



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:16 AM UTC

PDB ID : 5CQG / pdb_00005cqh
Title : Structure of Tribolium telomerase in complex with the highly specific inhibitor BIBR1532
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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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

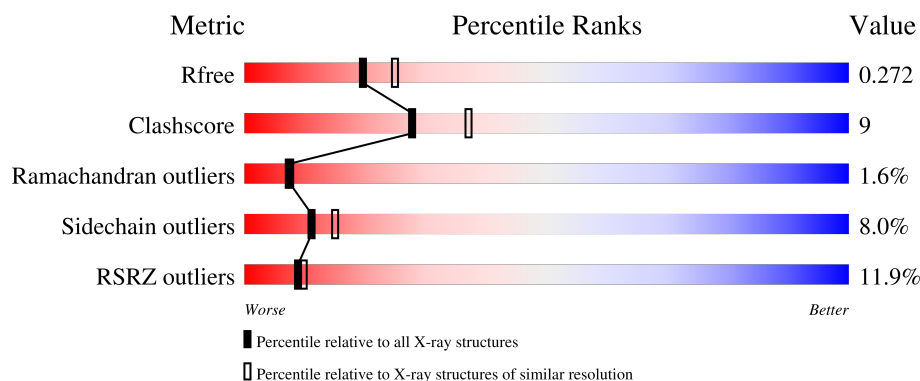
1 Overall quality at a glance

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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 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 $\leq 5\%$. 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	
1	B	596	

2 Entry composition [i](#)

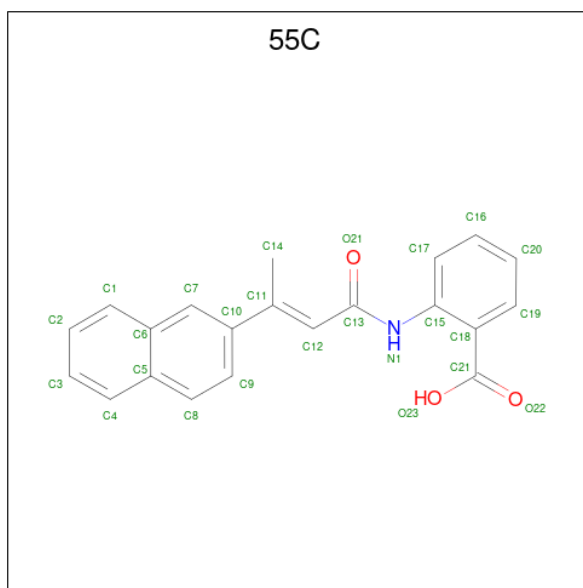
There are 3 unique types of molecules in this entry. The entry contains 10423 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: 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		

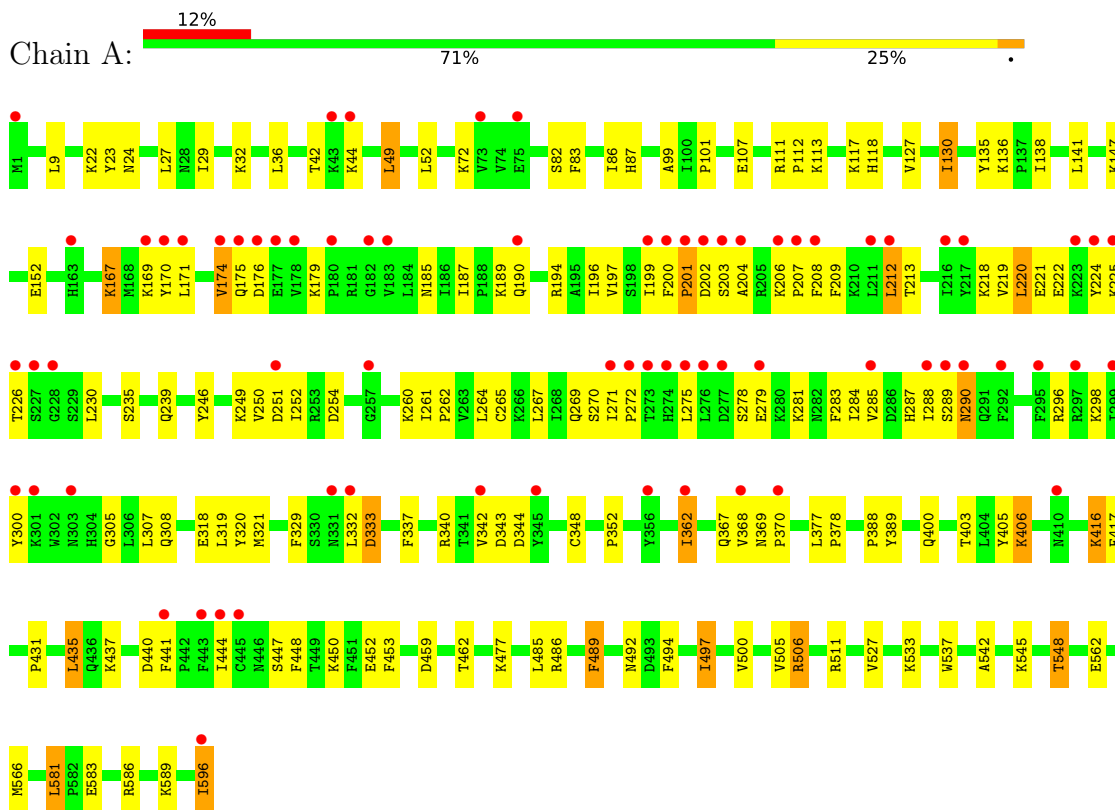
- Molecule 3 is water.

