



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:16 PM UTC

PDB ID : 1REV / pdb_00001rev
Title : HIV-1 REVERSE TRANSCRIPTASE
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Deposited on : 1995-09-17
Resolution : 2.60 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

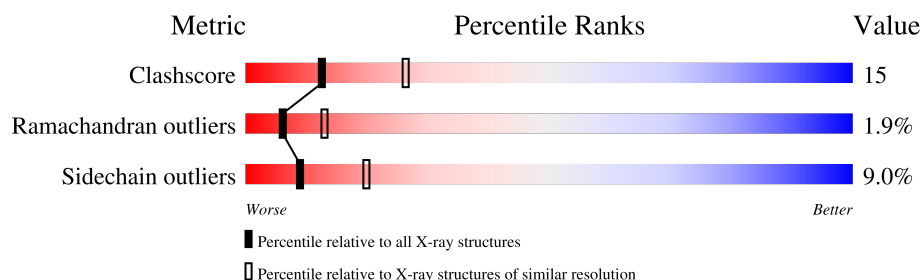
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

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	
2	B	440	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7844 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	525	Total	C	N	O	S	0	0	0
			4310	2792	714	796	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	CSD	CYS	conflict	UNP P04585

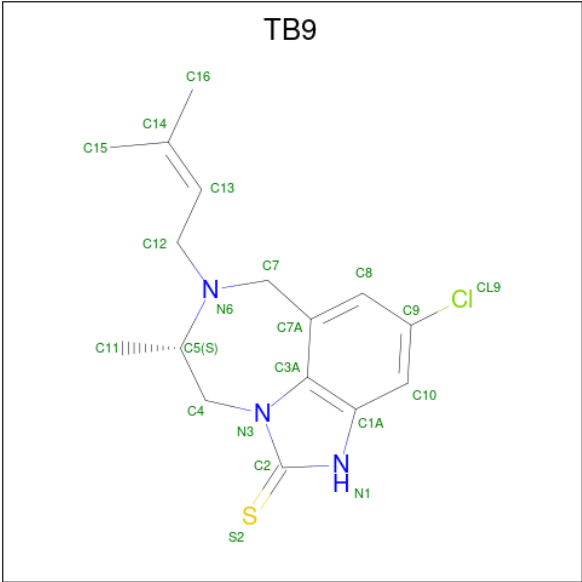
- Molecule 2 is a protein called HIV-1 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	412	Total	C	N	O	S	0	0	0
			3401	2212	565	617	7			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is 4-CHLORO-8-METHYL-7-(3-METHYL-BUT-2-ENYL)-6,7,8,9-TETRAHYDRO-2H-2,7,9A-TRIAZA-BENZO[CD]AZULENE-1-THIONE (CCD ID: TB9) (formula: C₁₆H₂₀ClN₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	S	0	0
			21	16	1	3	1		

- Molecule 5 is water.

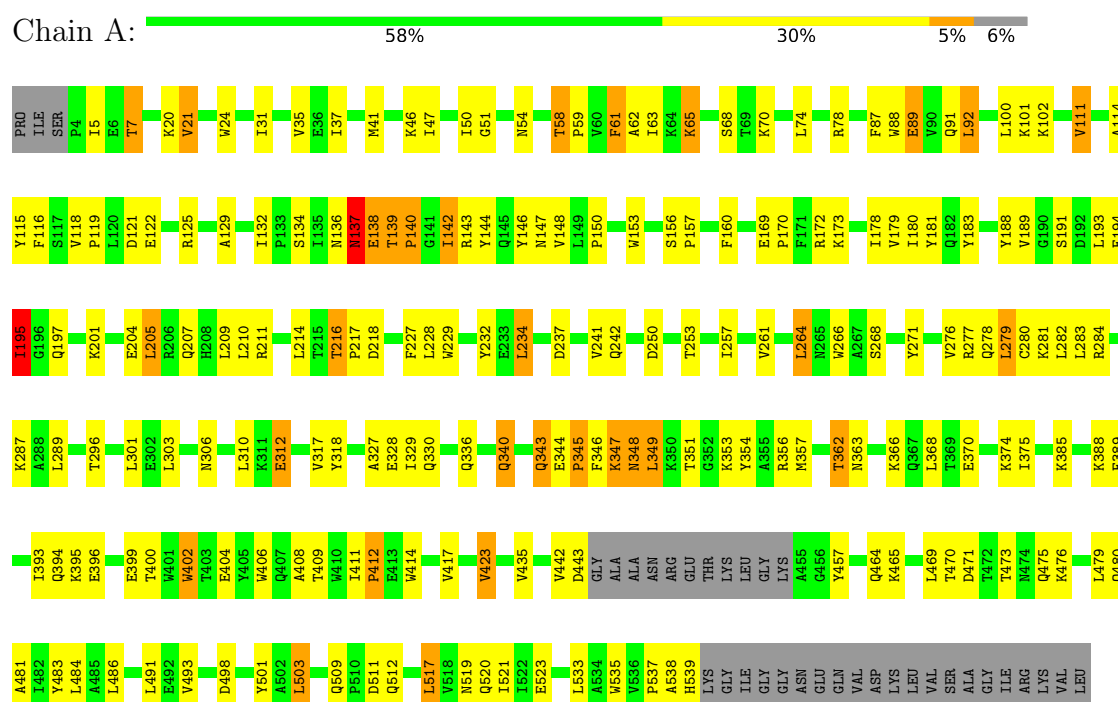
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	79	Total	O	0	0
			79	79		
5	B	32	Total	O	0	0
			32	32		

