



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 07:53 am GMT

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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

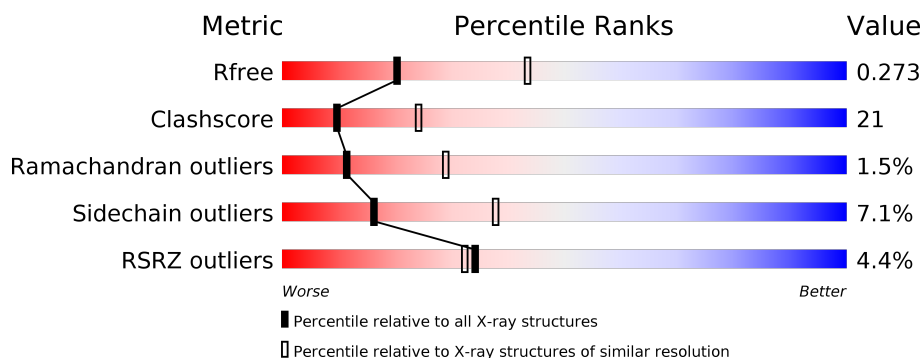
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	111664	2449 (2.70-2.70)
Clashscore	122126	2756 (2.70-2.70)
Ramachandran outliers	120053	2716 (2.70-2.70)
Sidechain outliers	120020	2716 (2.70-2.70)
RSRZ outliers	108989	2376 (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 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.

Mol	Chain	Length	Quality of chain
1	A	560	<div> <div>4%</div> <div> <div></div> <div>49%</div> <div>35%</div> <div>•</div> <div>12%</div> </div> </div>
2	B	440	<div> <div>3%</div> <div> <div></div> <div>51%</div> <div>31%</div> <div>•</div> <div>15%</div> </div> </div>

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.

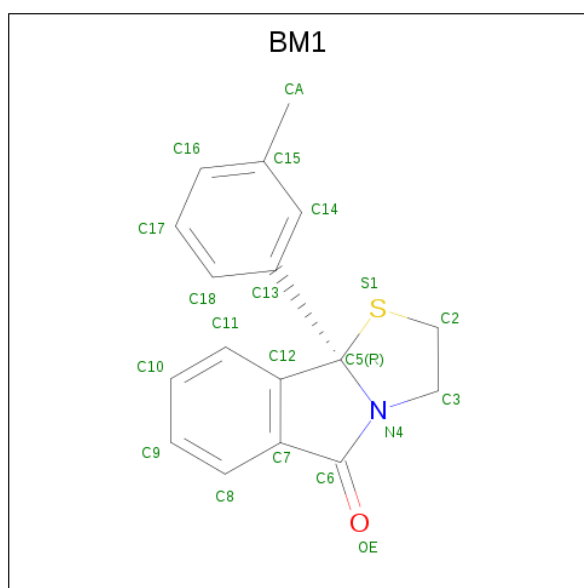
- Molecule 1 is a protein called HIV-1 REVERSE TRANSCRIPTASE (A-CHAIN).

