



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:59 AM UTC

PDB ID : 1RTH / pdb_00001rth
Title : HIGH RESOLUTION STRUCTURES OF HIV-1 RT FROM FOUR RT-INHIBITOR COMPLEXES
Authors : Ren, J.; Esnouf, R.; Garman, E.; Somers, D.; Ross, C.; Kirby, I.; Keeling, J.; Darby, G.; Jones, Y.; Stuart, D.; Stammers, D.
Deposited on : 1995-05-03
Resolution : 2.20 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

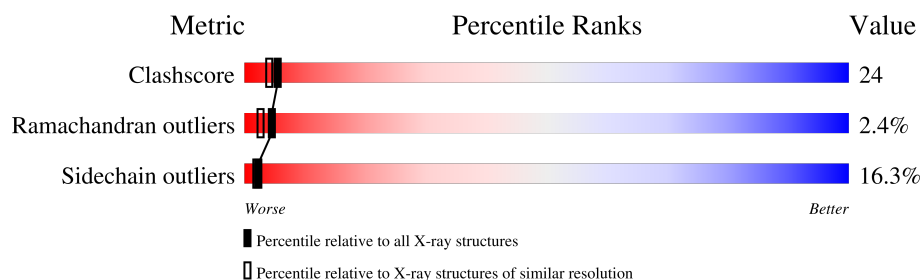
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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	560	 48% 36% 11% • •
2	B	440	 39% 43% 10% • 5%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8146 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.

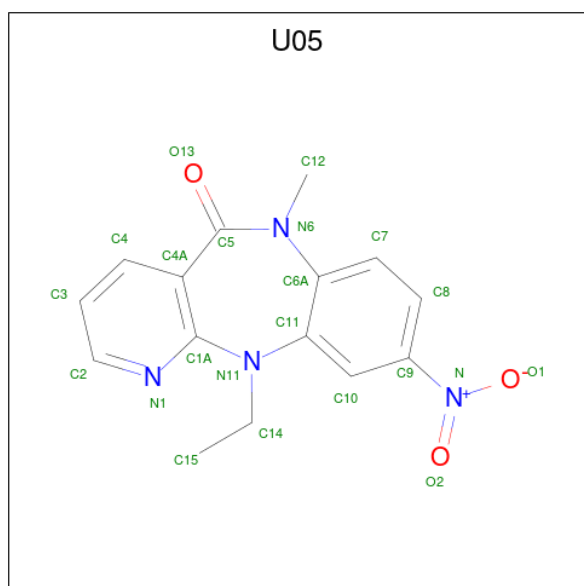
- Molecule 1 is a protein called HIV-1 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	543	Total	C	N	O	S	0	0	0
			4435	2869	739	819	8			

- Molecule 2 is a protein called HIV-1 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	420	Total	C	N	O	S	0	0	0
			3452	2242	573	630	7			

- Molecule 3 is 6,11-DIHYDRO-11-ETHYL-6-METHYL-9-NITRO-5H-PYRIDO[2,3-B][1,5]BENZODIAZEPIN-5-ONE (CCD ID: U05) (formula: $C_{15}H_{14}N_4O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			22	15	4	3		

- Molecule 4 is water.

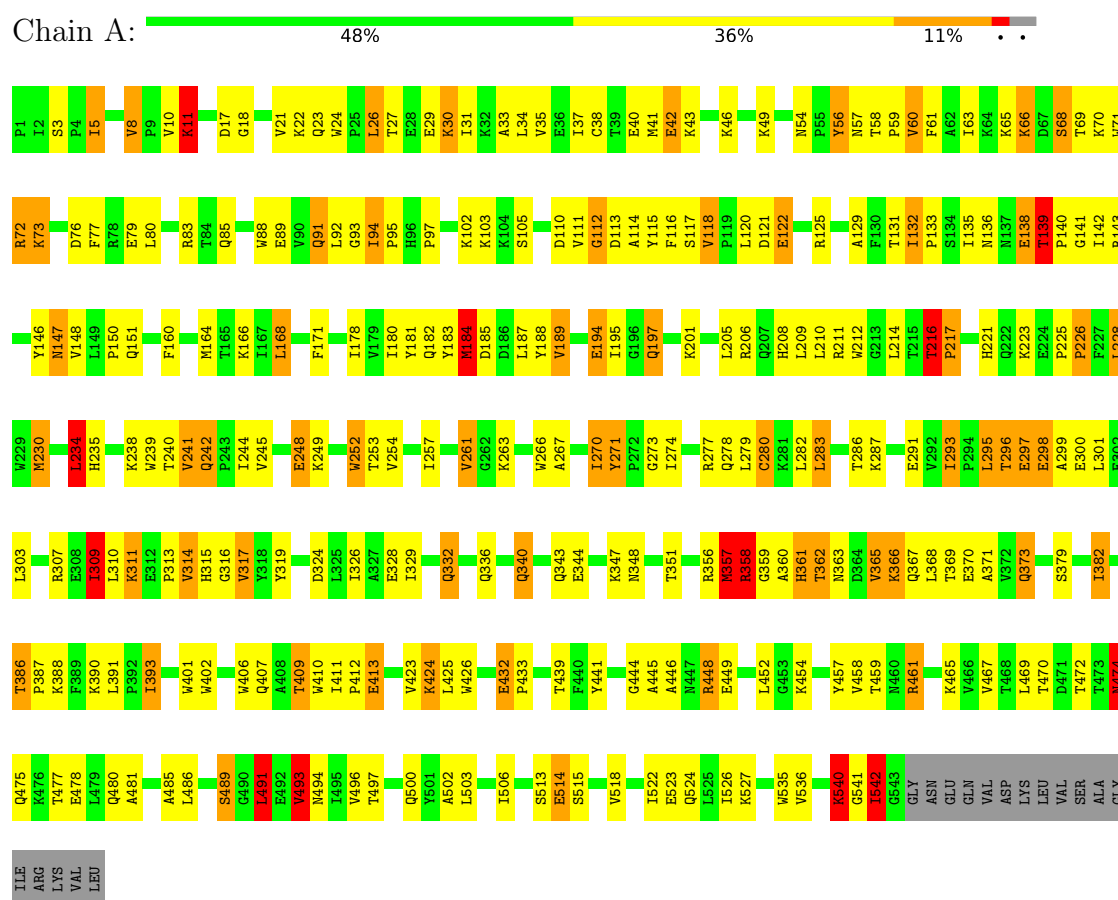
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	139	Total 139	O 139	0	0
4	B	98	Total 98	O 98	0	0

3 Residue-property plots

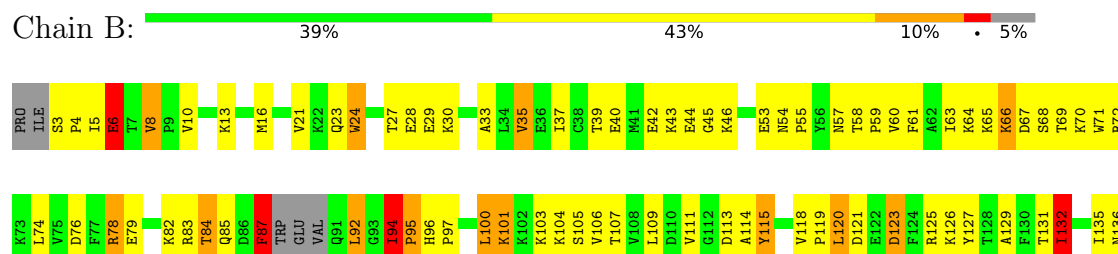
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: HIV-1 REVERSE TRANSCRIPTASE



