



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:53 PM UTC

PDB ID : 1C4V / pdb_00001c4v
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

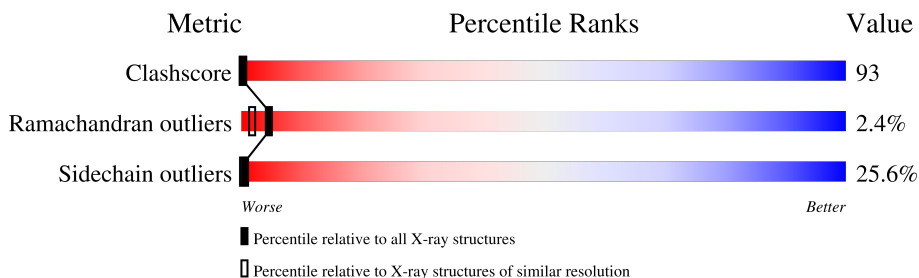
1 Overall quality at a glance

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	8% 22% 53% 17%
2	2	259	8% 31% 46% 13% .
3	3	15	7% 20% 20% 20% 33%

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
3	TYS	3	567	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 2548 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:SHORT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	36	Total	C	N	O	S	0	0	0
			287	177	48	61	1			

- Molecule 2 is a protein called THROMBIN:LONG CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	252	Total	C	N	O	S	0	0	0
			2035	1297	360	364	14			

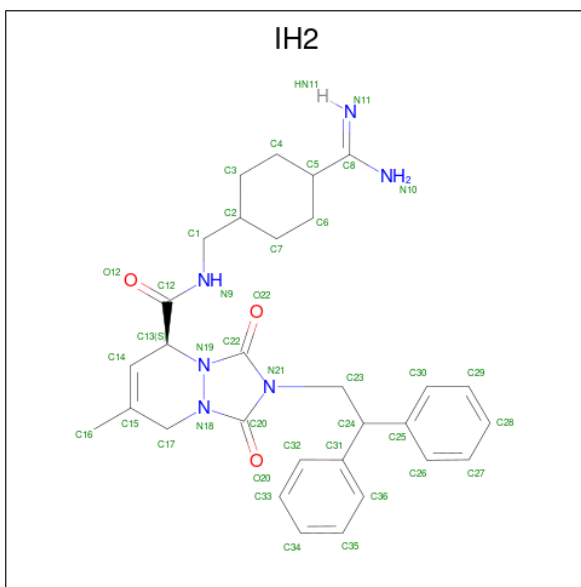
- Molecule 3 is a protein called HIRUGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	10	Total	C	N	O	S	0	0	0
			90	56	10	23	1			

- 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-(2,2-DIPHENYL-ETHYL)-7-METHYL-1,3-DIOXO-2,3,5,8-TETRAHYDR O-1H-[1,2,4]TRIAZOLO [1,2-A]PYRIDAZINE-5-CARBOXYLIC ACID(4-CARBAMIMID OYL-CYCLOHEXYLMETHYL)-AMIDE (CCD ID: IH2) (formula: C₃₀H₃₆N₆O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	2	1	Total	C	N	O	0	0
			39	30	6	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	1	13	Total	O	0	0
			13	13		
6	2	80	Total	O	0	0
			80	80		
6	3	3	Total	O	0	0
			3	3		

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.

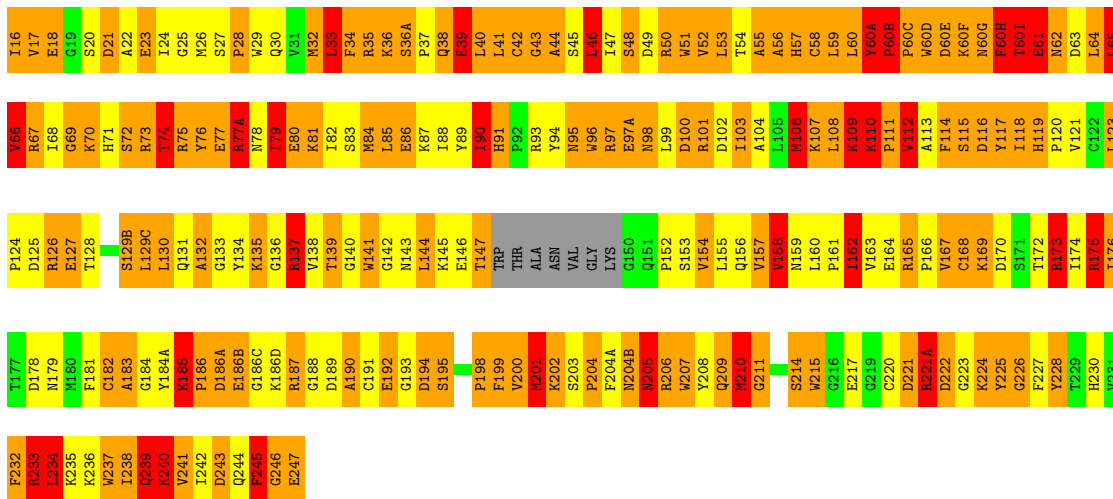
• Molecule 1: THROMBIN:SHORT CHAIN

Chain 1: 



• Molecule 2: THROMBIN:LONG CHAIN

Chain 2: 



• Molecule 3: 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	2548	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, IH2, 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	1.53	1/290 (0.3%)	3.54	44/384 (11.5%)
2	2	1.69	10/2087 (0.5%)	3.33	332/2818 (11.8%)
3	3	1.22	0/74	3.13	14/96 (14.6%)
All	All	1.66	11/2451 (0.4%)	3.35	390/3298 (11.8%)

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	5

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	221	ASP	C-N	19.83	1.79	1.34
2	2	137	ARG	NE-CZ	8.41	1.42	1.33
2	2	221(A)	ARG	C-N	8.36	1.44	1.33
2	2	103	ILE	N-CA	7.89	1.55	1.46
2	2	102	ASP	C-O	5.89	1.30	1.23
2	2	59	LEU	C-N	5.76	1.41	1.33
2	2	176	ILE	CA-CB	5.60	1.59	1.54
2	2	221(A)	ARG	N-CA	5.41	1.52	1.46
1	1	15	ARG	CD-NE	5.21	1.53	1.46
2	2	170	ASP	C-O	5.08	1.30	1.24
2	2	119	HIS	N-CA	5.05	1.53	1.46

