



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 10:20 PM GMT

PDB ID : 5CQG
Title : Structure of Tribolium telomerase in complex with the highly specific inhibitor BIBR1532
Authors : Bryan, C.; Rice, C.; Hoffman, H.; Harkisheimer, M.; Sweeney, M.; Skordalakes, E.
Deposited on : 2015-07-21
Resolution : 2.30 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20026982

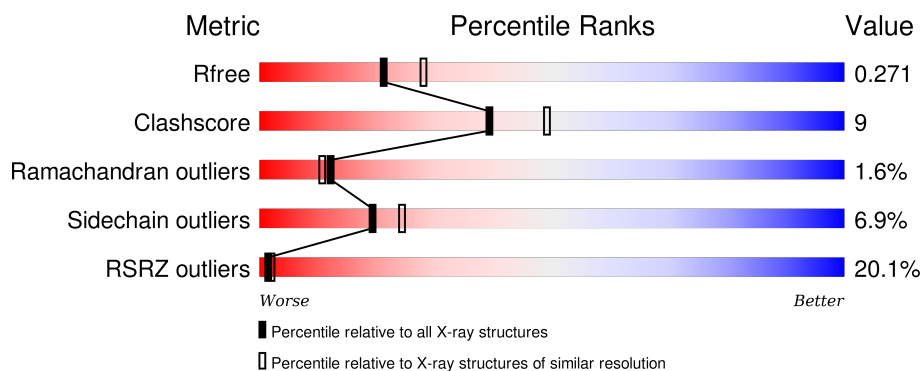
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	596	<div> <div>18%</div> <div>73%</div> <div>24%</div> <div>.</div> </div>
1	B	596	<div> <div>22%</div> <div>79%</div> <div>19%</div> <div>.</div> </div>

2 Entry composition [i](#)

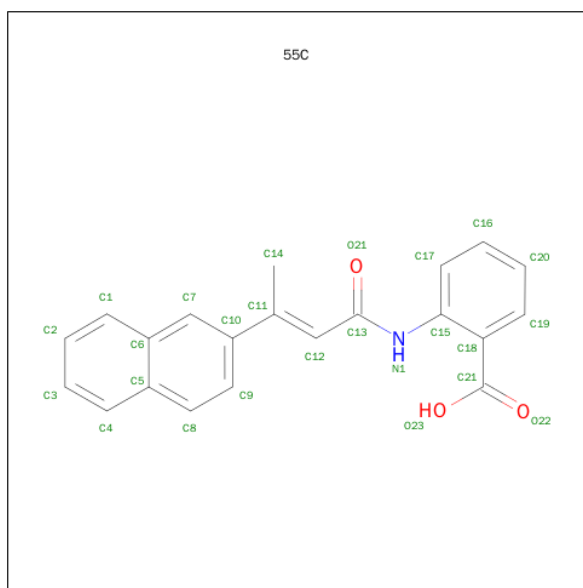
There are 3 unique types of molecules in this entry. The entry contains 10423 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Telomerase reverse transcriptase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	596	Total	C	N	O	S	0	0	0
			4982	3266	852	842	22			
1	B	596	Total	C	N	O	S	0	0	0
			4982	3266	852	842	22			

- Molecule 2 is 2-[[[(2E)-3-(naphthalen-2-yl)but-2-enoyl]amino]benzoic acid (three-letter code: 55C) (formula: C₂₁H₁₇NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			25	21	1	3		
2	B	1	Total	C	N	O	0	0
			25	21	1	3		