• Molecule 2: HIV-1 REVERSE TRANSCRIPTASE



P433	R357	Y271	K201	M137
I434	R358	Y274	I202	E138
G436	R361	I275	E203	T139
A437	T362	K276	E204	P140
E438	N363	R277	L205	
THR	D364	Q278	R206	R143
PHE	V365	L279	Q207	Y144
	K366	C280	H208	Q145
	Q367		L209	Y146
	L368		L210	N147
	T369		R211	V148
	E370	L283		L149
	A371	R284	L214	P150
	V372	G285	T215	Q151
		T286	T216	G152
	T376	K287	P217	W153
	T377	A288	ASP	K154
	E378	L289	LYS	G155
	S379	T290	LYS	S156
	I380	E291	HIS	P157
	V381		GLN	A158
	I382		LYS	I159
	W383	L295	GLU	F160
	G384	T296	PRO	Q161
	K385	A299	PRO	S162
	T386	E300	PHE	S163
	P387	L301	LEU	M164
	K388	E302	TRP	T165
	F389	L303	MET	K166
	K390	A304	G231	I167
	L391	E305	Y232	L168
	P392	N306	E233	E169
	I393		L234	P170
	W398	I309	H235	F171
	E399	L310	P236	R172
	T400	K311	D237	K173
	W401	E312	K238	Q174
	W402			
	T403	V317	Q242	I178
	E404	P321	P243	V179
	Y405	I326	I244	I180
			V245	Y181
		Q336	L246	Q182
	E415	W337	P247	Y183
	F416		E248	M184
	V417		K249	D185
	N418	I341	D250	D186
	P420	Y342	S251	L187
	P421	Q343		Y188
	L422	E344	N255	V189
	V423	P345		
	K424	F346	L260	D192
	L425	N348	V261	L193
	W426	K347	G262	E194
	Y427	I353	L264	I195
	Q428	Y354	K263	G196
	L429	A355	W265	Q197
		R356	W266	H198
			A267	R199
			S268	T200

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	141.10Å 110.90Å 73.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.20	Depositor
% Data completeness (in resolution range)	81.4 (25.00-2.20)	Depositor
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.214 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8146	wwPDB-VP
Average B, all atoms (Å ²)	61.0	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: U05, CSD

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	0.98	4/4544 (0.1%)	1.38	67/6175 (1.1%)
2	B	0.99	6/3547 (0.2%)	1.39	52/4818 (1.1%)
All	All	0.98	10/8091 (0.1%)	1.39	119/10993 (1.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	184	MET	SD-CE	7.85	1.99	1.79
2	B	317	VAL	CA-CB	6.97	1.61	1.53
1	A	393	ILE	CA-C	-5.88	1.45	1.52
2	B	434	ILE	CA-CB	5.86	1.61	1.54
1	A	365	VAL	CA-CB	-5.55	1.47	1.54
2	B	94	ILE	CA-CB	5.47	1.61	1.54
2	B	60	VAL	CA-CB	5.36	1.64	1.55
2	B	417	VAL	CA-C	-5.34	1.48	1.52
1	A	5	ILE	CA-CB	5.28	1.61	1.54
2	B	78	ARG	CA-C	-5.20	1.45	1.52