All (390) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	78	ASN	CA-CB-CG	20.08	132.68	112.60
1	1	1(C)	GLU	CA-CB-CG	16.23	146.57	114.10
2	2	233	ARG	CD-NE-CZ	15.85	146.59	124.40
2	2	221(A)	ARG	NE-CZ-NH2	14.96	132.67	119.20
2	2	35	ARG	CD-NE-CZ	14.84	145.18	124.40
2	2	246	GLY	N-CA-C	14.61	132.98	112.81
1	1	15	ARG	CD-NE-CZ	-13.62	105.33	124.40
2	2	186(A)	ASP	CA-CB-CG	13.52	126.12	112.60
2	2	74	THR	N-CA-C	13.39	125.96	111.36
1	1	14(G)	LEU	CB-CA-C	13.20	132.70	110.79
2	2	53	LEU	CA-C-O	-13.13	106.89	120.54
2	2	91	HIS	CA-CB-CG	-12.96	100.84	113.80
2	2	135	LYS	CA-C-N	12.94	132.69	121.82
2	2	135	LYS	C-N-CA	12.94	132.69	121.82
2	2	140	GLY	CA-C-N	12.89	142.23	122.37
2	2	140	GLY	C-N-CA	12.89	142.23	122.37
1	1	14(D)	ARG	CD-NE-CZ	12.64	142.10	124.40
2	2	126	ARG	CD-NE-CZ	12.49	141.89	124.40
2	2	238	ILE	CA-C-O	-11.86	108.60	121.17
2	2	224	LYS	CA-C-N	11.72	142.49	122.81
2	2	224	LYS	C-N-CA	11.72	142.49	122.81
2	2	185	LYS	N-CA-C	-11.63	96.36	110.31
2	2	173	ARG	NH1-CZ-NH2	-11.58	104.24	119.30
2	2	62	ASN	OD1-CG-ND2	11.54	134.14	122.60
2	2	42	CYS	CA-C-N	11.54	133.69	122.27
2	2	42	CYS	C-N-CA	11.54	133.69	122.27
2	2	175	ARG	CD-NE-CZ	-11.54	108.25	124.40
2	2	77	GLU	C-N-CA	11.43	150.28	121.70
2	2	154	VAL	CB-CA-C	11.33	128.26	110.82
2	2	190	ALA	N-CA-C	-11.29	92.86	110.36
1	1	1(A)	ASP	CA-CB-CG	-11.15	101.45	112.60
2	2	30	GLN	OE1-CD-NE2	11.10	133.70	122.60
2	2	160	LEU	O-C-N	11.07	133.57	121.94
2	2	137	ARG	CD-NE-CZ	-11.00	109.00	124.40
1	1	15	ARG	NH1-CZ-NH2	10.90	133.47	119.30
1	1	1(C)	GLU	CB-CG-CD	10.64	130.69	112.60
2	2	234	LEU	CB-CA-C	10.60	128.64	110.72
2	2	66	VAL	N-CA-CB	-10.50	96.92	111.41
2	2	120	PRO	CA-C-O	10.48	135.12	122.12
2	2	247	GLU	CB-CG-CD	10.44	130.34	112.60
2	2	232	PHE	CA-CB-CG	-10.38	103.42	113.80
2	2	114	PHE	CA-CB-CG	-10.26	103.54	113.80
2	2	226	GLY	CA-C-O	-10.23	111.61	120.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	562	GLU	CB-CG-CD	10.03	129.66	112.60
1	1	1(G)	PHE	CA-CB-CG	-9.93	103.87	113.80
2	2	173	ARG	CD-NE-CZ	9.92	138.29	124.40
2	2	80	GLU	CB-CG-CD	9.83	129.32	112.60
2	2	41	LEU	CB-CA-C	9.79	125.47	109.02
2	2	209	GLN	CA-C-N	9.77	133.73	120.44
2	2	209	GLN	C-N-CA	9.77	133.73	120.44
2	2	189	ASP	CA-CB-CG	9.75	122.35	112.60
2	2	84	MET	O-C-N	9.75	135.90	123.23
2	2	60(H)	PHE	CA-CB-CG	-9.65	104.15	113.80
2	2	28	PRO	N-CA-C	9.62	125.88	113.86
2	2	91	HIS	CA-C-O	-9.60	109.99	119.49
2	2	35	ARG	CA-C-N	9.59	133.48	120.54
2	2	35	ARG	C-N-CA	9.59	133.48	120.54
2	2	67	ARG	NE-CZ-NH1	9.54	131.04	121.50
2	2	66	VAL	CB-CA-C	9.50	124.69	110.63
2	2	60(B)	PRO	CB-CA-C	9.41	122.40	110.92
2	2	156	GLN	O-C-N	-9.41	112.28	123.10
2	2	227	PHE	CA-C-O	9.35	130.62	120.71
2	2	64	LEU	N-CA-C	9.32	124.22	109.50
1	1	1(C)	GLU	CA-C-O	-9.24	107.29	120.51
2	2	17	VAL	CA-C-N	9.20	135.16	122.19
2	2	17	VAL	C-N-CA	9.20	135.16	122.19
2	2	165	ARG	CD-NE-CZ	-9.09	111.67	124.40
2	2	18	GLU	CA-C-N	9.00	134.28	122.75
2	2	18	GLU	C-N-CA	9.00	134.28	122.75
2	2	129(C)	LEU	N-CA-C	8.93	124.89	112.04
2	2	73	ARG	NE-CZ-NH1	8.88	130.38	121.50
1	1	14(E)	GLU	CB-CG-CD	8.87	127.68	112.60
2	2	47	ILE	CA-C-O	8.83	127.34	118.96
2	2	165	ARG	NE-CZ-NH2	8.80	127.12	119.20
1	1	14(C)	GLU	CB-CA-C	-8.79	96.75	110.81
1	1	3	LEU	CA-C-O	-8.73	111.11	120.46
2	2	116	ASP	CA-CB-CG	8.72	121.32	112.60
2	2	135	LYS	O-C-N	-8.71	113.30	123.06
2	2	141	TRP	O-C-N	8.69	132.71	122.19
2	2	173	ARG	NE-CZ-NH1	8.66	130.16	121.50
1	1	1(A)	ASP	N-CA-C	-8.65	101.72	112.88
2	2	90	ILE	CB-CG1-CD1	8.55	131.75	113.80
2	2	139	THR	CA-C-O	8.54	130.96	121.06
2	2	215	TRP	CA-C-O	8.53	130.42	121.38
2	2	76	TYR	CA-C-N	8.51	137.79	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	76	TYR	C-N-CA	8.51	137.79	121.54
2	2	18	GLU	CA-CB-CG	8.48	131.05	114.10
1	1	15	ARG	NE-CZ-NH1	-8.46	113.04	121.50
1	1	1(D)	GLY	CA-C-O	8.43	133.78	122.06
2	2	232	PHE	CA-C-N	8.33	132.28	120.28
2	2	232	PHE	C-N-CA	8.33	132.28	120.28
2	2	32	MET	O-C-N	8.31	133.09	123.29
2	2	114	PHE	CA-C-O	-8.29	112.75	121.87
2	2	210	MET	CA-C-N	8.27	128.76	121.82
2	2	210	MET	C-N-CA	8.27	128.76	121.82
2	2	100	ASP	O-C-N	8.26	132.97	122.89
2	2	33	LEU	O-C-N	8.19	132.76	122.93
2	2	97	ARG	CD-NE-CZ	-8.17	112.96	124.40
2	2	118	ILE	CA-C-O	8.14	128.29	120.31
2	2	153	SER	N-CA-C	-8.13	101.14	112.45
2	2	184	GLY	CA-C-O	8.11	130.29	121.86
2	2	221(A)	ARG	NE-CZ-NH1	-8.11	113.39	121.50
2	2	239	GLN	CA-C-N	8.10	131.48	120.54
2	2	239	GLN	C-N-CA	8.10	131.48	120.54
2	2	30	GLN	CA-C-O	8.08	130.08	121.19
2	2	73	ARG	NE-CZ-NH2	-8.08	111.93	119.20
2	2	185	LYS	O-C-N	8.06	128.65	120.99
2	2	95	ASN	CA-CB-CG	8.05	120.66	112.60
2	2	222	ASP	CA-CB-CG	-8.05	104.55	112.60
2	2	100	ASP	CA-CB-CG	8.03	120.63	112.60
2	2	226	GLY	O-C-N	8.03	131.83	123.48
2	2	135	LYS	CA-C-O	8.03	130.99	121.36
2	2	158	VAL	CA-C-N	8.00	133.10	122.30
2	2	158	VAL	C-N-CA	8.00	133.10	122.30
2	2	104	ALA	O-C-N	7.95	131.93	123.42
2	2	154	VAL	N-CA-CB	-7.92	95.52	111.91
2	2	66	VAL	CA-CB-CG1	7.90	123.83	110.40
2	2	77	GLU	CA-C-O	7.83	131.71	120.51
2	2	33	LEU	N-CA-C	-7.79	95.87	108.41
2	2	170	ASP	O-C-N	7.78	133.90	122.39
1	1	14	ASP	CB-CA-C	7.73	123.35	109.83
2	2	64	LEU	CA-C-O	7.72	130.15	121.11
2	2	211	GLY	N-CA-C	7.70	122.38	111.14
1	1	12	LEU	CA-C-N	7.65	134.03	122.93
1	1	12	LEU	C-N-CA	7.65	134.03	122.93
1	1	1(C)	GLU	CA-C-N	7.62	133.96	117.20
2	2	129(B)	SER	CA-C-O	-7.60	111.52	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	48	SER	N-CA-CB	-7.59	99.77	111.46
2	2	21	ASP	O-C-N	7.58	132.14	122.89
