



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:02 PM GMT

PDB ID : 1RTH
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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

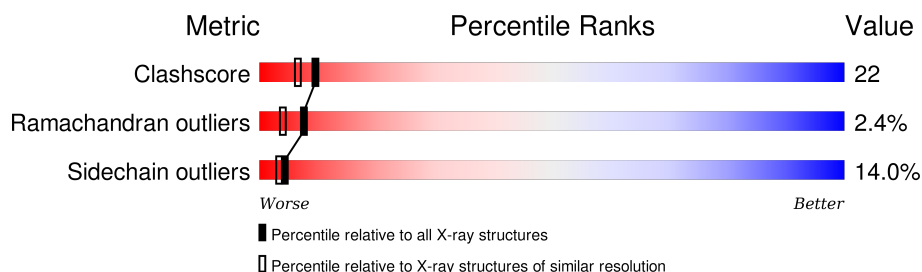
1 Overall quality at a glance ⓘ

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	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	560	
2	B	440	

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.

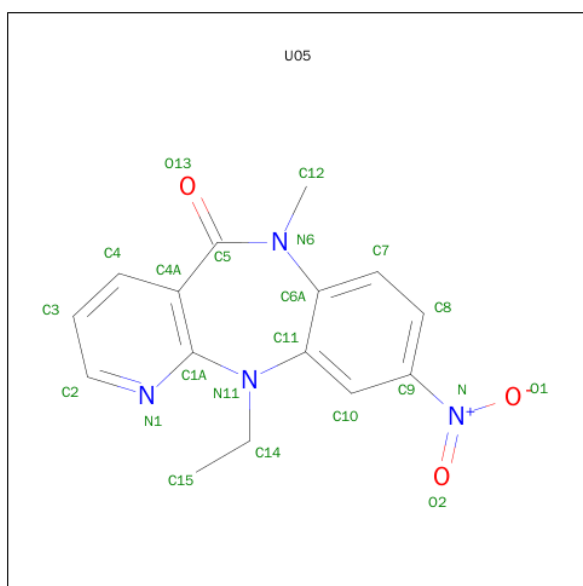
- Molecule 1 is a protein called HIV-1 REVERSE TRANSCRIPTASE.

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 (three-letter code: U05) (formula: C₁₅H₁₄N₄O₃).



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



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	141.10 Å 110.90 Å 73.30 Å 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

5.1 Standard geometry

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	0.79	0/4544	0.96	12/6175 (0.2%)
2	B	0.78	0/3547	0.95	2/4818 (0.0%)
All	All	0.79	0/8091	0.95	14/10993 (0.1%)

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

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	279	LEU	CA-CB-CG	7.41	132.34	115.30
1	A	493	VAL	CB-CA-C	-7.11	97.89	111.40
1	A	461	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	A	511	ASP	CB-CG-OD1	6.01	123.71	118.30
1	A	141	GLY	N-CA-C	-5.90	98.36	113.10
2	B	238	LYS	N-CA-C	-5.68	95.67	111.00
2	B	437	ALA	N-CA-C	-5.49	96.18	111.00
1	A	489	SER	N-CA-C	5.28	125.26	111.00
1	A	273	GLY	N-CA-C	-5.16	100.20	113.10
1	A	388	LYS	N-CA-C	-5.14	97.11	111.00
1	A	503	LEU	CA-CB-CG	5.14	127.12	115.30
1	A	92	LEU	CA-CB-CG	5.12	127.07	115.30
1	A	132	ILE	N-CA-C	-5.11	97.21	111.00
1	A	139	THR	C-N-CD	5.10	139.10	128.40

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	195	0
2	B	3452	0	3488	173	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	357	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 22.