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

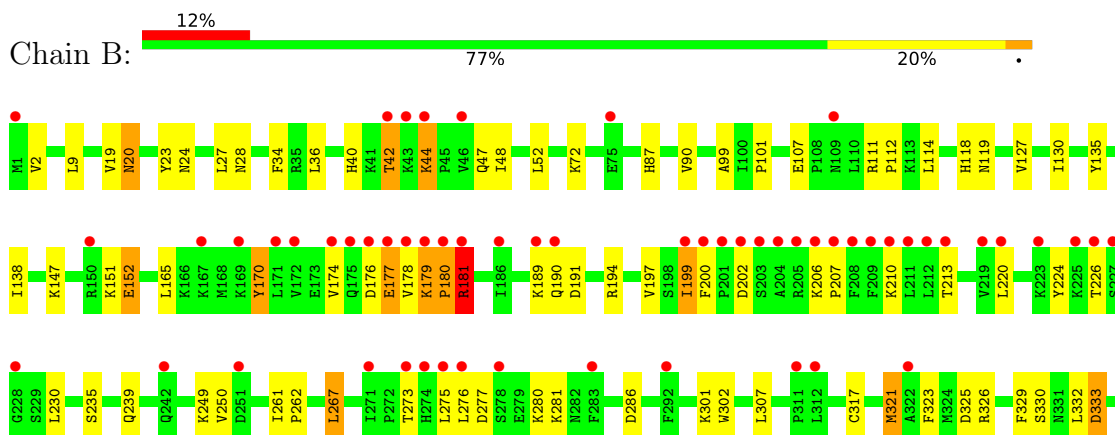
3 Residue-property plots [i](#)

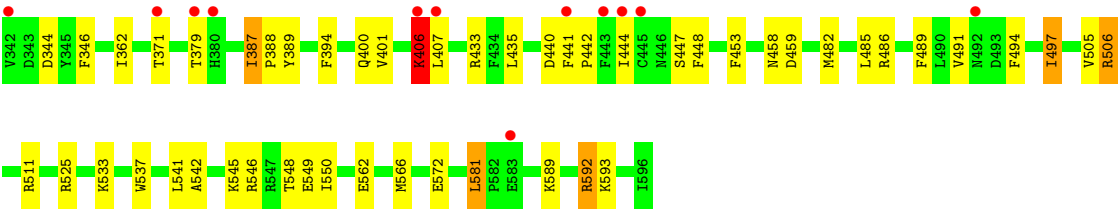
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 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 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (20.00-2.30) 99.3 (20.00-2.30)	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 , 0.272	Depositor DCC
R_{free} test set	4857 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	42.7	Xtriage
Anisotropy	0.598	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-h-l	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, 0.333 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: 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	0.72	0/5114	0.79	5/6893 (0.1%)
1	B	0.72	0/5114	0.78	3/6893 (0.0%)
All	All	0.72	0/10228	0.78	8/13786 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	491	VAL	N-CA-C	8.97	118.85	110.42
1	A	44	LYS	CA-C-N	6.27	127.68	119.84
1	A	44	LYS	C-N-CA	6.27	127.68	119.84
1	A	107	GLU	CA-C-N	5.37	126.56	119.84
1	A	107	GLU	C-N-CA	5.37	126.56	119.84
1	B	107	GLU	CA-C-N	5.25	126.40	119.84
1	B	107	GLU	C-N-CA	5.25	126.40	119.84
1	A	489	PHE	N-CA-C	-5.12	106.98	113.18

