



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:44 AM UTC

PDB ID : 1BKC / pdb_00001bkc
Title : CATALYTIC DOMAIN OF TNF-ALPHA CONVERTING ENZYME (TACE)
Authors : Maskos, K.; Fernandez-Catalan, C.; Bode, W.
Deposited on : 1998-04-23
Resolution : 2.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

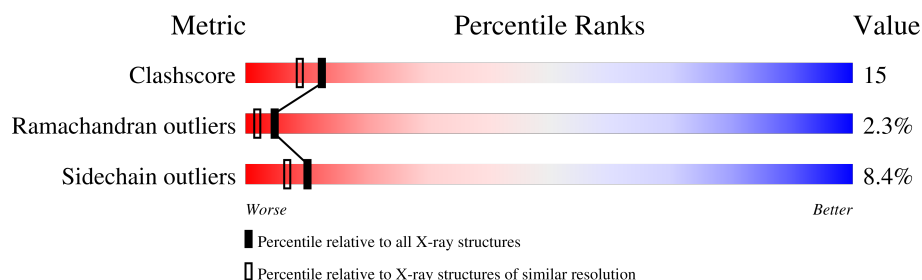
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	256	62% 30% 5% .
1	C	256	62% 25% 9% . .
2	E	256	61% 31% 6% .
3	I	256	62% 28% 7% . .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	INN	A	2	X	-	-	-
5	INN	C	2	X	-	-	-
5	INN	E	2	X	-	-	-
5	INN	I	2	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9822 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 TUMOR NECROSIS FACTOR-ALPHA-CONVERTING ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	9	0	0
			2025	1274	342	396	13			
1	C	254	Total	C	N	O	S	127	0	0
			2012	1265	340	394	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	266	ALA	SER	engineered mutation	UNP P78536
A	452	GLN	ASN	engineered mutation	UNP P78536
C	266	ALA	SER	engineered mutation	UNP P78536
C	452	GLN	ASN	engineered mutation	UNP P78536

- Molecule 2 is a protein called TUMOR NECROSIS FACTOR-ALPHA-CONVERTING ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	256	Total	C	N	O	S	18	0	0
			2028	1275	344	396	13			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	266	ALA	SER	engineered mutation	UNP P78536
E	420	LYS	LEU	conflict	UNP P78536
E	452	GLN	ASN	engineered mutation	UNP P78536

- Molecule 3 is a protein called TUMOR NECROSIS FACTOR-ALPHA-CONVERTING ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	254	Total	C	N	O	S	48	0	0
			2017	1269	341	394	13			

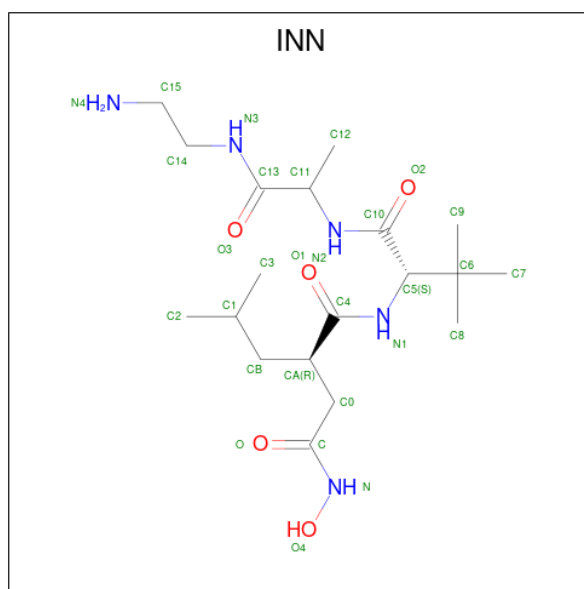
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	266	ALA	SER	engineered mutation	UNP P78536
I	428	GLU	ASP	conflict	UNP P78536
I	452	GLN	ASN	engineered mutation	UNP P78536

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		
4	C	1	Total	Zn	0	0
			1	1		
4	E	1	Total	Zn	0	0
			1	1		
4	I	1	Total	Zn	0	0
			1	1		

- Molecule 5 is N-{(2R)-2-[2-(hydroxyamino)-2-oxoethyl]-4-methylpentanoyl}-3-methyl-L-valyl-N-(2-aminoethyl)-L-alaninamide (CCD ID: INN) (formula: C₁₉H₃₇N₅O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			29	19	5	5		
5	C	1	Total	C	N	O	0	0
			29	19	5	5		
5	E	1	Total	C	N	O	0	0
			29	19	5	5		
5	I	1	Total	C	N	O	0	0
			29	19	5	5		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	572	Total	O	0	0
			572	572		
6	C	442	Total	O	0	0
			442	442		
6	E	368	Total	O	0	0
			368	368		
6	I	238	Total	O	0	0
			238	238		

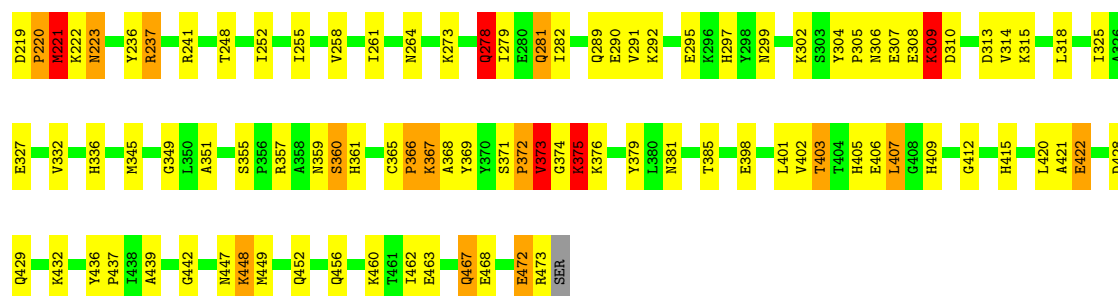
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

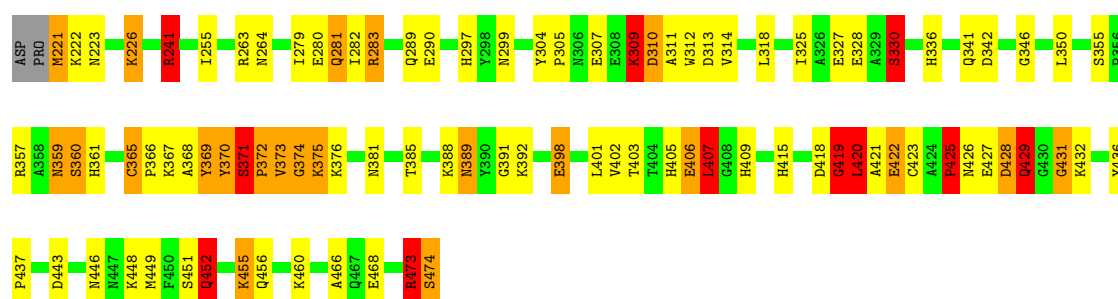
• Molecule 1: TUMOR NECROSIS FACTOR-ALPHA-CONVERTING ENZYME

Chain A: 



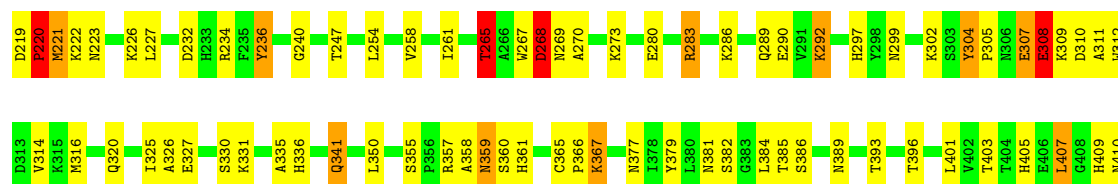
• Molecule 1: TUMOR NECROSIS FACTOR-ALPHA-CONVERTING ENZYME

Chain C: 



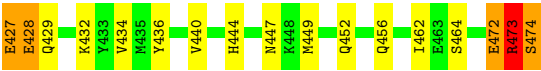
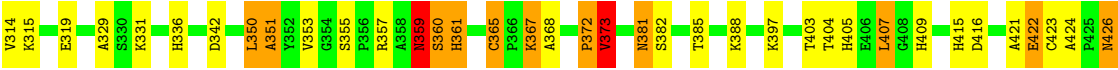
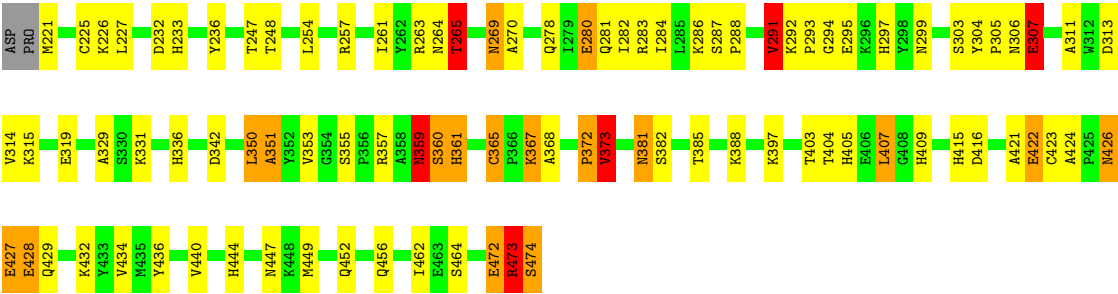
• Molecule 2: TUMOR NECROSIS FACTOR-ALPHA-CONVERTING ENZYME

Chain E: 





● Molecule 3: TUMOR NECROSIS FACTOR-ALPHA-CONVERTING ENZYME



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.38Å 126.27Å 81.27Å 90.00° 107.41° 90.00°	Depositor
Resolution (Å)	12.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (12.00-2.00)	Depositor
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.180 , 0.270	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9822	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.00	1/2071 (0.0%)	1.84	49/2795 (1.8%)
1	C	1.91	24/2056 (1.2%)	2.52	75/2773 (2.7%)
2	E	1.12	4/2074 (0.2%)	2.12	78/2798 (2.8%)
3	I	1.08	7/2062 (0.3%)	1.92	73/2781 (2.6%)
All	All	1.33	36/8263 (0.4%)	2.11	275/11147 (2.5%)

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	2
1	C	0	7
2	E	0	2
3	I	0	3
All	All	0	14