3	3	561	GLU	CG-CD-OE2	-7.57	100.98	118.40
2	2	186(D)	LYS	CB-CA-C	7.49	124.58	109.38
2	2	185	LYS	CA-CB-CG	7.45	128.99	114.10
2	2	199	PHE	N-CA-C	-7.40	94.89	107.99
1	1	1(G)	PHE	N-CA-CB	-7.37	98.03	110.49
2	2	185	LYS	N-CA-CB	7.32	118.07	109.72
2	2	204(B)	ASN	CA-C-N	7.29	135.47	121.54
2	2	204(B)	ASN	C-N-CA	7.29	135.47	121.54
2	2	240	LYS	O-C-N	7.27	129.65	122.09
2	2	60(G)	ASN	CA-CB-CG	-7.25	105.35	112.60
2	2	193	GLY	N-CA-C	-7.21	105.36	115.32
2	2	204(B)	ASN	CA-C-O	7.20	127.19	119.34
2	2	146	GLU	O-C-N	7.19	129.77	122.08
2	2	100	ASP	N-CA-C	-7.15	99.69	110.28
2	2	100	ASP	CA-C-O	-7.14	113.16	121.16
2	2	210	MET	CA-C-O	-7.10	113.39	120.70
2	2	147	THR	CA-C-O	7.08	132.84	120.80
2	2	21	ASP	N-CA-CB	7.07	120.37	109.97
2	2	137	ARG	NH1-CZ-NH2	7.04	128.45	119.30
2	2	205	ASN	CB-CA-C	7.03	124.42	110.42
1	1	1(A)	ASP	CA-C-O	6.99	127.83	119.59
2	2	74	THR	CA-CB-OG1	-6.96	99.16	109.60
2	2	245	PHE	CA-C-O	-6.94	112.34	120.53
2	2	52	VAL	CA-C-O	6.94	128.79	120.67
2	2	98	ASN	OD1-CG-ND2	-6.91	115.69	122.60
1	1	1(A)	ASP	CA-C-N	-6.91	102.00	117.20
2	2	112	VAL	O-C-N	6.90	131.24	122.61
2	2	225	TYR	CA-C-N	-6.90	115.67	122.36
2	2	225	TYR	C-N-CA	-6.90	115.67	122.36
2	2	233	ARG	CA-CB-CG	-6.89	100.32	114.10
2	2	101	ARG	NE-CZ-NH2	-6.89	113.00	119.20
2	2	137	ARG	NE-CZ-NH2	-6.85	113.04	119.20
2	2	181	PHE	CB-CA-C	6.84	124.52	109.94
2	2	62	ASN	CA-CB-CG	-6.83	105.77	112.60
2	2	110	LYS	N-CA-CB	6.83	120.27	110.77
2	2	153	SER	CA-C-O	6.83	128.34	120.00
1	1	7	PHE	CA-C-O	6.81	130.25	120.51
2	2	102	ASP	CA-C-N	-6.79	112.46	122.23
2	2	102	ASP	C-N-CA	-6.79	112.46	122.23
2	2	39	GLU	O-C-N	6.77	130.97	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	120	PRO	O-C-N	-6.75	114.90	123.14
2	2	129(B)	SER	CA-CB-OG	6.71	124.52	111.10
2	2	175	ARG	CA-C-N	6.69	129.64	120.35
2	2	175	ARG	C-N-CA	6.69	129.64	120.35
2	2	165	ARG	NE-CZ-NH1	-6.68	114.82	121.50
2	2	238	ILE	N-CA-CB	6.67	118.35	110.55
2	2	124	PRO	CB-CA-C	-6.65	102.27	110.98
2	2	110	LYS	CA-C-O	6.64	126.20	119.76
2	2	60	LEU	CB-CA-C	6.61	121.66	109.70
2	2	38	GLN	N-CA-CB	6.59	121.59	110.46
2	2	75	ARG	N-CA-CB	-6.58	100.29	110.29
2	2	210	MET	O-C-N	6.57	129.19	122.09
2	2	54	THR	CA-C-N	6.54	131.41	122.19
2	2	54	THR	C-N-CA	6.54	131.41	122.19
2	2	20	SER	CA-CB-OG	6.52	124.15	111.10
3	3	566	GLU	CA-CB-CG	6.52	127.14	114.10
1	1	14	ASP	CA-CB-CG	-6.51	106.09	112.60
2	2	194	ASP	CA-CB-CG	6.46	119.06	112.60
2	2	96	TRP	O-C-N	-6.46	114.78	122.15
2	2	175	ARG	NE-CZ-NH2	-6.42	113.43	119.20
2	2	97(A)	GLU	N-CA-C	6.40	124.43	110.80
2	2	57	HIS	CA-CB-CG	6.40	120.20	113.80
2	2	233	ARG	CA-C-N	-6.39	112.63	122.60
2	2	233	ARG	C-N-CA	-6.39	112.63	122.60
1	1	15	ARG	NE-CZ-NH2	-6.39	113.45	119.20
2	2	167	VAL	CA-C-O	6.39	127.92	121.27
2	2	157	VAL	CA-CB-CG2	6.35	121.20	110.40
2	2	140	GLY	CA-C-O	6.35	127.84	121.62
2	2	176	ILE	CA-C-O	-6.33	115.25	121.58
1	1	4	ARG	NE-CZ-NH2	6.33	124.89	119.20
2	2	110	LYS	CB-CA-C	-6.27	101.40	109.92
2	2	58	CYS	N-CA-C	-6.25	105.14	112.89
2	2	189	ASP	N-CA-C	-6.25	99.65	108.96
2	2	73	ARG	CD-NE-CZ	6.23	133.12	124.40
2	2	98	ASN	N-CA-CB	-6.22	100.71	110.98
1	1	1(B)	ALA	CB-CA-C	-6.22	98.05	110.42
2	2	141	TRP	CA-C-O	-6.20	112.16	119.48
2	2	109	LYS	CG-CD-CE	6.20	125.55	111.30
2	2	204(B)	ASN	CA-CB-CG	-6.20	106.40	112.60
2	2	27	SER	N-CA-CB	-6.19	101.21	110.99
2	2	24	ILE	CB-CA-C	6.19	120.12	111.34
2	2	201	MET	N-CA-C	-6.18	99.65	109.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	239	GLN	N-CA-CB	6.17	120.45	110.40
2	2	34	PHE	CA-C-O	6.16	127.02	120.36
2	2	100	ASP	CA-C-N	6.16	131.11	122.36
2	2	100	ASP	C-N-CA	6.16	131.11	122.36
2	2	173	ARG	CG-CD-NE	6.15	125.53	112.00
2	2	77(A)	ARG	CD-NE-CZ	-6.13	115.81	124.40
1	1	14(J)	TYR	N-CA-C	-6.13	97.74	110.80
1	1	1(F)	GLY	O-C-N	6.13	132.50	122.70
2	2	186(A)	ASP	N-CA-C	-6.13	103.75	111.11
2	2	144	LEU	CA-CB-CG	6.12	137.71	116.30
3	3	561	GLU	CA-C-N	6.11	130.41	121.31
3	3	561	GLU	C-N-CA	6.11	130.41	121.31
2	2	30	GLN	O-C-N	-6.10	115.37	122.87
2	2	27	SER	CA-C-N	6.09	125.71	119.56
2	2	27	SER	C-N-CA	6.09	125.71	119.56
2	2	236	LYS	CB-CA-C	6.06	121.15	110.85
2	2	25	GLY	CA-C-O	-6.05	111.71	119.58
2	2	232	PHE	CB-CA-C	6.01	120.43	110.81
2	2	64	LEU	N-CA-CB	-6.01	100.43	111.37
2	2	242	ILE	CB-CG1-CD1	6.01	126.42	113.80
1	1	3	LEU	O-C-N	6.00	130.69	123.13
1	1	1(B)	ALA	N-CA-CB	6.00	120.63	110.49
1	1	4	ARG	CD-NE-CZ	6.00	132.79	124.40
2	2	101	ARG	NH1-CZ-NH2	6.00	127.09	119.30
2	2	123	LEU	N-CA-C	-5.97	102.08	110.31
2	2	60(I)	THR	N-CA-C	-5.96	100.57	110.17
2	2	211	GLY	O-C-N	-5.95	118.42	123.60
2	2	128	THR	CA-C-N	5.94	129.73	120.82
2	2	128	THR	C-N-CA	5.94	129.73	120.82
2	2	214	SER	CB-CA-C	-5.94	103.22	112.31
3	3	559	ASP	CA-CB-CG	5.93	118.53	112.60
2	2	224	LYS	CA-C-O	-5.91	113.87	120.66
2	2	237	TRP	CB-CA-C	-5.88	100.68	110.68
2	2	72	SER	CA-CB-OG	5.88	122.85	111.10
1	1	9	LYS	N-CA-CB	-5.87	100.57	110.49
2	2	211	GLY	CA-C-O	5.87	127.85	121.57
2	2	121	VAL	CA-C-N	-5.86	111.66	121.39
2	2	121	VAL	C-N-CA	-5.86	111.66	121.39
2	2	186	PRO	N-CA-C	-5.86	105.89	113.57
1	1	2	GLY	CA-C-O	-5.85	112.26	119.69
1	1	1(D)	GLY	C-N-CA	5.85	136.32	121.70
1	1	13	GLU	CA-CB-CG	5.85	125.80	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	21	ASP	CA-CB-CG	5.85	118.45	112.60
2	2	36(A)	SER	N-CA-CB	-5.84	99.98	110.37
2	2	173	ARG	O-C-N	5.83	129.52	122.35
2	2	90	ILE	O-C-N	5.83	129.33	122.69
2	2	107	LYS	O-C-N	5.81	130.12	123.27
2	2	47	ILE	N-CA-CB	-5.79	105.84	112.21
