Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 08:36 PM EDT

PDB ID	:	1C0T
Title	:	CRYSTAL STRUCTURE OF HIV-1 REVERSE TRANSCRIPTASE IN COMPLEX WITH BM+21.1326
Authors	:	Ren, J.; Esnouf, R.M.; Hopkins, A.L.; Stuart, D.I.; Stammers, D.K.
Deposited on	:	1999-07-19
Resolution	:	2.70 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 (i) 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 (i)) were used in the production of this report:

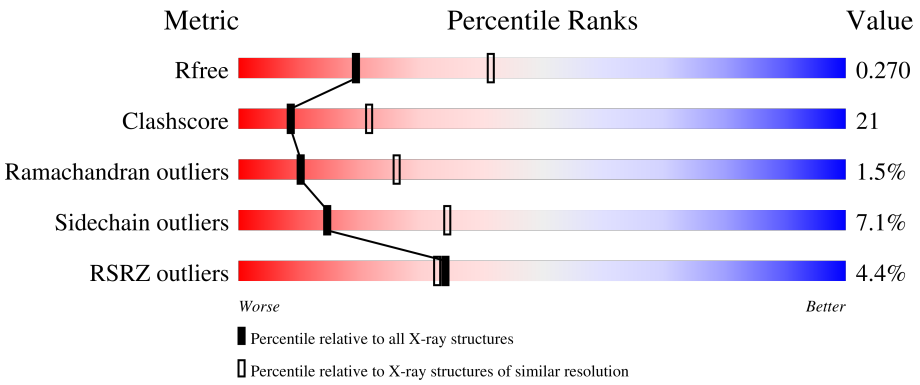
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 <=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	4% 49% 35% • 12%
2	B	440	3% 51% 31% • 15%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7166 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.

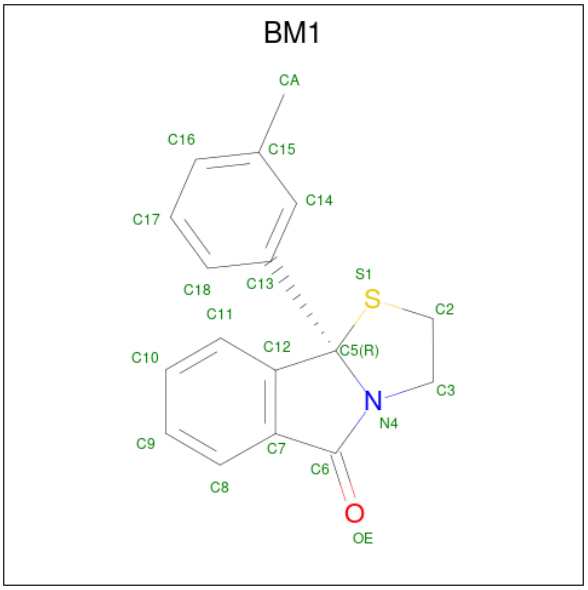
- Molecule 1 is a protein called HIV-1 REVERSE TRANSCRIPTASE (A-CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	491	4026	2611	669	740	6	0	0	0

- Molecule 2 is a protein called HIV-1 REVERSE TRANSCRIPTASE (B-CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	373	3077	2003	507	560	7	0	0	0

- Molecule 3 is (R)-(+)9B-(3-METHYL)PHENYL-2,3-DIHYDROTHIAZOLO[2,3-A]ISOINDOL-5(9BH)-ONE (three-letter code: BM1) (formula: $C_{17}H_{15}NOS$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	20	17	1	1	1	0	0

- Molecule 4 is water.

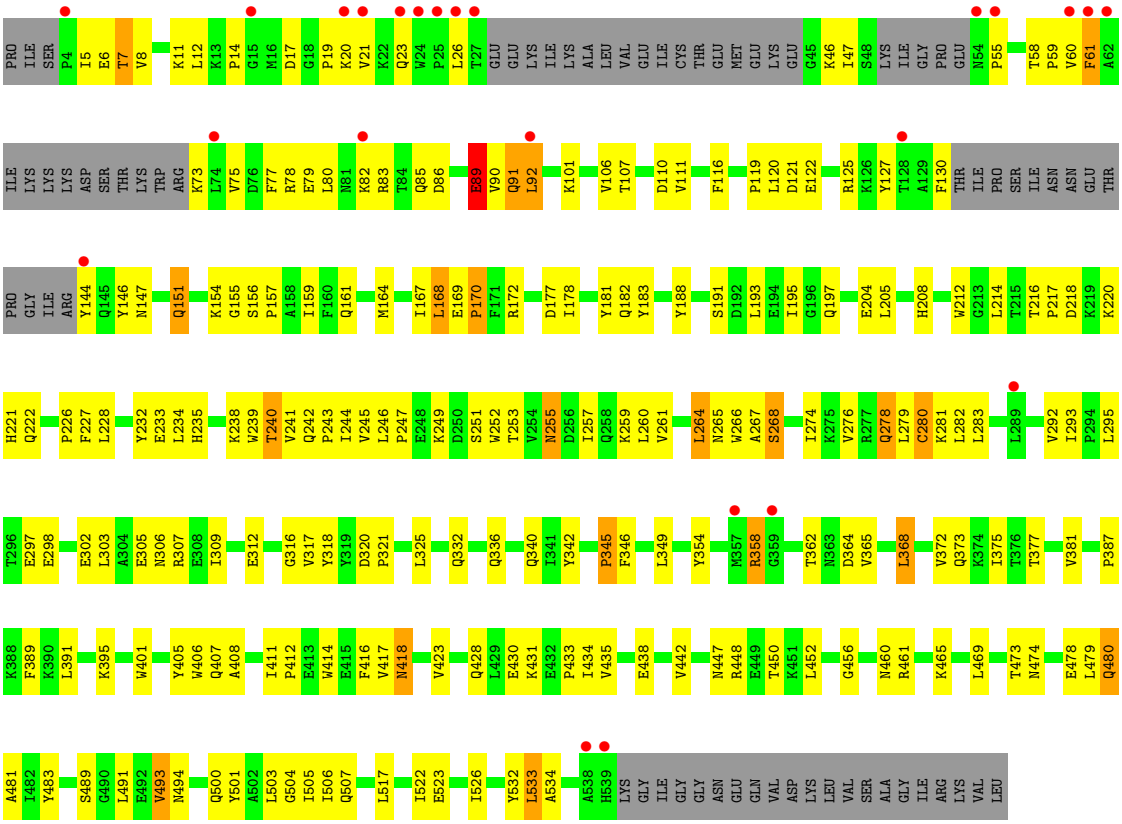
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	26	26	26	0	0
			Total	O		
4	B	17	17	17	0	0

3 Residue-property plots (i)

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.

