



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:43 PM UTC

PDB ID : 1RT3 / pdb\_00001rt3  
Title : AZT DRUG RESISTANT HIV-1 REVERSE TRANSCRIPTASE COM-  
PLEXED WITH 1051U91  
Authors : Ren, J.; Stammers, D.K.; Stuart, D.I.  
Deposited on : 1998-06-29  
Resolution : 3.00 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](mailto: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>.

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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) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

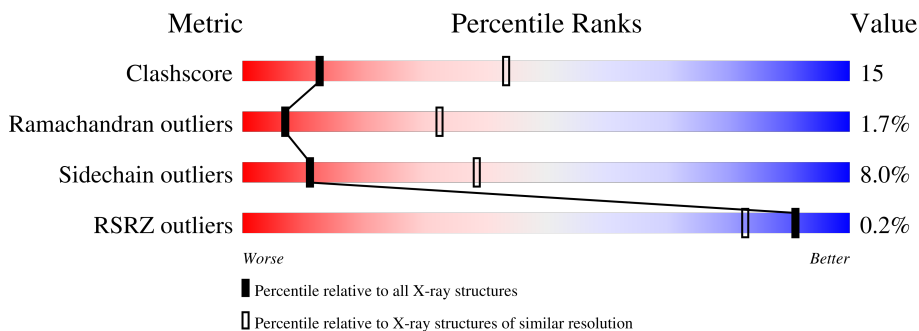
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	560	 57% 30% 6% • 7%
2	B	440	 55% 33% • 10%

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7599 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
			Total	C	N	O	S			
1	A	521	4283	2779	709	787	8	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	ASN	ASP	engineered mutation	UNP P04585
A	70	ARG	LYS	engineered mutation	UNP P04585
A	215	PHE	THR	engineered mutation	UNP P04585
A	219	GLN	LYS	engineered mutation	UNP P04585
A	280	CSD	CYS	modified residue	UNP P04585

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	398	3294	2143	547	597	7	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	67	ASN	ASP	engineered mutation	UNP P04585
B	70	ARG	LYS	engineered mutation	UNP P04585

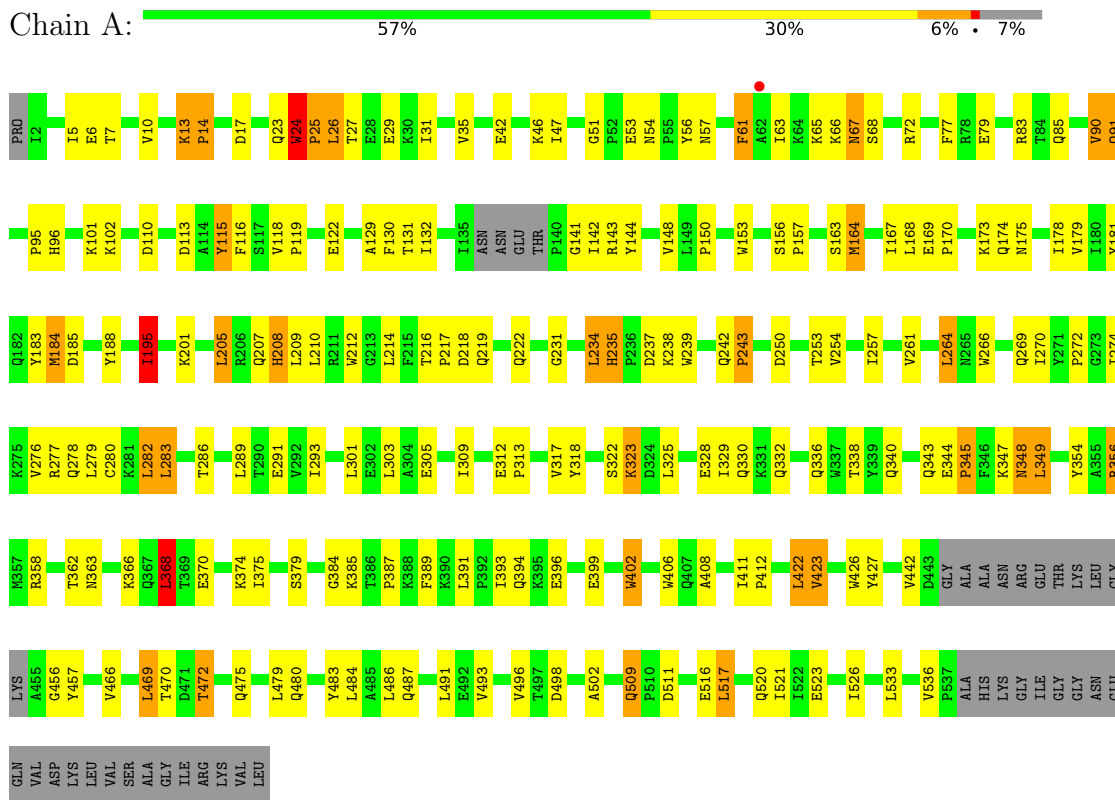
- Molecule 3 is 6,11-DIHYDRO-11-ETHYL-6-METHYL-9-NITRO-5H-PYRIDO[2,3-B][1,5]BENZODIAZEPIN-5-ONE (CCD ID: U05) (formula: C<sub>15</sub>H<sub>14</sub>N<sub>4</sub>O<sub>3</sub>).



