



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2021 – 10:26 PM EDT

PDB ID : 1RV7
Title : Crystal structures of a Multidrug-Resistant HIV-1 Protease Reveal an Expanded Active Site Cavity
Authors : Logsdon, B.C.; Vickrey, J.F.; Martin, P.; Proteasa, G.; Koepke, J.I.; Terlecky, S.R.; Wawrzak, Z.; Winters, M.A.; Merigan, T.C.; Kovari, L.C.
Deposited on : 2003-12-12
Resolution : 2.70 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (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) : 2.23.2

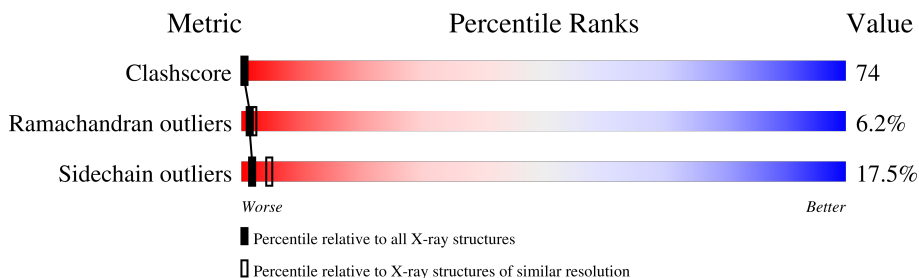
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	99	 9% 30% 43% 17%
1	B	99	 10% 29% 42% 18%

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
2	AB1	B	1001	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1592 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.

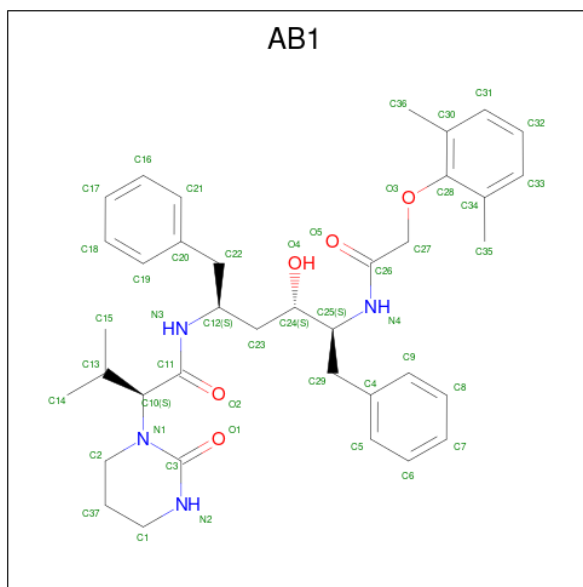
- Molecule 1 is a protein called protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	99	755	486	132	134	3	0	0	0
1	B	99	755	486	132	134	3	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	ASN	ASP	engineered mutation	UNP Q9QM22
A	36	VAL	MET	engineered mutation	UNP Q9QM22
A	84	VAL	ILE	engineered mutation	UNP Q9QM22
B	25	ASN	ASP	engineered mutation	UNP Q9QM22
B	36	VAL	MET	engineered mutation	UNP Q9QM22
B	84	VAL	ILE	engineered mutation	UNP Q9QM22

- Molecule 2 is N-{1-BENZYL-4-[2-(2,6-DIMETHYL-PHENOXY)-ACETYLAMINO]-3-HYDROXY-5-PHENYL-PENTYL}-3-METHYL-2-(2-OXO-TETRAHYDRO-PYRIMIDIN-1-YL)-BUTYRAMIDE (three-letter code: AB1) (formula: C₃₇H₄₈N₄O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	B	1	46	37	4	5	0	0

- Molecule 3 is water.

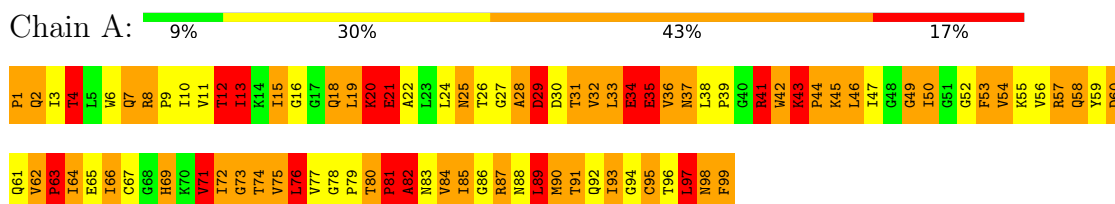
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	36	Total	O	0	0
			36	36		

3 Residue-property plots

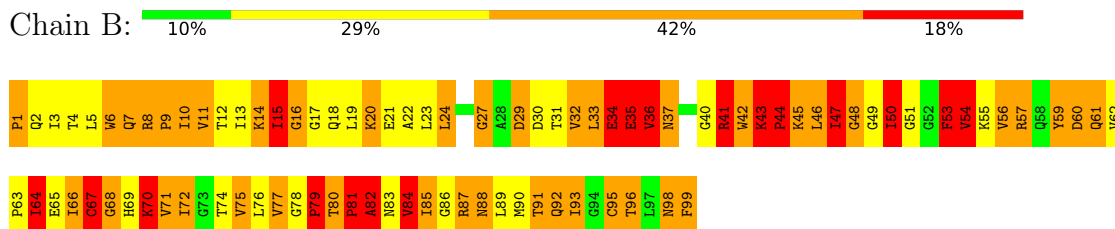
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



- Molecule 1: protease



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	44.98Å 44.98Å 103.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70	Depositor
% Data completeness (in resolution range)	97.3 (20.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.271 , 0.350	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	1592	wwPDB-VP
Average B, all atoms (Å ²)	41.0	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: AB1

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	4.01	134/769 (17.4%)	2.53	51/1044 (4.9%)
1	B	3.88	127/769 (16.5%)	2.44	47/1044 (4.5%)
All	All	3.94	261/1538 (17.0%)	2.49	98/2088 (4.7%)