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

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

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

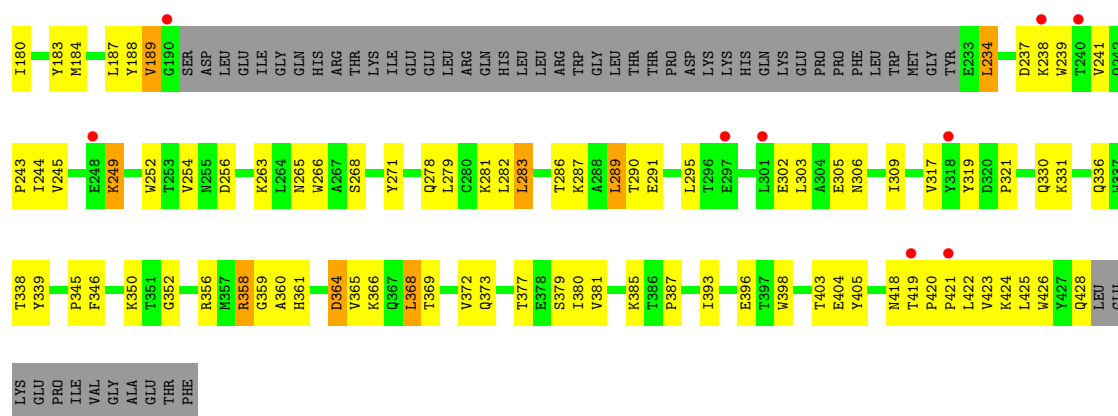
- Molecule 3 is (R)-(+)-9B-(3-METHYL)PHENYL-2,3-DIHYDROTHIAZOLO[2,3-A]ISOINDOL-5(9BH)-ONE (three-letter code: BM1) (formula: C₁₇H₁₅NOS).



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

- Molecule 4 is water.