2	2	108	LEU	CB-CA-C	5.79	119.98	109.62
2	2	50	ARG	O-C-N	5.77	128.52	122.23
2	2	26	MET	N-CA-C	5.76	119.49	112.23
3	3	559	ASP	CA-C-N	5.76	129.74	121.50
3	3	559	ASP	C-N-CA	5.76	129.74	121.50
2	2	86	GLU	N-CA-C	-5.75	105.03	112.68
2	2	190	ALA	CA-C-O	-5.75	114.87	121.82
2	2	30	GLN	CB-CA-C	5.74	119.25	109.72
2	2	78	ASN	CA-C-O	-5.74	112.49	119.32
2	2	129(B)	SER	N-CA-CB	5.74	119.05	110.22
2	2	128	THR	CA-CB-CG2	5.72	120.23	110.50
2	2	117	TYR	O-C-N	5.71	128.62	122.34
2	2	186(A)	ASP	C-N-CA	5.71	135.98	121.70
2	2	46	LEU	CB-CA-C	5.71	119.92	110.78
3	3	560	PHE	CA-CB-CG	-5.71	108.09	113.80
2	2	130	LEU	CA-C-N	5.70	131.91	122.33
2	2	130	LEU	C-N-CA	5.70	131.91	122.33
2	2	120	PRO	CA-C-N	5.68	132.71	122.43
2	2	120	PRO	C-N-CA	5.68	132.71	122.43
2	2	56	ALA	CA-C-O	-5.68	113.68	120.10
2	2	77(A)	ARG	CA-C-N	-5.67	113.70	122.49
2	2	77(A)	ARG	C-N-CA	-5.67	113.70	122.49
2	2	98	ASN	CB-CG-OD1	5.67	132.14	120.80
1	1	13	GLU	CG-CD-OE1	5.67	131.43	118.40
2	2	53	LEU	CB-CA-C	-5.66	101.73	110.78
2	2	56	ALA	CA-C-N	5.65	132.37	121.18
2	2	56	ALA	C-N-CA	5.65	132.37	121.18
2	2	26	MET	CB-CG-SD	-5.64	95.78	112.70
2	2	139	THR	CA-CB-CG2	5.64	120.08	110.50
2	2	223	GLY	O-C-N	5.64	129.22	122.34
2	2	83	SER	CA-C-O	5.63	128.33	121.68
2	2	36	LYS	CB-CA-C	-5.63	101.81	110.81
2	2	156	GLN	N-CA-C	5.62	119.22	110.17
2	2	189	ASP	CB-CA-C	5.62	123.85	111.09
2	2	214	SER	N-CA-C	5.62	119.71	111.34
2	2	211	GLY	CA-C-N	5.61	130.94	122.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	211	GLY	C-N-CA	5.61	130.94	122.98
3	3	561	GLU	CG-CD-OE1	5.61	131.29	118.40
2	2	199	PHE	CA-CB-CG	-5.59	108.20	113.80
1	1	4	ARG	NH1-CZ-NH2	-5.58	112.05	119.30
2	2	39	GLU	CG-CD-OE2	-5.57	105.58	118.40
2	2	190	ALA	O-C-N	5.57	129.10	122.20
1	1	12	LEU	N-CA-C	-5.56	100.63	109.59
2	2	95	ASN	CA-C-O	5.54	127.93	121.11
2	2	48	SER	CA-CB-OG	5.54	122.19	111.10
2	2	128	THR	N-CA-C	-5.54	104.93	110.97
3	3	561	GLU	CA-C-O	5.53	127.36	121.05
2	2	111	PRO	CA-C-O	-5.52	115.31	121.32
2	2	182	CYS	N-CA-CB	5.50	120.11	111.20
2	2	156	GLN	CA-C-O	5.50	127.77	121.28
2	2	50	ARG	CA-C-O	-5.49	112.82	119.03
2	2	36(A)	SER	N-CA-C	5.48	121.92	109.81
2	2	70	LYS	N-CA-C	5.48	118.17	110.23
2	2	239	GLN	CA-CB-CG	5.47	125.04	114.10
2	2	222	ASP	N-CA-C	5.45	117.93	110.24
2	2	84	MET	CA-C-O	-5.43	114.83	120.70
2	2	201	MET	CA-C-N	-5.43	115.78	122.84
2	2	201	MET	C-N-CA	-5.43	115.78	122.84
2	2	60(A)	TYR	CB-CG-CD1	-5.42	112.67	120.80
1	1	6	LEU	N-CA-C	5.41	119.87	113.16
2	2	106	MET	CA-C-N	-5.41	115.48	123.05
2	2	106	MET	C-N-CA	-5.41	115.48	123.05
2	2	137	ARG	CB-CG-CD	-5.39	98.89	111.30
2	2	21	ASP	CA-C-O	-5.38	115.13	121.16
2	2	217	GLU	CA-C-O	5.37	126.20	120.46
2	2	132	ALA	CB-CA-C	5.35	118.32	109.70
2	2	221(A)	ARG	O-C-N	5.35	129.32	123.27
2	2	77(A)	ARG	CG-CD-NE	-5.35	100.24	112.00
3	3	559	ASP	CB-CA-C	5.34	120.25	110.10
1	1	7	PHE	CA-CB-CG	-5.32	108.48	113.80
3	3	566	GLU	CB-CG-CD	5.31	121.63	112.60
2	2	113	ALA	CA-C-N	5.31	129.84	120.87
2	2	113	ALA	C-N-CA	5.31	129.84	120.87
2	2	207	TRP	CA-C-O	-5.30	114.66	120.43
2	2	221(A)	ARG	CA-C-N	-5.29	113.44	120.90
2	2	221(A)	ARG	C-N-CA	-5.29	113.44	120.90
2	2	69	GLY	N-CA-C	-5.29	108.40	114.69
2	2	76	TYR	CA-C-O	-5.26	115.30	120.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	43	GLY	N-CA-C	-5.26	104.52	112.41
2	2	199	PHE	CB-CA-C	5.26	119.36	110.79
2	2	144	LEU	N-CA-CB	-5.25	102.24	110.44
2	2	181	PHE	N-CA-C	-5.25	100.74	108.99
2	2	179	ASN	N-CA-C	-5.25	107.17	113.21
2	2	38	GLN	CA-C-N	-5.25	112.57	121.85
2	2	38	GLN	C-N-CA	-5.25	112.57	121.85
2	2	60(E)	ASP	CA-CB-CG	-5.24	107.36	112.60
2	2	80	GLU	CG-CD-OE2	-5.24	106.35	118.40
2	2	183	ALA	CA-C-N	5.24	129.00	121.56
2	2	183	ALA	C-N-CA	5.24	129.00	121.56
1	1	7	PHE	N-CA-CB	-5.23	101.66	110.49
2	2	130	LEU	CB-CA-C	5.22	120.03	111.41
2	2	147	THR	OG1-CB-CG2	5.22	119.74	109.30
2	2	65	LEU	CB-CA-C	5.22	120.49	109.79
2	2	145	LYS	CA-C-O	-5.21	115.15	120.99
2	2	225	TYR	CA-C-O	5.21	127.56	121.46
2	2	90	ILE	CA-C-O	-5.21	114.86	121.48
2	2	94	TYR	CB-CA-C	5.21	118.23	109.89
2	2	99	LEU	CA-C-O	-5.21	115.08	121.28
2	2	20	SER	CA-C-O	-5.19	115.72	121.33
2	2	192	GLU	CA-CB-CG	5.18	124.46	114.10
2	2	42	CYS	CA-CB-SG	5.18	126.31	114.40
2	2	204	PRO	CA-C-O	5.18	125.30	118.98
2	2	78	ASN	CB-CG-ND2	5.17	124.16	116.40
2	2	69	GLY	CA-C-N	5.15	128.02	120.71
2	2	69	GLY	C-N-CA	5.15	128.02	120.71
1	1	1(B)	ALA	CA-C-N	-5.13	105.91	117.20
2	2	226	GLY	N-CA-C	-5.13	102.07	111.25
2	2	243	ASP	CB-CA-C	5.12	119.48	110.37
2	2	23	GLU	CB-CG-CD	5.12	121.30	112.60
2	2	55	ALA	CA-C-O	-5.12	114.76	120.54
2	2	115	SER	CA-CB-OG	5.12	121.33	111.10
3	3	562	GLU	CA-C-O	5.11	126.59	121.07
2	2	186(B)	GLU	N-CA-C	5.11	118.99	112.34
2	2	81	LYS	N-CA-CB	5.11	120.25	111.00
2	2	162	ILE	O-C-N	5.11	128.24	122.67
2	2	228	TYR	N-CA-CB	-5.11	101.76	111.00
2	2	60(E)	ASP	OD1-CG-OD2	5.09	135.13	122.90
2	2	200	VAL	O-C-N	5.09	128.69	123.04
2	2	147	THR	N-CA-CB	-5.09	102.85	111.50
2	2	200	VAL	N-CA-C	-5.09	100.56	108.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	168	CYS	CB-CA-C	5.06	118.96	110.92
2	2	61	GLU	O-C-N	-5.05	115.87	122.59
2	2	206	ARG	NE-CZ-NH1	5.04	126.55	121.50
2	2	77(A)	ARG	O-C-N	5.03	129.28	122.59
2	2	165	ARG	CA-C-O	5.03	123.17	118.44
2	2	79	ILE	CA-CB-CG2	5.02	119.04	110.50
1	1	14(M)	GLY	N-CA-C	5.01	125.06	113.18
2	2	47	ILE	N-CA-C	-5.01	107.97	113.43
2	2	60(I)	THR	CA-CB-CG2	5.01	119.02	110.50
2	2	51	TRP	N-CA-C	5.00	117.22	108.76
2	2	227	PHE	N-CA-CB	5.00	118.74	110.69