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
1	B	0	3

All (261) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	21	GLU	CD-OE1	18.80	1.46	1.25
1	B	35	GLU	CD-OE1	18.48	1.46	1.25
1	B	42	TRP	CB-CG	-18.02	1.17	1.50
1	B	71	VAL	CB-CG2	17.70	1.90	1.52
1	A	34	GLU	CB-CG	16.81	1.84	1.52
1	A	34	GLU	CG-CD	15.86	1.75	1.51
1	A	7	GLN	CG-CD	15.37	1.86	1.51
1	A	35	GLU	C-O	15.14	1.52	1.23
1	A	35	GLU	CB-CG	14.01	1.78	1.52
1	B	34	GLU	CD-OE2	13.80	1.40	1.25
1	A	95	CYS	CB-SG	-13.58	1.59	1.82
1	A	36	VAL	CB-CG1	-13.20	1.25	1.52
1	B	41	ARG	NE-CZ	12.73	1.49	1.33
1	A	34	GLU	CD-OE2	12.55	1.39	1.25
1	A	35	GLU	CG-CD	12.44	1.70	1.51
1	A	35	GLU	CD-OE2	12.30	1.39	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	50	ILE	C-O	12.17	1.46	1.23
1	B	53	PHE	CE2-CZ	-12.14	1.14	1.37
1	B	53	PHE	CD1-CE1	-11.89	1.15	1.39
1	B	82	ALA	CA-CB	11.76	1.77	1.52
1	B	81	PRO	CA-C	11.65	1.76	1.52
1	B	1	PRO	CA-C	-11.47	1.29	1.52
1	A	8	ARG	C-O	11.30	1.44	1.23
1	B	57	ARG	C-O	-10.84	1.02	1.23
1	B	14	LYS	CE-NZ	10.75	1.75	1.49
1	A	34	GLU	CD-OE1	10.63	1.37	1.25
1	B	53	PHE	CD2-CE2	-10.62	1.18	1.39
1	A	35	GLU	CD-OE1	10.41	1.37	1.25
1	A	62	VAL	CB-CG2	-10.33	1.31	1.52
1	A	73	GLY	C-O	10.32	1.40	1.23
1	B	56	VAL	C-O	10.28	1.42	1.23
1	A	13	ILE	CB-CG2	-10.11	1.21	1.52
1	A	87	ARG	CB-CG	-10.09	1.25	1.52
1	B	78	GLY	C-O	10.05	1.39	1.23
1	B	20	LYS	CE-NZ	10.05	1.74	1.49
1	B	35	GLU	C-O	10.03	1.42	1.23
1	B	65	GLU	CD-OE2	10.03	1.36	1.25
1	A	89	LEU	C-O	-9.97	1.04	1.23
1	A	63	PRO	CG-CD	9.92	1.83	1.50
1	A	61	GLN	C-O	-9.84	1.04	1.23
1	B	59	TYR	C-O	-9.78	1.04	1.23
1	B	14	LYS	CD-CE	9.66	1.75	1.51
1	B	71	VAL	CB-CG1	9.63	1.73	1.52
1	A	29	ASP	CB-CG	-9.62	1.31	1.51
1	A	99	PHE	CE2-CZ	-9.57	1.19	1.37
1	A	56	VAL	C-O	9.55	1.41	1.23
1	B	80	THR	CA-CB	9.52	1.78	1.53
1	A	94	GLY	C-O	9.29	1.38	1.23
1	A	59	TYR	CG-CD2	9.26	1.51	1.39
1	B	59	TYR	CZ-OH	-9.23	1.22	1.37
1	A	98	ASN	C-O	9.21	1.40	1.23
1	A	29	ASP	CG-OD2	9.16	1.46	1.25
1	B	23	LEU	CG-CD2	-9.14	1.18	1.51
1	A	36	VAL	N-CA	8.94	1.64	1.46
1	A	78	GLY	N-CA	8.91	1.59	1.46
1	B	59	TYR	CB-CG	8.89	1.65	1.51
1	B	41	ARG	CG-CD	8.82	1.74	1.51
1	A	42	TRP	CB-CG	-8.79	1.34	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	6	TRP	CE3-CZ3	-8.76	1.23	1.38
1	B	66	ILE	C-O	-8.75	1.06	1.23
1	A	49	GLY	C-O	8.74	1.37	1.23
1	B	61	GLN	CB-CG	8.70	1.76	1.52
1	B	33	LEU	C-O	-8.61	1.06	1.23
1	A	69	HIS	C-O	-8.59	1.07	1.23
1	B	95	CYS	CB-SG	-8.57	1.67	1.82
1	B	48	GLY	C-O	8.54	1.37	1.23
1	A	1	PRO	CA-C	-8.49	1.35	1.52
1	B	99	PHE	CE2-CZ	-8.45	1.21	1.37
1	B	35	GLU	CG-CD	8.44	1.64	1.51
1	A	26	THR	CA-CB	-8.41	1.31	1.53
1	A	7	GLN	CD-NE2	8.39	1.53	1.32
1	A	71	VAL	CB-CG1	-8.39	1.35	1.52
1	B	20	LYS	CD-CE	8.37	1.72	1.51
1	B	1	PRO	CG-CD	8.31	1.78	1.50
1	A	6	TRP	CE2-CZ2	-8.30	1.25	1.39
1	B	72	ILE	C-O	8.29	1.39	1.23
1	B	20	LYS	C-O	-8.27	1.07	1.23
1	B	62	VAL	CB-CG1	8.24	1.70	1.52
1	B	78	GLY	CA-C	8.21	1.65	1.51
1	B	54	VAL	CB-CG2	-8.21	1.35	1.52
1	A	11	VAL	N-CA	-8.17	1.30	1.46
1	A	43	LYS	CD-CE	8.15	1.71	1.51
1	B	32	VAL	CA-CB	-8.11	1.37	1.54
1	A	11	VAL	CB-CG1	8.08	1.69	1.52
1	A	12	THR	CB-OG1	8.07	1.59	1.43
1	B	44	PRO	CA-C	8.06	1.69	1.52
1	B	61	GLN	C-O	-8.02	1.08	1.23
1	A	9	PRO	C-O	-8.01	1.07	1.23
1	A	60	ASP	CB-CG	7.98	1.68	1.51
1	B	6	TRP	CG-CD2	7.98	1.57	1.43
1	B	68	GLY	C-O	-7.92	1.10	1.23
1	B	19	LEU	N-CA	-7.86	1.30	1.46
1	A	60	ASP	N-CA	7.86	1.62	1.46
1	A	1	PRO	CG-CD	7.84	1.76	1.50
1	B	12	THR	N-CA	-7.68	1.30	1.46
1	A	53	PHE	CA-CB	7.64	1.70	1.53
1	B	41	ARG	CZ-NH2	7.61	1.43	1.33
1	B	90	MET	SD-CE	-7.51	1.35	1.77
1	A	49	GLY	N-CA	7.51	1.57	1.46
1	B	7	GLN	CD-OE1	7.50	1.40	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	56	VAL	CA-CB	7.48	1.70	1.54
1	A	99	PHE	CE1-CZ	7.46	1.51	1.37
1	B	64	ILE	CB-CG2	7.39	1.75	1.52
1	A	1	PRO	CB-CG	7.34	1.86	1.50
1	B	4	THR	N-CA	-7.34	1.31	1.46
1	A	42	TRP	CA-CB	-7.28	1.38	1.53
1	A	2	GLN	CG-CD	7.27	1.67	1.51
1	A	37	ASN	CG-OD1	7.25	1.40	1.24
1	A	44	PRO	CA-C	7.16	1.67	1.52
1	B	57	ARG	NE-CZ	-7.16	1.23	1.33
1	A	85	ILE	N-CA	7.06	1.60	1.46
1	A	37	ASN	CA-C	-7.04	1.34	1.52
1	B	50	ILE	N-CA	6.97	1.60	1.46
1	A	53	PHE	CG-CD2	6.93	1.49	1.38
1	B	84	VAL	CB-CG2	-6.92	1.38	1.52
1	B	62	VAL	CA-CB	6.85	1.69	1.54
1	A	80	THR	C-O	6.85	1.36	1.23
1	B	32	VAL	CB-CG1	6.80	1.67	1.52
1	A	90	MET	C-N	-6.76	1.18	1.34
1	A	59	TYR	CD1-CE1	-6.75	1.29	1.39
1	B	37	ASN	C-O	6.74	1.36	1.23
1	A	93	ILE	C-O	-6.74	1.10	1.23
1	B	35	GLU	CD-OE2	6.73	1.33	1.25
1	B	3	ILE	C-O	-6.69	1.10	1.23
1	A	15	ILE	CA-CB	-6.68	1.39	1.54
1	B	79	PRO	CB-CG	6.68	1.83	1.50
1	B	85	ILE	N-CA	6.65	1.59	1.46
1	A	31	THR	CA-C	-6.60	1.35	1.52