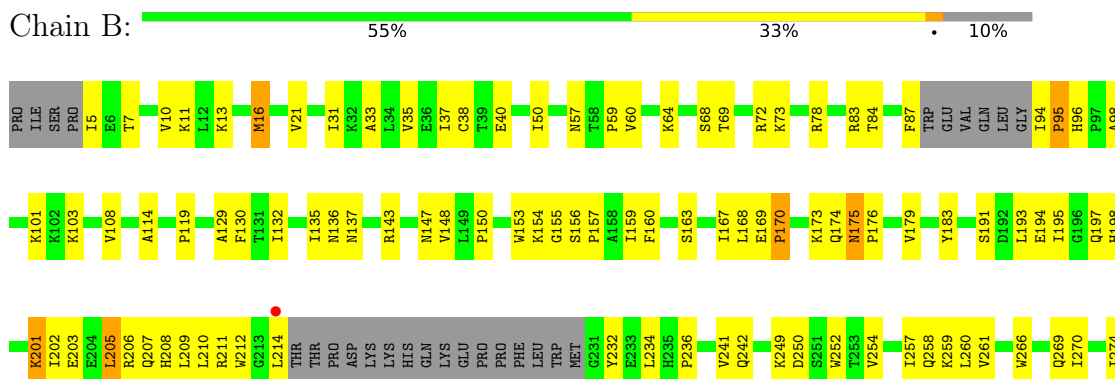
### 3 Residue-property plots

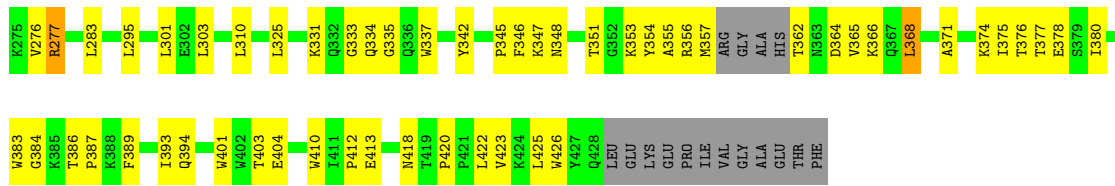
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

#### • Molecule 1: HIV-1 REVERSE TRANSCRIPTASE



#### • Molecule 2: HIV-1 REVERSE TRANSCRIPTASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	138.90Å 114.40Å 65.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 3.00 25.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	83.3 (25.00-3.00) 83.1 (25.00-3.00)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.94 (at 3.01Å)	Xtrriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.264 , 0.335 0.237 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.3	Xtrriage
Anisotropy	0.058	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 81.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	7599	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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: CSD, U05

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	0.38	0/4389	0.90	17/5965 (0.3%)
2	B	0.37	0/3384	0.86	5/4594 (0.1%)
All	All	0.37	0/7773	0.88	22/10559 (0.2%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	349	LEU	N-CA-C	-7.22	104.60	113.41
1	A	348	ASN	N-CA-C	6.92	119.67	110.53
1	A	234	LEU	N-CA-C	6.67	119.61	108.20
1	A	24	TRP	CB-CA-C	6.51	117.57	110.08
2	B	170	PRO	N-CA-C	-6.27	106.02	113.86
2	B	169	GLU	CA-C-N	-6.05	113.45	119.56
2	B	169	GLU	C-N-CA	-6.05	113.45	119.56
1	A	13	LYS	CA-C-N	5.84	127.14	119.84
1	A	13	LYS	C-N-CA	5.84	127.14	119.84
1	A	235	HIS	N-CA-C	-5.73	102.94	110.39
1	A	250	ASP	N-CA-C	-5.51	105.60	112.93
1	A	24	TRP	CA-C-N	5.43	126.62	119.84
1	A	24	TRP	C-N-CA	5.43	126.62	119.84
1	A	118	VAL	CA-C-N	5.37	125.66	119.92
1	A	118	VAL	C-N-CA	5.37	125.66	119.92
1	A	96	HIS	CA-C-N	5.36	126.54	119.84
1	A	96	HIS	C-N-CA	5.36	126.54	119.84
2	B	168	LEU	N-CA-C	5.32	119.83	113.23
2	B	147	ASN	N-CA-C	-5.24	107.02	113.41
1	A	208	HIS	N-CA-C	-5.15	105.67	111.28
1	A	368	LEU	N-CA-C	-5.09	105.63	111.07
1	A	487	GLN	N-CA-C	5.01	117.47	111.71

There are no chirality outliers.

There are no planarity outliers.

## 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	4283	0	4320	132	0
2	B	3294	0	3329	105	0
3	A	22	0	14	5	0
All	All	7599	0	7663	232	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 15.