All (357) 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:270:ILE:HD11	1:A:314:VAL:HG21	1.47	0.94
1:A:228:LEU:HD11	1:A:242:GLN:NE2	1.82	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
2:B:368:LEU:O	2:B:372:VAL:HG23	1.74	0.88
1:A:358:ARG:HB3	1:A:358:ARG:NH1	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:HA	1:A:332:GLN:NE2	2.03	0.72
2:B:247:PRO:HB2	2:B:249:LYS:HZ1	1.54	0.72
1:A:541:GLY:HA3	2:B:284:ARG:CZ	2.20	0.72
2:B:100:LEU:HD23	2:B:100:LEU:H	1.54	0.72
1:A:83:ARG:HH11	1:A:83:ARG:HG3	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:CZ	1:A:358:ARG:HB3	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:332:GLN:HA	1:A:332:GLN:HE21	1.62	0.65
1:A:72:ARG:HG2	1:A:73:LYS:N	2.11	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
2:B:390:LYS:HE2	2:B:415:GLU:OE2	1.97	0.64
2:B:65:LYS:O	2:B:68:SER:HB3	1.98	0.64
1:A:125:ARG:HD3	1:A:147:ASN:HA	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:N	2:B:132:ILE:HD12	2.16	0.60
1:A:340:GLN:HB3	1:A:351:THR:HG22	1.84	0.60
2:B:125:ARG:NE	2:B:147:ASN:HA	2.17	0.60
2:B:105:SER:HA	2:B:234:LEU:O	2.02	0.60
1:A:358:ARG:HH11	1:A:358:ARG:HB3	1.67	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: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
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:HA	1:A:300:GLU:OE1	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:400:THR:HG22	2:B:401:TRP:CD2	2.41	0.56
2:B:379:SER:CB	2:B:387:PRO:HD3	2.36	0.56
2:B:114:ALA:HB2	2:B:214:LEU:HD13	1.88	0.56
1:A:234:LEU:HD12	1:A:239:TRP:HB3	1.88	0.56
1:A:139:THR:HB	1:A:140:PRO:CD	2.35	0.56
2:B:363:ASN:ND2	2:B:366:LYS:HB2	2.21	0.56
1:A:541:GLY:HA3	2:B:284:ARG:NH2	2.21	0.56
1:A:122:GLU:CD	1:A:122:GLU:H	2.08	0.56
1:A:91:GLN:NE2	1:A:183:TYR:HE1	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:THR:HG23	1:A:217:PRO:CD	2.35	0.55
1:A:118:VAL:O	1:A:148:VAL:HG23	2.05	0.55
2:B:266:TRP:HZ3	2:B:426:TRP:CG	2.24	0.55
1:A:197:GLN:HE21	1:A:197:GLN:HA	1.70	0.55
2:B:206:ARG:C	2:B:210:LEU:HD13	2.26	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:485:ALA:O	1:A:489:SER:HB3	2.08	0.53
1:A:56:TYR:O	1:A:57:ASN:HB2	2.08	0.53
1:A:461:ARG:HH11	1:A:461:ARG:HG3	1.73	0.53
1:A:328:GLU:HG3	1:A:390:LYS:HB2	1.90	0.53
2:B:57:ASN:HD22	2:B:143:ARG:HH12	1.56	0.53
1:A:486:LEU:HB3	1:A:524:GLN:CG	2.39	0.53
1:A:164:MET:HG3	1:A:168:LEU:CD2	2.38	0.53
2:B:195:ILE:HG12	2:B:199:ARG:CZ	2.39	0.53
2:B:181:TYR:O	2:B:187:LEU:HA	2.09	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:HH11	1:A:448:ARG:HG2	1.73	0.53
2:B:369:THR:HG22	2:B:398:TRP:CZ3	2.44	0.52
2:B:344:GLU:HB3	2:B:347:LYS:HE3	1.90	0.52
1:A:226:PRO:HB3	1:A:235:HIS:HD2	1.72	0.52
1:A:486:LEU:HB3	1:A:524:GLN:HG3	1.91	0.52
1:A:444:GLY:HA3	1:A:477:THR:HG22	1.90	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