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	238	LYS	N-CA-C	-13.89	95.67	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	216	THR	CA-C-N	11.70	131.83	119.78
1	A	216	THR	C-N-CA	11.70	131.83	119.78
2	B	118	VAL	N-CA-C	11.05	118.13	108.63
1	A	489	SER	N-CA-C	11.03	125.26	111.69
1	A	94	ILE	N-CA-C	10.02	117.25	108.63
1	A	132	ILE	N-CA-C	-9.71	97.21	107.60
2	B	277	ARG	N-CA-C	9.60	121.75	111.28
2	B	363	ASN	N-CA-C	9.37	123.81	108.26
1	A	115	TYR	N-CA-C	-9.22	101.31	111.36
1	A	536	VAL	N-CA-C	-9.08	101.75	109.19
1	A	491	LEU	N-CA-C	8.95	121.85	111.11
2	B	214	LEU	N-CA-C	8.77	122.61	110.24
1	A	217	PRO	N-CA-C	8.28	124.38	111.21
1	A	388	LYS	N-CA-C	-8.28	97.11	110.20
2	B	66	LYS	N-CA-C	-8.26	99.12	110.35
1	A	242	GLN	CA-C-N	8.18	130.07	119.84
1	A	242	GLN	C-N-CA	8.18	130.07	119.84
1	A	271	TYR	CA-C-N	-7.97	111.80	119.85
1	A	271	TYR	C-N-CA	-7.97	111.80	119.85
1	A	139	THR	CA-C-N	-7.95	109.91	119.84
1	A	139	THR	C-N-CA	-7.95	109.91	119.84
1	A	386	THR	CA-C-N	7.93	127.94	119.78
1	A	386	THR	C-N-CA	7.93	127.94	119.78
1	A	194	GLU	N-CA-C	-7.79	98.75	110.28
1	A	54	ASN	CA-C-N	7.71	128.72	120.47
1	A	54	ASN	C-N-CA	7.71	128.72	120.47
1	A	402	TRP	N-CA-C	7.67	119.64	111.28
1	A	382	ILE	N-CA-C	7.42	118.35	111.45
1	A	493	VAL	CB-CA-C	-7.39	97.89	111.18
2	B	428	GLN	N-CA-C	-7.30	103.31	111.71
1	A	540	LYS	N-CA-C	-7.26	98.60	109.86
2	B	235	HIS	CA-C-N	7.18	128.82	119.84
2	B	235	HIS	C-N-CA	7.18	128.82	119.84
2	B	388	LYS	N-CA-C	-7.13	97.62	109.46
2	B	382	ILE	N-CA-C	7.09	117.69	110.82
2	B	115	TYR	N-CA-C	7.08	119.89	111.33
2	B	215	THR	N-CA-C	-7.03	99.09	110.20
1	A	147	ASN	N-CA-C	-7.02	104.75	113.38
1	A	298	GLU	N-CA-C	-6.95	103.75	111.82
1	A	195	ILE	N-CA-C	6.86	120.64	111.17
2	B	437	ALA	N-CA-C	-6.84	96.18	108.48
2	B	132	ILE	N-CA-C	-6.78	100.18	107.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	LYS	N-CA-C	6.59	119.20	109.24
1	A	252	TRP	N-CA-C	6.57	119.64	109.07
1	A	449	GLU	N-CA-C	6.56	118.23	111.14
1	A	93	GLY	N-CA-C	-6.48	100.79	110.38
2	B	419	THR	CA-C-N	-6.43	113.76	120.38
2	B	419	THR	C-N-CA	-6.43	113.76	120.38
2	B	276	VAL	CB-CA-C	6.27	117.83	110.93
2	B	391	LEU	N-CA-C	6.26	118.70	109.62
1	A	141	GLY	N-CA-C	-6.25	98.36	113.18
2	B	296	THR	N-CA-C	-6.25	101.68	110.50
2	B	343	GLN	N-CA-C	-6.25	106.29	114.04
1	A	474	ASN	N-CA-C	6.14	117.64	111.07
2	B	299	ALA	N-CA-C	-6.09	104.56	111.14
1	A	348	ASN	N-CA-C	6.08	119.42	109.76
1	A	166	LYS	N-CA-C	-6.02	104.41	110.97
1	A	245	VAL	N-CA-C	6.00	117.08	107.73
2	B	139	THR	CA-C-N	-5.97	114.61	120.52
2	B	139	THR	C-N-CA	-5.97	114.61	120.52
2	B	153	TRP	N-CA-C	-5.95	100.86	110.32
1	A	494	ASN	N-CA-C	-5.91	100.08	109.59
2	B	131	THR	N-CA-C	5.91	119.15	108.69
1	A	234	LEU	N-CA-C	5.88	118.31	108.96
2	B	168	LEU	N-CA-C	5.88	120.62	112.45
2	B	276	VAL	N-CA-CB	-5.86	104.74	112.36
2	B	372	VAL	CB-CA-C	-5.80	104.30	112.14
2	B	156	SER	N-CA-C	5.80	120.64	112.75
2	B	171	PHE	N-CA-C	-5.79	105.05	111.36
1	A	211	ARG	N-CA-C	-5.74	105.11	111.71
2	B	206	ARG	N-CA-C	-5.69	104.77	110.97
2	B	123	ASP	N-CA-C	5.66	119.81	113.01
2	B	336	GLN	N-CA-C	5.66	119.32	110.32
2	B	6	GLU	N-CA-C	-5.60	101.35	110.20
1	A	11	LYS	N-CA-C	5.58	118.32	109.50
1	A	458	VAL	N-CA-C	-5.55	99.81	108.81
1	A	248	GLU	N-CA-C	-5.54	100.95	109.76
1	A	226	PRO	CA-C-N	-5.53	115.37	123.00
1	A	226	PRO	C-N-CA	-5.53	115.37	123.00
1	A	266	TRP	N-CA-C	-5.53	105.15	111.07
2	B	156	SER	CA-C-N	-5.52	114.08	120.04
2	B	156	SER	C-N-CA	-5.52	114.08	120.04
2	B	250	ASP	N-CA-C	-5.52	105.18	111.14
2	B	70	LYS	N-CA-C	-5.49	99.33	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118	VAL	N-CA-C	5.49	113.35	108.63
1	A	273	GLY	N-CA-C	-5.48	100.20	113.18
1	A	69	THR	N-CA-C	-5.44	105.32	112.72
1	A	89	GLU	N-CA-C	5.43	117.19	107.80
1	A	441	TYR	N-CA-C	-5.42	98.39	107.99
2	B	42	GLU	N-CA-C	-5.41	105.47	111.36
1	A	8	VAL	CA-C-N	5.36	126.20	119.98
1	A	8	VAL	C-N-CA	5.36	126.20	119.98
1	A	212	TRP	N-CA-C	5.35	119.36	113.21
2	B	140	PRO	N-CA-C	-5.33	103.19	111.13
1	A	411	ILE	CA-C-N	5.32	125.61	119.92
1	A	411	ILE	C-N-CA	5.32	125.61	119.92
2	B	235	HIS	N-CA-C	5.32	117.79	108.75
2	B	366	LYS	N-CA-C	-5.31	105.19	110.97
2	B	87	PHE	CA-C-O	-5.27	111.84	120.80
2	B	186	ASP	N-CA-C	5.27	117.87	109.81
2	B	361	HIS	N-CA-C	5.24	121.97	110.80
2	B	101	LYS	N-CA-C	-5.22	105.59	111.28
1	A	309	ILE	N-CA-C	-5.21	105.42	110.42
1	A	71	TRP	N-CA-C	5.21	118.10	109.46
1	A	131	THR	N-CA-C	5.19	117.86	109.40
1	A	26	LEU	N-CA-C	5.17	117.67	109.50
1	A	267	ALA	N-CA-C	5.17	117.32	111.11
2	B	401	TRP	N-CA-C	5.14	120.68	113.02
1	A	366	LYS	N-CA-C	-5.14	104.95	111.11
2	B	233	GLU	N-CA-C	5.13	117.88	110.28
1	A	56	TYR	N-CA-C	5.11	117.12	110.53
1	A	73	LYS	N-CA-C	5.11	117.18	109.41
1	A	314	VAL	N-CA-C	5.07	115.43	108.12
1	A	80	LEU	N-CA-C	-5.07	105.75	111.28
2	B	193	LEU	N-CA-C	-5.07	103.65	110.24
1	A	10	VAL	N-CA-C	5.05	115.40	108.12
2	B	113	ASP	N-CA-C	5.03	117.41	111.33
2	B	276	VAL	N-CA-C	5.01	117.96	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	271	TYR	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	A	4435	0	4484	208	0
2	B	3452	0	3488	181	0
3	A	22	0	14	4	0
4	A	139	0	0	5	0
4	B	98	0	0	8	0
All	All	8146	0	7986	378	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (378) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:84:THR:HG22	2:B:154:LYS:HE2	1.37	1.05
1:A:59:PRO:HG2	1:A:76:ASP:HB3	1.39	1.00
1:A:410:TRP:CD1	2:B:363:ASN:HB2	2.01	0.95
1:A:228:LEU:HD11	1:A:242:GLN:NE2	1.82	0.94
1:A:270:ILE:HD11	1:A:314:VAL:HG21	1.47	0.94
2:B:79:GLU:O	2:B:83:ARG:HG3	1.69	0.93
1:A:239:TRP:CZ2	1:A:316:GLY:HA3	2.04	0.93
1:A:114:ALA:HA	1:A:117:SER:OG	1.69	0.92
1:A:171:PHE:HB2	1:A:208:HIS:HD2	1.34	0.91
1:A:257:ILE:O	1:A:261:VAL:HG23	1.71	0.91
1:A:358:ARG:NH1	1:A:358:ARG:HB3	1.89	0.88
2:B:368:LEU:O	2:B:372:VAL:HG23	1.74	0.88
1:A:278:GLN:HG2	1:A:298:GLU:HB3	1.55	0.86
1:A:171:PHE:HB2	1:A:208:HIS:CD2	2.09	0.86
1:A:216:THR:HG23	1:A:217:PRO:HD2	1.59	0.84
1:A:228:LEU:HD11	1:A:242:GLN:HE22	1.43	0.81
2:B:195:ILE:HG13	2:B:199:ARG:HG3	1.64	0.78
2:B:426:TRP:O	2:B:429:LEU:HB2	1.84	0.78
1:A:27:THR:HB	1:A:30:LYS:HG3	1.65	0.77
2:B:197:GLN:O	2:B:201:LYS:HB2	1.86	0.76
2:B:5:ILE:HG22	2:B:6:GLU:H	1.48	0.76
1:A:79:GLU:HG3	1:A:83:ARG:NH1	2.01	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:139:THR:HG22	2:B:140:PRO:HD2	1.66	0.75
2:B:203:GLU:HA	2:B:206:ARG:HD2	1.68	0.75
1:A:184:MET:HE3	1:A:184:MET:HA	1.69	0.75
2:B:180:ILE:HD11	2:B:189:VAL:HG13	1.69	0.75
2:B:369:THR:HG22	2:B:398:TRP:CH2	2.23	0.74
1:A:23:GLN:HE22	1:A:60:VAL:H	1.36	0.73
1:A:332:GLN:NE2	1:A:332:GLN:HA	2.03	0.72
1:A:541:GLY:HA3	2:B:284:ARG:CZ	2.20	0.72
2:B:247:PRO:HB2	2:B:249:LYS:HZ1	1.54	0.72
2:B:100:LEU:HD23	2:B:100:LEU:H	1.54	0.72
1:A:83:ARG:HG3	1:A:83:ARG:HH11	1.55	0.71
1:A:244:ILE:HG23	1:A:310:LEU:HD13	1.73	0.71
2:B:84:THR:CG2	2:B:154:LYS:HE2	2.21	0.69
2:B:365:VAL:O	2:B:369:THR:HG23	1.92	0.69
2:B:295:LEU:HB3	2:B:300:GLU:HG2	1.74	0.69
1:A:17:ASP:O	1:A:83:ARG:HD3	1.92	0.69
2:B:180:ILE:CD1	2:B:189:VAL:HG13	2.23	0.69
3:A:999:U05:O1	2:B:138:GLU:HG2	1.94	0.68
1:A:502:ALA:O	1:A:506:ILE:HD12	1.94	0.68
1:A:358:ARG:HB3	1:A:358:ARG:CZ	2.22	0.67
1:A:241:VAL:HG23	1:A:314:VAL:O	1.95	0.66
1:A:226:PRO:HB3	1:A:235:HIS:CD2	2.31	0.66
1:A:329:ILE:HD12	1:A:391:LEU:CD2	2.25	0.66
1:A:129:ALA:HB1	1:A:143:ARG:NH2	2.11	0.66
