	N59-C1P-C2P-O3
5	L	500	B13	N59-C1P-C2P-C3P
5	L	500	B13	C18-C60-C61-N62
5	L	500	B13	C18-C60-C61-O63
5	L	500	B13	C2-C3-C30-C31
5	D	500	B13	C1P-C2P-O3-P
5	D	500	B13	C18-C60-C61-N62
5	D	500	B13	C18-C60-C61-O63
5	D	500	B13	C2-C3-C30-C31
5	D	500	B13	C4-C3-C30-C31
5	D	500	B13	C7-C37-C38-O39
5	D	500	B13	C7-C37-C38-N40
5	H	500	B13	C3R-C4R-C5R-O8R
5	N	500	B13	C14-C13-C48-C49
5	J	500	B13	C42-C41-C8-C9
5	H	500	B13	C7-C37-C38-O39
5	B	500	B13	C7-C37-C38-N40
5	J	500	B13	C7-C37-C38-N40
5	L	500	B13	C7-C37-C38-N40
5	N	500	B13	C42-C41-C8-C9
5	F	500	B13	O6R-C4R-C5R-O8R
5	J	500	B13	O6R-C4R-C5R-O8R
5	N	500	B13	O6R-C4R-C5R-O8R
5	P	500	B13	C3R-C4R-C5R-O8R
5	H	500	B13	C42-C41-C8-C9
5	B	500	B13	C42-C41-C8-C9
5	N	500	B13	C25-C2-C26-C27
5	N	500	B13	C7-C37-C38-O39
5	L	500	B13	C7-C37-C38-O39
5	D	500	B13	O6R-C4R-C5R-O8R
5	N	500	B13	N59-C1P-C2P-O3
5	P	500	B13	C14-C13-C48-C49
5	F	500	B13	C14-C13-C48-C49
5	H	500	B13	C17-C55-C56-C57
5	F	500	B13	C3P-C2P-O3-P
5	D	500	B13	C3P-C2P-O3-P

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Mol	Chain	Res	Type	Atoms
5	P	500	B13	C12-C13-C48-C49
5	F	500	B13	C12-C13-C48-C49
5	P	500	B13	C42-C41-C8-C9
5	L	500	B13	O6R-C4R-C5R-O8R
5	J	500	B13	C8-C41-C42-C43
5	B	500	B13	O6R-C4R-C5R-O8R
5	J	500	B13	N59-C1P-C2P-C3P
5	F	500	B13	C8-C41-C42-C43
5	P	500	B13	C30-C31-C32-O34
5	D	500	B13	C12-C13-C48-C49
5	F	500	B13	C42-C41-C8-C9
5	N	500	B13	C17-C55-C56-C57
5	J	500	B13	C17-C55-C56-C57
5	H	500	B13	C30-C31-C32-O34
5	N	500	B13	C30-C31-C32-O34
5	J	500	B13	C42-C41-C8-C7
5	B	500	B13	C1P-C2P-O3-P
5	D	500	B13	C14-C13-C48-C49
5	P	500	B13	C30-C31-C32-N33
5	B	500	B13	C30-C31-C32-O34
5	J	500	B13	C3-C2-C26-C27
5	N	500	B13	C42-C41-C8-C7
5	J	500	B13	C38-C37-C7-C8
5	H	500	B13	C30-C31-C32-N33
5	N	500	B13	C30-C31-C32-N33
5	L	500	B13	C3-C30-C31-C32
5	P	500	B13	C4-C3-C30-C31
5	L	500	B13	C4-C3-C30-C31
5	L	500	B13	C30-C31-C32-O34
5	L	500	B13	C42-C41-C8-C9
5	D	500	B13	C42-C41-C8-C9
5	L	500	B13	C30-C31-C32-N33
5	L	500	B13	C17-C55-C56-C57
5	F	500	B13	C4R-C3R-O2-P
5	J	500	B13	C17-C18-C60-C61
5	L	500	B13	C3R-C4R-C5R-O8R
5	B	500	B13	C38-C37-C7-C8
5	B	500	B13	C30-C31-C32-N33
5	F	500	B13	C2R-C3R-O2-P
5	P	500	B13	C17-C18-C60-C61
5	P	500	B13	C19-C18-C60-C61
5	J	500	B13	C19-C18-C60-C61

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Mol	Chain	Res	Type	Atoms
5	D	500	B13	C19-C18-C60-C61
5	D	500	B13	C30-C31-C32-N33
5	B	500	B13	C3P-C2P-O3-P
5	L	500	B13	C4R-C3R-O2-P
5	D	500	B13	C17-C18-C60-C61
5	L	500	B13	C38-C37-C7-C36
5	D	500	B13	C54-C17-C55-C56
5	D	500	B13	C3R-C4R-C5R-O8R
5	F	500	B13	C17-C55-C56-C57
5	N	500	B13	C3R-C4R-C5R-O8R
5	D	500	B13	C30-C31-C32-O34
5	N	500	B13	C17-C18-C60-C61
5	H	500	B13	C42-C41-C8-C7
5	L	500	B13	C2R-C3R-O2-P

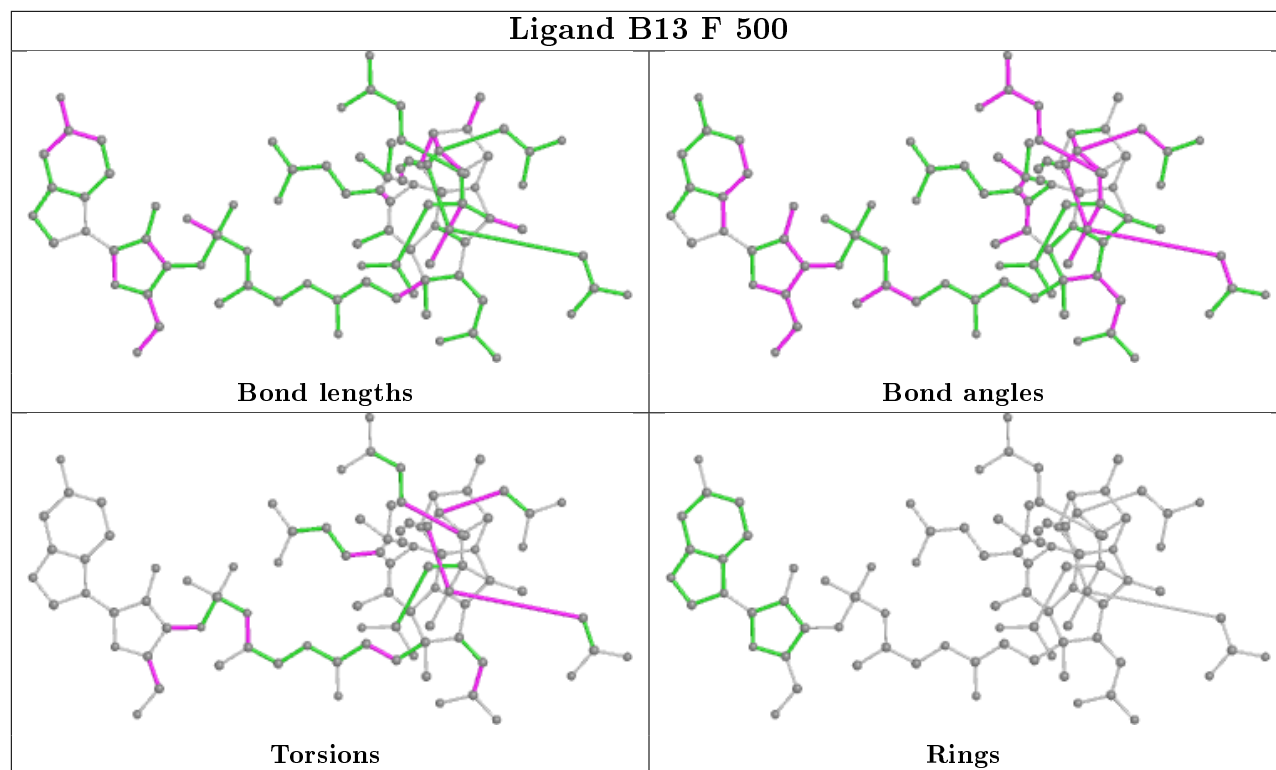
There are no ring outliers.

