



Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 08:41 pm BST

PDB ID : 1REV
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

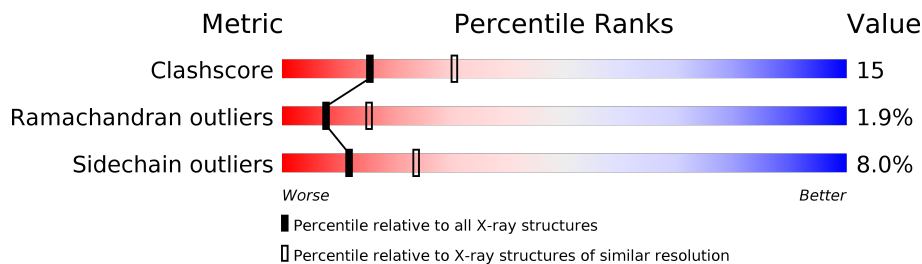
1 Overall quality at a glance

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	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (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 on 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 [i](#)

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
			Total	C	N	O	S			
1	A	525	4310	2792	714	796	8	0	0	0

There is a discrepancy between the modelled and reference sequences:

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

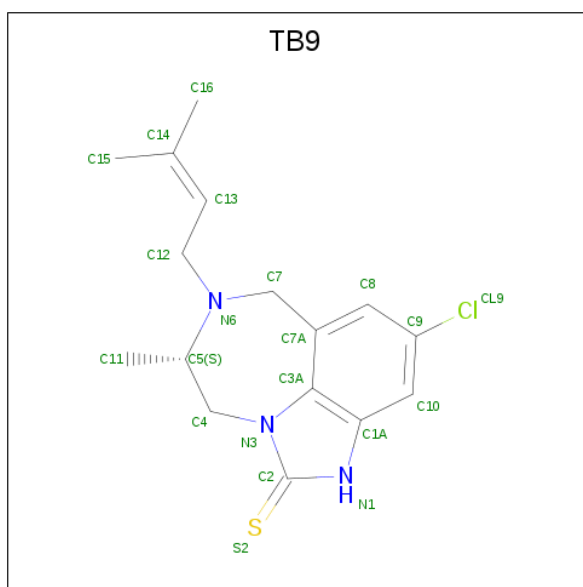
- Molecule 2 is a protein called HIV-1 REVERSE TRANSCRIPTASE.

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

- Molecule 3 is MAGNESIUM ION (three-letter code: 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 (three-letter code: TB9) (formula: C₁₆H₂₀ClN₃S).



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

- Molecule 5 is water.

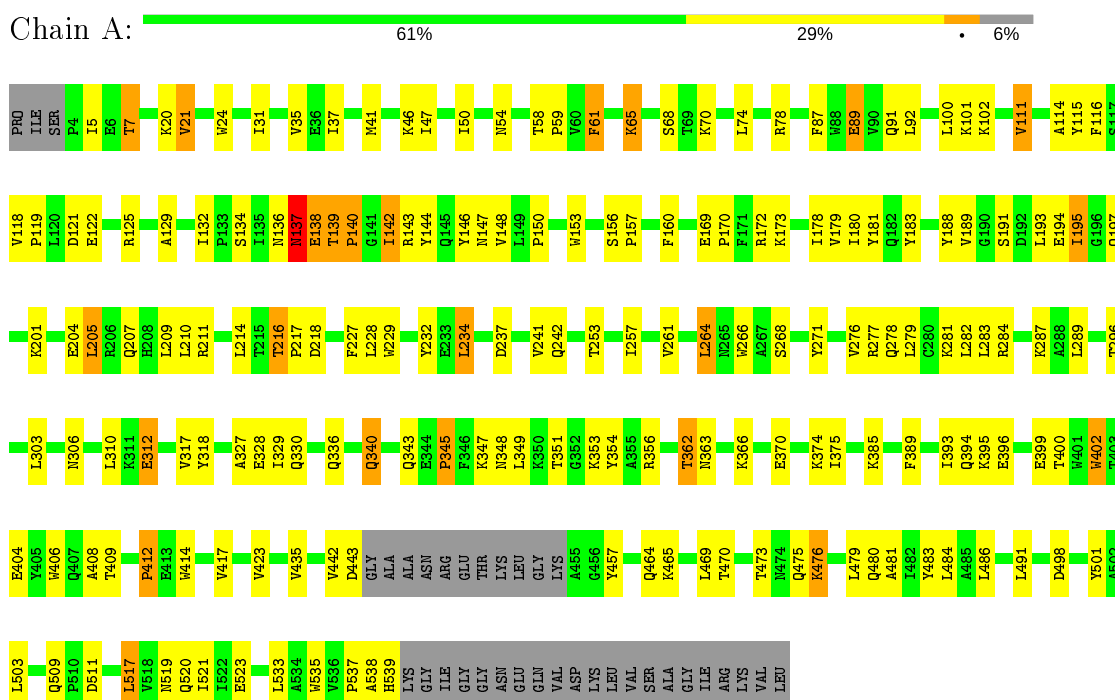
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	79	Total	O	0	0
			79	79		
5	B	32	Total	O	0	0
			32	32		