3 Residue-property plots

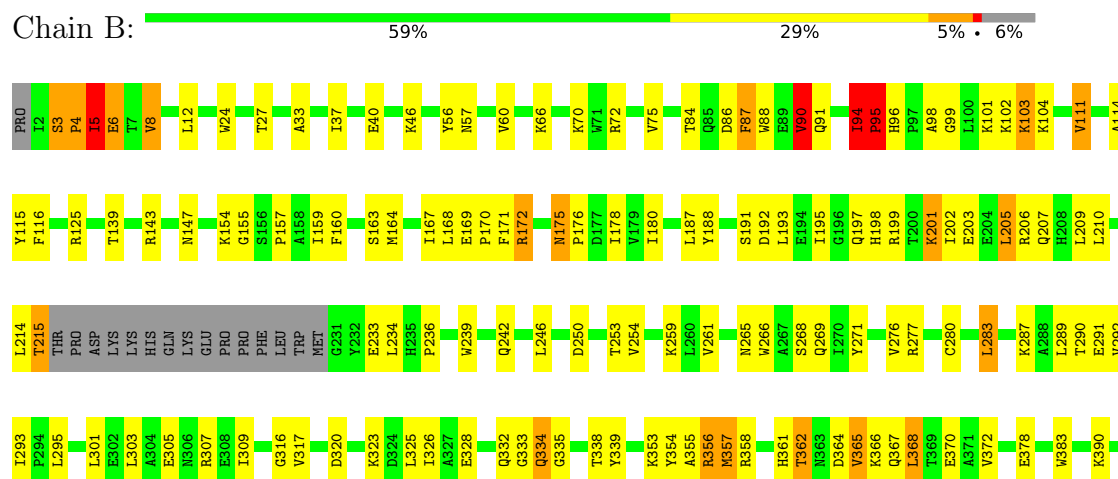
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



I393	Q394	W401	E413	M418	T419	P420	V423	K424	L425	Q428	LEU	GLU	LYS	GLU	PRO	ILE	VAL	GLY	ALA	GLU	THR	PHE
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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	138.80Å 115.80Å 66.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.60	Depositor
% Data completeness (in resolution range)	80.7 (25.00-2.60)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.224 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7844	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TB9, CSD, MG