8 monomers are involved in 82 short contacts:

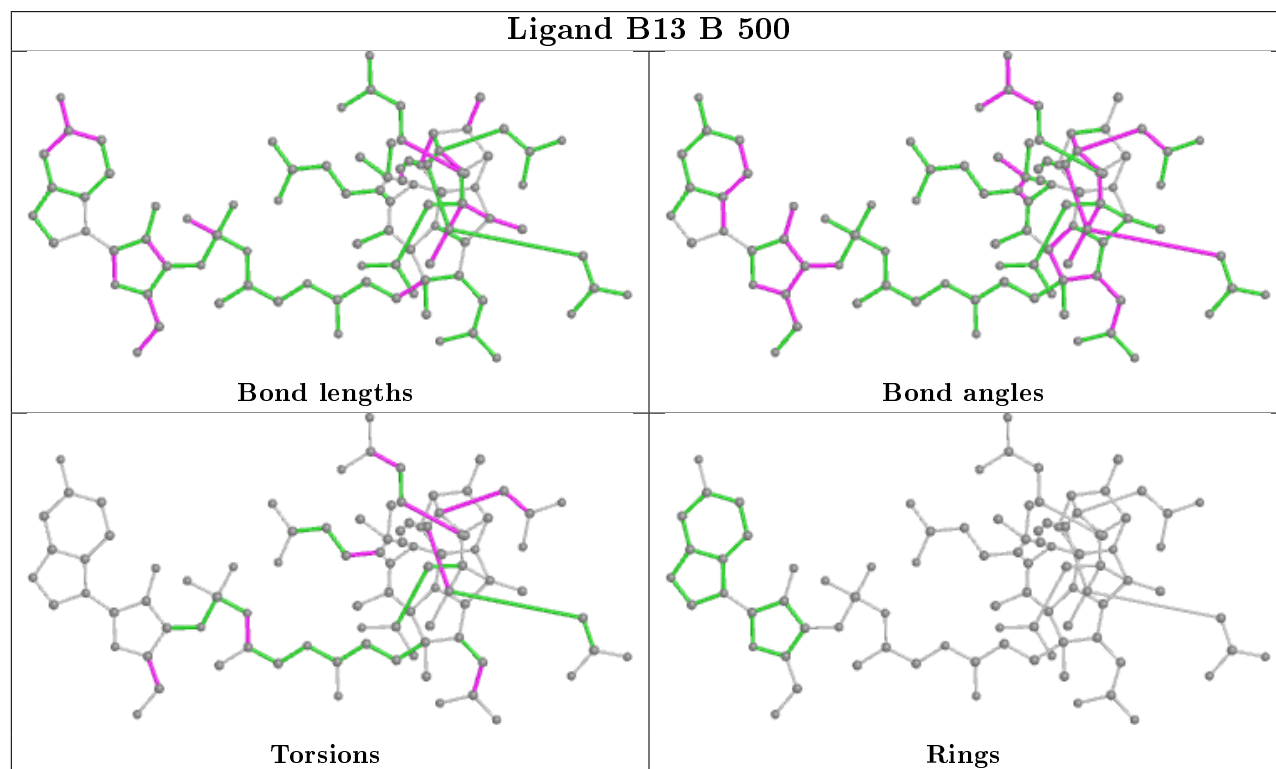
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	500	B13	7	0
5	B	500	B13	9	0
5	H	500	B13	10	0
5	N	500	B13	11	0
5	D	500	B13	13	0
5	J	500	B13	13	0
5	P	500	B13	9	0
5	L	500	B13	10	0

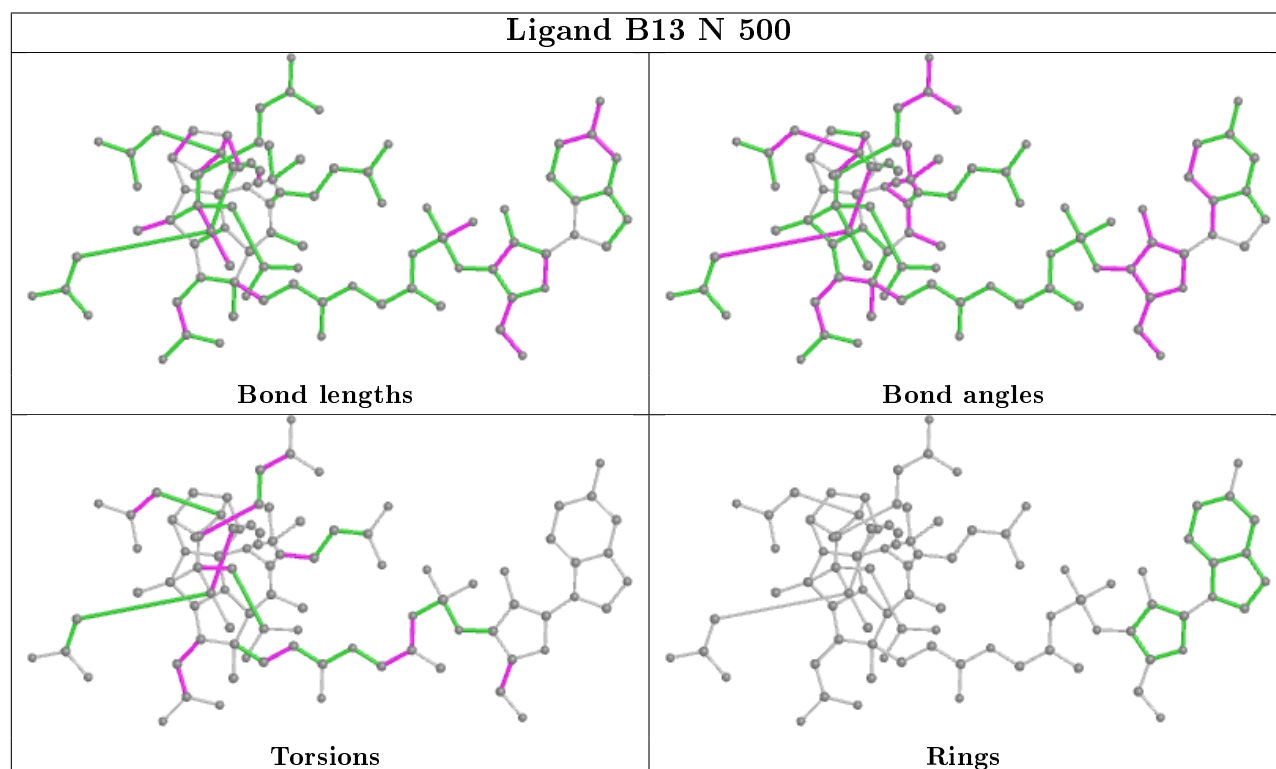
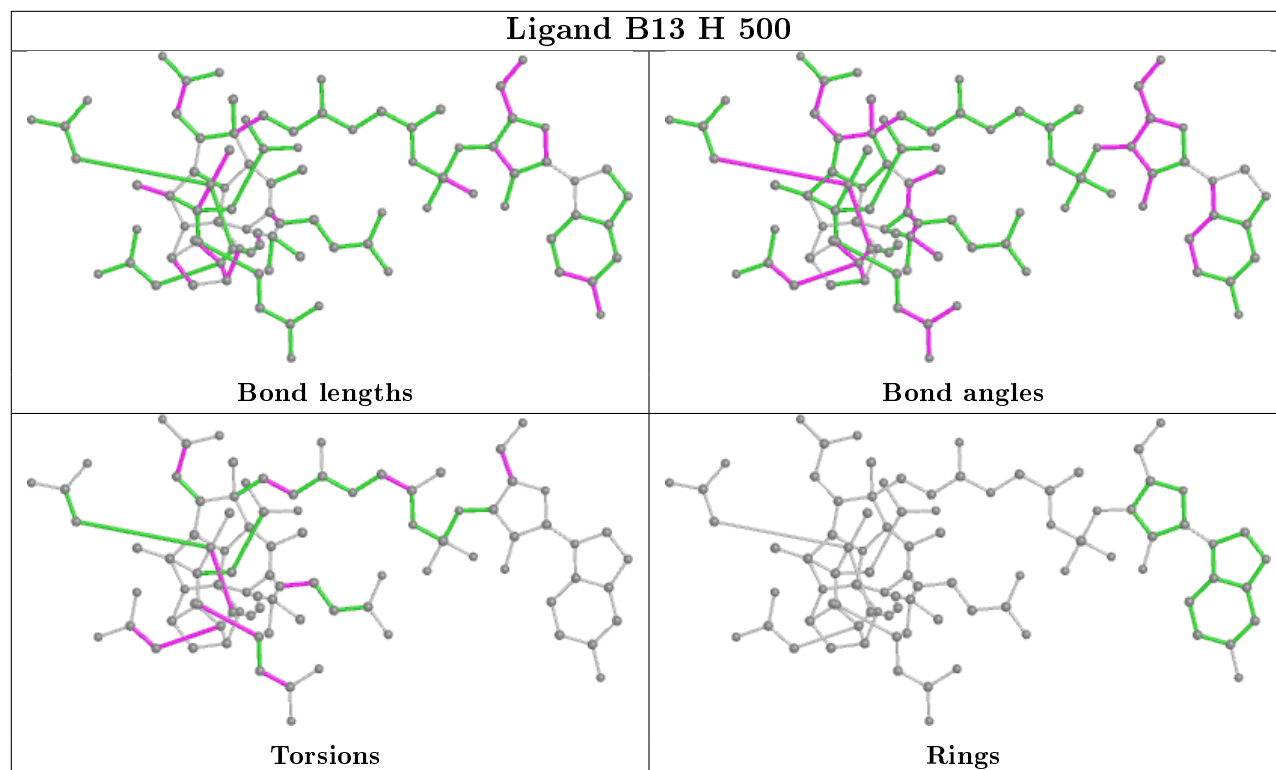
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 B13 F 500