3 Residue-property plots

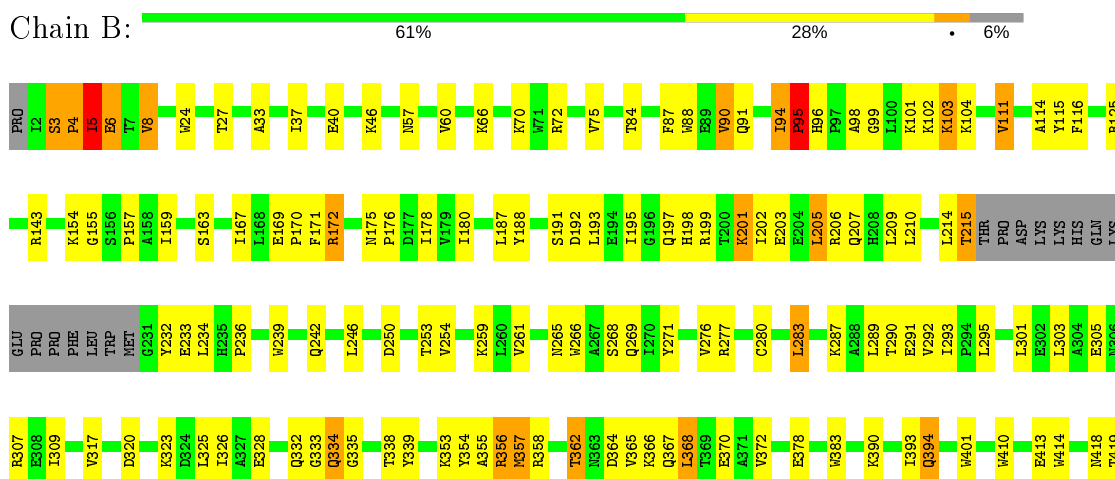
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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



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

Xtrriage (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.	Xtrriage
Total number of atoms	7844	wwPDB-VP
Average B, all atoms (Å ²)	66.0	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: 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	0.38	0/4417	0.64	1/6005 (0.0%)
2	B	0.38	0/3497	0.64	0/4752
All	All	0.38	0/7914	0.64	1/10757 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	537	PRO	N-CA-C	-5.80	97.03	112.10

