



# Full wwPDB X-ray Structure Validation Report ⓘ

May 19, 2020 – 02:33 am BST

PDB ID : 1AYP  
Title : A PROBE MOLECULE COMPOSED OF SEVENTEEN PERCENT OF TOTAL DIFFRACTING MATTER GIVES CORRECT SOLUTIONS IN MOLECULAR REPLACEMENT  
Authors : Oh, B.-H.  
Deposited on : 1994-07-19  
Resolution : 2.57 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

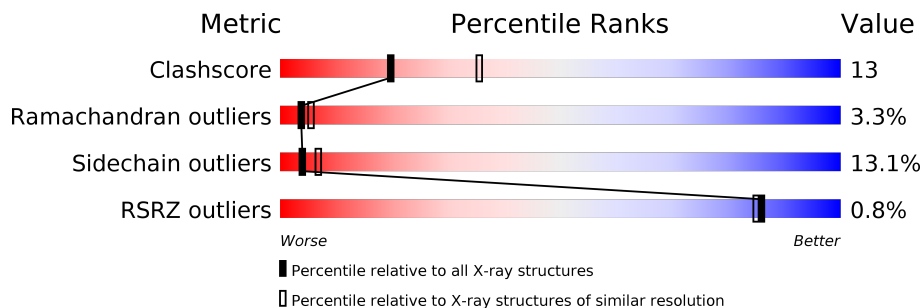
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.57 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))
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

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	124	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 56%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 27%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 16%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: grey; margin-right: 2px;"></div> </div> <p style="text-align: center; margin-top: 5px;">2%      56%      27%      16%      .</p>
1	B	124	<div style="display: flex; align-items: center;"> <div style="width: 58%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 31%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 8%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 3%; height: 10px; background-color: red; margin-right: 2px;"></div> </div> <p style="text-align: center; margin-top: 5px;">58%      31%      8%      .</p>
1	C	124	<div style="display: flex; align-items: center;"> <div style="width: 53%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 35%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 9%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 3%; height: 10px; background-color: red; margin-right: 2px;"></div> </div> <p style="text-align: center; margin-top: 5px;">53%      35%      9%      .</p>
1	D	124	<div style="display: flex; align-items: center;"> <div style="width: 63%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 27%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 8%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> </div> <p style="text-align: center; margin-top: 5px;">63%      27%      8%      .</p>
1	E	124	<div style="display: flex; align-items: center;"> <div style="width: 55%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 34%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 8%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 3%; height: 10px; background-color: red; margin-right: 2px;"></div> </div> <p style="text-align: center; margin-top: 5px;">%      55%      34%      8%      .</p>
1	F	124	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 57%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 35%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 7%; height: 10px; background-color: orange; margin-right: 2px;"></div> </div> <p style="text-align: center; margin-top: 5px;">2%      57%      35%      7%      .</p>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5988 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.

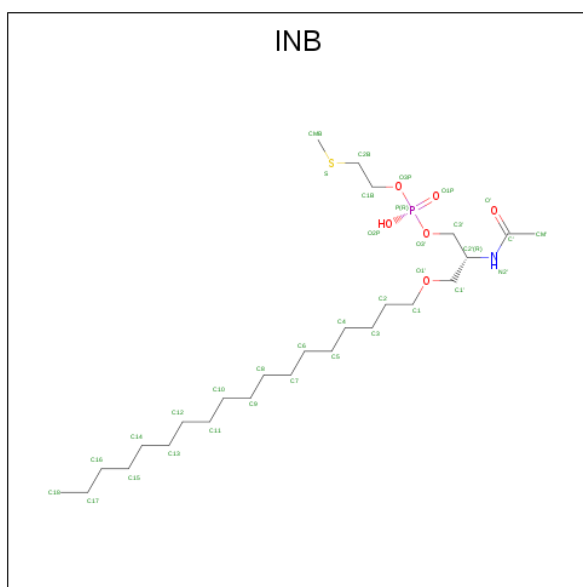
- Molecule 1 is a protein called PHOSPHOLIPASE A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	124	Total 960	C 586	N 181	O 178	S 15	0	0	0
1	B	124	Total 960	C 586	N 181	O 178	S 15	0	0	0
1	C	124	Total 960	C 586	N 181	O 178	S 15	0	0	0
1	D	124	Total 960	C 586	N 181	O 178	S 15	0	0	0
1	E	124	Total 960	C 586	N 181	O 178	S 15	0	0	0
1	F	124	Total 960	C 586	N 181	O 178	S 15	0	0	0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	2	Total Ca 2 2	0	0
2	E	2	Total Ca 2 2	0	0
2	B	2	Total Ca 2 2	0	0
2	C	2	Total Ca 2 2	0	0
2	A	2	Total Ca 2 2	0	0
2	F	2	Total Ca 2 2	0	0

- Molecule 3 is 1-OCTADECYL-2-ACETAMIDO-2-DEOXY-SN-GLYCEROL-3-PHOSPHOETHYLMETHYL SULFIDE (three-letter code: INB) (formula: C<sub>26</sub>H<sub>54</sub>NO<sub>6</sub>PS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
3	A	1	Total	C	N	O	P	S	0	0
			35	26	1	6	1	1		
3	B	1	Total	C	N	O	P	S	0	0
			35	26	1	6	1	1		
3	C	1	Total	C	N	O	P	S	0	0
			35	26	1	6	1	1		
3	D	1	Total	C	N	O	P	S	0	0
			35	26	1	6	1	1		
3	E	1	Total	C	N	O	P	S	0	0
			35	26	1	6	1	1		
3	F	1	Total	C	N	O	P	S	0	0
			35	26	1	6	1	1		

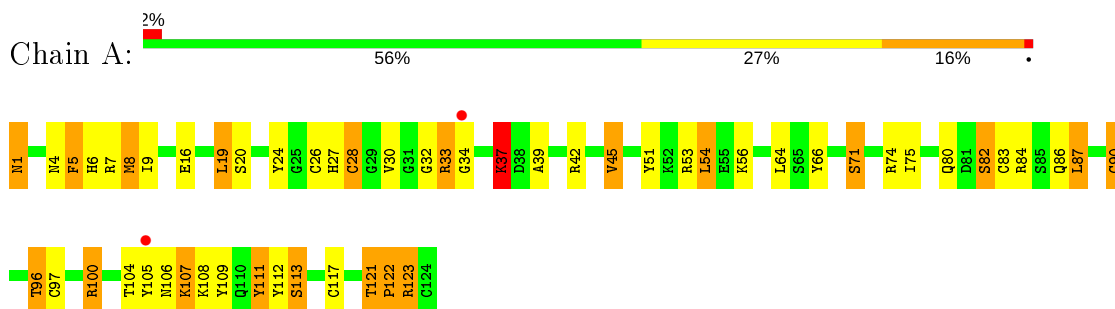
- Molecule 4 is water.

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

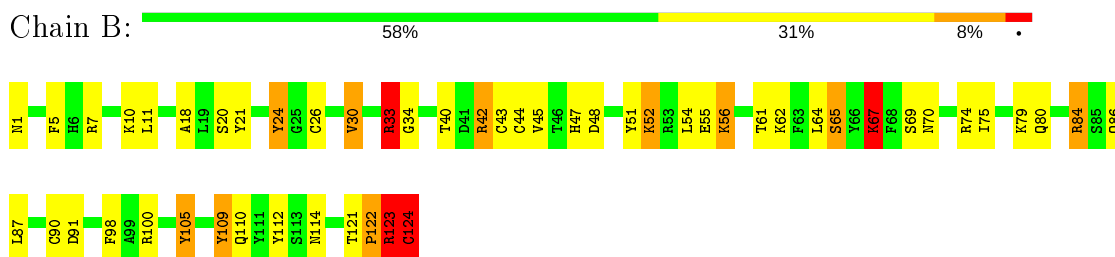
### 3 Residue-property plots [i](#)

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.

