



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 12:18 PM UTC

PDB ID : 1C4U / pdb_00001c4u
Title : SELECTIVE NON ELECTROPHILIC THROMBIN INHIBITORS WITH
CYCLOHEXYL MOIETIES.
Authors : Krishnan, R.; Mochalkin, I.; Arni, R.K.; Tulinsky, A.
Deposited on : 1999-09-25
Resolution : 2.10 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

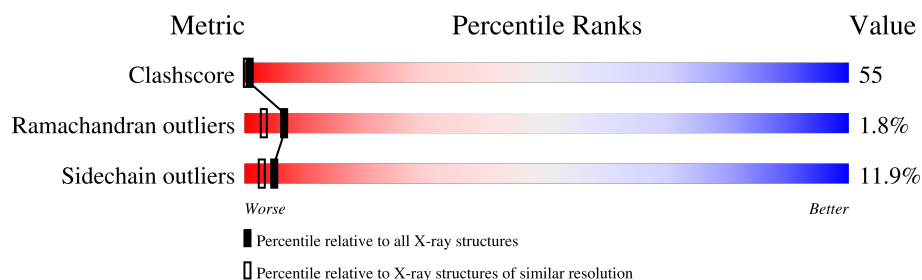
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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	1	36	19% 44% 19% 17%
2	2	259	14% 43% 32% 8% .
3	3	14	21% 7% 21% 7% 43%

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	IH1	2	370	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 2479 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 thrombin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	30	Total	C	N	O	S	0	0	0
			240	150	39	50	1			

- Molecule 2 is a protein called thrombin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	252	Total	C	N	O	S	0	0	0
			2039	1299	360	366	14			

- Molecule 3 is a protein called PROTEIN (HIRUGEN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	8	Total	C	N	O	S	0	0	0
			68	43	8	16	1			

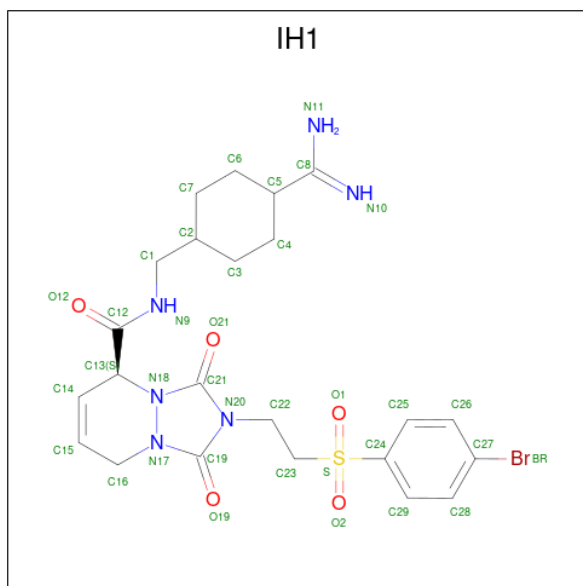
There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	554	ALA	-	insertion	UNP P28504
3	555	CYS	-	insertion	UNP P28504
3	556	GLU	-	insertion	UNP P28504
3	557	ASN	-	insertion	UNP P28504
3	558	GLU	-	insertion	UNP P28504
3	562	GLY	GLU	conflict	UNP P28504
3	565	GLY	GLU	conflict	UNP P28504

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	2	1	Total	Na	0	0
			1	1		

- Molecule 5 is 2-[2-(4-BROMO-BENZENESULFONYL)-ETHYL]-1-3-DIOXO-2,3,5,8-TETRAHYDRO-1H-[1,2,4]TRIAZOLO[1,2-A]PYRIDAZINE-5-CARBOXYLIC ACID (4-CARBAMIMIDOYL-CYCLOHEXYLMETHYL)-AMIDE (CCD ID: IH1) (formula: $C_{23}H_{29}BrN_6O_5S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	2	1	Total	Br	C	N	O	S	0	0
			36	1	23	6	5	1		

- Molecule 6 is water.

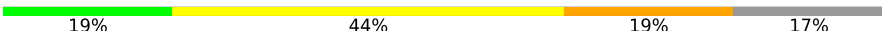
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	1	8	Total	O	0	0
			8	8		
6	2	85	Total	O	0	0
			85	85		
6	3	2	Total	O	0	0
			2	2		

3 Residue-property plots

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.

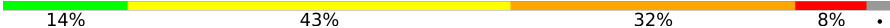
Note EDS was not executed.

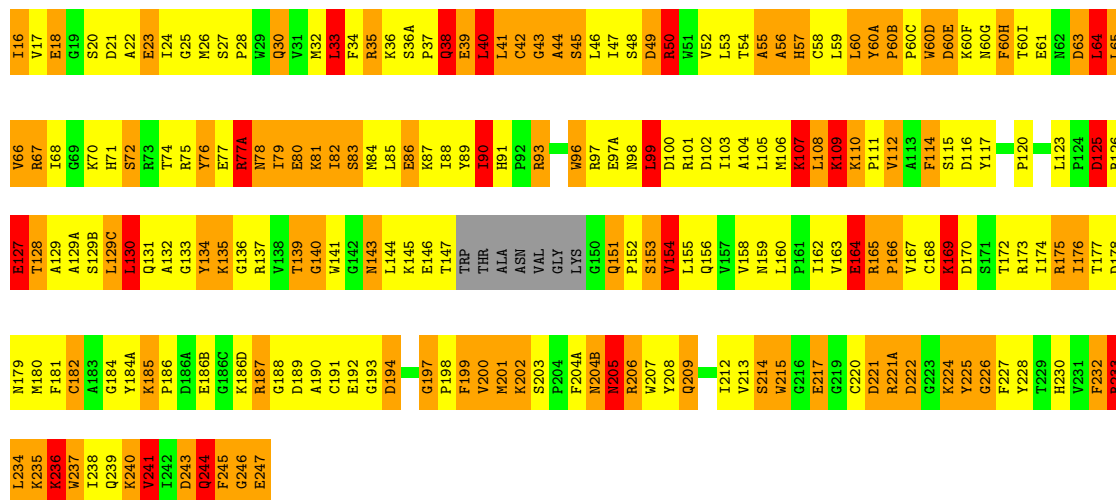
• Molecule 1: thrombin

Chain 1: 



• Molecule 2: thrombin

Chain 2: 



• Molecule 3: PROTEIN (HIRUGEN)

Chain 3: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	71.51Å 72.02Å 72.91Å 90.00° 100.80° 90.00°	Depositor
Resolution (Å)	7.00 – 2.10	Depositor
% Data completeness (in resolution range)	75.0 (7.00-2.10)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	0.12	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.167 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2479	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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: IH1, NA, TYS

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	1	1.30	0/242	2.83	20/322 (6.2%)
2	2	1.51	12/2091 (0.6%)	3.10	288/2823 (10.2%)
3	3	1.15	0/53	2.97	4/70 (5.7%)
All	All	1.48	12/2386 (0.5%)	3.07	312/3215 (9.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	2	0	3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	136	GLY	CA-C	8.34	1.61	1.52
2	2	217	GLU	N-CA	7.26	1.55	1.46
2	2	184	GLY	N-CA	7.21	1.52	1.45
2	2	209	GLN	CA-C	6.74	1.61	1.52
2	2	102	ASP	N-CA	6.44	1.54	1.46
2	2	140	GLY	CA-C	6.23	1.58	1.51
2	2	220	CYS	C-N	-5.97	1.25	1.33
2	2	30	GLN	C-O	5.71	1.30	1.23
2	2	96	TRP	NE1-CE2	-5.60	1.31	1.37
2	2	134	TYR	N-CA	5.46	1.53	1.46
2	2	128	THR	CB-OG1	5.35	1.52	1.43
2	2	47	ILE	C-N	-5.15	1.29	1.33