2:B:280:CYS:HB3	2:B:284:ARG:HH21	1.75	0.52
1:A:129:ALA:HB1	1:A:143:ARG:HH21	1.75	0.52
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.44	0.52
2:B:206:ARG:O	2:B:210:LEU:HD13	2.09	0.52
2:B:54:ASN:ND2	2:B:129:ALA:HB2	2.24	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:160:PHE:HE2	1:A:182:GLN:NE2	2.08	0.52
2:B:100:LEU:H	2:B:100:LEU:CD2	2.22	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:HIS:HE1	4:A:1047:HOH:O	1.91	0.51
2:B:92:LEU:HB3	2:B:161:GLN:OE1	2.10	0.51
2:B:92:LEU:HD22	2:B:165:THR:HG21	1.92	0.51
1:A:324:ASP:O	1:A:343:GLN:HG2	2.10	0.51
1:A:184:MET:CE	1:A:184:MET:HA	2.40	0.51
2:B:194:GLU:OE1	2:B:195:ILE:HG22	2.10	0.51
2:B:114:ALA:HB1	2:B:160:PHE:CZ	2.45	0.51
1:A:206:ARG:O	1:A:210:LEU:HB2	2.11	0.51
1:A:340:GLN:CB	1:A:351:THR:HG22	2.41	0.51
2:B:160:PHE:CD2	2:B:160:PHE:O	2.64	0.51
2:B:74:LEU:HD11	4:B:1209:HOH:O	2.11	0.51
1:A:523:GLU:O	1:A:527:LYS:HG2	2.10	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
1:A:77:PHE:CE2	1:A:150:PRO:HB2	2.45	0.50
2:B:35:VAL:O	2:B:39:THR:HG23	2.11	0.50
2:B:13:LYS:HE2	2:B:82:LYS:O	2.10	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
2:B:161:GLN:HA	2:B:161:GLN:NE2	2.26	0.50
1:A:252:TRP:CD1	1:A:295:LEU:CD1	2.95	0.50
2:B:78:ARG:O	2:B:82:LYS:HG3	2.11	0.50
1:A:373:GLN:HG2	4:B:1230:HOH:O	2.12	0.50
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
1:A:297:GLU:O	1:A:301:LEU:HD23	2.12	0.49
2:B:366:LYS:HG2	2:B:405:TYR:CD2	2.46	0.49
2:B:285:GLY:O	2:B:287:LYS:HG2	2.13	0.49
2:B:244:ILE:HG23	2:B:429:LEU:HB3	1.95	0.49
2:B:107:THR:O	2:B:189:VAL:N	2.38	0.49
2:B:58:THR:HG23	2:B:76:ASP:O	2.12	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
1:A:114:ALA:HB1	1:A:214:LEU:HD22	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:169:GLU:O	2:B:172:ARG:HB2	2.12	0.49
2:B:361:HIS:HD2	2:B:362:THR:CG2	2.26	0.49
2:B:24:TRP:CH2	2:B:61:PHE:CD1	3.00	0.49
2:B:288:ALA:O	2:B:291:GLU:HB3	2.12	0.49
1:A:432:GLU:HB2	1:A:433:PRO:HD2	1.94	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:206:ARG:O	2:B:209:LEU:N	2.46	0.48
2:B:155:GLY:O	2:B:158:ALA:HB3	2.12	0.48
2:B:101:LYS:HE2	2:B:382:ILE:HG23	1.94	0.48
1:A:448:ARG:HG2	4:A:1127:HOH:O	2.13	0.48
1:A:445:ALA:N	1:A:477:THR:HG21	2.28	0.48
1:A:253:THR:O	1:A:257:ILE:HG12	2.14	0.48
1:A:329:ILE:HD12	1:A:391:LEU:HD21	1.92	0.48
1:A:295:LEU:HD23	1:A:299:ALA:HB3	1.95	0.48
1:A:68:SER:C	1:A:70:LYS:H	2.17	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:HA	1:A:500:GLN:OE1	2.13	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
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
2:B:267:ALA:HB2	2:B:426:TRP:CZ3	2.49	0.47
2:B:24:TRP:CZ3	2:B:403:THR:HG21	2.50	0.47
1:A:344:GLU:O	1:A:347:LYS:HB2	2.14	0.47
1:A:357:MET:O	1:A:359:GLY:N	2.48	0.47
