Full wwPDB X-ray Structure Validation Report (i)

Aug 2, 2023 – 04:10 AM EDT

PDB ID	:	1C4V
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 (i) 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 (1)) were used in the production of this report:

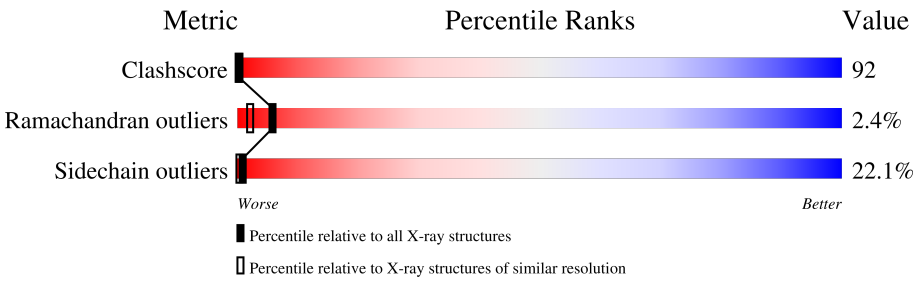
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	1	36	14% 28% 47% 11%
2	2	259	15% 39% 36% 8% •
3	3	15	7% 20% 33% 7% 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 (i)

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
			Total	C	N	O	S			
1	1	36	287	177	48	61	1	0	0	0

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

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

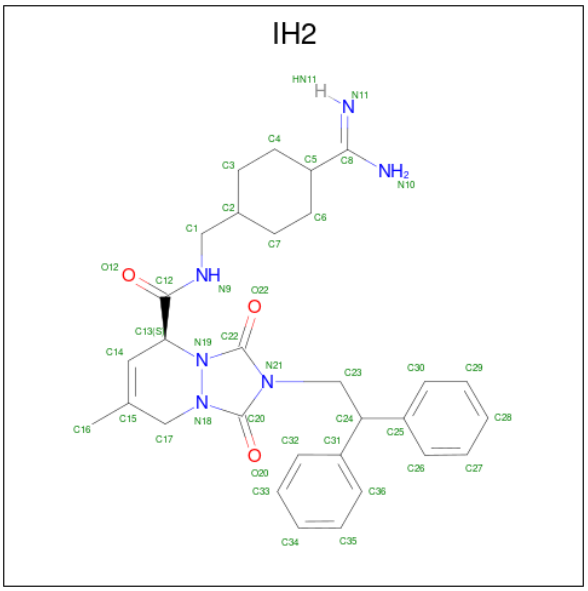
- Molecule 3 is a protein called HIRUGEN.

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

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 5 is 2-(2,2-DIPHENYL-ETHYL)-7-METHYL-1,3-DIOXO-2,3,5,8-TETRAHYDRO-1H-[1,2,4]TRIAZOLO [1,2-A]PYRIDAZINE-5-CARBOXYLIC ACID(4-CARBAMIMIDOYL-CYCLOHEXYLMETHYL)-AMIDE (three-letter code: IH2) (formula: $C_{30}H_{36}N_6O_3$).



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

- Molecule 6 is water.

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

3 Residue-property plots (i)

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

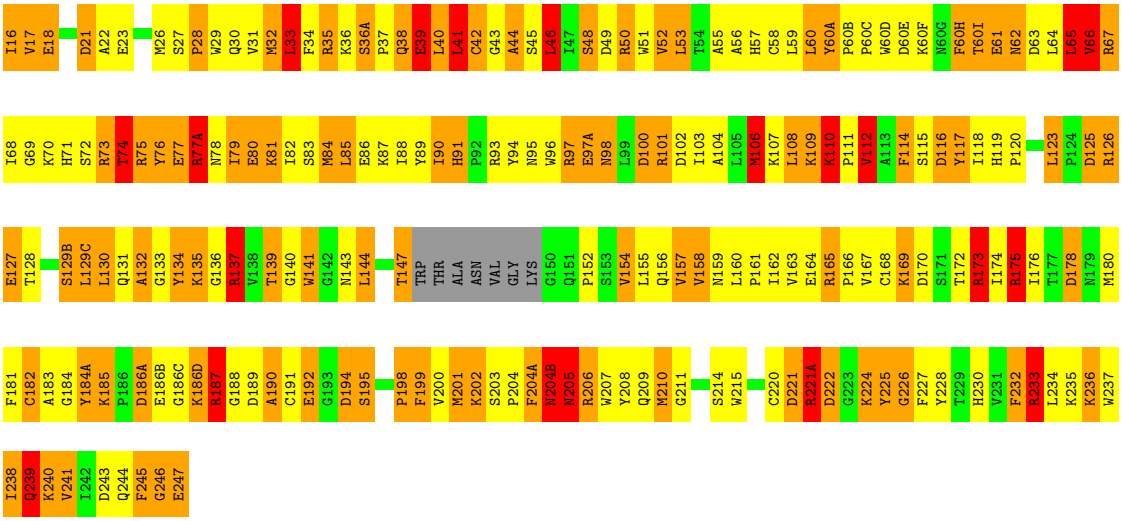
Note EDS was not executed.