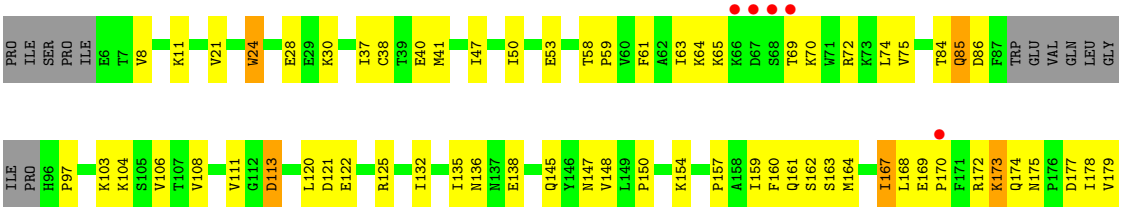
• Molecule 1: HIV-1 REVERSE TRANSCRIPTASE (A-CHAIN)

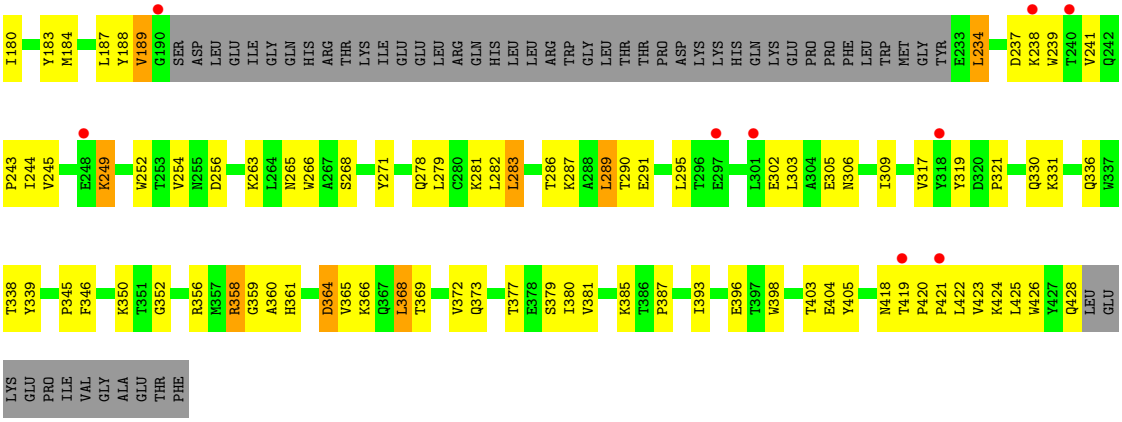
Chain A:



• Molecule 2: HIV-1 REVERSE TRANSCRIPTASE (B-CHAIN)

Chain B:




I180 Y183 M184 L187 Y188 V189 G190 SER ASP LEU GLU ILE GLY GLN HIS ARG THR LYS ILE GLU GLU LEU ARG GLN HIS LEU LEU ARG TRP GLY LEU THR THR PRO ASP LYS LYS HIS GLN LYS GLU PRO PRO PHE LEU TRP MET GLY TYR E233 L234 D237 K238 W239 T240 V241 Q242
P243 I244 V245 E248 K249 W252 T253 V254 N255 D256 K263 L264 N265 W266 A267 S268 Y271 Q278 L279 C280 K281 L282 L283 T286 K287 A288 L289 T290 E291 L295 T296 E297 L301 E302 L303 A304 E305 N306 I309 V317 Y318 Y319 D320 P321 Q330 K331 Q336 W337
T338 Y339 P345 F346 K350 T351 G352 R356 M357 R358 G359 A360 H361 D364 V365 K366 Q367 L368 T369 V372 Q373 T377 E378 S379 I380 V381 K385 T386 P387 I393 E396 T397 W398 T403 E404 Y405 N418 T419 P420 P421 L422 V423 K424 L425 W426 Y427 Q428 LEU GLU
LYS GLU PRO ILE VAL GLY ALA GLU THR PHE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	135.10Å 112.70Å 75.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 18.75 – 2.70	Depositor EDS
% Data completeness (in resolution range)	81.2 (20.00-2.70) 81.1 (18.75-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.99 (at 2.70Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.214 , 0.276 0.206 , 0.270	Depositor DCC
R_{free} test set	1259 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å^2)	54.1	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 67.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7166	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, BM1

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	0.41	0/4124	0.64	0/5604
2	B	0.40	0/3163	0.65	0/4296
All	All	0.41	0/7287	0.64	0/9900

There are no bond length outliers.

There are no bond angle outliers.

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	4026	0	4038	173	0
2	B	3077	0	3106	136	0
3	A	20	0	15	1	0
4	A	26	0	0	3	0
4	B	17	0	0	1	0
All	All	7166	0	7159	296	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 21.