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	0.46	0/4417	0.99	18/6005 (0.3%)
2	B	0.47	0/3497	0.96	9/4752 (0.2%)
All	All	0.46	0/7914	0.98	27/10757 (0.3%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	348	ASN	N-CA-C	9.96	123.47	110.43
1	A	349	LEU	N-CA-C	-9.23	102.53	113.88
1	A	537	PRO	N-CA-C	-9.03	97.03	111.38
1	A	411	ILE	CA-C-N	8.27	130.18	119.84
1	A	411	ILE	C-N-CA	8.27	130.18	119.84
1	A	250	ASP	N-CA-C	-7.26	104.04	113.12
1	A	346	PHE	N-CA-C	6.98	120.87	111.24
2	B	87	PHE	N-CA-C	6.07	119.89	107.69
1	A	88	TRP	N-CA-C	-5.96	104.86	111.71
1	A	58	THR	CA-C-N	5.94	125.88	119.76
1	A	58	THR	C-N-CA	5.94	125.88	119.76
1	A	195	ILE	N-CA-C	5.89	121.59	109.34
1	A	51	GLY	CA-C-N	5.77	125.47	119.82
1	A	51	GLY	C-N-CA	5.77	125.47	119.82
2	B	365	VAL	N-CA-C	5.41	115.61	110.53
2	B	147	ASN	N-CA-C	-5.33	107.33	113.88
1	A	343	GLN	N-CA-C	-5.31	106.86	113.55
2	B	12	LEU	N-CA-C	-5.29	103.40	110.55
2	B	316	GLY	N-CA-C	5.21	122.51	115.32
2	B	86	ASP	N-CA-C	-5.19	104.03	110.41
2	B	94	ILE	N-CA-C	5.16	120.02	108.88
1	A	137	ASN	N-CA-C	5.12	121.69	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	56	TYR	N-CA-C	5.04	117.35	110.55
1	A	388	LYS	N-CA-C	-5.03	101.56	109.25
2	B	401	TRP	N-CA-C	5.02	120.39	113.97
1	A	344	GLU	CA-C-N	5.01	126.10	119.84
1	A	344	GLU	C-N-CA	5.01	126.10	119.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4310	0	4343	135	0
2	B	3401	0	3434	109	0
3	A	1	0	0	0	0
4	A	21	0	20	3	0
5	A	79	0	0	3	0
5	B	32	0	0	2	0
All	All	7844	0	7797	238	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 (238) 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:139:THR:HB	1:A:140:PRO:CD	1.80	1.11
2:B:332:GLN:HB3	2:B:428:GLN:HE22	1.23	1.00
2:B:332:GLN:HB3	2:B:428:GLN:NE2	1.75	0.99
2:B:172:ARG:HG2	2:B:172:ARG:HH11	1.27	0.98
1:A:209:LEU:HB3	1:A:214:LEU:HB2	1.52	0.89
1:A:139:THR:HB	1:A:140:PRO:HD3	1.53	0.89
2:B:60:VAL:HG12	2:B:75:VAL:HG22	1.58	0.84
1:A:169:GLU:HB2	1:A:170:PRO:HD3	1.60	0.83
2:B:99:GLY:HA2	2:B:102:LYS:HE2	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:332:GLN:CB	2:B:428:GLN:HE22	1.93	0.80
2:B:332:GLN:CB	2:B:428:GLN:NE2	2.45	0.79
2:B:172:ARG:HG2	2:B:172:ARG:NH1	1.97	0.77
1:A:139:THR:HB	1:A:140:PRO:HD2	1.68	0.75
2:B:66:LYS:HE2	2:B:358:ARG:NH1	2.03	0.73
2:B:420:PRO:O	2:B:423:VAL:HG12	1.89	0.71
2:B:94:ILE:H	2:B:95:PRO:CD	2.04	0.71
2:B:362:THR:HB	2:B:367:GLN:HE21	1.55	0.71
1:A:264:LEU:HD23	1:A:276:VAL:HG12	1.71	0.70
1:A:61:PHE:CZ	1:A:74:LEU:HD23	2.26	0.70
2:B:114:ALA:HB2	2:B:214:LEU:HD13	1.73	0.70
1:A:138:GLU:O	1:A:139:THR:HG23	1.92	0.69
1:A:92:LEU:HD23	1:A:92:LEU:H	1.58	0.69
1:A:412:PRO:HG3	2:B:401:TRP:CZ2	2.29	0.68
1:A:179:VAL:HG23	4:A:999:TB9:H112	1.75	0.67
1:A:393:ILE:HB	1:A:423:VAL:HG22	1.76	0.67
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.75	0.67
2:B:57:ASN:HD22	2:B:143:ARG:HH12	1.43	0.66
1:A:412:PRO:HG3	2:B:401:TRP:HZ2	1.61	0.66
2:B:368:LEU:O	2:B:372:VAL:HG23	1.96	0.65
1:A:136:ASN:OD1	1:A:139:THR:HG21	1.98	0.64
2:B:57:ASN:HD22	2:B:143:ARG:NH1	1.96	0.64
1:A:191:SER:OG	1:A:193:LEU:HG	1.98	0.64
1:A:132:ILE:HB	1:A:142:ILE:HG13	1.80	0.64
2:B:94:ILE:H	2:B:95:PRO:HD2	1.62	0.64
1:A:271:TYR:HE2	1:A:312:GLU:O	1.82	0.63
2:B:175:ASN:HB3	2:B:178:ILE:HD13	1.81	0.63
1:A:257:ILE:O	1:A:261:VAL:HG23	1.99	0.63
2:B:3:SER:HB3	2:B:125:ARG:HH22	1.64	0.62
1:A:46:LYS:HD3	1:A:116:PHE:CD2	2.34	0.62
1:A:114:ALA:HB3	1:A:160:PHE:CE1	2.35	0.62
1:A:50:ILE:HD12	1:A:54:ASN:HB3	1.82	0.61
1:A:227:PHE:HB2	1:A:234:LEU:HB2	1.83	0.61
2:B:253:THR:HA	2:B:292:VAL:HA	1.82	0.61
1:A:399:GLU:HA	1:A:402:TRP:HE3	1.64	0.60
1:A:228:LEU:HD12	1:A:242:GLN:HG2	1.83	0.60
1:A:87:PHE:HB2	1:A:89:GLU:HG3	1.83	0.60
1:A:101:LYS:HD2	1:A:101:LYS:N	2.16	0.60
1:A:102:LYS:HG3	1:A:237:ASP:HA	1.83	0.60
1:A:277:ARG:HG3	1:A:277:ARG:HH11	1.65	0.60
1:A:457:TYR:OH	1:A:465:LYS:HD3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:TYR:CE2	4:A:999:TB9:H163	2.36	0.59
2:B:46:LYS:HE2	2:B:116:PHE:HB3	1.82	0.59
1:A:193:LEU:HD13	1:A:197:GLN:HG3	1.83	0.59
1:A:357:MET:HE2	1:A:512:GLN:NE2	2.17	0.59
1:A:519:ASN:O	1:A:523:GLU:HG2	2.04	0.58
2:B:169:GLU:N	2:B:170:PRO:HD2	2.19	0.58
1:A:21:VAL:HG13	1:A:59:PRO:HD3	1.86	0.57