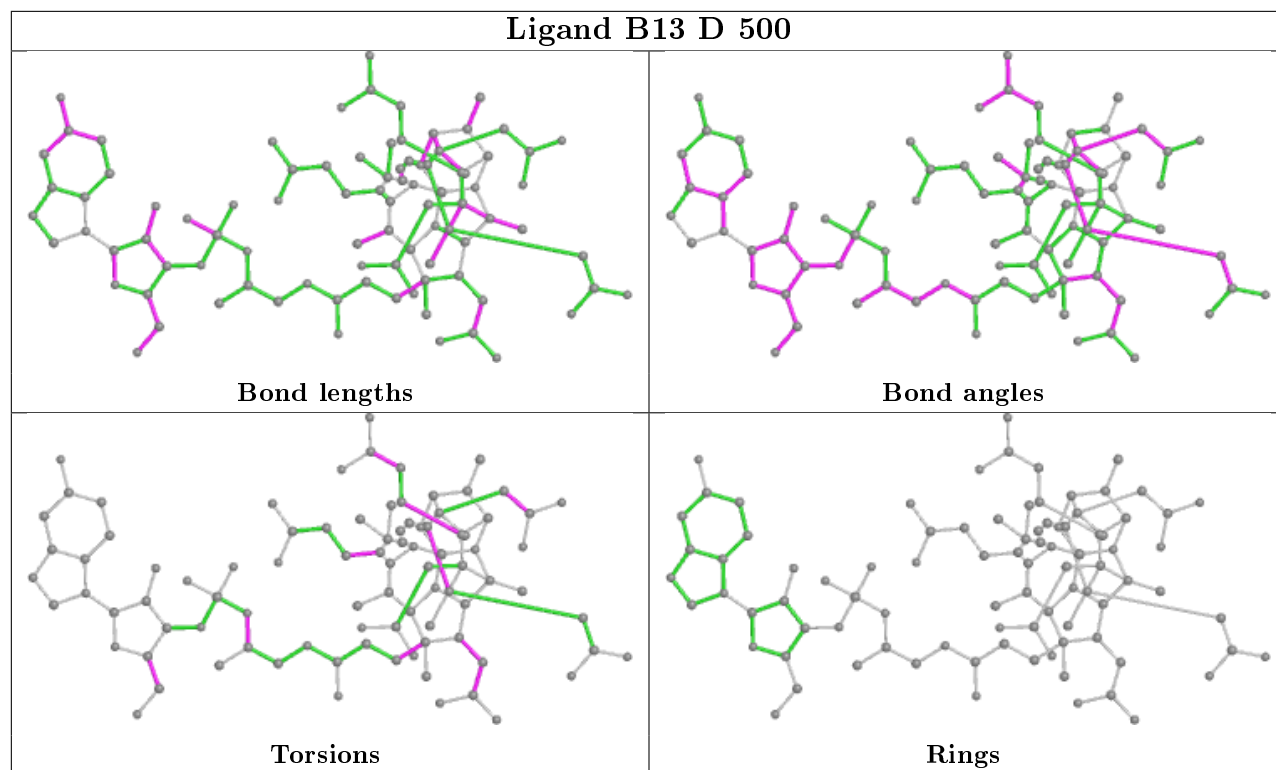


## Ligand B13 B 500

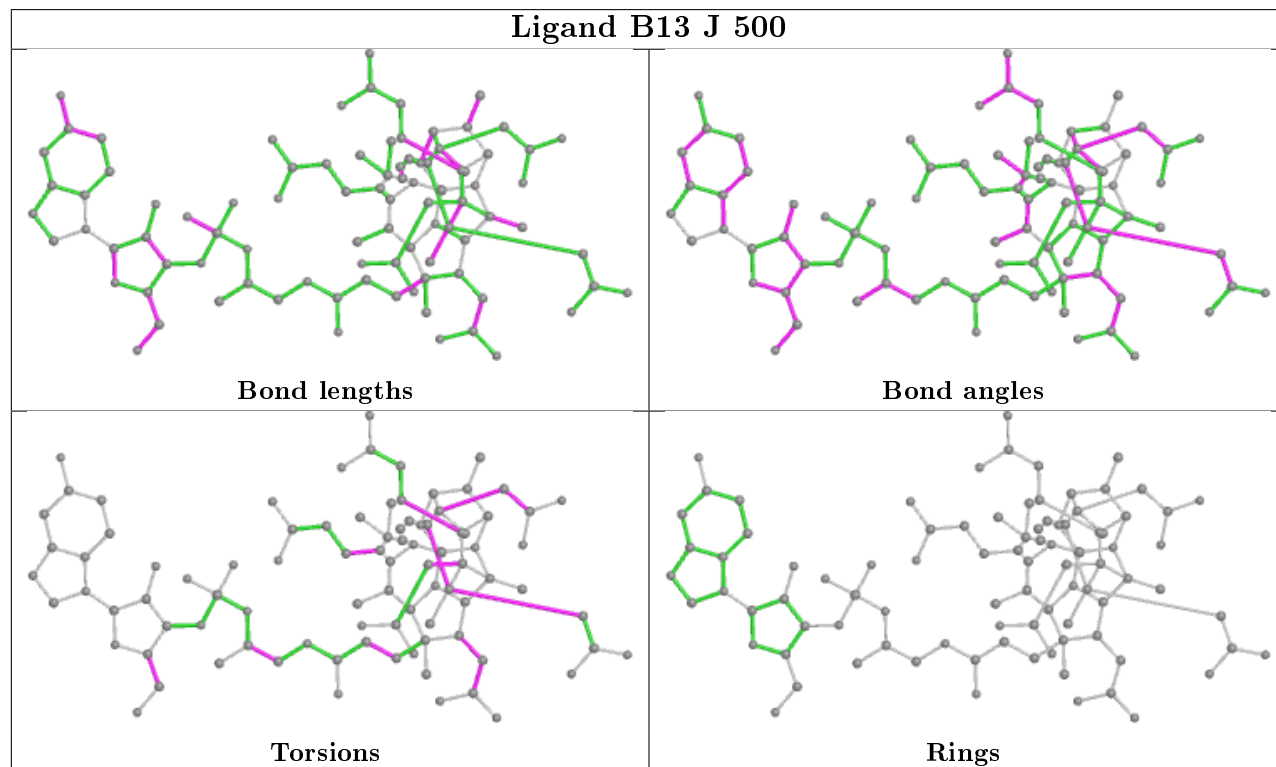


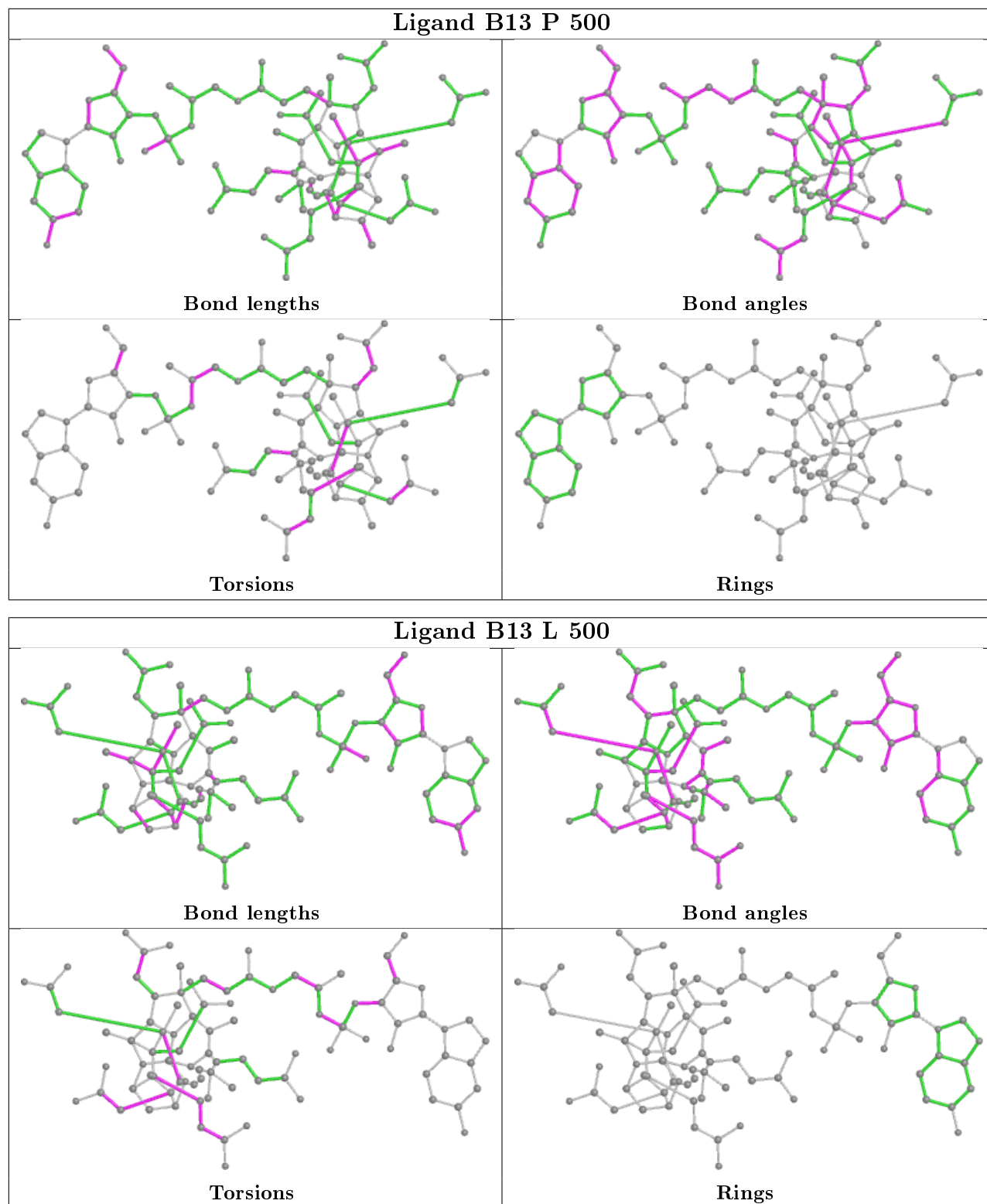


## Ligand B13 D 500



## Ligand B13 J 500





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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	459/461 (99%)	-0.25	0 <span>100</span> <span>100</span>	3, 11, 26, 38	0
1	C	459/461 (99%)	-0.25	0 <span>100</span> <span>100</span>	3, 10, 23, 39	0
1	E	459/461 (99%)	0.33	27 (5%) <span>22</span> <span>23</span>	25, 33, 42, 49	0
1	G	459/461 (99%)	0.02	11 (2%) <span>59</span> <span>62</span>	18, 29, 40, 49	0
1	I	459/461 (99%)	-0.17	4 (0%) <span>84</span> <span>86</span>	9, 20, 34, 50	0
1	K	459/461 (99%)	-0.16	3 (0%) <span>87</span> <span>89</span>	12, 20, 33, 46	0
1	M	459/461 (99%)	-0.20	1 (0%) <span>95</span> <span>95</span>	10, 20, 34, 48	0
1	O	459/461 (99%)	-0.20	1 (0%) <span>95</span> <span>95</span>	7, 18, 32, 45	0
2	B	258/258 (100%)	1.22	58 (22%) <span>0</span> <span>0</span>	4, 67, 100, 107	0
2	D	258/258 (100%)	1.31	71 (27%) <span>0</span> <span>0</span>	5, 66, 100, 110	0
2	F	258/258 (100%)	1.67	89 (34%) <span>0</span> <span>0</span>	18, 72, 102, 112	0
2	H	258/258 (100%)	2.10	116 (44%) <span>0</span> <span>0</span>	28, 73, 104, 110	0
2	J	258/258 (100%)	1.21	57 (22%) <span>0</span> <span>0</span>	17, 64, 97, 107	0
2	L	258/258 (100%)	1.63	97 (37%) <span>0</span> <span>0</span>	12, 71, 102, 113	0
2	N	258/258 (100%)	2.11	124 (48%) <span>0</span> <span>0</span>	12, 73, 103, 110	0
2	P	258/258 (100%)	1.25	51 (19%) <span>1</span> <span>1</span>	17, 67, 98, 108	0
All	All	5736/5752 (99%)	0.49	710 (12%) <span>4</span> <span>3</span>	3, 29, 92, 113	0

All (710) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	207	PHE	8.7
2	L	118	ALA	8.7
2	J	178	LEU	8.5
2	P	207	PHE	8.2
2	H	207	PHE	8.2

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Mol	Chain	Res	Type	RSRZ
2	F	207	PHE	8.0
2	P	208	ALA	8.0
2	L	119	THR	7.6
2	N	255	PHE	7.5
2	J	180	GLY	7.5
2	F	258	HIS	7.4
2	L	258	HIS	7.4
2	H	65	ALA	7.3
2	L	257	LYS	7.2
2	J	208	ALA	7.1
2	L	207	PHE	7.0
2	F	208	ALA	7.0
2	N	258	HIS	7.0
2	H	178	LEU	7.0
2	N	178	LEU	6.8
2	N	118	ALA	6.8
2	P	118	ALA	6.7
2	N	70	ILE	6.7
2	F	223	ALA	6.6
2	L	117	GLY	6.6
2	H	119	THR	6.6
2	B	119	THR	6.5
2	H	61	ALA	6.5
2	H	258	HIS	6.5
2	F	178	LEU	6.5
2	N	117	GLY	6.4
2	H	151	GLY	6.4
2	P	178	LEU	6.4
2	H	253	GLU	6.4
2	N	72	LEU	6.3
2	H	208	ALA	6.3