1	B	45	LYS	CD-CE	6.57	1.67	1.51
1	A	56	VAL	CB-CG1	-6.55	1.39	1.52
1	B	99	PHE	CE1-CZ	-6.54	1.25	1.37
1	A	74	THR	CA-C	6.47	1.69	1.52
1	B	87	ARG	CG-CD	-6.47	1.35	1.51
1	B	13	ILE	CB-CG2	-6.46	1.32	1.52
1	B	30	ASP	CB-CG	6.42	1.65	1.51
1	B	44	PRO	CB-CG	6.42	1.82	1.50
1	B	50	ILE	CA-CB	6.41	1.69	1.54
1	A	85	ILE	C-N	-6.41	1.21	1.33
1	A	9	PRO	CB-CG	-6.36	1.18	1.50
1	A	59	TYR	CE1-CZ	6.36	1.46	1.38
1	A	27	GLY	CA-C	6.35	1.62	1.51
1	B	87	ARG	CA-C	-6.35	1.36	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1	PRO	C-O	-6.34	1.10	1.23
1	A	59	TYR	CB-CG	6.31	1.61	1.51
1	A	19	LEU	CG-CD1	-6.30	1.28	1.51
1	B	82	ALA	C-O	6.28	1.35	1.23
1	A	79	PRO	CA-C	-6.28	1.40	1.52
1	B	43	LYS	N-CA	-6.24	1.33	1.46
1	A	3	ILE	CB-CG2	6.21	1.72	1.52
1	B	92	GLN	C-O	-6.19	1.11	1.23
1	B	93	ILE	CA-CB	6.19	1.69	1.54
1	A	66	ILE	CA-CB	6.15	1.69	1.54
1	A	74	THR	CB-CG2	-6.15	1.32	1.52
1	A	84	VAL	CA-CB	-6.13	1.41	1.54
1	A	7	GLN	C-O	6.13	1.35	1.23
1	A	99	PHE	CD2-CE2	6.12	1.51	1.39
1	A	77	VAL	CB-CG1	-6.11	1.40	1.52
1	A	32	VAL	CB-CG1	-6.10	1.40	1.52
1	A	18	GLN	CG-CD	6.09	1.65	1.51
1	A	86	GLY	C-O	-6.09	1.14	1.23
1	B	83	ASN	CG-OD1	6.09	1.37	1.24
1	B	99	PHE	CG-CD1	-6.08	1.29	1.38
1	B	75	VAL	CB-CG1	6.08	1.65	1.52
1	B	34	GLU	CG-CD	6.06	1.61	1.51
1	B	42	TRP	CA-CB	-6.06	1.40	1.53
1	A	65	GLU	CD-OE2	6.05	1.32	1.25
1	A	79	PRO	CG-CD	6.05	1.70	1.50
1	A	49	GLY	CA-C	6.04	1.61	1.51
1	A	32	VAL	N-CA	6.04	1.58	1.46
1	B	98	ASN	C-O	6.02	1.34	1.23
1	B	27	GLY	C-O	-6.01	1.14	1.23
1	A	41	ARG	CZ-NH2	6.00	1.40	1.33
1	A	92	GLN	C-O	-6.00	1.11	1.23
1	B	59	TYR	CA-CB	-5.99	1.40	1.53
1	B	68	GLY	N-CA	5.99	1.55	1.46
1	A	62	VAL	C-N	-5.98	1.22	1.34
1	B	42	TRP	CG-CD1	-5.98	1.28	1.36
1	A	54	VAL	C-O	-5.97	1.12	1.23
1	A	81	PRO	C-O	5.97	1.35	1.23
1	A	39	PRO	CG-CD	5.96	1.70	1.50
1	B	48	GLY	C-N	5.93	1.43	1.33
1	B	50	ILE	C-O	5.89	1.34	1.23
1	B	64	ILE	CG1-CD1	5.87	1.91	1.50
1	B	14	LYS	CG-CD	5.86	1.72	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	53	PHE	CD2-CE2	-5.86	1.27	1.39
1	A	28	ALA	C-O	-5.86	1.12	1.23
1	A	16	GLY	C-N	5.85	1.43	1.33
1	B	13	ILE	CA-CB	-5.84	1.41	1.54
1	A	6	TRP	N-CA	-5.82	1.34	1.46
1	B	16	GLY	CA-C	5.81	1.61	1.51
1	B	50	ILE	CB-CG2	5.81	1.70	1.52
1	A	99	PHE	C-OXT	5.79	1.34	1.23
1	B	87	ARG	C-O	-5.79	1.12	1.23
1	B	88	ASN	C-N	-5.76	1.20	1.34
1	A	25	ASN	N-CA	5.75	1.57	1.46
1	B	93	ILE	C-O	5.74	1.34	1.23
1	A	45	LYS	CB-CG	-5.71	1.37	1.52
1	B	29	ASP	CB-CG	5.71	1.63	1.51
1	A	38	LEU	CG-CD2	5.68	1.72	1.51
1	B	46	LEU	CG-CD1	-5.66	1.30	1.51
1	B	53	PHE	CB-CG	5.66	1.60	1.51
1	B	9	PRO	N-CA	-5.65	1.37	1.47
1	A	82	ALA	N-CA	-5.63	1.35	1.46
1	B	37	ASN	N-CA	5.63	1.57	1.46
1	B	30	ASP	CG-OD1	5.63	1.38	1.25
1	A	35	GLU	C-N	5.62	1.47	1.34
1	B	90	MET	C-O	-5.60	1.12	1.23
1	A	4	THR	CA-CB	-5.59	1.38	1.53
1	B	50	ILE	CG1-CD1	5.58	1.89	1.50
1	A	2	GLN	CA-CB	-5.57	1.41	1.53
1	B	42	TRP	CD2-CE3	5.57	1.48	1.40
1	A	57	ARG	C-O	-5.54	1.12	1.23
1	B	75	VAL	N-CA	-5.54	1.35	1.46
1	A	58	GLN	CG-CD	5.54	1.63	1.51
1	B	42	TRP	CE2-CZ2	5.53	1.49	1.39
1	A	20	LYS	CG-CD	-5.53	1.33	1.52
1	A	39	PRO	CB-CG	-5.51	1.22	1.50
1	B	91	THR	CB-CG2	-5.50	1.34	1.52
1	A	16	GLY	CA-C	5.47	1.60	1.51
1	A	8	ARG	CZ-NH1	5.47	1.40	1.33
1	A	77	VAL	C-O	5.46	1.33	1.23
1	B	54	VAL	CA-C	-5.46	1.38	1.52
1	A	82	ALA	C-N	5.43	1.46	1.34
1	B	11	VAL	CB-CG2	5.41	1.64	1.52
1	A	29	ASP	N-CA	-5.39	1.35	1.46
1	B	53	PHE	CG-CD1	-5.39	1.30	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	3	ILE	CB-CG2	-5.38	1.36	1.52
1	B	8	ARG	N-CA	-5.36	1.35	1.46
1	B	67	CYS	CA-C	-5.35	1.39	1.52
1	A	61	GLN	CA-C	-5.32	1.39	1.52
1	A	90	MET	CG-SD	5.32	1.95	1.81
1	B	60	ASP	C-O	-5.32	1.13	1.23
1	A	32	VAL	CA-CB	-5.32	1.43	1.54
1	A	71	VAL	CB-CG2	-5.30	1.41	1.52
1	A	55	LYS	C-O	5.30	1.33	1.23
1	A	76	LEU	N-CA	5.30	1.56	1.46
1	A	77	VAL	C-N	5.28	1.42	1.33
1	A	42	TRP	CG-CD2	-5.22	1.34	1.43
1	B	24	LEU	CA-CB	-5.21	1.41	1.53
1	A	50	ILE	CA-CB	5.18	1.66	1.54
1	A	74	THR	N-CA	5.16	1.56	1.46
1	B	99	PHE	C-OXT	5.15	1.33	1.23
1	B	70	LYS	CG-CD	5.15	1.70	1.52
1	A	74	THR	CB-OG1	-5.14	1.32	1.43
1	B	62	VAL	N-CA	-5.14	1.36	1.46
1	A	7	GLN	CD-OE1	5.14	1.35	1.24
1	A	75	VAL	CB-CG1	5.13	1.63	1.52
1	B	51	GLY	N-CA	5.13	1.53	1.46
1	B	93	ILE	N-CA	5.12	1.56	1.46
1	A	60	ASP	C-O	-5.09	1.13	1.23
1	A	10	ILE	CB-CG2	-5.08	1.37	1.52
1	B	55	LYS	CE-NZ	5.08	1.61	1.49
1	B	2	GLN	CD-OE1	-5.08	1.12	1.24
1	A	53	PHE	CE1-CZ	-5.07	1.27	1.37
1	A	81	PRO	CA-C	5.04	1.62	1.52
1	A	33	LEU	CG-CD2	5.04	1.70	1.51
1	A	93	ILE	CA-CB	5.04	1.66	1.54
1	B	10	ILE	CB-CG2	-5.03	1.37	1.52
1	B	40	GLY	CA-C	-5.02	1.43	1.51
1	B	79	PRO	CG-CD	5.02	1.67	1.50
1	B	20	LYS	N-CA	-5.00	1.36	1.46