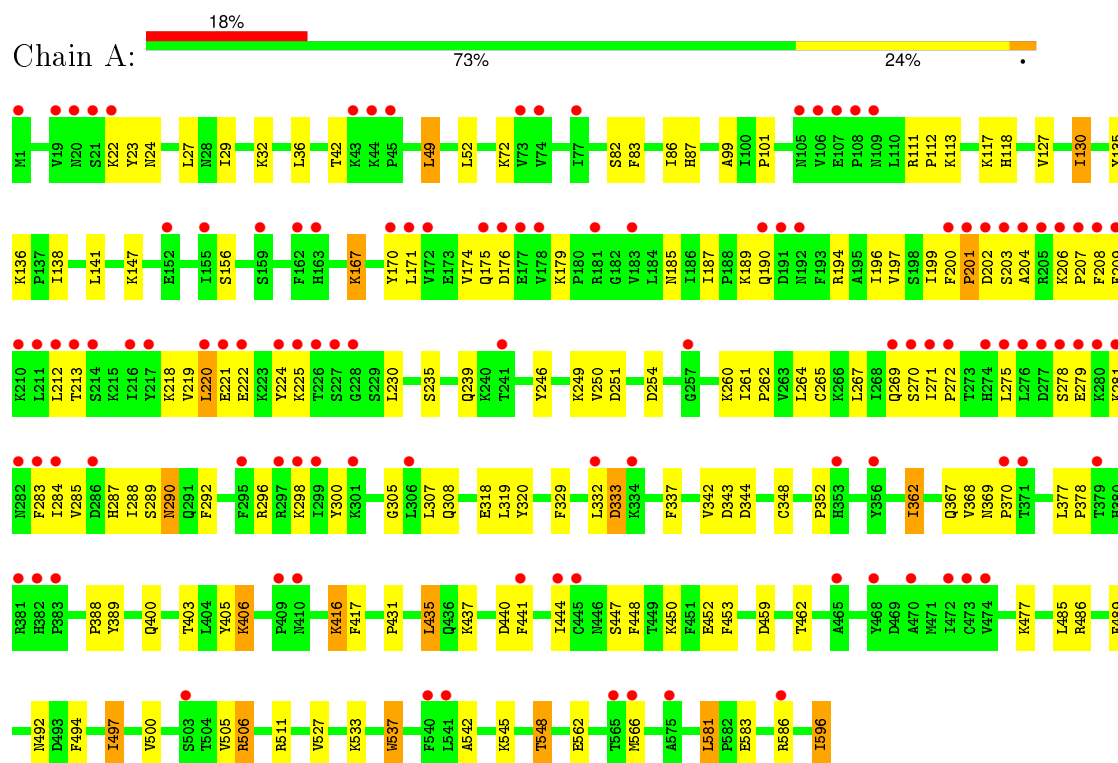
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	210	Total 210	O 210	0	0
3	B	199	Total 199	O 199	0	0

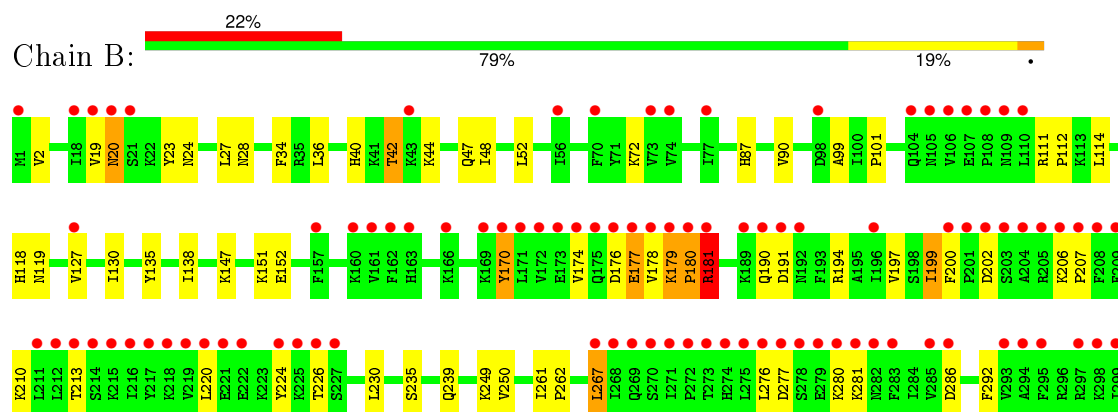
3 Residue-property plots

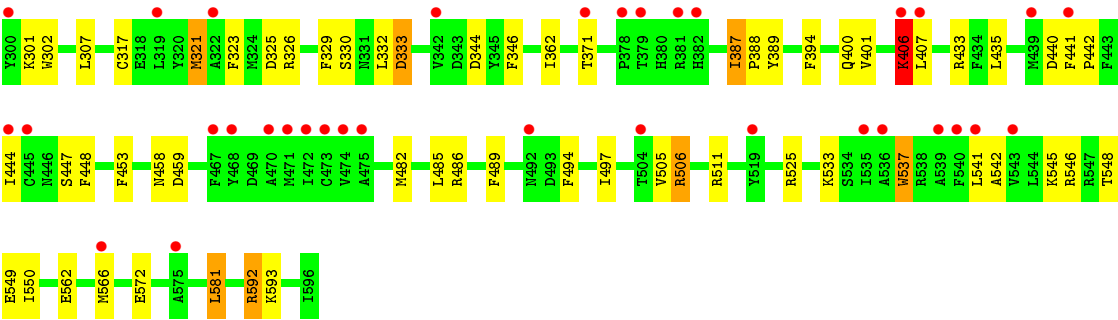
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Telomerase reverse transcriptase



• Molecule 1: Telomerase reverse transcriptase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	117.72Å 84.90Å 123.33Å 90.00° 116.20° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 33.83 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (20.00-2.30) 99.4 (33.83-2.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.235 , 0.273 0.233 , 0.271	Depositor DCC
R_{free} test set	4852 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	42.7	Xtriage
Anisotropy	0.598	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.0	EDS
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 96540 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10423	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.76% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 55C

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	0.53	1/5114 (0.0%)	0.53	0/6893
1	B	0.53	1/5114 (0.0%)	0.53	0/6893
All	All	0.53	2/10228 (0.0%)	0.53	0/13786

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	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	537	TRP	CD2-CE2	6.00	1.48	1.41
1	B	537	TRP	CD2-CE2	5.43	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	406	LYS	Peptide

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	4982	0	5126	99	0
1	B	4982	0	5126	83	0
2	A	25	0	16	2	0
2	B	25	0	16	1	0
3	A	210	0	0	5	0
3	B	199	0	0	5	0
All	All	10423	0	10284	180	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 9.