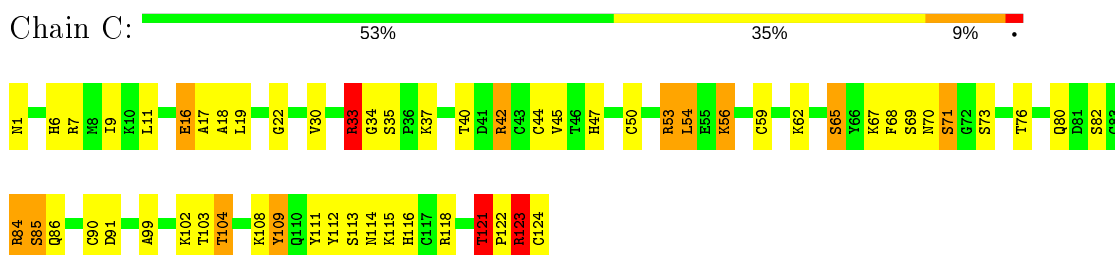
- Molecule 1: PHOSPHOLIPASE A2



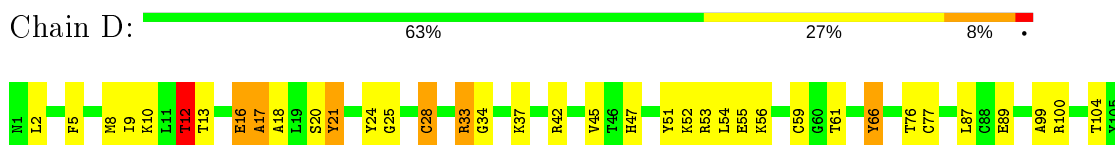
- Molecule 1: PHOSPHOLIPASE A2



- Molecule 1: PHOSPHOLIPASE A2

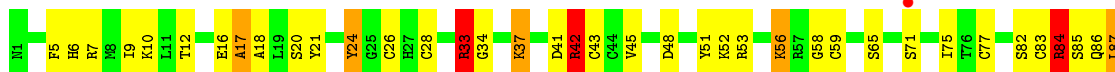


- Molecule 1: PHOSPHOLIPASE A2

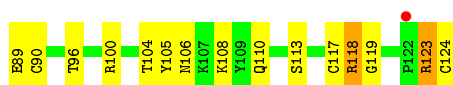




- Molecule 1: PHOSPHOLIPASE A2



- Molecule 1: PHOSPHOLIPASE A2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.51Å 114.72Å 64.43Å 90.00° 120.13° 90.00°	Depositor
Resolution (Å)	8.00 – 2.57 55.72 – 2.57	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.57) 85.9 (55.72-2.57)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.26 (at 2.58Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.214 , (Not available) 0.201 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.4	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 59.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.031 for l,k,-h-l 0.031 for -h-l,k,h 0.416 for l,-k,h 0.035 for -h-l,-k,l 0.039 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	5988	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.31% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, INB

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	1.12	2/978 (0.2%)	1.93	23/1305 (1.8%)
1	B	1.04	1/978 (0.1%)	1.89	26/1305 (2.0%)
1	C	1.04	0/978	2.02	30/1305 (2.3%)
1	D	1.02	0/978	1.87	24/1305 (1.8%)
1	E	1.07	3/978 (0.3%)	1.94	24/1305 (1.8%)
1	F	1.07	1/978 (0.1%)	1.95	21/1305 (1.6%)
All	All	1.06	7/5868 (0.1%)	1.93	148/7830 (1.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	C	0	2
1	D	0	2
1	E	0	1
All	All	0	8

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	16	GLU	CB-CG	5.65	1.62	1.52
1	A	71	SER	CB-OG	5.37	1.49	1.42
1	B	65	SER	CA-CB	-5.37	1.44	1.52
1	E	16	GLU	CG-CD	5.27	1.59	1.51
1	F	123	ARG	NE-CZ	5.20	1.39	1.33
1	A	53	ARG	NE-CZ	5.07	1.39	1.33
1	E	90	CYS	CA-CB	-5.01	1.43	1.53



All (148) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	53	ARG	NE-CZ-NH1	13.49	127.04	120.30
1	F	33	ARG	NE-CZ-NH1	13.07	126.83	120.30
1	C	123	ARG	CA-C-N	-11.88	91.07	117.20
1	C	42	ARG	NE-CZ-NH1	10.47	125.54	120.30
1	E	84	ARG	NE-CZ-NH1	10.39	125.50	120.30
1	C	123	ARG	NE-CZ-NH2	-10.29	115.16	120.30
1	E	84	ARG	NE-CZ-NH2	-10.22	115.19	120.30
1	C	7	ARG	NE-CZ-NH1	9.97	125.28	120.30
1	F	123	ARG	NE-CZ-NH1	9.80	125.20	120.30
1	F	123	ARG	CA-C-N	-9.38	96.56	117.20
1	D	21	TYR	CB-CG-CD1	-9.34	115.40	121.00
1	B	109	TYR	CB-CG-CD2	-9.30	115.42	121.00
1	A	74	ARG	NE-CZ-NH1	9.28	124.94	120.30
1	F	118	ARG	NE-CZ-NH1	8.84	124.72	120.30
1	C	84	ARG	NE-CZ-NH2	-8.83	115.88	120.30
1	B	44	CYS	CA-CB-SG	-8.76	98.23	114.00
1	B	123	ARG	NE-CZ-NH2	-8.71	115.94	120.30
1	A	33	ARG	NE-CZ-NH2	-8.66	115.97	120.30
1	D	109	TYR	CB-CG-CD2	-8.59	115.85	121.00
1	F	100	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	E	42	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	E	42	ARG	NE-CZ-NH2	-8.23	116.19	120.30
1	A	45	VAL	CG1-CB-CG2	-8.18	97.81	110.90
1	F	53	ARG	NE-CZ-NH2	-8.13	116.23	120.30
1	D	16	GLU	CA-C-N	-7.96	99.70	117.20
1	B	74	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	E	7	ARG	NE-CZ-NH1	7.81	124.20	120.30
1	D	33	ARG	NE-CZ-NH1	7.75	124.17	120.30
1	A	100	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	F	66	TYR	CB-CG-CD2	-7.74	116.36	121.00
1	A	8	MET	CG-SD-CE	7.71	112.54	100.20
1	F	53	ARG	CA-CB-CG	7.70	130.34	113.40
1	C	111	TYR	CB-CG-CD2	-7.68	116.39	121.00
1	B	124	CYS	CA-CB-SG	7.63	127.74	114.00
1	C	123	ARG	O-C-N	7.59	134.85	122.70
1	F	8	MET	CG-SD-CE	7.51	112.22	100.20
1	F	90	CYS	CA-CB-SG	7.35	127.23	114.00
1	A	112	TYR	CA-C-N	-7.21	101.33	117.20
1	B	91	ASP	CB-CG-OD1	7.15	124.74	118.30
1	A	123	ARG	CA-C-N	-7.13	101.51	117.20
1	B	84	ARG	NE-CZ-NH2	-7.05	116.77	120.30
1	D	33	ARG	NE-CZ-NH2	-7.01	116.79	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	30	VAL	CA-C-N	7.00	130.21	116.20
1	E	117	CYS	CA-CB-SG	-6.97	101.45	114.00
1	A	71	SER	N-CA-CB	-6.95	100.08	110.50
1	D	17	ALA	N-CA-C	6.91	129.65	111.00
1	F	118	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	D	120	SER	CA-C-N	-6.86	102.11	117.20
1	A	96	THR	CA-CB-CG2	6.84	121.98	112.40
1	E	90	CYS	N-CA-CB	-6.80	98.36	110.60
1	B	48	ASP	CB-CG-OD1	6.74	124.36	118.30
1	C	124	CYS	N-CA-C	6.73	129.18	111.00
1	A	28	CYS	CA-C-N	-6.71	102.78	116.20
1	E	43	CYS	CA-CB-SG	6.60	125.88	114.00
1	B	21	TYR	CB-CG-CD1	-6.60	117.04	121.00
1	F	21	TYR	CB-CG-CD1	-6.55	117.07	121.00
1	E	119	GLY	CA-C-N	-6.49	102.93	117.20
1	C	16	GLU	CA-C-N	-6.47	102.97	117.20
1	B	24	TYR	CB-CG-CD2	-6.46	117.12	121.00
1	A	53	ARG	CA-CB-CG	6.43	127.54	113.40
1	C	104	THR	CA-CB-OG1	-6.39	95.58	109.00
1	B	33	ARG	NE-CZ-NH1	6.39	123.49	120.30
1	C	104	THR	CA-CB-CG2	6.37	121.32	112.40
1	F	104	THR	N-CA-CB	-6.36	98.22	110.30
1	F	74	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	E	77	CYS	CA-CB-SG	-6.29	102.68	114.00
1	A	53	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	B	123	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	F	7	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	D	112	TYR	CA-C-N	-6.16	103.65	117.20
1	E	83	CYS	CA-CB-SG	-6.16	102.92	114.00
1	A	30	VAL	CG1-CB-CG2	-6.11	101.12	110.90
1	A	109	TYR	O-C-N	-6.11	112.92	122.70
1	D	33	ARG	CA-CB-CG	6.11	126.84	113.40
1	C	65	SER	CA-CB-OG	-6.09	94.76	111.20
1	B	7	ARG	CB-CG-CD	6.07	127.38	111.60
1	D	9	ILE	CA-C-N	6.07	130.56	117.20
1	E	42	ARG	CA-CB-CG	6.07	126.75	113.40
1	B	123	ARG	CA-C-N	-6.07	103.85	117.20
1	C	50	CYS	CA-CB-SG	6.06	124.92	114.00
1	D	51	TYR	CB-CG-CD2	-6.03	117.38	121.00
1	E	112	TYR	CA-C-N	-6.01	103.97	117.20
1	C	91	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	E	118	ARG	NE-CZ-NH1	5.97	123.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	33	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	E	53	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	A	90	CYS	CA-CB-SG	5.92	124.66	114.00
1	A	71	SER	CB-CA-C	5.91	121.33	110.10
1	D	9	ILE	O-C-N	-5.89	113.28	122.70
1	E	121	THR	N-CA-CB	5.88	121.47	110.30
1	C	53	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	E	51	TYR	CB-CG-CD2	-5.88	117.47	121.00
1	E	21	TYR	CB-CG-CD1	-5.87	117.48	121.00
1	A	112	TYR	O-C-N	5.86	132.08	122.70
1	F	123	ARG	CA-C-O	5.83	132.34	120.10
1	C	7	ARG	CG-CD-NE	5.82	124.03	111.80
1	D	100	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	F	3	VAL	CA-CB-CG1	-5.82	102.17	110.90
1	D	55	GLU	CA-CB-CG	5.80	126.17	113.40
1	D	66	TYR	CB-CG-CD2	-5.76	117.55	121.00
1	E	59	CYS	CA-CB-SG	5.74	124.33	114.00
1	A	71	SER	N-CA-C	-5.73	95.53	111.00
1	B	67	LYS	CA-CB-CG	5.73	126.00	113.40
1	C	99	ALA	CA-C-N	5.73	129.80	117.20
1	A	113	SER	N-CA-CB	-5.72	101.92	110.50
1	C	30	VAL	CA-C-N	5.71	127.61	116.20
1	A	7	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	B	33	ARG	CA-CB-CG	5.70	125.93	113.40
1	C	71	SER	N-CA-CB	-5.66	102.01	110.50
1	D	53	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	B	105	TYR	CB-CG-CD2	-5.60	117.64	121.00
1	C	91	ASP	CB-CG-OD1	5.54	123.28	118.30
1	E	17	ALA	N-CA-C	5.53	125.94	111.00
1	D	121	THR	N-CA-CB	-5.49	99.87	110.30
1	F	7	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	C	109	TYR	CB-CG-CD2	-5.45	117.73	121.00
1	D	28	CYS	CA-C-N	-5.44	105.32	116.20
1	C	33	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	D	21	TYR	CB-CG-CD2	5.43	124.26	121.00
1	F	100	ARG	CA-CB-CG	5.42	125.32	113.40
1	D	8	MET	CA-CB-CG	5.38	122.45	113.30
1	B	91	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	C	123	ARG	C-N-CA	5.27	134.87	121.70
1	C	53	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	B	100	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	A	96	THR	CA-CB-OG1	-5.24	98.00	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	CYS	O-C-N	5.23	132.08	123.20
1	E	87	LEU	CA-CB-CG	5.22	127.31	115.30
1	B	55	GLU	CA-C-O	5.21	131.04	120.10
1	E	41	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	64	LEU	CB-CG-CD1	-5.19	102.17	111.00
1	C	33	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	C	103	THR	N-CA-CB	-5.19	100.44	110.30
1	C	56	LYS	CB-CG-CD	-5.18	98.12	111.60
1	C	124	CYS	N-CA-CB	-5.17	101.29	110.60
1	D	5	PHE	CB-CG-CD2	-5.17	117.18	120.80
1	D	77	CYS	CA-CB-SG	-5.17	104.70	114.00
1	B	90	CYS	CB-CA-C	-5.12	100.17	110.40
1	B	98	PHE	CB-CG-CD2	-5.10	117.23	120.80
1	C	16	GLU	CA-C-O	5.09	130.79	120.10
1	C	123	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	E	118	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	B	84	ARG	CA-CB-CG	-5.06	102.27	113.40
1	B	30	VAL	O-C-N	-5.04	114.64	123.20
1	D	59	CYS	CA-CB-SG	5.04	123.06	114.00
1	D	12	THR	OG1-CB-CG2	-5.03	98.43	110.00
1	B	7	ARG	CA-CB-CG	5.03	124.46	113.40
1	F	71	SER	CA-CB-OG	-5.00	97.69	111.20