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	60	ASP	CB-CG-OD2	13.81	130.73	118.30
1	A	29	ASP	CB-CG-OD1	-12.86	106.72	118.30
1	A	8	ARG	NE-CZ-NH2	-12.57	114.01	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	71	VAL	CG1-CB-CG2	11.07	128.61	110.90
1	A	76	LEU	CB-CG-CD1	-10.30	93.49	111.00
1	B	87	ARG	NE-CZ-NH2	-10.05	115.27	120.30
1	B	19	LEU	CB-CG-CD1	9.63	127.37	111.00
1	A	8	ARG	NE-CZ-NH1	8.98	124.79	120.30
1	B	8	ARG	NE-CZ-NH2	-8.90	115.85	120.30
1	A	89	LEU	CB-CG-CD2	8.85	126.05	111.00
1	A	59	TYR	CZ-CE2-CD2	-8.83	111.86	119.80
1	B	41	ARG	NE-CZ-NH2	8.75	124.67	120.30
1	A	21	GLU	CG-CD-OE2	-8.56	101.17	118.30
1	A	96	THR	CA-CB-CG2	-8.05	101.13	112.40
1	B	86	GLY	CA-C-O	-7.85	106.48	120.60
1	B	57	ARG	NE-CZ-NH1	-7.80	116.40	120.30
1	A	64	ILE	CG1-CB-CG2	-7.70	94.47	111.40
1	B	59	TYR	CZ-CE2-CD2	-7.61	112.95	119.80
1	A	87	ARG	NE-CZ-NH2	-7.52	116.54	120.30
1	B	47	ILE	CG1-CB-CG2	-7.33	95.28	111.40
1	B	34	GLU	CG-CD-OE2	7.26	132.83	118.30
1	B	41	ARG	NH1-CZ-NH2	-7.21	111.47	119.40
1	A	37	ASN	CB-CA-C	-7.19	96.01	110.40
1	B	41	ARG	NE-CZ-NH1	7.09	123.84	120.30
1	A	76	LEU	CB-CG-CD2	6.94	122.80	111.00
1	B	63	PRO	N-CD-CG	6.92	113.58	103.20
1	A	41	ARG	NE-CZ-NH2	6.85	123.73	120.30
1	A	60	ASP	CB-CG-OD2	6.84	124.46	118.30
1	B	35	GLU	CG-CD-OE2	-6.76	104.79	118.30
1	A	21	GLU	OE1-CD-OE2	6.74	131.39	123.30
1	B	12	THR	OG1-CB-CG2	-6.66	94.69	110.00
1	A	42	TRP	CD1-NE1-CE2	-6.63	103.03	109.00
1	A	34	GLU	OE1-CD-OE2	-6.61	115.36	123.30
1	A	43	LYS	CD-CE-NZ	6.61	126.90	111.70
1	A	57	ARG	NE-CZ-NH2	6.58	123.59	120.30
1	B	65	GLU	N-CA-CB	-6.43	99.03	110.60
1	B	19	LEU	CB-CG-CD2	-6.40	100.12	111.00
1	B	34	GLU	CG-CD-OE1	-6.39	105.51	118.30
1	A	19	LEU	CB-CG-CD2	6.22	121.58	111.00
1	A	53	PHE	CA-C-O	-6.21	107.07	120.10
1	A	53	PHE	N-CA-CB	6.10	121.58	110.60
1	A	4	THR	CA-CB-CG2	-6.08	103.88	112.40
1	B	66	ILE	CB-CA-C	-6.08	99.44	111.60
1	B	77	VAL	C-N-CA	6.08	135.06	122.30
1	A	33	LEU	CB-CG-CD2	6.05	121.29	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	82	ALA	N-CA-CB	-6.04	101.64	110.10
1	A	62	VAL	CB-CA-C	-6.03	99.95	111.40
1	A	36	VAL	C-N-CA	-6.03	106.63	121.70
1	A	57	ARG	NH1-CZ-NH2	-5.99	112.81	119.40
1	A	29	ASP	OD1-CG-OD2	5.95	134.61	123.30
1	B	60	ASP	OD1-CG-OD2	-5.90	112.09	123.30
1	B	95	CYS	N-CA-CB	-5.88	100.01	110.60
1	A	35	GLU	N-CA-C	-5.84	95.22	111.00
1	A	77	VAL	N-CA-C	5.83	126.73	111.00
1	A	24	LEU	CB-CG-CD1	5.81	120.88	111.00
1	B	33	LEU	CB-CG-CD1	5.81	120.88	111.00
1	B	99	PHE	CB-CG-CD2	5.79	124.85	120.80
1	A	24	LEU	CB-CG-CD2	-5.78	101.17	111.00
1	B	7	GLN	CA-CB-CG	-5.78	100.69	113.40
1	A	12	THR	CA-CB-CG2	-5.76	104.34	112.40
1	B	35	GLU	OE1-CD-OE2	5.74	130.19	123.30
1	B	50	ILE	CG1-CB-CG2	5.73	124.01	111.40
1	B	36	VAL	CA-CB-CG1	5.71	119.47	110.90
1	B	70	LYS	CD-CE-NZ	-5.69	98.61	111.70
1	B	48	GLY	O-C-N	5.59	132.71	123.20
1	A	50	ILE	CA-C-N	-5.59	105.01	116.20
1	B	59	TYR	CA-C-N	5.55	129.41	117.20
1	B	79	PRO	N-CA-C	5.55	126.52	112.10
1	B	90	MET	CG-SD-CE	-5.52	91.37	100.20
1	A	72	ILE	CG1-CB-CG2	-5.48	99.35	111.40
1	A	49	GLY	CA-C-O	5.46	130.43	120.60
1	B	15	ILE	C-N-CA	-5.39	110.97	122.30
1	B	59	TYR	CB-CG-CD1	5.36	124.22	121.00
1	A	30	ASP	CB-CA-C	-5.30	99.80	110.40
1	A	91	THR	OG1-CB-CG2	-5.30	97.81	110.00
1	A	24	LEU	CA-CB-CG	5.24	127.34	115.30
1	B	45	LYS	CB-CA-C	5.24	120.87	110.40
1	A	46	LEU	CD1-CG-CD2	-5.23	94.82	110.50
1	A	85	ILE	C-N-CA	-5.20	111.37	122.30
1	B	37	ASN	CB-CA-C	-5.20	100.00	110.40
1	A	57	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	B	77	VAL	CA-CB-CG2	5.17	118.66	110.90
1	B	24	LEU	N-CA-CB	-5.16	100.07	110.40
1	A	3	ILE	CG1-CB-CG2	-5.14	100.09	111.40
1	B	96	THR	O-C-N	5.12	130.90	122.70
1	A	34	GLU	N-CA-C	-5.11	97.21	111.00
1	A	97	LEU	CB-CG-CD1	5.10	119.67	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	GLU	O-C-N	5.07	130.81	122.70
1	A	80	THR	OG1-CB-CG2	-5.07	98.34	110.00
1	A	3	ILE	CA-CB-CG1	5.07	120.62	111.00
1	B	32	VAL	CB-CA-C	-5.06	101.78	111.40
1	B	59	TYR	CG-CD2-CE2	5.06	125.35	121.30
1	A	53	PHE	CB-CG-CD2	5.05	124.33	120.80
1	A	12	THR	N-CA-C	-5.05	97.37	111.00
1	B	1	PRO	CB-CA-C	-5.05	99.38	112.00
1	B	76	LEU	CB-CG-CD1	-5.02	102.46	111.00
1	B	8	ARG	NH1-CZ-NH2	5.01	124.91	119.40
1	B	43	LYS	CD-CE-NZ	5.01	123.21	111.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	43	LYS	Mainchain
1	B	59	TYR	Sidechain
1	B	81	PRO	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	755	0	798	115	0
1	B	755	0	799	137	2
2	B	46	0	47	25	0
3	A	36	0	0	0	2
All	All	1592	0	1644	236	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 74.