All (180) 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:405:TYR:HA	1:A:406:LYS:CB	1.78	1.14
1:A:405:TYR:CA	1:A:406:LYS:HB2	1.77	1.14
1:B:406:LYS:HG3	1:B:407:LEU:HG	1.41	1.02
1:A:24:ASN:H	1:A:118:HIS:HE1	1.06	1.01
1:A:400:GLN:HE22	1:A:459:ASP:H	1.12	0.97
1:B:406:LYS:HB2	1:B:407:LEU:HA	1.49	0.94
1:B:406:LYS:CG	1:B:407:LEU:HG	1.98	0.92
1:B:400:GLN:HE22	1:B:459:ASP:H	1.13	0.90
1:B:401:VAL:H	1:B:458:ASN:HD21	1.21	0.89
1:B:24:ASN:H	1:B:118:HIS:HE1	1.19	0.85
1:B:20:ASN:H	1:B:20:ASN:HD22	1.28	0.81
1:A:405:TYR:HA	1:A:406:LYS:HB2	0.88	0.81
1:A:24:ASN:H	1:A:118:HIS:CE1	1.97	0.81
1:B:406:LYS:HB2	1:B:407:LEU:CA	2.14	0.77
1:A:261:ILE:HD12	1:A:288:ILE:HG22	1.68	0.73
1:B:332:LEU:O	1:B:333:ASP:HB2	1.89	0.72
1:A:332:LEU:O	1:A:333:ASP:HB2	1.89	0.71
1:B:24:ASN:H	1:B:118:HIS:CE1	2.05	0.71
1:B:400:GLN:NE2	1:B:459:ASP:H	1.89	0.69
1:B:40:HIS:CE1	1:B:42:THR:HG23	2.28	0.69
1:A:400:GLN:HE22	1:A:459:ASP:N	1.90	0.68
1:B:277:ASP:HB3	1:B:280:LYS:HB2	1.75	0.67
1:B:20:ASN:H	1:B:20:ASN:ND2	1.92	0.67
1:B:176:ASP:HB3	1:B:177:GLU:HB2	1.76	0.66
1:A:206:LYS:N	1:A:207:PRO:HD2	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:ARG:NH2	1:B:440:ASP:OD2	2.26	0.65
1:A:196:ILE:HG22	1:A:308:GLN:HB3	1.78	0.65
1:B:400:GLN:HE22	1:B:459:ASP:N	1.89	0.65
1:A:344:ASP:HB3	1:A:389:TYR:HE1	1.64	0.63
1:B:406:LYS:HG3	1:B:407:LEU:CG	2.25	0.61
1:A:261:ILE:HD12	1:A:288:ILE:CG2	2.31	0.61
1:B:542:ALA:HB1	1:B:581:LEU:HD13	1.83	0.61
1:B:206:LYS:N	1:B:207:PRO:HD2	2.17	0.60
1:A:417:PHE:CD1	1:A:477:LYS:HG3	2.36	0.60
1:B:47:GLN:HG2	3:B:861:HOH:O	2.00	0.59
1:B:448:PHE:HA	1:B:453:PHE:HE2	1.69	0.58
1:B:332:LEU:O	1:B:333:ASP:CB	2.52	0.58
1:A:440:ASP:OD2	1:B:506:ARG:NH2	2.36	0.57
1:B:549:GLU:HG2	1:B:550:ILE:N	2.19	0.56
1:A:368:VAL:O	1:A:370:PRO:HD3	2.05	0.56
1:B:24:ASN:N	1:B:118:HIS:HE1	1.99	0.55
1:A:537:TRP:CE2	1:A:562:GLU:HG3	2.42	0.55
1:A:200:PHE:N	1:A:201:PRO:HA	2.22	0.55
1:B:346:PHE:CZ	1:B:387:ILE:HD11	2.42	0.54
1:B:249:LYS:HD3	1:B:388:PRO:O	2.06	0.54
1:A:332:LEU:O	1:A:333:ASP:CB	2.57	0.53
1:B:48:ILE:CD1	1:B:135:TYR:HE2	2.21	0.53
1:A:444:ILE:O	1:A:444:ILE:HG13	2.08	0.53
1:A:283:PHE:O	1:A:287:HIS:HB2	2.09	0.53
1:A:23:TYR:HB3	1:A:27:LEU:HD12	1.90	0.52
1:A:406:LYS:HE3	1:A:416:LYS:HZ1	1.74	0.52
1:A:174:VAL:HG12	1:A:176:ASP:H	1.75	0.52
1:A:135:TYR:CZ	1:A:596:ILE:HB	2.45	0.52
1:B:170:TYR:HD2	1:B:170:TYR:H	1.56	0.52
1:B:486:ARG:HG2	2:B:601:55C:C20	2.39	0.52
1:A:29:ILE:O	1:A:32:LYS:HB3	2.11	0.51
1:B:549:GLU:HG2	1:B:550:ILE:H	1.76	0.51
1:B:546:ARG:HD2	1:B:581:LEU:HD21	1.93	0.50
1:A:208:PHE:O	1:A:212:LEU:HB2	2.10	0.50
1:A:494:PHE:O	1:A:497:ILE:HB	2.10	0.50
1:A:136:LYS:HD3	3:A:888:HOH:O	2.10	0.50