1:A:66:LYS:HA	1:A:66:LYS:HD2	1.67	0.47
2:B:65:LYS:NZ	2:B:72:ARG:HD3	2.30	0.47
2:B:72:ARG:HH11	2:B:72:ARG:HG3	1.79	0.47
1:A:319:TYR:CE1	1:A:343:GLN:NE2	2.82	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
2:B:326:ILE:O	2:B:341:ILE:HA	2.15	0.47
1:A:324:ASP:O	1:A:343:GLN:CG	2.63	0.47
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:347:LYS:HD3	1:A:347:LYS:HA	1.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:GLU:HA	1:A:307:ARG:NH2	2.30	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:110:ASP:C	1:A:112:GLY:H	2.19	0.46
2:B:169:GLU:HG2	2:B:173:LYS:HE2	1.97	0.46
1:A:295:LEU:HD23	1:A:299:ALA:CB	2.45	0.46
1:A:446:ALA:O	1:A:448:ARG:NH1	2.49	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
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:393:ILE:O	2:B:416:PHE:HB3	2.16	0.46
2:B:96:HIS:CD2	2:B:97:PRO:O	2.69	0.46
2:B:72:ARG:NH2	2:B:151:GLN:NE2	2.63	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:376:THR:CG2	2:B:386:THR:HG22	2.46	0.46
2:B:358:ARG:H	2:B:358:ARG:CD	2.29	0.46
1:A:424:LYS:HE3	1:A:426:TRP:CZ3	2.51	0.45
1:A:180:ILE:HG12	1:A:189:VAL:HG13	1.98	0.45
2:B:361:HIS:HD2	2:B:362:THR:HG22	1.81	0.45
1:A:41:MET:HB3	1:A:46:LYS:NZ	2.32	0.45
2:B:111:VAL:HG23	2:B:111:VAL:O	2.17	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:NH1	1:A:448:ARG:HG2	2.31	0.45
2:B:353:LYS:HG2	4:B:1205:HOH:O	2.16	0.45
2:B:202:ILE:O	2:B:205:LEU:HB3	2.16	0.45
1:A:187:LEU:HA	1:A:187:LEU:HD12	1.80	0.45
1:A:491:LEU:HD12	1:A:491:LEU:HA	1.72	0.45
1:A:357:MET:HG2	1:A:357:MET:O	2.17	0.44
1:A:24:TRP:CD1	1:A:61:PHE:HE1	2.35	0.44
2:B:8:VAL:HG22	2:B:8:VAL:O	2.17	0.44
1:A:328:GLU:HB3	1:A:340:GLN:OE1	2.17	0.44
1:A:91:GLN:HE22	1:A:183:TYR:HE1	1.63	0.44
2:B:43:LYS:C	2:B:45:GLY:H	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:ILE:O	1:A:526:ILE:HG13	2.17	0.44
1:A:454:LYS:HA	1:A:467:VAL:O	2.18	0.44
1:A:234:LEU:HD12	1:A:239:TRP:CB	2.47	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
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
2:B:354:TYR:CE2	2:B:371:ALA:HB2	2.53	0.44
1:A:514:GLU:HG3	1:A:514:GLU:H	1.60	0.44
1:A:366:LYS:O	1:A:370:GLU:HG3	2.18	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
2:B:201:LYS:HE3	4:B:1175:HOH:O	2.19	0.43
1:A:31:ILE:O	1:A:35:VAL:HG23	2.18	0.43
1:A:410:TRP:HZ3	2:B:401:TRP:CE2	2.36	0.43
1:A:287:LYS:HG2	1:A:291:GLU:OE1	2.18	0.43
2:B:170:PRO:O	2:B:174:GLN:HG2	2.18	0.43
2:B:271:TYR:HB2	2:B:274:ILE:HD11	2.00	0.43
2:B:66:LYS:HG3	2:B:67:ASP:OD1	2.18	0.43
2:B:178:ILE:HG22	2:B:179:VAL:N	2.33	0.43
2:B:195:ILE:HG23	2:B:196:GLY:N	2.32	0.43
1:A:72:ARG:CG	1:A:73:LYS:N	2.78	0.43
1:A:26:LEU:HD22	1:A:30:LYS:HE2	2.00	0.43
2:B:205:LEU:C	2:B:205:LEU:HD13	2.39	0.43
2:B:380:ILE:O	2:B:384:GLY:N	2.49	0.43
1:A:469:LEU:HB2	1:A:472:THR:HG21	2.00	0.43