2	L	179	THR	6.2
2	N	257	LYS	6.1
2	H	245	THR	6.1
2	J	209	CYS	6.1
2	P	119	THR	6.0
2	D	226	VAL	6.0
2	D	199	LEU	6.0
2	L	189	TYR	6.0
2	P	209	CYS	6.0
2	H	123	LYS	6.0
2	N	179	THR	6.0

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Mol	Chain	Res	Type	RSRZ
2	P	179	THR	5.9
2	D	65	ALA	5.8
2	N	250	GLU	5.8
2	H	242	ILE	5.8
2	J	119	THR	5.8
2	H	118	ALA	5.7
2	H	117	GLY	5.7
2	J	179	THR	5.7
2	F	179	THR	5.7
2	D	59	LEU	5.7
2	D	258	HIS	5.6
2	F	249	THR	5.6
2	N	121	LYS	5.6
2	N	207	PHE	5.6
2	N	243	ALA	5.5
2	L	243	ALA	5.5
2	N	151	GLY	5.5
2	N	227	TYR	5.5
2	D	243	ALA	5.5
2	N	113	LYS	5.4
2	H	250	GLU	5.4
2	H	77	LEU	5.4
2	N	36	LYS	5.4
2	H	113	LYS	5.4
2	N	59	LEU	5.4
2	H	79	VAL	5.3
2	N	56	VAL	5.3
2	F	244	GLY	5.3
2	F	119	THR	5.2
2	L	208	ALA	5.2
2	B	178	LEU	5.2
2	D	207	PHE	5.2
2	F	189	TYR	5.2
2	N	199	LEU	5.2
2	N	119	THR	5.2
2	D	77	LEU	5.2
2	F	123	LYS	5.1
2	H	116	SER	5.1
2	L	65	ALA	5.1
2	B	77	LEU	5.1
2	H	243	ALA	5.1
2	F	117	GLY	5.1

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Mol	Chain	Res	Type	RSRZ
2	N	246	THR	5.1
2	H	57	GLU	5.0
2	N	221	GLN	5.0
2	N	226	VAL	5.0
2	P	36	LYS	5.0
2	N	76	ALA	5.0
2	H	133	GLY	5.0
2	H	115	ASN	4.9
2	B	208	ALA	4.9
2	F	243	ALA	4.9
2	N	240	ALA	4.9
2	N	189	TYR	4.9
2	D	249	THR	4.9
2	N	168	ALA	4.9
2	D	68	ASP	4.9
2	F	67	LYS	4.9
2	L	174	LYS	4.9
2	B	207	PHE	4.9
2	B	65	ALA	4.9
2	L	242	ILE	4.9
2	N	242	ILE	4.9
2	H	244	GLY	4.8
2	N	114	GLU	4.8
2	F	247	ASP	4.8
2	P	77	LEU	4.8
2	H	121	LYS	4.8
2	P	121	LYS	4.8
2	B	253	GLU	4.8
1	E	97	TRP	4.8
2	N	77	LEU	4.8
2	J	226	VAL	4.8
2	H	179	THR	4.7
2	J	191	PHE	4.7
2	D	178	LEU	4.7
2	H	257	LYS	4.7
2	P	67	LYS	4.7
2	D	208	ALA	4.7
2	N	204	LYS	4.7
2	D	253	GLU	4.7
2	F	180	GLY	4.7
2	H	122	THR	4.7
2	P	226	VAL	4.7

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Mol	Chain	Res	Type	RSRZ
2	L	76	ALA	4.7
2	L	120	PRO	4.7
2	H	209	CYS	4.6
2	B	244	GLY	4.6
2	F	257	LYS	4.6
2	H	180	GLY	4.6
2	F	200	GLU	4.6
2	F	77	LEU	4.6
2	J	258	HIS	4.6
2	L	246	THR	4.6
2	N	247	ASP	4.6
2	P	243	ALA	4.6
2	N	208	ALA	4.6
2	B	226	VAL	4.6
2	D	223	ALA	4.5
2	F	219	VAL	4.5
2	N	112	CYS	4.5
2	N	69	PRO	4.5
2	N	220	SER	4.5
2	N	176	ILE	4.4
2	N	249	THR	4.4
2	N	123	LYS	4.4
2	N	200	GLU	4.4
2	B	179	THR	4.4
1	E	3	ALA	4.4
2	H	216	GLN	4.4
2	P	180	GLY	4.4
2	D	255	PHE	4.4
2	B	68	ASP	4.4
2	H	199	LEU	4.4
2	N	37	ASP	4.4
2	N	71	ASP	4.4
2	H	70	ILE	4.3
2	F	204	LYS	4.3
1	E	445	THR	4.3
2	L	249	THR	4.3
2	H	62	ALA	4.3
2	L	253	GLU	4.3
2	N	68	ASP	4.3
2	B	258	HIS	4.3
2	H	110	GLU	4.3
2	H	217	ASP	4.2