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	2	173	ARG	Sidechain
2	2	175	ARG	Sidechain
2	2	221(A)	ARG	Sidechain,Mainchain
2	2	77(A)	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	287	0	278	117	2
2	2	2035	0	2003	345	2
3	3	90	0	71	28	0
4	2	1	0	0	0	0
5	2	39	0	35	11	0
6	1	13	0	0	8	0
6	2	80	0	0	32	0
6	3	3	0	0	8	0
All	All	2548	0	2387	449	2

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 93.

All (449) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1(G):PHE:CD1	1:1:1(F):GLY:N	1.87	1.42
2:2:221:ASP:C	2:2:221(A):ARG:N	1.79	1.40
2:2:60(I):THR:CG2	2:2:62:ASN:HD22	1.42	1.31
1:1:1(G):PHE:HD1	1:1:1(F):GLY:N	1.20	1.27
3:3:564:PRO:HB2	3:3:566:GLU:OE1	1.36	1.24
1:1:1(E):SER:HA	2:2:123:LEU:O	1.35	1.22
3:3:564:PRO:HB2	3:3:566:GLU:CD	1.69	1.14
2:2:65:LEU:HD11	6:3:455:HOH:O	1.45	1.13
2:2:41:LEU:HB3	6:2:512:HOH:O	1.49	1.11
2:2:60(I):THR:HG23	2:2:62:ASN:ND2	1.65	1.10
2:2:152:PRO:HD3	6:2:479:HOH:O	1.50	1.09
1:1:14(G):LEU:HB3	6:1:458:HOH:O	1.51	1.07
2:2:33:LEU:HD22	2:2:41:LEU:HD11	1.30	1.07
2:2:60(I):THR:HG23	2:2:62:ASN:HD22	1.12	1.07
2:2:139:THR:HG22	2:2:157:VAL:HG12	1.34	1.07
2:2:33:LEU:HB3	2:2:41:LEU:HD12	1.27	1.06
1:1:1(H):THR:HG22	1:1:1(G):PHE:CB	1.86	1.06
2:2:175:ARG:NH1	2:2:175:ARG:HG2	1.70	1.05
1:1:1(H):THR:HG22	1:1:1(G):PHE:HB3	1.35	1.04
1:1:1(G):PHE:HD1	1:1:1(F):GLY:CA	1.72	1.03
2:2:60(I):THR:HG21	2:2:62:ASN:HD22	1.22	1.03
1:1:1(H):THR:HG22	1:1:1(G):PHE:N	1.73	1.01
2:2:79:ILE:HD12	2:2:117:TYR:CG	1.95	1.00
2:2:185:LYS:O	2:2:186(B):GLU:HB2	1.62	1.00
2:2:60(I):THR:CG2	2:2:62:ASN:ND2	2.22	0.99
1:1:15:ARG:CG	1:1:15:ARG:O	2.10	0.98
3:3:564:PRO:HG2	3:3:567:TYS:CE2	1.94	0.98
2:2:201:MET:HG3	2:2:210:MET:HG2	1.43	0.97
1:1:1(G):PHE:C	2:2:235:LYS:NZ	2.22	0.97
2:2:126:ARG:HD3	6:2:513:HOH:O	1.63	0.97
1:1:1(G):PHE:O	1:1:1(D):GLY:N	1.98	0.96
1:1:1(G):PHE:CD1	1:1:1(F):GLY:CA	2.47	0.96
1:1:14(M):GLY:N	6:1:458:HOH:O	1.98	0.96
1:1:14(I):SER:C	1:1:14(K):ILE:H	1.65	0.95
2:2:199:PHE:HE2	2:2:201:MET:HE2	1.28	0.95
3:3:564:PRO:HG2	3:3:567:TYS:CD2	1.96	0.95
2:2:174:ILE:O	6:2:414:HOH:O	1.85	0.94
3:3:564:PRO:CB	3:3:566:GLU:OE1	2.14	0.94
2:2:84:MET:CG	6:3:455:HOH:O	2.17	0.93
1:1:15:ARG:O	1:1:15:ARG:HG2	1.67	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:243:ASP:HB3	6:2:485:HOH:O	1.70	0.91
3:3:564:PRO:HB2	3:3:566:GLU:OE2	1.70	0.91
2:2:199:PHE:CE2	2:2:201:MET:HE2	2.05	0.91
1:1:14(M):GLY:CA	6:1:458:HOH:O	2.19	0.91
1:1:14(A):LYS:HG2	2:2:23:GLU:OE2	1.69	0.90
1:1:14(A):LYS:HG3	6:2:478:HOH:O	1.70	0.90
2:2:70:LYS:NZ	2:2:72:SER:O	2.05	0.89
2:2:247:GLU:HA	6:2:422:HOH:O	1.72	0.89
2:2:203:SER:O	2:2:205:ASN:HA	1.73	0.89
3:3:564:PRO:HG2	3:3:567:TYS:HE2	1.51	0.89
2:2:50:ARG:NH1	2:2:108:LEU:O	2.04	0.89
1:1:1(G):PHE:C	2:2:235:LYS:HZ2	1.82	0.88
1:1:1(G):PHE:HB2	2:2:239:GLN:HG3	1.55	0.88
1:1:1(G):PHE:HD1	1:1:1(F):GLY:H	0.92	0.88
2:2:175:ARG:HG2	2:2:175:ARG:HH11	1.39	0.88
1:1:1(E):SER:CA	2:2:123:LEU:O	2.21	0.87
2:2:73:ARG:NH2	3:3:559:ASP:OD1	2.08	0.87
2:2:97:ARG:NH1	6:2:518:HOH:O	2.08	0.87
2:2:93:ARG:O	2:2:101:ARG:HD2	1.76	0.86
1:1:1(H):THR:CG2	1:1:1(G):PHE:HB3	2.05	0.86
3:3:564:PRO:HG2	3:3:567:TYS:HD2	1.57	0.86
2:2:97:ARG:HD2	6:2:518:HOH:O	1.76	0.86
2:2:33:LEU:HB3	2:2:41:LEU:CD1	2.06	0.85
1:1:14(K):ILE:HG22	1:1:14(K):ILE:O	1.76	0.85
1:1:1(E):SER:OG	2:2:208:TYR:HE1	1.60	0.84
2:2:240:LYS:HE3	6:2:523:HOH:O	1.78	0.84
2:2:65:LEU:CD1	6:3:455:HOH:O	2.12	0.83
2:2:224:LYS:NZ	6:2:421:HOH:O	1.72	0.83
1:1:12:LEU:N	1:1:12:LEU:CD2	2.41	0.83
2:2:43:GLY:O	2:2:44:ALA:HB2	1.77	0.83
2:2:199:PHE:HE2	2:2:201:MET:CE	1.93	0.82
1:1:1(F):GLY:CA	2:2:235:LYS:HZ1	1.93	0.81
2:2:210:MET:N	2:2:210:MET:HE2	1.95	0.81
1:1:10:LYS:O	1:1:12:LEU:HD23	1.79	0.81
2:2:84:MET:HG2	6:3:455:HOH:O	1.80	0.81
2:2:203:SER:HB3	2:2:204(B):ASN:HD21	1.46	0.80
1:1:1(G):PHE:CD1	1:1:1(G):PHE:C	2.60	0.80
1:1:1(H):THR:CG2	1:1:1(G):PHE:N	2.39	0.80
2:2:79:ILE:HD12	2:2:117:TYR:CD2	2.16	0.80
2:2:201:MET:CG	2:2:210:MET:HG2	2.11	0.79
2:2:74:THR:HG22	2:2:75:ARG:HG3	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:65:LEU:HD11	2:2:84:MET:HG2	1.63	0.79
2:2:108:LEU:N	2:2:108:LEU:HD23	1.98	0.78
2:2:135:LYS:HE2	2:2:184(A):TYR:OH	1.82	0.78
3:3:563:ILE:HD12	3:3:567:TYS:HB3	1.65	0.78
3:3:564:PRO:CG	3:3:567:TYS:HE2	2.14	0.77
2:2:65:LEU:CD1	2:2:84:MET:HG2	2.14	0.77
2:2:46:LEU:HD22	2:2:48:SER:O	1.83	0.77
2:2:71:HIS:NE2	2:2:154:VAL:CG2	2.48	0.77
2:2:178:ASP:CG	6:2:435:HOH:O	2.27	0.77
1:1:1(G):PHE:O	2:2:235:LYS:NZ	2.17	0.76
2:2:71:HIS:NE2	2:2:154:VAL:HG22	1.99	0.76
1:1:1(F):GLY:N	2:2:235:LYS:HZ1	1.83	0.76
1:1:10:LYS:O	1:1:12:LEU:CD2	2.34	0.76
1:1:1(G):PHE:C	2:2:235:LYS:HZ1	1.92	0.75
2:2:35:ARG:HB2	2:2:41:LEU:HD23	1.66	0.75
2:2:49:ASP:HB3	2:2:114:PHE:CZ	2.20	0.75
2:2:175:ARG:HH11	2:2:175:ARG:CG	1.97	0.75
2:2:33:LEU:CD2	2:2:41:LEU:HD11	2.12	0.75
2:2:17:VAL:HG21	2:2:220:CYS:HB3	1.69	0.74
2:2:139:THR:CG2	2:2:157:VAL:HG12	2.14	0.74
2:2:178:ASP:OD1	6:2:435:HOH:O	2.05	0.74
2:2:215:TRP:CE3	5:2:370:IH2:H30	2.22	0.74
1:1:1(D):GLY:CA	6:2:401:HOH:O	2.35	0.74
1:1:5:PRO:HA	1:1:9:LYS:HD3	1.69	0.74
2:2:175:ARG:HG3	2:2:175:ARG:O	1.84	0.74
2:2:125:ASP:OD2	2:2:127:GLU:HG2	1.86	0.74
1:1:11:SER:C	1:1:12:LEU:HD22	2.13	0.74
1:1:1(E):SER:OG	2:2:208:TYR:CE1	2.37	0.73
2:2:74:THR:HG22	2:2:75:ARG:CG	2.19	0.73
1:1:1(A):ASP:O	2:2:119:HIS:NE2	2.21	0.73
1:1:14:ASP:OD2	1:1:14:ASP:C	2.30	0.73
2:2:130:LEU:CD2	2:2:162:ILE:HD12	2.18	0.72
1:1:1(G):PHE:CE2	6:1:481:HOH:O	2.42	0.72
2:2:201:MET:HE3	2:2:210:MET:HG3	1.72	0.72
2:2:17:VAL:O	2:2:188:GLY:HA2	1.89	0.72
2:2:202:LYS:HG3	2:2:207:TRP:CE2	2.25	0.72
2:2:203:SER:HB3	2:2:204(B):ASN:ND2	2.05	0.71
2:2:66:VAL:HG23	2:2:85:LEU:HD21	1.73	0.71
1:1:14(C):GLU:O	1:1:14(G):LEU:HD23	1.90	0.71
1:1:14(I):SER:C	1:1:14(K):ILE:N	2.41	0.71
1:1:14(D):ARG:HG2	1:1:14(E):GLU:N	2.04	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:50:ARG:HD2	2:2:111:PRO:HG3	1.73	0.70
2:2:84:MET:HE2	3:3:567:TYS:O	1.90	0.70
2:2:61:GLU:OE1	2:2:87:LYS:HA	1.90	0.70
2:2:33:LEU:HD13	2:2:41:LEU:HD13	1.72	0.70
1:1:1(F):GLY:N	2:2:235:LYS:NZ	2.39	0.69
1:1:1(D):GLY:HA3	6:2:401:HOH:O	1.91	0.69
1:1:1(G):PHE:CD1	1:1:1(F):GLY:HA3	2.25	0.69
2:2:184(A):TYR:HA	2:2:186(B):GLU:OE2	1.93	0.69
2:2:50:ARG:HB2	2:2:247:GLU:HG3	1.75	0.69
2:2:60(D):TRP:CH2	5:2:370:IH2:H171	2.27	0.69
1:1:12:LEU:N	1:1:12:LEU:HD23	2.09	0.68
2:2:185:LYS:N	2:2:186(B):GLU:OE2	2.27	0.68
1:1:1(H):THR:N	1:1:1(C):GLU:N	2.40	0.68
1:1:15:ARG:HB2	2:2:204:PRO:O	1.93	0.68
2:2:59:LEU:HD11	2:2:106:MET:HE3	1.74	0.68
1:1:11:SER:C	1:1:12:LEU:CD2	2.67	0.68
2:2:130:LEU:HD23	2:2:162:ILE:HD12	1.74	0.68
1:1:1(G):PHE:HB2	2:2:239:GLN:CG	2.23	0.68
2:2:84:MET:HG3	6:3:455:HOH:O	1.87	0.67
2:2:184(A):TYR:HB2	6:2:486:HOH:O	1.94	0.67
2:2:32:MET:HE3	2:2:70:LYS:HD3	1.77	0.67