1:B:505:VAL:HG12	1:B:533:LYS:HG3	1.92	0.50
1:A:218:LYS:O	1:A:222:GLU:HG2	2.12	0.50
1:A:406:LYS:NZ	1:A:416:LYS:HE2	2.27	0.50
1:A:82:SER:O	1:A:83:PHE:HB2	2.12	0.50
1:A:400:GLN:NE2	1:A:459:ASP:H	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:VAL:HG22	1:A:275:LEU:HD13	1.95	0.49
1:B:444:ILE:HG12	1:B:447:SER:HB2	1.94	0.49
1:A:246:TYR:CE2	1:A:352:PRO:HG3	2.48	0.49
1:A:284:ILE:O	1:A:288:ILE:HG12	2.12	0.49
1:B:220:LEU:O	1:B:224:TYR:HB2	2.12	0.49
1:A:344:ASP:HB3	1:A:389:TYR:CE1	2.46	0.49
2:A:601:55C:H5	2:A:601:55C:O21	2.12	0.48
1:B:199:ILE:HG22	1:B:200:PHE:H	1.78	0.48
1:B:170:TYR:N	1:B:170:TYR:CD2	2.81	0.48
1:B:210:LYS:HA	1:B:213:THR:HG22	1.96	0.48
1:B:197:VAL:HG13	1:B:307:LEU:HD22	1.95	0.48
1:A:329:PHE:HB3	1:A:332:LEU:HD11	1.96	0.48
1:A:261:ILE:HD11	1:A:305:GLY:HA2	1.97	0.47
1:B:206:LYS:H	1:B:207:PRO:HD2	1.79	0.47
1:A:448:PHE:HA	1:A:453:PHE:HE2	1.79	0.47
1:A:329:PHE:HZ	1:A:362:ILE:HG12	1.79	0.47
1:A:264:LEU:HD13	1:A:320:TYR:HB2	1.95	0.47
1:A:406:LYS:HE3	1:A:416:LYS:HE2	1.95	0.47
1:A:581:LEU:HB2	3:A:850:HOH:O	2.15	0.47
1:A:281:LYS:O	1:A:285:VAL:HG23	2.14	0.47
1:A:406:LYS:HE3	1:A:416:LYS:NZ	2.30	0.47
1:A:527:VAL:HA	3:A:786:HOH:O	2.14	0.47
1:B:387:ILE:O	1:B:387:ILE:HG12	2.15	0.47
1:B:127:VAL:O	1:B:130:ILE:HG22	2.15	0.47
1:A:400:GLN:NE2	1:A:462:THR:OG1	2.36	0.46
1:B:23:TYR:HB3	1:B:27:LEU:HD12	1.98	0.46
1:A:506:ARG:HH22	1:B:440:ASP:CG	2.16	0.46
1:B:151:LYS:HE3	3:B:888:HOH:O	2.16	0.46
1:B:2:VAL:HG22	3:B:817:HOH:O	2.15	0.46
1:A:171:LEU:HG	1:A:300:TYR:CD2	2.51	0.46
1:B:267:LEU:HD11	1:B:323:PHE:CB	2.46	0.46
1:A:111:ARG:HB2	1:A:112:PRO:HD3	1.97	0.46
1:B:448:PHE:HA	1:B:453:PHE:CE2	2.49	0.46
1:A:269:GLN:HA	1:A:281:LYS:HD3	1.96	0.46
1:A:197:VAL:HG13	1:A:307:LEU:HD22	1.98	0.46
1:A:206:LYS:N	1:A:207:PRO:CD	2.78	0.46
1:A:249:LYS:HE2	1:A:388:PRO:O	2.15	0.46
1:B:545:LYS:O	1:B:548:THR:HG23	2.16	0.46
1:A:265:CYS:O	1:A:269:GLN:HG2	2.15	0.46
1:A:583:GLU:OE1	1:A:586:ARG:NE	2.49	0.45
1:A:416:LYS:HA	1:A:416:LYS:HD2	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:593:LYS:HG3	3:B:896:HOH:O	2.16	0.45
1:A:220:LEU:HD11	1:A:318:GLU:HB3	1.98	0.45
1:A:417:PHE:CG	1:A:477:LYS:HG3	2.52	0.45
1:A:405:TYR:CA	1:A:406:LYS:CB	2.57	0.45
1:A:194:ARG:HE	1:A:308:GLN:NE2	2.14	0.45
1:A:437:LYS:HE2	3:A:742:HOH:O	2.17	0.45
1:B:152:GLU:CD	1:B:152:GLU:H	2.20	0.45
1:B:206:LYS:N	1:B:207:PRO:CD	2.80	0.44
1:B:537:TRP:CE2	1:B:562:GLU:HG3	2.52	0.44
1:A:261:ILE:HB	1:A:262:PRO:HD3	1.97	0.44
1:A:441:PHE:HB2	1:A:511:ARG:CZ	2.48	0.44
1:B:114:LEU:HA	1:B:114:LEU:HD23	1.86	0.44
1:A:377:LEU:HA	1:A:378:PRO:HD3	1.86	0.44
1:A:127:VAL:O	1:A:130:ILE:HG22	2.17	0.44
1:A:261:ILE:HD11	1:A:305:GLY:C	2.38	0.44