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Mol	Chain	Res	Type	RSRZ
2	F	177	MET	4.2
2	H	67	LYS	4.2
2	B	242	ILE	4.2
2	N	209	CYS	4.2
2	P	65	ALA	4.2
2	D	224	LEU	4.2
2	L	177	MET	4.2
2	L	178	LEU	4.2
2	F	225	GLY	4.2
2	F	246	THR	4.1
2	H	36	LYS	4.1
2	D	172	LYS	4.1
2	N	106	LEU	4.1
2	F	68	ASP	4.1
2	B	118	ALA	4.1
2	P	117	GLY	4.0
2	N	248	VAL	4.0
2	H	172	LYS	4.0
2	B	249	THR	4.0
2	D	219	VAL	4.0
2	N	236	LYS	4.0
2	N	120	PRO	4.0
2	L	110	GLU	4.0
2	B	110	GLU	4.0
2	H	255	PHE	4.0
2	N	116	SER	4.0
2	H	112	CYS	4.0
2	L	43	ILE	3.9
2	L	222	PHE	3.9
2	D	180	GLY	3.9
2	P	258	HIS	3.9
2	D	112	CYS	3.9
2	H	64	GLU	3.9
2	B	63	ILE	3.9
2	D	179	THR	3.9
2	F	193	GLU	3.9
2	H	226	VAL	3.9
2	J	59	LEU	3.9
2	D	189	TYR	3.8
2	J	117	GLY	3.8
2	N	203	ILE	3.8
2	F	220	SER	3.8

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Mol	Chain	Res	Type	RSRZ
2	N	202	GLY	3.8
2	B	209	CYS	3.8
2	J	67	LYS	3.8
2	L	221	GLN	3.8
2	P	69	PRO	3.8
2	F	59	LEU	3.8
2	L	59	LEU	3.8
2	N	186	THR	3.8
2	J	110	GLU	3.8
2	J	177	MET	3.7
2	L	200	GLU	3.7
2	N	154	VAL	3.7
2	N	217	ASP	3.7
2	P	177	MET	3.7
2	P	191	PHE	3.7
2	L	151	GLY	3.7
2	N	150	ASN	3.7
2	H	51	GLU	3.7
2	B	109	ILE	3.6
2	B	243	ALA	3.6
2	D	119	THR	3.6
2	H	248	VAL	3.6
2	L	36	LYS	3.6
2	F	84	VAL	3.6
2	N	201	ASN	3.6
2	F	222	PHE	3.6
2	N	206	PRO	3.6
2	N	256	HIS	3.6
2	D	200	GLU	3.6
2	N	124	GLY	3.6
2	P	110	GLU	3.6
2	N	174	LYS	3.6
2	F	116	SER	3.5
2	N	253	GLU	3.5
2	D	121	LYS	3.5
2	D	236	LYS	3.5
2	F	209	CYS	3.5
2	N	232	ALA	3.5
2	P	257	LYS	3.5
2	F	255	PHE	3.5
2	F	253	GLU	3.5
2	H	200	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	8	SER	3.5
2	L	202	GLY	3.5
2	N	53	ASP	3.5
2	B	151	GLY	3.5
2	F	251	LEU	3.5
1	K	53	ALA	3.5
2	N	194	VAL	3.5
2	L	171	GLN	3.5
1	G	56	GLU	3.5
2	N	110	GLU	3.5
2	H	53	ASP	3.5
2	J	194	VAL	3.5
2	H	38	GLU	3.5
2	L	226	VAL	3.5
2	F	242	ILE	3.4
2	N	218	PHE	3.4
2	F	133	GLY	3.4
2	D	250	GLU	3.4
2	H	52	GLU	3.4
2	H	174	LYS	3.4
2	J	118	ALA	3.4
2	H	204	LYS	3.4
2	N	239	ASP	3.4
2	L	69	PRO	3.4
2	N	44	ALA	3.4
2	N	192	LYS	3.4
2	N	215	ASN	3.4
2	P	122	THR	3.4
2	J	225	GLY	3.3
2	N	198	LEU	3.3
2	H	247	ASP	3.3
2	L	77	LEU	3.3
2	N	43	ILE	3.3
2	B	69	PRO	3.3
2	D	246	THR	3.3
2	H	120	PRO	3.3
2	J	257	LYS	3.3
2	P	116	SER	3.3
1	K	134	GLU	3.3
2	L	114	GLU	3.3
2	N	164	GLU	3.3
2	L	241	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
2	N	65	ALA	3.3
1	E	460	GLY	3.3
2	B	180	GLY	3.3
2	L	180	GLY	3.3
2	H	107	GLU	3.3
2	F	162	PRO	3.3
2	L	192	LYS	3.3
2	H	249	THR	3.3
2	N	122	THR	3.3
2	N	64	GLU	3.3
2	H	189	TYR	3.3
2	D	58	GLY	3.2
2	L	199	LEU	3.2
2	H	241	ILE	3.2
2	J	237	ILE	3.2
1	E	4	LYS	3.2
2	F	196	ASP	3.2
2	H	66	GLY	3.2
2	B	236	LYS	3.2
2	N	35	PRO	3.2
2	H	68	ASP	3.2
2	J	128	CYS	3.2
2	L	209	CYS	3.2
2	N	219	VAL	3.2
2	B	71	ASP	3.2
2	P	155	VAL	3.2
2	N	67	LYS	3.2
2	L	194	VAL	3.2
2	J	53	ASP	3.1
2	F	112	CYS	3.1
2	L	112	CYS	3.1
2	L	166	VAL	3.1
2	F	226	VAL	3.1
2	H	7	ALA	3.1
2	L	248	VAL	3.1
2	B	200	GLU	3.1
2	H	49	GLU	3.1
2	N	52	GLU	3.1
2	F	47	ILE	3.1
2	P	172	LYS	3.1
2	B	247	ASP	3.1
2	J	116	SER	3.1