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	420	LEU	C-N	-48.95	0.65	1.33
1	C	452	GLN	C-N	-26.75	1.00	1.33
1	C	376	LYS	C-N	-25.63	0.98	1.33
1	A	376	LYS	C-N	-16.62	1.09	1.33
1	C	371	SER	N-CA	-14.22	1.26	1.46
2	E	326	ALA	C-N	-13.85	1.15	1.33
1	C	374	GLY	N-CA	13.30	1.64	1.45
3	I	368	ALA	C-N	-13.14	1.16	1.33
2	E	455	LYS	C-N	-12.55	1.18	1.33
1	C	373	VAL	C-O	-12.17	1.09	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	426	ASN	C-N	-11.98	1.18	1.33
3	I	307	GLU	C-N	-10.86	1.17	1.33
1	C	419	GLY	C-N	10.78	1.48	1.33
3	I	444	HIS	C-N	-10.28	1.20	1.34
1	C	373	VAL	CA-C	9.98	1.65	1.52
1	C	373	VAL	C-N	8.83	1.46	1.33
1	C	422	GLU	C-N	-8.78	1.20	1.33
3	I	295	GLU	C-N	-8.25	1.22	1.33
1	C	371	SER	C-O	7.90	1.34	1.24
1	C	452	GLN	CA-C	-7.62	1.42	1.52
1	C	468	GLU	C-N	7.53	1.50	1.33
1	C	372	PRO	CA-CB	-7.52	1.43	1.53
1	C	371	SER	CA-C	-7.44	1.43	1.52
1	C	369	TYR	C-O	7.02	1.32	1.24
1	C	369	TYR	CA-C	-6.87	1.43	1.52
1	C	425	PRO	C-N	-6.63	1.24	1.33
1	C	466	ALA	C-N	-6.54	1.25	1.34
2	E	468	GLU	N-CA	-6.52	1.38	1.46
1	C	373	VAL	N-CA	6.29	1.54	1.46
1	C	372	PRO	N-CA	-6.06	1.39	1.47
3	I	294	GLY	C-N	-6.04	1.24	1.33
1	C	370	TYR	CA-C	-5.84	1.45	1.52
3	I	292	LYS	C-N	5.65	1.47	1.33
1	C	368	ALA	C-N	-5.64	1.25	1.33
2	E	327	GLU	C-N	-5.21	1.26	1.33
3	I	415	HIS	CE1-NE2	-5.07	1.27	1.32