2:B:57:ASN:HD22	2:B:143:ARG:NH1	1.94	0.66
1:A:139:THR:HB	1:A:140:PRO:HD3	1.78	0.65
2:B:158:ALA:O	2:B:161:GLN:HB2	1.95	0.65
1:A:72:ARG:HG2	1:A:73:LYS:N	2.11	0.65
1:A:332:GLN:HA	1:A:332:GLN:HE21	1.62	0.65
1:A:40:GLU:O	1:A:43:LYS:HG2	1.97	0.64
1:A:37:ILE:O	1:A:40:GLU:HB3	1.97	0.64
1:A:188:TYR:CD2	3:A:999:U05:H122	2.32	0.64
1:A:125:ARG:HD3	1:A:147:ASN:HA	1.78	0.64
2:B:65:LYS:O	2:B:68:SER:HB3	1.98	0.64
2:B:390:LYS:HE2	2:B:415:GLU:OE2	1.97	0.64
2:B:33:ALA:O	2:B:37:ILE:HG13	1.97	0.63
1:A:497:THR:O	1:A:535:TRP:HA	1.99	0.63
2:B:420:PRO:HB2	2:B:423:VAL:HG13	1.81	0.63
2:B:247:PRO:HB2	2:B:249:LYS:NZ	2.13	0.62
2:B:5:ILE:HG22	2:B:6:GLU:N	2.15	0.62
1:A:79:GLU:HG3	1:A:83:ARG:HH12	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:SER:CB	1:A:214:LEU:HD23	2.30	0.61
2:B:103:LYS:HE3	2:B:192:ASP:OD2	2.00	0.61
2:B:54:ASN:HD21	2:B:129:ALA:HB2	1.66	0.61
2:B:125:ARG:HE	2:B:147:ASN:HA	1.66	0.61
2:B:132:ILE:HD12	2:B:132:ILE:N	2.16	0.60
1:A:340:GLN:HB3	1:A:351:THR:HG22	1.84	0.60
2:B:105:SER:HA	2:B:234:LEU:O	2.02	0.60
2:B:125:ARG:NE	2:B:147:ASN:HA	2.17	0.60
1:A:358:ARG:HB3	1:A:358:ARG:HH11	1.67	0.60
2:B:206:ARG:C	2:B:210:LEU:HD13	2.26	0.60
1:A:489:SER:HB2	1:A:493:VAL:HG13	1.84	0.59
2:B:157:PRO:HG2	2:B:184:MET:HA	1.84	0.59
1:A:27:THR:HG22	1:A:29:GLU:H	1.68	0.59
1:A:122:GLU:H	1:A:122:GLU:CD	2.08	0.59
1:A:164:MET:HG3	1:A:168:LEU:HD22	1.84	0.59
2:B:163:SER:O	2:B:167:ILE:HG13	2.03	0.59
2:B:183:TYR:HB3	2:B:188:TYR:HE2	1.67	0.58
2:B:251:SER:HA	4:B:1192:HOH:O	2.03	0.58
2:B:421:PRO:O	2:B:425:LEU:HD22	2.03	0.58
1:A:33:ALA:O	1:A:37:ILE:HD13	2.03	0.58
2:B:3:SER:N	2:B:4:PRO:HD3	2.18	0.58
1:A:94:ILE:HD12	1:A:230:MET:HE1	1.85	0.57
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.86	0.57
2:B:84:THR:HG22	2:B:154:LYS:CE	2.24	0.57
1:A:300:GLU:OE1	1:A:300:GLU:HA	2.04	0.57
2:B:422:LEU:HB2	4:B:1208:HOH:O	2.05	0.57
1:A:114:ALA:O	1:A:117:SER:HB2	2.04	0.56
2:B:126:LYS:HG3	2:B:127:TYR:N	2.19	0.56
1:A:541:GLY:HA3	2:B:284:ARG:NE	2.20	0.56
2:B:379:SER:CB	2:B:387:PRO:HD3	2.36	0.56
2:B:400:THR:HG22	2:B:401:TRP:CD2	2.41	0.56
1:A:164:MET:HE1	1:A:214:LEU:HD13	1.88	0.56
2:B:114:ALA:HB2	2:B:214:LEU:HD13	1.88	0.56
1:A:139:THR:HB	1:A:140:PRO:CD	2.35	0.56
1:A:234:LEU:HD12	1:A:239:TRP:HB3	1.88	0.56
1:A:541:GLY:HA3	2:B:284:ARG:NH2	2.21	0.56
2:B:363:ASN:ND2	2:B:366:LYS:HB2	2.21	0.56
1:A:91:GLN:NE2	1:A:183:TYR:HE1	2.04	0.56
1:A:118:VAL:O	1:A:148:VAL:HG23	2.05	0.55
1:A:216:THR:HG23	1:A:217:PRO:CD	2.35	0.55
1:A:197:GLN:HE21	1:A:197:GLN:HA	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:266:TRP:HZ3	2:B:426:TRP:CG	2.24	0.55
1:A:216:THR:CG2	1:A:217:PRO:HD2	2.35	0.55
2:B:101:LYS:NZ	2:B:101:LYS:HB3	2.22	0.55
2:B:311:LYS:O	2:B:312:GLU:HG3	2.06	0.54
1:A:282:LEU:HB3	1:A:293:ILE:HG21	1.88	0.54
1:A:58:THR:HG23	1:A:59:PRO:HD2	1.90	0.54
1:A:34:LEU:HD21	1:A:73:LYS:HB2	1.90	0.54
1:A:142:ILE:N	1:A:142:ILE:HD12	2.23	0.54
1:A:11:LYS:NZ	1:A:11:LYS:HB3	2.23	0.54
1:A:56:TYR:O	1:A:57:ASN:HB2	2.08	0.53
1:A:485:ALA:O	1:A:489:SER:HB3	2.08	0.53
1:A:461:ARG:HG3	1:A:461:ARG:HH11	1.73	0.53
1:A:328:GLU:HG3	1:A:390:LYS:HB2	1.90	0.53
1:A:486:LEU:HB3	1:A:524:GLN:CG	2.39	0.53
2:B:57:ASN:HD22	2:B:143:ARG:HH12	1.56	0.53
1:A:164:MET:HG3	1:A:168:LEU:CD2	2.38	0.53
2:B:181:TYR:O	2:B:187:LEU:HA	2.09	0.53
2:B:195:ILE:HG12	2:B:199:ARG:CZ	2.39	0.53
1:A:68:SER:C	1:A:70:LYS:H	2.17	0.53
2:B:28:GLU:HG3	2:B:135:ILE:CD1	2.39	0.53
2:B:280:CYS:HB3	2:B:284:ARG:NH2	2.24	0.53
1:A:448:ARG:HG2	1:A:448:ARG:HH11	1.73	0.53
2:B:344:GLU:HB3	2:B:347:LYS:HE3	1.90	0.52
2:B:369:THR:HG22	2:B:398:TRP:CZ3	2.44	0.52
1:A:226:PRO:HB3	1:A:235:HIS:HD2	1.72	0.52
1:A:444:GLY:HA3	1:A:477:THR:HG22	1.90	0.52
1:A:486:LEU:HB3	1:A:524:GLN:HG3	1.91	0.52
2:B:341:ILE:N	2:B:341:ILE:HD12	2.24	0.52
1:A:540:LYS:HG2	2:B:280:CYS:SG	2.50	0.52
1:A:129:ALA:HB1	1:A:143:ARG:HH21	1.75	0.52
2:B:280:CYS:HB3	2:B:284:ARG:HH21	1.75	0.52
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.44	0.52
2:B:54:ASN:ND2	2:B:129:ALA:HB2	2.24	0.52
1:A:160:PHE:HE2	1:A:182:GLN:NE2	2.08	0.52
1:A:168:LEU:HD11	1:A:209:LEU:HD21	1.91	0.52
1:A:424:LYS:HE3	1:A:426:TRP:CE3	2.45	0.52
1:A:24:TRP:H	1:A:24:TRP:CD1	2.28	0.51
1:A:235:HIS:HE1	4:A:1047:HOH:O	1.91	0.51
2:B:100:LEU:H	2:B:100:LEU:CD2	2.22	0.51
2:B:92:LEU:HB3	2:B:161:GLN:OE1	2.10	0.51
1:A:324:ASP:O	1:A:343:GLN:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:92:LEU:HD22	2:B:165:THR:HG21	1.92	0.51
2:B:114:ALA:HB1	2:B:160:PHE:CZ	2.45	0.51
2:B:194:GLU:OE1	2:B:195:ILE:HG22	2.10	0.51
1:A:206:ARG:O	1:A:210:LEU:HB2	2.11	0.51
1:A:110:ASP:C	1:A:112:GLY:H	2.19	0.51
1:A:340:GLN:CB	1:A:351:THR:HG22	2.41	0.51
1:A:523:GLU:O	1:A:527:LYS:HG2	2.10	0.51
2:B:74:LEU:HD11	4:B:1209:HOH:O	2.11	0.51
2:B:160:PHE:O	2:B:160:PHE:CD2	2.64	0.51
2:B:205:LEU:O	2:B:208:HIS:HB3	2.11	0.51
1:A:356:ARG:HH22	1:A:371:ALA:HB2	1.76	0.51
1:A:270:ILE:HD12	1:A:270:ILE:O	2.10	0.51
1:A:239:TRP:CE2	1:A:316:GLY:HA3	2.44	0.50
2:B:206:ARG:O	2:B:210:LEU:HD13	2.09	0.50
1:A:77:PHE:CE2	1:A:150:PRO:HB2	2.45	0.50
2:B:13:LYS:HE2	2:B:82:LYS:O	2.10	0.50
2:B:35:VAL:O	2:B:39:THR:HG23	2.11	0.50
1:A:164:MET:O	1:A:168:LEU:HD22	2.11	0.50
1:A:168:LEU:CD1	1:A:209:LEU:HD21	2.42	0.50
1:A:356:ARG:NH1	1:A:367:GLN:O	2.45	0.50
2:B:198:HIS:HD2	2:B:233:GLU:OE1	1.95	0.50
1:A:235:HIS:HB2	1:A:238:LYS:O	2.11	0.50
1:A:252:TRP:CD1	1:A:295:LEU:CD1	2.95	0.50
2:B:161:GLN:HA	2:B:161:GLN:NE2	2.26	0.50
1:A:373:GLN:HG2	4:B:1230:HOH:O	2.12	0.50
2:B:78:ARG:O	2:B:82:LYS:HG3	2.11	0.50
1:A:297:GLU:O	1:A:301:LEU:HD23	2.12	0.49
1:A:324:ASP:HA	4:A:1087:HOH:O	2.11	0.49
2:B:40:GLU:O	2:B:43:LYS:HB2	2.12	0.49
2:B:87:PHE:CD1	2:B:87:PHE:N	2.80	0.49
2:B:285:GLY:O	2:B:287:LYS:HG2	2.13	0.49
2:B:366:LYS:HG2	2:B:405:TYR:CD2	2.46	0.49
2:B:58:THR:HG23	2:B:76:ASP:O	2.12	0.49
2:B:107:THR:O	2:B:189:VAL:N	2.38	0.49
2:B:244:ILE:HG23	2:B:429:LEU:HB3	1.95	0.49
2:B:266:TRP:CZ3	2:B:426:TRP:CG	3.00	0.49
1:A:197:GLN:HG3	4:A:1065:HOH:O	2.12	0.49
2:B:43:LYS:C	2:B:45:GLY:H	2.21	0.49
1:A:114:ALA:HB1	1:A:214:LEU:HD22	1.94	0.49
1:A:432:GLU:HB2	1:A:433:PRO:HD2	1.94	0.49
1:A:489:SER:HB2	1:A:493:VAL:CG1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:TRP:CH2	2:B:61:PHE:CD1	3.00	0.49
2:B:169:GLU:O	2:B:172:ARG:HB2	2.12	0.49
2:B:288:ALA:O	2:B:291:GLU:HB3	2.12	0.49
2:B:361:HIS:HD2	2:B:362:THR:CG2	2.26	0.49
2:B:85:GLN:O	2:B:85:GLN:HG3	2.12	0.49
1:A:117:SER:HB3	1:A:214:LEU:HD23	1.95	0.49
2:B:16:MET:HE3	2:B:83:ARG:HA	1.95	0.48
1:A:445:ALA:N	1:A:477:THR:HG21	2.28	0.48
1:A:448:ARG:HG2	4:A:1127:HOH:O	2.13	0.48
2:B:101:LYS:HE2	2:B:382:ILE:HG23	1.94	0.48
2:B:155:GLY:O	2:B:158:ALA:HB3	2.12	0.48
2:B:206:ARG:O	2:B:209:LEU:N	2.46	0.48
1:A:253:THR:O	1:A:257:ILE:HG12	2.14	0.48
1:A:295:LEU:HD23	1:A:299:ALA:HB3	1.95	0.48
1:A:329:ILE:HD12	1:A:391:LEU:HD21	1.92	0.48
1:A:184:MET:HA	1:A:184:MET:CE	2.40	0.48
1:A:439:THR:HG21	2:B:289:LEU:HD13	1.96	0.48
1:A:116:PHE:HE1	1:A:151:GLN:HB2	1.77	0.48
2:B:255:ASN:ND2	4:B:1199:HOH:O	2.46	0.48
1:A:500:GLN:OE1	1:A:500:GLN:HA	2.13	0.48
2:B:205:LEU:HD13	2:B:205:LEU:C	2.39	0.48
1:A:125:ARG:NH1	1:A:147:ASN:HB3	2.28	0.47
2:B:261:VAL:HG22	2:B:276:VAL:HG22	1.95	0.47
1:A:41:MET:HB3	1:A:46:LYS:HZ1	1.79	0.47
1:A:365:VAL:O	1:A:366:LYS:C	2.57	0.47
2:B:268:SER:HA	2:B:271:TYR:O	2.14	0.47
2:B:336:GLN:OE1	2:B:336:GLN:N	2.46	0.47
2:B:28:GLU:HG3	2:B:135:ILE:HD11	1.95	0.47