• Molecule 1: THROMBIN:SHORT CHAIN

Chain 1: 14% 28% 47% 11%

• Molecule 2: THROMBIN:LONG CHAIN

Chain 2: 15% 39% 36% 8% •



• Molecule 3: HIRUGEN

Chain 3: 7% 20% 33% 7% 33%

4 Data and refinement statistics (i)

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: IH2, TYS, NA

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	1.36	0/290	3.43	38/384 (9.9%)
2	2	1.34	3/2087 (0.1%)	2.85	179/2818 (6.4%)
3	3	1.16	0/74	2.54	5/96 (5.2%)
All	All	1.33	3/2451 (0.1%)	2.91	222/3298 (6.7%)

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	5

All (3) 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	7.12	1.42	1.33
2	2	27	SER	CB-OG	-7.07	1.33	1.42

All (222) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	221(A)	ARG	NE-CZ-NH2	24.73	132.67	120.30
2	2	67	ARG	NE-CZ-NH1	21.48	131.04	120.30
2	2	73	ARG	NE-CZ-NH1	20.17	130.38	120.30
2	2	173	ARG	NE-CZ-NH1	19.72	130.16	120.30
2	2	73	ARG	NE-CZ-NH2	-16.74	111.93	120.30
2	2	233	ARG	CD-NE-CZ	16.42	146.59	123.60
2	2	35	ARG	CD-NE-CZ	15.41	145.18	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	1(C)	GLU	CA-CB-CG	15.08	146.57	113.40
2	2	101	ARG	NE-CZ-NH2	-14.60	113.00	120.30
1	1	15	ARG	NE-CZ-NH1	-14.53	113.04	120.30
2	2	137	ARG	NE-CZ-NH2	-14.53	113.04	120.30
2	2	60(A)	TYR	CB-CG-CD1	-13.88	112.67	121.00
2	2	221(A)	ARG	NE-CZ-NH1	-13.82	113.39	120.30
2	2	173	ARG	NH1-CZ-NH2	-13.78	104.24	119.40
2	2	175	ARG	NE-CZ-NH2	-13.75	113.43	120.30
1	1	15	ARG	NE-CZ-NH2	-13.70	113.45	120.30
2	2	165	ARG	NE-CZ-NH2	13.64	127.12	120.30
1	1	14(D)	ARG	CD-NE-CZ	13.21	142.10	123.60
2	2	126	ARG	CD-NE-CZ	13.06	141.89	123.60
1	1	15	ARG	CD-NE-CZ	-13.05	105.33	123.60
1	1	15	ARG	NH1-CZ-NH2	12.79	133.47	119.40
2	2	206	ARG	NE-CZ-NH1	12.49	126.55	120.30
1	1	14	ASP	CB-CG-OD2	-12.19	107.33	118.30
2	2	222	ASP	CB-CG-OD2	-12.00	107.50	118.30
1	1	14(G)	LEU	CB-CA-C	11.84	132.70	110.20
2	2	189	ASP	CB-CG-OD2	11.72	128.85	118.30
2	2	77	GLU	C-N-CA	11.43	150.28	121.70
2	2	184(A)	TYR	CB-CG-CD2	-10.98	114.41	121.00
2	2	165	ARG	NE-CZ-NH1	-10.97	114.82	120.30
2	2	175	ARG	CD-NE-CZ	-10.97	108.25	123.60
2	2	187	ARG	NE-CZ-NH1	10.96	125.78	120.30
2	2	184(A)	TYR	CB-CG-CD1	10.72	127.43	121.00
2	2	67	ARG	NE-CZ-NH2	-10.60	115.00	120.30
2	2	50	ARG	NE-CZ-NH2	-10.60	115.00	120.30
2	2	173	ARG	CD-NE-CZ	10.49	138.29	123.60
2	2	137	ARG	CD-NE-CZ	-10.43	109.00	123.60
2	2	126	ARG	NE-CZ-NH1	10.30	125.45	120.30
2	2	144	LEU	CA-CB-CG	9.74	137.71	115.30
2	2	234	LEU	CB-CA-C	9.70	128.64	110.20
2	2	97(A)	GLU	OE1-CD-OE2	9.45	134.64	123.30
2	2	178	ASP	CB-CG-OD1	9.36	126.72	118.30
1	1	4	ARG	NE-CZ-NH2	9.19	124.89	120.30
2	2	154	VAL	CB-CA-C	8.88	128.26	111.40
2	2	126	ARG	NE-CZ-NH2	-8.81	115.89	120.30
2	2	78	ASN	CA-CB-CG	8.76	132.68	113.40
2	2	60(E)	ASP	CB-CG-OD1	-8.74	110.43	118.30
1	1	14(L)	ASP	CB-CG-OD2	-8.74	110.43	118.30
3	3	561	GLU	CG-CD-OE2	-8.66	100.98	118.30
2	2	66	VAL	CA-CB-CG1	8.62	123.83	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	165	ARG	CD-NE-CZ	-8.52	111.67	123.60
2	2	224	LYS	C-N-CA	8.32	142.49	121.70
2	2	60(H)	PHE	CB-CG-CD1	-8.28	115.00	120.80
2	2	84	MET	O-C-N	8.25	135.90	122.70
2	2	137	ARG	NH1-CZ-NH2	8.23	128.45	119.40
2	2	140	GLY	C-N-CA	8.21	142.23	121.70
2	2	247	GLU	OE1-CD-OE2	-8.16	113.50	123.30
2	2	178	ASP	CB-CG-OD2	-8.11	111.00	118.30
2	2	41	LEU	CB-CA-C	8.04	125.47	110.20
1	1	1(B)	ALA	CB-CA-C	-8.04	98.05	110.10
2	2	18	GLU	CA-CB-CG	8.02	131.05	113.40