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	100	0
1	B	4982	0	5126	84	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	182	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 (182) 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:24:ASN:H	1:A:118:HIS:CE1	1.97	0.81
1:A:405:TYR:HA	1:A:406:LYS:HB2	0.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:261:ILE:HD12	1:A:288:ILE:CG2	2.31	0.61
1:B:406:LYS:HG3	1:B:407:LEU:CG	2.25	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:283:PHE:O	1:A:287:HIS:HB2	2.09	0.53
1:A:444:ILE:HG13	1:A:444:ILE:O	2.08	0.53
1:A:23:TYR:HB3	1:A:27:LEU:HD12	1.90	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:H	1:B:170:TYR:HD2	1.56	0.52
1:B:486:ARG:HG2	2:B:601:55C:C20	2.39	0.52
1:A:506:ARG:HH22	1:B:440:ASP:CG	2.16	0.51
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:PHE:O	1:A:212:LEU:HB2	2.10	0.50
1:A:136:LYS:HD3	3:A:888:HOH:O	2.10	0.50
1:A:494:PHE:O	1:A:497:ILE:HB	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:400:GLN:NE2	1:A:459:ASP:H	1.95	0.49
1:A:82:SER:O	1:A:83:PHE:HB2	2.12	0.49
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:B:152:GLU:H	1:B:152:GLU:CD	2.20	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:261:ILE:HD11	1:A:305:GLY:C	2.38	0.49
1:A:344:ASP:HB3	1:A:389:TYR:CE1	2.46	0.49
2:A:601:55C:O21	2:A:601:55C:H5	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:A:448:PHE:HA	1:A:453:PHE:HE2	1.79	0.47
1:B:206:LYS:H	1:B:207:PRO:HD2	1.79	0.47
1:A:264:LEU:HD13	1:A:320:TYR:HB2	1.95	0.47
1:A:329:PHE:HZ	1:A:362:ILE:HG12	1.79	0.47
1:A:296:ARG:C	1:A:298:LYS:H	2.22	0.47
1:A:406:LYS:HE3	1:A:416:LYS:HE2	1.95	0.47
1:A:281:LYS:O	1:A:285:VAL:HG23	2.14	0.47
1:A:581:LEU:HB2	3:A:850:HOH:O	2.15	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:127:VAL:O	1:B:130:ILE:HG22	2.15	0.47
1:B:387:ILE:O	1:B:387:ILE:HG12	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:B:151:LYS:HE3	3:B:888:HOH:O	2.16	0.46
1:A:171:LEU:HG	1:A:300:TYR:CD2	2.51	0.46
1:B:2:VAL:HG22	3:B:817:HOH:O	2.15	0.46
1:A:111:ARG:HB2	1:A:112:PRO:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:LEU:HD11	1:B:323:PHE:CB	2.46	0.46
1:A:197:VAL:HG13	1:A:307:LEU:HD22	1.98	0.46
1:A:269:GLN:HA	1:A:281:LYS:HD3	1.96	0.46
1:B:448:PHE:HA	1:B:453:PHE:CE2	2.49	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:HD2	1:A:416:LYS:HA	1.79	0.45
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:194:ARG:HE	1:A:308:GLN:NE2	2.14	0.45