All (236) 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:A:1:PRO:CG	1:A:1:PRO:CD	1.76	1.61
1:B:64:ILE:CB	1:B:64:ILE:CG2	1.75	1.59
1:B:82:ALA:CB	1:B:82:ALA:CA	1.77	1.57
1:B:14:LYS:CE	1:B:14:LYS:CD	1.75	1.56
1:B:80:THR:CB	1:B:80:THR:CA	1.78	1.55
1:A:35:GLU:CB	1:A:35:GLU:CG	1.78	1.55
1:B:61:GLN:CB	1:B:61:GLN:CG	1.76	1.55
1:B:81:PRO:C	1:B:81:PRO:CA	1.76	1.53
1:A:1:PRO:CG	1:A:1:PRO:CB	1.86	1.52
1:A:34:GLU:CD	1:A:34:GLU:CG	1.75	1.52
1:B:50:ILE:CD1	1:B:50:ILE:CG1	1.89	1.51
1:A:34:GLU:CG	1:A:34:GLU:CB	1.84	1.51
1:B:20:LYS:CE	1:B:20:LYS:NZ	1.74	1.50
1:B:64:ILE:CD1	1:B:64:ILE:CG1	1.90	1.49
1:B:71:VAL:CB	1:B:71:VAL:CG2	1.90	1.48
1:B:14:LYS:CE	1:B:14:LYS:NZ	1.75	1.47
1:B:79:PRO:CB	1:B:79:PRO:CG	1.83	1.47
1:A:63:PRO:CD	1:A:63:PRO:CG	1.83	1.46
1:B:1:PRO:CD	1:B:1:PRO:CG	1.78	1.44
1:A:7:GLN:CD	1:A:7:GLN:CG	1.86	1.44
1:B:44:PRO:CG	1:B:44:PRO:CB	1.82	1.36
1:B:49:GLY:O	1:B:50:ILE:HG23	1.29	1.26
1:B:15:ILE:HD13	1:B:16:GLY:N	1.49	1.25
1:B:81:PRO:HG2	2:B:1001:AB1:C37	1.87	1.03
1:B:82:ALA:HB3	2:B:1001:AB1:C1	1.87	1.03
1:B:81:PRO:CG	2:B:1001:AB1:H6	1.92	0.98
1:A:95:CYS:HA	1:B:98:ASN:O	1.63	0.97
1:B:49:GLY:O	1:B:50:ILE:CG2	2.13	0.95
1:B:80:THR:HG23	1:B:82:ALA:O	1.68	0.94
1:A:34:GLU:HA	1:A:80:THR:HG22	1.50	0.90
1:B:81:PRO:HG2	2:B:1001:AB1:H6	0.96	0.90
1:A:58:GLN:NE2	1:A:60:ASP:OD1	2.06	0.89
1:B:82:ALA:HB3	2:B:1001:AB1:C37	2.02	0.88
1:B:82:ALA:HB3	2:B:1001:AB1:H3	1.55	0.88
1:B:82:ALA:HB3	2:B:1001:AB1:H7	1.54	0.88
1:A:80:THR:OG1	2:B:1001:AB1:H43	1.73	0.88
1:B:34:GLU:O	1:B:35:GLU:O	1.92	0.86
1:B:15:ILE:HD13	1:B:16:GLY:H	1.40	0.84
1:A:99:PHE:OXT	1:B:1:PRO:HD2	1.80	0.82
1:A:87:ARG:O	1:A:91:THR:HG23	1.82	0.80
1:A:73:GLY:O	1:A:75:VAL:HG23	1.83	0.79
1:A:98:ASN:HD22	1:B:98:ASN:CG	1.85	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:ILE:HG23	1:A:15:ILE:O	1.81	0.78
1:A:34:GLU:HG3	1:A:35:GLU:O	1.83	0.78
1:A:25:ASN:HB3	1:A:28:ALA:HB3	1.65	0.78
1:B:29:ASP:OD1	1:B:87:ARG:NH2	2.17	0.78
1:B:82:ALA:CB	2:B:1001:AB1:H3	2.15	0.76
1:B:64:ILE:CG2	1:B:64:ILE:CG1	2.63	0.76
1:A:20:LYS:HE3	1:A:36:VAL:HG21	1.66	0.75
1:B:20:LYS:HZ1	1:B:36:VAL:HB	1.51	0.74
1:B:32:VAL:H	1:B:84:VAL:HG12	1.51	0.74
1:B:35:GLU:CD	1:B:57:ARG:HH12	1.90	0.73
1:B:15:ILE:HD13	1:B:15:ILE:C	2.09	0.72
1:B:82:ALA:CB	2:B:1001:AB1:H7	2.19	0.72
1:A:15:ILE:O	1:A:15:ILE:CG2	2.38	0.71
1:B:61:GLN:CB	1:B:61:GLN:CD	2.58	0.70
1:B:15:ILE:CD1	1:B:16:GLY:N	2.42	0.70
1:A:20:LYS:CE	1:A:36:VAL:HG21	2.22	0.70
1:A:35:GLU:CG	1:A:35:GLU:H	2.06	0.68
1:B:5:LEU:C	1:B:7:GLN:H	1.97	0.68
1:A:35:GLU:CG	1:A:35:GLU:CA	2.70	0.68
1:A:98:ASN:HD22	1:B:98:ASN:ND2	1.92	0.68
1:B:71:VAL:CG2	1:B:71:VAL:CA	2.72	0.68
1:A:15:ILE:HD13	1:A:33:LEU:HD22	1.76	0.68
1:A:80:THR:HG23	1:A:80:THR:O	1.93	0.67
1:B:80:THR:CG2	1:B:82:ALA:O	2.42	0.67
1:B:47:ILE:HD11	1:B:56:VAL:HG21	1.77	0.66
1:A:19:LEU:HD12	1:A:19:LEU:N	2.09	0.66
1:B:47:ILE:HD11	1:B:56:VAL:CG2	2.26	0.66
1:B:61:GLN:CG	1:B:61:GLN:CA	2.71	0.65
1:B:82:ALA:CA	2:B:1001:AB1:H3	2.27	0.65
1:A:67:CYS:C	1:A:69:HIS:H	1.99	0.65
1:B:46:LEU:N	1:B:46:LEU:HD12	2.12	0.65
2:B:1001:AB1:H16	2:B:1001:AB1:O5	1.97	0.65
1:A:25:ASN:OD1	1:B:27:GLY:HA3	1.97	0.65
1:A:63:PRO:N	1:A:72:ILE:HG13	2.12	0.65
1:A:34:GLU:HA	1:A:80:THR:CG2	2.24	0.64
1:B:20:LYS:NZ	1:B:36:VAL:HB	2.11	0.64
1:B:70:LYS:HB3	1:B:70:LYS:HZ2	1.61	0.64
1:A:8:ARG:HG3	1:B:87:ARG:NH2	2.13	0.64
1:B:35:GLU:OE1	1:B:57:ARG:NH1	2.30	0.64
1:A:1:PRO:CG	1:A:1:PRO:CA	2.74	0.63
1:B:80:THR:CA	1:B:80:THR:HB	2.15	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:ILE:C	1:B:64:ILE:HD13	2.20	0.63
1:A:81:PRO:O	1:A:82:ALA:HB2	1.98	0.62
1:B:70:LYS:HZ2	1:B:70:LYS:CB	2.09	0.62
1:A:2:GLN:HG3	1:B:98:ASN:OD1	1.98	0.62
1:A:98:ASN:O	1:B:95:CYS:HA	2.00	0.62
1:A:42:TRP:HE3	1:A:43:LYS:N	1.98	0.61
1:B:16:GLY:C	1:B:18:GLN:H	2.03	0.61
1:B:71:VAL:HG22	1:B:72:ILE:H	1.64	0.61
1:B:43:LYS:HE3	1:B:60:ASP:OD2	2.01	0.61
1:B:84:VAL:CG2	2:B:1001:AB1:O1	2.50	0.60
1:A:35:GLU:CG	1:A:35:GLU:N	2.64	0.60
1:A:66:ILE:O	1:A:69:HIS:HB2	2.01	0.60
1:B:47:ILE:N	1:B:47:ILE:HD13	2.16	0.60
1:B:66:ILE:O	1:B:68:GLY:N	2.35	0.59
1:A:1:PRO:HD2	1:B:99:PHE:OXT	2.03	0.59
1:A:49:GLY:HA2	1:A:52:GLY:O	2.02	0.58
1:B:54:VAL:HG23	1:B:54:VAL:O	2.02	0.58
1:B:81:PRO:CA	1:B:82:ALA:N	2.62	0.57
1:A:42:TRP:CE3	1:A:42:TRP:C	2.77	0.57
1:A:15:ILE:HD12	1:A:64:ILE:HG23	1.86	0.57
1:B:84:VAL:HG21	2:B:1001:AB1:O1	2.04	0.57
1:A:7:GLN:OE1	1:A:7:GLN:N	2.38	0.57
1:B:45:LYS:C	1:B:46:LEU:HD12	2.24	0.57
1:A:72:ILE:O	1:A:72:ILE:HG23	2.03	0.57
1:B:53:PHE:CD1	1:B:53:PHE:N	2.72	0.56
1:A:49:GLY:HA3	1:A:53:PHE:CD1	2.41	0.56
1:A:63:PRO:C	1:A:64:ILE:HG13	2.26	0.56
1:B:80:THR:CA	1:B:80:THR:CG2	2.74	0.55
1:A:42:TRP:HE3	1:A:43:LYS:CA	2.19	0.55
2:B:1001:AB1:C14	2:B:1001:AB1:H34	2.37	0.55
1:B:34:GLU:OE2	1:B:79:PRO:HA	2.06	0.55
1:A:62:VAL:C	1:A:72:ILE:HG13	2.27	0.55
1:A:72:ILE:O	1:A:72:ILE:CG2	2.55	0.55
1:B:64:ILE:HD11	1:B:66:ILE:HG12	1.89	0.55
1:B:98:ASN:ND2	1:B:98:ASN:N	2.53	0.55
1:A:42:TRP:HZ3	1:A:44:PRO:HD3	1.72	0.54