2	2	246	GLY	N-CA-C	7.95	132.98	113.10
2	2	60(A)	TYR	CB-CG-CD2	7.70	125.62	121.00
1	1	1(C)	GLU	CA-C-N	7.62	133.96	117.20
2	2	97	ARG	CD-NE-CZ	-7.60	112.96	123.60
1	1	1(B)	ALA	N-CA-CB	7.52	120.63	110.10
2	2	91	HIS	CA-CB-CG	-7.50	100.84	113.60
2	2	233	ARG	NE-CZ-NH1	7.44	124.02	120.30
2	2	175	ARG	NE-CZ-NH1	-7.42	116.59	120.30
2	2	102	ASP	CB-CG-OD2	-7.40	111.64	118.30
2	2	225	TYR	CB-CG-CD2	-7.36	116.59	121.00
1	1	1(D)	GLY	CA-C-O	7.32	133.78	120.60
2	2	154	VAL	N-CA-CB	-7.26	95.52	111.50
2	2	186(A)	ASP	CB-CG-OD1	7.22	124.80	118.30
2	2	134	TYR	CB-CG-CD1	-7.20	116.68	121.00
2	2	50	ARG	NE-CZ-NH1	7.18	123.89	120.30
2	2	48	SER	N-CA-CB	-7.15	99.77	110.50
2	2	186(D)	LYS	CB-CA-C	7.09	124.58	110.40
2	2	185	LYS	CA-CB-CG	7.09	128.99	113.40
2	2	181	PHE	CB-CA-C	7.06	124.52	110.40
2	2	36(A)	SER	N-CA-CB	-7.01	99.98	110.50
2	2	205	ASN	CB-CA-C	7.01	124.42	110.40
2	2	170	ASP	O-C-N	7.00	133.90	122.70
2	2	66	VAL	CB-CA-C	7.00	124.69	111.40
2	2	125	ASP	CB-CG-OD1	7.00	124.60	118.30
2	2	101	ARG	NH1-CZ-NH2	6.99	127.09	119.40
1	1	1(G)	PHE	N-CA-CB	-6.98	98.03	110.60
1	1	1(A)	ASP	CA-C-N	-6.91	102.00	117.20
2	2	157	VAL	CA-CB-CG2	6.87	121.20	110.90
2	2	42	CYS	CA-CB-SG	6.84	126.31	114.00
1	1	14(C)	GLU	CB-CA-C	-6.83	96.75	110.40
2	2	73	ARG	CD-NE-CZ	6.80	133.12	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	134	TYR	CB-CG-CD2	6.77	125.06	121.00
2	2	189	ASP	CB-CA-C	6.73	123.85	110.40
2	2	190	ALA	N-CA-C	-6.72	92.86	111.00
1	1	4	ARG	NH1-CZ-NH2	-6.68	112.05	119.40
2	2	66	VAL	N-CA-CB	-6.63	96.92	111.50
1	1	14(D)	ARG	NE-CZ-NH2	6.61	123.61	120.30
1	1	14(G)	LEU	CB-CG-CD2	6.59	122.20	111.00
2	2	21	ASP	CB-CG-OD2	-6.57	112.39	118.30
1	1	4	ARG	CD-NE-CZ	6.57	132.79	123.60
1	1	13	GLU	CG-CD-OE1	6.56	131.43	118.30
2	2	160	LEU	O-C-N	6.56	133.57	121.10
2	2	173	ARG	CG-CD-NE	6.54	125.53	111.80
2	2	156	GLN	O-C-N	-6.51	112.28	122.70
3	3	561	GLU	CG-CD-OE1	6.50	131.29	118.30
2	2	32	MET	O-C-N	6.50	133.09	122.70
1	1	14	ASP	CB-CA-C	6.48	123.35	110.40
2	2	76	TYR	C-N-CA	6.44	137.79	121.70
2	2	100	ASP	O-C-N	6.42	132.97	122.70
2	2	90	ILE	CB-CG1-CD1	6.38	131.75	113.90
2	2	39	GLU	CG-CD-OE2	-6.36	105.58	118.30
2	2	117	TYR	CB-CG-CD2	-6.35	117.19	121.00
2	2	173	ARG	NE-CZ-NH2	6.32	123.46	120.30
2	2	97	ARG	NE-CZ-NH1	-6.31	117.14	120.30
2	2	53	LEU	CA-C-O	-6.29	106.89	120.10
2	2	33	LEU	O-C-N	6.29	132.76	122.70
1	1	14(L)	ASP	CB-CG-OD1	6.28	123.95	118.30
3	3	566	GLU	CA-CB-CG	6.24	127.14	113.40
2	2	204(A)	PHE	CZ-CE2-CD2	-6.24	112.62	120.10
2	2	60(E)	ASP	OD1-CG-OD2	6.22	135.13	123.30
2	2	120	PRO	CA-C-O	6.21	135.12	120.20
2	2	27	SER	N-CA-CB	-6.20	101.21	110.50
2	2	77(A)	ARG	NE-CZ-NH2	-6.20	117.20	120.30
2	2	123	LEU	CB-CG-CD2	-6.18	100.50	111.00
1	1	1(F)	GLY	O-C-N	6.13	132.50	122.70
1	1	1(C)	GLU	CB-CG-CD	6.11	130.69	114.20
2	2	38	GLN	N-CA-CB	6.11	121.59	110.60
1	1	1(C)	GLU	CA-C-O	-6.10	107.29	120.10
2	2	147	THR	CA-C-O	6.07	132.84	120.10
2	2	60	LEU	CB-CA-C	6.03	121.66	110.20
2	2	247	GLU	CB-CG-CD	5.98	130.34	114.20
2	2	80	GLU	CG-CD-OE2	-5.98	106.35	118.30
2	2	199	PHE	N-CA-C	-5.97	94.89	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	114	PHE	CB-CG-CD1	-5.96	116.63	120.80
2	2	233	ARG	CA-CB-CG	-5.95	100.32	113.40
2	2	21	ASP	O-C-N	5.90	132.14	122.70
1	1	1(D)	GLY	C-N-CA	5.85	136.32	121.70
2	2	135	LYS	O-C-N	-5.82	113.30	123.20
2	2	80	GLU	CG-CD-OE1	5.79	129.89	118.30
2	2	186(A)	ASP	CA-CB-CG	5.78	126.12	113.40
2	2	104	ALA	O-C-N	5.77	131.93	122.70