All (296) 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:406:TRP:CH2	2:B:418:ASN:HA	2.06	0.91
1:A:448:ARG:HH12	1:A:474:ASN:H	1.11	0.91
2:B:61:PHE:CZ	2:B:74:LEU:HD23	2.08	0.89
1:A:60:VAL:HG12	1:A:75:VAL:HG22	1.58	0.84
1:A:448:ARG:NH1	1:A:474:ASN:H	1.79	0.81
2:B:161:GLN:HE21	2:B:161:GLN:HA	1.46	0.81
1:A:279:LEU:HA	1:A:282:LEU:HD23	1.63	0.79
2:B:369:THR:HG22	2:B:398:TRP:CZ3	2.18	0.79
1:A:448:ARG:HH12	1:A:474:ASN:N	1.81	0.79
1:A:500:GLN:HG2	2:B:422:LEU:HD11	1.63	0.78
2:B:65:LYS:HE3	2:B:72:ARG:HG2	1.65	0.78
2:B:163:SER:O	2:B:167:ILE:HG22	1.83	0.77
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.68	0.76
2:B:358:ARG:HD3	2:B:359:GLY:H	1.52	0.74
1:A:253:THR:HG22	1:A:292:VAL:HG22	1.72	0.70
1:A:47:ILE:HG22	1:A:146:TYR:HA	1.74	0.69
2:B:120:LEU:HD23	2:B:125:ARG:HG2	1.74	0.69
1:A:125:ARG:HG2	1:A:146:TYR:O	1.93	0.69
2:B:365:VAL:O	2:B:369:THR:HG23	1.93	0.69
1:A:406:TRP:HH2	2:B:418:ASN:HA	1.55	0.69
2:B:358:ARG:HG3	2:B:358:ARG:HH11	1.57	0.68
1:A:406:TRP:CE3	2:B:419:THR:HB	2.28	0.68
2:B:63:ILE:HD13	2:B:74:LEU:HD22	1.76	0.67
2:B:161:GLN:HA	2:B:161:GLN:NE2	2.10	0.67
2:B:169:GLU:N	2:B:170:PRO:HD2	2.09	0.67
1:A:233:GLU:HB3	1:A:240:THR:HG23	1.75	0.67
2:B:11:LYS:O	2:B:85:GLN:HB3	1.96	0.66
2:B:420:PRO:HB2	2:B:423:VAL:HG12	1.78	0.66
1:A:218:ASP:O	1:A:222:GLN:HG3	1.96	0.65
1:A:188:TYR:HB3	3:A:999:BM1:S1	2.36	0.65
1:A:408:ALA:HA	2:B:364:ASP:OD1	1.96	0.65
2:B:356:ARG:NH2	2:B:361:HIS:HB2	2.11	0.65
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.37	0.64
1:A:257:ILE:O	1:A:261:VAL:HG23	1.97	0.64
2:B:369:THR:HG22	2:B:398:TRP:CH2	2.33	0.64
1:A:21:VAL:CG1	1:A:59:PRO:HD3	2.27	0.64
1:A:125:ARG:HE	1:A:147:ASN:HA	1.61	0.64
1:A:503:LEU:HD21	1:A:507:GLN:HE21	1.64	0.62
1:A:155:GLY:O	1:A:159:ILE:HG13	1.99	0.62
1:A:151:GLN:N	1:A:151:GLN:HE21	1.97	0.62
1:A:280:CSD:C	1:A:281:LYS:N	2.62	0.62
1:A:167:ILE:O	1:A:170:PRO:HD2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:266:TRP:CZ3	2:B:426:TRP:HB3	2.36	0.61
1:A:279:LEU:HD13	1:A:302:GLU:OE1	1.99	0.61
1:A:345:PRO:O	1:A:346:PHE:HB2	1.99	0.61
2:B:64:LYS:HE3	2:B:69:THR:O	2.00	0.61
1:A:391:LEU:C	1:A:417:VAL:HG12	2.22	0.60
1:A:244:ILE:CD1	1:A:267:ALA:HB2	2.32	0.60
1:A:325:LEU:HB3	1:A:387:PRO:HB3	1.84	0.59
1:A:303:LEU:HD21	1:A:307:ARG:NH2	2.18	0.59
2:B:266:TRP:CE3	2:B:426:TRP:HB3	2.36	0.59
1:A:280:CSD:O	1:A:281:LYS:N	2.35	0.59
2:B:85:GLN:HG2	2:B:86:ASP:N	2.17	0.59
1:A:247:PRO:HB3	1:A:249:LYS:HE3	1.83	0.59
2:B:103:LYS:HE3	2:B:179:VAL:CG2	2.33	0.58
1:A:8:VAL:HG21	1:A:159:ILE:HG23	1.86	0.58
1:A:178:ILE:HD13	1:A:191:SER:HB2	1.85	0.58
1:A:494:ASN:HB3	2:B:289:LEU:HD22	1.85	0.58
1:A:283:LEU:HD22	1:A:283:LEU:N	2.18	0.58
1:A:395:LYS:HD3	1:A:414:TRP:CH2	2.38	0.58
1:A:430:GLU:HG3	1:A:434:ILE:HD11	1.84	0.58
2:B:358:ARG:HG3	2:B:358:ARG:NH1	2.18	0.58
1:A:501:TYR:CZ	1:A:505:ILE:HD11	2.39	0.58
1:A:418:ASN:C	1:A:418:ASN:HD22	2.07	0.58
2:B:104:LYS:HA	2:B:237:ASP:OD1	2.04	0.57
2:B:339:TYR:CZ	2:B:352:GLY:HA3	2.39	0.57
1:A:450:THR:OG1	1:A:452:LEU:HB2	2.04	0.57
1:A:19:PRO:HA	1:A:83:ARG:HH12	1.70	0.57
2:B:154:LYS:HA	2:B:184:MET:HE1	1.87	0.57
1:A:101:LYS:HD2	1:A:101:LYS:N	2.19	0.56
1:A:26:LEU:HD11	1:A:61:PHE:HB3	1.88	0.56
1:A:522:ILE:O	1:A:526:ILE:HG13	2.06	0.56
1:A:21:VAL:HG11	1:A:59:PRO:HD3	1.88	0.56
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.40	0.56