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	111	TYR	Sidechain
1	B	105	TYR	Sidechain
1	B	51	TYR	Sidechain
1	C	121	THR	Peptide
1	C	123	ARG	Mainchain
1	D	112	TYR	Sidechain
1	D	66	TYR	Sidechain
1	E	24	TYR	Sidechain

## 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	960	0	920	28	0
1	B	960	0	920	27	0
1	C	960	0	920	25	0
1	D	960	0	920	20	0
1	E	960	0	920	24	0
1	F	960	0	920	26	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	35	0	53	4	0
3	B	35	0	53	5	0
3	C	35	0	53	3	0
3	D	35	0	53	4	0
3	E	35	0	53	4	0
3	F	35	0	53	6	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
All	All	5988	0	5838	150	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 13.

All (150) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:106:ASN:HD21	1:F:108:LYS:HD2	1.50	0.77
1:C:53:ARG:HA	1:C:56:LYS:HD2	1.67	0.76
1:C:65:SER:O	1:C:84:ARG:HD3	1.90	0.72
1:E:26:CYS:SG	1:E:37:LYS:NZ	2.64	0.71
1:D:47:HIS:HB3	3:D:204:INB:HM'2	1.73	0.69
3:A:201:INB:H162	3:A:201:INB:H32	1.75	0.68
1:B:52:LYS:HB2	3:B:202:INB:S	2.34	0.68
1:D:24:TYR:HB3	1:D:28:CYS:HB2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:52:LYS:HE3	3:D:204:INB:S	2.35	0.66
1:E:96:THR:HG22	1:E:100:ARG:NH1	2.10	0.66
1:E:65:SER:O	1:E:84:ARG:HD2	1.96	0.66
1:E:122:PRO:O	1:E:123:ARG:HB3	1.94	0.65
1:E:12:THR:HG22	1:E:99:ALA:HB2	1.77	0.65
1:F:33:ARG:HG3	1:F:117:CYS:HB2	1.78	0.65
1:E:18:ALA:HB2	3:E:205:INB:H92	1.78	0.65
1:E:33:ARG:HB3	1:E:33:ARG:NH1	2.13	0.64
1:F:33:ARG:HH11	1:F:33:ARG:HB3	1.63	0.64
1:C:86:GLN:O	1:C:90:CYS:HB2	1.97	0.63
1:E:24:TYR:HB3	1:E:28:CYS:SG	2.39	0.63
1:B:64:LEU:HD11	1:E:58:GLY:HA2	1.80	0.63
1:C:82:SER:HA	1:C:85:SER:OG	1.99	0.62
1:A:1:ASN:HB3	1:A:4:ASN:ND2	2.15	0.62
1:C:9:ILE:HD12	1:C:17:ALA:HB1	1.82	0.61
1:C:80:GLN:HG3	1:C:84:ARG:HB3	1.81	0.61
1:E:52:LYS:O	1:E:56:LYS:HD3	2.01	0.61
1:E:33:ARG:HB3	1:E:33:ARG:HH11	1.66	0.60
1:E:86:GLN:O	1:E:90:CYS:HB2	2.02	0.59
1:F:1:ASN:ND2	1:F:65:SER:HB3	2.16	0.59
1:C:116:HIS:HA	1:C:118:ARG:HH12	1.65	0.59
1:F:54:LEU:HD11	1:F:86:GLN:HB3	1.85	0.59
1:A:100:ARG:HH11	1:A:100:ARG:HG3	1.67	0.58
1:A:105:TYR:HE1	1:A:107:LYS:HG2	1.68	0.58
1:D:12:THR:HB	1:D:99:ALA:HB2	1.85	0.57
1:B:34:GLY:O	1:B:121:THR:HA	2.04	0.57
1:D:54:LEU:HD23	1:D:61:THR:HG22	1.87	0.57
1:F:24:TYR:HD2	1:F:110:GLN:HA	1.70	0.57
1:E:18:ALA:CB	3:E:205:INB:H92	2.35	0.57
3:A:201:INB:H121	3:A:201:INB:H81	1.86	0.56
1:B:52:LYS:HE2	1:B:124:CYS:SG	2.46	0.56
1:B:109:TYR:HA	1:B:112:TYR:HB2	1.87	0.56
1:E:42:ARG:HA	1:E:45:VAL:HG23	1.86	0.56
1:D:24:TYR:HB3	1:D:28:CYS:CB	2.36	0.55
1:A:51:TYR:CD2	3:A:201:INB:H3'1	2.41	0.55
1:C:1:ASN:HA	1:C:62:LYS:O	2.06	0.55
1:F:106:ASN:ND2	1:F:108:LYS:HD2	2.22	0.55
1:F:105:TYR:OH	1:F:110:GLN:HG3	2.07	0.55
1:C:6:HIS:HD2	1:C:17:ALA:HB3	1.71	0.54
1:F:68:PHE:HD2	1:F:75:ILE:CG2	2.20	0.54
1:A:54:LEU:HD11	1:A:86:GLN:HB3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:203:INB:H32	3:C:203:INB:H81	1.89	0.54
1:B:47:HIS:HB3	3:B:202:INB:HM'2	1.89	0.54
1:D:123:ARG:HD3	1:D:124:CYS:H	1.73	0.53
1:C:33:ARG:HD3	1:C:114:ASN:HB3	1.90	0.53
1:F:47:HIS:HB3	3:F:206:INB:HM'2	1.90	0.53
1:A:42:ARG:HA	1:A:45:VAL:HG12	1.90	0.53
1:B:54:LEU:HD23	1:B:61:THR:HG22	1.90	0.53
1:F:6:HIS:CD2	1:F:17:ALA:HB3	2.44	0.53
1:A:83:CYS:O	1:A:87:LEU:HB2	2.08	0.53
1:F:6:HIS:HD2	1:F:17:ALA:HB3	1.73	0.53
1:C:69:SER:HB2	1:C:76:THR:HB	1.91	0.53
1:A:66:TYR:CD2	1:A:87:LEU:HD13	2.44	0.52
1:B:33:ARG:HH21	1:F:32:GLY:H	1.57	0.52
1:F:61:THR:HA	1:F:87:LEU:HD13	1.90	0.52
1:D:18:ALA:HB1	3:D:204:INB:H81	1.90	0.52
1:F:18:ALA:HB1	3:F:206:INB:H82	1.90	0.52
1:E:48:ASP:O	3:E:205:INB:H2'2	2.10	0.52
1:C:6:HIS:CD2	1:C:17:ALA:HB3	2.45	0.51
1:B:40:THR:HA	1:B:43:CYS:SG	2.50	0.51
1:D:45:VAL:HG21	1:D:122:PRO:HB2	1.93	0.51
1:A:19:LEU:HG	1:A:111:TYR:OH	2.11	0.51
1:D:2:LEU:HD22	3:D:204:INB:H11	1.93	0.50