1:A:22:ALA:HB1	1:A:85:ILE:HG13	1.89	0.54
1:B:15:ILE:C	1:B:15:ILE:CD1	2.75	0.54
1:B:88:ASN:O	1:B:92:GLN:HG2	2.08	0.54
1:A:49:GLY:HA3	1:A:53:PHE:CE1	2.43	0.54
1:A:7:GLN:CD	1:A:7:GLN:CB	2.70	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:PRO:HB2	1:B:24:LEU:HB2	1.90	0.53
1:B:81:PRO:HG2	2:B:1001:AB1:C1	2.37	0.53
1:A:34:GLU:CG	1:A:35:GLU:O	2.54	0.53
1:A:45:LYS:HG2	1:A:76:LEU:HD22	1.89	0.53
1:A:35:GLU:H	1:A:35:GLU:HG2	1.73	0.52
1:B:66:ILE:O	1:B:67:CYS:C	2.47	0.52
1:B:81:PRO:C	1:B:81:PRO:CB	2.73	0.52
1:B:64:ILE:CG2	1:B:64:ILE:CA	2.82	0.52
1:B:82:ALA:HB3	2:B:1001:AB1:N2	2.24	0.52
1:A:4:THR:HA	1:B:96:THR:HG22	1.93	0.51
1:A:99:PHE:CE2	1:B:1:PRO:HG2	2.45	0.51
1:A:33:LEU:C	1:A:34:GLU:O	2.41	0.51
1:B:8:ARG:O	1:B:10:ILE:N	2.43	0.51
1:A:98:ASN:HB2	1:B:98:ASN:ND2	2.26	0.51
1:B:87:ARG:O	1:B:91:THR:HG23	2.11	0.50
1:B:66:ILE:C	1:B:68:GLY:N	2.63	0.50
1:A:93:ILE:HD11	1:A:95:CYS:HB2	1.94	0.50
1:A:29:ASP:OD1	1:A:29:ASP:C	2.46	0.50
1:A:98:ASN:ND2	1:B:98:ASN:ND2	2.58	0.50
1:B:47:ILE:HG12	1:B:54:VAL:CG2	2.42	0.50
1:A:41:ARG:HG3	1:A:42:TRP:N	2.26	0.50
1:A:12:THR:OG1	1:A:21:GLU:OE1	2.26	0.50
1:A:50:ILE:HG13	2:B:1001:AB1:H20	1.93	0.50
1:B:16:GLY:C	1:B:18:GLN:N	2.65	0.50
1:A:82:ALA:O	2:B:1001:AB1:H42	2.11	0.49
1:A:36:VAL:CG1	1:A:37:ASN:N	2.75	0.49
1:B:5:LEU:C	1:B:7:GLN:N	2.59	0.49
1:A:21:GLU:OE1	1:A:21:GLU:HA	2.13	0.49
1:A:1:PRO:CG	1:A:1:PRO:N	2.69	0.49
1:B:35:GLU:HA	1:B:77:VAL:CG1	2.43	0.49
1:A:80:THR:C	1:A:82:ALA:H	2.17	0.48
1:B:15:ILE:HD13	1:B:16:GLY:CA	2.40	0.48
1:B:20:LYS:NZ	1:B:20:LYS:CD	2.71	0.48
1:A:93:ILE:HD12	1:B:99:PHE:CD2	2.49	0.48
1:A:60:ASP:HA	1:A:74:THR:HA	1.97	0.47
1:A:99:PHE:OXT	1:B:1:PRO:CD	2.58	0.47
1:B:98:ASN:O	1:B:99:PHE:HB3	2.14	0.47
1:B:64:ILE:CB	1:B:64:ILE:CD1	2.87	0.47
1:A:43:LYS:HB2	1:A:43:LYS:NZ	2.29	0.47
1:A:49:GLY:CA	1:A:52:GLY:O	2.63	0.47
1:A:87:ARG:HD2	1:B:5:LEU:HB3	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:PHE:HD2	1:B:69:HIS:CE1	2.32	0.47
1:B:47:ILE:O	1:B:48:GLY:O	2.31	0.47
1:B:82:ALA:N	2:B:1001:AB1:H3	2.30	0.47
1:B:88:ASN:ND2	1:B:89:LEU:HG	2.29	0.47
1:A:25:ASN:HB3	1:A:28:ALA:CB	2.40	0.47
1:A:18:GLN:C	1:A:19:LEU:HD12	2.35	0.46
1:A:35:GLU:O	1:A:36:VAL:HG23	2.15	0.46
1:B:80:THR:CB	1:B:80:THR:C	2.75	0.46
1:B:80:THR:CB	1:B:80:THR:HA	2.20	0.46
1:A:67:CYS:C	1:A:69:HIS:N	2.66	0.46
1:A:43:LYS:O	1:A:58:GLN:HB3	2.15	0.45
1:B:47:ILE:CD1	1:B:56:VAL:CG2	2.94	0.45
1:A:97:LEU:HD22	1:B:5:LEU:HD21	1.98	0.45
1:A:89:LEU:HD13	1:A:89:LEU:HA	1.81	0.45
1:B:53:PHE:H	1:B:53:PHE:HD1	1.65	0.45
1:B:71:VAL:CG2	1:B:71:VAL:HB	2.24	0.45
1:A:49:GLY:HA2	1:A:52:GLY:C	2.37	0.45
1:A:19:LEU:N	1:A:19:LEU:CD1	2.77	0.44
1:A:80:THR:OG1	1:A:82:ALA:O	2.34	0.44
1:A:34:GLU:CA	1:A:80:THR:CG2	2.93	0.44
1:B:47:ILE:HB	1:B:48:GLY:H	1.67	0.44
1:B:80:THR:CB	1:B:80:THR:N	2.68	0.44
1:B:81:PRO:CD	2:B:1001:AB1:H21	2.48	0.44
1:B:36:VAL:HG13	1:B:36:VAL:O	2.18	0.44
1:A:34:GLU:CG	1:A:34:GLU:C	2.86	0.44
1:A:35:GLU:N	1:A:35:GLU:HG2	2.31	0.44
1:A:72:ILE:HG21	1:A:72:ILE:HD13	1.67	0.44
1:B:11:VAL:HB	1:B:67:CYS:SG	2.57	0.43
1:B:46:LEU:N	1:B:46:LEU:CD1	2.79	0.43
1:A:42:TRP:CE3	1:A:43:LYS:CA	3.00	0.43
1:A:87:ARG:CD	1:B:5:LEU:HB3	2.48	0.43
1:B:47:ILE:HG23	1:B:47:ILE:HD12	1.34	0.43
1:B:47:ILE:HG12	1:B:54:VAL:HG21	2.01	0.43
1:A:13:ILE:O	1:A:13:ILE:CG1	2.64	0.43
1:A:42:TRP:C	1:A:42:TRP:CD2	2.88	0.43
1:A:62:VAL:HA	1:A:63:PRO:HD2	1.79	0.43
1:B:82:ALA:CB	1:B:82:ALA:C	2.79	0.43
1:B:66:ILE:C	1:B:68:GLY:H	2.23	0.42
1:B:47:ILE:HD11	1:B:56:VAL:HG22	1.99	0.42
1:A:33:LEU:HD12	1:A:33:LEU:N	2.34	0.42
1:A:46:LEU:HD22	1:A:53:PHE:HB2	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:ILE:HG13	1:B:93:ILE:HG21	2.01	0.42
1:A:64:ILE:HD11	1:A:75:VAL:CG2	2.50	0.42
1:A:88:ASN:ND2	1:A:89:LEU:HD22	2.35	0.42
1:B:60:ASP:O	1:B:61:GLN:C	2.50	0.42
1:A:34:GLU:CA	1:A:80:THR:HG22	2.35	0.42
1:A:42:TRP:CE3	1:A:43:LYS:N	2.81	0.42
1:B:31:THR:HG23	1:B:84:VAL:O	2.19	0.42
2:B:1001:AB1:H10	2:B:1001:AB1:H4	1.71	0.42
1:A:42:TRP:CE2	1:A:57:ARG:HD2	2.55	0.41
1:B:34:GLU:C	1:B:35:GLU:O	2.58	0.41
1:B:64:ILE:CD1	1:B:64:ILE:C	2.89	0.41
1:B:15:ILE:HG12	1:B:64:ILE:HB	2.01	0.41
1:A:4:THR:H	1:A:4:THR:HG23	1.32	0.41
1:B:41:ARG:CZ	1:B:41:ARG:HB3	2.50	0.41
1:B:47:ILE:CD1	1:B:56:VAL:HG22	2.50	0.41
1:B:84:VAL:HG23	2:B:1001:AB1:O1	2.19	0.41
1:A:36:VAL:HG12	1:A:37:ASN:N	2.36	0.41
1:A:46:LEU:C	1:A:47:ILE:HG23	2.41	0.41
1:A:71:VAL:HG13	1:A:72:ILE:N	2.34	0.41
1:A:80:THR:OG1	2:B:1001:AB1:C33	2.58	0.41
1:A:67:CYS:O	1:A:69:HIS:N	2.54	0.41
1:A:90:MET:HB3	1:A:95:CYS:HB3	2.02	0.41
1:B:6:TRP:O	1:B:7:GLN:HG3	2.20	0.41
1:B:22:ALA:HB3	1:B:85:ILE:HD11	2.03	0.41
1:B:33:LEU:HD12	1:B:75:VAL:HG11	2.03	0.41
1:A:31:THR:HG23	1:A:84:VAL:O	2.21	0.40
1:A:33:LEU:O	1:A:34:GLU:O	2.39	0.40
1:B:70:LYS:HZ3	1:B:70:LYS:HG2	1.48	0.40
1:A:21:GLU:O	1:A:83:ASN:HB2	2.21	0.40
1:B:81:PRO:HD2	2:B:1001:AB1:H21	2.03	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:B:42:TRP:O	3:A:118:HOH:O[3_565]	1.64	0.56
1:B:41:ARG:NH1	3:A:125:HOH:O[3_565]	2.16	0.04