All (312) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	126	ARG	CD-NE-CZ	20.67	153.33	124.40
2	2	143	ASN	OD1-CG-ND2	17.09	139.69	122.60
2	2	226	GLY	O-C-N	16.52	139.87	123.35
2	2	187	ARG	NE-CZ-NH1	13.71	135.21	121.50
2	2	221(A)	ARG	NE-CZ-NH2	13.05	130.95	119.20
2	2	205	ASN	CB-CA-C	12.68	129.74	111.73
1	1	14(J)	TYR	CA-C-O	12.35	138.17	120.51
2	2	222	ASP	CA-CB-CG	12.08	124.68	112.60
2	2	77	GLU	CA-C-O	12.02	137.67	122.64
1	1	14(A)	LYS	CA-C-O	-11.88	105.12	119.49
2	2	116	ASP	CA-CB-CG	11.88	124.47	112.60
2	2	154	VAL	N-CA-CB	-11.14	96.92	112.52
2	2	100	ASP	CA-CB-CG	10.98	123.58	112.60
2	2	23	GLU	CA-C-O	-10.96	109.62	121.56
2	2	102	ASP	CA-CB-CG	-10.82	101.78	112.60
2	2	206	ARG	CA-C-O	-10.80	108.40	121.36
3	3	561	GLU	CA-C-N	10.78	131.86	120.43
3	3	561	GLU	C-N-CA	10.78	131.86	120.43
2	2	205	ASN	CA-C-N	10.76	140.46	122.07
2	2	205	ASN	C-N-CA	10.76	140.46	122.07
2	2	176	ILE	CA-CB-CG2	10.72	128.73	110.50
2	2	204(B)	ASN	CA-C-N	10.69	137.26	122.19
2	2	204(B)	ASN	C-N-CA	10.69	137.26	122.19
2	2	156	GLN	OE1-CD-NE2	10.69	133.29	122.60
2	2	65	LEU	O-C-N	10.68	135.66	123.27
2	2	170	ASP	CA-CB-CG	-10.62	101.98	112.60
2	2	79	ILE	CA-C-O	-10.50	110.65	120.73
1	1	1(A)	ASP	CA-CB-CG	-10.21	102.39	112.60
2	2	76	TYR	CA-C-O	-9.99	110.15	120.54
2	2	221(A)	ARG	NE-CZ-NH1	-9.97	111.53	121.50
2	2	243	ASP	CA-CB-CG	-9.96	102.64	112.60
2	2	164	GLU	CB-CG-CD	9.96	129.53	112.60
2	2	126	ARG	NE-CZ-NH1	9.71	131.21	121.50
2	2	177	THR	CA-CB-CG2	9.70	126.99	110.50
2	2	130	LEU	CB-CA-C	9.67	127.37	111.50
2	2	167	VAL	O-C-N	9.65	132.38	121.96
2	2	110	LYS	N-CA-CB	9.65	127.57	111.17
2	2	36	LYS	CA-C-O	-9.18	110.82	120.55
1	1	14(K)	ILE	CA-CB-CG1	9.17	125.99	110.40
2	2	66	VAL	CA-C-N	9.10	136.03	123.11
2	2	66	VAL	C-N-CA	9.10	136.03	123.11
2	2	180	MET	CA-C-O	-9.03	110.87	121.44
2	2	35	ARG	CA-C-O	8.94	131.20	120.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	99	LEU	O-C-N	-8.93	106.76	122.21
2	2	180	MET	O-C-N	8.91	134.73	123.15
2	2	226	GLY	CA-C-O	-8.88	113.36	121.18
2	2	42	CYS	CA-C-N	8.83	131.39	122.30
2	2	42	CYS	C-N-CA	8.83	131.39	122.30
2	2	201	MET	CA-C-O	-8.83	111.11	121.44
2	2	167	VAL	CA-C-O	-8.71	112.35	121.41
2	2	66	VAL	CA-C-O	8.63	129.76	120.53
2	2	93	ARG	CD-NE-CZ	8.44	136.21	124.40
2	2	194	ASP	CA-C-N	8.38	132.72	120.90
2	2	194	ASP	C-N-CA	8.38	132.72	120.90
2	2	185	LYS	CB-CA-C	-8.23	96.29	109.37
2	2	172	THR	N-CA-CB	-8.22	98.56	111.56
2	2	238	ILE	CA-C-N	8.20	131.26	120.28
2	2	238	ILE	C-N-CA	8.20	131.26	120.28
2	2	84	MET	O-C-N	8.19	132.52	123.10
2	2	115	SER	N-CA-C	-8.19	96.76	107.73
2	2	222	ASP	N-CA-CB	8.19	122.01	109.97
2	2	232	PHE	CA-CB-CG	-8.19	105.61	113.80
2	2	61	GLU	O-C-N	8.15	130.75	122.12
2	2	41	LEU	N-CA-CB	-8.13	98.61	110.40
2	2	190	ALA	N-CA-C	-8.09	98.86	110.59
2	2	233	ARG	NE-CZ-NH2	-8.09	111.92	119.20
2	2	201	MET	O-C-N	8.02	133.58	123.15
3	3	560	PHE	CA-CB-CG	8.02	121.82	113.80
2	2	205	ASN	N-CA-CB	-7.98	100.09	112.13
2	2	177	THR	CA-CB-OG1	-7.94	97.69	109.60
2	2	64	LEU	N-CA-C	7.93	120.96	109.14
2	2	175	ARG	CA-C-N	7.93	131.93	120.91
2	2	175	ARG	C-N-CA	7.93	131.93	120.91
2	2	54	THR	CA-C-N	7.90	133.78	122.09
2	2	54	THR	C-N-CA	7.90	133.78	122.09
2	2	79	ILE	O-C-N	7.88	128.99	121.98
2	2	108	LEU	N-CA-CB	-7.84	98.44	109.97
2	2	201	MET	CA-C-N	-7.79	112.25	123.00
2	2	201	MET	C-N-CA	-7.79	112.25	123.00
2	2	49	ASP	CA-CB-CG	-7.78	104.82	112.60
2	2	129(A)	ALA	CB-CA-C	7.73	123.61	110.79
1	1	4	ARG	CA-C-O	7.68	125.38	119.46
2	2	225	TYR	CA-CB-CG	-7.61	100.20	113.90
2	2	230	HIS	N-CA-CB	-7.58	99.25	110.24
2	2	174	ILE	CA-C-O	-7.56	112.11	121.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	209	GLN	CB-CA-C	-7.56	98.28	111.05
2	2	83	SER	CA-C-O	7.54	129.63	121.11
2	2	185	LYS	CA-C-O	-7.54	112.74	120.96
2	2	199	PHE	CA-CB-CG	-7.54	106.26	113.80
2	2	221(A)	ARG	CA-C-O	-7.54	112.80	121.47
2	2	114	PHE	N-CA-CB	7.50	121.16	110.44
2	2	34	PHE	CA-C-O	7.47	128.61	120.32
1	1	4	ARG	CD-NE-CZ	-7.44	113.98	124.40
2	2	80	GLU	CG-CD-OE2	-7.43	101.30	118.40
2	2	169	LYS	CB-CG-CD	7.38	128.26	111.30
2	2	109	LYS	CG-CD-CE	7.36	128.22	111.30
1	1	14(J)	TYR	CA-C-N	-7.33	101.08	117.20
2	2	241	VAL	N-CA-C	7.29	118.06	110.62
2	2	66	VAL	CB-CA-C	7.28	121.59	110.96
2	2	184	GLY	CA-C-O	-7.27	114.54	121.96
1	1	14(H)	GLU	CB-CG-CD	7.24	124.90	112.60
2	2	139	THR	O-C-N	-7.22	114.43	123.17
2	2	244	GLN	N-CA-CB	7.22	121.55	110.14