All (275) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	452	GLN	O-C-N	-32.62	77.45	122.46
1	C	419	GLY	O-C-N	-30.91	82.52	122.70
1	C	420	LEU	CA-C-N	27.73	174.51	121.54
1	C	420	LEU	C-N-CA	27.73	174.51	121.54
1	C	420	LEU	O-C-N	-26.24	87.13	123.07
1	C	369	TYR	O-C-N	25.88	157.01	122.59
2	E	467	GLN	CA-C-N	25.02	154.47	120.44
2	E	467	GLN	C-N-CA	25.02	154.47	120.44
1	C	376	LYS	CA-C-N	19.72	148.63	120.82
1	C	376	LYS	C-N-CA	19.72	148.63	120.82
1	C	373	VAL	O-C-N	-17.57	100.61	122.57
1	C	426	ASN	CA-C-N	17.27	146.72	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	426	ASN	C-N-CA	17.27	146.72	120.82
2	E	468	GLU	N-CA-C	-14.10	95.91	111.14
1	C	241	ARG	CD-NE-CZ	13.60	143.44	124.40
1	C	370	TYR	O-C-N	13.54	140.60	122.59
2	E	326	ALA	CA-C-O	-13.00	106.99	120.90
2	E	467	GLN	CA-C-O	12.02	137.70	120.51
3	I	368	ALA	O-C-N	11.94	137.54	122.97
1	C	426	ASN	O-C-N	-11.88	109.31	122.85
2	E	341	GLN	OE1-CD-NE2	11.75	134.35	122.60
2	E	455	LYS	CA-C-O	-11.35	106.92	119.97
1	C	428	ASP	N-CA-CB	11.25	128.77	110.43
1	A	368	ALA	N-CA-C	11.21	126.05	110.24
1	C	304	TYR	CA-C-O	-10.97	109.33	119.86
3	I	368	ALA	CA-C-O	-10.63	109.46	121.15
3	I	263	ARG	CD-NE-CZ	10.54	139.16	124.40
1	C	376	LYS	O-C-N	-10.54	104.62	122.11
1	C	373	VAL	CB-CA-C	10.37	128.29	111.29
1	A	304	TYR	CA-C-O	-9.85	108.32	120.23
3	I	307	GLU	O-C-N	-9.83	108.90	122.46
3	I	415	HIS	CE1-NE2-CD2	9.77	118.77	109.00
1	A	278	GLN	OE1-CD-NE2	9.73	132.33	122.60
2	E	307	GLU	CA-C-O	-9.72	110.50	121.19
1	C	452	GLN	CA-C-N	9.67	133.59	120.54
1	C	452	GLN	C-N-CA	9.67	133.59	120.54
2	E	467	GLN	O-C-N	-9.60	109.83	122.59
1	A	366	PRO	CA-C-N	9.59	138.39	122.76
1	A	366	PRO	C-N-CA	9.59	138.39	122.76
2	E	220	PRO	N-CA-C	9.46	131.97	112.47
3	I	405	HIS	CE1-NE2-CD2	9.24	118.24	109.00
1	C	371	SER	CA-C-O	-9.21	107.54	120.16
2	E	415	HIS	CE1-NE2-CD2	9.17	118.17	109.00
1	C	452	GLN	N-CA-C	-9.12	101.58	112.89
1	C	409	HIS	CE1-NE2-CD2	9.04	118.04	109.00
1	C	311	ALA	N-CA-C	9.02	124.17	108.75
1	A	405	HIS	CE1-NE2-CD2	8.75	117.75	109.00
1	C	369	TYR	CA-C-N	8.71	138.19	121.54
1	C	369	TYR	C-N-CA	8.71	138.19	121.54
1	A	366	PRO	CB-CA-C	8.68	121.97	111.46
3	I	304	TYR	CA-C-O	-8.61	109.82	120.23
3	I	291	VAL	CA-C-O	-8.52	112.64	121.67
1	C	405	HIS	CE1-NE2-CD2	8.43	117.43	109.00
3	I	405	HIS	CG-CD2-NE2	-8.32	98.88	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	368	ALA	O-C-N	-8.24	112.67	122.81
3	I	264	ASN	CA-CB-CG	-8.20	104.40	112.60
2	E	405	HIS	CE1-NE2-CD2	8.19	117.19	109.00
2	E	358	ALA	CA-C-O	8.17	132.20	120.51
1	A	278	GLN	CB-CG-CD	-8.15	98.74	112.60
1	A	304	TYR	O-C-N	8.07	129.63	121.72
2	E	304	TYR	CA-C-O	-8.06	110.47	120.23
2	E	415	HIS	CG-CD2-NE2	-8.05	99.15	107.20
2	E	327	GLU	CA-C-N	8.03	134.12	120.71
2	E	327	GLU	C-N-CA	8.03	134.12	120.71
1	A	375	LYS	O-C-N	-7.95	108.45	122.21
3	I	361	HIS	CA-C-O	7.92	130.06	121.11
2	E	467	GLN	N-CA-CB	7.92	123.87	110.49
2	E	415	HIS	CA-CB-CG	-7.91	105.89	113.80
2	E	267	TRP	CA-C-N	7.89	134.09	120.68
2	E	267	TRP	C-N-CA	7.89	134.09	120.68
1	A	409	HIS	CE1-NE2-CD2	7.86	116.86	109.00
1	C	428	ASP	CA-CB-CG	-7.83	104.77	112.60
1	A	415	HIS	CE1-NE2-CD2	7.75	116.75	109.00
1	C	372	PRO	N-CA-CB	7.75	111.39	103.25
1	C	405	HIS	CG-CD2-NE2	-7.71	99.49	107.20
1	A	405	HIS	CG-CD2-NE2	-7.60	99.60	107.20
1	C	409	HIS	CG-CD2-NE2	-7.57	99.63	107.20
2	E	311	ALA	N-CA-CB	-7.56	99.03	111.66
2	E	311	ALA	N-CA-C	7.39	120.30	109.07
3	I	372	PRO	N-CA-C	-7.38	99.91	111.34
2	E	310	ASP	CA-C-O	7.32	128.35	119.49
3	I	444	HIS	CA-C-O	-7.27	112.70	121.28
1	C	409	HIS	ND1-CE1-NE2	-7.13	101.27	108.40
2	E	360	SER	CA-C-O	-7.00	113.97	121.88
2	E	409	HIS	CA-CB-CG	-6.97	106.83	113.80
3	I	415	HIS	CG-CD2-NE2	-6.95	100.25	107.20
2	E	418	ASP	N-CA-CB	6.88	121.62	110.41
3	I	415	HIS	ND1-CE1-NE2	-6.84	101.56	108.40
1	C	452	GLN	CA-C-O	6.82	127.77	119.31
1	C	290	GLU	CB-CG-CD	6.82	124.20	112.60
3	I	282	ILE	N-CA-CB	6.80	120.50	111.25
2	E	470	PHE	CA-CB-CG	6.78	120.58	113.80
1	C	314	VAL	O-C-N	-6.72	115.35	121.87
3	I	473	ARG	CD-NE-CZ	6.67	133.73	124.40
2	E	405	HIS	CG-CD2-NE2	-6.63	100.57	107.20
3	I	307	GLU	CA-C-O	-6.62	110.44	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	326	ALA	O-C-N	6.62	128.97	122.09
2	E	468	GLU	N-CA-CB	6.58	119.61	110.07
1	C	330	SER	CB-CA-C	-6.57	99.51	110.68
2	E	427	GLU	CA-C-N	6.55	130.27	120.31
2	E	427	GLU	C-N-CA	6.55	130.27	120.31
3	I	306	ASN	OD1-CG-ND2	-6.54	116.06	122.60
1	A	255	ILE	CA-C-O	6.53	127.75	120.95
3	I	305	PRO	N-CD-CG	6.50	111.60	103.80
1	A	314	VAL	N-CA-C	6.49	117.24	110.62
2	E	359	ASN	N-CA-CB	-6.48	99.55	110.49
1	C	389	ASN	OD1-CG-ND2	-6.47	116.13	122.60
3	I	447	ASN	CA-CB-CG	6.47	119.07	112.60
3	I	473	ARG	CA-C-N	6.45	133.30	121.70
3	I	473	ARG	C-N-CA	6.45	133.30	121.70
1	A	309	LYS	CG-CD-CE	6.43	126.09	111.30
1	A	220	PRO	N-CA-C	-6.41	99.28	112.47
3	I	359	ASN	N-CA-CB	6.39	121.30	110.49
1	A	264	ASN	CA-CB-CG	-6.38	106.22	112.60
1	A	374	GLY	N-CA-C	-6.38	106.75	113.58
2	E	410	ASN	CA-CB-CG	6.37	118.97	112.60
1	C	381	ASN	CA-CB-CG	6.36	118.96	112.60
1	A	351	ALA	CA-C-O	-6.35	113.91	120.89
1	A	409	HIS	CG-CD2-NE2	-6.34	100.86	107.20
1	C	406	GLU	CA-C-O	6.34	127.14	120.42
2	E	268	ASP	CB-CA-C	-6.34	97.45	110.38
2	E	320	GLN	OE1-CD-NE2	6.32	128.92	122.60
1	C	381	ASN	OD1-CG-ND2	-6.28	116.32	122.60
1	A	442	GLY	N-CA-C	-6.24	106.48	115.27
2	E	419	GLY	N-CA-C	-6.23	98.42	113.18
3	I	409	HIS	CE1-NE2-CD2	6.18	115.18	109.00
1	A	305	PRO	N-CD-CG	6.18	111.22	103.80
3	I	472	GLU	CA-C-O	-6.16	114.84	121.56
2	E	415	HIS	ND1-CE1-NE2	-6.16	102.24	108.40
3	I	355	SER	N-CA-CB	-6.11	104.68	111.10
1	C	283	ARG	NE-CZ-NH2	-6.11	113.70	119.20
2	E	418	ASP	CA-CB-CG	6.11	118.71	112.60
2	E	455	LYS	O-C-N	6.09	129.76	122.27
2	E	418	ASP	N-CA-C	-6.02	100.74	110.32
3	I	449	MET	CA-CB-CG	6.01	126.12	114.10
1	A	373	VAL	N-CA-CB	5.99	121.11	111.23
2	E	409	HIS	CE1-NE2-CD2	5.99	114.99	109.00
1	A	415	HIS	CG-CD2-NE2	-5.98	101.22	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	403	THR	CA-C-O	-5.95	114.24	120.55
1	A	409	HIS	CA-CB-CG	-5.95	107.85	113.80
2	E	361	HIS	N-CA-CB	5.92	119.89	110.65
1	A	372	PRO	N-CA-C	-5.92	100.50	110.21
1	C	473	ARG	NE-CZ-NH2	5.91	124.52	119.20
2	E	307	GLU	N-CA-C	-5.91	101.66	110.23
2	E	310	ASP	CA-CB-CG	-5.91	106.69	112.60
1	A	369	TYR	CA-C-O	-5.90	114.45	120.71
1	A	405	HIS	ND1-CE1-NE2	-5.89	102.51	108.40
1	C	309	LYS	CA-C-N	-5.88	110.30	121.54
1	C	309	LYS	C-N-CA	-5.88	110.30	121.54
2	E	325	ILE	O-C-N	-5.88	115.22	122.57
1	C	264	ASN	CA-CB-CG	-5.87	106.73	112.60
3	I	294	GLY	O-C-N	-5.86	115.08	122.70
3	I	388	LYS	CA-C-O	-5.86	113.99	120.38
3	I	305	PRO	N-CA-CB	5.84	109.03	102.60
3	I	359	ASN	N-CA-C	-5.84	98.36	110.80
2	E	386	SER	CA-C-O	-5.83	114.53	120.71
3	I	264	ASN	CA-C-N	-5.83	113.98	122.19
3	I	264	ASN	C-N-CA	-5.83	113.98	122.19
3	I	305	PRO	CA-N-CD	-5.83	103.34	111.50
3	I	292	LYS	CA-C-N	5.82	127.12	119.84
3	I	292	LYS	C-N-CA	5.82	127.12	119.84
2	E	310	ASP	O-C-N	-5.79	114.86	122.39
1	C	305	PRO	N-CD-CG	5.79	110.75	103.80
3	I	427	GLU	CA-C-O	-5.77	115.43	122.41
2	E	314	VAL	N-CA-C	5.77	115.96	110.42
1	C	373	VAL	N-CA-C	-5.76	97.35	109.34
1	A	415	HIS	ND1-CE1-NE2	-5.75	102.65	108.40
2	E	309	LYS	O-C-N	-5.74	116.50	123.10
1	C	415	HIS	CA-CB-CG	-5.74	108.06	113.80
3	I	307	GLU	CA-C-N	5.71	131.13	121.14
3	I	307	GLU	C-N-CA	5.71	131.13	121.14
1	A	351	ALA	O-C-N	5.69	129.85	123.48
3	I	462	ILE	CB-CA-C	-5.69	104.69	111.97
1	A	412	GLY	CA-C-O	5.68	125.46	119.04
3	I	409	HIS	CB-CA-C	-5.67	101.98	110.88
3	I	269	ASN	OD1-CG-ND2	5.67	128.27	122.60
2	E	445	GLU	N-CA-C	5.66	118.18	111.33
1	C	451	SER	O-C-N	-5.63	115.10	122.59
2	E	360	SER	CA-C-N	-5.63	115.06	123.00
2	E	360	SER	C-N-CA	-5.63	115.06	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	422	GLU	N-CA-C	-5.63	105.00	112.94
3	I	404	THR	O-C-N	5.62	127.86	122.07
2	E	409	HIS	CG-CD2-NE2	-5.61	101.59	107.20
1	C	422	GLU	CA-C-O	5.59	126.08	119.48
3	I	382	SER	N-CA-C	5.58	117.46	109.14
1	C	468	GLU	CA-C-N	-5.58	111.61	120.70
1	C	468	GLU	C-N-CA	-5.58	111.61	120.70
1	A	447	ASN	N-CA-CB	5.55	118.38	110.06
1	A	313	ASP	CA-C-O	-5.54	114.61	120.92
2	E	265	THR	N-CA-CB	5.53	119.19	110.23
3	I	232	ASP	CA-CB-CG	5.53	118.13	112.60
3	I	225	CYS	CA-C-O	-5.53	114.66	120.58
1	A	403	THR	O-C-N	5.52	127.97	122.12
1	C	409	HIS	CA-CB-CG	-5.50	108.31	113.80
2	E	377	ASN	OD1-CG-ND2	5.49	128.09	122.60
1	A	381	ASN	OD1-CG-ND2	-5.46	117.14	122.60
2	E	232	ASP	CA-CB-CG	5.46	118.06	112.60
2	E	384	LEU	O-C-N	5.45	129.49	123.33
2	E	389	ASN	OD1-CG-ND2	-5.44	117.16	122.60
3	I	409	HIS	CA-CB-CG	-5.43	108.37	113.80
3	I	351	ALA	CA-C-O	-5.43	114.92	120.89
2	E	359	ASN	N-CA-C	5.42	122.34	110.80
3	I	434	VAL	N-CA-C	5.42	117.82	111.05
3	I	440	VAL	CA-C-O	-5.41	116.13	122.13
3	I	314	VAL	N-CA-C	5.41	116.13	110.62
1	A	310	ASP	CA-CB-CG	-5.40	107.20	112.60
1	A	409	HIS	CB-CA-C	-5.40	102.40	110.88
1	A	318	LEU	CA-C-O	5.40	126.49	120.82
1	A	369	TYR	N-CA-CB	5.39	119.37	110.69
3	I	426	ASN	OD1-CG-ND2	-5.38	117.22	122.60
3	I	473	ARG	NE-CZ-NH2	-5.38	114.36	119.20
2	E	381	ASN	CA-CB-CG	5.37	117.97	112.60
1	C	281	GLN	OE1-CD-NE2	-5.36	117.24	122.60
2	E	360	SER	N-CA-C	-5.36	102.96	110.35
2	E	393	THR	CA-CB-OG1	-5.36	101.57	109.60
3	I	247	THR	CA-C-N	5.36	127.77	120.54
3	I	247	THR	C-N-CA	5.36	127.77	120.54
1	A	361	HIS	CA-CB-CG	5.34	119.14	113.80
2	E	320	GLN	CA-C-O	5.34	126.08	120.42
3	I	265	THR	N-CA-CB	5.34	118.97	110.16
1	C	405	HIS	N-CA-CB	-5.33	102.28	110.01
1	C	428	ASP	N-CA-C	-5.33	100.56	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	443	ASP	CA-CB-CG	5.31	117.91	112.60
1	A	409	HIS	ND1-CE1-NE2	-5.31	103.09	108.40
2	E	305	PRO	N-CA-CB	5.31	108.44	102.60
1	C	313	ASP	N-CA-C	-5.31	101.79	109.59
2	E	223	ASN	CA-C-N	-5.31	115.51	122.99
2	E	223	ASN	C-N-CA	-5.31	115.51	122.99
3	I	405	HIS	ND1-CE1-NE2	-5.28	103.12	108.40
2	E	426	ASN	CA-C-N	5.27	127.60	120.38
2	E	426	ASN	C-N-CA	5.27	127.60	120.38
3	I	304	TYR	O-C-N	5.26	126.88	121.72
1	C	307	GLU	N-CA-C	5.26	117.09	111.36
3	I	373	VAL	N-CA-CB	5.25	119.89	111.23
2	E	409	HIS	CB-CA-C	-5.24	102.65	110.88
1	C	255	ILE	O-C-N	5.24	127.72	121.80
1	C	407	LEU	CA-C-N	5.23	125.75	119.94
1	C	407	LEU	C-N-CA	5.23	125.75	119.94
1	A	258	VAL	O-C-N	-5.23	116.79	121.91
3	I	280	GLU	N-CA-C	-5.23	104.52	112.04
1	C	398	GLU	CA-C-O	5.21	125.95	120.42
3	I	397	LYS	CA-C-N	5.21	127.53	120.44
3	I	397	LYS	C-N-CA	5.21	127.53	120.44
1	C	310	ASP	CB-CA-C	5.21	120.78	110.42
1	C	431	GLY	O-C-N	-5.19	117.98	122.91
2	E	236	TYR	CA-CB-CG	5.19	123.25	113.90
1	A	313	ASP	N-CA-C	-5.18	102.39	110.10
2	E	220	PRO	N-CA-CB	-5.17	97.83	103.25
1	C	415	HIS	CE1-NE2-CD2	5.16	114.16	109.00
1	A	349	GLY	CA-C-O	-5.16	116.60	121.60
1	A	462	ILE	CB-CA-C	-5.15	105.38	111.97
3	I	257	ARG	NE-CZ-NH2	-5.14	114.58	119.20
1	A	373	VAL	N-CA-C	-5.13	98.66	109.34
2	E	361	HIS	CA-C-O	5.12	125.78	120.30
1	C	429	GLN	N-CA-C	-5.11	99.92	110.80
3	I	313	ASP	N-CA-C	-5.11	102.30	109.96
2	E	405	HIS	N-CA-CB	-5.10	102.62	110.16
1	C	409	HIS	CB-CA-C	-5.09	102.19	110.85
3	I	365	CYS	CA-C-O	5.09	127.13	120.16
1	C	310	ASP	CA-C-O	-5.08	113.24	120.51
3	I	353	VAL	CA-C-O	-5.08	114.97	120.71
3	I	424	ALA	CA-C-N	5.08	125.35	119.92
3	I	424	ALA	C-N-CA	5.08	125.35	119.92
3	I	416	ASP	CA-C-O	5.06	124.86	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	415	HIS	O-C-N	5.05	128.66	122.75
1	C	318	LEU	O-C-N	-5.05	116.77	122.12
2	E	227	LEU	CB-CA-C	-5.05	100.13	109.37
1	C	455	LYS	CA-CB-CG	5.04	124.18	114.10
3	I	409	HIS	CG-CD2-NE2	-5.04	102.16	107.20
1	C	330	SER	CA-CB-OG	-5.03	101.03	111.10
3	I	342	ASP	CA-C-O	-5.03	116.59	122.37
2	E	366	PRO	CB-CA-C	5.02	117.89	111.21
1	A	305	PRO	CA-N-CD	-5.02	104.47	111.50
3	I	265	THR	CA-CB-CG2	5.01	119.02	110.50
2	E	467	GLN	CB-CG-CD	5.00	121.10	112.60

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	278	GLN	Mainchain
1	A	375	LYS	Mainchain
1	C	371	SER	Peptide,Mainchain
1	C	375	LYS	Peptide
1	C	419	GLY	Mainchain
1	C	420	LEU	Peptide
1	C	425	PRO	Mainchain
1	C	452	GLN	Mainchain
2	E	268	ASP	Mainchain
2	E	467	GLN	Peptide
3	I	270	ALA	Mainchain
3	I	291	VAL	Mainchain
3	I	307	GLU	Mainchain

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	2025	0	1937	67	2
1	C	2012	0	1916	61	4
2	E	2028	0	1940	58	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	2017	0	1933	53	4
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	I	1	0	0	0	0
5	A	29	0	34	1	1
5	C	29	0	35	1	0
5	E	29	0	35	1	1
5	I	29	0	35	0	1
6	A	572	0	0	21	18
6	C	442	0	0	16	8
6	E	368	0	0	9	18
6	I	238	0	0	7	9
All	All	9822	0	7865	240	34

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 15.