All (232) 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:114:ALA:HB2	2:B:214:LEU:HD13	1.57	0.85
1:A:90:VAL:HG12	1:A:91:GLN:H	1.41	0.83
1:A:181:TYR:HD2	3:A:999:U05:H141	1.46	0.79
1:A:469:LEU:H	1:A:469:LEU:HD22	1.50	0.76
1:A:264:LEU:HD23	1:A:276:VAL:HG12	1.68	0.76
2:B:16:MET:HE3	2:B:83:ARG:HA	1.68	0.75
1:A:277:ARG:NH1	1:A:336:GLN:HE22	1.84	0.75
1:A:354:TYR:HD1	1:A:374:LYS:HD2	1.53	0.73
2:B:193:LEU:HD23	2:B:197:GLN:HG3	1.71	0.71
1:A:517:LEU:HA	1:A:520:GLN:HE21	1.55	0.70
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.73	0.69
1:A:90:VAL:HG12	1:A:91:GLN:N	2.08	0.69
2:B:119:PRO:HA	2:B:148:VAL:HA	1.75	0.68
2:B:242:GLN:HE21	2:B:353:LYS:HE3	1.58	0.68
2:B:261:VAL:HG13	2:B:276:VAL:HG11	1.74	0.68
1:A:181:TYR:HD2	3:A:999:U05:H10	1.59	0.67
1:A:393:ILE:HB	1:A:423:VAL:HG22	1.77	0.66
1:A:181:TYR:CD2	3:A:999:U05:H10	2.30	0.66
2:B:274:ILE:HD11	2:B:310:LEU:HD21	1.78	0.66
2:B:203:GLU:HG3	2:B:207:GLN:HE22	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:38:CYS:SG	2:B:73:LYS:HE2	2.37	0.65
1:A:279:LEU:HA	1:A:282:LEU:HD23	1.80	0.63
1:A:90:VAL:CG1	1:A:91:GLN:H	2.08	0.63
1:A:456:GLY:HA3	1:A:466:VAL:HG22	1.79	0.63
2:B:7:THR:HG22	2:B:119:PRO:HG2	1.82	0.62
2:B:242:GLN:NE2	2:B:353:LYS:HE3	2.14	0.62
2:B:13:LYS:HE3	2:B:84:THR:O	2.00	0.61
2:B:362:THR:HA	2:B:366:LYS:HD3	1.80	0.61
1:A:181:TYR:CD2	3:A:999:U05:H141	2.33	0.61
2:B:365:VAL:HG11	2:B:401:TRP:HB2	1.81	0.61
1:A:195:ILE:HD12	1:A:195:ILE:H	1.66	0.60
1:A:329:ILE:HD11	1:A:375:ILE:HD12	1.83	0.59
2:B:362:THR:HG22	2:B:366:LYS:HD3	1.83	0.59
2:B:191:SER:HB2	2:B:193:LEU:HD13	1.85	0.59
2:B:154:LYS:O	2:B:157:PRO:HD2	2.02	0.59
1:A:235:HIS:HB2	1:A:238:LYS:O	2.03	0.59
2:B:37:ILE:O	2:B:40:GLU:HG2	2.03	0.58
2:B:420:PRO:O	2:B:423:VAL:HG12	2.03	0.58
1:A:132:ILE:HB	1:A:142:ILE:HD11	1.86	0.58
2:B:342:TYR:HB3	2:B:348:ASN:HA	1.85	0.58
1:A:209:LEU:HB3	1:A:214:LEU:HB2	1.84	0.58
1:A:115:TYR:CE2	1:A:156:SER:HB3	2.38	0.58
2:B:254:VAL:O	2:B:258:GLN:HG3	2.03	0.58
2:B:201:LYS:HE3	2:B:201:LYS:HA	1.86	0.57
1:A:366:LYS:O	1:A:370:GLU:HG3	2.04	0.57
1:A:427:TYR:OH	1:A:509:GLN:HA	2.05	0.57
2:B:193:LEU:HB3	2:B:197:GLN:HB3	1.88	0.56
2:B:354:TYR:CZ	2:B:357:MET:SD	2.99	0.56
2:B:57:ASN:HD22	2:B:143:ARG:NH1	2.03	0.56
1:A:498:ASP:HA	1:A:536:VAL:O	2.06	0.55
1:A:131:THR:OG1	1:A:143:ARG:HD2	2.07	0.55
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.88	0.55
1:A:132:ILE:HB	1:A:142:ILE:CD1	2.37	0.55
1:A:207:GLN:HA	1:A:210:LEU:HB2	1.88	0.55
2:B:64:LYS:HE2	2:B:68:SER:O	2.07	0.54
1:A:270:ILE:O	1:A:272:PRO:HD3	2.07	0.54
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.90	0.54
1:A:77:PHE:CE2	1:A:150:PRO:HB3	2.43	0.53