1:A:405:TYR:CA	1:A:406:LYS:CB	2.57	0.45
1:A:437:LYS:HE2	3:A:742:HOH:O	2.17	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:A:377:LEU:HA	1:A:378:PRO:HD3	1.86	0.44
1:B:114:LEU:HD23	1:B:114:LEU:HA	1.86	0.44
1:A:127:VAL:O	1:A:130:ILE:HG22	2.17	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:252:ILE:HD13	1:A:321:MET:HE1	2.01	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:A:270:SER:HA	1:A:271:ILE:HA	1.64	0.43
1:B:179:LYS:O	1:B:179:LYS:HD2	2.18	0.43
1:B:494:PHE:O	1:B:497:ILE:HB	2.18	0.43
1:B:42:THR:HB	1:B:44:LYS:H	1.83	0.43
1:A:435:LEU:HD13	1:A:500:VAL:HG11	2.00	0.43
1:B:387:ILE:HD13	1:B:394:PHE:O	2.18	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:99:ALA:O	1:A:101:PRO:HD3	2.19	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:185:ASN:HD22	1:A:187:ILE:HD11	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:48:ILE:HD11	1:B:135:TYR:HE2	1.84	0.42
1:B:346:PHE:HZ	1:B:387:ILE:HD11	1.85	0.42
1:B:111:ARG:HB2	1:B:112:PRO:HD3	2.01	0.42
1:A:22:LYS:HE2	1:A:117:LYS:HE2	2.02	0.42
1:A:174:VAL:CG1	1:A:175:GLN:N	2.82	0.42
1:A:290:ASN:OD1	1:A:290:ASN:N	2.51	0.42
1:A:545:LYS:O	1:A:548:THR:HG23	2.19	0.42
1:B:317:CYS:O	1:B:321:MET:HB2	2.20	0.42
1:B:387:ILE:HD11	1:B:394:PHE:HB2	2.02	0.42
1:B:261:ILE:HB	1:B:262:PRO:HD3	2.02	0.42
1:A:49:LEU:HB2	3:A:814: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:B:592:ARG:HD2	3:B:835: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:A:505:VAL:HG12	1:A:533:LYS:HG3	2.01	0.41
1:B:302:TRP:CD1	1:B:307:LEU:HG	2.55	0.41
1:B:119:ASN:HD22	1:B:119:ASN:HA	1.61	0.41
1:A:337:PHE:HB3	1:A:348:CYS:HB2	2.02	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:224:TYR:C	1:A:226:THR:H	2.28	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:A:170:TYR:N	1:A:170:TYR:CD1	2.89	0.41
1:B:34:PHE:CE1	1:B:130:ILE:HD13	2.56	0.41
1:B:273:THR:C	1:B:275:LEU:H	2.29	0.41
1:B:325:ASP:HA	1:B:329:PHE:HD2	1.86	0.41
1:A:209:PHE:O	1:A:213:THR:HG22	2.20	0.41
1:B:34:PHE:HE1	1:B:130:ILE:CD1	2.34	0.41
1:B:72:LYS:HA	1:B:72:LYS:HE2	2.03	0.41
1:B:441:PHE:N	1:B:442:PRO:HD2	2.36	0.40
1:A:141:LEU:HD12	1:A:189:LYS:NZ	2.36	0.40
1:A:270:SER:HB3	1:A:271:ILE:HG13	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:VAL:HG11	1:A:307:LEU:HD13	2.02	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	594/596 (100%)	542 (91%)	40 (7%)	12 (2%)	6	5
1	B	594/596 (100%)	547 (92%)	40 (7%)	7 (1%)	10	12
All	All	1188/1192 (100%)	1089 (92%)	80 (7%)	19 (2%)	7	7