1:A:220:LEU:O	1:A:224:TYR:HB2	2.18	0.43
1:A:542:ALA:HB1	1:A:581:LEU:HD13	1.99	0.43
1:A:289:SER:HA	1:A:290:ASN:HA	1.76	0.43
1:A:167:LYS:HD3	1:A:167:LYS:HA	1.76	0.43
1:B:179:LYS:HD2	1:B:179:LYS:O	2.18	0.43
1:B:494:PHE:O	1:B:497:ILE:HB	2.18	0.43
1:A:270:SER:HA	1:A:271:ILE:HA	1.64	0.43
1:B:42:THR:HB	1:B:44:LYS:H	1.83	0.43
1:B:387:ILE:HD13	1:B:394:PHE:O	2.18	0.43
1:A:435:LEU:HD13	1:A:500:VAL:HG11	2.00	0.43
1:B:435:LEU:HD13	1:B:482:MET:CE	2.49	0.43
1:A:406:LYS:HE3	1:A:416:LYS:CE	2.49	0.43
1:B:344:ASP:HB2	1:B:389:TYR:HE1	1.84	0.43
1:A:296:ARG:C	1:A:298:LYS:H	2.22	0.42
1:A:278:SER:HA	1:A:281:LYS:HE3	2.02	0.42
1:B:99:ALA:O	1:B:101:PRO:HD3	2.19	0.42
1:A:99:ALA:O	1:A:101:PRO:HD3	2.19	0.42
1:A:406:LYS:CE	1:A:416:LYS:HE2	2.50	0.42
1:B:235:SER:O	1:B:239:GLN:HG2	2.19	0.42
1:A:185:ASN:HD22	1:A:187:ILE:HD11	1.84	0.42
1:B:346:PHE:HZ	1:B:387:ILE:HD11	1.85	0.42
1:B:48:ILE:HD11	1:B:135:TYR:HE2	1.84	0.42
1:A:290:ASN:N	1:A:290:ASN:OD1	2.51	0.42
1:B:111:ARG:HB2	1:B:112:PRO:HD3	2.01	0.42
1:A:174:VAL:CG1	1:A:175:GLN:N	2.82	0.42
1:A:545:LYS:O	1:A:548:THR:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:LYS:HE2	1:A:117:LYS:HE2	2.02	0.42
1:B:387:ILE:HD11	1:B:394:PHE:HB2	2.02	0.42
1:B:317:CYS:O	1:B:321:MET:HB2	2.20	0.42
1:B:261:ILE:HB	1:B:262:PRO:HD3	2.02	0.42
1:B:592:ARG:HD2	3:B:835:HOH:O	2.20	0.42
1:A:235:SER:O	1:A:239:GLN:HG2	2.20	0.42
1:B:441:PHE:HB2	1:B:511:ARG:CZ	2.49	0.42
1:A:49:LEU:HB2	3:A:814:HOH:O	2.20	0.42
1:B:326:ARG:HA	1:B:330:SER:HB2	2.02	0.41
1:A:403:THR:OG1	1:A:452:GLU:OE1	2.33	0.41
1:B:302:TRP:CD1	1:B:307:LEU:HG	2.55	0.41
1:A:505:VAL:HG12	1:A:533:LYS:HG3	2.01	0.41
1:B:119:ASN:HA	1:B:119:ASN:HD22	1.61	0.41
1:A:486:ARG:HG2	2:A:601:55C:C20	2.50	0.41
1:B:87:HIS:HE1	1:B:489:PHE:CZ	2.38	0.41
1:A:337:PHE:HB3	1:A:348:CYS:HB2	2.02	0.41
1:B:387:ILE:CD1	1:B:394:PHE:HB2	2.51	0.41
1:A:250:VAL:HG21	1:A:362:ILE:HG21	2.03	0.41
1:A:431:PRO:CB	1:A:485:LEU:HD22	2.51	0.41
1:B:34:PHE:CE1	1:B:130:ILE:HD13	2.56	0.41
1:A:170:TYR:N	1:A:170:TYR:CD1	2.89	0.41
1:B:325:ASP:HA	1:B:329:PHE:HD2	1.86	0.41
1:B:34:PHE:HE1	1:B:130:ILE:CD1	2.34	0.41
1:B:72:LYS:HE2	1:B:72:LYS:HA	2.03	0.41
1:A:209:PHE:O	1:A:213:THR:HG22	2.20	0.41
1:B:441:PHE:N	1:B:442:PRO:HD2	2.36	0.40
1:A:270:SER:HB3	1:A:271:ILE:HG13	2.03	0.40
1:A:141:LEU:HD12	1:A:189:LYS:NZ	2.36	0.40
1:B:19:VAL:HG22	1:B:28:ASN:OD1	2.21	0.40
1:B:180:PRO:O	1:B:181:ARG:CB	2.69	0.40
1:A:87:HIS:HE1	1:A:489:PHE:CE1	2.39	0.40
1:A:197:VAL:HG11	1:A:307:LEU:HD13	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	594/596 (100%)	542 (91%)	40 (7%)	12 (2%)	9	7
1	B	594/596 (100%)	547 (92%)	40 (7%)	7 (1%)	16	16
All	All	1188/1192 (100%)	1089 (92%)	80 (7%)	19 (2%)	12	11