2	2	232	PHE	CB-CG-CD1	-5.74	116.78	120.80
2	2	75	ARG	N-CA-CB	-5.73	100.29	110.60
3	3	562	GLU	CB-CG-CD	5.72	129.66	114.20
2	2	186(A)	ASP	C-N-CA	5.71	135.98	121.70
2	2	226	GLY	O-C-N	5.71	131.83	122.70
2	2	18	GLU	C-N-CA	5.70	134.28	122.30
2	2	129(B)	SER	N-CA-CB	5.70	119.05	110.50
2	2	227	PHE	CA-C-N	-5.67	104.72	117.20
2	2	31	VAL	CG1-CB-CG2	5.65	119.94	110.90
1	1	13	GLU	CA-CB-CG	5.63	125.80	113.40
2	2	33	LEU	N-CA-C	-5.60	95.87	111.00
2	2	80	GLU	CB-CG-CD	5.60	129.32	114.20
2	2	128	THR	CA-CB-CG2	5.59	120.23	112.40
2	2	141	TRP	O-C-N	5.59	132.71	123.20
1	1	9	LYS	N-CA-CB	-5.57	100.57	110.60
2	2	77(A)	ARG	CD-NE-CZ	-5.56	115.81	123.60
2	2	74	THR	N-CA-C	5.54	125.96	111.00
2	2	26	MET	CB-CG-SD	-5.54	95.78	112.40
2	2	77	GLU	CA-C-O	5.53	131.71	120.10
2	2	18	GLU	CG-CD-OE1	5.52	129.34	118.30
1	1	4	ARG	NE-CZ-NH1	5.52	123.06	120.30
2	2	77(A)	ARG	CG-CD-NE	-5.51	100.24	111.80
2	2	204(B)	ASN	C-N-CA	5.51	135.47	121.70
2	2	98	ASN	N-CA-CB	-5.49	100.71	110.60
3	3	568	LEU	CA-C-O	-5.49	108.57	120.10
2	2	139	THR	CA-CB-CG2	5.49	120.08	112.40
2	2	132	ALA	CB-CA-C	5.48	118.32	110.10
2	2	238	ILE	CA-C-O	-5.47	108.60	120.10
2	2	239	GLN	N-CA-CB	5.47	120.45	110.60
1	1	1(A)	ASP	CA-CB-CG	-5.43	101.45	113.40
2	2	21	ASP	N-CA-CB	5.43	120.37	110.60
2	2	42	CYS	C-N-CA	5.42	133.69	122.30
2	2	185	LYS	N-CA-C	-5.42	96.36	111.00
2	2	46	LEU	CB-CG-CD1	5.42	120.21	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	65	LEU	CB-CA-C	5.41	120.49	110.20
2	2	84	MET	CA-CB-CG	-5.40	104.11	113.30
2	2	184	GLY	CA-C-O	5.38	130.29	120.60
2	2	17	VAL	C-N-CA	5.38	135.16	121.70
1	1	14(G)	LEU	CA-CB-CG	5.38	127.68	115.30
2	2	236	LYS	CB-CA-C	5.38	121.15	110.40
2	2	110	LYS	N-CA-CB	5.37	120.27	110.60
2	2	225	TYR	CZ-CE2-CD2	-5.37	114.97	119.80
2	2	81	LYS	N-CA-CB	5.36	120.25	110.60
2	2	112	VAL	O-C-N	5.34	131.24	122.70
2	2	199	PHE	CZ-CE2-CD2	-5.33	113.70	120.10
2	2	62	ASN	OD1-CG-ND2	5.32	134.14	121.90
2	2	106	MET	CA-CB-CG	5.32	122.34	113.30
1	1	14(D)	ARG	NH1-CZ-NH2	-5.31	113.56	119.40
2	2	28	PRO	N-CA-C	5.30	125.88	112.10
2	2	239	GLN	CA-CB-CG	5.29	125.04	113.40
2	2	182	CYS	N-CA-CB	5.28	120.11	110.60
2	2	241	VAL	CG1-CB-CG2	5.27	119.34	110.90
2	2	98	ASN	CB-CG-OD1	5.27	132.14	121.60
2	2	83	SER	CA-C-N	-5.27	105.61	117.20
2	2	241	VAL	CA-CB-CG1	-5.27	103.00	110.90
2	2	189	ASP	CB-CG-OD1	-5.22	113.60	118.30
2	2	222	ASP	CB-CG-OD1	5.22	123.00	118.30
2	2	180	MET	CG-SD-CE	5.22	108.55	100.20
2	2	187	ARG	NE-CZ-NH2	-5.20	117.70	120.30
2	2	52	VAL	CA-CB-CG1	5.20	118.70	110.90
2	2	75	ARG	NE-CZ-NH1	5.20	122.90	120.30
2	2	135	LYS	CA-C-O	5.19	130.99	120.10
2	2	21	ASP	CB-CG-OD1	5.17	122.96	118.30
2	2	130	LEU	CB-CA-C	5.17	120.03	110.20
2	2	139	THR	CA-C-O	5.17	130.96	120.10
2	2	39	GLU	O-C-N	5.17	130.97	122.70
2	2	108	LEU	CB-CA-C	5.15	119.98	110.20
2	2	129(C)	LEU	N-CA-C	5.14	124.89	111.00
1	1	1(B)	ALA	CA-C-N	-5.13	105.91	117.20
2	2	30	GLN	OE1-CD-NE2	5.13	133.70	121.90
1	1	12	LEU	CB-CG-CD2	-5.13	102.28	111.00
2	2	46	LEU	CB-CA-C	5.11	119.92	110.20
1	1	6	LEU	CA-CB-CG	5.10	127.04	115.30
2	2	194	ASP	CB-CG-OD2	5.10	122.89	118.30
2	2	221(A)	ARG	NH1-CZ-NH2	-5.09	113.80	119.40
1	1	13	GLU	OE1-CD-OE2	-5.08	117.21	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	32	MET	CG-SD-CE	5.07	108.31	100.20
2	2	192	GLU	CA-CB-CG	5.03	124.46	113.40
2	2	232	PHE	CB-CA-C	5.02	120.43	110.40
2	2	227	PHE	CA-C-O	5.01	130.62	120.10
2	2	67	ARG	NH1-CZ-NH2	-5.00	113.90	119.40