2	2	204(B)	ASN	CA-C-O	7.21	126.99	118.69
1	1	1(A)	ASP	OD1-CG-OD2	7.19	140.16	122.90
2	2	207	TRP	O-C-N	7.18	131.60	123.19
2	2	186(D)	LYS	CA-C-O	-7.16	112.75	121.06
2	2	127	GLU	CB-CG-CD	7.16	124.77	112.60
2	2	77	GLU	CB-CG-CD	7.14	124.74	112.60
2	2	67	ARG	NE-CZ-NH1	7.12	128.62	121.50
2	2	224	LYS	CA-C-N	7.08	133.71	122.59
2	2	224	LYS	C-N-CA	7.08	133.71	122.59
2	2	204(A)	PHE	CA-C-O	-7.07	111.45	119.79
2	2	67	ARG	CA-C-N	7.05	132.37	123.14
2	2	67	ARG	C-N-CA	7.05	132.37	123.14
2	2	67	ARG	NH1-CZ-NH2	-7.04	110.15	119.30
2	2	90	ILE	CA-C-O	-7.04	112.08	121.02
1	1	13	GLU	CA-C-O	-7.00	113.03	120.80
2	2	237	TRP	CA-C-N	6.99	129.44	120.70
2	2	237	TRP	C-N-CA	6.99	129.44	120.70
2	2	187	ARG	NE-CZ-NH2	-6.97	112.93	119.20
2	2	48	SER	O-C-N	-6.93	117.91	123.11
2	2	221	ASP	CB-CA-C	6.92	121.55	111.73
2	2	49	ASP	CA-C-O	-6.91	111.27	119.35
2	2	38	GLN	CA-C-O	-6.90	110.64	120.51
2	2	81	LYS	O-C-N	-6.86	115.14	123.30
1	1	14(B)	THR	CA-C-O	-6.86	111.39	119.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	93	ARG	NE-CZ-NH2	-6.84	113.04	119.20
2	2	99	LEU	CA-C-N	6.84	130.58	120.87
2	2	99	LEU	C-N-CA	6.84	130.58	120.87
2	2	239	GLN	OE1-CD-NE2	-6.80	115.80	122.60
2	2	110	LYS	O-C-N	6.76	126.58	121.85
2	2	144	LEU	O-C-N	6.76	131.54	122.49
2	2	244	GLN	CA-C-O	-6.74	112.65	120.20
2	2	244	GLN	CA-C-N	-6.68	111.86	122.08
2	2	244	GLN	C-N-CA	-6.68	111.86	122.08
2	2	217	GLU	CB-CG-CD	6.66	123.92	112.60
2	2	41	LEU	CB-CA-C	6.66	119.66	109.34
2	2	68	ILE	N-CA-CB	-6.64	102.24	111.41
2	2	34	PHE	O-C-N	-6.63	115.55	123.31
2	2	143	ASN	CA-C-O	-6.63	114.28	121.44
2	2	166	PRO	CA-C-N	6.59	129.40	120.77
2	2	166	PRO	C-N-CA	6.59	129.40	120.77
2	2	93	ARG	O-C-N	-6.57	114.43	122.25
2	2	26	MET	N-CA-C	6.56	119.25	111.71
2	2	158	VAL	CA-C-N	6.52	131.32	122.84
2	2	158	VAL	C-N-CA	6.52	131.32	122.84
2	2	57	HIS	CA-CB-CG	6.52	120.32	113.80
2	2	93	ARG	CA-CB-CG	-6.52	101.06	114.10
2	2	182	CYS	CA-CB-SG	6.51	129.38	114.40
2	2	115	SER	CA-C-O	-6.51	114.17	120.94
2	2	135	LYS	CA-C-N	6.47	129.79	122.67
2	2	135	LYS	C-N-CA	6.47	129.79	122.67
2	2	35	ARG	CA-C-N	6.46	128.93	120.28
2	2	35	ARG	C-N-CA	6.46	128.93	120.28
2	2	143	ASN	CA-CB-CG	-6.44	106.16	112.60
2	2	187	ARG	NH1-CZ-NH2	-6.44	110.92	119.30
2	2	220	CYS	CA-C-O	-6.44	113.42	120.24
2	2	205	ASN	OD1-CG-ND2	6.43	129.03	122.60
2	2	33	LEU	O-C-N	6.40	130.62	122.93
2	2	189	ASP	CA-CB-CG	6.40	119.00	112.60
2	2	126	ARG	NE-CZ-NH2	-6.37	113.47	119.20
2	2	47	ILE	CA-C-O	6.34	124.98	118.96
2	2	63	ASP	CA-CB-CG	6.33	118.94	112.60
2	2	230	HIS	CA-CB-CG	-6.30	107.50	113.80
2	2	78	ASN	O-C-N	6.30	129.74	122.25
2	2	77	GLU	N-CA-C	6.29	119.39	109.39
2	2	189	ASP	N-CA-C	-6.28	99.91	108.38
1	1	14	ASP	N-CA-C	-6.26	102.09	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	200	VAL	CA-C-O	-6.26	114.36	121.75
2	2	115	SER	O-C-N	6.25	130.00	122.75
2	2	60(E)	ASP	N-CA-CB	-6.24	102.74	112.41
2	2	46	LEU	CA-C-O	-6.19	113.74	120.36
2	2	159	ASN	OD1-CG-ND2	6.18	128.78	122.60
2	2	35	ARG	CA-CB-CG	6.17	126.45	114.10
2	2	60(A)	TYR	CB-CG-CD2	6.17	130.05	120.80
2	2	173	ARG	N-CA-C	-6.13	105.83	113.38
2	2	169	LYS	CA-CB-CG	6.13	126.36	114.10
2	2	128	THR	N-CA-C	-6.12	104.53	111.14
2	2	47	ILE	CA-CB-CG2	6.11	120.89	110.50
2	2	109	LYS	CA-C-O	-6.11	114.08	120.55
2	2	200	VAL	CA-CB-CG1	6.10	120.77	110.40
2	2	209	GLN	CA-CB-CG	-6.08	101.93	114.10
2	2	204(A)	PHE	O-C-N	6.08	132.43	122.70
2	2	35	ARG	CD-NE-CZ	6.07	132.89	124.40
2	2	243	ASP	CB-CA-C	6.06	120.86	110.86
1	1	3	LEU	O-C-N	6.06	130.76	123.13
2	2	214	SER	N-CA-C	6.05	123.69	110.80
2	2	35	ARG	CG-CD-NE	-6.05	98.69	112.00
2	2	160	LEU	O-C-N	6.02	127.32	121.66
2	2	27	SER	N-CA-CB	-6.02	102.97	110.79
2	2	60(H)	PHE	CA-CB-CG	6.01	119.81	113.80
2	2	239	GLN	CA-C-O	-6.01	114.18	120.55
3	3	566	GLU	CB-CG-CD	5.99	122.79	112.60
2	2	127	GLU	N-CA-CB	-5.99	101.00	110.28
2	2	163	VAL	O-C-N	-5.98	115.13	122.61
2	2	86	GLU	CA-CB-CG	-5.97	102.15	114.10
2	2	204(B)	ASN	CB-CA-C	5.97	119.06	109.27
2	2	137	ARG	O-C-N	5.95	130.27	123.31
2	2	173	ARG	CD-NE-CZ	-5.95	116.08	124.40
2	2	178	ASP	CB-CG-OD2	-5.93	104.75	118.40
1	1	14	ASP	N-CA-CB	5.92	119.45	110.45
2	2	20	SER	CA-C-O	-5.90	114.90	121.51
2	2	186(D)	LYS	N-CA-C	-5.89	100.09	109.23
2	2	194	ASP	O-C-N	-5.84	114.39	122.46
2	2	204(A)	PHE	CA-CB-CG	-5.83	107.97	113.80
2	2	217	GLU	CG-CD-OE2	5.81	131.76	118.40