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Mol	Chain	Res	Type	RSRZ
2	F	156	ASP	3.1
2	F	38	GLU	3.1
2	B	59	LEU	3.1
2	F	65	ALA	3.1
2	P	194	VAL	3.1
2	N	42	PRO	3.1
2	N	222	PHE	3.1
2	H	75	ASP	3.0
2	D	109	ILE	3.0
2	P	112	CYS	3.0
2	H	59	LEU	3.0
2	N	38	GLU	3.0
2	F	113	LYS	3.0
1	E	53	ALA	3.0
2	H	223	ALA	3.0
2	F	22	LYS	3.0
2	H	162	PRO	3.0
2	D	242	ILE	3.0
1	O	53	ALA	3.0
2	B	56	VAL	3.0
2	D	225	GLY	3.0
2	L	255	PHE	3.0
2	P	242	ILE	3.0
2	N	172	LYS	3.0
2	H	41	TYR	3.0
2	D	251	LEU	3.0
2	H	108	GLY	3.0
2	L	113	LYS	3.0
2	D	191	PHE	3.0
2	H	191	PHE	3.0
2	B	227	TYR	3.0
2	L	227	TYR	3.0
2	H	251	LEU	3.0
2	N	205	ILE	2.9
2	B	246	THR	2.9
2	F	23	ALA	2.9
2	F	118	ALA	2.9
2	H	227	TYR	2.9
2	J	251	LEU	2.9
2	F	201	ASN	2.9
2	N	107	GLU	2.9
2	P	253	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
2	H	78	MET	2.9
2	D	222	PHE	2.9
1	E	93	ASN	2.9
1	I	3	ALA	2.9
2	B	37	ASP	2.9
2	J	68	ASP	2.9
2	N	60	GLN	2.9
2	N	63	ILE	2.9
2	F	194	VAL	2.9
2	H	155	VAL	2.9
1	E	135	PHE	2.9
1	E	431	ALA	2.9
2	B	60	GLN	2.9
2	J	254	LYS	2.9
2	N	241	ILE	2.9
2	F	174	LYS	2.9
2	L	129	HIS	2.9
2	F	248	VAL	2.8
2	H	156	ASP	2.8
2	P	210	GLY	2.8
2	D	174	LYS	2.8
2	L	39	LEU	2.8
2	D	116	SER	2.8
2	H	80	GLY	2.8
2	B	67	LYS	2.8
2	B	191	PHE	2.8
2	F	160	ASP	2.8
2	D	201	ASN	2.8
2	H	153	ASN	2.8
2	N	254	LYS	2.8
2	F	171	GLN	2.8
2	H	63	ILE	2.8
2	N	129	HIS	2.8
2	F	36	LYS	2.8
2	J	200	GLU	2.8
2	N	41	TYR	2.8
2	B	121	LYS	2.8
2	P	206	PRO	2.8
2	B	217	ASP	2.8
2	L	217	ASP	2.8
2	N	223	ALA	2.8
2	F	164	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	248	VAL	2.8
2	B	255	PHE	2.8
2	D	37	ASP	2.8
2	J	69	PRO	2.8
1	E	133	ARG	2.7
2	H	86	ARG	2.7
2	F	132	GLU	2.7
2	N	133	GLY	2.7
2	H	252	ARG	2.7
2	N	104	ALA	2.7
2	F	199	LEU	2.7
2	F	217	ASP	2.7
2	F	129	HIS	2.7
2	F	221	GLN	2.7
2	J	172	LYS	2.7
2	P	236	LYS	2.7
2	J	234	ALA	2.7
2	N	237	ILE	2.7
2	D	192	LYS	2.7
2	L	67	LYS	2.7
2	P	70	ILE	2.7
2	P	129	HIS	2.7
2	B	51	GLU	2.7
2	J	162	PRO	2.7
2	L	193	GLU	2.7
2	D	204	LYS	2.7
2	N	125	THR	2.7
2	H	222	PHE	2.7
2	P	59	LEU	2.7
2	D	206	PRO	2.7
2	D	257	LYS	2.7
2	L	254	LYS	2.7
2	D	209	CYS	2.7
2	F	110	GLU	2.7
2	H	232	ALA	2.7
1	I	133	ARG	2.7
2	D	205	ILE	2.7
2	L	70	ILE	2.7
2	L	198	LEU	2.7
1	E	208	LYS	2.7
2	H	45	LYS	2.7
2	F	37	ASP	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	N	245	THR	2.6
2	H	47	ILE	2.6
2	J	199	LEU	2.6
2	J	244	GLY	2.6
2	H	132	GLU	2.6
2	B	257	LYS	2.6
2	N	50	GLY	2.6
2	N	167	LEU	2.6
2	H	43	ILE	2.6
2	N	177	MET	2.6
2	N	51	GLU	2.6
2	P	52	GLU	2.6
2	H	56	VAL	2.6
2	L	56	VAL	2.6
2	L	80	GLY	2.6
2	L	251	LEU	2.6
2	P	53	ASP	2.6
2	N	73	ILE	2.6
2	H	60	GLN	2.6
1	E	452	LYS	2.6
2	N	244	GLY	2.6
2	L	155	VAL	2.6
2	H	114	GLU	2.6
2	P	225	GLY	2.6
2	F	250	GLU	2.6
2	H	106	LEU	2.6
2	H	202	GLY	2.6
2	B	114	GLU	2.6
2	F	51	GLU	2.6
2	J	65	ALA	2.5
2	D	247	ASP	2.5
1	E	148	GLU	2.5
2	B	116	SER	2.5
2	L	225	GLY	2.5
1	G	3	ALA	2.5
2	H	149	ALA	2.5
2	J	60	GLN	2.5
2	P	181	THR	2.5
2	H	167	LEU	2.5
2	D	66	GLY	2.5
2	N	75	ASP	2.5
2	L	63	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	105	MET	2.5
2	N	162	PRO	2.5
2	P	166	VAL	2.5
2	B	58	GLY	2.5
2	L	244	GLY	2.5
2	D	64	GLU	2.5
2	D	69	PRO	2.5
2	J	181	THR	2.5
2	B	189	TYR	2.5
2	D	256	HIS	2.5
1	E	457	GLU	2.5
2	L	52	GLU	2.5
1	I	4	LYS	2.5
1	G	437	ASP	2.5
2	H	76	ALA	2.5
2	J	206	PRO	2.5
2	L	23	ALA	2.5
2	H	160	ASP	2.5
2	N	23	ALA	2.5
2	L	250	GLU	2.5
2	J	127	VAL	2.4
2	D	196	ASP	2.4
2	N	105	MET	2.4
2	N	197	MET	2.4
2	F	69	PRO	2.4
2	F	108	GLY	2.4
2	J	202	GLY	2.4
2	F	224	LEU	2.4
2	N	147	LEU	2.4
2	J	189	TYR	2.4
1	G	461	PHE	2.4
2	H	203	ILE	2.4
2	J	64	GLU	2.4
2	L	109	ILE	2.4
2	F	120	PRO	2.4
2	P	158	GLY	2.4
2	L	58	GLY	2.4
2	N	216	GLN	2.4
2	L	234	ALA	2.4
2	D	164	GLU	2.4
1	E	449	SER	2.4
2	L	146	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	P	227	TYR	2.4
2	J	210	GLY	2.4
2	H	42	PRO	2.4
2	J	243	ALA	2.4
1	K	141	ASP	2.4
2	L	233	ASP	2.4
2	D	133	GLY	2.4
2	D	215	ASN	2.4
1	E	443	CYS	2.4
2	N	185	THR	2.4
2	P	202	GLY	2.4
2	J	129	HIS	2.4
2	N	191	PHE	2.4
2	L	37	ASP	2.4
2	D	221	GLN	2.4
2	L	72	LEU	2.4
2	B	70	ILE	2.3
2	B	177	MET	2.3
2	H	109	ILE	2.3
2	L	38	GLU	2.3
2	F	154	VAL	2.3
1	E	435	ASP	2.3
2	D	177	MET	2.3
2	D	230	GLU	2.3
2	F	203	ILE	2.3
2	F	205	ILE	2.3
2	H	81	MET	2.3
2	H	168	ALA	2.3
2	D	71	ASP	2.3
2	D	217	ASP	2.3
2	H	214	VAL	2.3
2	L	218	PHE	2.3
1	E	5	ARG	2.3
2	H	20	LEU	2.3
2	N	251	LEU	2.3
2	F	172	LYS	2.3
2	L	130	VAL	2.3
2	P	127	VAL	2.3
2	J	242	ILE	2.3
2	B	232	ALA	2.3
1	E	210	THR	2.3
2	F	54	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	52	GLU	2.3
2	L	164	GLU	2.3
2	D	203	ILE	2.3
2	L	247	ASP	2.3
2	H	111	TYR	2.3
2	B	206	PRO	2.3
2	F	114	GLU	2.3
2	F	80	GLY	2.3
1	G	133	ARG	2.2
2	L	197	MET	2.2
2	L	216	GLN	2.2
2	L	57	GLU	2.2
2	H	224	LEU	2.2
2	P	71	ASP	2.2
2	F	43	ILE	2.2
1	E	27	LYS	2.2
2	B	36	LYS	2.2
2	L	123	LYS	2.2
2	L	167	LEU	2.2
2	J	120	PRO	2.2
2	H	239	ASP	2.2
2	N	180	GLY	2.2
2	F	81	MET	2.2
2	J	121	LYS	2.2
2	D	57	GLU	2.2
2	D	78	MET	2.2
2	H	154	VAL	2.2
2	L	79	VAL	2.2
2	N	57	GLU	2.2
2	B	74	ASP	2.2
2	N	212	GLY	2.2
2	B	55	VAL	2.2
2	J	76	ALA	2.2
1	G	438	LYS	2.2
2	F	128	CYS	2.2
2	H	206	PRO	2.2
2	J	77	LEU	2.2
2	N	146	LEU	2.2
1	E	209	LYS	2.2
1	E	427	ALA	2.2
2	H	238	ALA	2.2
1	E	7	THR	2.2

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Mol	Chain	Res	Type	RSRZ
2	L	68	ASP	2.2
2	N	109	ILE	2.2
2	L	210	GLY	2.2
2	P	255	PHE	2.2
2	H	72	LEU	2.2
2	L	224	LEU	2.2
2	F	74	ASP	2.1
2	H	37	ASP	2.1
2	J	5	THR	2.1
2	J	38	GLU	2.1
2	J	224	LEU	2.1
2	P	113	LYS	2.1
1	E	441	ASP	2.1
2	D	53	ASP	2.1
2	H	195	ASN	2.1
1	G	409	ALA	2.1
2	D	210	GLY	2.1
2	H	19	ALA	2.1
2	H	193	GLU	2.1
2	D	245	THR	2.1
2	J	236	LYS	2.1
2	L	203	ILE	2.1
2	N	39	LEU	2.1
2	F	52	GLU	2.1
1	G	423	ALA	2.1
2	F	121	LYS	2.1
2	L	50	GLY	2.1
2	N	171	GLN	2.1
2	F	230	GLU	2.1
2	J	174	LYS	2.1
2	F	234	ALA	2.1
2	H	35	PRO	2.1
2	H	142	ILE	2.1
2	L	47	ILE	2.1
1	M	134	GLU	2.1
1	E	387	ASP	2.1
2	F	236	LYS	2.1
2	B	201	ASN	2.1
2	N	169	ALA	2.1
1	G	416	ARG	2.1
2	L	116	SER	2.1
2	J	36	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	J	190	ALA	2.1
2	L	121	LYS	2.1
2	D	55	VAL	2.1
2	J	47	ILE	2.1
2	L	256	HIS	2.1
1	E	461	PHE	2.1
1	G	135	PHE	2.1
2	D	72	LEU	2.1
2	H	198	LEU	2.1
2	L	51	GLU	2.1
2	B	113	LYS	2.1
2	B	172	LYS	2.1
2	F	252	ARG	2.1
2	F	168	ALA	2.0
2	L	175	PRO	2.0
2	D	130	VAL	2.0
2	H	246	THR	2.0
2	L	55	VAL	2.0
2	N	79	VAL	2.0
2	P	205	ILE	2.0
1	G	460	GLY	2.0
2	D	108	GLY	2.0
2	B	248	VAL	2.0
2	H	221	GLN	2.0
2	L	220	SER	2.0
2	D	198	LEU	2.0
2	P	228	GLY	2.0
2	F	191	PHE	2.0
2	B	174	LYS	2.0
2	L	168	ALA	2.0
2	P	128	CYS	2.0
1	I	460	GLY	2.0
2	L	156	ASP	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