All (240) 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)
3:I:350:LEU:HG	6:I:1289:HOH:O	1.60	1.00
3:I:281:GLN:HE21	3:I:283:ARG:HE	0.99	0.97
1:C:279:ILE:HG23	6:C:838:HOH:O	1.64	0.95
1:A:219:ASP:N	1:A:467:GLN:HE22	1.67	0.91
1:C:281:GLN:HE21	1:C:283:ARG:NE	1.68	0.91
3:I:278:GLN:HE22	3:I:474:SER:H	0.95	0.89
1:C:421:ALA:HB1	1:C:423:CYS:H	1.36	0.88
1:A:449:MET:HG3	6:A:676:HOH:O	1.75	0.87
1:C:388:LYS:HG2	6:C:879:HOH:O	1.75	0.86
3:I:281:GLN:NE2	3:I:283:ARG:HH21	1.74	0.84
1:A:278:GLN:HE22	1:A:473:ARG:NH1	1.76	0.84
1:C:223:ASN:ND2	1:C:473:ARG:HH12	1.75	0.83
1:C:223:ASN:HD21	1:C:473:ARG:HH12	1.25	0.83
1:A:219:ASP:HB3	1:A:222:LYS:H	1.43	0.82
1:C:346:GLY:HA2	1:C:389:ASN:HD21	1.45	0.82
2:E:467:GLN:HB2	2:E:470:PHE:O	1.79	0.81
1:C:281:GLN:NE2	1:C:283:ARG:NE	2.29	0.80
1:A:279:ILE:HD13	1:A:282:ILE:HD11	1.62	0.80
3:I:278:GLN:HE22	3:I:474:SER:N	1.78	0.79
2:E:302:LYS:HB3	2:E:307:GLU:HG3	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:HIS:HD2	1:C:299:ASN:H	1.30	0.78
3:I:297:HIS:HD2	3:I:299:ASN:H	1.33	0.76
3:I:281:GLN:NE2	3:I:283:ARG:HE	1.80	0.76
2:E:307:GLU:O	2:E:308:GLU:HB3	1.83	0.76
3:I:281:GLN:HE22	3:I:283:ARG:HH21	1.34	0.74
3:I:297:HIS:CD2	3:I:299:ASN:H	2.06	0.74
3:I:281:GLN:HE21	3:I:283:ARG:NE	1.81	0.74
1:A:297:HIS:HD2	1:A:299:ASN:H	1.35	0.74
3:I:278:GLN:NE2	3:I:474:SER:H	1.80	0.74
1:C:473:ARG:O	1:C:474:SER:HB2	1.89	0.73
1:A:279:ILE:HG21	1:A:282:ILE:HG13	1.70	0.72
3:I:381:ASN:HD22	3:I:381:ASN:H	1.38	0.71
2:E:359:ASN:HB3	2:E:367:LYS:CD	2.21	0.70
2:E:297:HIS:CD2	2:E:299:ASN:H	2.09	0.70
2:E:297:HIS:HD2	2:E:299:ASN:H	1.37	0.70
1:A:315:LYS:HB3	6:A:991:HOH:O	1.90	0.69
3:I:372:PRO:O	3:I:373:VAL:HB	1.93	0.69
2:E:467:GLN:HA	2:E:470:PHE:H	1.56	0.69
1:C:425:PRO:HB3	1:C:429:GLN:HB3	1.74	0.69
2:E:269:ASN:HD21	2:E:452:GLN:HE22	1.39	0.68
3:I:473:ARG:O	3:I:474:SER:HB2	1.93	0.68
1:A:297:HIS:CD2	1:A:299:ASN:H	2.11	0.68
1:C:281:GLN:NE2	1:C:283:ARG:HE	1.91	0.68
1:A:278:GLN:HE22	1:A:473:ARG:HH11	1.41	0.66
1:A:220:PRO:HD3	6:A:1046:HOH:O	1.95	0.66
1:C:342:ASP:OD1	6:C:614:HOH:O	2.14	0.66
3:I:227:LEU:HB3	6:I:2206:HOH:O	1.96	0.66
1:A:282:ILE:HB	6:A:944:HOH:O	1.95	0.66
3:I:269:ASN:HD21	3:I:452:GLN:HE22	1.44	0.65
1:A:448:LYS:O	1:A:449:MET:HE2	1.95	0.65
1:C:312:TRP:H	1:C:341:GLN:NE2	1.94	0.64
1:C:297:HIS:CD2	1:C:299:ASN:H	2.14	0.64
3:I:359:ASN:HA	3:I:367:LYS:HD3	1.80	0.64
3:I:360:SER:H	3:I:367:LYS:HD3	1.63	0.64
1:A:403:THR:HG22	1:A:407:LEU:HD22	1.80	0.63
5:C:2:INN:H142	6:C:798:HOH:O	2.00	0.62
2:E:261:ILE:O	2:E:265:THR:HG22	2.00	0.62
2:E:234:ARG:NH1	6:E:805:HOH:O	2.33	0.61
1:A:278:GLN:NE2	1:A:473:ARG:NH1	2.48	0.61
2:E:312:TRP:H	2:E:341:GLN:NE2	1.99	0.61
2:E:307:GLU:O	2:E:308:GLU:OE1	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:GLN:HG3	6:A:923:HOH:O	2.02	0.60
1:C:281:GLN:HG3	6:C:738:HOH:O	2.00	0.60
3:I:281:GLN:NE2	3:I:283:ARG:NH2	2.50	0.59
3:I:248:THR:OG1	3:I:284:ILE:HD11	2.02	0.59
1:A:357:ARG:O	1:A:360:SER:HB3	2.02	0.59
2:E:307:GLU:O	2:E:308:GLU:CB	2.51	0.59
1:A:220:PRO:HG2	6:A:815:HOH:O	2.03	0.59
1:C:223:ASN:HD21	1:C:473:ARG:NH1	1.97	0.58
3:I:359:ASN:HA	3:I:367:LYS:CE	2.34	0.58
1:C:226:LYS:HB3	1:C:280:GLU:HB2	1.85	0.58
2:E:467:GLN:HA	2:E:469:CYS:N	2.19	0.58
3:I:233:HIS:H	3:I:299:ASN:HD21	1.52	0.57
3:I:429:GLN:NE2	6:I:1353:HOH:O	2.38	0.57
2:E:222:LYS:CE	2:E:467:GLN:HB3	2.35	0.56
2:E:226:LYS:HB3	2:E:280:GLU:HB2	1.86	0.56
1:C:388:LYS:HE2	6:C:879:HOH:O	2.05	0.56
1:A:241:ARG:HH11	1:A:241:ARG:HB3	1.69	0.56
1:C:401:LEU:HD21	1:C:448:LYS:HG2	1.87	0.56
2:E:222:LYS:CD	2:E:467:GLN:HB3	2.36	0.56
1:C:336:HIS:HE1	1:C:385:THR:OG1	1.87	0.56
3:I:329:ALA:HB1	3:I:381:ASN:HD21	1.70	0.55
1:A:219:ASP:N	1:A:467:GLN:NE2	2.47	0.55
2:E:336:HIS:HE1	2:E:385:THR:OG1	1.90	0.55
2:E:240:GLY:HA3	2:E:247:THR:OG1	2.08	0.54
3:I:226:LYS:HB3	3:I:280:GLU:HB2	1.89	0.54
1:A:302:LYS:HG2	6:A:539:HOH:O	2.07	0.54
1:A:292:LYS:HB2	1:A:295:GLU:CD	2.32	0.53
2:E:269:ASN:HD21	2:E:452:GLN:NE2	2.06	0.53
1:C:456:GLN:O	1:C:460:LYS:HG3	2.09	0.53
2:E:258:VAL:HG13	6:E:827:HOH:O	2.08	0.53
2:E:403:THR:HG22	2:E:407:LEU:HD22	1.89	0.53
1:A:372:PRO:O	1:A:373:VAL:HB	2.07	0.53
2:E:467:GLN:HA	2:E:470:PHE:N	2.22	0.53
3:I:233:HIS:H	3:I:299:ASN:ND2	2.06	0.53
1:C:456:GLN:HG3	6:C:903:HOH:O	2.09	0.53
3:I:221:MET:HB3	3:I:472:GLU:HG2	1.91	0.53
1:A:336:HIS:HD2	6:A:569:HOH:O	1.90	0.53
1:A:308:GLU:HG2	1:A:309:LYS:HE2	1.90	0.52
3:I:261:ILE:O	3:I:265:THR:HG22	2.08	0.52
2:E:467:GLN:H	2:E:470:PHE:HB2	1.75	0.52
3:I:357:ARG:O	3:I:360:SER:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:381:ASN:HD22	3:I:381:ASN:N	2.06	0.52
1:C:403:THR:HG22	1:C:407:LEU:HD22	1.91	0.52
2:E:359:ASN:HB3	2:E:367:LYS:HD2	1.92	0.52
2:E:331:LYS:HE2	6:E:821:HOH:O	2.10	0.51
1:A:336:HIS:HE1	1:A:385:THR:OG1	1.92	0.51
2:E:222:LYS:HE2	2:E:467:GLN:HB3	1.92	0.51
1:A:223:ASN:HD22	1:A:223:ASN:H	1.57	0.51
1:A:359:ASN:HB3	6:A:896:HOH:O	2.10	0.50
1:A:468:GLU:HG2	6:A:790:HOH:O	2.11	0.50
1:A:222:LYS:HE2	6:A:814:HOH:O	2.12	0.50
2:E:467:GLN:NE2	2:E:470:PHE:O	2.44	0.50
3:I:421:ALA:O	3:I:423:CYS:N	2.39	0.50
1:A:237:ARG:HA	1:A:237:ARG:HH11	1.77	0.49
1:C:446:ASN:HA	1:C:449:MET:HE3	1.94	0.49
2:E:336:HIS:HD2	6:E:485:HOH:O	1.94	0.49
2:E:268:ASP:HB3	2:E:270:ALA:H	1.77	0.49
1:C:391:GLY:N	6:C:879:HOH:O	2.37	0.49
1:C:421:ALA:HB1	1:C:423:CYS:N	2.17	0.49
2:E:221:MET:HE3	2:E:472:GLU:CD	2.37	0.49
3:I:432:LYS:HD3	3:I:436:TYR:CD2	2.47	0.49
1:A:306:ASN:HB3	1:A:308:GLU:OE2	2.12	0.49
1:C:419:GLY:O	1:C:421:ALA:N	2.45	0.49
1:C:402:VAL:O	1:C:406:GLU:HG2	2.12	0.49
1:C:281:GLN:NE2	1:C:283:ARG:CZ	2.76	0.49
1:A:452:GLN:HE21	1:A:456:GLN:HG3	1.77	0.48
2:E:429:GLN:HG3	6:E:770:HOH:O	2.12	0.48
3:I:359:ASN:HA	3:I:367:LYS:CD	2.41	0.48
3:I:287:SER:HB2	3:I:288:PRO:HD2	1.95	0.48
1:A:359:ASN:HB2	6:A:895:HOH:O	2.14	0.48
1:A:398:GLU:HA	1:A:401:LEU:HD12	1.95	0.48
1:A:241:ARG:HB3	1:A:241:ARG:NH1	2.29	0.47
2:E:304:TYR:HE2	2:E:316:MET:HE1	1.78	0.47
2:E:432:LYS:HD2	2:E:436:TYR:CD1	2.50	0.47
1:C:221:MET:HG2	1:C:222:LYS:N	2.29	0.47
2:E:270:ALA:O	2:E:273:LYS:HE2	2.15	0.47
2:E:307:GLU:HB3	6:E:627:HOH:O	2.14	0.47
3:I:315:LYS:HA	6:I:1289:HOH:O	2.14	0.47
1:A:436:TYR:CG	1:A:437:PRO:HD2	2.50	0.47
1:A:460:LYS:HA	1:A:460:LYS:HD3	1.73	0.47
1:A:332:VAL:O	1:A:366:PRO:HG3	2.16	0.46
1:A:448:LYS:HB2	6:A:933:HOH:O	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:315:LYS:O	3:I:319:GLU:HG3	2.15	0.46
2:E:254:LEU:HD23	2:E:254:LEU:C	2.40	0.46
2:E:467:GLN:HA	2:E:469:CYS:H	1.80	0.46
1:A:241:ARG:HG3	6:A:983:HOH:O	2.16	0.46
1:C:223:ASN:CG	1:C:473:ARG:HH12	2.23	0.46
1:C:289:GLN:HG2	1:C:297:HIS:CG	2.51	0.46
1:C:428:ASP:O	1:C:429:GLN:HB2	2.16	0.46
2:E:439:ALA:HA	5:E:2:INN:H21	1.98	0.46
3:I:336:HIS:HE1	3:I:385:THR:OG1	1.99	0.46
2:E:359:ASN:HB3	2:E:367:LYS:HD3	1.98	0.46
2:E:424:ALA:N	2:E:425:PRO:HD3	2.30	0.45
2:E:292:LYS:HA	2:E:292:LYS:HD3	1.87	0.45
1:C:241:ARG:HA	1:C:241:ARG:HD2	1.84	0.45
1:C:342:ASP:CG	6:C:879:HOH:O	2.59	0.45
1:A:371:SER:OG	1:A:373:VAL:O	2.34	0.45
3:I:336:HIS:HD2	6:I:1169:HOH:O	1.99	0.45
3:I:359:ASN:HA	3:I:367:LYS:HE2	1.97	0.45
1:A:299:ASN:ND2	6:A:865:HOH:O	2.50	0.45
3:I:236:TYR:CZ	3:I:286:LYS:HG2	2.52	0.45
1:A:367:LYS:HD3	6:A:970:HOH:O	2.16	0.44
1:A:297:HIS:HE1	6:A:747:HOH:O	2.00	0.44
1:A:375:LYS:HG3	6:A:961:HOH:O	2.17	0.44
1:C:456:GLN:HG3	6:C:683:HOH:O	2.17	0.44
2:E:330:SER:HB3	2:E:379:TYR:CE2	2.53	0.44
1:C:327:GLU:O	1:C:330:SER:HB2	2.17	0.44
1:C:398:GLU:O	1:C:402:VAL:HG23	2.17	0.44
2:E:222:LYS:HE2	2:E:467:GLN:HG2	2.00	0.44
3:I:359:ASN:CA	3:I:367:LYS:HD3	2.45	0.44
3:I:427:GLU:O	3:I:428:GLU:CD	2.61	0.44
1:A:366:PRO:HB2	1:A:379:TYR:CD2	2.53	0.44
2:E:283:ARG:HG2	6:E:582:HOH:O	2.18	0.44
1:A:237:ARG:HH11	1:A:237:ARG:CG	2.31	0.44
1:C:325:ILE:HD11	1:C:328:GLU:OE1	2.17	0.44
1:C:421:ALA:HB1	1:C:423:CYS:HB2	1.98	0.44
1:C:221:MET:HE2	1:C:221:MET:N	2.33	0.43
1:C:428:ASP:O	1:C:429:GLN:CB	2.65	0.43
1:C:309:LYS:HG3	6:C:754:HOH:O	2.18	0.43
1:A:223:ASN:H	1:A:223:ASN:ND2	2.14	0.43
1:C:223:ASN:HD21	1:C:473:ARG:HH22	1.65	0.43
1:C:336:HIS:HD2	6:C:609:HOH:O	2.02	0.43
2:E:289:GLN:HG2	2:E:297:HIS:CG	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:ALA:HA	6:A:1022:HOH:O	2.17	0.43
3:I:422:GLU:H	3:I:422:GLU:HG3	1.59	0.43
1:A:402:VAL:O	1:A:406:GLU:HG2	2.18	0.43
1:C:421:ALA:CB	1:C:423:CYS:HB2	2.49	0.43
1:C:446:ASN:HA	1:C:449:MET:CE	2.49	0.43
1:A:309:LYS:HA	1:A:309:LYS:HD3	1.78	0.43
1:C:389:ASN:ND2	6:C:614:HOH:O	2.44	0.43
1:C:392:LYS:HD2	6:C:619:HOH:O	2.17	0.43
1:C:431:GLY:HA2	6:C:795:HOH:O	2.19	0.42
1:A:221:MET:O	1:A:472:GLU:HA	2.19	0.42
1:A:261:ILE:HD11	1:A:448:LYS:HD3	2.00	0.42
2:E:236:TYR:CZ	2:E:286:LYS:HG2	2.54	0.42
2:E:401:LEU:HD21	2:E:448:LYS:HG2	2.02	0.42
1:C:357:ARG:O	1:C:360:SER:HB3	2.20	0.42
2:E:297:HIS:HE1	6:E:608:HOH:O	2.02	0.42
2:E:307:GLU:N	6:E:625:HOH:O	2.44	0.42
3:I:360:SER:N	3:I:367:LYS:HD3	2.33	0.42
1:A:355:SER:HB3	1:A:360:SER:HB2	2.01	0.42
1:A:421:ALA:O	1:A:422:GLU:CB	2.66	0.42
1:A:452:GLN:NE2	1:A:456:GLN:HG3	2.34	0.42
1:A:439:ALA:HA	5:A:2:INN:H21	2.01	0.42
1:C:361:HIS:CE1	1:C:367:LYS:HD3	2.55	0.42
3:I:221:MET:HB3	3:I:221:MET:HE3	1.96	0.42
1:A:289:GLN:HG2	1:A:297:HIS:CG	2.54	0.42
1:C:279:ILE:HG21	1:C:282:ILE:HG13	2.02	0.42
1:C:418:ASP:OD2	1:C:436:TYR:OH	2.38	0.42
2:E:465:LYS:O	2:E:466:ALA:C	2.63	0.42
3:I:421:ALA:O	6:I:1350:HOH:O	2.20	0.42
1:A:372:PRO:O	1:A:373:VAL:CB	2.67	0.42
1:A:281:GLN:HG3	1:A:282:ILE:N	2.34	0.41
2:E:335:ALA:O	2:E:382:SER:HA	2.20	0.41
1:A:456:GLN:NE2	6:A:805:HOH:O	2.53	0.41
1:C:403:THR:O	1:C:407:LEU:HB2	2.20	0.41
2:E:219:ASP:HA	2:E:220:PRO:HD3	1.84	0.41
2:E:422:GLU:H	2:E:422:GLU:HG3	1.15	0.41
3:I:456:GLN:HG3	6:I:2223:HOH:O	2.19	0.41
1:A:432:LYS:HD3	1:A:436:TYR:CD2	2.55	0.41
1:C:297:HIS:HE1	6:C:533:HOH:O	2.02	0.41
3:I:403:THR:HG22	3:I:407:LEU:HD22	2.02	0.41
1:A:302:LYS:HB3	1:A:307:GLU:HG2	2.01	0.41
3:I:254:LEU:HD23	3:I:254:LEU:C	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:436:TYR:CD1	1:C:437:PRO:HD2	2.55	0.41
1:A:236:TYR:HD2	1:A:237:ARG:HD2	1.85	0.41
1:C:359:ASN:HD22	1:C:359:ASN:HA	1.65	0.41
2:E:234:ARG:HH11	2:E:234:ARG:HD3	1.72	0.41
3:I:303:SER:HB2	3:I:311:ALA:C	2.45	0.41
2:E:222:LYS:CG	2:E:467:GLN:HB3	2.51	0.41
2:E:467:GLN:N	2:E:470:PHE:H	2.19	0.41
1:A:473:ARG:NH1	6:A:700:HOH:O	2.54	0.41
1:C:361:HIS:ND1	1:C:367:LYS:HD3	2.36	0.41
3:I:350:LEU:CD1	3:I:351:ALA:H	2.34	0.41
1:A:248:THR:O	1:A:252:ILE:HG13	2.21	0.40
1:C:365:CYS:HA	1:C:366:PRO:HD2	1.89	0.40
3:I:297:HIS:HD2	3:I:299:ASN:N	2.08	0.40
3:I:381:ASN:H	3:I:381:ASN:ND2	2.11	0.40
2:E:357:ARG:O	2:E:359:ASN:N	2.55	0.40