1:A:344:GLU:O	1:A:347:LYS:HB2	2.14	0.47
2:B:24:TRP:CZ3	2:B:403:THR:HG21	2.50	0.47
2:B:267:ALA:HB2	2:B:426:TRP:CZ3	2.49	0.47
1:A:66:LYS:HD2	1:A:66:LYS:HA	1.67	0.47
1:A:357:MET:O	1:A:359:GLY:N	2.48	0.47
1:A:319:TYR:CE1	1:A:343:GLN:NE2	2.82	0.47
2:B:65:LYS:NZ	2:B:72:ARG:HD3	2.30	0.47
2:B:72:ARG:HG3	2:B:72:ARG:HH11	1.79	0.47
2:B:271:TYR:HB2	2:B:274:ILE:CD1	2.44	0.47
2:B:120:LEU:HD12	2:B:150:PRO:HD3	1.97	0.47
1:A:235:HIS:ND1	1:A:238:LYS:HE3	2.30	0.47
1:A:324:ASP:O	1:A:343:GLN:CG	2.63	0.47
2:B:326:ILE:O	2:B:341:ILE:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:LYS:HG2	1:A:23:GLN:N	2.30	0.46
1:A:102:LYS:HG2	4:A:1053:HOH:O	2.16	0.46
1:A:248:GLU:HA	1:A:307:ARG:NH2	2.30	0.46
1:A:347:LYS:HA	1:A:347:LYS:HD3	1.54	0.46
1:A:540:LYS:HB3	1:A:542:ILE:CD1	2.44	0.46
2:B:182:GLN:HB2	2:B:187:LEU:CD1	2.46	0.46
1:A:295:LEU:HD23	1:A:299:ALA:CB	2.45	0.46
2:B:169:GLU:HG2	2:B:173:LYS:HE2	1.97	0.46
1:A:8:VAL:HG13	2:B:53:GLU:OE1	2.16	0.46
1:A:38:CYS:O	1:A:42:GLU:HB3	2.16	0.46
1:A:446:ALA:O	1:A:448:ARG:NH1	2.49	0.46
2:B:169:GLU:HA	2:B:172:ARG:HB2	1.97	0.46
3:A:999:U05:N1	3:A:999:U05:H153	2.30	0.46
2:B:96:HIS:CD2	2:B:97:PRO:O	2.69	0.46
2:B:393:ILE:O	2:B:416:PHE:HB3	2.16	0.46
1:A:307:ARG:O	1:A:311:LYS:HE2	2.15	0.46
1:A:474:ASN:O	1:A:478:GLU:HG3	2.16	0.46
2:B:72:ARG:NH2	2:B:151:GLN:NE2	2.63	0.46
2:B:358:ARG:H	2:B:358:ARG:CD	2.29	0.46
2:B:376:THR:CG2	2:B:386:THR:HG22	2.46	0.46
1:A:180:ILE:HG12	1:A:189:VAL:HG13	1.98	0.45
1:A:424:LYS:HE3	1:A:426:TRP:CZ3	2.51	0.45
1:A:41:MET:HB3	1:A:46:LYS:NZ	2.32	0.45
2:B:361:HIS:HD2	2:B:362:THR:HG22	1.81	0.45
1:A:278:GLN:HG2	1:A:298:GLU:CB	2.35	0.45
1:A:116:PHE:CE2	1:A:146:TYR:HE2	2.34	0.45
1:A:280:CSD:O	1:A:283:LEU:HB2	2.17	0.45
2:B:66:LYS:O	2:B:67:ASP:HB2	2.16	0.45
1:A:34:LEU:HD21	1:A:73:LYS:CB	2.47	0.45
1:A:296:THR:O	1:A:299:ALA:HB3	2.17	0.45
1:A:461:ARG:HH11	1:A:461:ARG:CG	2.30	0.45
1:A:448:ARG:HG2	1:A:448:ARG:NH1	2.31	0.45
2:B:353:LYS:HG2	4:B:1205:HOH:O	2.16	0.45
1:A:187:LEU:HD12	1:A:187:LEU:HA	1.80	0.45
2:B:202:ILE:O	2:B:205:LEU:HB3	2.16	0.45
1:A:491:LEU:HD12	1:A:491:LEU:HA	1.72	0.45
1:A:357:MET:O	1:A:357:MET:HG2	2.17	0.44
2:B:111:VAL:O	2:B:111:VAL:HG23	2.17	0.44
1:A:24:TRP:CD1	1:A:61:PHE:HE1	2.35	0.44
2:B:8:VAL:O	2:B:8:VAL:HG22	2.17	0.44
1:A:91:GLN:HE22	1:A:183:TYR:HE1	1.63	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:GLU:HB3	1:A:340:GLN:OE1	2.17	0.44
1:A:454:LYS:HA	1:A:467:VAL:O	2.18	0.44
1:A:522:ILE:O	1:A:526:ILE:HG13	2.17	0.44
1:A:234:LEU:HD12	1:A:239:TRP:CB	2.47	0.44
1:A:412:PRO:O	1:A:413:GLU:C	2.60	0.44
1:A:540:LYS:HB3	1:A:542:ILE:HD11	1.99	0.44
1:A:22:LYS:HG2	1:A:23:GLN:H	1.82	0.44
1:A:118:VAL:O	1:A:148:VAL:CG2	2.65	0.44
1:A:283:LEU:O	1:A:286:THR:HG23	2.17	0.44
1:A:120:LEU:O	1:A:121:ASP:C	2.59	0.44
2:B:377:THR:O	2:B:380:ILE:HB	2.18	0.44
1:A:228:LEU:HD22	1:A:228:LEU:HA	1.88	0.44
2:B:126:LYS:HG3	2:B:127:TYR:H	1.82	0.44
2:B:433:PRO:CG	2:B:436:GLY:HA2	2.48	0.44
1:A:366:LYS:O	1:A:370:GLU:HG3	2.18	0.44
1:A:514:GLU:H	1:A:514:GLU:HG3	1.60	0.44
2:B:354:TYR:CE2	2:B:371:ALA:HB2	2.53	0.44
1:A:382:ILE:O	2:B:136:ASN:HB2	2.18	0.43
2:B:23:GLN:OE1	2:B:59:PRO:HA	2.17	0.43
1:A:31:ILE:O	1:A:35:VAL:HG23	2.18	0.43
2:B:201:LYS:HE3	4:B:1175:HOH:O	2.19	0.43
1:A:287:LYS:HG2	1:A:291:GLU:OE1	2.18	0.43
1:A:410:TRP:HZ3	2:B:401:TRP:CE2	2.36	0.43
2:B:66:LYS:HG3	2:B:67:ASP:OD1	2.18	0.43
2:B:170:PRO:O	2:B:174:GLN:HG2	2.18	0.43
2:B:178:ILE:HG22	2:B:179:VAL:N	2.33	0.43
2:B:271:TYR:HB2	2:B:274:ILE:HD11	2.00	0.43
1:A:72:ARG:CG	1:A:73:LYS:N	2.78	0.43
2:B:195:ILE:HG23	2:B:196:GLY:N	2.32	0.43
1:A:26:LEU:HD22	1:A:30:LYS:HE2	2.00	0.43
1:A:164:MET:HE2	1:A:164:MET:HB2	1.89	0.43
1:A:469:LEU:HB2	1:A:472:THR:HG21	2.00	0.43
2:B:380:ILE:O	2:B:384:GLY:N	2.49	0.43
1:A:27:THR:HB	1:A:30:LYS:CG	2.42	0.43
1:A:181:TYR:CE2	1:A:183:TYR:HB2	2.53	0.43
1:A:252:TRP:CD1	1:A:295:LEU:HD12	2.54	0.43
1:A:425:LEU:HD23	1:A:425:LEU:HA	1.87	0.43
2:B:5:ILE:CG2	2:B:6:GLU:H	2.26	0.43
2:B:115:TYR:N	2:B:115:TYR:CD1	2.81	0.43
2:B:242:GLN:HA	2:B:242:GLN:HE21	1.83	0.43
2:B:336:GLN:C	2:B:337:TRP:CD1	2.97	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:ARG:HB2	1:A:367:GLN:NE2	2.34	0.43
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.54	0.43
2:B:104:LYS:HB2	2:B:192:ASP:HA	2.00	0.43
1:A:239:TRP:HE1	1:A:317:VAL:C	2.26	0.42
2:B:120:LEU:C	2:B:120:LEU:HD23	2.44	0.42
1:A:83:ARG:NH1	1:A:83:ARG:HG3	2.30	0.42
1:A:362:THR:HG22	1:A:363:ASN:H	1.83	0.42
2:B:5:ILE:H	2:B:119:PRO:HG3	1.84	0.42
2:B:65:LYS:HZ3	2:B:72:ARG:HD3	1.84	0.42
2:B:232:TYR:CD1	2:B:232:TYR:C	2.96	0.42
1:A:254:VAL:HG13	1:A:283:LEU:HD12	2.01	0.42
1:A:94:ILE:HG22	1:A:95:PRO:O	2.19	0.42
1:A:223:LYS:HB2	1:A:223:LYS:HE3	1.85	0.42
2:B:21:VAL:HB	2:B:59:PRO:HD3	2.00	0.42
1:A:34:LEU:HB3	1:A:132:ILE:HD12	2.01	0.42
1:A:114:ALA:HA	1:A:117:SER:HG	1.79	0.42
2:B:92:LEU:CD2	2:B:165:THR:HG21	2.49	0.42
2:B:149:LEU:HA	2:B:150:PRO:HD3	1.90	0.42
2:B:274:ILE:HG23	2:B:306:ASN:CG	2.43	0.42
2:B:27:THR:OG1	2:B:30:LYS:HG2	2.20	0.42
2:B:101:LYS:HB3	2:B:101:LYS:HZ3	1.83	0.42
2:B:28:GLU:O	2:B:29:GLU:C	2.63	0.42
2:B:157:PRO:CG	2:B:184:MET:HA	2.49	0.42
2:B:195:ILE:CG2	2:B:196:GLY:N	2.82	0.42
1:A:239:TRP:CH2	1:A:316:GLY:HA3	2.53	0.42
1:A:95:PRO:HB3	2:B:136:ASN:ND2	2.35	0.42
1:A:410:TRP:NE1	2:B:363:ASN:HB2	2.33	0.42
2:B:64:LYS:HD2	2:B:71:TRP:CE2	2.55	0.42
2:B:120:LEU:HD23	2:B:121:ASP:O	2.20	0.42
2:B:278:GLN:HB2	2:B:302:GLU:OE1	2.20	0.42
1:A:407:GLN:HG2	2:B:393:ILE:HA	2.01	0.42
1:A:361:HIS:ND1	1:A:361:HIS:N	2.68	0.41
2:B:363:ASN:CG	2:B:366:LYS:HB2	2.45	0.41
2:B:423:VAL:O	2:B:427:TYR:HD2	2.02	0.41
2:B:311:LYS:HE2	4:B:1194:HOH:O	2.20	0.41
1:A:274:ILE:HG12	1:A:309:ILE:HG21	2.02	0.41
1:A:478:GLU:O	1:A:481:ALA:HB3	2.20	0.41
2:B:193:LEU:CD1	2:B:193:LEU:H	2.34	0.41
1:A:184:MET:HB3	1:A:185:ASP:H	1.61	0.41
1:A:178:ILE:HD11	1:A:201:LYS:HG3	2.03	0.41
1:A:357:MET:O	1:A:358:ARG:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:TYR:CE2	1:A:465:LYS:HB3	2.55	0.41
2:B:107:THR:HG23	2:B:232:TYR:HE1	1.85	0.41
1:A:42:GLU:OE1	1:A:49:LYS:HE3	2.20	0.41
1:A:58:THR:HG23	1:A:76:ASP:O	2.20	0.41
1:A:142:ILE:N	1:A:142:ILE:CD1	2.84	0.41
2:B:5:ILE:CG2	2:B:6:GLU:N	2.84	0.41
2:B:94:ILE:HD12	2:B:94:ILE:HA	1.93	0.41
2:B:305:GLU:O	2:B:309:ILE:HG13	2.20	0.41
1:A:11:LYS:O	1:A:85:GLN:HB3	2.20	0.41
1:A:116:PHE:CE1	1:A:151:GLN:HB2	2.56	0.41
3:A:999:U05:N1	3:A:999:U05:C15	2.84	0.41
2:B:356:ARG:CZ	2:B:361:HIS:HB3	2.51	0.41
1:A:37:ILE:N	1:A:37:ILE:HD12	2.36	0.41
1:A:103:LYS:HA	1:A:103:LYS:HD3	1.70	0.41
1:A:444:GLY:CA	1:A:477:THR:HG22	2.50	0.41
1:A:457:TYR:CD1	1:A:457:TYR:C	2.99	0.41
1:A:515:SER:HB3	1:A:518:VAL:HG23	2.03	0.41
2:B:356:ARG:NH2	2:B:361:HIS:HB3	2.36	0.41
1:A:401:TRP:CZ3	1:A:409:THR:HG21	2.56	0.40
2:B:345:PRO:O	2:B:346:PHE:HB2	2.20	0.40
1:A:270:ILE:HD12	1:A:270:ILE:C	2.46	0.40
2:B:106:VAL:HG12	2:B:107:THR:N	2.36	0.40
1:A:116:PHE:O	1:A:148:VAL:HG21	2.21	0.40
1:A:379:SER:CB	1:A:387:PRO:HD3	2.51	0.40
2:B:342:TYR:HB3	2:B:348:ASN:HA	2.03	0.40
1:A:3:SER:OG	1:A:5:ILE:HG22	2.21	0.40
2:B:162:SER:O	2:B:163:SER:C	2.64	0.40
2:B:260:LEU:O	2:B:264:LEU:HG	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	540/560 (96%)	479 (89%)	47 (9%)	14 (3%)	4	2
2	B	414/440 (94%)	378 (91%)	27 (6%)	9 (2%)	5	3
All	All	954/1000 (95%)	857 (90%)	74 (8%)	23 (2%)	4	3