1:A:27:THR:HB	1:A:30:LYS:CG	2.42	0.43
2:B:5:ILE:CG2	2:B:6:GLU:H	2.26	0.43
2:B:65:LYS:HZ1	2:B:72:ARG:HE	1.65	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:365:VAL:O	1:A:366:LYS:C	2.57	0.43
2:B:115:TYR:CD1	2:B:115:TYR:N	2.81	0.43
1:A:425:LEU:HA	1:A:425:LEU:HD23	1.87	0.43
2:B:242:GLN:HE21	2:B:242:GLN:HA	1.83	0.43
2:B:104:LYS:HB2	2:B:192:ASP:HA	2.00	0.43
1:A:356:ARG:HB2	1:A:367:GLN:NE2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.54	0.43
2:B:5:ILE:H	2:B:119:PRO:HG3	1.84	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
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
2:B:21:VAL:HB	2:B:59:PRO:HD3	2.00	0.42
1:A:223:LYS:HB2	1:A:223:LYS:HE3	1.85	0.42
2:B:92:LEU:CD2	2:B:165:THR:HG21	2.49	0.42
1:A:34:LEU:HB3	1:A:132:ILE:HD12	2.01	0.42
2:B:149:LEU:HA	2:B:150:PRO:HD3	1.90	0.42
2:B:27:THR:OG1	2:B:30:LYS:HG2	2.20	0.42
2:B:195:ILE:CG2	2:B:196:GLY:N	2.82	0.42
2:B:157:PRO:CG	2:B:184:MET:HA	2.49	0.42
1:A:239:TRP:CH2	1:A:316:GLY:HA3	2.53	0.42
1:A:410:TRP:NE1	2:B:363:ASN:HB2	2.33	0.42
2:B:120:LEU:HD23	2:B:121:ASP:O	2.20	0.42
1:A:95:PRO:HB3	2:B:136:ASN:ND2	2.35	0.42
2:B:278:GLN:HB2	2:B:302:GLU:OE1	2.20	0.42
2:B:64:LYS:HD2	2:B:71:TRP:CE2	2.55	0.42
1:A:407:GLN:HG2	2:B:393:ILE:HA	2.01	0.42
2:B:423:VAL:O	2:B:427:TYR:HD2	2.02	0.41
1:A:361:HIS:ND1	1:A:361:HIS:N	2.68	0.41
2:B:311:LYS:HE2	4:B:1194:HOH:O	2.20	0.41
1:A:478:GLU:O	1:A:481:ALA:HB3	2.20	0.41
2:B:193:LEU:H	2:B:193:LEU:CD1	2.34	0.41
1:A:274:ILE:HG12	1:A:309:ILE:HG21	2.02	0.41
1:A:184:MET:HB3	1:A:185:ASP:H	1.61	0.41
2:B:107:THR:HG23	2:B:232:TYR:HE1	1.85	0.41
1:A:178:ILE:HD11	1:A:201:LYS:HG3	2.03	0.41
1:A:457:TYR:CE2	1:A:465:LYS:HB3	2.55	0.41
1:A:58:THR:HG23	1:A:76:ASP:O	2.20	0.41
2:B:5:ILE:CG2	2:B:6:GLU:N	2.84	0.41
1:A:142:ILE:N	1:A:142:ILE:CD1	2.84	0.41
1:A:42:GLU:OE1	1:A:49:LYS:HE3	2.20	0.41
2:B:94:ILE:HA	2:B:94:ILE:HD12	1.93	0.41
2:B:305:GLU:O	2:B:309:ILE:HG13	2.20	0.41
3:A:999:U05:N1	3:A:999:U05:C15	2.84	0.41
1:A:116:PHE:CE1	1:A:151:GLN:HB2	2.56	0.41
1:A:11:LYS:O	1:A:85:GLN:HB3	2.20	0.41
2:B:356:ARG:CZ	2:B:361:HIS:HB3	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ILE:HD12	1:A:37:ILE:N	2.36	0.41
1:A:444:GLY:CA	1:A:477:THR:HG22	2.50	0.41
2:B:356:ARG:NH2	2:B:361:HIS:HB3	2.36	0.41
1:A:515:SER:HB3	1:A:518:VAL:HG23	2.03	0.41
1:A:103:LYS:HA	1:A:103:LYS:HD3	1.70	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
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
2:B:418:ASN:N	2:B:418:ASN:OD1	2.55	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
2:B:260:LEU:O	2:B:264:LEU:HG	2.21	0.40
1:A:3:SER:OG	1:A:5:ILE:HG22	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%)	7	3
2	B	414/440 (94%)	378 (91%)	27 (6%)	9 (2%)	8	4
All	All	954/1000 (95%)	857 (90%)	74 (8%)	23 (2%)	7	4