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

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Mol	Chain	Res	Type
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%)	509 (92%)	43 (8%)	11	16
1	B	552/552 (100%)	507 (92%)	45 (8%)	10	14
All	All	1104/1104 (100%)	1016 (92%)	88 (8%)	11	15

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
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	152	GLU
1	A	167	LYS
1	A	169	LYS
1	A	174	VAL
1	A	199	ILE
1	A	212	LEU
1	A	220	LEU
1	A	221	GLU
1	A	230	LEU
1	A	251	ASP

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Mol	Chain	Res	Type
1	A	260	LYS
1	A	267	LEU
1	A	279	GLU
1	A	290	ASN
1	A	319	LEU
1	A	340	ARG
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
1	A	581	LEU
1	A	589	LYS
1	A	596	ILE
1	B	9	LEU
1	B	20	ASN
1	B	36	LEU
1	B	42	THR
1	B	44	LYS
1	B	52	LEU
1	B	90	VAL
1	B	138	ILE
1	B	147	LYS
1	B	152	GLU
1	B	165	LEU
1	B	170	TYR
1	B	177	GLU
1	B	178	VAL
1	B	179	LYS
1	B	181	ARG
1	B	189	LYS
1	B	191	ASP
1	B	194	ARG
1	B	199	ILE

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Mol	Chain	Res	Type
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	301	LYS
1	B	321	MET
1	B	362	ILE
1	B	371	THR
1	B	379	THR
1	B	387	ILE
1	B	406	LYS
1	B	433	ARG
1	B	485	LEU
1	B	497	ILE
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	589	LYS
1	B	592	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	118	HIS
1	A	119	ASN
1	A	125	ASN
1	A	185	ASN
1	A	258	ASN
1	A	282	ASN
1	A	304	HIS
1	A	308	GLN
1	A	351	HIS
1	A	382	HIS
1	A	400	GLN
1	B	20	ASN

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Mol	Chain	Res	Type
1	B	47	GLN
1	B	118	HIS
1	B	119	ASN
1	B	258	ASN
1	B	291	GLN
1	B	331	ASN
1	B	351	HIS
1	B	400	GLN
1	B	436	GLN
1	B	458	ASN
1	B	492	ASN
1	B	569	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](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	B	601	-	27,27,27	0.94	0	36,37,37	0.99	2 (5%)
2	55C	A	601	-	27,27,27	0.94	0	36,37,37	0.81	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
2	55C	B	601	-	-	0/16/16/16	0/3/3/3
2	55C	A	601	-	-	0/16/16/16	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	55C	O21-C13-N1	2.37	126.23	123.11
2	B	601	55C	C7-C10-C11	-2.24	119.64	121.12

There are no chirality outliers.

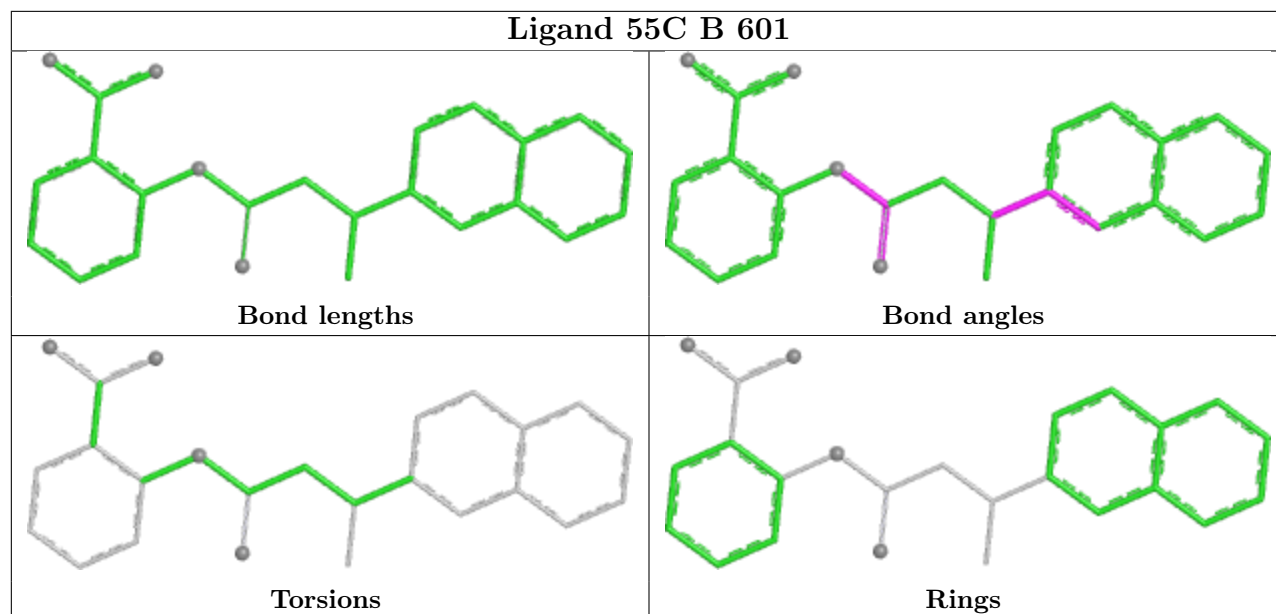
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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%)	0.71	72 (12%)  	24, 50, 126, 192	0
1	B	596/596 (100%)	0.68	70 (11%)  	25, 51, 144, 187	0
All	All	1192/1192 (100%)	0.69	142 (11%)  	24, 51, 138, 192	0