1:A:60:VAL:HG11	1:A:130:PHE:CD1	2.41	0.55
1:A:253:THR:O	1:A:257:ILE:HG13	2.06	0.55
1:A:164:MET:HG3	1:A:168:LEU:HD22	1.88	0.55
1:A:77:PHE:CD2	1:A:80:LEU:HD23	2.41	0.55
1:A:78:ARG:O	1:A:82:LYS:HG3	2.07	0.55
1:A:83:ARG:HG3	1:A:83:ARG:HH11	1.70	0.55
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.87	0.55
2:B:103:LYS:HE3	2:B:179:VAL:HG23	1.89	0.55
1:A:358:ARG:HG3	1:A:358:ARG:HH11	1.70	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.88	0.54
2:B:305:GLU:O	2:B:309:ILE:HG13	2.07	0.54
1:A:90:VAL:CG1	1:A:91:GLN:N	2.70	0.54
2:B:125:ARG:HH11	2:B:147:ASN:HD22	1.54	0.54
1:A:252:TRP:NE1	1:A:295:LEU:HD11	2.23	0.54
1:A:504:GLY:HA2	2:B:421:PRO:HG2	1.89	0.54
2:B:65:LYS:CE	2:B:72:ARG:HG2	2.34	0.54
2:B:237:ASP:OD2	2:B:238:LYS:HE3	2.09	0.53
1:A:239:TRP:NE1	1:A:316:GLY:HA3	2.24	0.53
1:A:247:PRO:CB	1:A:249:LYS:HE3	2.38	0.53
1:A:456:GLY:HA3	1:A:465:LYS:O	2.08	0.53
2:B:279:LEU:HG	2:B:302:GLU:OE2	2.09	0.53
2:B:61:PHE:CE2	2:B:74:LEU:HD23	2.42	0.53
2:B:65:LYS:HD3	2:B:72:ARG:HE	1.74	0.53
2:B:37:ILE:O	2:B:40:GLU:HG2	2.08	0.52
1:A:120:LEU:O	1:A:121:ASP:C	2.47	0.52
1:A:220:LYS:HE3	1:A:221:HIS:CE1	2.44	0.52
2:B:174:GLN:HG3	2:B:175:ASN:OD1	2.09	0.52
2:B:234:LEU:H	2:B:234:LEU:HD22	1.72	0.52
2:B:28:GLU:HG3	2:B:135:ILE:HD11	1.90	0.52
1:A:12:LEU:HD11	1:A:127:TYR:CE2	2.44	0.52
1:A:246:LEU:HD22	1:A:260:LEU:CD1	2.40	0.52
1:A:260:LEU:O	1:A:264:LEU:HD13	2.10	0.52
1:A:101:LYS:HG2	4:A:1041:HOH:O	2.09	0.51
1:A:358:ARG:NH2	2:B:396:GLU:OE2	2.44	0.51
1:A:534:ALA:HB1	4:A:1054:HOH:O	2.11	0.51
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.91	0.51
1:A:246:LEU:HD22	1:A:260:LEU:HD11	1.92	0.51
1:A:438:GLU:HG3	1:A:461:ARG:HD2	1.93	0.51
2:B:172:ARG:HD3	2:B:180:ILE:HB	1.93	0.51
2:B:358:ARG:CD	2:B:359:GLY:H	2.23	0.51
2:B:234:LEU:HD22	2:B:234:LEU:N	2.26	0.51
2:B:319:TYR:OH	2:B:385:LYS:HD3	2.10	0.51
1:A:7:THR:HG21	1:A:121:ASP:HA	1.92	0.51
1:A:21:VAL:HG13	1:A:59:PRO:HD3	1.90	0.51
1:A:245:VAL:HG13	1:A:245:VAL:O	2.11	0.51
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.93	0.51
1:A:235:HIS:HB2	1:A:238:LYS:O	2.10	0.50
2:B:84:THR:HB	2:B:154:LYS:HE2	1.94	0.50
1:A:317:VAL:HG22	1:A:318:TYR:H	1.76	0.50
1:A:242:GLN:HB2	1:A:243:PRO:HD2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:LEU:HD12	1:A:293:ILE:CG2	2.41	0.50
2:B:64:LYS:HE3	2:B:69:THR:C	2.32	0.50
1:A:354:TYR:HE2	1:A:375:ILE:HG13	1.76	0.50
1:A:298:GLU:H	1:A:298:GLU:CD	2.14	0.50
1:A:342:TYR:CD1	1:A:342:TYR:C	2.86	0.49
2:B:154:LYS:HA	2:B:184:MET:CE	2.42	0.49
2:B:169:GLU:N	2:B:170:PRO:CD	2.74	0.49
2:B:24:TRP:HH2	2:B:61:PHE:CE1	2.31	0.49
2:B:164:MET:O	2:B:167:ILE:HG23	2.11	0.49
2:B:173:LYS:HB2	2:B:173:LYS:NZ	2.28	0.49
2:B:183:TYR:CD1	2:B:380:ILE:HD13	2.48	0.49
1:A:332:GLN:O	1:A:336:GLN:HB2	2.12	0.49
2:B:120:LEU:O	2:B:121:ASP:C	2.49	0.49
1:A:253:THR:HA	1:A:292:VAL:HA	1.94	0.49
2:B:177:ASP:CG	2:B:178:ILE:N	2.66	0.49
2:B:249:LYS:HE2	2:B:256:ASP:OD1	2.13	0.49
2:B:393:ILE:HD13	2:B:398:TRP:HB2	1.95	0.48
2:B:254:VAL:HG23	2:B:291:GLU:O	2.14	0.48
2:B:24:TRP:CH2	2:B:61:PHE:CD1	3.01	0.48
2:B:177:ASP:CG	2:B:178:ILE:H	2.16	0.48
1:A:7:THR:CG2	1:A:121:ASP:HA	2.43	0.48
1:A:8:VAL:CG2	1:A:159:ILE:HG23	2.42	0.48
1:A:389:PHE:HB2	1:A:414:TRP:HB3	1.95	0.48
2:B:404:GLU:HG2	4:B:1017:HOH:O	2.13	0.48
1:A:506:ILE:HG21	1:A:533:LEU:HD12	1.95	0.48