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	130	0
2	B	3401	0	3434	106	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	230	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 (230) 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:HH11	2:B:172:ARG:HG2	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
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:NH1	2:B:172:ARG:HG2	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:362:THR:HB	2:B:367:GLN:HE21	1.55	0.71
2:B:94:ILE:H	2:B:95:PRO:CD	2.04	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:H	1:A:92:LEU:HD23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:A:101:LYS:HD2	2.16	0.60
1:A:102:LYS:HG3	1:A:237:ASP:HA	1.83	0.60
1:A:277:ARG:HH11	1:A:277:ARG:HG3	1.65	0.60
1:A:457:TYR:OH	1:A:465:LYS:HD3	2.02	0.60
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:136:ASN:O	1:A:139:THR:OG1	2.18	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:476:LYS:HD3	1:A:517:LEU:HD12	1.85	0.57
1:A:21:VAL:HG13	1:A:59:PRO:HD3	1.86	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
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:N	1:A:61:PHE:CD1	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:HA	2:B:201:LYS:HE3	1.88	0.54
2:B:305:GLU:O	2:B:309:ILE:HG13	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:210:LEU:HD22	2:B:215:THR:HA	1.89	0.54
1:A:181:TYR:CE2	1:A:183:TYR:HB2	2.42	0.54
1:A:65:LYS:HB3	1:A:68:SER:HB3	1.89	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: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:HD12	2:B:295:LEU:H	1.74	0.52
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:306:ASN:O	1:A:310:LEU:HG	2.09	0.51
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: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:ND2	1:A:137:ASN:H	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:103:LYS:HG2	2:B:191:SER:N	2.27	0.50
2:B:87:PHE:CE2	2:B:155:GLY:HA2	2.47	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:242:GLN:NE2	2:B:353:LYS:HE3	2.28	0.49
2:B:8:VAL:HG11	2:B:159:ILE:HG23	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:CG	2:B:172:ARG:NH1	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
2:B:209:LEU:HD22	2:B:214:LEU:HD23	1.98	0.45
1:A:435:VAL:HG22	2:B:290:THR:HG21	1.97	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:NH1	1:A:277:ARG:HG3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:278:GLN:HA	1:A:278:GLN:NE2	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:400:THR:O	1:A:404:GLU:HG2	2.19	0.43
1:A:70:LYS:HD2	1:A:70:LYS:HA	1.78	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
1:A:417:VAL:O	1:A:417:VAL:HG13	2.18	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:201:LYS:HA	1:A:201:LYS:HD2	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:HA	2:B:70:LYS:HD3	1.81	0.42
2:B:104:LYS:HG3	2:B:192:ASP:OD1	2.19	0.42
2:B:6:GLU:O	2:B:6:GLU:HG2	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:78:ARG:NH2	5:A:1090:HOH:O	2.53	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
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
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:469:LEU:HD21	1:A:480:GLN:HG3	2.03	0.40
1:A:5:ILE:HG22	1:A:119:PRO:HD2	2.03	0.40
2:B:332:GLN:HG3	2:B:338:THR:HG23	2.03	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
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%)	10	21
2	B	408/440 (93%)	366 (90%)	32 (8%)	10 (2%)	5	9
All	All	928/1000 (93%)	847 (91%)	63 (7%)	18 (2%)	8	15

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 [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	473/499 (95%)	432 (91%)	41 (9%)	10	20
2	B	374/400 (94%)	347 (93%)	27 (7%)	14	29
All	All	847/899 (94%)	779 (92%)	68 (8%)	12	24

All (68) 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	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	283	LEU
1	A	287	LYS
1	A	296	THR
1	A	303	LEU
1	A	312	GLU
1	A	317	VAL
1	A	340	GLN
1	A	345	PRO
1	A	348	ASN
1	A	356	ARG
1	A	362	THR
1	A	396	GLU
1	A	402	TRP
1	A	443	ASP
1	A	470	THR
1	A	473	THR
1	A	476	LYS
1	A	484	LEU
1	A	491	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

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Mol	Chain	Res	Type
2	B	6	GLU
2	B	8	VAL
2	B	27	THR
2	B	72	ARG
2	B	95	PRO
2	B	103	LYS
2	B	172	ARG
2	B	201	LYS
2	B	205	LEU
2	B	215	THR
2	B	232	TYR
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	368	LEU
2	B	394	GLN
2	B	410	TRP
2	B	413	GLU
2	B	414	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	ASN
1	A	222	GLN
1	A	278	GLN
1	A	336	GLN
1	A	373	GLN
1	A	507	GLN
1	A	512	GLN
1	A	520	GLN
2	B	57	ASN
2	B	147	ASN
2	B	207	GLN
2	B	242	GLN
2	B	278	GLN

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Mol	Chain	Res	Type
2	B	336	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	3,7,8	0.98	0	1,8,10	6.98	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(°)	Ideal(°)
1	A	280	CSD	OD1-SG-CB	6.98	118.81	105.54

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 carbohydrates 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	-	19,23,23	5.50	8 (42%)	18,34,34	4.92	9 (50%)

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	-	-	2/4/17/17	0/2/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	999	TB9	C8-C9	-11.54	1.38	1.52
4	A	999	TB9	C10-C9	-11.51	1.38	1.52
4	A	999	TB9	C3A-N3	-8.86	1.35	1.47
4	A	999	TB9	C10-C1A	-8.50	1.40	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	999	TB9	C1A-N1	-6.89	1.35	1.46
4	A	999	TB9	C7A-C3A	-6.57	1.41	1.53
4	A	999	TB9	C8-C7A	-6.49	1.38	1.53
4	A	999	TB9	C9-CL9	-4.87	1.69	1.81