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.43	0.53
2:B:94:ILE:N	2:B:95:PRO:CD	2.71	0.53
1:A:17:ASP:O	1:A:83:ARG:HD3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:LEU:HD12	1:A:422:LEU:H	1.74	0.53
1:A:61:PHE:CD1	1:A:61:PHE:N	2.77	0.53
2:B:401:TRP:O	2:B:404:GLU:HB2	2.07	0.53
1:A:469:LEU:HD23	1:A:472:THR:HG21	1.90	0.53
2:B:266:TRP:O	2:B:269:GLN:HG2	2.09	0.53
1:A:42:GLU:HA	1:A:47:ILE:O	2.09	0.53
2:B:31:ILE:O	2:B:35:VAL:HG23	2.09	0.53
2:B:103:LYS:O	2:B:236:PRO:HG2	2.09	0.53
2:B:16:MET:CE	2:B:83:ARG:HA	2.39	0.53
2:B:211:ARG:HG2	2:B:212:TRP:CZ3	2.43	0.52
1:A:384:GLY:HA3	2:B:135:ILE:HD12	1.90	0.52
1:A:95:PRO:HB3	2:B:136:ASN:O	2.10	0.52
1:A:282:LEU:HD12	1:A:293:ILE:CG2	2.40	0.52
1:A:379:SER:CB	1:A:387:PRO:HD3	2.39	0.52
1:A:26:LEU:N	1:A:26:LEU:HD12	2.25	0.52
1:A:27:THR:HG22	1:A:29:GLU:H	1.75	0.52
2:B:103:LYS:HE2	2:B:179:VAL:HG21	1.91	0.51
1:A:46:LYS:HD3	1:A:116:PHE:CD2	2.45	0.51
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.45	0.51
1:A:354:TYR:CD1	1:A:374:LYS:HD2	2.39	0.51
2:B:84:THR:HB	2:B:154:LYS:HE2	1.91	0.51
2:B:163:SER:O	2:B:167:ILE:HG13	2.10	0.51
1:A:27:THR:HG22	1:A:29:GLU:N	2.25	0.51
1:A:368:LEU:HD21	1:A:391:LEU:HD22	1.92	0.51
2:B:193:LEU:HD23	2:B:197:GLN:CG	2.38	0.51
2:B:259:LYS:HE3	2:B:425:LEU:HD11	1.93	0.51
1:A:239:TRP:HZ2	1:A:349:LEU:O	1.94	0.50
1:A:174:GLN:HG3	1:A:175:ASN:ND2	2.27	0.50
1:A:31:ILE:O	1:A:35:VAL:HG23	2.12	0.50
2:B:156:SER:HB2	2:B:157:PRO:HD3	1.93	0.50
1:A:266:TRP:O	1:A:269:GLN:HG2	2.12	0.49
1:A:90:VAL:CG1	1:A:91:GLN:N	2.73	0.49
1:A:178:ILE:HG22	1:A:179:VAL:N	2.27	0.49
1:A:26:LEU:HD12	1:A:26:LEU:H	1.78	0.49
2:B:10:VAL:HG21	2:B:159:ILE:HD11	1.95	0.48
2:B:295:LEU:H	2:B:295:LEU:HD12	1.77	0.48
1:A:475:GLN:O	1:A:479:LEU:HD13	2.14	0.48
2:B:393:ILE:HG12	2:B:394:GLN:N	2.27	0.48
1:A:23:GLN:NE2	1:A:24:TRP:O	2.46	0.48
2:B:57:ASN:HA	2:B:129:ALA:O	2.13	0.48
2:B:355:ALA:O	2:B:357:MET:SD	2.72	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:371:ALA:O	2:B:375:ILE:HG13	2.14	0.47
1:A:115:TYR:HE2	1:A:156:SER:HB3	1.78	0.47
1:A:208:HIS:O	1:A:212:TRP:HD1	1.97	0.47
1:A:27:THR:O	1:A:31:ILE:HG13	2.14	0.47
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.95	0.47
1:A:323:LYS:O	1:A:343:GLN:NE2	2.48	0.47
1:A:442:VAL:HG22	1:A:496:VAL:O	2.15	0.47
1:A:164:MET:HE3	1:A:214:LEU:CD1	2.45	0.47
1:A:24:TRP:CD1	1:A:24:TRP:C	2.93	0.47
1:A:317:VAL:HG12	1:A:318:TYR:O	2.15	0.47
2:B:50:ILE:HG13	2:B:143:ARG:HB3	1.97	0.47
1:A:516:GLU:O	1:A:520:GLN:HG3	2.15	0.46
1:A:183:TYR:HB3	1:A:188:TYR:CE2	2.50	0.46
1:A:257:ILE:O	1:A:261:VAL:HG23	2.14	0.46
2:B:13:LYS:HD2	2:B:16:MET:HE2	1.96	0.46