All (34) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:452:GLN:CD	6:A:1012:HOH:O[1_655]	1.08	1.12
1:C:452:GLN:CG	6:A:1012:HOH:O[1_655]	1.20	1.00
6:A:920:HOH:O	6:E:606:HOH:O[2_546]	1.55	0.65
6:A:710:HOH:O	6:I:1189:HOH:O[2_656]	1.56	0.64
6:A:600:HOH:O	6:E:628:HOH:O[2_546]	1.66	0.54
3:I:426:ASN:CB	6:A:1011:HOH:O[2_545]	1.69	0.51
5:I:2:INN:N4	6:C:862:HOH:O[2_545]	1.85	0.35
6:A:733:HOH:O	6:E:737:HOH:O[2_646]	1.86	0.34
6:A:870:HOH:O	6:I:1257:HOH:O[2_656]	1.89	0.31
1:C:452:GLN:NE2	6:A:1012:HOH:O[1_655]	1.89	0.31
1:C:452:GLN:OE1	6:A:1012:HOH:O[1_655]	1.91	0.29
6:A:876:HOH:O	6:E:730:HOH:O[2_646]	1.94	0.26
6:E:822:HOH:O	6:I:1234:HOH:O[2_555]	1.95	0.25
6:A:721:HOH:O	6:E:521:HOH:O[2_646]	1.98	0.22
6:C:823:HOH:O	6:I:1194:HOH:O[2_655]	1.98	0.22
3:I:331:LYS:CD	6:E:751:HOH:O[2_646]	2.00	0.20
3:I:421:ALA:CB	6:C:593:HOH:O[2_545]	2.02	0.18
1:A:421:ALA:CB	6:E:638:HOH:O[2_546]	2.03	0.17
6:E:822:HOH:O	6:I:1229:HOH:O[2_555]	2.03	0.17
6:A:983:HOH:O	6:E:521:HOH:O[2_646]	2.04	0.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:947:HOH:O	6:E:729:HOH:O[2_646]	2.05	0.15
2:E:429:GLN:NE2	6:I:1244:HOH:O[2_656]	2.07	0.13
3:I:456:GLN:OE1	6:E:715:HOH:O[2_545]	2.09	0.11
6:A:530:HOH:O	6:I:1252:HOH:O[2_656]	2.10	0.10
5:E:2:INN:N4	6:C:907:HOH:O[2_656]	2.10	0.10
6:C:857:HOH:O	6:I:1287:HOH:O[2_555]	2.14	0.06
6:A:920:HOH:O	6:E:605:HOH:O[2_546]	2.15	0.05
6:A:917:HOH:O	6:E:620:HOH:O[2_546]	2.16	0.04
1:A:421:ALA:N	6:E:638:HOH:O[2_546]	2.17	0.03
5:A:2:INN:N4	6:E:602:HOH:O[2_546]	2.17	0.03
6:C:847:HOH:O	6:E:589:HOH:O[2_545]	2.17	0.03
6:A:505:HOH:O	6:E:737:HOH:O[2_646]	2.18	0.02
6:C:543:HOH:O	6:I:1279:HOH:O[2_555]	2.18	0.02
2:E:290:GLU:CD	6:C:848:HOH:O[2_555]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	253/256 (99%)	241 (95%)	8 (3%)	4 (2%)	7	3
1	C	250/256 (98%)	228 (91%)	14 (6%)	8 (3%)	3	1
2	E	254/256 (99%)	238 (94%)	11 (4%)	5 (2%)	6	2
3	I	252/256 (98%)	243 (96%)	3 (1%)	6 (2%)	4	2
All	All	1009/1024 (98%)	950 (94%)	36 (4%)	23 (2%)	5	2