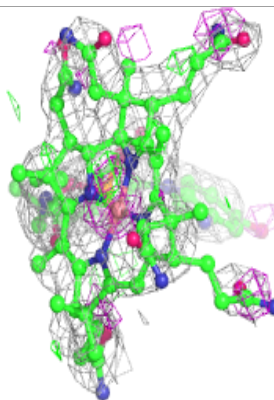
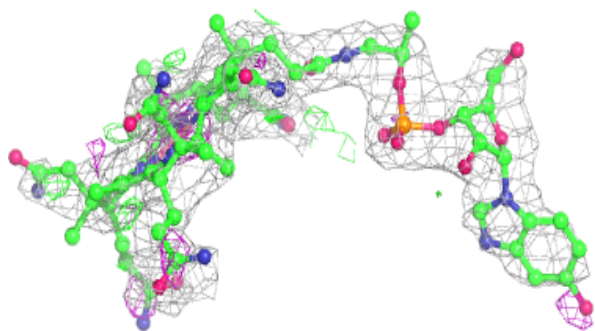
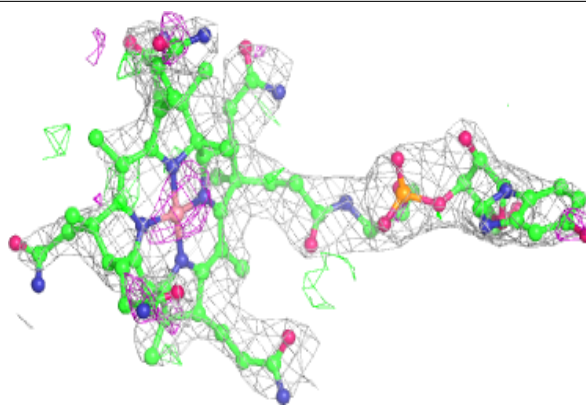
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	K	G	514	1/1	0.82	0.20	39,39,39,39	1
5	B13	N	500	90/90	0.91	0.22	60,66,72,73	0
3	ZN	E	503	1/1	0.91	0.11	36,36,36,36	1
4	K	E	513	1/1	0.91	0.12	33,33,33,33	1
4	K	O	518	1/1	0.92	0.12	35,35,35,35	1
4	K	I	515	1/1	0.92	0.09	28,28,28,28	1
5	B13	F	500	90/90	0.92	0.21	53,63,71,72	0
5	B13	L	500	90/90	0.94	0.21	41,47,58,59	0
5	B13	H	500	90/90	0.94	0.18	45,58,68,69	0
5	B13	P	500	90/90	0.94	0.18	31,40,45,52	0
4	K	M	517	1/1	0.95	0.11	33,33,33,33	1
4	K	C	512	1/1	0.95	0.15	22,22,22,22	1
5	B13	J	500	90/90	0.95	0.17	32,37,50,57	0
5	B13	D	500	90/90	0.96	0.17	20,30,40,42	0
3	ZN	O	508	1/1	0.96	0.07	33,33,33,33	0
4	K	A	511	1/1	0.97	0.09	23,23,23,23	1
5	B13	B	500	90/90	0.97	0.14	9,24,48,49	0
3	ZN	G	504	1/1	0.97	0.09	33,33,33,33	1
3	ZN	I	505	1/1	0.98	0.09	30,30,30,30	0
3	ZN	A	501	1/1	0.98	0.11	20,20,20,20	0
3	ZN	C	502	1/1	0.99	0.11	19,19,19,19	0
3	ZN	K	506	1/1	0.99	0.11	33,33,33,33	0
3	ZN	E	522	1/1	0.99	0.08	37,37,37,37	0
3	ZN	M	523	1/1	0.99	0.10	21,21,21,21	0
3	ZN	M	507	1/1	0.99	0.13	33,33,33,33	0
3	ZN	I	521	1/1	0.99	0.08	16,16,16,16	0
4	K	K	516	1/1	0.99	0.07	31,31,31,31	1
3	ZN	A	524	1/1	1.00	0.09	9,9,9,9	0

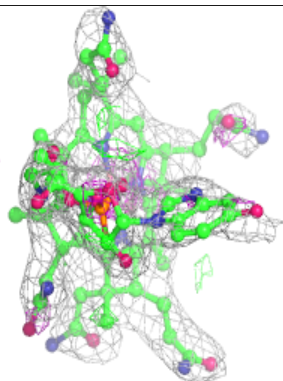
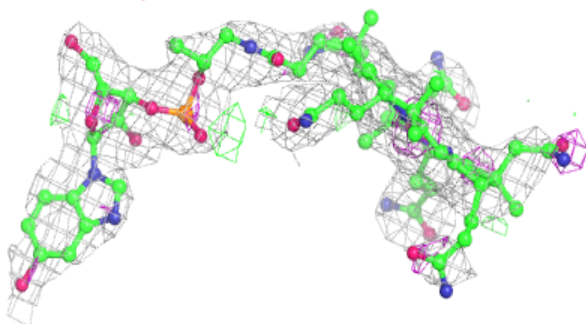
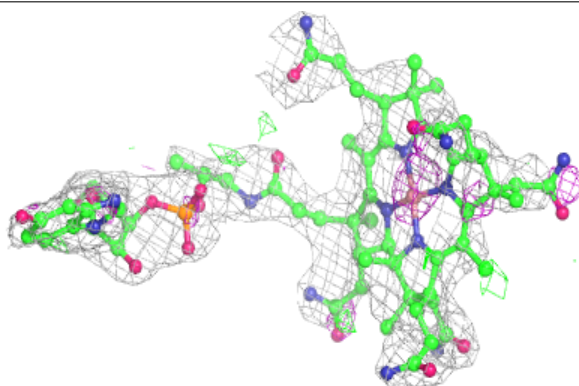
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around B13 N 500:**

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

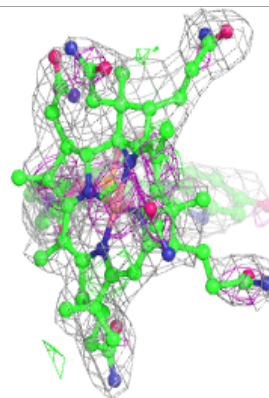
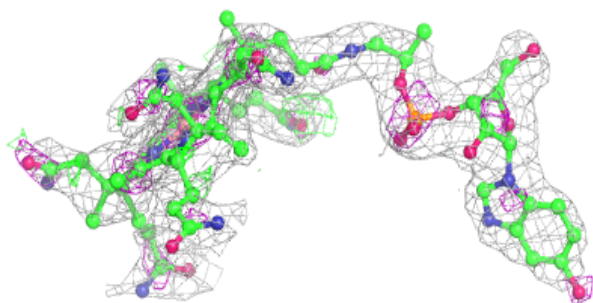
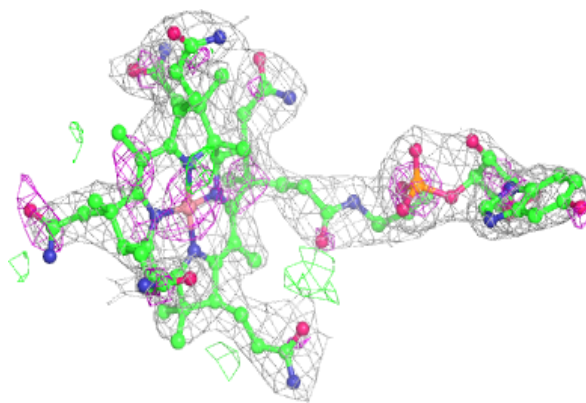
**Electron density around B13 F 500:**