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



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 2.70Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.214 , 0.276 0.213 , 0.273	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	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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:448:ARG:HH12	1:A:474:ASN:H	1.11	0.91
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.06	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:HA	2:B:161:GLN:HE21	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:HH11	2:B:358:ARG:HG3	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
2:B:356:ARG:NH2	2:B:361:HIS:HB2	2.11	0.65
1:A:408:ALA:HA	2:B:364:ASP:OD1	1.96	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:125:ARG:HE	1:A:147:ASN:HA	1.61	0.64
1:A:21:VAL:CG1	1:A:59:PRO:HD3	2.27	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:HE21	1:A:151:GLN:N	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:N	1:A:283:LEU:HD22	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:NH1	2:B:358:ARG:HG3	2.18	0.58
1:A:501:TYR:CZ	1:A:505:ILE:HD11	2.39	0.58
1:A:418:ASN:HD22	1:A:418:ASN:C	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:N	1:A:101:LYS:HD2	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:253:THR:O	1:A:257:ILE:HG13	2.06	0.55
1:A:60:VAL:HG11	1:A:130:PHE:CD1	2.41	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:169:GLU:HB3	1:A:170:PRO:HD3	1.87	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
2:B:103:LYS:HE3	2:B:179:VAL:HG23	1.89	0.55
1:A:358:ARG:HH11	1:A:358:ARG:HG3	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:65:LYS:HD3	2:B:72:ARG:HE	1.74	0.53
2:B:61:PHE:CE2	2:B:74:LEU:HD23	2.42	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:HD22	2:B:234:LEU:H	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:N	2:B:234:LEU:HD22	2.26	0.51
2:B:319:TYR:OH	2:B:385:LYS:HD3	2.10	0.51
1:A:245:VAL:HG13	1:A:245:VAL:O	2.11	0.51
1:A:21:VAL:HG13	1:A:59:PRO:HD3	1.90	0.51
1:A:7:THR:HG21	1:A:121:ASP:HA	1.92	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:169:GLU:N	2:B:170:PRO:CD	2.74	0.49
2:B:154:LYS:HA	2:B:184:MET:CE	2.42	0.49
2:B:164:MET:O	2:B:167:ILE:HG23	2.11	0.49
2:B:173:LYS:NZ	2:B:173:LYS:HB2	2.28	0.49
2:B:183:TYR:CD1	2:B:380:ILE:HD13	2.48	0.49
2:B:24:TRP:HH2	2:B:61:PHE:CE1	2.31	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:177:ASP:CG	2:B:178:ILE:H	2.16	0.48
2:B:24:TRP:CH2	2:B:61:PHE:CD1	3.01	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:HD22	1:A:234:LEU:N	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:345:PRO:O	2:B:346:PHE:HB2	2.14	0.48
2:B:239:TRP:CH2	2:B:381:VAL:HG11	2.48	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:CA	2:B:161:GLN:HE21	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:O	2:B:423:VAL:HG13	2.14	0.47
1:A:151:GLN:CA	1:A:151:GLN:HE21	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
2:B:172:ARG:C	2:B:173:LYS:HZ2	2.18	0.47
1:A:407:GLN:HG2	2:B:393:ILE:HA	1.96	0.47
1:A:317:VAL:HG22	1:A:318:TYR:N	2.29	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:HZ3	2:B:173:LYS:HB2	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:HG23	2:B:245:VAL:O	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:278:GLN:HB2	1:A:302:GLU:OE2	2.15	0.46
1:A:252:TRP:CD1	1:A:295:LEU:HD11	2.51	0.46
2:B:125:ARG:HD3	2:B:147:ASN:HA	1.95	0.46
1:A:469:LEU:N	1:A:469:LEU:HD22	2.31	0.46
1:A:73:LYS:HE2	1:A:75:VAL:CG2	2.46	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:239:TRP:CD1	1:A:316:GLY:O	2.69	0.45
1:A:23:GLN:HE22	1:A:60:VAL:H	1.62	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:532:TYR:CE2	1:A:534:ALA:HB2	2.52	0.45
1:A:89:GLU:HB2	1:A:92:LEU:HD23	1.99	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:282:LEU:CD1	2:B:295:LEU:HD23	2.47	0.45
2:B:65:LYS:HZ2	2:B:72:ARG:NE	2.15	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:CD1	2:B:160:PHE:O	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: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
1:A:86:ASP:OD2	1:A:154:LYS:NZ	2.45	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:489:SER:HB2	1:A:493:VAL:HG13	1.99	0.44
1:A:8:VAL:O	1:A:121:ASP:HB2	2.17	0.44
2:B:317:VAL:O	2:B:317:VAL:HG23	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:368:LEU:O	2:B:372:VAL:HG23	2.19	0.43
2:B:58:THR:HG21	2:B:75:VAL:HG12	2.00	0.43
2:B:104:LYS:HB2	2:B:104:LYS:HE3	1.92	0.43
2:B:30:LYS:HE2	2:B:404:GLU:OE1	2.18	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:CD1	1:A:264:LEU:N	2.82	0.41
1:A:228:LEU:HA	1:A:232:TYR:O	2.20	0.41
1:A:58:THR:HA	1:A:59:PRO:HD3	1.94	0.41
2:B:70:LYS:N	2:B:70:LYS:HD2	2.35	0.41
2:B:113:ASP:OD2	2:B:113:ASP:N	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:391:LEU:O	1:A:416:PHE:HA	2.20	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
2:B:356:ARG:CZ	2:B:361:HIS:HB2	2.51	0.41
2:B:69:THR:CG2	2:B:70:LYS:HD2	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: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
1:A:90:VAL:O	1:A:92:LEU:N	2.54	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%)	8	20
2	B	367/440 (83%)	334 (91%)	30 (8%)	3 (1%)	21	47
All	All	846/1000 (85%)	767 (91%)	66 (8%)	13 (2%)	11	29

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 ⓘ

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%)	13	30
2	B	339/400 (85%)	319 (94%)	20 (6%)	21	47
All	All	777/899 (86%)	722 (93%)	55 (7%)	16	38

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

Some 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 ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	CSD	A	280	1	4,7,8	1.28	1 (25%)	2,8,10	3.60	1 (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
1	CSD	A	280	1	-	1/2/6/8	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	280	CSD	CA-C	2.34	1.53	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	CSD	OD1-SG-CB	4.92	114.90	105.54

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 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	280	CSD	2	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	BM1	A	999	-	21,23,23	1.38	2 (9%)	26,35,35	0.52	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	-4.02	1.39	1.51
3	A	999	BM1	C6-N4	2.67	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

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

6.1 Protein, DNA and RNA chains

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 32	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(\AA^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 carbohydrates 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(\AA^2)	Q<0.9
3	BM1	A	999	20/20	0.97	0.15	25,44,57,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.