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	999	TB9	C10-C9-CL9	11.63	120.30	109.77
4	A	999	TB9	C8-C9-CL9	10.04	118.86	109.77
4	A	999	TB9	C10-C9-C8	7.73	120.84	111.79
4	A	999	TB9	C12-N6-C7	6.58	123.70	111.98
4	A	999	TB9	C4-N3-C3A	5.67	132.25	123.06
4	A	999	TB9	C3A-C1A-N1	4.43	107.53	102.22
4	A	999	TB9	C8-C7A-C3A	3.78	119.95	109.47
4	A	999	TB9	C1A-C3A-N3	3.53	107.28	102.58
4	A	999	TB9	C10-C1A-N1	3.26	133.28	118.26

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	999	TB9	C13-C12-N6-C7
4	A	999	TB9	N6-C12-C13-C14

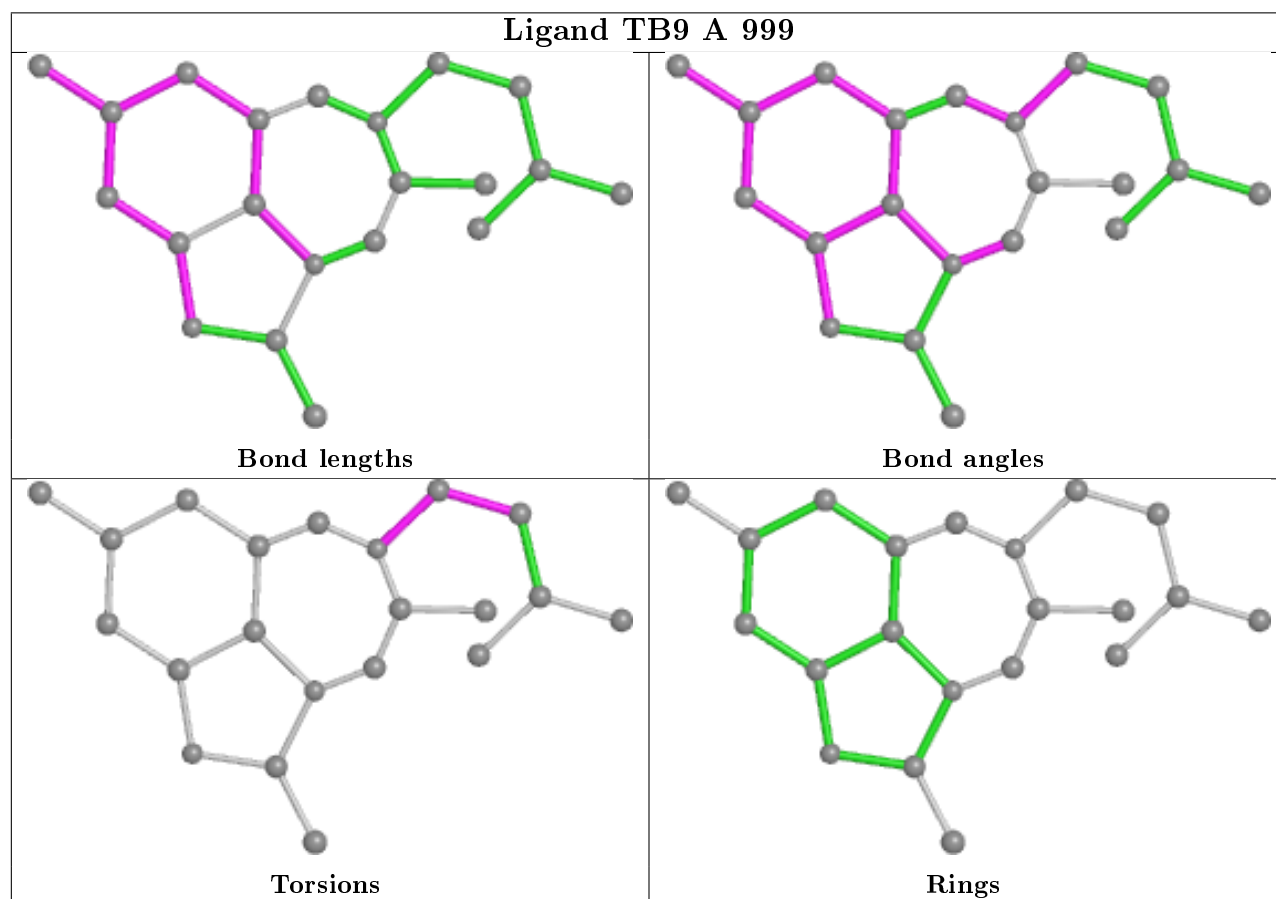
There are no ring outliers.

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.