2:B:148:VAL:O	2:B:150:PRO:HD3	2.14	0.48
1:A:234:LEU:N	1:A:234:LEU:HD22	2.28	0.48
1:A:297:GLU:HB3	1:A:298:GLU:OE2	2.13	0.48
1:A:448:ARG:HH22	1:A:474:ASN:N	2.11	0.48
2:B:239:TRP:CH2	2:B:381:VAL:HG11	2.48	0.48
2:B:345:PRO:O	2:B:346:PHE:HB2	2.14	0.48
1:A:106:VAL:HG12	1:A:227:PHE:CE2	2.49	0.48
1:A:89:GLU:OE2	1:A:92:LEU:HD21	2.14	0.47
1:A:448:ARG:CZ	1:A:474:ASN:H	2.26	0.47
2:B:161:GLN:HE21	2:B:161:GLN:CA	2.16	0.47
1:A:168:LEU:O	1:A:172:ARG:HG3	2.14	0.47
2:B:63:ILE:HG13	2:B:72:ARG:HB3	1.96	0.47
2:B:50:ILE:HG23	2:B:145:GLN:HG2	1.96	0.47
2:B:180:ILE:CD1	2:B:189:VAL:HG13	2.44	0.47
2:B:423:VAL:HG13	2:B:423:VAL:O	2.14	0.47
1:A:151:GLN:HE21	1:A:151:GLN:CA	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:LEU:N	1:A:282:LEU:HD22	2.30	0.47
1:A:79:GLU:O	1:A:83:ARG:HG2	2.15	0.47
1:A:317:VAL:HG22	1:A:318:TYR:N	2.29	0.47
1:A:407:GLN:HG2	2:B:393:ILE:HA	1.96	0.47
2:B:172:ARG:C	2:B:173:LYS:HZ2	2.18	0.47
1:A:406:TRP:CH2	1:A:407:GLN:NE2	2.83	0.47
1:A:274:ILE:HG23	1:A:306:ASN:OD1	2.15	0.47
2:B:173:LYS:HB2	2:B:173:LYS:HZ3	1.79	0.47
2:B:263:LYS:HA	2:B:426:TRP:CD1	2.50	0.47
1:A:85:GLN:O	1:A:154:LYS:NZ	2.40	0.46
2:B:245:VAL:O	2:B:245:VAL:HG23	2.15	0.46
2:B:282:LEU:HD11	2:B:295:LEU:HD23	1.97	0.46
1:A:111:VAL:HG11	1:A:214:LEU:HD22	1.96	0.46
2:B:379:SER:CB	2:B:387:PRO:HD3	2.45	0.46
2:B:178:ILE:CG2	2:B:189:VAL:HG12	2.45	0.46
1:A:252:TRP:CD1	1:A:295:LEU:HD11	2.51	0.46
1:A:278:GLN:HB2	1:A:302:GLU:OE2	2.15	0.46
2:B:125:ARG:HD3	2:B:147:ASN:HA	1.95	0.46
1:A:73:LYS:HE2	1:A:75:VAL:CG2	2.46	0.46
1:A:469:LEU:N	1:A:469:LEU:HD22	2.31	0.46
2:B:268:SER:HA	2:B:271:TYR:O	2.16	0.46
2:B:428:GLN:O	2:B:428:GLN:HG3	2.16	0.46
1:A:193:LEU:HB3	1:A:197:GLN:HB2	1.97	0.46
1:A:298:GLU:CD	1:A:298:GLU:N	2.69	0.46
2:B:241:VAL:O	2:B:243:PRO:HD3	2.16	0.46
1:A:240:THR:OG1	1:A:241:VAL:N	2.49	0.46
1:A:448:ARG:HH22	1:A:474:ASN:H	1.63	0.46
2:B:369:THR:O	2:B:373:GLN:HG3	2.16	0.45
1:A:23:GLN:HE22	1:A:60:VAL:H	1.62	0.45
1:A:239:TRP:CD1	1:A:316:GLY:O	2.69	0.45
2:B:157:PRO:HG3	2:B:184:MET:HE1	1.97	0.45
2:B:241:VAL:HG22	2:B:350:LYS:HG3	1.97	0.45
2:B:169:GLU:H	2:B:170:PRO:HD2	1.80	0.45
1:A:317:VAL:HG13	1:A:349:LEU:HD23	1.99	0.45
2:B:41:MET:HB3	2:B:47:ILE:HG12	1.98	0.45
1:A:372:VAL:HG11	1:A:411:ILE:HG23	1.98	0.45
1:A:474:ASN:O	1:A:478:GLU:HG3	2.16	0.45
2:B:108:VAL:HG23	2:B:234:LEU:HD21	1.97	0.45
2:B:330:GLN:HB2	2:B:338:THR:OG1	2.16	0.45
1:A:89:GLU:HB2	1:A:92:LEU:HD23	1.99	0.45
1:A:532:TYR:CE2	1:A:534:ALA:HB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:LEU:HD23	1:A:276:VAL:HG12	1.99	0.45
2:B:65:LYS:HZ2	2:B:72:ARG:NE	2.15	0.45
2:B:282:LEU:CD1	2:B:295:LEU:HD23	2.47	0.45
1:A:417:VAL:O	1:A:417:VAL:HG13	2.16	0.44
1:A:480:GLN:O	1:A:483:TYR:HB3	2.17	0.44
1:A:448:ARG:NH2	1:A:474:ASN:H	2.15	0.44
2:B:160:PHE:O	2:B:160:PHE:CD1	2.71	0.44
2:B:103:LYS:HE3	2:B:179:VAL:HG21	1.98	0.44
2:B:356:ARG:HH12	2:B:358:ARG:HA	1.83	0.44
2:B:339:TYR:CE1	2:B:352:GLY:HA3	2.52	0.44
1:A:86:ASP:OD2	1:A:154:LYS:NZ	2.45	0.44
1:A:122:GLU:HA	1:A:125:ARG:HD2	1.99	0.44
1:A:345:PRO:C	1:A:346:PHE:HD1	2.21	0.44
1:A:377:THR:O	1:A:381:VAL:HG23	2.18	0.44
2:B:381:VAL:O	2:B:381:VAL:CG1	2.65	0.44
2:B:425:LEU:HD23	2:B:425:LEU:O	2.18	0.44
1:A:8:VAL:O	1:A:121:ASP:HB2	2.17	0.44
1:A:489:SER:HB2	1:A:493:VAL:HG13	1.99	0.44