1:F:24:TYR:CD2	1:F:110:GLN:HA	2.46	0.50
1:A:37:LYS:HE2	1:A:37:LYS:HA	1.92	0.50
1:A:87:LEU:O	1:A:90:CYS:HB2	2.11	0.50
1:A:34:GLY:HA3	1:A:117:CYS:HB3	1.94	0.50
1:F:18:ALA:CB	3:F:206:INB:H82	2.42	0.50
1:A:97:CYS:HA	1:A:100:ARG:HD2	1.94	0.50
1:B:67:LYS:HE2	1:B:80:GLN:OE1	2.12	0.50
1:E:114:ASN:O	1:E:117:CYS:HB2	2.12	0.50
1:B:1:ASN:ND2	1:B:65:SER:HB3	2.27	0.49
1:D:34:GLY:H	1:D:121:THR:HB	1.76	0.49
1:C:34:GLY:O	1:C:121:THR:HA	2.13	0.49
1:A:32:GLY:H	1:D:33:ARG:HH21	1.59	0.49
1:D:13:THR:HG22	1:D:99:ALA:HA	1.95	0.49
1:A:80:GLN:HG3	1:A:84:ARG:HB2	1.95	0.49
1:D:106:ASN:OD1	1:D:108:LYS:HG2	2.13	0.48
1:B:54:LEU:HD21	1:B:87:LEU:HB2	1.94	0.48
1:A:6:HIS:HB2	3:A:201:INB:H131	1.95	0.48
1:D:21:TYR:O	1:D:28:CYS:HB3	2.13	0.48
1:C:113:SER:HB2	1:C:115:LYS:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:LYS:HG2	1:C:68:PHE:N	2.28	0.48
1:F:21:TYR:HB3	3:F:206:INB:H182	1.96	0.48
1:D:54:LEU:HD21	1:D:87:LEU:HB2	1.96	0.47
1:A:66:TYR:HD2	1:A:87:LEU:HD13	1.80	0.46
1:A:24:TYR:O	1:A:28:CYS:HB2	2.15	0.46
1:C:44:CYS:SG	3:C:203:INB:HM'1	2.56	0.46
1:D:42:ARG:HA	1:D:45:VAL:HG12	1.96	0.46
1:B:18:ALA:HB1	3:B:202:INB:H82	1.97	0.46
1:D:109:TYR:HA	1:D:112:TYR:HB2	1.97	0.46
1:E:33:ARG:HB2	1:E:117:CYS:HB3	1.97	0.46
1:C:116:HIS:HA	1:C:118:ARG:NH1	2.31	0.46
1:A:39:ALA:HB3	1:A:104:THR:HG21	1.96	0.46
1:F:1:ASN:HB3	1:F:64:LEU:O	2.15	0.46
3:B:202:INB:H122	3:B:202:INB:H91	1.63	0.45
1:B:70:ASN:HB3	1:B:75:ILE:HG13	1.98	0.45
1:C:54:LEU:O	1:C:59:CYS:HB2	2.17	0.45
1:E:10:LYS:NZ	1:E:10:LYS:HB3	2.30	0.45
1:B:5:PHE:CE2	3:B:202:INB:H162	2.52	0.45
1:F:42:ARG:O	1:F:45:VAL:HG22	2.16	0.45
1:C:33:ARG:HD2	1:C:33:ARG:N	2.32	0.45
1:B:61:THR:HA	1:B:87:LEU:HD13	1.99	0.45
1:A:27:HIS:HE1	1:A:121:THR:HG23	1.82	0.44
1:A:37:LYS:HA	1:A:37:LYS:CE	2.48	0.43
1:B:65:SER:O	1:B:84:ARG:HD3	2.18	0.43
1:B:79:LYS:HA	1:B:79:LYS:HD3	1.79	0.43
1:D:54:LEU:CD2	1:D:61:THR:HG22	2.48	0.43
1:E:37:LYS:HD3	1:E:109:TYR:CE1	2.53	0.43
1:F:11:LEU:HD13	1:F:70:ASN:HB3	2.00	0.43
1:A:8:MET:CE	1:A:75:ILE:HG21	2.49	0.43
1:B:24:TYR:CD2	1:B:110:GLN:HA	2.54	0.43
1:A:26:CYS:HB3	1:A:33:ARG:O	2.19	0.43
1:C:11:LEU:HD13	1:C:70:ASN:CG	2.38	0.43
1:E:5:PHE:O	1:E:9:ILE:HG13	2.17	0.43
1:A:80:GLN:HG3	1:A:84:ARG:CB	2.49	0.42
1:B:10:LYS:HA	1:B:10:LYS:HD2	1.75	0.42
1:C:47:HIS:HB3	3:C:203:INB:HM'2	2.00	0.42
1:F:35:SER:OG	1:F:119:GLY:HA3	2.20	0.42
1:B:64:LEU:HD21	1:B:84:ARG:HG3	2.01	0.42
1:A:106:ASN:C	1:A:108:LYS:H	2.22	0.41
1:B:33:ARG:HB2	1:B:33:ARG:HH11	1.85	0.41
1:B:40:THR:O	1:B:43:CYS:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:86:GLN:HE21	1:F:89:GLU:HB2	1.85	0.41
1:C:42:ARG:HA	1:C:45:VAL:HG13	2.03	0.41
1:A:5:PHE:O	1:A:9:ILE:HG13	2.20	0.41
1:B:26:CYS:O	1:B:114:ASN:ND2	2.54	0.41
1:A:8:MET:HE2	1:A:75:ILE:HG21	2.03	0.41
1:C:18:ALA:O	1:C:22:GLY:HA3	2.21	0.41
1:D:121:THR:HA	1:D:122:PRO:HD3	1.71	0.41
1:F:21:TYR:CB	3:F:206:INB:H182	2.50	0.41
1:B:42:ARG:HH21	1:B:45:VAL:HG21	1.86	0.41
1:C:37:LYS:HD3	1:C:37:LYS:HA	1.87	0.41
1:E:52:LYS:HG2	1:E:56:LYS:HE2	2.03	0.41
1:C:109:TYR:HA	1:C:112:TYR:HB2	2.02	0.40
1:F:51:TYR:CD2	3:F:206:INB:H3'1	2.56	0.40
1:F:26:CYS:HB3	1:F:33:ARG:O	2.21	0.40
1:E:6:HIS:HB2	3:E:205:INB:H132	2.03	0.40
1:B:67:LYS:CE	1:B:80:GLN:HG2	2.51	0.40
1:B:84:ARG:NH2	1:E:58:GLY:N	2.70	0.40
1:A:82:SER:O	1:A:86:GLN:HB2	2.21	0.40
1:E:96:THR:HG22	1:E:100:ARG:HH11	1.86	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	122/124 (98%)	108 (88%)	9 (7%)	5 (4%)	3	3
1	B	122/124 (98%)	112 (92%)	7 (6%)	3 (2%)	5	9
1	C	122/124 (98%)	107 (88%)	11 (9%)	4 (3%)	4	5
1	D	122/124 (98%)	114 (93%)	5 (4%)	3 (2%)	5	9
1	E	122/124 (98%)	108 (88%)	7 (6%)	7 (6%)	1	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	122/124 (98%)	114 (93%)	6 (5%)	2 (2%)	9	18
All	All	732/744 (98%)	663 (91%)	45 (6%)	24 (3%)	4	5