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	201	PRO
1	A	272	PRO
1	A	333	ASP
1	A	406	LYS
1	B	333	ASP
1	A	190	GLN
1	A	203	SER
1	B	181	ARG
1	B	190	GLN
1	A	204	ALA
1	B	180	PRO
1	B	406	LYS
1	A	179	LYS
1	A	254	ASP
1	B	276	LEU
1	A	202	ASP
1	A	225	LYS
1	B	174	VAL
1	A	369	ASN

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	552/552 (100%)	514 (93%)	38 (7%)	19	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	552/552 (100%)	514 (93%)	38 (7%)	19	24
All	All	1104/1104 (100%)	1028 (93%)	76 (7%)	19	24

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

Mol	Chain	Res	Type
1	A	36	LEU
1	A	42	THR
1	A	49	LEU
1	A	52	LEU
1	A	72	LYS
1	A	86	ILE
1	A	113	LYS
1	A	130	ILE
1	A	138	ILE
1	A	147	LYS
1	A	156	SER
1	A	167	LYS
1	A	199	ILE
1	A	220	LEU
1	A	221	GLU
1	A	230	LEU
1	A	251	ASP
1	A	260	LYS
1	A	267	LEU
1	A	279	GLU
1	A	290	ASN
1	A	292	PHE
1	A	319	LEU
1	A	342	VAL
1	A	343	ASP
1	A	362	ILE
1	A	367	GLN
1	A	416	LYS
1	A	435	LEU
1	A	447	SER
1	A	450	LYS
1	A	492	ASN
1	A	497	ILE
1	A	506	ARG
1	A	548	THR
1	A	566	MET

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Mol	Chain	Res	Type
1	A	581	LEU
1	A	596	ILE
1	B	20	ASN
1	B	36	LEU
1	B	42	THR
1	B	52	LEU
1	B	90	VAL
1	B	138	ILE
1	B	147	LYS
1	B	170	TYR
1	B	177	GLU
1	B	178	VAL
1	B	179	LYS
1	B	181	ARG
1	B	191	ASP
1	B	194	ARG
1	B	199	ILE
1	B	202	ASP
1	B	226	THR
1	B	230	LEU
1	B	250	VAL
1	B	267	LEU
1	B	281	LYS
1	B	286	ASP
1	B	292	PHE
1	B	301	LYS
1	B	321	MET
1	B	362	ILE
1	B	371	THR
1	B	387	ILE
1	B	406	LYS
1	B	433	ARG
1	B	485	LEU
1	B	506	ARG
1	B	525	ARG
1	B	541	LEU
1	B	566	MET
1	B	572	GLU
1	B	581	LEU
1	B	592	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	118	HIS
1	A	119	ASN
1	A	185	ASN
1	A	258	ASN
1	A	308	GLN
1	A	351	HIS
1	A	400	GLN
1	B	20	ASN
1	B	40	HIS
1	B	118	HIS
1	B	119	ASN
1	B	258	ASN
1	B	291	GLN
1	B	400	GLN
1	B	436	GLN
1	B	458	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands are 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
2	55C	A	601	-	24,27,27	0.87	0	31,37,37	0.75	0
2	55C	B	601	-	24,27,27	0.88	0	31,37,37	0.86	1 (3%)