1:A:476:LYS:HD3	1:A:517:LEU:HD12	1.85	0.57
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.85	0.57
2:B:163:SER:O	2:B:167:ILE:HG13	2.04	0.57
1:A:362:THR:HG22	1:A:366:LYS:HD3	1.87	0.57
1:A:139:THR:CB	1:A:140:PRO:CD	2.69	0.57
1:A:136:ASN:O	1:A:139:THR:OG1	2.18	0.56
2:B:326:ILE:HG21	2:B:390:LYS:HE2	1.87	0.56
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.40	0.56
1:A:61:PHE:CD1	1:A:61:PHE:N	2.74	0.56
2:B:33:ALA:O	2:B:37:ILE:HG13	2.06	0.56
1:A:111:VAL:HG11	1:A:160:PHE:CZ	2.41	0.55
2:B:90:VAL:HG12	2:B:91:GLN:H	1.69	0.55
2:B:203:GLU:HG3	2:B:207:GLN:HE22	1.72	0.55
2:B:37:ILE:O	2:B:40:GLU:HG2	2.07	0.55
1:A:114:ALA:O	1:A:118:VAL:HG23	2.07	0.54
1:A:277:ARG:NH2	1:A:336:GLN:HE22	2.05	0.54
1:A:399:GLU:HG3	1:A:402:TRP:CZ3	2.42	0.54
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.41	0.54
2:B:154:LYS:O	2:B:157:PRO:HD2	2.07	0.54
2:B:365:VAL:HG11	2:B:401:TRP:HB2	1.89	0.54
2:B:201:LYS:HE3	2:B:201:LYS:HA	1.88	0.54
2:B:305:GLU:O	2:B:309:ILE:HG13	2.07	0.54
2:B:210:LEU:HD22	2:B:215:THR:HA	1.89	0.54
1:A:65:LYS:HB3	1:A:68:SER:HB3	1.89	0.54
1:A:181:TYR:CE2	1:A:183:TYR:HB2	2.42	0.54
1:A:24:TRP:HZ3	1:A:61:PHE:CG	2.25	0.54
1:A:517:LEU:HA	1:A:520:GLN:HE21	1.73	0.54
2:B:180:ILE:HA	2:B:188:TYR:O	2.08	0.53
2:B:328:GLU:HG2	2:B:390:LYS:HD2	1.90	0.53
2:B:160:PHE:HE2	2:B:164:MET:HE2	1.74	0.53
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.44	0.53
2:B:239:TRP:CH2	2:B:378:GLU:HG2	2.44	0.53
2:B:320:ASP:OD2	2:B:323:LYS:HG2	2.08	0.53
2:B:295:LEU:H	2:B:295:LEU:HD12	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:236:PRO:HA	2:B:239:TRP:CE2	2.44	0.52
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.91	0.52
1:A:216:THR:HG22	1:A:217:PRO:HD2	1.90	0.52
2:B:254:VAL:HG23	2:B:291:GLU:O	2.10	0.52
1:A:31:ILE:O	1:A:35:VAL:HG23	2.11	0.51
1:A:47:ILE:HD12	1:A:144:TYR:CD2	2.45	0.51
1:A:306:ASN:O	1:A:310:LEU:HG	2.09	0.51
1:A:279:LEU:HA	1:A:282:LEU:HD23	1.91	0.51
1:A:329:ILE:HD11	1:A:375:ILE:HD12	1.92	0.51
1:A:137:ASN:H	1:A:137:ASN:ND2	2.09	0.51
1:A:170:PRO:O	1:A:173:LYS:HG2	2.11	0.51
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.93	0.51
2:B:115:TYR:OH	2:B:157:PRO:HG3	2.10	0.51
2:B:266:TRP:O	2:B:269:GLN:HG2	2.11	0.51
1:A:328:GLU:HG2	1:A:330:GLN:NE2	2.26	0.51
1:A:479:LEU:HB3	1:A:517:LEU:HD13	1.92	0.50
1:A:399:GLU:HA	1:A:402:TRP:CE3	2.45	0.50
2:B:87:PHE:CE2	2:B:155:GLY:HA2	2.47	0.50
2:B:103:LYS:HG2	2:B:191:SER:N	2.27	0.50
1:A:169:GLU:HB2	1:A:170:PRO:CD	2.38	0.50
2:B:24:TRP:HB2	5:B:1064:HOH:O	2.12	0.49
1:A:24:TRP:HZ3	1:A:61:PHE:CD1	2.30	0.49
2:B:8:VAL:HG11	2:B:159:ILE:HG23	1.94	0.49
2:B:242:GLN:NE2	2:B:353:LYS:HE3	2.28	0.49
1:A:134:SER:HB2	1:A:139:THR:OG1	2.12	0.49
1:A:366:LYS:O	1:A:370:GLU:HG3	2.12	0.49
2:B:175:ASN:N	2:B:176:PRO:HD3	2.28	0.49
1:A:483:TYR:O	1:A:486:LEU:HB2	2.13	0.49
2:B:393:ILE:HG12	2:B:394:GLN:N	2.27	0.49
2:B:170:PRO:HG2	2:B:171:PHE:H	1.77	0.49
2:B:261:VAL:HG13	2:B:276:VAL:HG11	1.94	0.49
2:B:328:GLU:O	2:B:339:TYR:HA	2.13	0.48
1:A:65:LYS:HB2	1:A:65:LYS:NZ	2.28	0.48
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.48	0.48
2:B:5:ILE:HB	2:B:6:GLU:H	1.56	0.48
1:A:181:TYR:HE2	1:A:183:TYR:HB2	1.77	0.48
2:B:84:THR:HB	2:B:154:LYS:HE2	1.95	0.48
1:A:253:THR:O	1:A:257:ILE:HG13	2.13	0.48
1:A:394:GLN:HG2	5:A:1045:HOH:O	2.13	0.48
1:A:172:ARG:HH21	1:A:180:ILE:HB	1.79	0.47
1:A:189:VAL:HG21	1:A:205:LEU:HD12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:ASN:OD1	1:A:139:THR:CG2	2.62	0.47
1:A:54:ASN:ND2	1:A:129:ALA:HB2	2.29	0.47
1:A:328:GLU:HG2	1:A:330:GLN:HE21	1.79	0.47
2:B:160:PHE:CE2	2:B:164:MET:HE2	2.50	0.47
2:B:354:TYR:CE1	2:B:357:MET:SD	3.08	0.47
1:A:480:GLN:HG2	1:A:517:LEU:HD11	1.97	0.47
2:B:172:ARG:NH1	2:B:172:ARG:CG	2.72	0.47
2:B:4:PRO:HB2	2:B:5:ILE:HD13	1.97	0.47
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.97	0.47
1:A:61:PHE:N	1:A:61:PHE:HD1	2.12	0.46
2:B:335:GLY:O	2:B:355:ALA:HA	2.16	0.46
2:B:261:VAL:HG22	2:B:276:VAL:CG1	2.46	0.46
2:B:246:LEU:HD12	2:B:307:ARG:HG2	1.97	0.46
1:A:241:VAL:HB	1:A:266:TRP:HE1	1.81	0.46
2:B:198:HIS:O	2:B:202:ILE:HG12	2.16	0.46
2:B:253:THR:HG22	2:B:292:VAL:HG22	1.97	0.46