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	LYS
1	A	122	PRO
1	A	123	ARG
1	C	123	ARG
1	D	17	ALA
1	E	17	ALA
1	B	123	ARG
1	E	120	SER
1	E	121	THR
1	F	22	GLY
1	F	123	ARG
1	A	107	LYS
1	C	121	THR
1	D	37	LYS
1	A	121	THR
1	B	56	LYS
1	C	102	LYS
1	E	56	LYS
1	E	123	ARG
1	E	34	GLY
1	B	122	PRO
1	E	122	PRO
1	C	122	PRO
1	D	25	GLY

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	104/105 (99%)	90 (86%)	14 (14%)	4	6
1	B	104/105 (99%)	90 (86%)	14 (14%)	4	6
1	C	104/105 (99%)	93 (89%)	11 (11%)	6	12
1	D	104/105 (99%)	94 (90%)	10 (10%)	8	15
1	E	104/105 (99%)	88 (85%)	16 (15%)	2	4
1	F	104/105 (99%)	87 (84%)	17 (16%)	2	3
All	All	624/630 (99%)	542 (87%)	82 (13%)	4	7

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ASN
1	A	5	PHE
1	A	16	GLU
1	A	19	LEU
1	A	20	SER
1	A	37	LYS
1	A	54	LEU
1	A	56	LYS
1	A	71	SER
1	A	82	SER
1	A	87	LEU
1	A	96	THR
1	A	113	SER
1	A	122	PRO
1	B	11	LEU
1	B	20	SER
1	B	30	VAL
1	B	33	ARG
1	B	42	ARG
1	B	52	LYS
1	B	56	LYS
1	B	62	LYS
1	B	67	LYS
1	B	69	SER
1	B	86	GLN
1	B	122	PRO
1	B	123	ARG
1	B	124	CYS
1	C	16	GLU
1	C	19	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	33	ARG
1	C	35	SER
1	C	40	THR
1	C	54	LEU
1	C	71	SER
1	C	73	SER
1	C	85	SER
1	C	104	THR
1	C	108	LYS
1	D	10	LYS
1	D	12	THR
1	D	16	GLU
1	D	20	SER
1	D	56	LYS
1	D	76	THR
1	D	89	GLU
1	D	104	THR
1	D	108	LYS
1	D	124	CYS
1	E	20	SER
1	E	33	ARG
1	E	37	LYS
1	E	42	ARG
1	E	71	SER
1	E	75	ILE
1	E	82	SER
1	E	84	ARG
1	E	85	SER
1	E	87	LEU
1	E	103	THR
1	E	108	LYS
1	E	113	SER
1	E	115	LYS
1	E	118	ARG
1	E	122	PRO
1	F	3	VAL
1	F	7	ARG
1	F	16	GLU
1	F	19	LEU
1	F	30	VAL
1	F	33	ARG
1	F	46	THR

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Mol	Chain	Res	Type
1	F	54	LEU
1	F	55	GLU
1	F	71	SER
1	F	74	ARG
1	F	82	SER
1	F	86	GLN
1	F	96	THR
1	F	113	SER
1	F	118	ARG
1	F	124	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	6	HIS
1	C	6	HIS
1	C	116	HIS
1	D	116	HIS
1	F	6	HIS
1	F	86	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 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
3	INB	D	204	2	34,34,34	0.77	0	35,38,38	1.17	2 (5%)
3	INB	B	202	2	34,34,34	0.81	0	35,38,38	1.02	1 (2%)
3	INB	C	203	2	34,34,34	0.81	0	35,38,38	1.29	4 (11%)
3	INB	F	206	2	34,34,34	0.79	0	35,38,38	1.27	3 (8%)
3	INB	A	201	2	34,34,34	0.95	2 (5%)	35,38,38	1.41	5 (14%)
3	INB	E	205	2	34,34,34	1.06	2 (5%)	35,38,38	1.44	5 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	INB	D	204	2	-	15/36/36/36	-
3	INB	B	202	2	-	15/36/36/36	-
3	INB	C	203	2	-	12/36/36/36	-
3	INB	F	206	2	-	9/36/36/36	-
3	INB	A	201	2	-	12/36/36/36	-
3	INB	E	205	2	-	11/36/36/36	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	201	INB	P-O3'	3.17	1.72	1.59
3	E	205	INB	C2-C1	2.56	1.61	1.51
3	A	201	INB	C3'-C2'	2.17	1.56	1.51
3	E	205	INB	C3'-C2'	-2.10	1.47	1.51

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	205	INB	C2'-N2'-C'	-5.20	115.94	122.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	201	INB	C3'-C2'-N2'	3.96	117.36	109.58
3	C	203	INB	C2'-N2'-C'	-3.45	118.24	122.78
3	A	201	INB	O3P-C1B-C2B	3.24	120.84	109.41
3	D	204	INB	C2'-N2'-C'	-2.99	118.85	122.78
3	D	204	INB	CM'-C'-N2'	-2.87	111.24	116.10
3	F	206	INB	C2'-N2'-C'	-2.77	119.13	122.78
3	E	205	INB	CM'-C'-N2'	-2.72	111.50	116.10
3	A	201	INB	C16-C15-C14	-2.71	100.65	114.42
3	F	206	INB	CM'-C'-N2'	2.65	120.59	116.10
3	A	201	INB	C7-C6-C5	-2.59	101.29	114.42
3	E	205	INB	O'-C'-CM'	2.56	126.82	122.06
3	B	202	INB	O3P-C1B-C2B	2.47	118.13	109.41
3	C	203	INB	C3'-C2'-N2'	2.43	114.37	109.58
3	E	205	INB	C9-C8-C7	2.38	126.50	114.42
3	C	203	INB	O2P-P-O3P	2.30	118.42	107.75
3	A	201	INB	C1'-C2'-N2'	-2.28	105.10	109.58
3	C	203	INB	C10-C9-C8	2.26	125.91	114.42
3	E	205	INB	C15-C14-C13	-2.22	103.15	114.42
3	F	206	INB	P-O3P-C1B	-2.07	111.41	121.59

There are no chirality outliers.

All (74) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	204	INB	C2'-C3'-O3'-P
3	D	204	INB	C1B-O3P-P-O1P
3	E	205	INB	O1'-C1'-C2'-C3'
3	E	205	INB	O1'-C1'-C2'-N2'
3	A	201	INB	O1'-C1'-C2'-C3'
3	A	201	INB	O1'-C1'-C2'-N2'
3	A	201	INB	C2'-C3'-O3'-P
3	A	201	INB	C1B-O3P-P-O1P
3	C	203	INB	C2-C3-C4-C5
3	E	205	INB	C4-C5-C6-C7
3	D	204	INB	C6-C7-C8-C9
3	F	206	INB	C11-C10-C9-C8
3	A	201	INB	C12-C13-C14-C15
3	C	203	INB	C11-C12-C13-C14
3	F	206	INB	C12-C13-C14-C15
3	E	205	INB	C13-C14-C15-C16
3	C	203	INB	C3-C4-C5-C6
3	B	202	INB	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
3	B	202	INB	C4-C5-C6-C7
3	D	204	INB	C9-C10-C11-C12
3	B	202	INB	C13-C14-C15-C16
3	A	201	INB	C10-C11-C12-C13
3	E	205	INB	C14-C15-C16-C17
3	D	204	INB	C4-C5-C6-C7
3	E	205	INB	C11-C10-C9-C8
3	C	203	INB	C2'-C1'-O1'-C1
3	A	201	INB	C4-C5-C6-C7
3	D	204	INB	C7-C8-C9-C10
3	A	201	INB	C11-C12-C13-C14
3	D	204	INB	C13-C14-C15-C16
3	D	204	INB	C2'-C1'-O1'-C1
3	E	205	INB	C2'-C1'-O1'-C1
3	E	205	INB	C1B-C2B-S-CMB
3	A	201	INB	C1B-O3P-P-O3'
3	D	204	INB	C15-C16-C17-C18
3	C	203	INB	C9-C10-C11-C12
3	B	202	INB	O1'-C1'-C2'-C3'
3	C	203	INB	O1'-C1'-C2'-N2'
3	D	204	INB	C12-C13-C14-C15
3	F	206	INB	C2'-C1'-O1'-C1
3	F	206	INB	C4-C5-C6-C7
3	A	201	INB	C11-C10-C9-C8
3	F	206	INB	C2'-C3'-O3'-P
3	E	205	INB	C2'-C3'-O3'-P
3	C	203	INB	N2'-C2'-C3'-O3'
3	D	204	INB	N2'-C2'-C3'-O3'
3	B	202	INB	N2'-C2'-C3'-O3'
3	E	205	INB	N2'-C2'-C3'-O3'
3	A	201	INB	N2'-C2'-C3'-O3'
3	B	202	INB	O1'-C1-C2-C3
3	C	203	INB	C1B-O3P-P-O3'
3	C	203	INB	C10-C11-C12-C13
3	B	202	INB	C3-C4-C5-C6
3	C	203	INB	C7-C8-C9-C10
3	B	202	INB	C2-C3-C4-C5
3	D	204	INB	C1B-O3P-P-O3'
3	B	202	INB	C1B-O3P-P-O3'
3	B	202	INB	C9-C10-C11-C12
3	C	203	INB	C1B-C2B-S-CMB
3	F	206	INB	C1B-C2B-S-CMB