2:2:33:LEU:CD2	2:2:64:LEU:HD22	2.25	0.67
2:2:50:ARG:HD3	2:2:247:GLU:CG	2.24	0.67
2:2:194:ASP:O	2:2:195:SER:C	2.38	0.67
1:1:1(E):SER:HG	2:2:208:TYR:HE1	0.78	0.67
2:2:200:VAL:HA	2:2:208:TYR:O	1.95	0.66
2:2:57:HIS:NE2	2:2:195:SER:HB3	2.10	0.66
2:2:40:LEU:HD23	2:2:40:LEU:C	2.19	0.66
2:2:51:TRP:HE1	2:2:247:GLU:H	1.42	0.66
1:1:1(H):THR:HG22	1:1:1(G):PHE:CD2	2.31	0.66
2:2:50:ARG:HD3	2:2:247:GLU:CD	2.21	0.66
2:2:204(B):ASN:HD22	2:2:205:ASN:N	1.93	0.66
2:2:50:ARG:NH1	2:2:86:GLU:OE1	2.28	0.66
2:2:71:HIS:CD2	2:2:154:VAL:CG2	2.79	0.66
3:3:566:GLU:OE2	3:3:567:TYS:CE2	2.44	0.66
2:2:89:TYR:CE2	2:2:245:PHE:CE1	2.84	0.66
2:2:50:ARG:HG2	2:2:111:PRO:HA	1.78	0.65
2:2:41:LEU:O	2:2:42:CYS:SG	2.54	0.65
2:2:33:LEU:HD13	2:2:41:LEU:CD1	2.25	0.65
2:2:33:LEU:CB	2:2:41:LEU:HD12	2.16	0.65
2:2:60(B):PRO:N	2:2:60(C):PRO:CD	2.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1(G):PHE:CG	1:1:1(F):GLY:N	2.52	0.64
2:2:65:LEU:CG	6:3:455:HOH:O	2.40	0.64
2:2:230:HIS:HE1	2:2:232:PHE:HB3	1.63	0.64
2:2:246:GLY:O	6:2:422:HOH:O	2.15	0.64
2:2:201:MET:HG3	2:2:210:MET:CG	2.25	0.64
1:1:14(B):THR:HA	1:1:14(D):ARG:NE	2.14	0.63
1:1:1(H):THR:HG22	1:1:1(G):PHE:CG	2.32	0.63
2:2:65:LEU:HD21	3:3:567:TYS:O	1.99	0.63
1:1:14(A):LYS:CG	6:2:478:HOH:O	2.37	0.63
1:1:14(A):LYS:CG	2:2:23:GLU:OE2	2.43	0.63
2:2:240:LYS:O	2:2:244:GLN:HB2	1.99	0.62
2:2:230:HIS:CE1	2:2:232:PHE:HB3	2.34	0.62
1:1:1(G):PHE:HA	2:2:123:LEU:HD12	1.80	0.62
1:1:5:PRO:HG2	2:2:115:SER:O	1.99	0.62
1:1:11:SER:O	1:1:12:LEU:HD22	2.00	0.62
2:2:175:ARG:NH1	2:2:175:ARG:CG	2.41	0.62
2:2:244:GLN:NE2	2:2:245:PHE:CZ	2.67	0.62
1:1:1(H):THR:CG2	1:1:1(G):PHE:HD2	2.13	0.62
1:1:1(H):THR:H2	1:1:1(C):GLU:N	1.98	0.62
2:2:43:GLY:O	2:2:44:ALA:CB	2.47	0.62
2:2:46:LEU:CD2	2:2:48:SER:O	2.48	0.62
1:1:1(E):SER:N	2:2:235:LYS:HZ1	1.97	0.61
5:2:370:IH2:H72	5:2:370:IH2:O12	2.00	0.61
2:2:77:GLU:O	2:2:79:ILE:N	2.33	0.61
1:1:14(D):ARG:NH1	1:1:14(E):GLU:HB2	2.15	0.61
2:2:215:TRP:HB2	5:2:370:IH2:O22	2.00	0.61
2:2:36:LYS:HE2	2:2:65:LEU:HD13	1.82	0.61
2:2:174:ILE:HD11	5:2:370:IH2:C32	2.30	0.60
2:2:136:GLY:HA3	2:2:199:PHE:CZ	2.36	0.60
1:1:1(H):THR:HG22	1:1:1(G):PHE:CA	2.31	0.60
2:2:183:ALA:HB3	2:2:228:TYR:CE1	2.37	0.60
2:2:129(B):SER:OG	2:2:204(A):PHE:CE2	2.55	0.60
2:2:21:ASP:CG	2:2:154:VAL:CG1	2.75	0.60
2:2:204(B):ASN:ND2	2:2:206:ARG:H	2.00	0.60
2:2:91:HIS:ND1	2:2:91:HIS:C	2.60	0.59
2:2:64:LEU:O	6:2:460:HOH:O	2.16	0.59
1:1:1(H):THR:CG2	1:1:1(G):PHE:CD2	2.85	0.59
2:2:56:ALA:HB2	2:2:103:ILE:O	2.02	0.59
2:2:60(I):THR:HG21	2:2:62:ASN:ND2	2.04	0.59
2:2:235:LYS:HE3	2:2:239:GLN:OE1	2.02	0.59
2:2:50:ARG:HB2	2:2:247:GLU:CG	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:183:ALA:HB3	2:2:228:TYR:HE1	1.67	0.59
2:2:209:GLN:C	2:2:210:MET:HE2	2.28	0.59
2:2:114:PHE:N	2:2:114:PHE:CD1	2.66	0.59
3:3:563:ILE:CD1	3:3:567:TYS:HB3	2.31	0.59
2:2:51:TRP:CZ3	2:2:107:LYS:HB3	2.38	0.58
2:2:49:ASP:HB2	2:2:112:VAL:O	2.04	0.58
2:2:186(C):GLY:C	6:2:468:HOH:O	2.45	0.58
1:1:1(G):PHE:CB	2:2:239:GLN:HG3	2.32	0.58
1:1:14(D):ARG:HH11	1:1:14(E):GLU:HB2	1.69	0.58
1:1:14(J):TYR:OH	2:2:201:MET:HB3	2.03	0.58
2:2:50:ARG:HD2	2:2:111:PRO:CG	2.34	0.57
2:2:57:HIS:NE2	2:2:195:SER:CB	2.67	0.57
2:2:69:GLY:O	2:2:79:ILE:HD11	2.04	0.57
3:3:563:ILE:HB	3:3:564:PRO:HD2	1.85	0.57
2:2:33:LEU:CB	2:2:41:LEU:CD1	2.79	0.57
2:2:86:GLU:HB2	2:2:109:LYS:HA	1.86	0.57
1:1:7:PHE:O	1:1:11:SER:N	2.38	0.57
2:2:85:LEU:HD13	2:2:106:MET:HE2	1.86	0.57
3:3:564:PRO:C	3:3:566:GLU:OE1	2.48	0.57
2:2:208:TYR:HB3	2:2:210:MET:HE1	1.87	0.56
2:2:86:GLU:HB2	2:2:109:LYS:HG3	1.87	0.56
2:2:57:HIS:CE1	2:2:195:SER:HB3	2.41	0.56
2:2:60(I):THR:HG23	2:2:62:ASN:H	1.70	0.56
2:2:71:HIS:CE1	2:2:154:VAL:HG22	2.40	0.56
2:2:134:TYR:HD1	2:2:134:TYR:N	2.04	0.56
2:2:204(B):ASN:HD22	2:2:204(B):ASN:C	2.12	0.56
2:2:172:THR:OG1	2:2:173:ARG:N	2.39	0.55
2:2:71:HIS:CD2	2:2:154:VAL:HG22	2.40	0.55
1:1:10:LYS:C	1:1:12:LEU:HD23	2.30	0.55
2:2:203:SER:O	2:2:205:ASN:CA	2.51	0.55
2:2:84:MET:CE	3:3:567:TYS:O	2.55	0.55
2:2:210:MET:HE2	2:2:210:MET:CA	2.36	0.55
1:1:1(G):PHE:CE1	1:1:1(F):GLY:HA3	2.42	0.55
1:1:1(D):GLY:HA2	6:2:401:HOH:O	2.02	0.55
2:2:132:ALA:CB	2:2:164:GLU:HG3	2.37	0.55
2:2:141:TRP:CE2	2:2:155:LEU:HB2	2.42	0.55
2:2:50:ARG:HD2	2:2:111:PRO:CD	2.37	0.54
2:2:129(B):SER:OG	2:2:204(A):PHE:HE2	1.89	0.54
1:1:15:ARG:NH1	2:2:204(A):PHE:O	2.40	0.54
1:1:14(D):ARG:HD3	6:1:457:HOH:O	2.08	0.54
2:2:161:PRO:HG3	2:2:184(A):TYR:CE2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:127:GLU:CD	2:2:127:GLU:H	2.16	0.54
2:2:230:HIS:O	2:2:233:ARG:HB2	2.08	0.54
2:2:71:HIS:NE2	2:2:154:VAL:HG21	2.23	0.54
2:2:154:VAL:HG12	6:2:515:HOH:O	2.07	0.53
2:2:174:ILE:HD11	5:2:370:IH2:C33	2.38	0.53
2:2:130:LEU:HD23	2:2:162:ILE:CD1	2.39	0.53
3:3:564:PRO:CB	3:3:566:GLU:OE2	2.50	0.53
2:2:204(B):ASN:ND2	2:2:204(B):ASN:C	2.65	0.53
3:3:564:PRO:CA	3:3:566:GLU:OE1	2.57	0.53
1:1:1(G):PHE:CE1	1:1:1(F):GLY:CA	2.92	0.53
2:2:65:LEU:HG	6:3:455:HOH:O	2.07	0.53
2:2:192:GLU:HG3	6:2:483:HOH:O	2.09	0.53
1:1:1(H):THR:N	1:1:1(C):GLU:CA	2.71	0.52
2:2:66:VAL:HG23	2:2:85:LEU:CD2	2.39	0.52
2:2:65:LEU:HD12	2:2:84:MET:HG2	1.90	0.52
2:2:79:ILE:CD1	2:2:117:TYR:CD2	2.90	0.52
1:1:1(G):PHE:O	1:1:1(D):GLY:CA	2.57	0.52
2:2:50:ARG:HD3	2:2:247:GLU:HG2	1.91	0.52
2:2:77:GLU:HB2	2:2:80:GLU:HG2	1.90	0.52
2:2:161:PRO:HG3	2:2:184(A):TYR:CD2	2.45	0.52
2:2:91:HIS:HB2	2:2:103:ILE:HG23	1.91	0.52
1:1:1(E):SER:H	2:2:235:LYS:HZ1	1.58	0.52
1:1:14(D):ARG:CG	1:1:14(E):GLU:N	2.73	0.52
2:2:134:TYR:N	2:2:134:TYR:CD1	2.78	0.52
1:1:14(G):LEU:O	1:1:14(L):ASP:N	2.39	0.52
2:2:34:PHE:CZ	2:2:38:GLN:HB3	2.45	0.51
1:1:3:LEU:O	2:2:119:HIS:CD2	2.63	0.51
2:2:182:CYS:HA	2:2:226:GLY:O	2.10	0.51
2:2:237:TRP:O	2:2:241:VAL:CG1	2.58	0.51
2:2:141:TRP:NE1	2:2:155:LEU:HB2	2.25	0.51
2:2:202:LYS:HG3	2:2:207:TRP:NE1	2.25	0.51
2:2:36:LYS:CE	2:2:65:LEU:HD13	2.40	0.51
2:2:36(A):SER:HA	2:2:37:PRO:C	2.36	0.51
1:1:1(G):PHE:O	1:1:1(F):GLY:C	2.54	0.51
2:2:33:LEU:HD22	2:2:64:LEU:HD22	1.93	0.51
2:2:176:ILE:N	2:2:176:ILE:HD13	2.25	0.51
2:2:136:GLY:O	2:2:159:ASN:HA	2.12	0.50
3:3:564:PRO:CG	3:3:567:TYS:CE2	2.78	0.50
2:2:93:ARG:C	2:2:101:ARG:HD2	2.36	0.50
3:3:561:GLU:HG2	3:3:562:GLU:N	2.18	0.50
2:2:45:SER:O	2:2:52:VAL:HA	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:167:VAL:O	2:2:168:CYS:C	2.52	0.50
1:1:1(E):SER:H	2:2:235:LYS:NZ	2.09	0.50
2:2:35:ARG:CD	2:2:39:GLU:OE1	2.60	0.50
2:2:60(I):THR:HG22	2:2:63:ASP:OD2	2.12	0.50
2:2:85:LEU:HD13	2:2:106:MET:CE	2.41	0.50
2:2:33:LEU:HD21	2:2:64:LEU:HD22	1.94	0.50
2:2:70:LYS:HB2	6:2:403:HOH:O	2.11	0.49
5:2:370:IH2:C7	5:2:370:IH2:C12	2.88	0.49
2:2:77(A):ARG:CB	6:2:475:HOH:O	2.60	0.49
2:2:50:ARG:CG	2:2:111:PRO:HA	2.41	0.49
2:2:60(A):TYR:HB3	2:2:60(F):LYS:HB3	1.93	0.49