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 (i)

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	2002	340	2
3	3	90	0	71	27	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	9	0
All	All	2548	0	2386	443	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 92.

All (443) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:221:ASP:C	2:2:221(A):ARG:N	1.79	1.35
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
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
3:3:564:PRO:HB2	3:3:566:GLU:CD	1.69	1.09
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
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
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
1:1:15:ARG:O	1:1:15:ARG:HG2	1.67	0.93
2:2:84:MET:CG	6:3:455:HOH:O	2.17	0.93
1:1:1(G):PHE:C	2:2:235:LYS:NZ	2.22	0.92
1:1:14(I):SER:C	1:1:14(K):ILE:H	1.65	0.92
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
1:1:14(M):GLY:CA	6:1:458:HOH:O	2.19	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:2:199:PHE:HE2	2:2:201:MET:HE3	1.38	0.87
2:2:93:ARG:O	2:2:101:ARG:HD2	1.76	0.86
2:2:224:LYS:NZ	6:2:421:HOH:O	1.72	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(H):THR:CG2	1:1:1(G):PHE:N	2.39	0.84
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
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
1:1:1(G):PHE:C	2:2:235:LYS:HZ2	1.82	0.82
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:2:85:LEU:HD13	2:2:106:MET:HE2	1.67	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
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
1:1:1(G):PHE:CD1	1:1:1(G):PHE:C	2.60	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
1:1:1(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
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
2:2:17: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
1:1:1(G):PHE:C	2:2:235:LYS:HZ1	1.92	0.71
1:1:14(C):GLU:O	1:1:14(G):LEU:HD23	1.90	0.71
2:2:178:ASP:CG	6:2:435:HOH:O	2.27	0.71
1:1:14(D):ARG:HG2	1:1:14(E):GLU:N	2.04	0.70
2:2:50:ARG:HD2	2:2:111:PRO:HG3	1.73	0.70
1:1:14(I):SER:C	1:1:14(K):ILE:N	2.41	0.70
2:2:61:GLU:OE1	2:2:87:LYS:HA	1.90	0.70
1:1:14:ASP:OD2	1:1:14:ASP:C	2.30	0.70
2:2:33:LEU:HD13	2:2:41:LEU:HD13	1.72	0.70
2:2:208:TYR:HB3	2:2:210:MET:HE1	1.73	0.69
1:1:1(F):GLY:N	2:2:235:LYS:NZ	2.39	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1(D):GLY:HA3	6:2:401:HOH:O	1.91	0.69
1:1:11:SER:C	1:1:12:LEU:HD22	2.13	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
2:2:130: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
2:2:33: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
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
2:2:51: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
2:2:204(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
1:1:12:LEU:N	1:1:12:LEU:HD22	2.09	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
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
1:1:11:SER:C	1:1:12:LEU:CD2	2.67	0.63
2:2:65:LEU:HD21	3:3:567:TYS:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:2:194:ASP:O	2:2:195:SER:C	2.38	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
2:2:40:LEU:HD23	2:2:40:LEU:C	2.19	0.62
2:2:84:MET:HE2	3:3:567:TYS:O	2.00	0.62
1:1:5:PRO:HG2	2:2:115:SER:O	1.99	0.62
2:2:130:LEU:HD23	2:2:201:MET:HE1	1.81	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
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
1:1:1(H):THR:H2	1:1:1(C):GLU:N	1.99	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
2:2:50:ARG:HD3	2:2:247:GLU:CD	2.21	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
2:2:199:PHE:CE2	2:2:201:MET:HE3	2.29	0.60
2:2:204(B):ASN:ND2	2:2:206:ARG:H	2.00	0.60
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
2:2:183:ALA:HB3	2:2:228:TYR:HE1	1.67	0.59
2:2:32:MET:HE3	2:2:70:LYS:HD3	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:32:MET:HE1	2:2:70:LYS:HE3	1.84	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
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
3:3:561:GLU:HG2	3:3:562:GLU:N	2.18	0.56
2:2:86:GLU:HB2	2:2:109:LYS:HG3	1.87	0.56