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	178	VAL	8.9
1	B	178	VAL	8.0
1	A	200	PHE	5.8
1	A	201	PRO	5.7
1	B	174	VAL	5.7
1	B	204	ALA	5.4
1	A	211	LEU	5.3
1	A	271	ILE	5.2
1	B	342	VAL	5.2
1	A	204	ALA	4.8
1	B	211	LEU	4.7
1	B	169	LYS	4.4
1	A	444	ILE	4.3
1	B	379	THR	4.3
1	B	276	LEU	4.0
1	A	170	TYR	4.0
1	B	406	LYS	3.9
1	B	226	THR	3.9
1	A	272	PRO	3.9
1	A	169	LYS	3.9
1	A	225	LYS	3.9
1	B	206	LYS	3.9
1	B	172	VAL	3.8
1	B	180	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	278	SER	3.8
1	B	223	LYS	3.8
1	B	273	THR	3.8
1	A	228	GLY	3.8
1	A	276	LEU	3.7
1	B	209	PHE	3.7
1	A	182	GLY	3.7
1	B	1	MET	3.7
1	B	199	ILE	3.6
1	B	201	PRO	3.6
1	A	290	ASN	3.5
1	A	177	GLU	3.5
1	B	43	LYS	3.5
1	A	445	CYS	3.5
1	B	200	PHE	3.5
1	B	189	LYS	3.4
1	A	171	LEU	3.4
1	B	179	LYS	3.4
1	B	225	LYS	3.3
1	B	219	VAL	3.3
1	B	275	LEU	3.2
1	A	206	LYS	3.2
1	B	207	PRO	3.2
1	B	227	SER	3.2
1	A	176	ASP	3.2
1	A	288	ILE	3.2
1	B	444	ILE	3.1
1	A	279	GLU	3.1
1	B	190	GLN	3.1
1	A	273	THR	3.1
1	A	410	ASN	3.1
1	A	301	LYS	3.1
1	B	407	LEU	3.1
1	A	289	SER	3.0
1	B	46	VAL	3.0
1	A	224	TYR	3.0
1	A	208	PHE	3.0
1	B	274	HIS	3.0
1	A	207	PRO	3.0
1	B	292	PHE	2.9
1	A	332	LEU	2.9
1	A	285	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	356	TYR	2.9
1	A	342	VAL	2.9
1	A	596	ILE	2.9
1	B	181	ARG	2.8
1	A	226	THR	2.8
1	A	223	LYS	2.8
1	A	174	VAL	2.8
1	A	299	ILE	2.8
1	B	441	PHE	2.8
1	A	275	LEU	2.7
1	B	205	ARG	2.7
1	B	283	PHE	2.7
1	B	177	GLU	2.7
1	B	445	CYS	2.7
1	A	295	PHE	2.7
1	B	220	LEU	2.7
1	B	312	LEU	2.6
1	A	292	PHE	2.6
1	A	274	HIS	2.6
1	B	171	LEU	2.6
1	B	443	PHE	2.6
1	A	251	ASP	2.5
1	B	210	LYS	2.5
1	B	212	LEU	2.5
1	A	443	PHE	2.5
1	B	322	ALA	2.5
1	B	213	THR	2.5
1	A	1	MET	2.5
1	A	73	VAL	2.4
1	A	257	GLY	2.4
1	A	203	SER	2.4
1	A	199	ILE	2.4
1	B	492	ASN	2.4
1	B	167	LYS	2.4
1	A	175	GLN	2.4
1	B	208	PHE	2.3
1	A	303	ASN	2.3
1	A	217	TYR	2.3
1	B	44	LYS	2.3
1	A	202	ASP	2.3
1	A	368	VAL	2.3
1	A	441	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	297	ARG	2.3
1	A	370	PRO	2.2
1	B	311	PRO	2.2
1	A	212	LEU	2.2
1	A	43	LYS	2.2
1	A	190	GLN	2.2
1	B	242	GLN	2.2
1	B	371	THR	2.2
1	A	227	SER	2.2
1	A	183	VAL	2.2
1	B	203	SER	2.2
1	B	186	ILE	2.2
1	A	44	LYS	2.2
1	B	380	HIS	2.2
1	B	202	ASP	2.1
1	A	277	ASP	2.1
1	A	331	ASN	2.1
1	B	75	GLU	2.1
1	A	180	PRO	2.1
1	B	228	GLY	2.1
1	A	75	GLU	2.1
1	A	300	TYR	2.1
1	B	251	ASP	2.1
1	B	583	GLU	2.1
1	A	163	HIS	2.1
1	B	271	ILE	2.1
1	A	345	TYR	2.1
1	B	150	ARG	2.1
1	B	175	GLN	2.0
1	B	176	ASP	2.0
1	A	216	ILE	2.0
1	A	362	ILE	2.0
1	B	42	THR	2.0
1	B	109	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