2:2:85:LEU:N	2:2:85:LEU:HD23	2.27	0.49
2:2:77(A):ARG:HB3	6:2:475:HOH:O	2.12	0.49
2:2:198:PRO:HB3	2:2:209:GLN:NE2	2.26	0.49
1:1:1(F):GLY:HA2	2:2:235:LYS:HE2	1.94	0.49
1:1:14(J):TYR:HE1	2:2:135:LYS:O	1.95	0.49
2:2:36:LYS:O	2:2:38:GLN:HG3	2.11	0.49
2:2:215:TRP:CD2	5:2:370:IH2:H30	2.48	0.49
2:2:66:VAL:CG2	2:2:85:LEU:CD2	2.90	0.49
2:2:204(B):ASN:HD22	2:2:204(B):ASN:N	2.10	0.49
2:2:130:LEU:CD2	2:2:162:ILE:CD1	2.91	0.49
1:1:14(M):GLY:HA3	6:1:458:HOH:O	1.96	0.48
2:2:60(B):PRO:N	2:2:60(C):PRO:HD2	2.27	0.48
2:2:237:TRP:O	2:2:241:VAL:HG13	2.12	0.48
1:1:11:SER:C	1:1:12:LEU:HD23	2.38	0.48
2:2:59:LEU:HD11	2:2:106:MET:CE	2.42	0.48
2:2:59:LEU:HD13	2:2:88:ILE:CG2	2.42	0.48
2:2:204(B):ASN:HD22	2:2:204(B):ASN:H	1.61	0.48
3:3:565:GLY:C	3:3:567:TYS:N	2.70	0.48
1:1:5:PRO:HA	1:1:9:LYS:CD	2.42	0.48
2:2:49:ASP:CB	2:2:114:PHE:CZ	2.94	0.48
2:2:52:VAL:CG2	2:2:108:LEU:HD11	2.43	0.48
2:2:95:ASN:HD21	2:2:97(A):GLU:HB3	1.79	0.48
1:1:4:ARG:HG2	2:2:28:PRO:HG2	1.95	0.48
2:2:88:ILE:HG12	2:2:106:MET:CE	2.43	0.48
2:2:192:GLU:CG	6:2:483:HOH:O	2.60	0.48
2:2:16:ILE:N	2:2:194:ASP:OD1	2.46	0.48
2:2:36(A):SER:CA	2:2:37:PRO:O	2.61	0.48
2:2:174:ILE:CD1	5:2:370:IH2:C32	2.92	0.48
2:2:230:HIS:CE1	2:2:233:ARG:HG3	2.49	0.48
2:2:143:ASN:HB2	2:2:191:CYS:SG	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:187:ARG:HH22	2:2:222:ASP:CG	2.23	0.47
1:1:14:ASP:OD1	2:2:137:ARG:NH1	2.47	0.47
2:2:191:CYS:N	2:2:194:ASP:OD1	2.48	0.47
2:2:32:MET:CE	2:2:70:LYS:HE3	2.45	0.47
2:2:87:LYS:HB3	2:2:89:TYR:CE1	2.49	0.47
1:1:14(J):TYR:CE1	2:2:135:LYS:O	2.68	0.47
2:2:51:TRP:CH2	2:2:107:LYS:HB3	2.49	0.47
2:2:60(F):LYS:HB2	2:2:60(F):LYS:HE2	1.70	0.47
2:2:221:ASP:C	2:2:221(A):ARG:CA	2.80	0.47
2:2:135:LYS:CE	2:2:184(A):TYR:OH	2.59	0.47
2:2:32:MET:HE1	2:2:70:LYS:HE3	1.97	0.46
2:2:162:ILE:HD11	2:2:201:MET:CE	2.45	0.46
2:2:208:TYR:HB3	2:2:210:MET:CE	2.46	0.46
1:1:1(F):GLY:C	2:2:235:LYS:HZ1	2.23	0.46
2:2:36:LYS:O	2:2:38:GLN:CG	2.63	0.46
2:2:84:MET:CE	6:3:455:HOH:O	2.63	0.46
2:2:60(I):THR:HG22	2:2:63:ASP:CG	2.41	0.46
2:2:60(A):TYR:HD2	2:2:60(D):TRP:HB2	1.80	0.46
2:2:129(B):SER:O	2:2:131:GLN:NE2	2.48	0.46
2:2:59:LEU:HD13	2:2:88:ILE:HG23	1.98	0.46
2:2:91:HIS:CE1	2:2:93:ARG:H	2.34	0.46
2:2:97:ARG:CD	6:2:518:HOH:O	2.46	0.46
2:2:158:VAL:O	2:2:158:VAL:CG1	2.63	0.46
2:2:50:ARG:CB	2:2:247:GLU:HG3	2.45	0.45
2:2:60(B):PRO:HD2	2:2:60(C):PRO:HD3	1.98	0.45
2:2:163:VAL:HG21	2:2:225:TYR:CE2	2.51	0.45
2:2:16:ILE:HD12	2:2:190:ALA:HA	1.98	0.45
2:2:17:VAL:CG2	2:2:220:CYS:HB3	2.44	0.45
2:2:133:GLY:C	6:2:517:HOH:O	2.60	0.45
2:2:152:PRO:CD	6:2:479:HOH:O	2.32	0.45
2:2:191:CYS:O	2:2:194:ASP:HB2	2.17	0.45
2:2:233:ARG:C	2:2:234:LEU:HG	2.41	0.45
2:2:17:VAL:HG21	2:2:220:CYS:CB	2.44	0.45
2:2:61:GLU:OE1	2:2:87:LYS:CA	2.61	0.45
2:2:56:ALA:HB1	2:2:90:ILE:HG23	1.99	0.44
1:1:10:LYS:HG3	1:1:12:LEU:HD23	1.99	0.44
2:2:91:HIS:HB2	2:2:103:ILE:CG2	2.46	0.44
2:2:198:PRO:HB3	2:2:209:GLN:CD	2.42	0.44
2:2:74:THR:HG22	2:2:75:ARG:HG2	1.95	0.44
2:2:126:ARG:HA	2:2:232:PHE:CZ	2.51	0.44
1:1:1(H):THR:H1	1:1:1(C):GLU:CB	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:67:ARG:HB3	2:2:70:LYS:HD2	1.98	0.44
2:2:87:LYS:HA	2:2:87:LYS:HD2	1.63	0.44
2:2:158:VAL:O	2:2:158:VAL:HG13	2.16	0.44
1:1:14(K):ILE:O	1:1:14(L):ASP:HB2	2.16	0.44
2:2:71:HIS:HE2	2:2:154:VAL:HG21	1.83	0.44
2:2:76:TYR:CZ	3:3:564:PRO:HG3	2.53	0.44
2:2:186:PRO:O	2:2:186(A):ASP:C	2.60	0.44
1:1:1(H):THR:HB	1:1:1(G):PHE:CD2	2.52	0.44
1:1:6:LEU:HA	1:1:10:LYS:HD2	1.99	0.44
2:2:106:MET:HE2	2:2:106:MET:HB3	1.40	0.44
2:2:172:THR:HG21	2:2:176:ILE:HD11	2.00	0.43
2:2:33:LEU:CG	2:2:41:LEU:CD1	2.96	0.43
2:2:161:PRO:HD3	2:2:184(A):TYR:CZ	2.53	0.43
2:2:201:MET:HE3	2:2:210:MET:CG	2.46	0.43
2:2:210:MET:HE2	2:2:210:MET:HA	1.99	0.43
2:2:126:ARG:HB3	6:2:513:HOH:O	2.18	0.43
2:2:182:CYS:HB2	2:2:225:TYR:HB3	2.01	0.43
1:1:1(G):PHE:O	1:1:1(E):SER:N	2.51	0.43
2:2:204(B):ASN:ND2	2:2:204(B):ASN:H	2.15	0.43
5:2:370:IH2:H72	5:2:370:IH2:C12	2.49	0.43
3:3:564:PRO:CG	3:3:567:TYS:HD2	2.40	0.43
1:1:1(H):THR:N	1:1:1(D):GLY:C	2.76	0.43
2:2:129(C):LEU:HD21	2:2:204:PRO:HD3	2.00	0.43
1:1:14(C):GLU:O	1:1:14(G):LEU:CD2	2.64	0.43
1:1:1(H):THR:HB	1:1:1(G):PHE:HD2	1.84	0.42
1:1:5:PRO:HA	1:1:9:LYS:HB2	2.01	0.42
2:2:49:ASP:HA	2:2:112:VAL:HG22	2.01	0.42
2:2:230:HIS:ND1	2:2:233:ARG:HG3	2.34	0.42
1:1:1(A):ASP:OD1	1:1:9:LYS:NZ	2.42	0.42
2:2:134:TYR:HD1	2:2:134:TYR:H	1.66	0.42
2:2:86:GLU:CB	2:2:109:LYS:HG3	2.49	0.42
2:2:35:ARG:HB2	2:2:41:LEU:CD2	2.45	0.42
2:2:110:LYS:HB3	2:2:111:PRO:HD2	2.02	0.42
2:2:165:ARG:N	2:2:166:PRO:CD	2.83	0.42
2:2:49:ASP:HB3	2:2:114:PHE:HZ	1.80	0.42
2:2:175:ARG:CG	2:2:175:ARG:O	2.63	0.42
1:1:14(A):LYS:HE3	1:1:14(B):THR:HG23	2.02	0.42
2:2:35:ARG:HD3	2:2:39:GLU:OE1	2.20	0.42
2:2:53:LEU:HA	2:2:53:LEU:HD12	1.71	0.42
2:2:55:ALA:O	2:2:58:CYS:HB2	2.19	0.42
2:2:144:LEU:HG	6:2:479:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:162:ILE:HD11	2:2:201:MET:HE1	2.02	0.42
2:2:187:ARG:NH2	2:2:222:ASP:OD1	2.53	0.42
3:3:561:GLU:CG	3:3:562:GLU:N	2.75	0.42
2:2:22:ALA:O	2:2:71:HIS:HE1	2.02	0.41
1:1:14(D):ARG:CZ	1:1:14(E):GLU:HB2	2.50	0.41
2:2:21:ASP:HB3	2:2:154:VAL:HG13	2.03	0.41
2:2:60(H):PHE:HB3	2:2:64:LEU:HD11	2.01	0.41
2:2:60(C):PRO:HD3	2:2:96:TRP:CE3	2.55	0.41
2:2:63:ASP:OD2	2:2:63:ASP:N	2.52	0.41
2:2:95:ASN:ND2	2:2:98:ASN:OD1	2.53	0.41
2:2:95:ASN:N	2:2:100:ASP:O	2.47	0.41
2:2:174:ILE:CD1	5:2:370:IH2:C33	2.98	0.41
1:1:1(F):GLY:N	2:2:235:LYS:CE	2.84	0.41
2:2:75:ARG:HA	3:3:561:GLU:HB3	2.02	0.41
1:1:5:PRO:HB2	2:2:116:ASP:HA	2.02	0.41
2:2:36(A):SER:N	2:2:37:PRO:O	2.54	0.41
1:1:14(B):THR:HB	1:1:14(D):ARG:NH1	2.36	0.41
1:1:14(G):LEU:CA	6:1:458:HOH:O	2.66	0.41
2:2:204(B):ASN:ND2	2:2:204(B):ASN:N	2.66	0.41
2:2:50:ARG:HE	2:2:50:ARG:HB3	1.50	0.41
2:2:103:ILE:HD11	2:2:238:ILE:HD11	2.03	0.41
2:2:142:GLY:O	2:2:143:ASN:C	2.63	0.41
2:2:178:ASP:O	2:2:233:ARG:HD3	2.20	0.41
2:2:33:LEU:CD1	2:2:41:LEU:CD1	2.98	0.41
2:2:50:ARG:HD2	2:2:111:PRO:HD3	2.03	0.41
2:2:199:PHE:HB3	2:2:211:GLY:HA3	2.03	0.41
2:2:238:ILE:O	2:2:238:ILE:CG2	2.69	0.41
2:2:50:ARG:CD	2:2:111:PRO:HG3	2.47	0.40
2:2:87:LYS:NZ	2:2:88:ILE:O	2.54	0.40
2:2:115:SER:N	2:2:118:ILE:O	2.53	0.40
1:1:1(F):GLY:HA2	2:2:235:LYS:CE	2.51	0.40
1:1:14(K):ILE:O	1:1:14(K):ILE:CG2	2.47	0.40
2:2:98:ASN:ND2	2:2:175:ARG:O	2.35	0.40
3:3:561:GLU:HG3	3:3:562:GLU:CD	2.47	0.40
1:1:1(C):GLU:HA	6:1:481:HOH:O	2.20	0.40
2:2:66:VAL:HG21	2:2:85:LEU:HD22	2.04	0.40
1:1:4:ARG:HG2	2:2:28:PRO:CG	2.52	0.40
1:1:14(E):GLU:HG2	2:2:135:LYS:HD3	2.04	0.40
2:2:35:ARG:O	2:2:38:GLN:HA	2.21	0.40
2:2:49:ASP:O	2:2:112:VAL:HG13	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:15:ARG:NH2	2:2:169:LYS:O[4_556]	2.06	0.14
1:1:14(L):ASP:O	2:2:173:ARG:NH2[4_556]	2.15	0.05