2:2:208:TYR:CB	2:2:210:MET:HE1	2.35	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
2:2:172:THR:OG1	2:2:173:ARG:N	2.39	0.55
2:2:199:PHE:CE2	2:2:201:MET:CE	2.83	0.55
2:2:71:HIS:CD2	2:2:154:VAL:HG22	2.40	0.55
2:2:21:ASP:CG	2:2:154:VAL:CG1	2.75	0.55
2:2:91:HIS:ND1	2:2:91:HIS:C	2.60	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
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
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
2:2:186(C):GLY:C	6:2:468:HOH:O	2.45	0.53
2:2:174:ILE:HD11	5:2:370:IH2:C33	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:3:564:PRO:C	3:3:566:GLU:OE1	2.48	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
2:2:204(B):ASN:HD22	2:2:204(B):ASN:C	2.12	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
2:2:33: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
1:1:10:LYS:C	1:1:12:LEU:HD23	2.30	0.50
2:2:45:SER:O	2:2:52:VAL:HA	2.11	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
2:2:33:LEU:HD21	2:2:64:LEU:HD22	1.94	0.50
3:3:561:GLU:CG	3:3:562:GLU:N	2.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:2:204(B):ASN:ND2	2:2:204(B):ASN:C	2.65	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
2:2:59:LEU:HD11	2:2:106:MET:HE3	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
2:2:127:GLU:CD	2:2:127:GLU:H	2.16	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:135:LYS:CE	2:2:184(A):TYR:OH	2.59	0.47
2:2:162:ILE:HD11	2:2:201:MET:CE	2.45	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
2:2:36(A):SER:HA	2:2:37:PRO:C	2.36	0.46
2:2:60(A):TYR:HD2	2:2:60(D):TRP:HB2	1.80	0.46
1:1:1(G):PHE:O	1:1:1(F):GLY:C	2.54	0.46
2:2:129(B):SER:O	2:2:131:GLN:NE2	2.48	0.46
2:2:93:ARG:C	2:2:101:ARG:HD2	2.36	0.46
2:2:59:LEU:HD13	2:2:88:ILE:HG23	1.98	0.46
2:2:84:MET:HE3	6:3:455:HOH:O	2.16	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
2:2:167:VAL:O	2:2:168:CYS:C	2.52	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
2:2:152: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
2:2:199:PHE:CE2	2:2:201:MET:HE2	2.52	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
2:2:210:MET:N	2:2:210:MET:CE	2.80	0.44
3:3:565:GLY:C	3:3:567:TYS:N	2.70	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
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
1:1:11:SER:C	1:1:12:LEU:HD23	2.38	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1(H):THR:H1	1:1:1(C):GLU:CB	2.31	0.43
2:2:172:THR:HG21	2:2:176:ILE:HD11	2.00	0.43
2:2:204(B):ASN:ND2	2:2:204(B):ASN:N	2.66	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
2:2:126: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
2:2:59:LEU:HD21	2:2:106:MET:HE1	2.01	0.43
2:2:129(C):LEU:HD21	2:2:204:PRO:HD3	2.00	0.43
2:2:210:MET:N	2:2:210:MET:HE2	2.34	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
2:2:187:ARG:HH22	2:2:222:ASP:CG	2.23	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
2:2:85:LEU:HD13	2:2:106:MET:CE	2.41	0.42
2:2:175:ARG:CG	2:2:175:ARG:O	2.63	0.42
2:2:221:ASP:C	2:2:221(A):ARG:CA	2.80	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
2:2:187:ARG:NH2	2:2:222:ASP:OD1	2.53	0.42
2:2:22:ALA:O	2:2:71:HIS:HE1	2.02	0.41
1:1:1(F):GLY:C	2:2:235:LYS:HZ1	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:60(C):PRO:HD3	2:2:96:TRP:CE3	2.55	0.41
2:2:60(I):THR:HG22	2:2:63:ASP:CG	2.41	0.41
2:2:63:ASP:OD2	2:2:63:ASP:N	2.52	0.41
2:2:95:ASN:N	2:2:100:ASP:O	2.47	0.41
2:2:95:ASN:ND2	2:2:98:ASN:OD1	2.53	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
2:2:50: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
2:2:178: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
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
2:2:133:GLY:C	6:2:517:HOH:O	2.60	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 symmetry 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%)	13 8
3	3	7/15 (47%)	4 (57%)	3 (43%)	0	100 100
All	All	289/310 (93%)	249 (86%)	33 (11%)	7 (2%)	6 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%)	24 (77%)	7 (23%)	1 0
2	2	219/225 (97%)	172 (78%)	47 (22%)	1 0
3	3	8/12 (67%)	5 (62%)	3 (38%)	0 0
All	All	258/268 (96%)	201 (78%)	57 (22%)	1 0