2	2	215	TRP	CA-C-O	5.79	127.59	121.33
2	2	185	LYS	O-C-N	5.79	128.87	121.34
2	2	130	LEU	N-CA-CB	-5.77	100.84	110.42
2	2	49	ASP	N-CA-C	-5.76	105.91	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	81	LYS	CG-CD-CE	5.76	124.55	111.30
2	2	185	LYS	N-CA-C	-5.75	102.65	110.36
2	2	245	PHE	CA-C-O	-5.72	112.03	118.55
2	2	240	LYS	N-CA-CB	5.70	118.49	109.82
2	2	127	GLU	N-CA-C	5.69	118.42	111.82
2	2	60(D)	TRP	N-CA-CB	5.67	118.83	110.56
2	2	167	VAL	N-CA-CB	5.67	116.57	110.62
2	2	84	MET	CA-C-O	-5.66	114.60	121.28
2	2	40	LEU	O-C-N	5.66	129.66	123.04
2	2	26	MET	CA-C-N	5.66	129.08	122.85
2	2	26	MET	C-N-CA	5.66	129.08	122.85
1	1	1(A)	ASP	CB-CG-OD1	-5.66	105.39	118.40
2	2	202	LYS	CA-C-O	-5.65	114.22	120.38
1	1	1(A)	ASP	CA-C-O	5.65	126.04	119.32
1	1	3	LEU	CA-C-O	-5.64	114.42	120.46
2	2	45	SER	O-C-N	-5.64	116.96	123.33
2	2	104	ALA	N-CA-C	-5.63	99.43	108.55
2	2	221(A)	ARG	CD-NE-CZ	-5.63	116.52	124.40
2	2	245	PHE	O-C-N	5.63	128.06	122.10
2	2	143	ASN	CB-CG-OD1	-5.62	109.55	120.80
2	2	129(A)	ALA	N-CA-C	5.62	117.40	111.28
2	2	43	GLY	N-CA-C	-5.61	103.71	112.58
2	2	234	LEU	CA-C-N	5.61	128.12	120.54
2	2	234	LEU	C-N-CA	5.61	128.12	120.54
2	2	125	ASP	N-CA-C	-5.61	102.16	110.46
2	2	215	TRP	CA-C-N	5.60	128.20	120.92
2	2	215	TRP	C-N-CA	5.60	128.20	120.92
2	2	57	HIS	CA-C-N	5.59	128.04	120.44
2	2	57	HIS	C-N-CA	5.59	128.04	120.44
2	2	68	ILE	CA-C-O	-5.57	114.54	120.39
2	2	179	ASN	CA-C-O	-5.57	112.69	119.43
2	2	90	ILE	CB-CG1-CD1	5.56	125.47	113.80
2	2	55	ALA	CA-C-O	-5.55	114.54	120.92
2	2	193	GLY	N-CA-C	-5.54	108.09	114.69
2	2	50	ARG	O-C-N	5.53	128.11	122.09
2	2	60(B)	PRO	N-CA-C	5.51	117.43	110.70
2	2	52	VAL	O-C-N	-5.50	117.24	123.18
2	2	60(I)	THR	O-C-N	5.50	130.62	122.97
2	2	21	ASP	CA-CB-CG	5.49	118.09	112.60
2	2	56	ALA	CA-C-O	-5.49	112.63	119.38
2	2	167	VAL	N-CA-C	-5.48	104.53	110.23
2	2	136	GLY	N-CA-C	-5.48	102.97	112.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	72	SER	CA-C-O	5.47	127.22	120.92
2	2	112	VAL	O-C-N	5.46	129.44	122.61
2	2	60(I)	THR	N-CA-CB	5.46	118.83	110.70
2	2	97	ARG	NE-CZ-NH2	5.45	124.10	119.20
2	2	180	MET	N-CA-CB	5.44	121.01	111.55
1	1	14(K)	ILE	CB-CG1-CD1	-5.42	102.42	113.80
2	2	104	ALA	O-C-N	5.42	129.66	123.48
2	2	133	GLY	CA-C-N	-5.39	113.71	121.42
2	2	133	GLY	C-N-CA	-5.39	113.71	121.42
2	2	25	GLY	CA-C-N	5.39	128.04	120.28
2	2	25	GLY	C-N-CA	5.39	128.04	120.28
2	2	175	ARG	NE-CZ-NH2	5.39	124.05	119.20
2	2	192	GLU	CB-CG-CD	5.39	121.76	112.60
2	2	60(C)	PRO	O-C-N	5.37	131.30	122.70
2	2	23	GLU	N-CA-CB	5.36	117.89	110.17
2	2	151	GLN	O-C-N	5.36	126.16	121.39
2	2	207	TRP	N-CA-CB	5.35	119.34	110.52
2	2	59	LEU	N-CA-CB	-5.34	102.30	110.26
2	2	194	ASP	N-CA-C	5.33	119.50	112.89
2	2	107	LYS	N-CA-CB	5.31	119.61	110.68
2	2	60	LEU	O-C-N	5.31	131.19	122.70
2	2	164	GLU	N-CA-CB	-5.30	102.18	109.97
2	2	18	GLU	CB-CA-C	-5.29	103.19	111.39
2	2	16	ILE	CA-CB-CG1	5.27	119.36	110.40
2	2	77	GLU	O-C-N	-5.26	114.28	122.70
1	1	14(C)	GLU	CG-CD-OE2	5.26	130.50	118.40
2	2	246	GLY	N-CA-C	5.26	125.64	113.18
2	2	166	PRO	CA-C-O	5.25	130.16	120.60
2	2	77(A)	ARG	CA-C-N	-5.23	114.44	122.60
2	2	77(A)	ARG	C-N-CA	-5.23	114.44	122.60
2	2	46	LEU	CB-CA-C	5.22	118.65	110.19
2	2	238	ILE	CA-C-O	-5.22	115.70	121.29
2	2	243	ASP	N-CA-C	-5.22	104.51	111.24
2	2	76	TYR	CA-C-N	5.21	130.26	122.23
2	2	76	TYR	C-N-CA	5.21	130.26	122.23
2	2	233	ARG	CB-CG-CD	-5.21	99.31	111.30
2	2	64	LEU	CA-C-O	5.20	127.33	121.51
2	2	129(C)	LEU	N-CA-CB	-5.19	102.48	110.42
2	2	200	VAL	O-C-N	5.17	128.50	122.97
2	2	41	LEU	N-CA-C	-5.16	107.05	113.55
2	2	236	LYS	CA-C-O	-5.15	113.71	119.79
2	2	77	GLU	C-N-CA	5.15	134.58	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	129(C)	LEU	O-C-N	5.15	129.72	122.20
2	2	60(C)	PRO	N-CA-C	-5.15	106.08	113.75
2	2	209	GLN	CA-C-O	-5.13	115.44	120.98
1	1	14(E)	GLU	CA-CB-CG	5.13	124.36	114.10
2	2	44	ALA	CA-C-O	-5.13	113.17	120.51
2	2	181	PHE	N-CA-CB	5.10	121.01	111.52
2	2	21	ASP	CA-C-O	-5.09	115.46	121.16
2	2	153	SER	CA-C-N	5.08	130.23	122.92
2	2	153	SER	C-N-CA	5.08	130.23	122.92
2	2	39	GLU	CB-CG-CD	5.07	121.22	112.60
2	2	30	GLN	CB-CG-CD	5.07	121.21	112.60
2	2	116	ASP	O-C-N	5.06	129.81	122.43
2	2	65	LEU	N-CA-CB	5.05	120.92	111.53
2	2	23	GLU	O-C-N	5.04	128.81	122.86
2	2	199	PHE	N-CA-C	-5.03	97.59	107.69
2	2	128	THR	N-CA-CB	5.02	117.34	110.07
2	2	60(C)	PRO	N-CA-CB	5.01	108.97	103.26