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	34/36 (94%)	22 (65%)	8 (24%)	4 (12%)	0	0
2	2	248/259 (96%)	223 (90%)	22 (9%)	3 (1%)	10	7
3	3	7/15 (47%)	4 (57%)	3 (43%)	0	100	100
All	All	289/310 (93%)	249 (86%)	33 (11%)	7 (2%)	4	2

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	1(B)	ALA
1	1	14(M)	GLY
2	2	77(A)	ARG
1	1	1(F)	GLY
2	2	44	ALA
2	2	195	SER
1	1	14(L)	ASP

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	31/31 (100%)	22 (71%)	9 (29%)	0	0
2	2	219/225 (97%)	166 (76%)	53 (24%)	1	0
3	3	8/12 (67%)	4 (50%)	4 (50%)	0	0
All	All	258/268 (96%)	192 (74%)	66 (26%)	0	0

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	1(H)	THR
1	1	1(G)	PHE
1	1	1(E)	SER
1	1	1(C)	GLU
1	1	1(A)	ASP
1	1	1	CYS
1	1	6	LEU
1	1	10	LYS
1	1	13	GLU
2	2	16	ILE
2	2	18	GLU
2	2	29	TRP
2	2	33	LEU
2	2	39	GLU
2	2	40	LEU
2	2	46	LEU
2	2	60	LEU
2	2	60(A)	TYR
2	2	60(B)	PRO
2	2	60(C)	PRO
2	2	60(D)	TRP
2	2	60(E)	ASP
2	2	60(F)	LYS
2	2	60(G)	ASN
2	2	60(H)	PHE
2	2	60(I)	THR
2	2	61	GLU
2	2	65	LEU
2	2	66	VAL
2	2	68	ILE
2	2	74	THR
2	2	79	ILE
2	2	81	LYS
2	2	82	ILE

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Mol	Chain	Res	Type
2	2	85	LEU
2	2	90	ILE
2	2	106	MET
2	2	109	LYS
2	2	110	LYS
2	2	112	VAL
2	2	127	GLU
2	2	137	ARG
2	2	138	VAL
2	2	147	THR
2	2	158	VAL
2	2	162	ILE
2	2	169	LYS
2	2	175	ARG
2	2	185	LYS
2	2	187	ARG
2	2	198	PRO
2	2	201	MET
2	2	202	LYS
2	2	205	ASN
2	2	210	MET
2	2	214	SER
2	2	233	ARG
2	2	234	LEU
2	2	239	GLN
2	2	240	LYS
2	2	241	VAL
2	2	245	PHE
3	3	559	ASP
3	3	562	GLU
3	3	563	ILE
3	3	566	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	2	38	GLN
2	2	62	ASN
2	2	78	ASN
2	2	95	ASN
2	2	156	GLN
2	2	204(B)	ASN

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Mol	Chain	Res	Type
2	2	205	ASN
2	2	244	GLN

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	1.59	2 (13%)	15,22,24	1.37	1 (6%)

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-CZ	-4.03	1.36	1.42
3	3	567	TYS	OH-S	3.40	1.65	1.58

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	567	TYS	CB-CG-CD1	-2.41	116.42	120.90

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	3	567	TYS	CA-CB-CG-CD1

There are no ring outliers.

1 monomer is involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	3	567	TYS	14	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	IH2	2	370	-	41,43,43	4.32	27 (65%)	51,61,61	3.80	26 (50%)

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	IH2	2	370	-	-	4/23/47/47	0/5/5/5

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	2	370	IH2	O12-C12	9.65	1.41	1.23
5	2	370	IH2	N19-N18	-7.82	1.32	1.42
5	2	370	IH2	C1-C2	-7.24	1.38	1.52
5	2	370	IH2	C17-C15	6.24	1.56	1.50
5	2	370	IH2	C17-N18	-6.16	1.36	1.46
5	2	370	IH2	C32-C31	6.16	1.48	1.39
5	2	370	IH2	C29-C30	6.04	1.49	1.38
5	2	370	IH2	C27-C26	6.03	1.49	1.38
5	2	370	IH2	C5-C8	-5.97	1.38	1.49
5	2	370	IH2	C30-C25	5.63	1.48	1.39
5	2	370	IH2	C1-N9	5.31	1.60	1.46
5	2	370	IH2	C26-C25	-5.28	1.30	1.39
5	2	370	IH2	C35-C34	5.02	1.49	1.38
5	2	370	IH2	C3-C4	-4.99	1.40	1.52
5	2	370	IH2	C27-C28	4.74	1.48	1.38
5	2	370	IH2	C20-N21	-4.50	1.30	1.39
5	2	370	IH2	O22-C22	-4.44	1.14	1.22
5	2	370	IH2	C22-N19	-4.29	1.28	1.38
5	2	370	IH2	C29-C28	-4.20	1.29	1.38
5	2	370	IH2	C8-N11	3.91	1.35	1.27
5	2	370	IH2	C16-C15	-3.88	1.41	1.50
5	2	370	IH2	C6-C7	-3.19	1.45	1.52
5	2	370	IH2	C36-C31	2.89	1.43	1.39
5	2	370	IH2	C25-C24	2.88	1.60	1.53
5	2	370	IH2	C14-C15	-2.82	1.28	1.32
5	2	370	IH2	C23-N21	-2.79	1.41	1.47
5	2	370	IH2	C4-C5	-2.64	1.46	1.53

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	2	370	IH2	O20-C20-N18	12.39	134.87	126.69
5	2	370	IH2	C3-C4-C5	8.29	125.78	111.18
5	2	370	IH2	C6-C5-C8	7.98	121.48	111.29
5	2	370	IH2	C4-C5-C8	6.80	119.97	111.29
5	2	370	IH2	C29-C30-C25	6.66	128.62	120.65
5	2	370	IH2	C5-C8-N10	5.88	127.06	116.59
5	2	370	IH2	C28-C27-C26	5.41	126.91	120.24
5	2	370	IH2	C16-C15-C14	-5.24	115.88	122.46
5	2	370	IH2	C26-C25-C30	-5.16	111.90	118.30
5	2	370	IH2	C23-N21-C22	4.93	130.82	122.83
5	2	370	IH2	C27-C28-C29	-4.59	113.58	119.87
5	2	370	IH2	C6-C7-C2	-4.53	103.80	112.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	2	370	IH2	C4-C5-C6	4.03	118.48	110.00
5	2	370	IH2	C30-C25-C24	3.97	131.76	120.83
5	2	370	IH2	C33-C34-C35	3.70	124.93	119.87
5	2	370	IH2	C34-C33-C32	-3.46	115.97	120.24
5	2	370	IH2	C13-C12-N9	3.46	121.71	114.86
5	2	370	IH2	C20-N18-N19	3.24	110.84	107.89
5	2	370	IH2	C22-N21-C20	-3.10	108.92	111.45
5	2	370	IH2	C23-C24-C25	2.96	125.36	112.32
5	2	370	IH2	N19-C22-N21	2.73	108.47	106.00
5	2	370	IH2	C7-C2-C1	-2.72	105.94	111.47
5	2	370	IH2	C4-C3-C2	-2.66	107.34	112.36
5	2	370	IH2	C1-N9-C12	2.36	127.14	122.65
5	2	370	IH2	O12-C12-C13	-2.35	117.62	120.96
5	2	370	IH2	O20-C20-N21	-2.18	120.22	125.69

There are no chirality outliers.

All (4) torsion outliers are listed below:

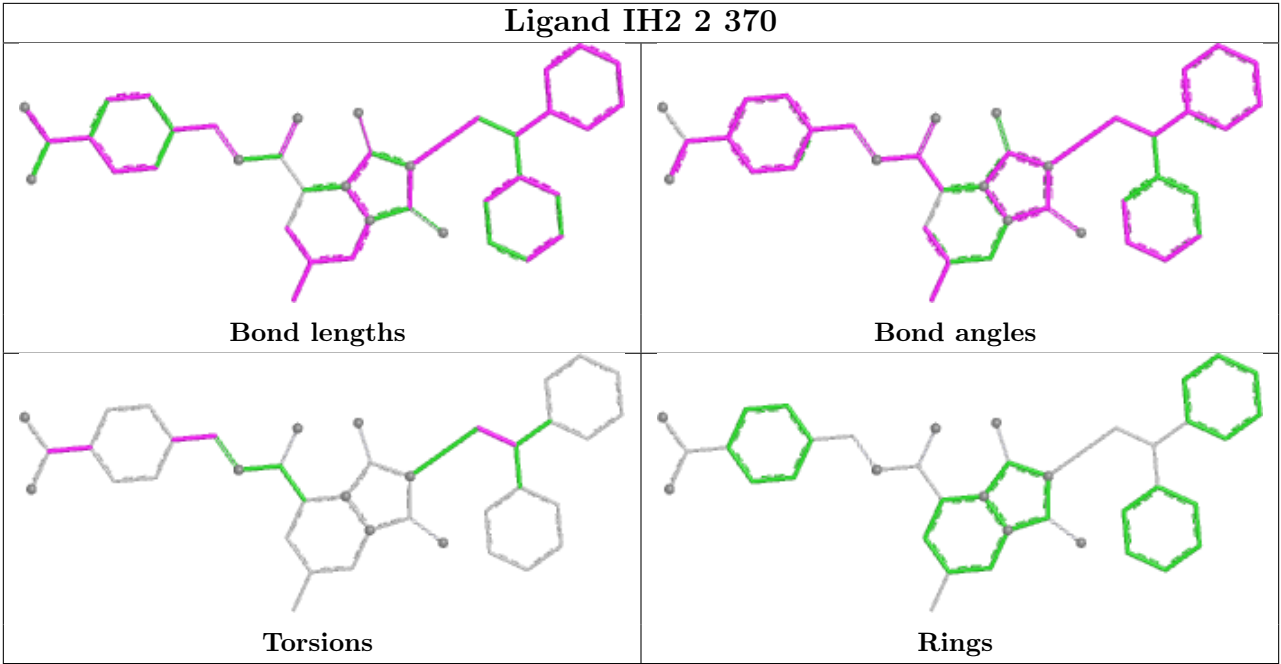
Mol	Chain	Res	Type	Atoms
5	2	370	IH2	N9-C1-C2-C7
5	2	370	IH2	C6-C5-C8-N10
5	2	370	IH2	N9-C1-C2-C3
5	2	370	IH2	N21-C23-C24-C25

There are no ring outliers.

1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	2	370	IH2	11	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	221:ASP	C	221(A):ARG	N	1.79

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.