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	1(H)	THR
1	1	6	LEU
1	1	10	LYS
1	1	14(A)	LYS
1	1	14(D)	ARG
1	1	14(J)	TYR
1	1	14(L)	ASP
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	41	LEU
2	2	46	LEU
2	2	60	LEU
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	77(A)	ARG
2	2	79	ILE
2	2	81	LYS
2	2	82	ILE
2	2	85	LEU
2	2	94	TYR
2	2	106	MET
2	2	109	LYS
2	2	110	LYS
2	2	112	VAL
2	2	116	ASP
2	2	127	GLU
2	2	137	ARG
2	2	147	THR
2	2	158	VAL
2	2	169	LYS
2	2	175	ARG
2	2	186(A)	ASP
2	2	186(D)	LYS
2	2	187	ARG

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Mol	Chain	Res	Type
2	2	198	PRO
2	2	201	MET
2	2	202	LYS
2	2	204(B)	ASN
2	2	205	ASN
2	2	210	MET
2	2	214	SER
2	2	233	ARG
2	2	236	LYS
2	2	239	GLN
2	2	240	LYS
2	2	245	PHE
3	3	559	ASP
3	3	562	GLU
3	3	563	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) 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
2	2	244	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	1.72	2 (13%)	18,22,24	1.68	2 (11%)

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	4.47	1.65	1.58
3	3	567	TYS	OH-CZ	-3.94	1.36	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	3	567	TYS	CG-CB-CA	-4.53	104.92	114.10
3	3	567	TYS	CB-CG-CD1	-2.26	116.42	120.91

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 monosaccharides 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	-	38,43,43	4.43	26 (68%)	39,61,61	3.72	22 (56%)

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	-	-	4/19/47/47	0/4/5/5

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	2	370	IH2	C17-N18	-11.82	1.36	1.46
5	2	370	IH2	O12-C12	9.32	1.41	1.23
5	2	370	IH2	C23-N21	-7.06	1.41	1.48
5	2	370	IH2	C1-C2	-6.57	1.38	1.51
5	2	370	IH2	C32-C31	6.05	1.48	1.39
5	2	370	IH2	C13-C14	-5.83	1.38	1.50
5	2	370	IH2	C30-C25	5.53	1.48	1.39
5	2	370	IH2	C1-N9	5.16	1.60	1.46
5	2	370	IH2	C17-C15	5.13	1.56	1.50
5	2	370	IH2	C26-C25	-5.07	1.30	1.39
5	2	370	IH2	C29-C30	4.90	1.49	1.38
5	2	370	IH2	C5-C8	-4.89	1.38	1.49
5	2	370	IH2	C27-C26	4.89	1.49	1.38
5	2	370	IH2	C13-C12	4.85	1.60	1.54
5	2	370	IH2	C3-C4	-4.85	1.40	1.52
5	2	370	IH2	C35-C34	4.25	1.49	1.38
5	2	370	IH2	C27-C28	4.01	1.48	1.38
5	2	370	IH2	C16-C15	-3.67	1.41	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	2	370	IH2	C29-C28	-3.39	1.29	1.38
5	2	370	IH2	C8-N11	3.11	1.35	1.27
5	2	370	IH2	C6-C7	-3.09	1.45	1.52
5	2	370	IH2	C36-C31	2.87	1.43	1.39
5	2	370	IH2	C25-C24	2.64	1.60	1.53
5	2	370	IH2	C14-C15	-2.62	1.28	1.32
5	2	370	IH2	C4-C5	-2.58	1.46	1.53
5	2	370	IH2	C20-N21	-2.17	1.30	1.35