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	88	TRP
1	A	135	ILE
1	A	138	GLU
1	A	358	ARG
1	A	112	GLY
1	A	139	THR
1	A	542	ILE
2	B	237	ASP
1	A	18	GLY
1	A	91	GLN
1	A	230	MET
1	A	360	ALA
2	B	44	GLU
2	B	172	ARG
2	B	162	SER
2	B	185	ASP
2	B	236	PRO
2	B	361	HIS
1	A	357	MET
2	B	94	ILE
2	B	95	PRO
1	A	133	PRO
1	A	111	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	485/499 (97%)	405 (84%)	80 (16%)	2	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	380/400 (95%)	319 (84%)	61 (16%)	2	2
All	All	865/899 (96%)	724 (84%)	141 (16%)	2	2

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LYS
1	A	21	VAL
1	A	30	LYS
1	A	42	GLU
1	A	60	VAL
1	A	63	ILE
1	A	65	LYS
1	A	66	LYS
1	A	68	SER
1	A	72	ARG
1	A	92	LEU
1	A	97	PRO
1	A	105	SER
1	A	113	ASP
1	A	122	GLU
1	A	136	ASN
1	A	138	GLU
1	A	168	LEU
1	A	184	MET
1	A	189	VAL
1	A	194	GLU
1	A	197	GLN
1	A	205	LEU
1	A	216	THR
1	A	221	HIS
1	A	225	PRO
1	A	228	LEU
1	A	234	LEU
1	A	240	THR
1	A	241	VAL
1	A	261	VAL
1	A	263	LYS
1	A	270	ILE
1	A	277	ARG
1	A	279	LEU
1	A	283	LEU