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	2	165	ARG	Sidechain
2	2	197	GLY	Mainchain
2	2	233	ARG	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	1	240	0	239	46	0
2	2	2039	0	2010	242	0
3	3	68	0	53	8	0
4	2	1	0	0	0	0
5	2	36	0	26	5	0
6	1	8	0	0	2	0
6	2	85	0	0	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	3	2	0	0	0	0
All	All	2479	0	2328	261	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 55.

All (261) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:86:GLU:CG	2:2:109:LYS:HZ2	1.22	1.52
2:2:86:GLU:HG3	2:2:109:LYS:NZ	1.16	1.47
1:1:14(K):ILE:CG2	2:2:134:TYR:OH	1.73	1.36
1:1:14(K):ILE:HG22	2:2:134:TYR:CZ	1.62	1.34
1:1:14(K):ILE:HG22	2:2:134:TYR:CE1	1.70	1.26
2:2:86:GLU:CG	2:2:109:LYS:NZ	1.86	1.24
1:1:1(C):GLU:CB	1:1:1:CYS:HB3	1.68	1.22
2:2:205:ASN:HB3	6:2:532:HOH:O	1.05	1.19
2:2:215:TRP:CH2	6:2:529:HOH:O	2.00	1.12
2:2:187:ARG:HD3	2:2:221:ASP:OD2	1.50	1.10
2:2:75:ARG:NH2	3:3:561:GLU:HB2	1.67	1.07
2:2:18:GLU:HG3	2:2:187:ARG:HG3	1.35	1.05
1:1:1(C):GLU:HB3	1:1:1:CYS:CB	1.86	1.05
2:2:215:TRP:CZ3	6:2:529:HOH:O	2.08	1.05
2:2:75:ARG:NH2	6:2:510:HOH:O	1.91	1.04
1:1:14(K):ILE:CG2	2:2:134:TYR:CZ	2.36	1.03
2:2:105:LEU:HD12	2:2:241:VAL:HG21	1.39	1.02
2:2:78:ASN:N	6:2:448:HOH:O	1.78	1.02
2:2:217:GLU:OE1	6:2:527:HOH:O	1.76	1.01
2:2:50:ARG:NH1	2:2:86:GLU:OE1	1.93	1.01
2:2:85:LEU:HD13	2:2:106:MET:HE2	1.43	1.01
2:2:185:LYS:N	2:2:186(B):GLU:OE1	1.92	1.00
1:1:1(E):SER:HB2	2:2:123:LEU:O	1.60	1.00
1:1:14(K):ILE:HG23	2:2:134:TYR:OH	1.64	0.96
1:1:1(D):GLY:HA3	2:2:123:LEU:H	1.27	0.96
2:2:86:GLU:CD	2:2:109:LYS:NZ	2.23	0.95
2:2:236:LYS:HD2	2:2:237:TRP:N	1.82	0.94
1:1:1(D):GLY:CA	2:2:123:LEU:H	1.81	0.92
2:2:105:LEU:CD1	2:2:241:VAL:HG21	2.00	0.92
2:2:86:GLU:HG3	2:2:109:LYS:HZ3	1.29	0.90
1:1:1(C):GLU:HB3	1:1:1:CYS:HB3	0.94	0.90
2:2:236:LYS:HD2	2:2:237:TRP:H	1.33	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1(E):SER:CB	2:2:123:LEU:O	2.21	0.88
2:2:86:GLU:CB	2:2:109:LYS:HZ2	1.86	0.88
1:1:1(D):GLY:HA3	2:2:123:LEU:N	1.88	0.88
1:1:1(C):GLU:HG3	2:2:120:PRO:HG2	1.55	0.87
2:2:70:LYS:HE3	2:2:72:SER:O	1.74	0.87
2:2:40:LEU:HD12	2:2:41:LEU:N	1.91	0.86
2:2:18:GLU:HG3	2:2:187:ARG:CG	2.06	0.86
1:1:14(K):ILE:CG2	2:2:134:TYR:CE1	2.59	0.85
2:2:153:SER:HA	6:2:503:HOH:O	1.76	0.85
2:2:57:HIS:O	2:2:60(F):LYS:CE	2.25	0.85
2:2:80:GLU:O	2:2:81:LYS:HD3	1.77	0.85
2:2:236:LYS:HD2	2:2:236:LYS:N	1.91	0.85
2:2:86:GLU:CD	2:2:109:LYS:HZ2	1.82	0.85
2:2:57:HIS:O	2:2:60(F):LYS:HE3	1.77	0.83
2:2:86:GLU:HG3	2:2:109:LYS:HZ1	1.41	0.83
1:1:14(K):ILE:HG21	2:2:134:TYR:OH	1.77	0.82
2:2:60(D):TRP:O	2:2:60(E):ASP:HB2	1.81	0.81
1:1:14(H):GLU:OE1	6:1:445:HOH:O	1.99	0.81
1:1:14(K):ILE:HA	6:1:427:HOH:O	1.81	0.81
1:1:1(D):GLY:N	2:2:123:LEU:H	1.76	0.80
1:1:1(D):GLY:H	2:2:123:LEU:H	1.29	0.80
2:2:236:LYS:CD	2:2:237:TRP:N	2.44	0.80
2:2:117:TYR:HD2	6:2:451:HOH:O	1.64	0.79
2:2:221(A):ARG:HH11	2:2:221(A):ARG:CG	1.95	0.78
2:2:86:GLU:HB3	2:2:107:LYS:HG3	1.65	0.78
2:2:74:THR:OG1	6:2:530:HOH:O	2.01	0.77
2:2:70:LYS:NZ	2:2:80:GLU:OE1	2.17	0.77
1:1:14(I):SER:O	1:1:14(K):ILE:N	2.17	0.76
2:2:221(A):ARG:NH1	2:2:221(A):ARG:HG3	2.00	0.76
2:2:37:PRO:O	2:2:39:GLU:HG2	1.86	0.75
2:2:105:LEU:CD1	2:2:241:VAL:CG2	2.63	0.75
2:2:45:SER:HB3	2:2:198:PRO:HG3	1.66	0.75
2:2:77(A):ARG:CA	6:2:448:HOH:O	2.34	0.74
2:2:87:LYS:HG3	2:2:89:TYR:CE1	2.22	0.74
2:2:237:TRP:HZ2	6:2:531:HOH:O	1.71	0.74
1:1:14(A):LYS:HG3	2:2:23:GLU:OE2	1.88	0.74
1:1:14(I):SER:C	1:1:14(K):ILE:N	2.43	0.73
2:2:205:ASN:CB	6:2:532:HOH:O	1.85	0.73
1:1:14(I):SER:C	1:1:14(K):ILE:H	1.90	0.72
2:2:176:ILE:HD12	2:2:227:PHE:CE1	2.24	0.72
1:1:14(D):ARG:O	1:1:14(H):GLU:HG3	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:40:LEU:HD12	2:2:41:LEU:H	1.54	0.72
1:1:1(C):GLU:CB	1:1:1:CYS:CB	2.57	0.71
2:2:86:GLU:CD	2:2:109:LYS:HZ1	1.97	0.71
1:1:1(C):GLU:HG3	2:2:120:PRO:CG	2.21	0.71
2:2:87:LYS:HD3	2:2:88:ILE:H	1.55	0.70
2:2:184(A):TYR:O	6:2:522:HOH:O	2.08	0.70
2:2:50:ARG:HH11	2:2:107:LYS:HE2	1.57	0.70
2:2:130:LEU:CD2	2:2:162:ILE:HD13	2.23	0.69