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	221	MET
1	A	373	VAL
1	C	370	TYR

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Mol	Chain	Res	Type
1	C	371	SER
1	C	372	PRO
1	C	373	VAL
1	C	429	GLN
2	E	220	PRO
2	E	420	LYS
2	E	467	GLN
3	I	359	ASN
3	I	422	GLU
3	I	428	GLU
1	A	420	LEU
1	C	369	TYR
2	E	308	GLU
1	A	365	CYS
1	C	365	CYS
2	E	365	CYS
3	I	365	CYS
3	I	293	PRO
3	I	373	VAL
1	C	374	GLY

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	218/219 (100%)	197 (90%)	21 (10%)	8	5
1	C	216/219 (99%)	194 (90%)	22 (10%)	7	4
2	E	218/219 (100%)	200 (92%)	18 (8%)	10	7
3	I	217/219 (99%)	205 (94%)	12 (6%)	19	17
All	All	869/876 (99%)	796 (92%)	73 (8%)	10	7

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	221	MET

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Mol	Chain	Res	Type
1	A	223	ASN
1	A	237	ARG
1	A	273	LYS
1	A	278	GLN
1	A	281	GLN
1	A	290	GLU
1	A	291	VAL
1	A	309	LYS
1	A	325	ILE
1	A	327	GLU
1	A	345	MET
1	A	360	SER
1	A	367	LYS
1	A	407	LEU
1	A	422	GLU
1	A	428	ASP
1	A	448	LYS
1	A	463	GLU
1	A	467	GLN
1	A	472	GLU
1	C	221	MET
1	C	226	LYS
1	C	241	ARG
1	C	263	ARG
1	C	309	LYS
1	C	310	ASP
1	C	330	SER
1	C	350	LEU
1	C	355	SER
1	C	359	ASN
1	C	360	SER
1	C	371	SER
1	C	375	LYS
1	C	407	LEU
1	C	420	LEU
1	C	422	GLU
1	C	427	GLU
1	C	432	LYS
1	C	452	GLN
1	C	455	LYS
1	C	473	ARG
1	C	474	SER

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Mol	Chain	Res	Type
2	E	220	PRO
2	E	221	MET
2	E	265	THR
2	E	268	ASP
2	E	283	ARG
2	E	292	LYS
2	E	308	GLU
2	E	350	LEU
2	E	355	SER
2	E	367	LYS
2	E	396	THR
2	E	407	LEU
2	E	422	GLU
2	E	432	LYS
2	E	445	GLU
2	E	465	LYS
2	E	467	GLN
2	E	474	SER
3	I	265	THR
3	I	291	VAL
3	I	307	GLU
3	I	350	LEU
3	I	360	SER
3	I	361	HIS
3	I	367	LYS
3	I	381	ASN
3	I	407	LEU
3	I	464	SER
3	I	473	ARG
3	I	474	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	223	ASN
1	A	269	ASN
1	A	278	GLN
1	A	297	HIS
1	A	336	HIS
1	A	410	ASN
1	A	452	GLN
1	A	456	GLN

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Mol	Chain	Res	Type
1	A	471	GLN
1	C	223	ASN
1	C	249	ASN
1	C	281	GLN
1	C	297	HIS
1	C	336	HIS
1	C	341	GLN
1	C	359	ASN
1	C	389	ASN
1	C	429	GLN
1	C	444	HIS
1	C	456	GLN
1	C	471	GLN
2	E	223	ASN
2	E	264	ASN
2	E	297	HIS
2	E	336	HIS
2	E	341	GLN
2	E	452	GLN
3	I	278	GLN
3	I	281	GLN
3	I	297	HIS
3	I	299	ASN
3	I	336	HIS
3	I	361	HIS
3	I	381	ASN
3	I	410	ASN
3	I	452	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	INN	A	2	4	28,28,28	3.51	4 (14%)	35,38,38	5.13	21 (60%)
5	INN	E	2	4	28,28,28	3.62	6 (21%)	35,38,38	3.91	14 (40%)
5	INN	C	2	4	28,28,28	3.75	6 (21%)	35,38,38	5.03	20 (57%)
5	INN	I	2	4	28,28,28	3.85	7 (25%)	35,38,38	4.57	17 (48%)

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	INN	A	2	4	1/1/9/13	9/40/40/40	-
5	INN	E	2	4	1/1/9/13	8/40/40/40	-
5	INN	C	2	4	1/1/9/13	8/40/40/40	-
5	INN	I	2	4	1/1/9/13	6/40/40/40	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	2	INN	C4-N1	14.07	1.64	1.34
5	C	2	INN	C4-N1	13.25	1.62	1.34
5	E	2	INN	C4-N1	12.65	1.61	1.34
5	A	2	INN	C4-N1	12.27	1.60	1.34
5	A	2	INN	C11-C13	-9.45	1.29	1.52
5	C	2	INN	C11-C13	-9.18	1.29	1.52
5	C	2	INN	C10-N2	-9.01	1.14	1.34
5	E	2	INN	C11-C13	-8.96	1.30	1.52
5	I	2	INN	C11-C13	-8.85	1.30	1.52
5	E	2	INN	C10-N2	-8.74	1.15	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	2	INN	C10-N2	-8.15	1.16	1.34
5	A	2	INN	C10-N2	-8.07	1.16	1.34
5	I	2	INN	C0-CA	-5.28	1.42	1.53
5	C	2	INN	C0-CA	-4.43	1.44	1.53
5	E	2	INN	C0-CA	-4.30	1.44	1.53
5	A	2	INN	C0-CA	-3.74	1.45	1.53
5	C	2	INN	C6-C5	2.32	1.59	1.55
5	C	2	INN	CB-CA	2.29	1.58	1.53
5	I	2	INN	C-N	2.22	1.34	1.32
5	E	2	INN	O4-N	-2.16	1.34	1.40
5	I	2	INN	CA-C4	2.10	1.55	1.51
5	E	2	INN	C5-N1	-2.05	1.42	1.45
5	I	2	INN	C11-N2	2.03	1.49	1.45