2:B:103:LYS:O	2:B:236:PRO:HG2	2.15	0.46
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.16	0.45
1:A:435:VAL:HG22	2:B:290:THR:HG21	1.97	0.45
2:B:209:LEU:HD22	2:B:214:LEU:HD23	1.98	0.45
1:A:100:LEU:HB2	1:A:318:TYR:CE1	2.51	0.45
2:B:94:ILE:N	2:B:95:PRO:CD	2.75	0.45
1:A:347:LYS:HD2	1:A:347:LYS:HA	1.65	0.45
1:A:354:TYR:HD1	1:A:374:LYS:HD2	1.81	0.45
1:A:229:TRP:CD2	4:A:999:TB9:H151	2.51	0.45
1:A:277:ARG:HG3	1:A:277:ARG:NH1	2.29	0.45
2:B:191:SER:HB2	2:B:193:LEU:HD13	1.97	0.45
1:A:47:ILE:HG22	1:A:146:TYR:HA	1.99	0.45
2:B:333:GLY:O	2:B:334:GLN:HG2	2.16	0.45
1:A:111:VAL:HG11	1:A:160:PHE:HZ	1.78	0.45
2:B:90:VAL:HG12	2:B:91:GLN:N	2.32	0.45
1:A:475:GLN:HB3	1:A:501:TYR:CD2	2.51	0.45
1:A:253:THR:HG22	1:A:289:LEU:O	2.17	0.45
1:A:503:LEU:HG	1:A:535:TRP:HB2	1.97	0.45
1:A:268:SER:OG	1:A:353:LYS:HE2	2.17	0.45
1:A:340:GLN:HB3	1:A:351:THR:HG22	1.99	0.45
1:A:150:PRO:HB2	1:A:153:TRP:HB2	1.99	0.45
2:B:325:LEU:HD21	2:B:383:TRP:CE3	2.51	0.44
1:A:486:LEU:CD1	1:A:521:ILE:HG23	2.47	0.44
1:A:125:ARG:NE	1:A:147:ASN:HA	2.33	0.44
2:B:335:GLY:HA3	2:B:356:ARG:HE	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:GLN:NE2	1:A:278:GLN:HA	2.33	0.44
1:A:178:ILE:HD11	1:A:201:LYS:HG2	2.00	0.44
2:B:366:LYS:O	2:B:370:GLU:HG3	2.18	0.44
1:A:271:TYR:CE2	1:A:312:GLU:O	2.67	0.43
2:B:169:GLU:HG2	2:B:170:PRO:HD3	1.99	0.43
1:A:70:LYS:HA	1:A:70:LYS:HD2	1.78	0.43
1:A:400:THR:O	1:A:404:GLU:HG2	2.19	0.43
2:B:326:ILE:CG2	2:B:390:LYS:HE2	2.47	0.43
1:A:100:LEU:O	1:A:318:TYR:HB3	2.18	0.43
2:B:259:LYS:HB3	2:B:259:LYS:HE2	1.69	0.43
1:A:399:GLU:HG3	1:A:402:TRP:CE3	2.54	0.43
1:A:115:TYR:OH	1:A:157:PRO:HG3	2.18	0.43
1:A:409:THR:O	2:B:364:ASP:HB2	2.19	0.43
1:A:277:ARG:HH22	1:A:336:GLN:HE22	1.67	0.43
1:A:354:TYR:CD1	1:A:374:LYS:HD2	2.54	0.43
2:B:3:SER:HA	2:B:4:PRO:HD3	1.76	0.43
2:B:95:PRO:O	2:B:96:HIS:HB2	2.18	0.43
1:A:62:ALA:C	1:A:63:ILE:HD12	2.43	0.42
1:A:201:LYS:HD2	1:A:201:LYS:HA	1.79	0.42
1:A:116:PHE:O	1:A:148:VAL:HG11	2.19	0.42
1:A:50:ILE:CG1	1:A:143:ARG:HB3	2.50	0.42
2:B:193:LEU:HD23	2:B:197:GLN:HB3	2.01	0.42
2:B:287:LYS:HD3	2:B:291:GLU:OE2	2.20	0.42
1:A:138:GLU:O	1:A:139:THR:CG2	2.64	0.42
2:B:70:LYS:HD3	2:B:70:LYS:HA	1.81	0.42
2:B:6:GLU:O	2:B:6:GLU:HG2	2.20	0.42
2:B:104:LYS:HG3	2:B:192:ASP:OD1	2.19	0.42
1:A:417:VAL:O	1:A:417:VAL:HG13	2.18	0.42
1:A:464:GLN:O	1:A:465:LYS:HD2	2.19	0.42
1:A:180:ILE:HA	1:A:188:TYR:O	2.19	0.42
2:B:98:ALA:O	2:B:101:LYS:HG2	2.19	0.42
1:A:281:LYS:HE2	1:A:284:ARG:CZ	2.49	0.42
2:B:171:PHE:CE2	2:B:205:LEU:HA	2.54	0.41
1:A:37:ILE:O	1:A:41:MET:HG3	2.20	0.41
2:B:268:SER:HA	2:B:271:TYR:O	2.19	0.41
1:A:78:ARG:NH2	5:A:1090:HOH:O	2.53	0.41
1:A:201:LYS:O	1:A:204:GLU:HB3	2.20	0.41
1:A:207:GLN:O	1:A:211:ARG:HG3	2.20	0.41
1:A:229:TRP:O	1:A:232:TYR:HB2	2.21	0.41
2:B:205:LEU:O	2:B:209:LEU:HG	2.20	0.41
2:B:261:VAL:O	2:B:265:ASN:HB2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:259:LYS:HE3	2:B:425:LEU:HD21	2.03	0.41
1:A:327:ALA:HB3	1:A:389:PHE:CD1	2.56	0.41
1:A:402:TRP:CD1	1:A:402:TRP:C	2.98	0.41
2:B:101:LYS:O	2:B:236:PRO:HB2	2.20	0.41
1:A:100:LEU:HB2	1:A:318:TYR:CD1	2.56	0.41
1:A:498:ASP:HB3	1:A:538:ALA:HB2	2.03	0.41
2:B:169:GLU:N	2:B:170:PRO:CD	2.84	0.41
2:B:283:LEU:HD12	2:B:283:LEU:HA	1.85	0.41
2:B:287:LYS:HD2	2:B:293:ILE:HD11	2.02	0.41
1:A:7:THR:HG21	1:A:121:ASP:HA	2.03	0.41
2:B:195:ILE:HD11	2:B:233:GLU:OE2	2.21	0.41
2:B:419:THR:HA	2:B:420:PRO:HD3	1.88	0.41
1:A:58:THR:HA	1:A:59:PRO:HD3	1.91	0.40
1:A:5:ILE:HG22	1:A:119:PRO:HD2	2.03	0.40
1:A:469:LEU:HD21	1:A:480:GLN:HG3	2.03	0.40
2:B:168:LEU:C	2:B:170:PRO:HD2	2.45	0.40
2:B:332:GLN:HG3	2:B:338:THR:HG23	2.03	0.40
1:A:138:GLU:C	1:A:139:THR:HG23	2.46	0.40
2:B:195:ILE:HG13	2:B:199:ARG:HE	1.85	0.40
2:B:203:GLU:O	2:B:206:ARG:HB2	2.22	0.40
1:A:385:LYS:HD2	5:A:1032:HOH:O	2.21	0.40
1:A:464:GLN:C	1:A:465:LYS:HD2	2.46	0.40
2:B:163:SER:HB2	5:B:1077:HOH:O	2.20	0.40
2:B:234:LEU:HD23	2:B:239:TRP:CZ2	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	520/560 (93%)	481 (92%)	31 (6%)	8 (2%)	8 18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	408/440 (93%)	366 (90%)	32 (8%)	10 (2%)	4 8
All	All	928/1000 (93%)	847 (91%)	63 (7%)	18 (2%)	6 13