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

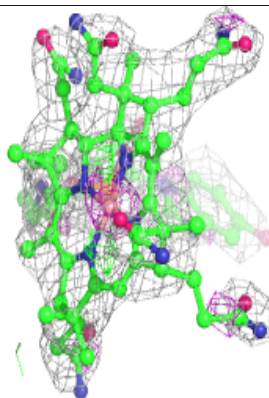
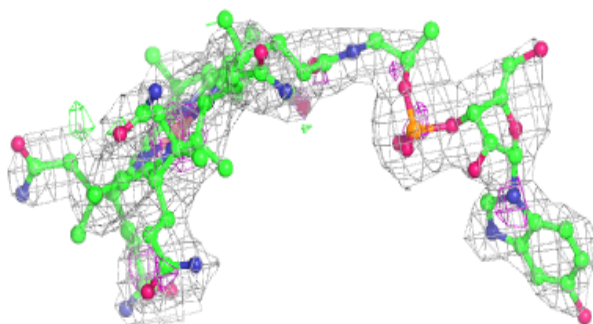
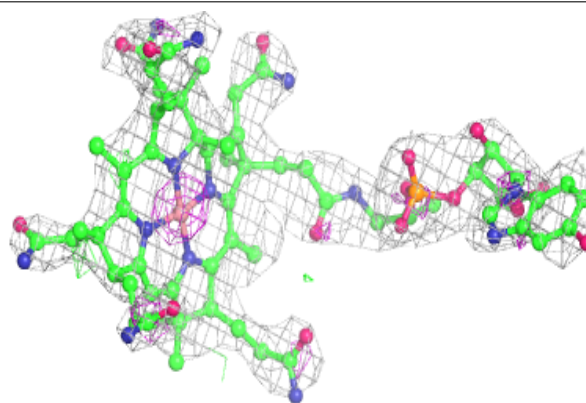


**Electron density around B13 L 500:**

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

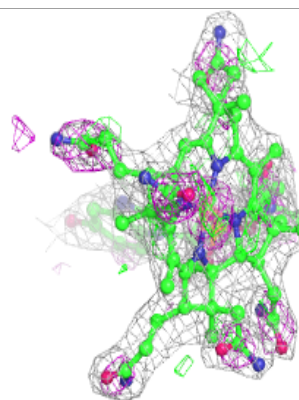
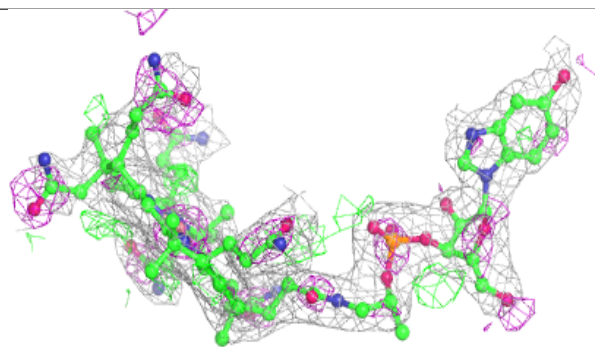
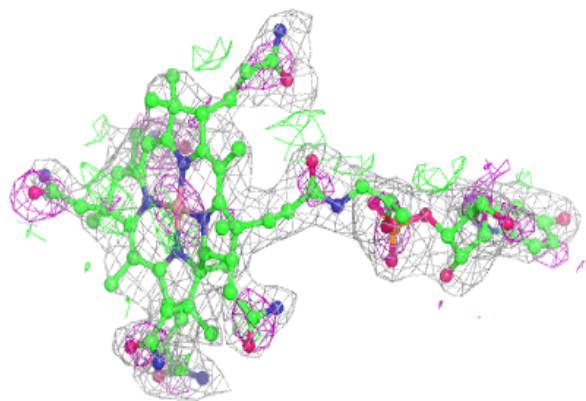
**Electron density around B13 H 500:**

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

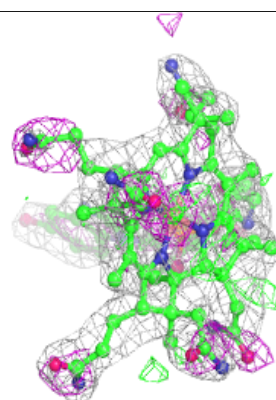
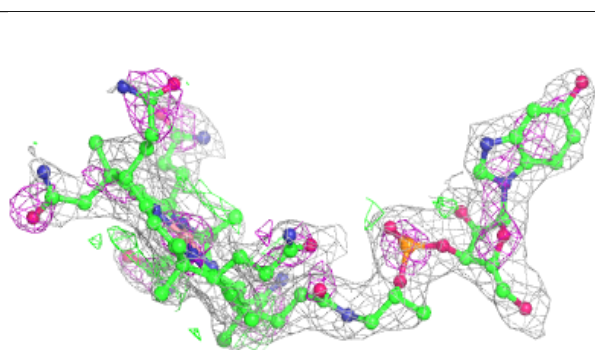
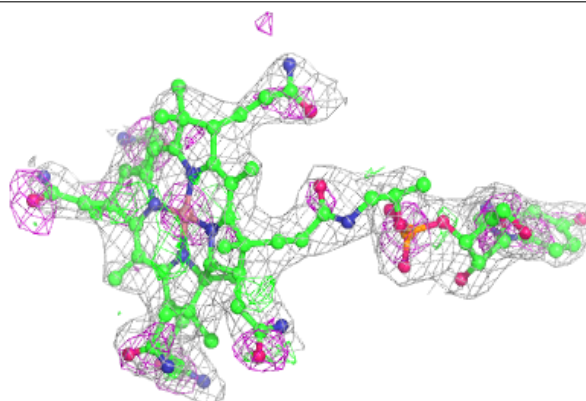


**Electron density around B13 P 500:**

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

**Electron density around B13 J 500:**

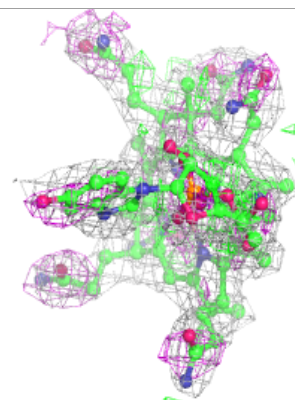
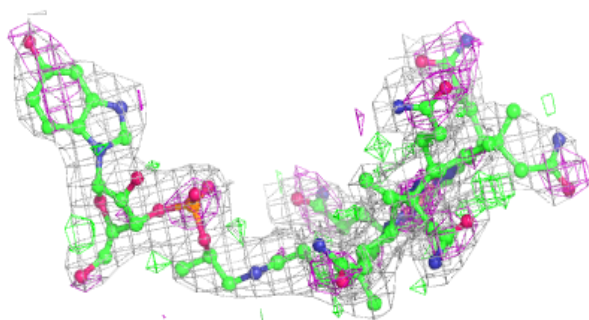
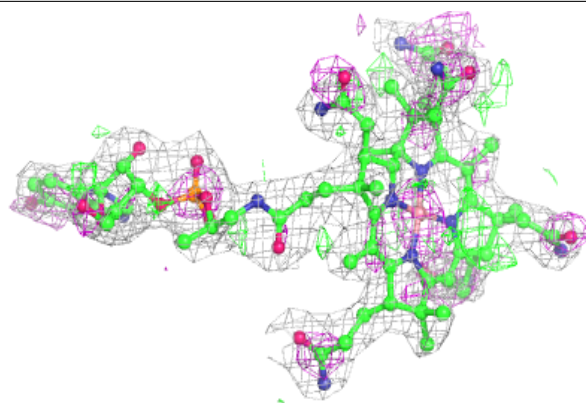
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



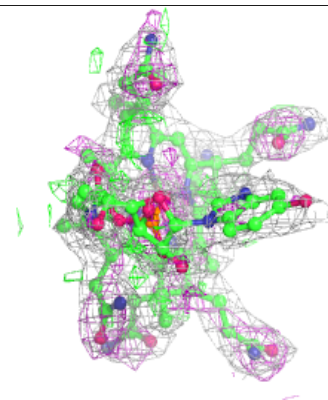
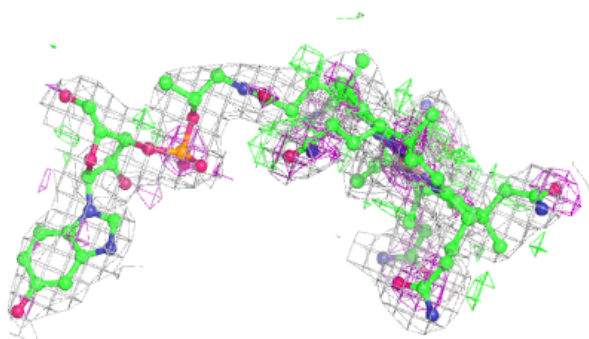
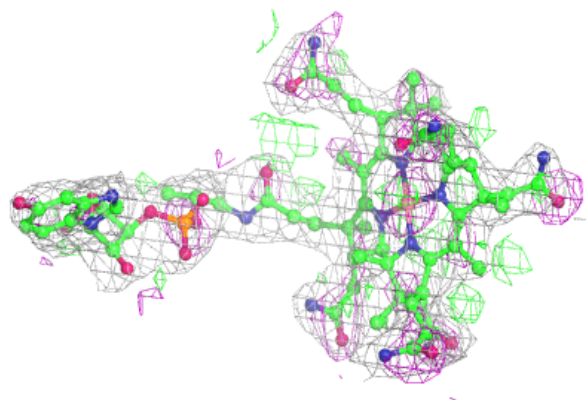


**Electron density around B13 D 500:**

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

**Electron density around B13 B 500:**

$2mF_o-DF_c$  (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.