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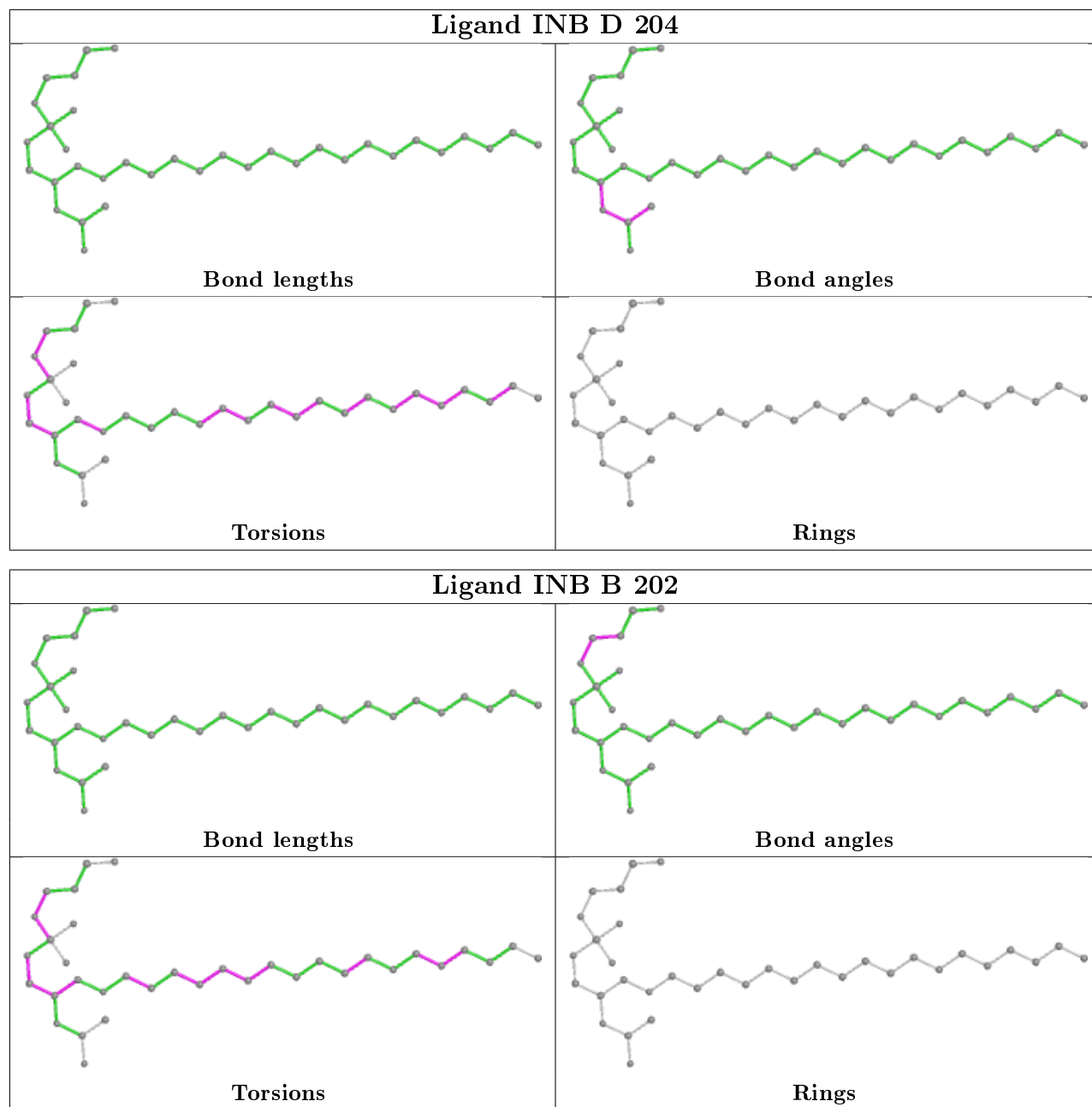
Mol	Chain	Res	Type	Atoms
3	B	202	INB	C12-C13-C14-C15
3	D	204	INB	C2B-C1B-O3P-P
3	B	202	INB	C2B-C1B-O3P-P
3	A	201	INB	C5-C6-C7-C8
3	F	206	INB	C5-C6-C7-C8
3	D	204	INB	C3-C4-C5-C6
3	B	202	INB	O1'-C1'-C2'-N2'
3	C	203	INB	C5-C6-C7-C8
3	D	204	INB	C11-C12-C13-C14
3	B	202	INB	C2'-C3'-O3'-P
3	F	206	INB	C9-C10-C11-C12
3	F	206	INB	N2'-C2'-C3'-O3'
3	E	205	INB	C15-C16-C17-C18
3	B	202	INB	C1B-O3P-P-O1P

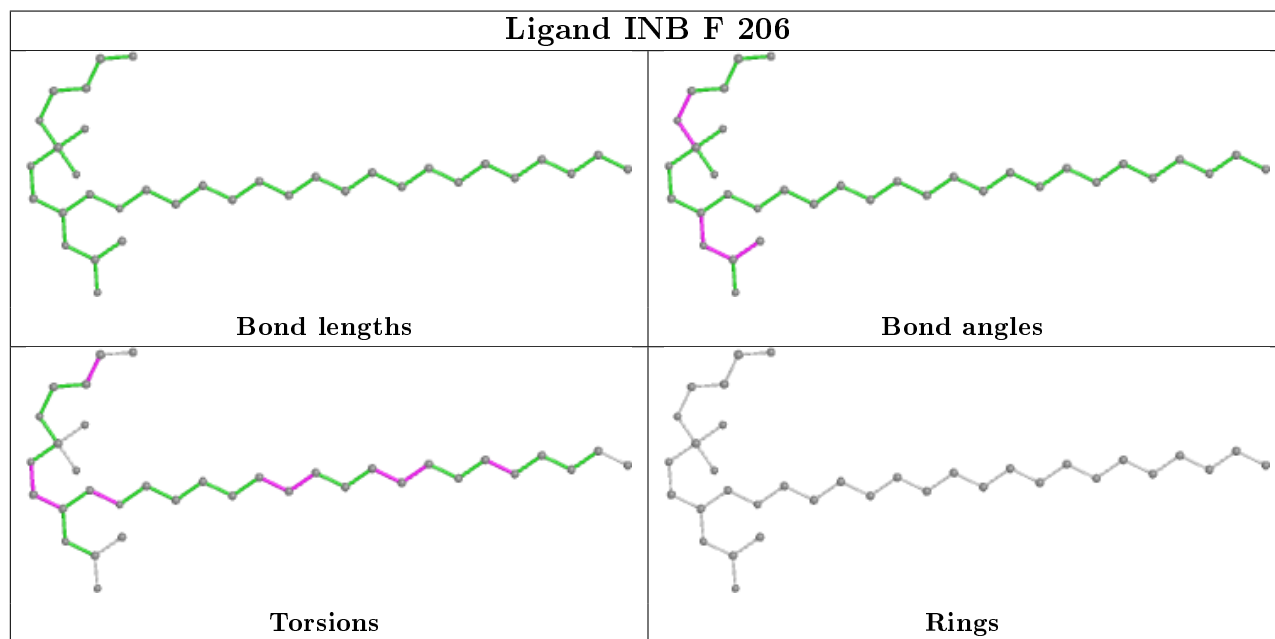
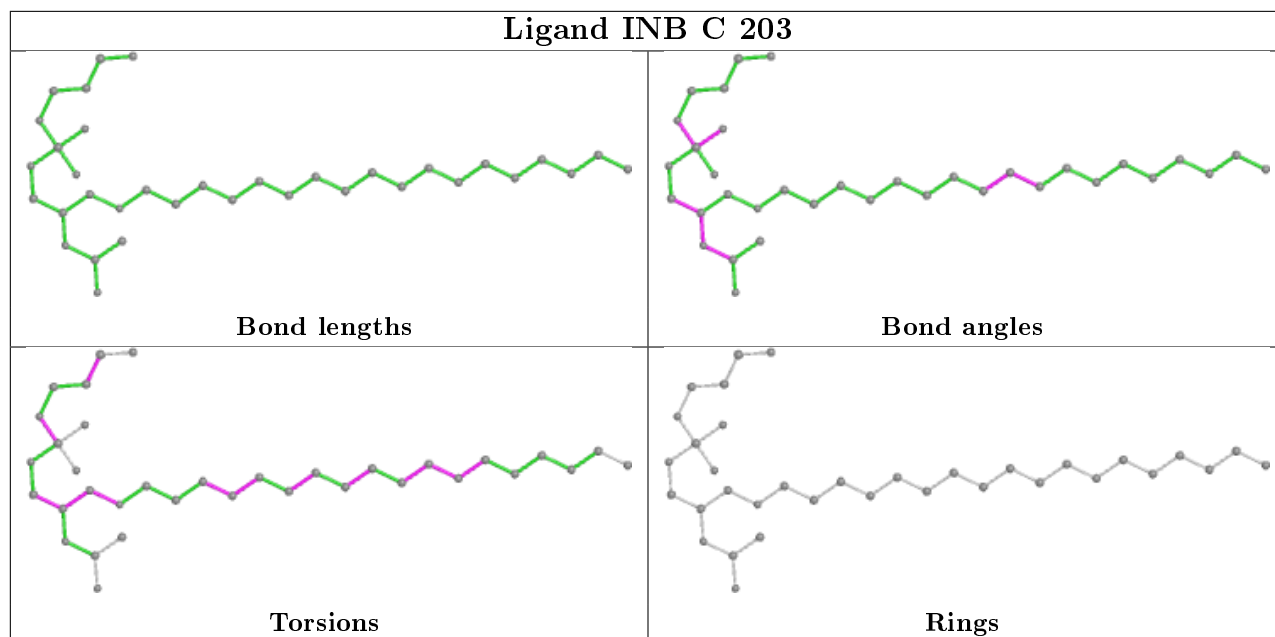
There are no ring outliers.