2:B:317:VAL:HG23	2:B:317:VAL:O	2.18	0.44
2:B:366:LYS:HA	2:B:405:TYR:CD1	2.52	0.44
1:A:435:VAL:HG22	2:B:290:THR:HG21	1.99	0.44
1:A:73:LYS:HE2	1:A:75:VAL:HG22	1.99	0.43
1:A:83:ARG:HG3	1:A:83:ARG:NH1	2.33	0.43
1:A:106:VAL:HG12	1:A:227:PHE:HE2	1.82	0.43
1:A:364:ASP:O	1:A:368:LEU:HB2	2.18	0.43
2:B:106:VAL:O	2:B:234:LEU:N	2.46	0.43
2:B:249:LYS:HG2	2:B:252:TRP:CE2	2.54	0.43
2:B:302:GLU:O	2:B:306:ASN:ND2	2.51	0.43
1:A:5:ILE:CG2	1:A:119:PRO:HD2	2.49	0.43
1:A:20:LYS:HE3	1:A:55:PRO:O	2.19	0.43
2:B:234:LEU:HD11	2:B:377:THR:HG21	2.00	0.43
1:A:90:VAL:HG12	1:A:91:GLN:N	2.33	0.43
2:B:278:GLN:HB2	2:B:302:GLU:OE2	2.19	0.43
1:A:46:LYS:HD3	1:A:116:PHE:HB3	2.01	0.43
2:B:58:THR:HG21	2:B:75:VAL:HG12	2.00	0.43
2:B:368:LEU:O	2:B:372:VAL:HG23	2.19	0.43
2:B:30:LYS:HE2	2:B:404:GLU:OE1	2.18	0.43
2:B:104:LYS:HE3	2:B:104:LYS:HB2	1.92	0.43
2:B:281:LYS:C	2:B:283:LEU:H	2.22	0.42
1:A:265:ASN:O	1:A:267:ALA:N	2.52	0.42
1:A:249:LYS:HB2	1:A:252:TRP:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:LEU:N	1:A:283:LEU:CD2	2.81	0.42
1:A:302:GLU:O	1:A:305:GLU:HB3	2.20	0.42
1:A:460:ASN:HA	2:B:286:THR:O	2.19	0.42
2:B:163:SER:O	2:B:167:ILE:CG2	2.59	0.42
2:B:168:LEU:HD13	2:B:180:ILE:HG21	2.01	0.42
2:B:265:ASN:O	2:B:268:SER:OG	2.27	0.42
1:A:503:LEU:CD2	1:A:507:GLN:HE21	2.30	0.42
2:B:159:ILE:C	2:B:161:GLN:H	2.23	0.42
2:B:379:SER:OG	2:B:387:PRO:HD3	2.19	0.42
1:A:255:ASN:O	1:A:259:LYS:HD3	2.20	0.42
1:A:5:ILE:HG23	1:A:119:PRO:HD2	2.01	0.42
1:A:405:TYR:O	2:B:331:LYS:HD3	2.20	0.42
1:A:309:ILE:O	1:A:312:GLU:HG3	2.20	0.42
1:A:244:ILE:O	1:A:244:ILE:HG22	2.19	0.42
1:A:265:ASN:O	1:A:268:SER:N	2.53	0.42
1:A:365:VAL:HG11	1:A:401:TRP:CD1	2.55	0.42
2:B:136:ASN:HB3	2:B:138:GLU:HG3	2.02	0.42
1:A:447:ASN:OD1	1:A:450:THR:HG23	2.19	0.42
2:B:183:TYR:HB3	2:B:188:TYR:HE1	1.85	0.42
2:B:422:LEU:HB3	2:B:426:TRP:CH2	2.55	0.42
1:A:226:PRO:HB3	1:A:235:HIS:CE1	2.55	0.41
1:A:264:LEU:N	1:A:264:LEU:CD1	2.82	0.41
1:A:58:THR:HA	1:A:59:PRO:HD3	1.94	0.41
1:A:228:LEU:HA	1:A:232:TYR:O	2.20	0.41
2:B:70:LYS:HD2	2:B:70:LYS:N	2.35	0.41
2:B:113:ASP:N	2:B:113:ASP:OD2	2.50	0.41
1:A:106:VAL:HG12	1:A:107:THR:N	2.36	0.41
1:A:216:THR:HB	1:A:217:PRO:HD2	2.02	0.41
2:B:244:ILE:HG22	2:B:263:LYS:HE2	2.02	0.41
1:A:433:PRO:HB3	2:B:289:LEU:HD23	2.03	0.41
1:A:181:TYR:CE1	1:A:183:TYR:HB2	2.55	0.41
1:A:208:HIS:CE1	1:A:212:TRP:CZ3	3.07	0.41
1:A:208:HIS:CE1	1:A:212:TRP:HZ3	2.39	0.41
1:A:260:LEU:HD23	1:A:279:LEU:HD23	2.03	0.41
1:A:391:LEU:O	1:A:416:PHE:HA	2.20	0.41
2:B:69:THR:CG2	2:B:70:LYS:HD2	2.51	0.41
2:B:356:ARG:CZ	2:B:361:HIS:HB2	2.51	0.41
1:A:358:ARG:HH11	1:A:358:ARG:CG	2.34	0.41
2:B:161:GLN:O	2:B:162:SER:C	2.59	0.41
1:A:412:PRO:O	1:A:414:TRP:HD1	2.04	0.40
1:A:503:LEU:HD11	1:A:507:GLN:NE2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:178:ILE:HG21	2:B:189:VAL:HG12	2.03	0.40
2:B:281:LYS:C	2:B:283:LEU:N	2.74	0.40
2:B:319:TYR:CE1	2:B:321:PRO:HD3	2.56	0.40
1:A:204:GLU:HG3	4:A:1043:HOH:O	2.22	0.40
1:A:320:ASP:HA	1:A:321:PRO:HD2	1.97	0.40
1:A:90:VAL:O	1:A:92:LEU:N	2.54	0.40
1:A:244:ILE:HD13	1:A:267:ALA:HB2	2.01	0.40
1:A:278:GLN:HB2	1:A:302:GLU:CD	2.42	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	479/560 (86%)	433 (90%)	36 (8%)	10 (2%)	7 18
2	B	367/440 (83%)	334 (91%)	30 (8%)	3 (1%)	19 43
All	All	846/1000 (85%)	767 (91%)	66 (8%)	13 (2%)	10 26