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	139	THR
1	A	412	PRO
2	B	94	ILE
2	B	95	PRO
1	A	137	ASN
2	B	5	ILE
2	B	90	VAL
2	B	277	ARG
1	A	140	PRO
2	B	4	PRO
1	A	89	GLU
1	A	195	ILE
1	A	345	PRO
2	B	88	TRP
2	B	356	ARG
2	B	362	THR
1	A	111	VAL
2	B	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	473/499 (95%)	424 (90%)	49 (10%)	7 14
2	B	374/400 (94%)	347 (93%)	27 (7%)	13 30
All	All	847/899 (94%)	771 (91%)	76 (9%)	9 20

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	20	LYS
1	A	21	VAL
1	A	61	PHE
1	A	65	LYS
1	A	91	GLN
1	A	92	LEU
1	A	122	GLU
1	A	137	ASN
1	A	138	GLU
1	A	142	ILE
1	A	194	GLU
1	A	195	ILE
1	A	205	LEU
1	A	210	LEU
1	A	216	THR
1	A	218	ASP
1	A	234	LEU
1	A	264	LEU
1	A	279	LEU
1	A	283	LEU
1	A	287	LYS
1	A	296	THR
1	A	301	LEU
1	A	303	LEU
1	A	312	GLU
1	A	317	VAL
1	A	340	GLN
1	A	345	PRO
1	A	347	LYS
1	A	348	ASN
1	A	356	ARG
1	A	362	THR
1	A	368	LEU
1	A	396	GLU
1	A	402	TRP
1	A	423	VAL
1	A	443	ASP
1	A	470	THR
1	A	471	ASP
1	A	473	THR
1	A	484	LEU
1	A	491	LEU