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	97/99 (98%)	81 (84%)	13 (13%)	3 (3%)	4	9
1	B	97/99 (98%)	77 (79%)	11 (11%)	9 (9%)	0	0
All	All	194/198 (98%)	158 (81%)	24 (12%)	12 (6%)	1	2

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	GLU
1	A	81	PRO
1	B	35	GLU
1	B	36	VAL
1	B	50	ILE
1	B	82	ALA
1	A	82	ALA
1	B	17	GLY
1	B	67	CYS
1	B	74	THR
1	B	81	PRO
1	B	79	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	83/83 (100%)	67 (81%)	16 (19%)	1 3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	83/83 (100%)	70 (84%)	13 (16%)	2 6
All	All	166/166 (100%)	137 (82%)	29 (18%)	2 4

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	12	THR
1	A	13	ILE
1	A	20	LYS
1	A	21	GLU
1	A	29	ASP
1	A	32	VAL
1	A	35	GLU
1	A	41	ARG
1	A	43	LYS
1	A	54	VAL
1	A	63	PRO
1	A	71	VAL
1	A	76	LEU
1	A	89	LEU
1	A	97	LEU
1	B	15	ILE
1	B	21	GLU
1	B	34	GLU
1	B	37	ASN
1	B	41	ARG
1	B	44	PRO
1	B	47	ILE
1	B	50	ILE
1	B	53	PHE
1	B	54	VAL
1	B	64	ILE
1	B	70	LYS
1	B	84	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	ASN
1	B	69	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	98	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand 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
2	AB1	B	1001	-	48,49,49	4.47	32 (66%)	56,66,66	3.09	30 (53%)

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
2	AB1	B	1001	-	-	4/41/52/52	0/4/4/4