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	424	LYS
1	A	91	GLN
1	A	251	SER
1	A	266	TRP
1	A	240	THR
2	B	360	ALA
1	A	89	GLU
1	A	268	SER
2	B	97	PRO
1	A	195	ILE

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Mol	Chain	Res	Type
1	A	14	PRO
1	A	170	PRO
1	A	345	PRO

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	438/499 (88%)	403 (92%)	35 (8%)	12	27
2	B	339/400 (85%)	319 (94%)	20 (6%)	19	43
All	All	777/899 (86%)	722 (93%)	55 (7%)	14	34

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	7	THR
1	A	11	LYS
1	A	17	ASP
1	A	61	PHE
1	A	89	GLU
1	A	92	LEU
1	A	110	ASP
1	A	144	TYR
1	A	151	GLN
1	A	161	GLN
1	A	168	LEU
1	A	177	ASP
1	A	182	GLN
1	A	205	LEU
1	A	255	ASN
1	A	264	LEU
1	A	278	GLN
1	A	340	GLN
1	A	358	ARG

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Mol	Chain	Res	Type
1	A	362	THR
1	A	368	LEU
1	A	373	GLN
1	A	418	ASN
1	A	423	VAL
1	A	428	GLN
1	A	431	LYS
1	A	473	THR
1	A	479	LEU
1	A	480	GLN
1	A	491	LEU
1	A	493	VAL
1	A	517	LEU
1	A	523	GLU
1	A	533	LEU
2	B	8	VAL
2	B	24	TRP
2	B	53	GLU
2	B	85	GLN
2	B	113	ASP
2	B	122	GLU
2	B	167	ILE
2	B	173	LYS
2	B	189	VAL
2	B	234	LEU
2	B	249	LYS
2	B	283	LEU
2	B	287	LYS
2	B	289	LEU
2	B	303	LEU
2	B	336	GLN
2	B	358	ARG
2	B	364	ASP
2	B	368	LEU
2	B	403	THR

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

Mol	Chain	Res	Type
1	A	23	GLN
1	A	57	ASN
1	A	147	ASN

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Mol	Chain	Res	Type
1	A	151	GLN
1	A	197	GLN
1	A	222	GLN
1	A	255	ASN
1	A	278	GLN
1	A	315	HIS
1	A	332	GLN
1	A	334	GLN
1	A	407	GLN
1	A	418	ASN
1	A	464	GLN
1	A	475	GLN
1	A	480	GLN
1	A	507	GLN
1	A	520	GLN
2	B	147	ASN
2	B	151	GLN
2	B	161	GLN
2	B	336	GLN
2	B	361	HIS

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	0.65	0	1,8,10	4.92	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(^{o})	Ideal(^{o})
1	A	280	CSD	OD1-SG-CB	4.92	114.90	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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	280	CSD	2	0

5.5 Carbohydrates (i)

There are no monosaccharides 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	BM1	A	999	-	21,23,23	1.41	2 (9%)	27,35,35	0.53	0

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	BM1	A	999	-	-	0/6/33/33	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	BM1	C2-C3	-4.16	1.39	1.51
3	A	999	BM1	C6-N4	2.80	1.40	1.36

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

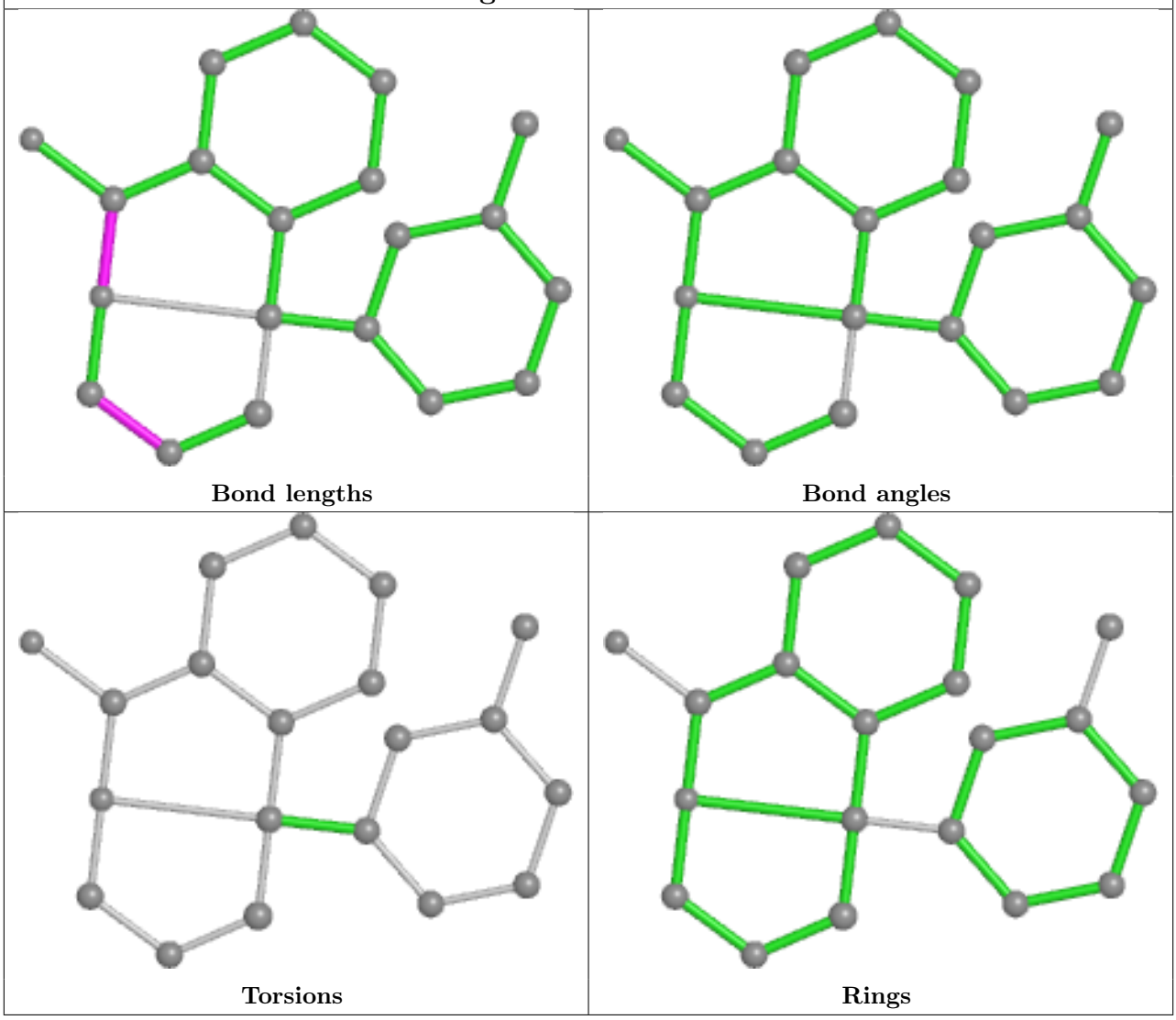
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	BM1	1	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 then 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.