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	2	370	IH2	C3-C4-C5	8.71	125.78	111.18
5	2	370	IH2	C6-C5-C8	7.68	121.48	111.44
5	2	370	IH2	C23-C24-C25	6.72	125.36	111.99
5	2	370	IH2	C4-C5-C8	6.52	119.97	111.44
5	2	370	IH2	C29-C30-C25	6.45	128.62	120.65
5	2	370	IH2	C5-C8-N10	5.98	127.06	116.66
5	2	370	IH2	C6-C7-C2	-5.21	103.80	112.42
5	2	370	IH2	C26-C25-C30	-5.12	111.90	118.29
5	2	370	IH2	C16-C15-C14	-4.92	115.88	122.46
5	2	370	IH2	C13-C12-N9	4.49	121.71	115.68
5	2	370	IH2	C28-C27-C26	4.41	126.91	120.19
5	2	370	IH2	C4-C5-C6	4.03	118.48	109.97
5	2	370	IH2	C30-C25-C24	4.03	131.76	120.81
5	2	370	IH2	C27-C28-C29	-3.42	113.58	119.93
5	2	370	IH2	C12-C13-N19	3.20	118.37	110.95
5	2	370	IH2	C4-C3-C2	-3.07	107.34	112.42
5	2	370	IH2	C34-C33-C32	-2.77	115.97	120.19
5	2	370	IH2	C33-C34-C35	2.69	124.93	119.93
5	2	370	IH2	C7-C2-C1	-2.61	105.94	111.47
5	2	370	IH2	O12-C12-C13	-2.38	117.62	120.98
5	2	370	IH2	C1-N9-C12	2.34	127.14	122.67
5	2	370	IH2	C16-C15-C17	2.07	119.17	114.83

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	N9-C1-C2-C3
5	2	370	IH2	C6-C5-C8-N10

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Mol	Chain	Res	Type	Atoms
5	2	370	IH2	N21-C23-C24-C25

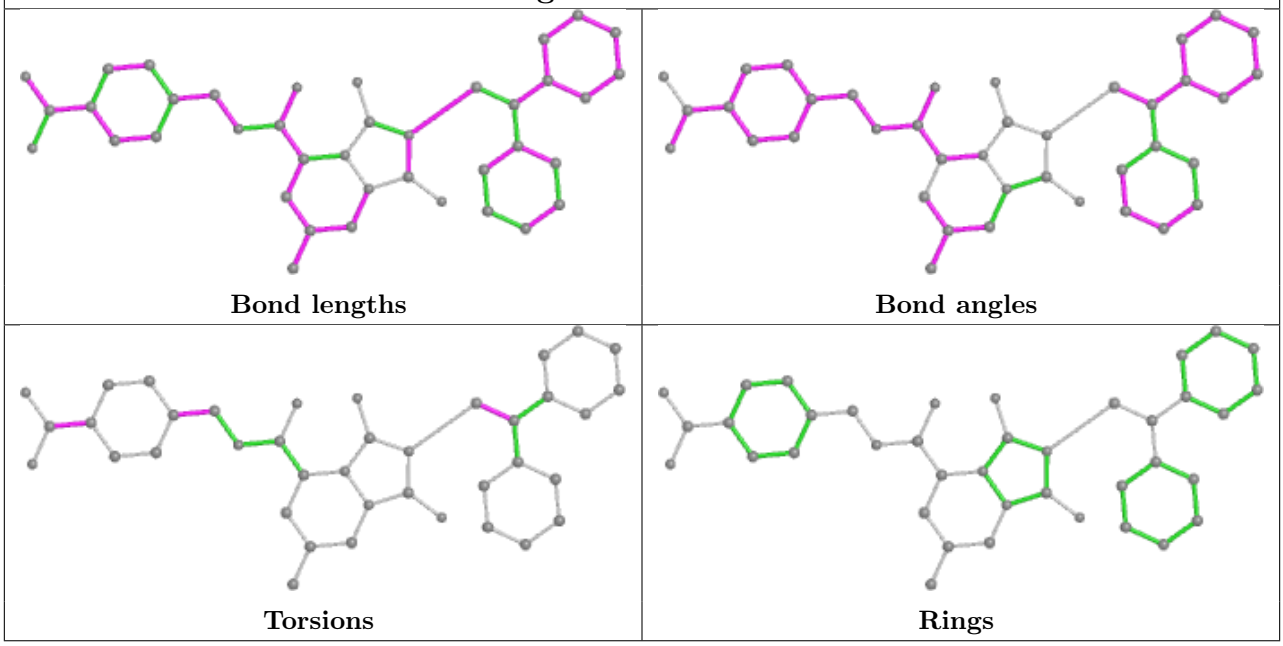
There are no ring outliers.

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand IH2 2 370



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.