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
2	55C	A	601	-	-	0/12/16/16	0/3/3/3
2	55C	B	601	-	-	0/12/16/16	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	55C	O21-C13-N1	2.54	126.23	122.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	55C	2	0
2	B	601	55C	1	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

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	596/596 (100%)	1.08	110 (18%) 2 2	24, 50, 126, 192	0
1	B	596/596 (100%)	1.30	129 (21%) 1 2	25, 51, 144, 187	0
All	All	1192/1192 (100%)	1.19	239 (20%) 1 2	24, 51, 138, 192	0

All (239) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	178	VAL	19.8
1	A	178	VAL	16.3
1	A	204	ALA	12.4
1	B	211	LEU	11.5
1	B	220	LEU	11.2
1	B	205	ARG	9.8
1	A	205	ARG	9.0
1	A	201	PRO	8.6
1	B	174	VAL	8.3
1	B	200	PHE	8.2
1	A	177	GLU	7.8
1	B	175	GLN	7.8
1	B	204	ALA	7.8
1	B	177	GLU	7.1
1	A	211	LEU	6.8
1	B	225	LYS	6.8
1	A	200	PHE	6.6
1	B	190	GLN	6.6
1	B	279	GLU	6.6
1	B	221	GLU	6.5
1	B	226	THR	6.4
1	B	219	VAL	6.4
1	A	190	GLN	6.3
1	B	218	LYS	6.3