1:A:54:ASN:ND2	1:A:129:ALA:HB2	2.31	0.46
1:A:67:ASN:C	1:A:67:ASN:HD22	2.24	0.46
2:B:132:ILE:HD12	2:B:132:ILE:N	2.31	0.46
1:A:63:ILE:O	1:A:72:ARG:N	2.49	0.46
1:A:163:SER:O	1:A:167:ILE:HG13	2.15	0.46
1:A:332:GLN:HB2	1:A:338:THR:HG23	1.97	0.46
2:B:331:LYS:HB2	2:B:337:TRP:CZ3	2.50	0.46
2:B:57:ASN:HD22	2:B:143:ARG:HH12	1.63	0.46
1:A:170:PRO:O	1:A:173:LYS:HB3	2.15	0.46
1:A:235:HIS:HB2	1:A:238:LYS:HG3	1.97	0.46
1:A:282:LEU:HD12	1:A:293:ILE:HG22	1.97	0.46
1:A:234:LEU:HD23	3:A:999:U05:C5	2.47	0.45
1:A:13:LYS:HG3	1:A:85:GLN:HA	1.97	0.45
1:A:426:TRP:CE3	1:A:526:ILE:HD13	2.52	0.45
1:A:102:LYS:HG3	1:A:237:ASP:HA	1.98	0.45
1:A:167:ILE:HG23	1:A:212:TRP:CD1	2.52	0.45
1:A:253:THR:HG22	1:A:289:LEU:O	2.17	0.45
1:A:79:GLU:OE1	1:A:79:GLU:HA	2.16	0.45
1:A:278:GLN:O	1:A:282:LEU:HD22	2.17	0.45
2:B:167:ILE:O	2:B:208:HIS:HE1	2.00	0.45
2:B:241:VAL:HG13	2:B:351:THR:OG1	2.17	0.45
2:B:94:ILE:N	2:B:95:PRO:HD3	2.32	0.45
2:B:103:LYS:HE2	2:B:179:VAL:CG2	2.46	0.45
2:B:335:GLY:HA3	2:B:356:ARG:HE	1.81	0.45
2:B:60:VAL:HG11	2:B:130:PHE:CD2	2.52	0.45
2:B:183:TYR:OH	2:B:386:THR:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:170:PRO:HG2	2:B:208:HIS:NE2	2.32	0.45
2:B:362:THR:HA	2:B:366:LYS:CD	2.46	0.45
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.52	0.44
1:A:363:ASN:HA	1:A:511:ASP:CG	2.43	0.44
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.17	0.44
1:A:205:LEU:O	1:A:205:LEU:HD22	2.17	0.44
2:B:205:LEU:O	2:B:209:LEU:HG	2.18	0.44
1:A:254:VAL:HG23	1:A:291:GLU:O	2.18	0.44
2:B:150:PRO:HG2	2:B:153:TRP:HB2	1.99	0.44
1:A:24:TRP:O	1:A:24:TRP:CD1	2.70	0.44
1:A:317:VAL:HG12	1:A:318:TYR:N	2.33	0.44
1:A:408:ALA:HB2	2:B:337:TRP:HH2	1.82	0.44
1:A:442:VAL:HG12	1:A:457:TYR:HB3	1.99	0.44
2:B:98:ALA:O	2:B:101:LYS:HG2	2.18	0.44
2:B:270:ILE:HG12	2:B:346:PHE:HB3	2.00	0.44
1:A:102:LYS:HD2	1:A:237:ASP:HB2	2.00	0.44
1:A:24:TRP:HA	1:A:25:PRO:HD2	1.70	0.43
1:A:231:GLY:O	1:A:242:GLN:HG2	2.17	0.43
1:A:347:LYS:HD3	1:A:347:LYS:HA	1.71	0.43
1:A:366:LYS:NZ	1:A:370:GLU:OE2	2.51	0.43
1:A:389:PHE:CE2	1:A:412:PRO:HG2	2.53	0.43
2:B:33:ALA:O	2:B:37:ILE:HG13	2.18	0.43
2:B:114:ALA:HB1	2:B:160:PHE:CZ	2.54	0.43
2:B:208:HIS:O	2:B:211:ARG:HB3	2.19	0.43
2:B:295:LEU:HD12	2:B:295:LEU:N	2.34	0.43
2:B:325:LEU:HD21	2:B:383:TRP:CE3	2.53	0.43
2:B:368:LEU:HD23	2:B:368:LEU:HA	1.77	0.43
2:B:380:ILE:O	2:B:384:GLY:HA2	2.18	0.43
1:A:54:ASN:HB3	1:A:143:ARG:HH21	1.84	0.43
2:B:13:LYS:HB2	2:B:16:MET:HG3	2.01	0.43
1:A:54:ASN:HD21	1:A:129:ALA:HB2	1.83	0.43
1:A:57:ASN:OD1	1:A:143:ARG:NH1	2.51	0.43
1:A:150:PRO:HB2	1:A:153:TRP:HB2	1.99	0.43
1:A:283:LEU:O	1:A:286:THR:HG23	2.18	0.43