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Mol	Chain	Res	Type
1	A	293	ILE
1	A	295	LEU
1	A	296	THR
1	A	297	GLU
1	A	303	LEU
1	A	309	ILE
1	A	311	LYS
1	A	313	PRO
1	A	315	HIS
1	A	317	VAL
1	A	326	ILE
1	A	332	GLN
1	A	336	GLN
1	A	340	GLN
1	A	357	MET
1	A	358	ARG
1	A	361	HIS
1	A	362	THR
1	A	368	LEU
1	A	369	THR
1	A	373	GLN
1	A	386	THR
1	A	393	ILE
1	A	409	THR
1	A	413	GLU
1	A	423	VAL
1	A	424	LYS
1	A	432	GLU
1	A	448	ARG
1	A	452	LEU
1	A	459	THR
1	A	461	ARG
1	A	470	THR
1	A	474	ASN
1	A	475	GLN
1	A	480	GLN
1	A	491	LEU
1	A	493	VAL
1	A	496	VAL
1	A	503	LEU
1	A	513	SER
1	A	514	GLU

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Mol	Chain	Res	Type
1	A	540	LYS
1	A	542	ILE
2	B	6	GLU
2	B	8	VAL
2	B	10	VAL
2	B	24	TRP
2	B	35	VAL
2	B	46	LYS
2	B	55	PRO
2	B	63	ILE
2	B	69	THR
2	B	84	THR
2	B	87	PHE
2	B	92	LEU
2	B	94	ILE
2	B	95	PRO
2	B	100	LEU
2	B	109	LEU
2	B	120	LEU
2	B	123	ASP
2	B	132	ILE
2	B	139	THR
2	B	145	GLN
2	B	161	GLN
2	B	162	SER
2	B	163	SER
2	B	170	PRO
2	B	174	GLN
2	B	179	VAL
2	B	180	ILE
2	B	186	ASP
2	B	193	LEU
2	B	194	GLU
2	B	197	GLN
2	B	201	LYS
2	B	206	ARG
2	B	211	ARG
2	B	232	TYR
2	B	233	GLU
2	B	236	PRO
2	B	242	GLN
2	B	245	VAL