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Mol	Chain	Res	Type	RSRZ
1	A	277	ASP	6.3
1	B	275	LEU	6.2
1	B	286	ASP	6.2
1	B	209	PHE	6.1
1	B	271	ILE	6.0
1	B	272	PRO	5.9
1	B	203	SER	5.8
1	A	163	HIS	5.8
1	A	203	SER	5.8
1	A	271	ILE	5.8
1	B	172	VAL	5.7
1	B	176	ASP	5.7
1	A	207	PRO	5.6
1	A	382	HIS	5.5
1	A	175	GLN	5.5
1	A	227	SER	5.5
1	B	43	LYS	5.4
1	B	299	ILE	5.2
1	B	109	ASN	5.2
1	A	208	PHE	5.2
1	A	21	SER	5.2
1	B	278	SER	5.1
1	B	274	HIS	5.1
1	A	191	ASP	5.1
1	B	201	PRO	5.0
1	A	170	TYR	5.0
1	B	281	LYS	5.0
1	B	282	ASN	4.9
1	B	189	LYS	4.8
1	B	382	HIS	4.8
1	B	212	LEU	4.8
1	B	277	ASP	4.7
1	A	279	GLU	4.7
1	A	225	LYS	4.7
1	B	270	SER	4.7
1	B	191	ASP	4.7
1	B	269	GLN	4.7
1	A	222	GLU	4.7
1	B	192	ASN	4.6
1	B	276	LEU	4.6
1	B	107	GLU	4.6
1	A	176	ASP	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	267	LEU	4.5
1	B	207	PRO	4.5
1	B	21	SER	4.4
1	A	445	CYS	4.4
1	A	275	LEU	4.4
1	A	444	ILE	4.4
1	B	163	HIS	4.4
1	A	73	VAL	4.4
1	B	217	TYR	4.4
1	B	283	PHE	4.4
1	A	171	LEU	4.3
1	B	171	LEU	4.3
1	B	181	ARG	4.3
1	A	106	VAL	4.3
1	A	206	LYS	4.2
1	B	273	THR	4.2
1	B	342	VAL	4.2
1	B	180	PRO	4.1
1	B	300	TYR	4.1
1	A	43	LYS	4.1
1	B	222	GLU	4.0
1	B	474	VAL	4.0
1	A	283	PHE	4.0
1	A	105	ASN	4.0
1	A	370	PRO	3.9
1	B	297	ARG	3.9
1	A	298	LYS	3.9
1	B	285	VAL	3.9
1	A	281	LYS	3.9
1	B	73	VAL	3.9
1	B	213	THR	3.8
1	B	444	ILE	3.8
1	B	379	THR	3.8
1	B	208	PHE	3.8
1	B	20	ASN	3.8
1	A	276	LEU	3.7
1	A	202	ASP	3.7
1	A	214	SER	3.7
1	B	74	VAL	3.7
1	A	332	LEU	3.6
1	A	192	ASN	3.6
1	A	356	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	299	ILE	3.5
1	B	470	ALA	3.5
1	A	381	ARG	3.5
1	A	213	THR	3.5
1	A	278	SER	3.5
1	B	105	ASN	3.5
1	B	173	GLU	3.5
1	B	468	TYR	3.5
1	B	1	MET	3.5
1	B	169	LYS	3.5
1	B	206	LYS	3.5
1	A	74	VAL	3.4
1	B	202	ASP	3.4
1	B	445	CYS	3.4
1	B	298	LYS	3.3
1	B	294	ALA	3.3
1	A	172	VAL	3.3
1	B	540	PHE	3.3
1	A	107	GLU	3.2
1	A	282	ASN	3.2
1	A	306	LEU	3.2
1	A	474	VAL	3.2
1	A	280	LYS	3.2
1	A	410	ASN	3.2
1	A	220	LEU	3.2
1	B	539	ALA	3.2
1	A	1	MET	3.2
1	B	214	SER	3.2
1	B	179	LYS	3.1
1	A	109	ASN	3.1
1	B	519	TYR	3.1
1	B	319	LEU	3.1
1	B	473	CYS	3.1
1	B	322	ALA	3.1
1	A	221	GLU	3.1
1	A	371	THR	3.1
1	B	293	VAL	3.0
1	B	19	VAL	3.0
1	B	216	ILE	3.0
1	B	106	VAL	3.0
1	A	272	PRO	2.9
1	A	212	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	20	ASN	2.9
1	B	227	SER	2.9
1	B	170	TYR	2.9
1	B	472	ILE	2.9
1	A	257	GLY	2.8
1	A	270	SER	2.8
1	B	166	LYS	2.8
1	A	224	TYR	2.8
1	B	108	PRO	2.8
1	B	110	LEU	2.7
1	B	104	GLN	2.7
1	A	209	PHE	2.7
1	B	160	LYS	2.7
1	B	541	LEU	2.7
1	A	301	LYS	2.7
1	A	217	TYR	2.7
1	A	44	LYS	2.6
1	A	269	GLN	2.6
1	B	475	ALA	2.6
1	B	575	ALA	2.6
1	B	162	PHE	2.6
1	B	268	ILE	2.6
1	B	406	LYS	2.6
1	A	470	ALA	2.6
1	B	543	VAL	2.6
1	A	473	CYS	2.5
1	B	371	THR	2.5
1	B	157	PHE	2.5
1	B	492	ASN	2.5
1	A	541	LEU	2.5
1	A	565	THR	2.4
1	A	241	THR	2.4
1	B	535	ILE	2.4
1	A	566	MET	2.4
1	A	228	GLY	2.4
1	A	108	PRO	2.4
1	B	98	ASP	2.4
1	A	441	PHE	2.4
1	A	274	HIS	2.3
1	A	575	ALA	2.3
1	B	215	LYS	2.3
1	A	162	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	183	VAL	2.3
1	B	56	ILE	2.3
1	A	45	PRO	2.3
1	B	70	PHE	2.3
1	B	467	PHE	2.3
1	A	155	ILE	2.3
1	A	379	THR	2.3
1	B	536	ALA	2.3
1	A	19	VAL	2.3
1	A	295	PHE	2.3
1	A	540	PHE	2.3
1	B	378	PRO	2.2
1	B	224	TYR	2.2
1	A	226	THR	2.2
1	A	152	GLU	2.2
1	B	161	VAL	2.2
1	B	77	ILE	2.2
1	A	210	LYS	2.2
1	A	353	HIS	2.2
1	B	504	THR	2.2
1	B	18	ILE	2.2
1	B	471	MET	2.2
1	A	465	ALA	2.1
1	A	586	ARG	2.1
1	B	441	PHE	2.1
1	A	472	ILE	2.1
1	B	407	LEU	2.1
1	A	286	ASP	2.1
1	A	503	SER	2.1
1	B	439	MET	2.1
1	A	468	TYR	2.1
1	A	216	ILE	2.1
1	B	280	LYS	2.1
1	B	381	ARG	2.1
1	A	159	SER	2.1
1	A	334	LYS	2.1
1	A	284	ILE	2.1
1	B	196	ILE	2.1
1	A	297	ARG	2.0
1	A	22	LYS	2.0
1	A	409	PRO	2.0
1	B	127	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	295	PHE	2.0
1	A	77	ILE	2.0
1	B	566	MET	2.0
1	A	181	ARG	2.0
1	A	383	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	55C	A	601	25/25	0.88	0.13	-0.69	42,48,60,67	0
2	55C	B	601	25/25	0.86	0.14	-0.84	44,49,58,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.