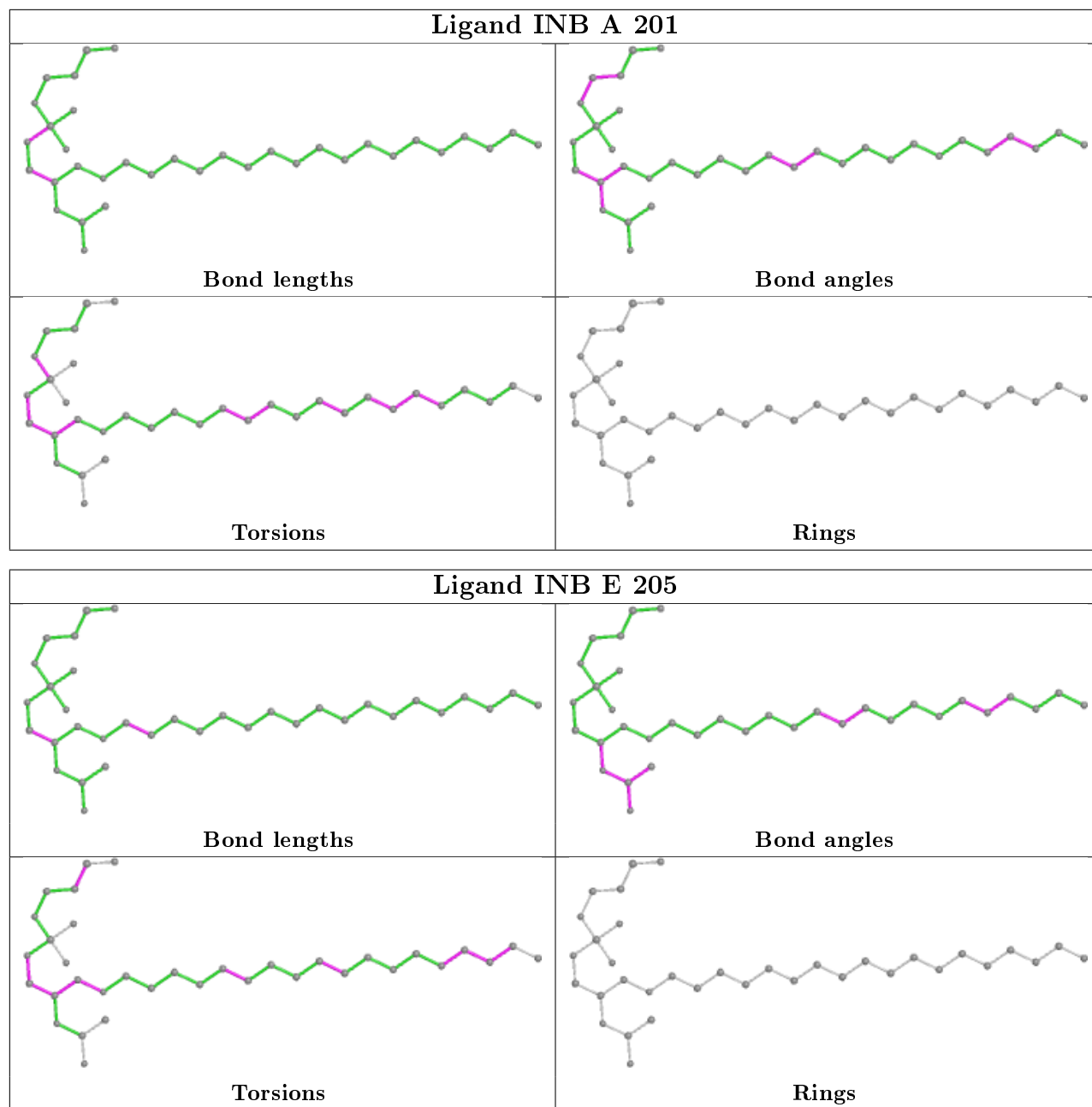
6 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	204	INB	4	0
3	B	202	INB	5	0
3	C	203	INB	3	0
3	F	206	INB	6	0
3	A	201	INB	4	0
3	E	205	INB	4	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.







## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	124/124 (100%)	-0.10	2 (1%) 72 69	7, 18, 39, 47	0
1	B	124/124 (100%)	-0.27	0 100 100	7, 18, 40, 51	0
1	C	124/124 (100%)	-0.07	0 100 100	7, 16, 32, 44	0
1	D	124/124 (100%)	-0.20	0 100 100	6, 17, 41, 49	0
1	E	124/124 (100%)	-0.25	1 (0%) 86 85	7, 17, 32, 42	0
1	F	124/124 (100%)	-0.08	3 (2%) 59 55	7, 18, 38, 47	0
All	All	744/744 (100%)	-0.16	6 (0%) 86 85	6, 17, 38, 51	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	122	PRO	3.9
1	E	71	SER	2.5
1	F	31	GLY	2.4
1	F	33	ARG	2.3
1	A	105	TYR	2.3
1	A	34	GLY	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands

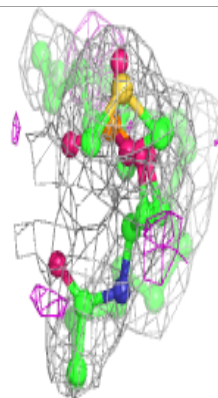
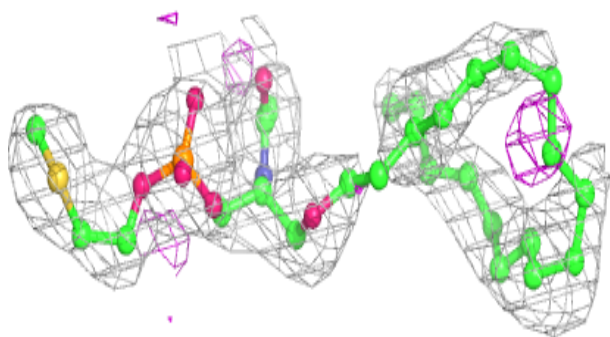
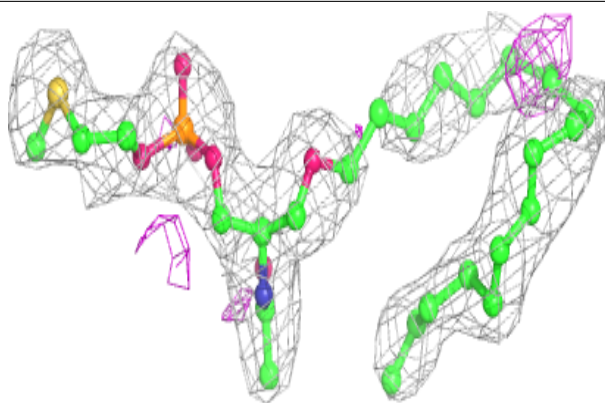
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	INB	E	205	35/35	0.93	0.20	6,10,26,33	0
3	INB	A	201	35/35	0.93	0.24	6,10,31,35	0
3	INB	B	202	35/35	0.95	0.18	6,11,31,39	0
2	CA	C	306	1/1	0.95	0.08	21,21,21,21	0
3	INB	D	204	35/35	0.95	0.19	6,10,31,38	0
3	INB	C	203	35/35	0.96	0.16	6,10,22,23	0
3	INB	F	206	35/35	0.96	0.19	6,13,29,34	0
2	CA	F	311	1/1	0.97	0.06	14,14,14,14	0
2	CA	D	308	1/1	0.97	0.08	19,19,19,19	0
2	CA	E	310	1/1	0.97	0.07	21,21,21,21	0
2	CA	C	305	1/1	0.98	0.07	18,18,18,18	0
2	CA	A	302	1/1	0.98	0.07	24,24,24,24	0
2	CA	B	304	1/1	0.98	0.08	18,18,18,18	0
2	CA	A	301	1/1	0.98	0.04	7,7,7,7	0
2	CA	B	303	1/1	0.98	0.08	13,13,13,13	0
2	CA	F	312	1/1	0.99	0.08	21,21,21,21	0
2	CA	D	307	1/1	0.99	0.08	10,10,10,10	0
2	CA	E	309	1/1	0.99	0.09	10,10,10,10	0