2:2:236:LYS:CD	2:2:237:TRP:H	2.03	0.69
2:2:130:LEU:HD23	2:2:162:ILE:CD1	2.22	0.69
1:1:1(D):GLY:CA	2:2:123:LEU:HB2	2.23	0.68
2:2:87:LYS:CG	2:2:89:TYR:CE1	2.77	0.68
2:2:112:VAL:O	6:2:517:HOH:O	2.12	0.68
2:2:165:ARG:NH1	2:2:169:LYS:HE3	2.08	0.68
2:2:64:LEU:HD12	2:2:85:LEU:HD12	1.75	0.67
2:2:146:GLU:HG2	2:2:147:THR:HG22	1.76	0.67
2:2:202:LYS:HE2	2:2:205:ASN:CG	2.19	0.67
2:2:75:ARG:CZ	3:3:561:GLU:HB2	2.24	0.66
2:2:85:LEU:HD13	2:2:106:MET:CE	2.21	0.66
2:2:204(B):ASN:HD22	2:2:205:ASN:N	1.93	0.65
1:1:14(K):ILE:HG22	2:2:134:TYR:HE1	1.55	0.65
2:2:85:LEU:CD1	2:2:106:MET:HE2	2.23	0.65
2:2:86:GLU:CG	2:2:109:LYS:HZ1	1.95	0.65
2:2:202:LYS:HE2	2:2:205:ASN:OD1	1.97	0.65
2:2:236:LYS:CD	2:2:236:LYS:C	2.70	0.64
2:2:87:LYS:HD3	2:2:88:ILE:N	2.12	0.64
2:2:146:GLU:CD	2:2:221(A):ARG:HE	2.04	0.64
2:2:235:LYS:HD2	2:2:235:LYS:O	1.97	0.63
2:2:17:VAL:O	2:2:188:GLY:HA2	1.99	0.63
1:1:1(D):GLY:H	2:2:123:LEU:N	1.98	0.62
2:2:81:LYS:NZ	3:3:567:TYS:O3	2.29	0.62
2:2:187:ARG:CD	2:2:221:ASP:OD2	2.39	0.62
2:2:191:CYS:O	2:2:194:ASP:HB2	1.98	0.62
2:2:91:HIS:CE1	2:2:93:ARG:HB2	2.35	0.61
2:2:105:LEU:HD12	2:2:241:VAL:CG2	2.21	0.61
2:2:203:SER:HB3	2:2:204(B):ASN:ND2	2.16	0.61
2:2:130:LEU:HD23	2:2:162:ILE:HD13	1.82	0.61
2:2:215:TRP:CE3	5:2:370:IH1:HC29	2.37	0.60
2:2:71:HIS:HD2	6:2:436:HOH:O	1.83	0.60
2:2:85:LEU:HD22	2:2:106:MET:HB3	1.83	0.59
2:2:60(G):ASN:OD1	2:2:60(G):ASN:C	2.43	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:127:GLU:CD	2:2:127:GLU:N	2.60	0.59
2:2:233:ARG:O	2:2:236:LYS:NZ	2.30	0.59
2:2:77(A):ARG:N	6:2:448:HOH:O	2.35	0.59
1:1:1(D):GLY:HA3	2:2:123:LEU:HB2	1.85	0.58
2:2:76:TYR:HE1	2:2:82:ILE:HD11	1.68	0.58
2:2:87:LYS:HG2	2:2:89:TYR:CZ	2.38	0.58
2:2:93:ARG:CB	2:2:101:ARG:HD2	2.33	0.58
1:1:1(E):SER:HB3	2:2:123:LEU:O	2.03	0.58
1:1:14(D):ARG:NE	1:1:14(H):GLU:CD	2.62	0.58
2:2:86:GLU:HB3	2:2:107:LYS:O	2.03	0.57
2:2:241:VAL:O	2:2:245:PHE:N	2.35	0.57
2:2:33:LEU:HB2	2:2:42:CYS:O	2.05	0.57
2:2:24:ILE:O	6:2:441:HOH:O	2.18	0.56
2:2:153:SER:CA	6:2:503:HOH:O	2.44	0.56
1:1:4:ARG:HG2	2:2:28:PRO:HG3	1.86	0.56
2:2:93:ARG:HB2	2:2:101:ARG:CD	2.35	0.56
2:2:130:LEU:C	2:2:131:GLN:HG2	2.31	0.56
2:2:109:LYS:HE3	2:2:109:LYS:HA	1.86	0.55
2:2:49:ASP:O	2:2:111:PRO:HA	2.06	0.55
2:2:234:LEU:HA	2:2:236:LYS:HE2	1.88	0.55
1:1:14(K):ILE:HG23	2:2:134:TYR:HH	1.71	0.54
2:2:200:VAL:HG12	2:2:209:GLN:HA	1.90	0.54
2:2:97(A):GLU:OE2	2:2:175:ARG:NH2	2.34	0.54
2:2:244:GLN:HA	2:2:244:GLN:NE2	2.21	0.54
2:2:64:LEU:HD12	2:2:85:LEU:CD1	2.37	0.54
2:2:236:LYS:HD3	2:2:237:TRP:N	2.23	0.54
2:2:50:ARG:NH1	2:2:107:LYS:HE2	2.21	0.54
2:2:85:LEU:CD1	2:2:106:MET:CE	2.85	0.54
2:2:204(B):ASN:ND2	2:2:204(B):ASN:C	2.66	0.54
2:2:75:ARG:HD2	2:2:75:ARG:N	2.22	0.54
2:2:240:LYS:O	2:2:244:GLN:N	2.31	0.54
1:1:14(D):ARG:NE	1:1:14(H):GLU:OE2	2.41	0.53
2:2:243:ASP:O	2:2:244:GLN:C	2.51	0.53
2:2:93:ARG:HB2	2:2:101:ARG:HD3	1.91	0.53
2:2:225:TYR:N	2:2:225:TYR:CD1	2.73	0.53
2:2:50:ARG:NH1	2:2:108:LEU:O	2.41	0.53
2:2:237:TRP:O	2:2:241:VAL:HG13	2.09	0.53
2:2:204(B):ASN:HD22	2:2:204(B):ASN:N	2.05	0.53
2:2:33:LEU:HD12	2:2:42:CYS:HB2	1.90	0.53
2:2:107:LYS:HG3	2:2:107:LYS:O	2.08	0.53
2:2:60:LEU:HG	2:2:60(B):PRO:HD3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:93:ARG:HB3	2:2:101:ARG:HD2	1.89	0.52
2:2:246:GLY:O	2:2:247:GLU:OE2	2.27	0.52
2:2:127:GLU:CD	2:2:127:GLU:H	2.00	0.52
2:2:236:LYS:CD	2:2:236:LYS:H	2.23	0.52
2:2:32:MET:HG3	2:2:40:LEU:HD13	1.91	0.52
2:2:75:ARG:HH21	3:3:561:GLU:HB2	1.68	0.52
2:2:87:LYS:HG2	2:2:89:TYR:CE1	2.44	0.52
2:2:57:HIS:O	2:2:60(F):LYS:NZ	2.42	0.51
2:2:80:GLU:C	2:2:81:LYS:HD3	2.35	0.51
1:1:4:ARG:HG2	2:2:28:PRO:CG	2.40	0.51
2:2:197:GLY:O	2:2:213:VAL:HG23	2.11	0.51
1:1:14(G):LEU:HD21	2:2:202:LYS:HD3	1.93	0.51
2:2:182:CYS:HA	2:2:226:GLY:O	2.11	0.51
2:2:204(B):ASN:HD22	2:2:204(B):ASN:C	2.14	0.51
1:1:3:LEU:HB3	1:1:9:LYS:HD3	1.92	0.50
2:2:246:GLY:C	2:2:247:GLU:HG3	2.36	0.50
2:2:236:LYS:HD2	2:2:236:LYS:H	1.70	0.50
1:1:14(A):LYS:HG3	2:2:23:GLU:CD	2.37	0.50
2:2:30:GLN:NE2	2:2:139:THR:OG1	2.45	0.50