2:B:375:ILE:HD12	2:B:389:PHE:HE2	1.83	0.43
1:A:195:ILE:HD12	1:A:195:ILE:N	2.32	0.43
1:A:110:ASP:H	1:A:217:PRO:HG3	1.84	0.43
1:A:305:GLU:O	1:A:309:ILE:HG13	2.18	0.43
1:A:24:TRP:O	1:A:24:TRP:HD1	2.02	0.43
2:B:206:ARG:O	2:B:210:LEU:HD23	2.19	0.43
1:A:17:ASP:OD1	1:A:56:TYR:HE1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:175:ASN:N	2:B:176:PRO:HD3	2.34	0.43
1:A:486:LEU:CD1	1:A:521:ILE:HG23	2.49	0.42
2:B:94:ILE:HG13	2:B:94:ILE:O	2.19	0.42
1:A:264:LEU:O	1:A:274:ILE:HG21	2.19	0.42
2:B:87:PHE:CE2	2:B:155:GLY:HA2	2.54	0.42
1:A:399:GLU:HA	1:A:402:TRP:HE3	1.84	0.42
2:B:31:ILE:HD12	2:B:135:ILE:HD11	2.01	0.42
2:B:276:VAL:O	2:B:277:ARG:C	2.63	0.42
2:B:422:LEU:HB3	2:B:426:TRP:CH2	2.55	0.42
1:A:479:LEU:HD12	1:A:502:ALA:HB2	2.02	0.42
2:B:170:PRO:O	2:B:174:GLN:HB2	2.20	0.42
1:A:325:LEU:HD12	1:A:385:LYS:HG3	2.02	0.42
2:B:374:LYS:O	2:B:378:GLU:HG3	2.19	0.42
1:A:119:PRO:HA	1:A:148:VAL:HA	2.02	0.41
2:B:234:LEU:HD21	2:B:377:THR:CG2	2.49	0.41
2:B:333:GLY:O	2:B:334:GLN:HG2	2.21	0.41
2:B:342:TYR:CB	2:B:348:ASN:HA	2.50	0.41
2:B:78:ARG:NH1	2:B:412:PRO:O	2.54	0.41
2:B:95:PRO:O	2:B:96:HIS:HB2	2.20	0.41
2:B:198:HIS:O	2:B:202:ILE:HG12	2.19	0.41
1:A:219:GLN:HA	1:A:222:GLN:NE2	2.35	0.41
1:A:253:THR:O	1:A:257:ILE:HG13	2.19	0.41
2:B:108:VAL:HB	2:B:232:TYR:HB3	2.03	0.41
1:A:483:TYR:CZ	1:A:520:GLN:HB3	2.55	0.41
2:B:234:LEU:N	2:B:234:LEU:HD12	2.35	0.41
1:A:184:MET:HB3	1:A:185:ASP:H	1.68	0.41
1:A:168:LEU:HD21	1:A:209:LEU:HD21	2.03	0.41
1:A:293:ILE:N	1:A:293:ILE:HD12	2.35	0.41
2:B:150:PRO:HG2	2:B:153:TRP:CB	2.50	0.41
2:B:269:GLN:HE21	2:B:269:GLN:HB3	1.67	0.41
1:A:164:MET:HE2	1:A:164:MET:HA	2.02	0.41
1:A:328:GLU:HG2	1:A:330:GLN:NE2	2.36	0.41
1:A:484:LEU:HD23	1:A:484:LEU:HA	1.94	0.41
2:B:249:LYS:HG3	2:B:252:TRP:CE2	2.56	0.41
2:B:252:TRP:CZ3	2:B:260:LEU:HD22	2.56	0.41
1:A:10:VAL:HG11	1:A:153:TRP:CH2	2.54	0.40
1:A:257:ILE:HD13	1:A:282:LEU:HB3	2.03	0.40
2:B:365:VAL:HG11	2:B:401:TRP:CB	2.49	0.40
1:A:51:GLY:C	1:A:53:GLU:H	2.29	0.40
1:A:101:LYS:N	1:A:101:LYS:HD2	2.36	0.40
1:A:113:ASP:C	1:A:115:TYR:N	2.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:ILE:HD11	1:A:201:LYS:HD2	2.03	0.40
1:A:183:TYR:HB3	1:A:188:TYR:HE2	1.85	0.40
2:B:257:ILE:O	2:B:261:VAL:HG23	2.21	0.40
2:B:425:LEU:HD23	2:B:425:LEU:O	2.21	0.40
1:A:358:ARG:HD3	1:A:370:GLU:CD	2.47	0.40
2:B:345:PRO:C	2:B:347:LYS:H	2.29	0.40
2:B:376:THR:HB	2:B:410:TRP:CH2	2.57	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	514/560 (92%)	471 (92%)	32 (6%)	11 (2%)	<b>5</b> 27
2	B	390/440 (89%)	363 (93%)	23 (6%)	4 (1%)	12 <b>45</b>
All	All	904/1000 (90%)	834 (92%)	55 (6%)	15 (2%)	<b>7</b> 32