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

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Mol	Chain	Res	Type
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%)	420 (87%)	65 (13%)	5	4
2	B	380/400 (95%)	324 (85%)	56 (15%)	4	3
All	All	865/899 (96%)	744 (86%)	121 (14%)	4	3

All (121) 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

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Mol	Chain	Res	Type
1	A	60	VAL
1	A	63	ILE
1	A	65	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	168	LEU
1	A	184	MET
1	A	194	GLU
1	A	197	GLN
1	A	205	LEU
1	A	208	HIS
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	263	LYS
1	A	270	ILE
1	A	279	LEU
1	A	283	LEU
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	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

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Mol	Chain	Res	Type
1	A	373	GLN
1	A	386	THR
1	A	423	VAL
1	A	424	LYS
1	A	432	GLU
1	A	448	ARG
1	A	452	LEU
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	503	LEU
1	A	513	SER
1	A	514	GLU
1	A	540	LYS
1	A	542	ILE
2	B	6	GLU
2	B	10	VAL
2	B	24	TRP
2	B	46	LYS
2	B	53	GLU
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	139	THR
2	B	145	GLN
2	B	161	GLN
2	B	162	SER
2	B	163	SER
2	B	170	PRO

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Mol	Chain	Res	Type
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	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
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	368	LEU
2	B	379	SER
2	B	390	LYS
2	B	399	GLU
2	B	418	ASN
2	B	420	PRO
2	B	424	LYS
2	B	425	LEU
2	B	429	LEU

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	23	GLN
1	A	91	GLN
1	A	174	GLN
1	A	197	GLN
1	A	242	GLN

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Mol	Chain	Res	Type
1	A	332	GLN
1	A	336	GLN
1	A	475	GLN
1	A	480	GLN
1	A	512	GLN
2	B	57	ASN
2	B	85	GLN
2	B	151	GLN
2	B	242	GLN
2	B	269	GLN
2	B	361	HIS

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	3,7,8	1.25	0	3,8,10	3.69	1 (33%)

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	-	1/2/6/8	0/0/0/0

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	6.09	115.55	105.40

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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 carbohydrates 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	-	16,24,24	1.63	3 (18%)	15,35,35	1.46	3 (20%)

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	0/2/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	U05	C2-N1	2.87	1.38	1.32
3	A	999	U05	C7-C8	3.12	1.43	1.36
3	A	999	U05	C3-C4	3.61	1.44	1.36

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	U05	C4-C4A-C1A	2.22	119.07	117.00
3	A	999	U05	C10-C11-C6A	2.35	121.44	119.06
3	A	999	U05	C8-C9-N	2.39	121.42	119.48

There are no chirality outliers.

There are no torsion outliers.

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

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.