2:2:97(A):GLU:HG2	2:2:98:ASN:N	2.26	0.50
2:2:201:MET:N	2:2:208:TYR:O	2.41	0.50
2:2:55:ALA:O	2:2:58:CYS:HB2	2.11	0.50
2:2:204(B):ASN:HD22	2:2:204(B):ASN:H	1.60	0.50
2:2:35:ARG:O	2:2:38:GLN:HA	2.11	0.49
2:2:185:LYS:HG2	2:2:186(B):GLU:OE1	2.13	0.49
2:2:96:TRP:HA	2:2:99:LEU:HD12	1.95	0.49
2:2:204(B):ASN:HD22	2:2:205:ASN:H	1.61	0.49
2:2:232:PHE:O	2:2:235:LYS:HB3	2.12	0.49
2:2:49:ASP:C	2:2:49:ASP:OD1	2.51	0.49
2:2:71:HIS:CD2	6:2:436:HOH:O	2.64	0.49
2:2:40:LEU:HD12	2:2:40:LEU:C	2.36	0.49
2:2:165:ARG:O	2:2:168:CYS:HB2	2.12	0.49
2:2:76:TYR:CE1	2:2:82:ILE:HD11	2.46	0.48
2:2:146:GLU:OE1	2:2:221(A):ARG:NE	2.46	0.48
2:2:165:ARG:NH1	6:2:464:HOH:O	2.43	0.48
2:2:134:TYR:N	2:2:134:TYR:CD1	2.81	0.48
2:2:90:ILE:O	6:2:531:HOH:O	2.20	0.48
2:2:22:ALA:N	2:2:155:LEU:O	2.36	0.47
2:2:60(A):TYR:CE1	5:2:370:IH1:HC15	2.49	0.47
2:2:244:GLN:HA	2:2:244:GLN:HE21	1.78	0.47
2:2:71:HIS:ND1	2:2:154:VAL:HG22	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:134:TYR:N	2:2:134:TYR:HD1	2.12	0.47
2:2:56:ALA:CB	2:2:90:ILE:HG23	2.43	0.47
2:2:125:ASP:OD1	2:2:127:GLU:HG2	2.14	0.47
2:2:105:LEU:CD1	2:2:241:VAL:HG22	2.44	0.47
3:3:565:GLY:C	3:3:567:TYS:N	2.68	0.47
2:2:146:GLU:O	2:2:147:THR:HB	2.14	0.47
2:2:71:HIS:O	2:2:154:VAL:HA	2.15	0.47
2:2:205:ASN:CG	6:2:532:HOH:O	2.34	0.47
2:2:43:GLY:O	2:2:44:ALA:HB2	2.15	0.46
2:2:60:LEU:HD12	2:2:60(G):ASN:HB2	1.98	0.46
1:1:1(D):GLY:HA2	2:2:123:LEU:HB2	1.98	0.46
1:1:14(F):LEU:HD12	2:2:135:LYS:HB3	1.98	0.46
2:2:37:PRO:O	2:2:39:GLU:N	2.49	0.46
2:2:199:PHE:CD1	2:2:199:PHE:C	2.94	0.46
2:2:132:ALA:HA	2:2:162:ILE:O	2.17	0.45
2:2:141:TRP:CZ2	2:2:155:LEU:HD13	2.52	0.45
3:3:565:GLY:O	3:3:566:GLU:C	2.59	0.45
2:2:228:TYR:CD1	2:2:228:TYR:N	2.84	0.45
1:1:4:ARG:HA	1:1:5:PRO:HD3	1.90	0.45
2:2:232:PHE:O	2:2:235:LYS:CB	2.65	0.44
1:1:14(K):ILE:HG21	1:1:14(K):ILE:HD13	1.58	0.44
2:2:130:LEU:O	2:2:131:GLN:HG2	2.17	0.44
2:2:164:GLU:H	2:2:164:GLU:CD	2.14	0.44
2:2:165:ARG:O	2:2:166:PRO:C	2.61	0.44
2:2:67:ARG:HG2	2:2:82:ILE:HG23	2.00	0.44
1:1:5:PRO:HA	1:1:9:LYS:HG3	1.98	0.44
2:2:36(A):SER:HA	2:2:37:PRO:C	2.43	0.44
2:2:37:PRO:O	2:2:38:GLN:C	2.61	0.43
2:2:75:ARG:HA	3:3:561:GLU:HB3	2.00	0.43
2:2:217:GLU:OE2	2:2:224:LYS:NZ	2.51	0.43
2:2:203:SER:HB3	2:2:204(B):ASN:HD21	1.81	0.43
1:1:1(D):GLY:HA3	2:2:123:LEU:CB	2.48	0.43
2:2:202:LYS:CE	2:2:205:ASN:OD1	2.63	0.43
2:2:60(H):PHE:HA	2:2:63:ASP:OD2	2.19	0.43
2:2:74:THR:HA	3:3:560:PHE:CD1	2.54	0.42
2:2:91:HIS:CE1	2:2:101:ARG:HD3	2.53	0.42
2:2:204(B):ASN:ND2	2:2:204(B):ASN:N	2.67	0.42
2:2:50:ARG:O	2:2:108:LEU:HG	2.19	0.42
2:2:99:LEU:HD12	2:2:99:LEU:HA	1.81	0.42
2:2:87:LYS:HG3	2:2:89:TYR:CD1	2.54	0.42
2:2:75:ARG:HA	2:2:75:ARG:NE	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:107:LYS:HB2	2:2:107:LYS:HE3	1.28	0.41
2:2:235:LYS:HZ2	2:2:235:LYS:HG2	1.51	0.41
2:2:93:ARG:CB	2:2:101:ARG:CD	2.97	0.41
2:2:151:GLN:HA	2:2:152:PRO:HD3	1.80	0.41
2:2:17:VAL:O	2:2:18:GLU:HB2	2.19	0.41
2:2:60(A):TYR:OH	5:2:370:IH1:H161	2.21	0.41
2:2:60(A):TYR:CZ	5:2:370:IH1:HC15	2.55	0.41
2:2:143:ASN:HB2	2:2:191:CYS:SG	2.60	0.41
2:2:114:PHE:CZ	2:2:120:PRO:HG3	2.56	0.41
2:2:240:LYS:NZ	2:2:244:GLN:OE1	2.49	0.41
5:2:370:IH1:H111	5:2:370:IH1:HC61	1.54	0.41
2:2:53:LEU:HD11	2:2:103:ILE:HG13	2.03	0.41
2:2:70:LYS:CE	2:2:72:SER:O	2.57	0.41
2:2:206:ARG:HH11	2:2:206:ARG:HD3	1.73	0.41
2:2:140:GLY:HA3	2:2:194:ASP:OD1	2.21	0.41
2:2:186:PRO:HB3	2:2:222:ASP:HB3	2.03	0.41
2:2:212:ILE:HD13	2:2:212:ILE:HG21	1.93	0.41
2:2:227:PHE:CE2	6:2:529:HOH:O	2.57	0.41
2:2:246:GLY:O	2:2:247:GLU:CG	2.69	0.41
2:2:16:ILE:N	6:2:413:HOH:O	2.53	0.40
2:2:79:ILE:HG23	2:2:117:TYR:CD2	2.56	0.40
2:2:128:THR:O	2:2:129:ALA:C	2.62	0.40
2:2:203:SER:O	2:2:205:ASN:HA	2.20	0.40
2:2:185:LYS:HA	2:2:185:LYS:HD2	1.73	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	1	28/36 (78%)	23 (82%)	2 (7%)	3 (11%)	0 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	2	248/259 (96%)	232 (94%)	14 (6%)	2 (1%)	16	12
3	3	6/14 (43%)	6 (100%)	0	0	100	100
All	All	282/309 (91%)	261 (93%)	16 (6%)	5 (2%)	6	3