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Mol	Chain	Res	Type
1	A	493	VAL
1	A	503	LEU
1	A	509	GLN
1	A	517	LEU
1	A	533	LEU
1	A	539	HIS
2	B	3	SER
2	B	5	ILE
2	B	6	GLU
2	B	8	VAL
2	B	27	THR
2	B	72	ARG
2	B	90	VAL
2	B	95	PRO
2	B	103	LYS
2	B	139	THR
2	B	172	ARG
2	B	175	ASN
2	B	201	LYS
2	B	205	LEU
2	B	215	THR
2	B	250	ASP
2	B	280	CYS
2	B	283	LEU
2	B	289	LEU
2	B	301	LEU
2	B	303	LEU
2	B	317	VAL
2	B	334	GLN
2	B	357	MET
2	B	361	HIS
2	B	368	LEU
2	B	413	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	ASN
1	A	145	GLN
1	A	222	GLN
1	A	265	ASN
1	A	278	GLN

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Mol	Chain	Res	Type
1	A	332	GLN
1	A	336	GLN
1	A	373	GLN
1	A	475	GLN
1	A	480	GLN
1	A	509	GLN
1	A	512	GLN
1	A	520	GLN
1	A	524	GLN
2	B	57	ASN
2	B	137	ASN
2	B	147	ASN
2	B	207	GLN
2	B	242	GLN
2	B	278	GLN
2	B	334	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	1.55	1 (25%)	1,8,10	7.17	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	2.58	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	7.17	118.81	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	TB9	A	999	-	22,23,23	0.93	2 (9%)	22,34,34	2.47	5 (22%)