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	AB1	C28-C34	16.30	1.68	1.40
2	B	1001	AB1	C28-C30	12.45	1.61	1.40
2	B	1001	AB1	C9-C4	7.65	1.55	1.38
2	B	1001	AB1	C5-C4	7.23	1.54	1.38
2	B	1001	AB1	C19-C20	5.95	1.51	1.38
2	B	1001	AB1	C17-C16	5.68	1.53	1.38
2	B	1001	AB1	C29-C4	5.16	1.63	1.51
2	B	1001	AB1	C32-C31	5.02	1.49	1.38
2	B	1001	AB1	C6-C5	5.02	1.49	1.38
2	B	1001	AB1	C35-C34	-4.55	1.41	1.51
2	B	1001	AB1	C27-C26	4.52	1.60	1.51
2	B	1001	AB1	C8-C9	4.44	1.48	1.38
2	B	1001	AB1	C8-C7	4.02	1.48	1.38
2	B	1001	AB1	C32-C33	3.93	1.47	1.38
2	B	1001	AB1	C13-C10	3.91	1.64	1.54
2	B	1001	AB1	O3-C28	3.73	1.46	1.39
2	B	1001	AB1	C26-N4	3.69	1.41	1.34
2	B	1001	AB1	C31-C30	-3.63	1.32	1.39
2	B	1001	AB1	C15-C13	3.52	1.65	1.52
2	B	1001	AB1	C21-C20	3.48	1.46	1.38
2	B	1001	AB1	C10-C11	-3.42	1.48	1.53
2	B	1001	AB1	O3-C27	3.28	1.50	1.42
2	B	1001	AB1	O4-C24	-3.17	1.36	1.43
2	B	1001	AB1	O2-C11	-2.66	1.18	1.23
2	B	1001	AB1	C16-C21	2.66	1.44	1.38
2	B	1001	AB1	C22-C20	2.64	1.57	1.51
2	B	1001	AB1	C11-N3	-2.56	1.28	1.34
2	B	1001	AB1	O5-C26	2.33	1.28	1.23
2	B	1001	AB1	C18-C19	2.32	1.43	1.38
2	B	1001	AB1	C12-N3	2.25	1.51	1.46
2	B	1001	AB1	C14-C13	2.23	1.60	1.52
2	B	1001	AB1	C23-C12	2.02	1.58	1.53

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	AB1	C33-C32-C31	8.62	132.49	120.25
2	B	1001	AB1	C16-C21-C20	-6.09	111.29	120.63
2	B	1001	AB1	C36-C30-C28	5.99	130.48	120.82
2	B	1001	AB1	C2-C37-C1	5.67	129.59	111.31
2	B	1001	AB1	C27-O3-C28	5.56	130.69	114.73
2	B	1001	AB1	C32-C33-C34	-5.34	112.28	121.11
2	B	1001	AB1	O2-C11-N3	5.18	132.53	122.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	AB1	C27-C26-N4	-5.08	107.53	116.37
2	B	1001	AB1	C17-C16-C21	4.49	127.03	120.19
2	B	1001	AB1	C37-C1-N2	-4.30	100.79	110.24
2	B	1001	AB1	C22-C20-C21	-4.24	112.50	120.91
2	B	1001	AB1	C18-C19-C20	3.99	126.75	120.63
2	B	1001	AB1	C12-N3-C11	-3.88	117.01	123.20
2	B	1001	AB1	C17-C18-C19	-3.68	114.59	120.19
2	B	1001	AB1	C10-C11-N3	-3.19	109.54	115.57
2	B	1001	AB1	O1-C3-N1	3.10	126.99	123.11
2	B	1001	AB1	C25-N4-C26	-2.98	118.47	123.48
2	B	1001	AB1	C22-C20-C19	2.92	126.71	120.91
2	B	1001	AB1	O5-C26-N4	2.74	127.58	122.95
2	B	1001	AB1	C7-C8-C9	2.71	124.31	120.19
2	B	1001	AB1	C35-C34-C28	2.68	125.14	120.82
2	B	1001	AB1	C23-C12-C22	-2.64	109.09	112.42
2	B	1001	AB1	C29-C25-C24	2.64	116.07	111.65
2	B	1001	AB1	C8-C9-C4	-2.59	116.66	120.63
2	B	1001	AB1	C31-C30-C28	-2.57	113.64	117.68
2	B	1001	AB1	C22-C12-N3	2.54	115.28	110.39
2	B	1001	AB1	C20-C22-C12	-2.39	108.36	113.78
2	B	1001	AB1	C35-C34-C33	-2.37	115.68	120.31
2	B	1001	AB1	C36-C30-C31	-2.28	115.85	120.31
2	B	1001	AB1	C29-C25-N4	-2.10	107.00	110.07

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1001	AB1	C13-C10-N1-C2
2	B	1001	AB1	C34-C28-O3-C27
2	B	1001	AB1	C11-C10-C13-C14
2	B	1001	AB1	N3-C12-C22-C20

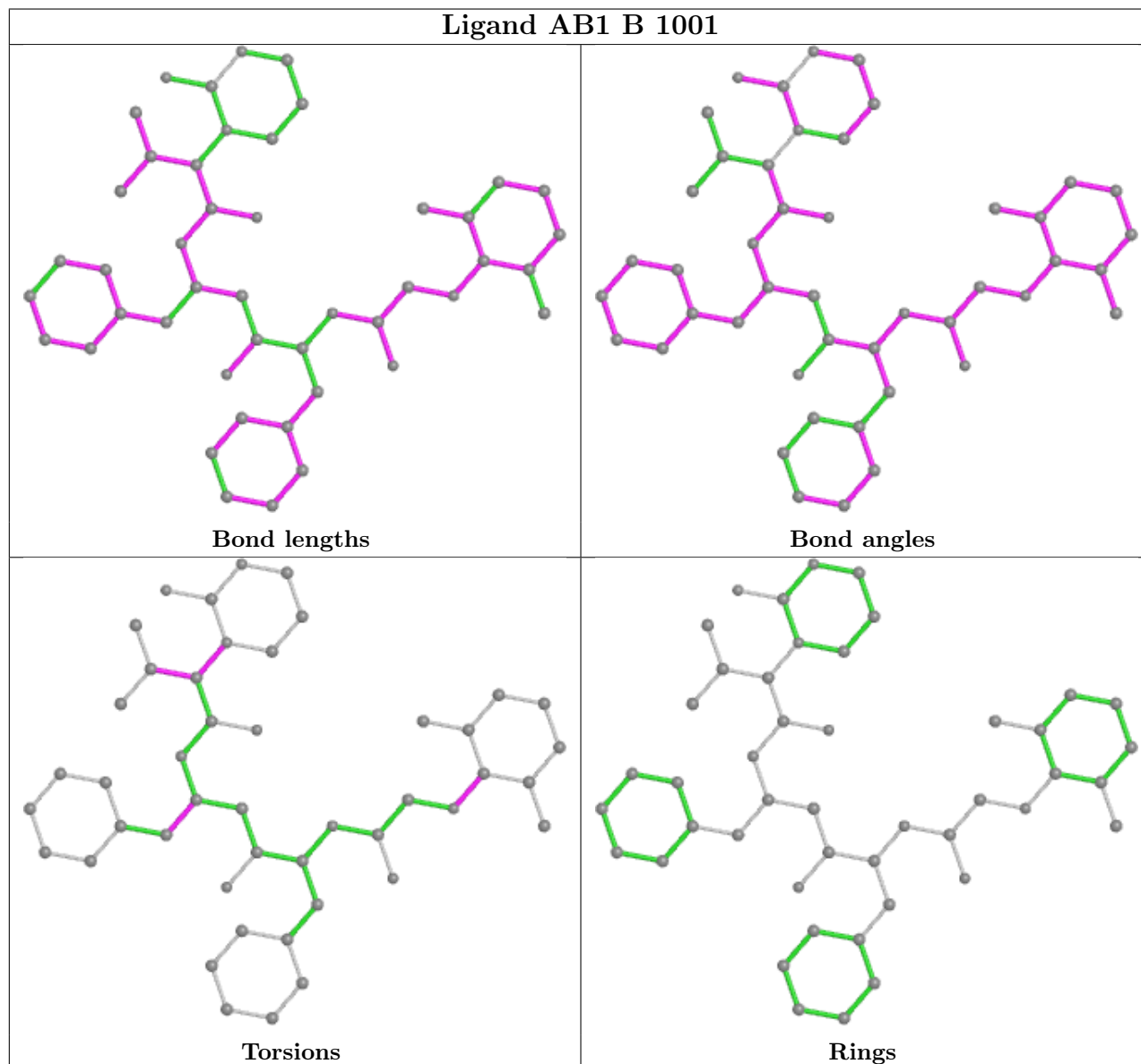
There are no ring outliers.

1 monomer is involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1001	AB1	25	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	90:MET	C	91:THR	N	1.18

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.