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	2	INN	C11-C13-N3	17.97	157.88	116.47
5	A	2	INN	C11-C13-N3	15.79	152.85	116.47
5	I	2	INN	C11-C13-N3	15.10	151.27	116.47
5	C	2	INN	O3-C13-C11	-13.09	91.70	120.57
5	E	2	INN	O3-C13-C11	-12.94	92.04	120.57
5	A	2	INN	O3-C13-C11	-12.49	93.04	120.57
5	I	2	INN	O3-C13-C11	-12.11	93.88	120.57
5	A	2	INN	O4-N-C	10.40	135.16	119.79
5	C	2	INN	O4-N-C	9.65	134.06	119.79
5	A	2	INN	C5-N1-C4	-8.63	104.55	121.98
5	I	2	INN	C13-C11-N2	8.50	132.64	111.59
5	E	2	INN	C11-C13-N3	7.87	134.61	116.47
5	E	2	INN	O4-N-C	7.86	131.41	119.79
5	C	2	INN	C13-C11-N2	7.50	130.17	111.59
5	E	2	INN	CA-C0-C	-7.10	98.39	112.33
5	A	2	INN	C13-C11-N2	6.99	128.89	111.59
5	E	2	INN	C5-N1-C4	-6.78	108.28	121.98
5	A	2	INN	CA-C0-C	-6.64	99.30	112.33
5	C	2	INN	CA-C0-C	-6.63	99.32	112.33
5	A	2	INN	C14-N3-C13	-6.55	110.78	122.55
5	I	2	INN	C5-N1-C4	-6.53	108.79	121.98
5	E	2	INN	C13-C11-N2	6.39	127.41	111.59
5	C	2	INN	O3-C13-N3	-6.09	110.09	122.98
5	I	2	INN	O-C-C0	-6.05	112.68	121.54
5	E	2	INN	C0-CA-C4	-5.79	101.47	109.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	2	INN	CA-C0-C	-5.27	101.99	112.33
5	A	2	INN	O3-C13-N3	-5.15	112.09	122.98
5	I	2	INN	O4-N-C	5.10	127.33	119.79
5	A	2	INN	CA-C4-N1	5.03	124.85	116.19
5	C	2	INN	C0-CA-C4	-5.02	102.57	109.71
5	A	2	INN	C0-C-N	4.60	122.10	115.14
5	C	2	INN	C5-N1-C4	-4.55	112.80	121.98
5	I	2	INN	C10-C5-N1	-4.37	99.35	109.47
5	I	2	INN	O-C-N	-4.24	118.06	123.27
5	A	2	INN	C11-N2-C10	4.12	129.99	121.32
5	A	2	INN	O1-C4-N1	-4.09	115.63	122.96
5	A	2	INN	O-C-C0	-4.06	115.60	121.54
5	C	2	INN	O-C-C0	-4.05	115.61	121.54
5	A	2	INN	C10-C5-N1	-3.98	100.28	109.47
5	I	2	INN	O2-C10-C5	-3.92	114.43	120.85
5	I	2	INN	O3-C13-N3	-3.90	114.72	122.98
5	I	2	INN	C0-C-N	3.90	121.06	115.14
5	I	2	INN	C0-CA-C4	-3.52	104.70	109.71
5	A	2	INN	O2-C10-C5	-3.49	115.14	120.85
5	C	2	INN	C11-N2-C10	3.39	128.46	121.32
5	C	2	INN	CA-C4-N1	3.34	121.93	116.19
5	E	2	INN	C12-C11-C13	3.32	116.44	110.14
5	I	2	INN	C6-C5-C10	-3.25	109.40	112.97
5	E	2	INN	C6-C5-C10	-3.21	109.44	112.97
5	E	2	INN	C12-C11-N2	2.94	115.77	110.38
5	C	2	INN	O1-C4-N1	-2.88	117.81	122.96
5	A	2	INN	C5-C10-N2	2.80	121.24	116.22
5	C	2	INN	C5-C10-N2	2.77	121.20	116.22
5	A	2	INN	C0-CA-C4	-2.72	105.84	109.71
5	A	2	INN	C6-C5-C10	-2.68	110.02	112.97
5	C	2	INN	O1-C4-CA	-2.55	118.25	122.19
5	C	2	INN	C6-C5-C10	-2.54	110.18	112.97
5	I	2	INN	O1-C4-N1	-2.52	118.44	122.96
5	E	2	INN	C0-C-N	2.38	118.75	115.14
5	E	2	INN	C6-C5-N1	-2.35	108.27	111.94
5	C	2	INN	O2-C10-C5	-2.34	117.01	120.85
5	A	2	INN	C12-C11-N2	2.31	114.62	110.38
5	C	2	INN	C12-C11-C13	2.28	114.47	110.14
5	I	2	INN	C14-N3-C13	-2.26	118.48	122.55
5	C	2	INN	C14-N3-C13	2.26	126.60	122.55
5	C	2	INN	C10-C5-N1	-2.24	104.30	109.47
5	C	2	INN	CA-CB-C1	-2.23	110.97	115.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	2	INN	C10-C5-N1	-2.22	104.34	109.47
5	I	2	INN	O2-C10-N2	2.19	126.88	122.96
5	A	2	INN	O1-C4-CA	-2.16	118.85	122.19
5	A	2	INN	C12-C11-C13	2.09	114.11	110.14
5	E	2	INN	O-C-N	-2.08	120.71	123.27

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	2	INN	C11
5	C	2	INN	C11
5	E	2	INN	C11
5	I	2	INN	C11

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2	INN	C0-C-N-O4
5	A	2	INN	O-C-N-O4
5	A	2	INN	N3-C14-C15-N4
5	C	2	INN	O-C-N-O4
5	C	2	INN	C13-C11-N2-C10
5	E	2	INN	O-C-N-O4
5	E	2	INN	C13-C11-N2-C10
5	E	2	INN	N3-C14-C15-N4
5	I	2	INN	O-C-N-O4
5	C	2	INN	O3-C13-N3-C14
5	C	2	INN	O2-C10-N2-C11
5	A	2	INN	C11-C13-N3-C14
5	C	2	INN	C11-C13-N3-C14
5	A	2	INN	O2-C10-N2-C11
5	E	2	INN	O2-C10-N2-C11
5	E	2	INN	C11-C13-N3-C14
5	E	2	INN	N2-C11-C13-O3
5	E	2	INN	C12-C11-C13-N3
5	A	2	INN	N2-C11-C13-O3
5	I	2	INN	O2-C10-N2-C11
5	C	2	INN	N2-C11-C13-O3
5	E	2	INN	N-C-C0-CA
5	I	2	INN	N-C-C0-CA
5	C	2	INN	N2-C11-C13-N3
5	I	2	INN	N2-C11-C13-O3

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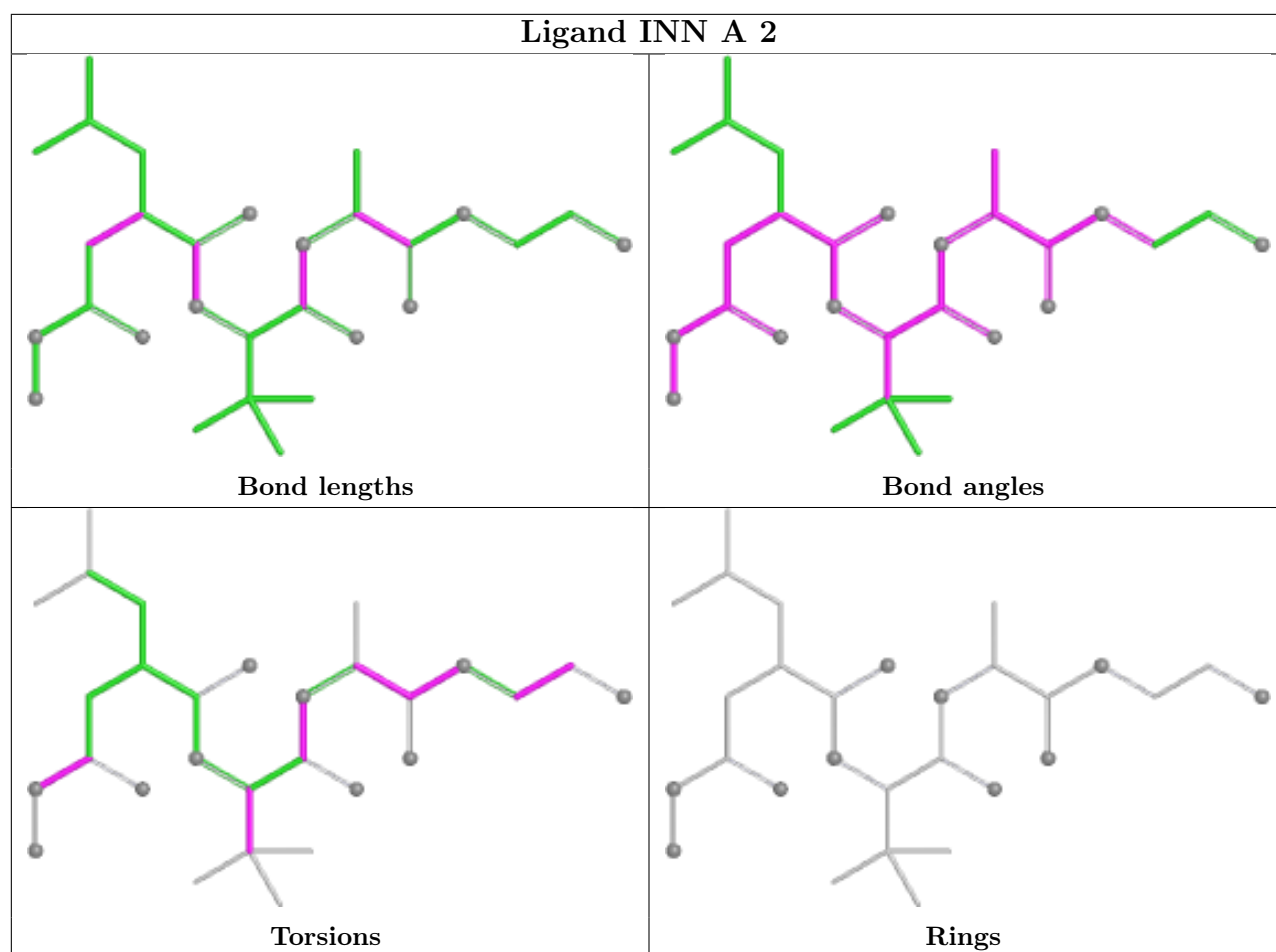
Mol	Chain	Res	Type	Atoms
5	I	2	INN	N2-C11-C13-N3
5	C	2	INN	N-C-C0-CA
5	A	2	INN	N1-C5-C6-C8
5	I	2	INN	CA-C4-N1-C5
5	A	2	INN	N1-C5-C6-C9
5	A	2	INN	N2-C11-C13-N3