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Mol	Chain	Res	Type
2	B	263	LYS
2	B	276	VAL
2	B	283	LEU
2	B	284	ARG
2	B	287	LYS
2	B	291	GLU
2	B	303	LEU
2	B	321	PRO
2	B	358	ARG
2	B	362	THR
2	B	363	ASN
2	B	366	LYS
2	B	368	LEU
2	B	379	SER
2	B	390	LYS
2	B	399	GLU
2	B	418	ASN
2	B	420	PRO
2	B	423	VAL
2	B	425	LEU
2	B	429	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	91	GLN
1	A	174	GLN
1	A	175	ASN
1	A	197	GLN
1	A	207	GLN
1	A	222	GLN
1	A	242	GLN
1	A	332	GLN
1	A	336	GLN
1	A	363	ASN
1	A	428	GLN
1	A	475	GLN
1	A	480	GLN
1	A	512	GLN
2	B	57	ASN
2	B	85	GLN

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Mol	Chain	Res	Type
2	B	96	HIS
2	B	151	GLN
2	B	242	GLN
2	B	269	GLN
2	B	361	HIS
2	B	428	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	$\# Z > 2$
1	CSD	A	280	1	4,7,8	1.78	1 (25%)	1,8,10	5.40	1 (100%)

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
1	CSD	A	280	1	-	2/2/6/8	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	280	CSD	OD1-SG	2.74	1.50	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	CSD	OD1-SG-CB	5.40	115.55	105.60

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	280	CSD	N-CA-CB-SG
1	A	280	CSD	CA-CB-SG-OD1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	280	CSD	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	$\# Z > 2$
3	U05	A	999	-	22,24,24	1.84	5 (22%)	26,35,35	2.16	5 (19%)

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	U05	A	999	-	-	1/4/6/6	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	U05	C9-N	3.84	1.54	1.45
3	A	999	U05	C3-C4	3.52	1.44	1.38
3	A	999	U05	C14-N11	3.03	1.55	1.47
3	A	999	U05	C8-C7	2.72	1.43	1.38
3	A	999	U05	C4A-C5	2.03	1.53	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	U05	N1-C1A-N11	5.27	121.60	114.94
3	A	999	U05	C6A-C11-N11	-4.97	116.23	121.47
3	A	999	U05	C4A-C1A-N11	-4.46	115.60	120.93
3	A	999	U05	C12-N6-C6A	-3.19	113.38	118.38
3	A	999	U05	C8-C9-N	2.38	121.42	119.34

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	999	U05	C15-C14-N11-C1A

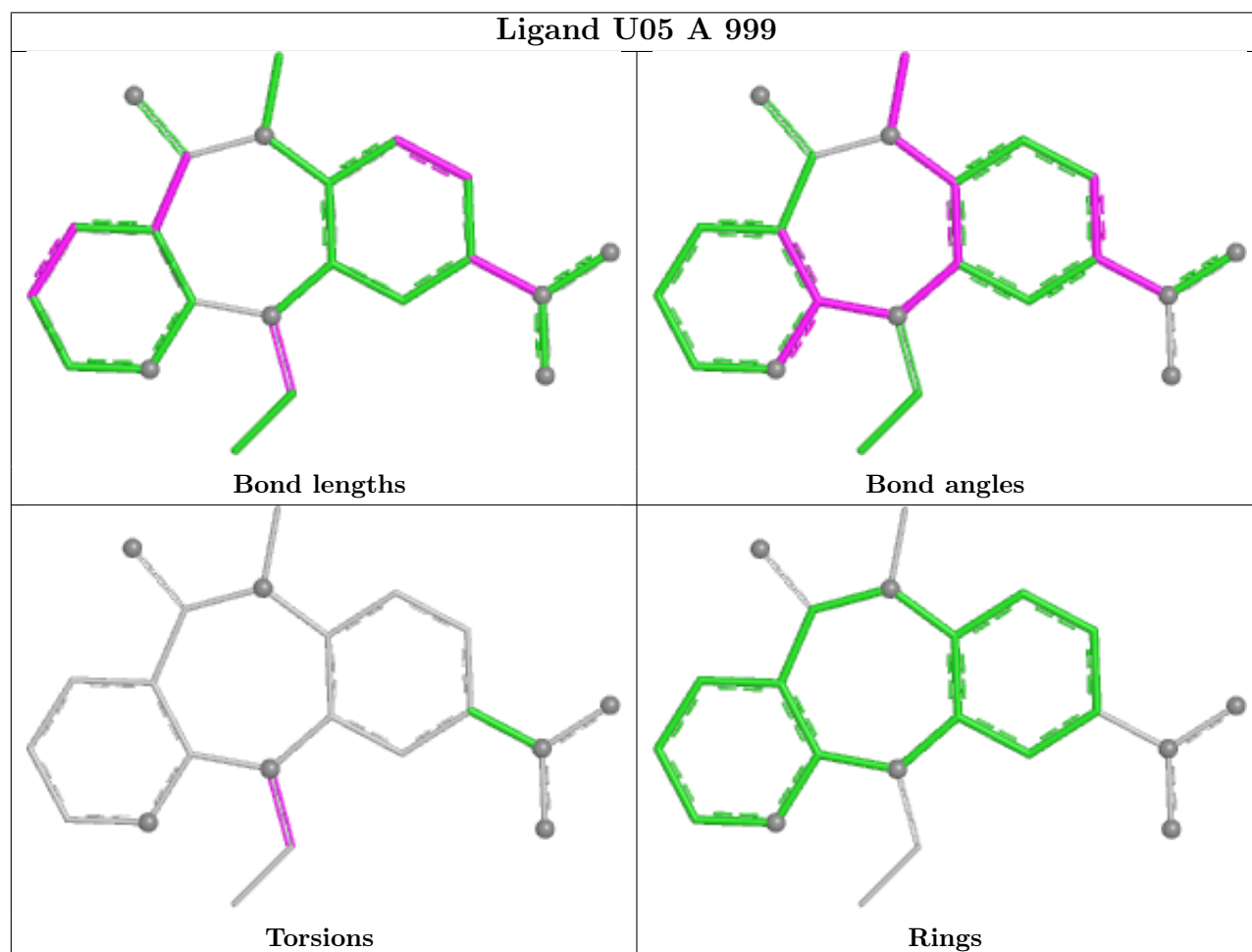
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	U05	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.