Ligand BM1 A 999



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	280:CSD	C	281:LYS	N	2.62

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, 95th 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^2)	Q<0.9
1	A	490/560 (87%)	-0.15	24 (4%)	29	28	22, 53, 107, 149	0
2	B	373/440 (84%)	-0.22	14 (3%)	40	39	23, 56, 98, 133	0
All	All	863/1000 (86%)	-0.18	38 (4%)	34	33	22, 54, 105, 149	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	539	HIS	4.9
1	A	27	THR	4.3
1	A	26	LEU	4.2
2	B	421	PRO	4.2
1	A	24	TRP	4.1
2	B	67	ASP	4.0
1	A	20	LYS	3.9
1	A	54	ASN	3.7
1	A	359	GLY	3.5
1	A	144	TYR	3.5
1	A	74	LEU	3.4
2	B	248	GLU	3.4
1	A	61	PHE	3.4
1	A	62	ALA	3.4
2	B	68	SER	3.3
1	A	4	PRO	3.3
2	B	301	LEU	3.1
1	A	23	GLN	3.1
2	B	419	THR	3.0
1	A	357	MET	2.9
2	B	190	GLY	2.7
2	B	318	TYR	2.6
1	A	128	THR	2.5
1	A	82	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	55	PRO	2.5
2	B	69	THR	2.5
2	B	66	LYS	2.4
1	A	25	PRO	2.4
2	B	240	THR	2.4
1	A	538	ALA	2.3
1	A	15	GLY	2.3
2	B	238	LYS	2.2
2	B	297	GLU	2.2
1	A	289	LEU	2.1
1	A	21	VAL	2.1
1	A	92	LEU	2.0
1	A	60	VAL	2.0
2	B	170	PRO	2.0

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, 95th 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^2)	Q<0.9
1	CSD	A	280	8/9	0.92	0.14	74,83,86,87	0

6.3 Carbohydrates (i)

There are no monosaccharides 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, 95th 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.

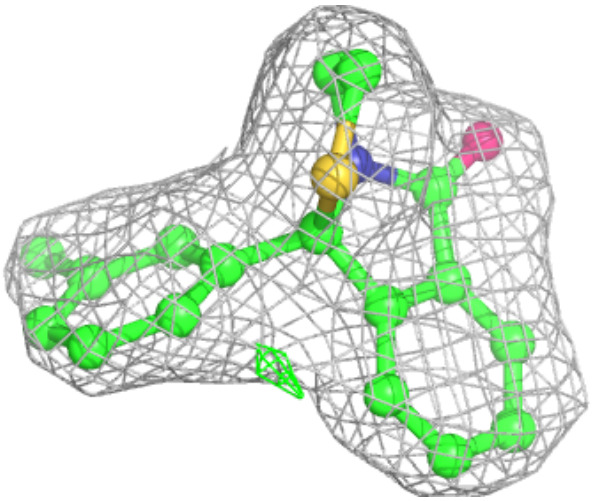
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BM1	A	999	20/20	0.97	0.15	25,44,57,68	0

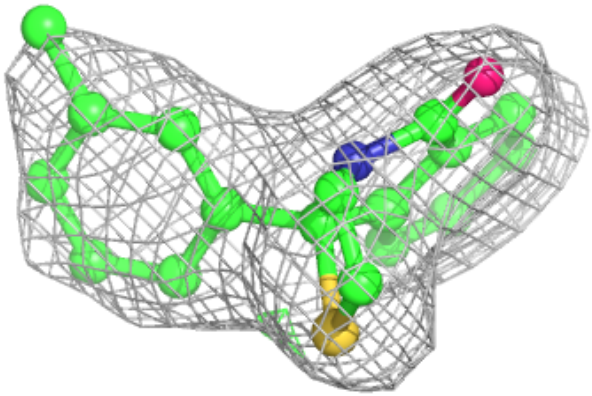
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

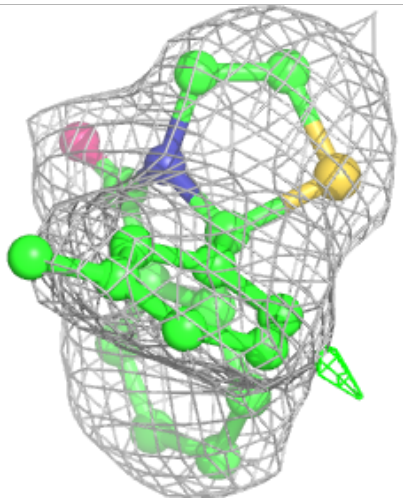
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around BM1 A 999:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.