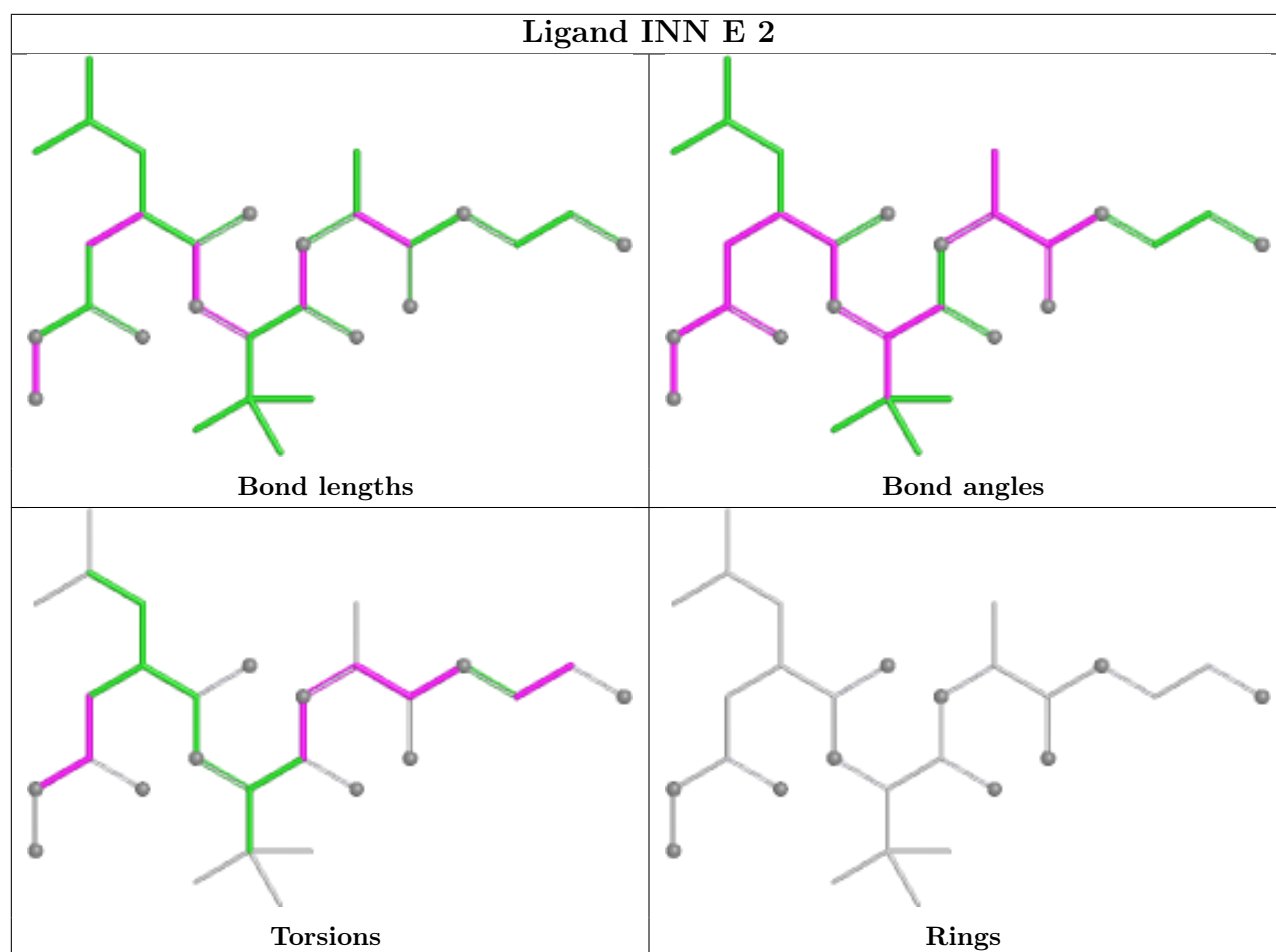
There are no ring outliers.

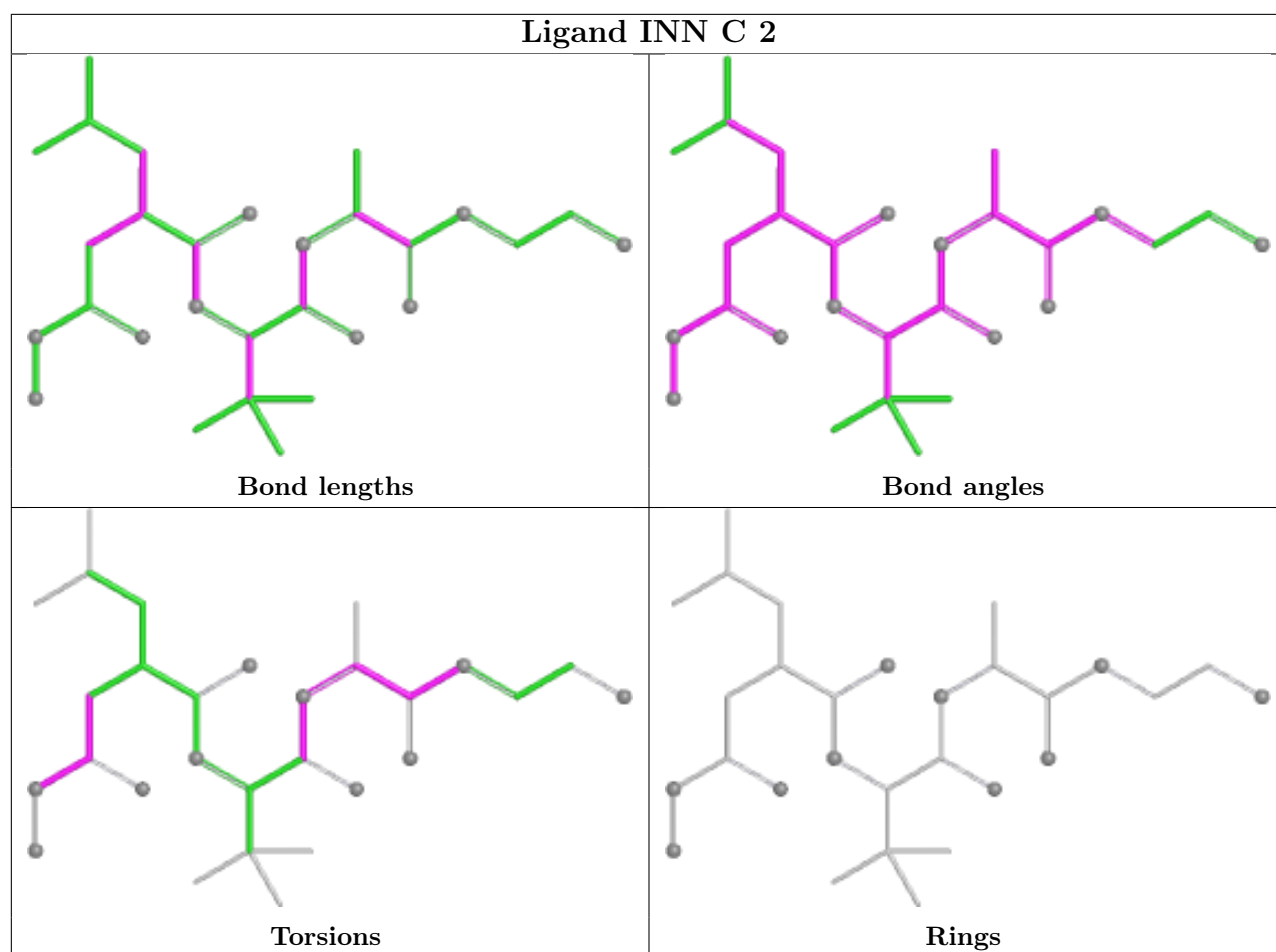
4 monomers are involved in 6 short contacts:

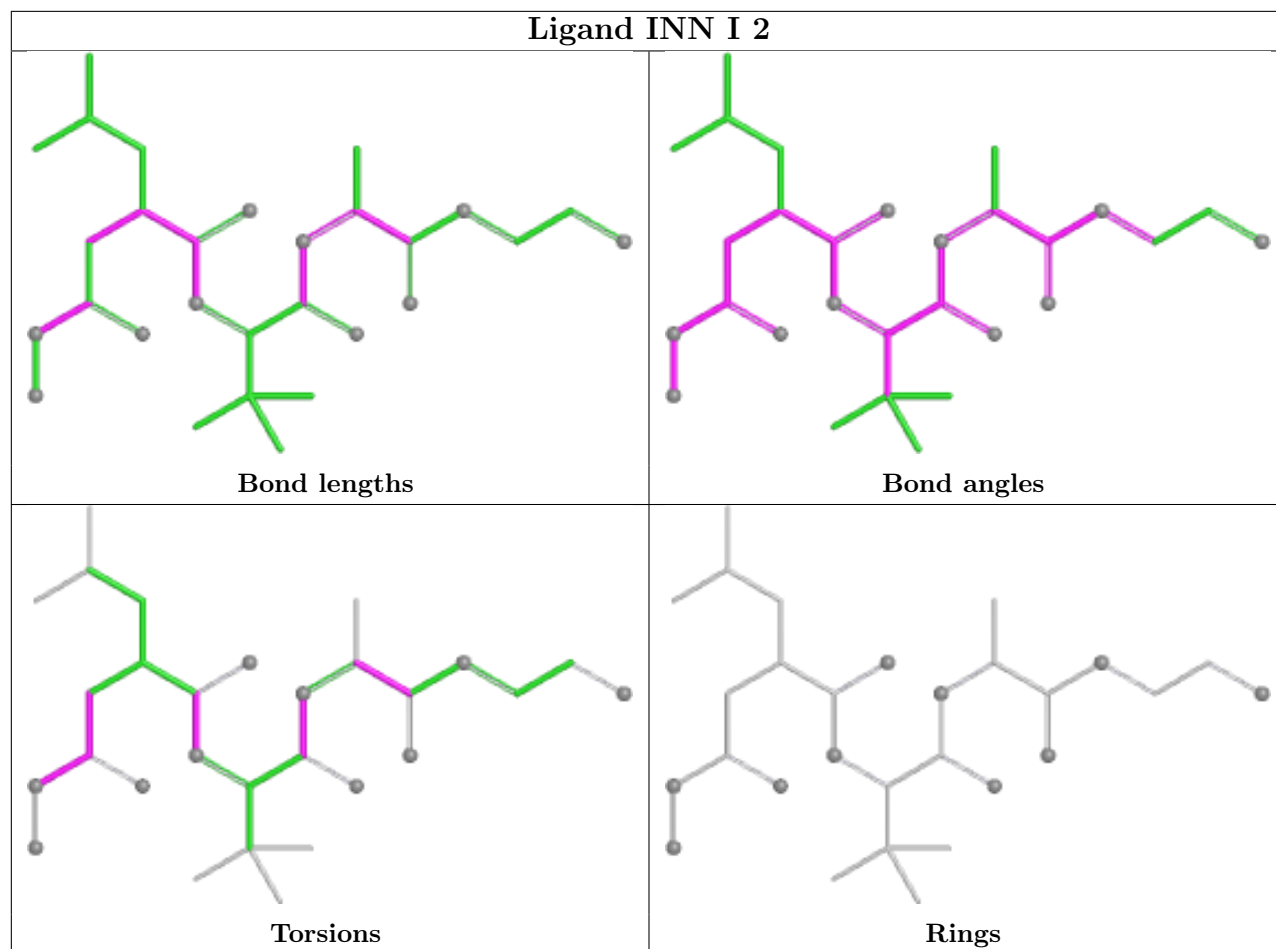
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2	INN	1	1
5	E	2	INN	1	1
5	C	2	INN	1	0
5	I	2	INN	0	1

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	6
3	I	3
2	E	2
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	421:ALA	C	422:GLU	N	2.06
1	C	422:GLU	C	423:CYS	N	1.20

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	444:HIS	C	445:GLU	N	1.20
1	C	426:ASN	C	427:GLU	N	1.18
1	E	455:LYS	C	456:GLN	N	1.18
1	I	307:GLU	C	308:GLU	N	1.17
1	I	368:ALA	C	369:TYR	N	1.16
1	E	326:ALA	C	327:GLU	N	1.15
1	A	376:LYS	C	377:ASN	N	1.09
1	C	452:GLN	C	453:CYS	N	1.00
1	C	376:LYS	C	377:ASN	N	0.98
1	C	420:LEU	C	421:ALA	N	0.65

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.