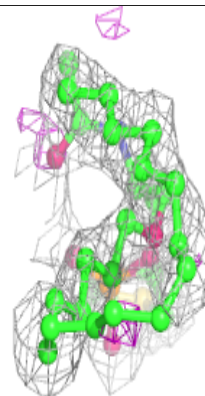
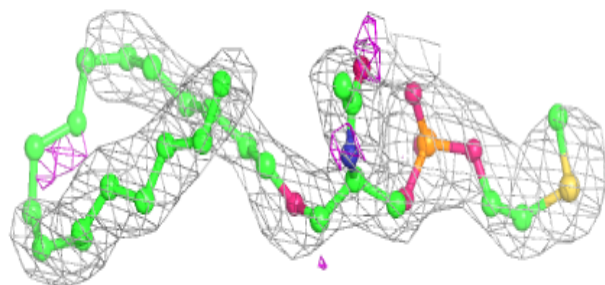
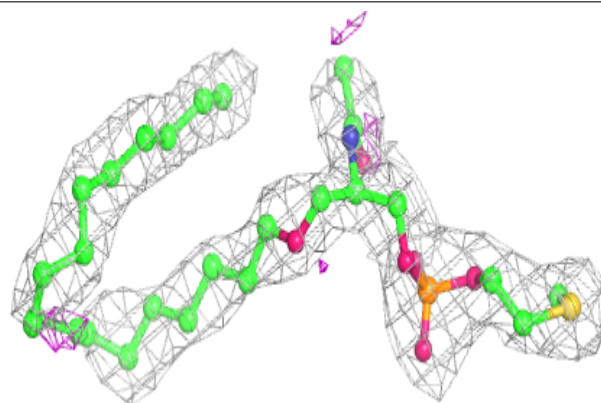
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around INB E 205:**

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

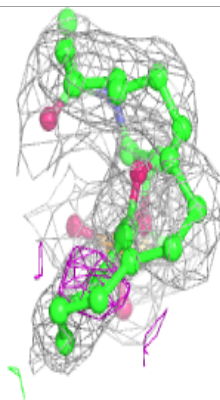
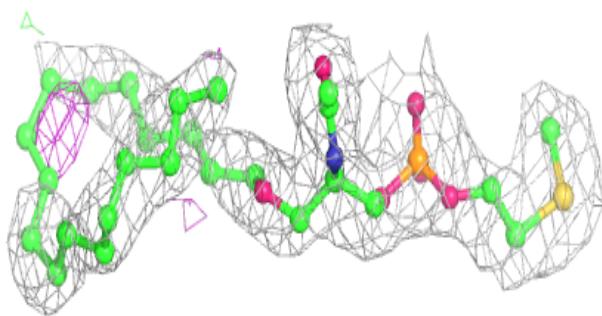
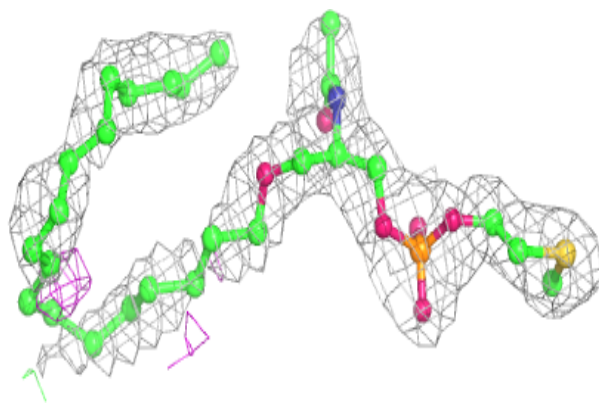
**Electron density around INB A 201:**

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

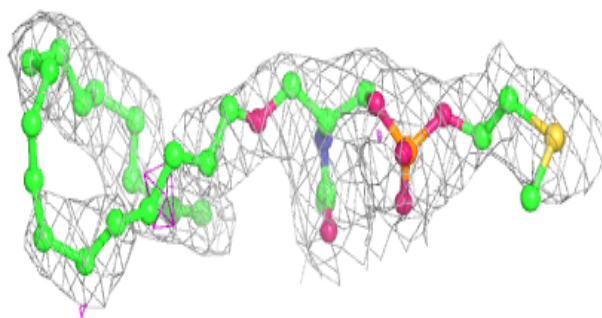
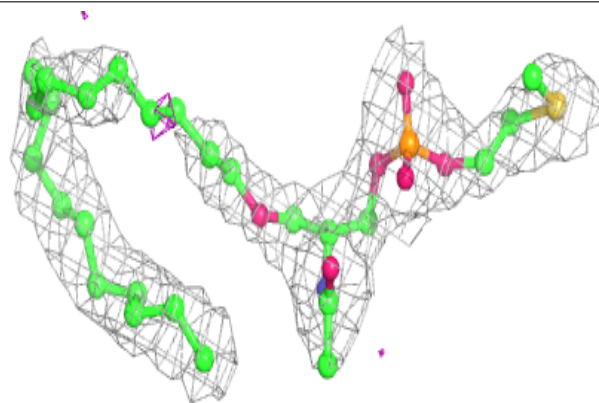


**Electron density around INB B 202:**

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

**Electron density around INB D 204:**

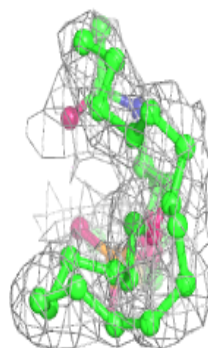
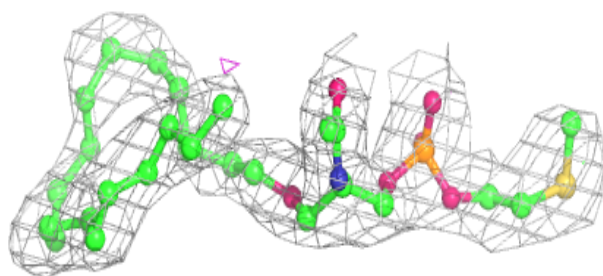
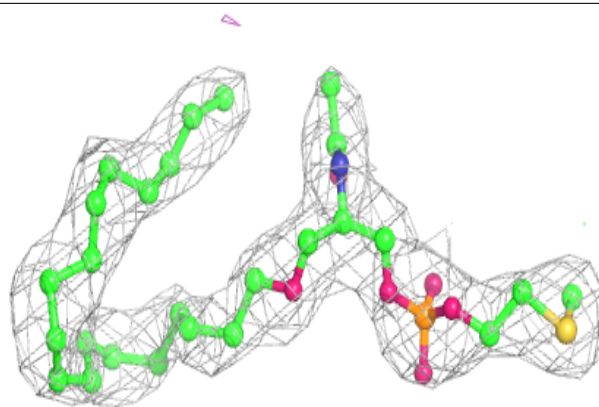
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



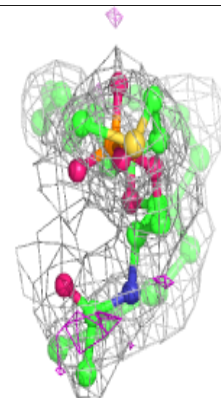
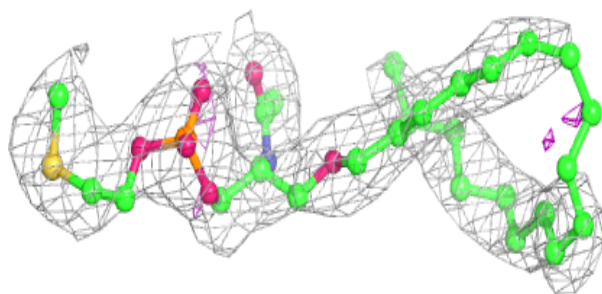
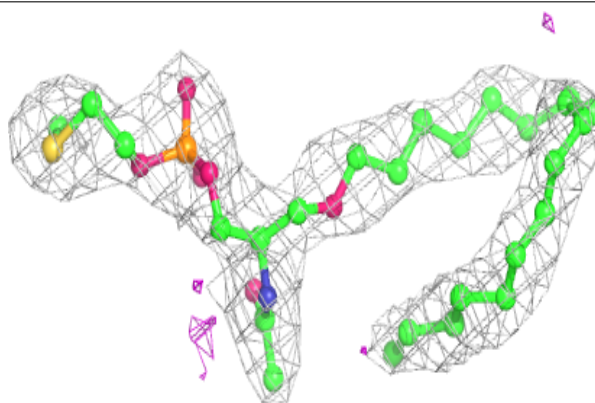


**Electron density around INB C 203:**

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

**Electron density around INB F 206:**

$2mF_o-DF_c$  (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.