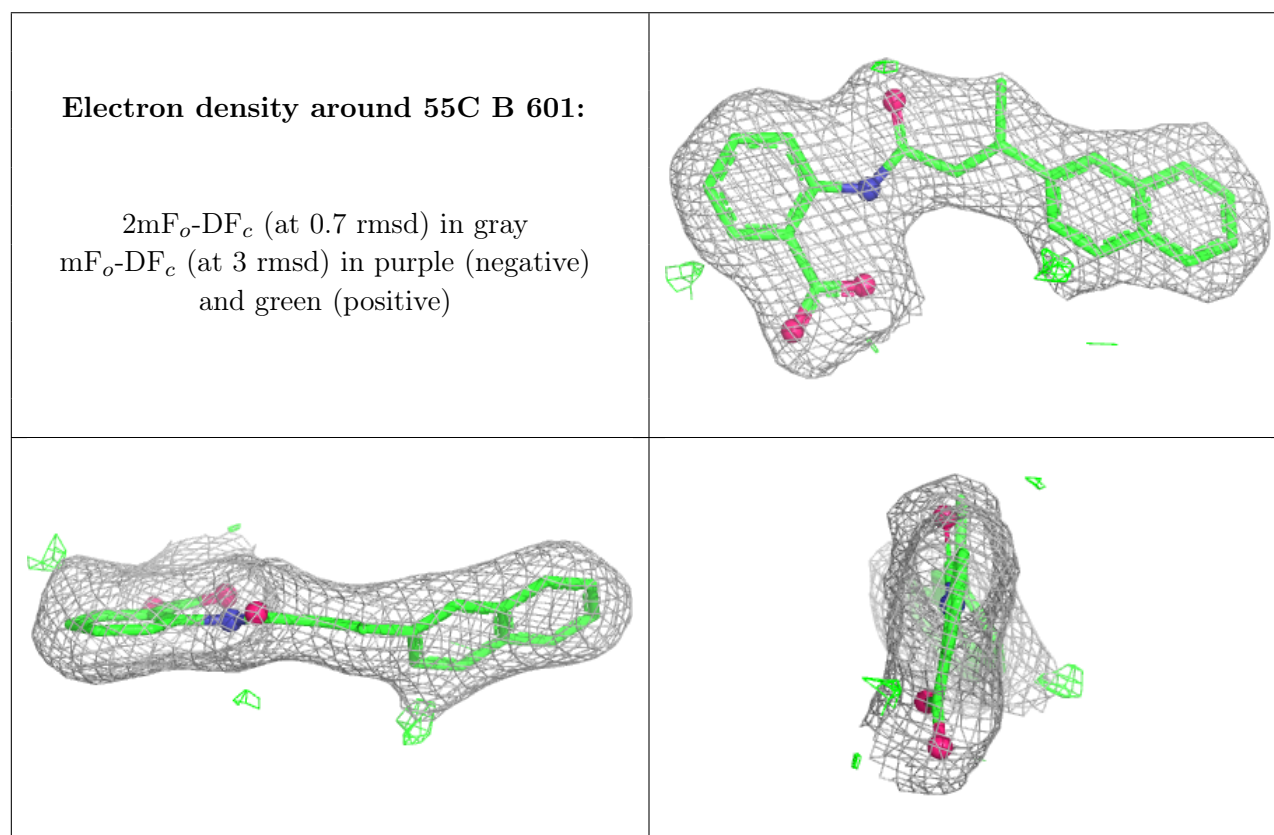
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
2	55C	A	601	25/25	0.91	0.10	42,48,60,67	0
2	55C	B	601	25/25	0.91	0.10	44,49,58,63	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.