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	VAL
1	A	472	THR
1	A	195	ILE
1	A	313	PRO
2	B	95	PRO
2	B	195	ILE
2	B	277	ARG
1	A	14	PRO
1	A	356	ARG
1	A	243	PRO
1	A	345	PRO

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Mol	Chain	Res	Type
1	A	402	TRP
1	A	25	PRO
2	B	69	THR
1	A	141	GLY

### 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	470/499 (94%)	420 (89%)	50 (11%)	6	27
2	B	363/400 (91%)	346 (95%)	17 (5%)	23	58
All	All	833/899 (93%)	766 (92%)	67 (8%)	11	38

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	6	GLU
1	A	7	THR
1	A	14	PRO
1	A	24	TRP
1	A	26	LEU
1	A	61	PHE
1	A	65	LYS
1	A	66	LYS
1	A	67	ASN
1	A	68	SER
1	A	91	GLN
1	A	115	TYR
1	A	122	GLU
1	A	164	MET
1	A	184	MET
1	A	195	ILE
1	A	205	LEU
1	A	216	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	218	ASP
1	A	243	PRO
1	A	264	LEU
1	A	282	LEU
1	A	283	LEU
1	A	301	LEU
1	A	303	LEU
1	A	312	GLU
1	A	322	SER
1	A	323	LYS
1	A	340	GLN
1	A	344	GLU
1	A	345	PRO
1	A	348	ASN
1	A	356	ARG
1	A	362	THR
1	A	368	LEU
1	A	394	GLN
1	A	396	GLU
1	A	411	ILE
1	A	422	LEU
1	A	423	VAL
1	A	469	LEU
1	A	470	THR
1	A	480	GLN
1	A	491	LEU
1	A	493	VAL
1	A	509	GLN
1	A	517	LEU
1	A	523	GLU
1	A	533	LEU
2	B	5	ILE
2	B	11	LYS
2	B	16	MET
2	B	72	ARG
2	B	137	ASN
2	B	173	LYS
2	B	175	ASN
2	B	194	GLU
2	B	201	LYS
2	B	205	LEU
2	B	250	ASP

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Mol	Chain	Res	Type
2	B	283	LEU
2	B	301	LEU
2	B	303	LEU
2	B	368	LEU
2	B	403	THR
2	B	413	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	91	GLN
1	A	174	GLN
1	A	197	GLN
1	A	255	ASN
1	A	258	GLN
1	A	265	ASN
1	A	336	GLN
1	A	487	GLN
1	A	512	GLN
1	A	520	GLN
1	A	524	GLN
2	B	57	ASN
2	B	67	ASN
2	B	151	GLN
2	B	161	GLN
2	B	207	GLN
2	B	242	GLN
2	B	269	GLN
2	B	278	GLN
2	B	407	GLN
2	B	428	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
1	CSD	A	280	1	4,7,8	1.06	0	1,8,10	3.15	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	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	280	CSD	OD1-SG-CB	3.15	111.41	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.

No monomer is involved in short contacts.

## 5.5 Carbohydrates

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

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	0.83	1 (4%)	26,35,35	1.38	2 (7%)

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	-	-	0/4/6/6	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	U05	O1-N	-2.10	1.21	1.35

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	U05	N1-C1A-N11	3.56	119.44	114.94
3	A	999	U05	C12-N6-C6A	-3.13	113.48	118.38

There are no chirality outliers.

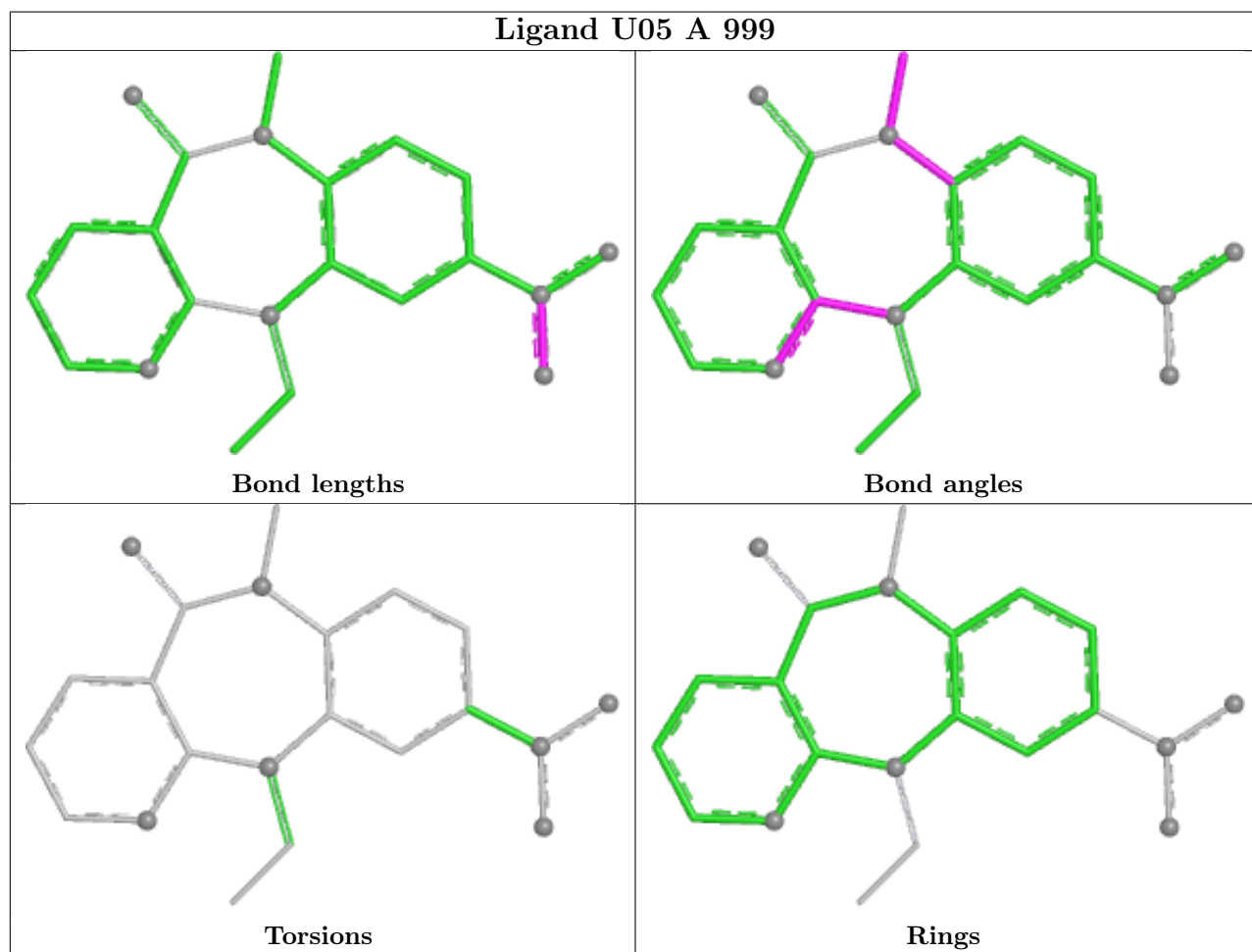
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	U05	5	0