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	1(C)	GLU
1	1	1(D)	GLY
1	1	1(B)	ALA
2	2	38	GLN
2	2	77(A)	ARG

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	1	27/31 (87%)	27 (100%)	0	100	100
2	2	220/225 (98%)	191 (87%)	29 (13%)	4	2
3	3	5/10 (50%)	4 (80%)	1 (20%)	1	0
All	All	252/266 (95%)	222 (88%)	30 (12%)	5	3

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	2	33	LEU
2	2	40	LEU
2	2	50	ARG
2	2	64	LEU
2	2	65	LEU
2	2	66	VAL
2	2	82	ILE
2	2	83	SER
2	2	90	ILE

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Mol	Chain	Res	Type
2	2	99	LEU
2	2	107	LYS
2	2	109	LYS
2	2	110	LYS
2	2	125	ASP
2	2	127	GLU
2	2	129(B)	SER
2	2	129(C)	LEU
2	2	130	LEU
2	2	145	LYS
2	2	154	VAL
2	2	164	GLU
2	2	169	LYS
2	2	205	ASN
2	2	214	SER
2	2	235	LYS
2	2	236	LYS
2	2	241	VAL
2	2	244	GLN
2	2	247	GLU
3	3	566	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	2	30	GLN
2	2	78	ASN
2	2	156	GLN
2	2	179	ASN
2	2	204(B)	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	TYS	3	567	3	15,16,17	1.53	2 (13%)	15,22,24	1.81	5 (33%)

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	TYS	3	567	3	-	1/10/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	567	TYS	OH-S	4.07	1.66	1.58
3	3	567	TYS	OH-CZ	-3.50	1.37	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	567	TYS	OH-S-O2	-3.96	95.49	107.56
3	3	567	TYS	CD1-CE1-CZ	-3.35	115.91	119.73
3	3	567	TYS	O2-S-O1	2.43	121.59	112.24
3	3	567	TYS	CE2-CD2-CG	-2.08	118.27	121.00
3	3	567	TYS	CE2-CZ-CE1	2.01	123.09	120.16

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	3	567	TYS	CZ-OH-S-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	3	567	TYS	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	IH1	2	370	-	38,39,39	4.38	24 (63%)	51,57,57	4.15	32 (62%)

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	IH1	2	370	-	-	10/23/45/45	0/4/4/4

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	2	370	IH1	C1-N9	-12.42	1.13	1.46
5	2	370	IH1	C16-N17	-11.83	1.35	1.46
5	2	370	IH1	C7-C6	-6.95	1.36	1.52
5	2	370	IH1	BR-C27	-6.57	1.77	1.90
5	2	370	IH1	N18-N17	-5.90	1.35	1.42
5	2	370	IH1	C19-N20	-5.78	1.28	1.39
5	2	370	IH1	C1-C2	-5.41	1.42	1.52
5	2	370	IH1	C5-C8	-5.21	1.40	1.49
5	2	370	IH1	C21-N18	-4.57	1.28	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	2	370	IH1	C25-C24	-4.46	1.32	1.38
5	2	370	IH1	C22-N20	-4.37	1.38	1.47
5	2	370	IH1	O21-C21	-4.33	1.14	1.22
5	2	370	IH1	C13-C14	-4.30	1.41	1.51
5	2	370	IH1	C4-C3	-4.17	1.42	1.52
5	2	370	IH1	C12-N9	3.35	1.41	1.33
5	2	370	IH1	C4-C5	3.30	1.61	1.53
5	2	370	IH1	C8-N11	-3.11	1.28	1.33
5	2	370	IH1	C22-C23	3.09	1.60	1.52
5	2	370	IH1	C28-C27	-3.03	1.32	1.38
5	2	370	IH1	O2-S	2.98	1.48	1.44
5	2	370	IH1	O12-C12	2.94	1.29	1.23
5	2	370	IH1	C26-C25	-2.35	1.35	1.38
5	2	370	IH1	C19-N17	2.34	1.39	1.37
5	2	370	IH1	C24-S	-2.19	1.73	1.76

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	2	370	IH1	O19-C19-N17	-10.94	119.46	126.69
5	2	370	IH1	C1-N9-C12	8.53	138.91	122.65
5	2	370	IH1	O12-C12-N9	-8.21	105.62	122.98
5	2	370	IH1	C13-C12-N9	7.66	130.01	114.86
5	2	370	IH1	C7-C6-C5	7.54	124.45	111.18
5	2	370	IH1	C25-C24-S	-6.48	112.81	119.50
5	2	370	IH1	C6-C5-C8	-6.13	103.46	111.29
5	2	370	IH1	C4-C5-C8	-5.81	103.87	111.29
5	2	370	IH1	C2-C1-N9	5.72	122.71	112.77
5	2	370	IH1	C3-C2-C1	5.71	123.11	111.47
5	2	370	IH1	O1-S-C24	-5.45	103.12	108.33
5	2	370	IH1	C6-C5-C4	-5.29	98.84	110.00
5	2	370	IH1	C29-C28-C27	-4.86	113.37	119.18
5	2	370	IH1	C29-C24-S	4.72	124.37	119.50
5	2	370	IH1	O19-C19-N20	4.58	137.22	125.69
5	2	370	IH1	C23-S-C24	4.53	111.22	105.09
5	2	370	IH1	O2-S-O1	-4.50	113.63	118.45
5	2	370	IH1	C16-C15-C14	-3.87	115.30	123.06
5	2	370	IH1	O2-S-C24	-3.77	104.73	108.33
5	2	370	IH1	N17-C19-N20	-3.47	102.84	105.98
5	2	370	IH1	C5-C8-N11	3.43	122.69	116.59
5	2	370	IH1	C13-C14-C15	3.20	132.79	123.11
5	2	370	IH1	C26-C27-C28	2.89	125.72	121.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	2	370	IH1	C28-C29-C24	2.88	122.24	119.44
5	2	370	IH1	C7-C2-C1	-2.84	105.69	111.47
5	2	370	IH1	N18-C21-N20	2.83	108.56	106.00
5	2	370	IH1	O2-S-C23	2.75	112.68	108.18
5	2	370	IH1	C7-C2-C3	2.67	115.81	109.29
5	2	370	IH1	C21-N18-N17	-2.64	104.63	108.44
5	2	370	IH1	C26-C25-C24	-2.49	117.02	119.44
5	2	370	IH1	BR-C27-C28	-2.41	116.01	119.30
5	2	370	IH1	C22-N20-C19	2.07	126.09	122.91

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	2	370	IH1	C23-C22-N20-C19
5	2	370	IH1	O12-C12-C13-N18
5	2	370	IH1	N9-C1-C2-C3
5	2	370	IH1	C6-C5-C8-N11
5	2	370	IH1	C25-C24-S-O2
5	2	370	IH1	C29-C24-S-O2
5	2	370	IH1	C25-C24-S-C23
5	2	370	IH1	C29-C24-S-C23
5	2	370	IH1	C23-C22-N20-C21
5	2	370	IH1	N9-C1-C2-C7

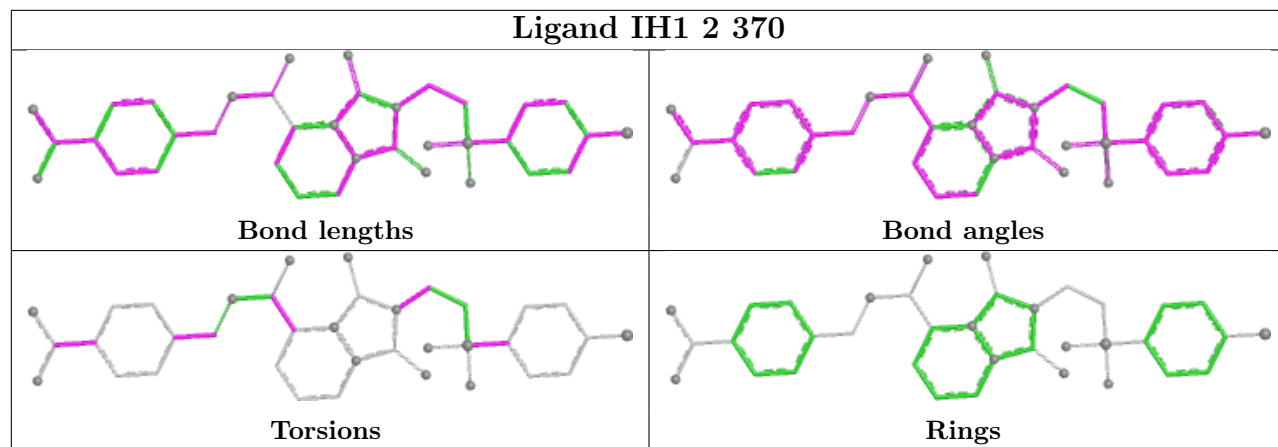
There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	2	370	IH1	5	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

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.