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
4	TB9	A	999	-	-	1/5/17/17	0/2/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	999	TB9	C3A-N3	-2.53	1.35	1.40
4	A	999	TB9	C9-CL9	-2.10	1.69	1.74

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	999	TB9	C12-N6-C7	6.68	123.70	112.07
4	A	999	TB9	C3A-N3-C2	-6.50	106.96	109.95
4	A	999	TB9	C1A-N1-C2	-4.54	107.29	110.67
4	A	999	TB9	C10-C1A-C3A	-2.43	119.17	121.74
4	A	999	TB9	C7-C7A-C3A	-2.20	119.08	122.45

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	999	TB9	C13-C12-N6-C7

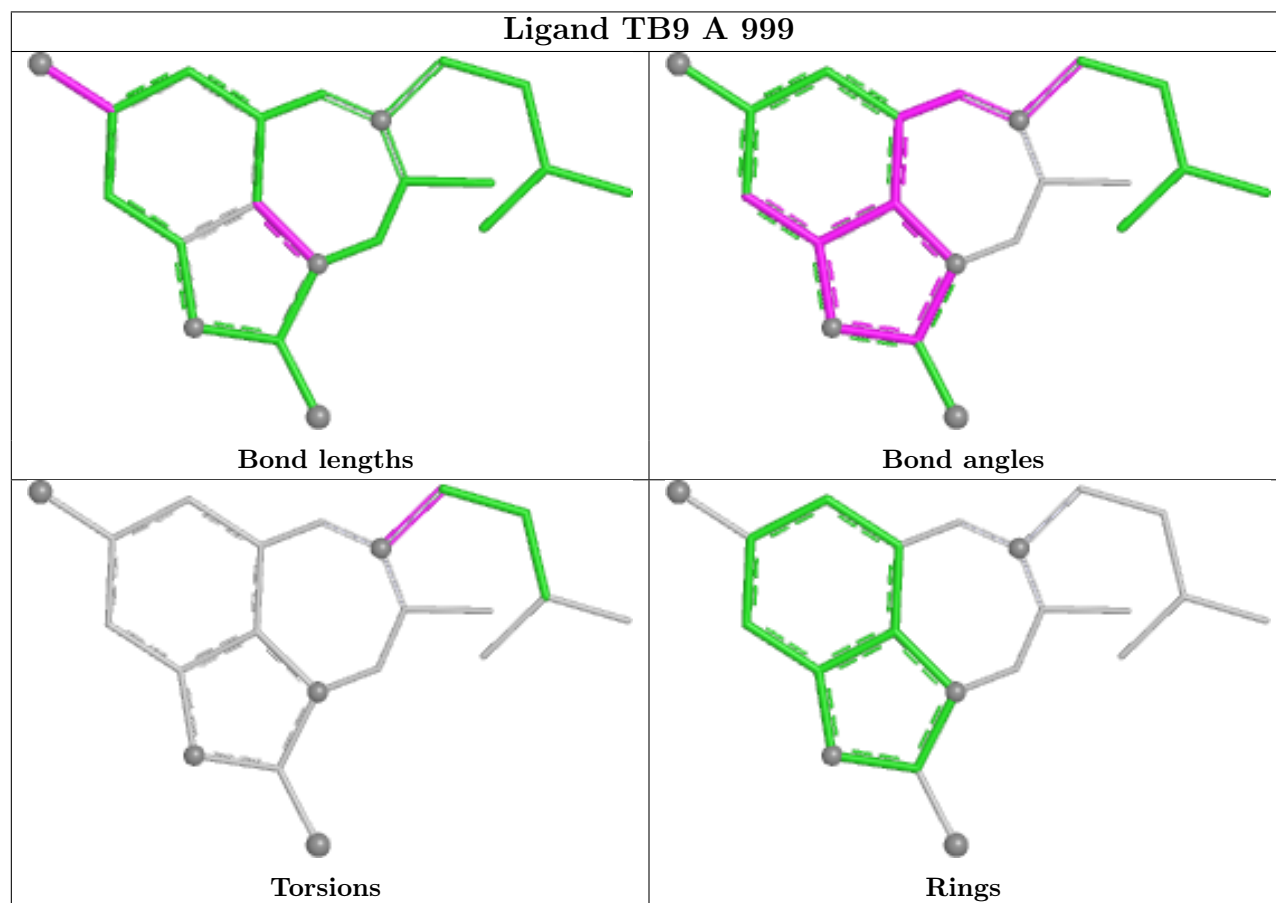
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	999	TB9	3	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.