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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	520/560 (92%)	-0.16	1 (0%) 91 83	6, 49, 106, 147	0
2	B	398/440 (90%)	-0.33	1 (0%) 90 79	11, 42, 92, 128	0
All	All	918/1000 (91%)	-0.24	2 (0%) 91 83	6, 47, 101, 147	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	214	LEU	2.1
1	A	62	ALA	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	CSD	A	280	8/9	0.94	0.07	34,45,52,60	0

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

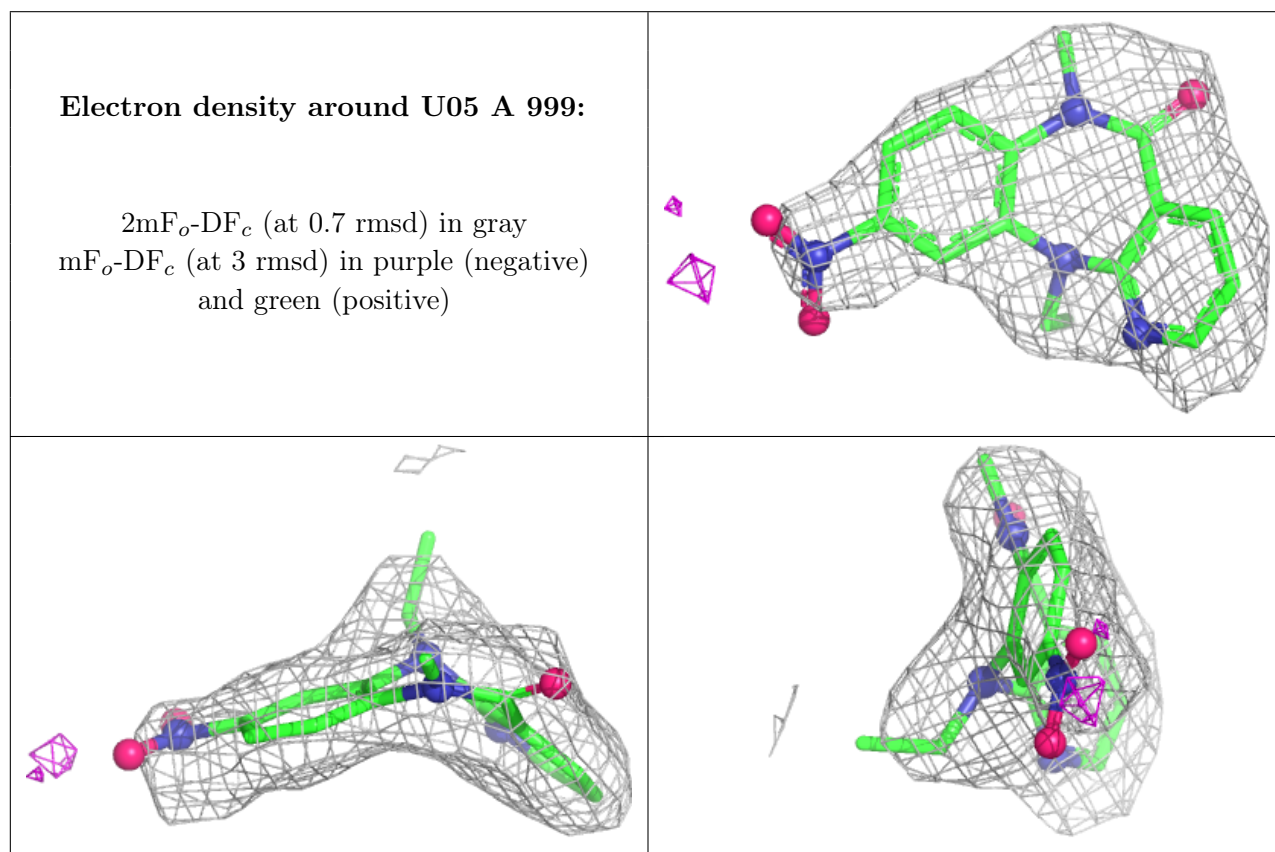
### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	U05	A	999	22/22	0.93	0.09	12,34,85,94	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



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

There are no such residues in this entry.