Full wwPDB X-ray Structure Validation Report (i)

Sep 18, 2023 – 07:16 PM EDT

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
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:

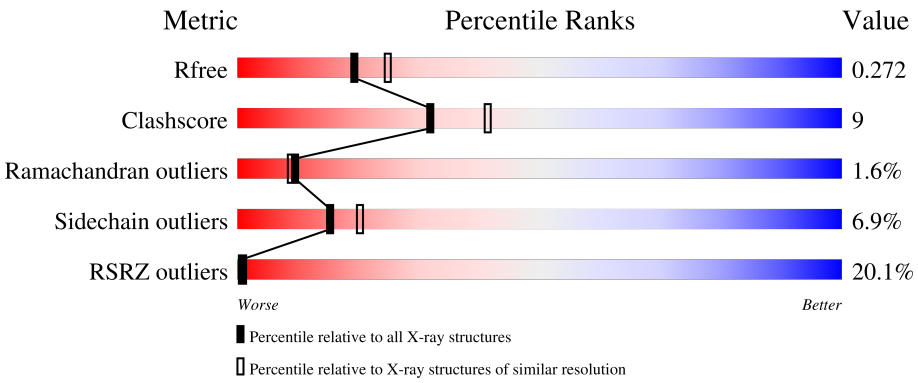
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.30 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 <=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	18% 73% 24% •
1	B	596	22% 79% 19% •

2 Entry composition (i)

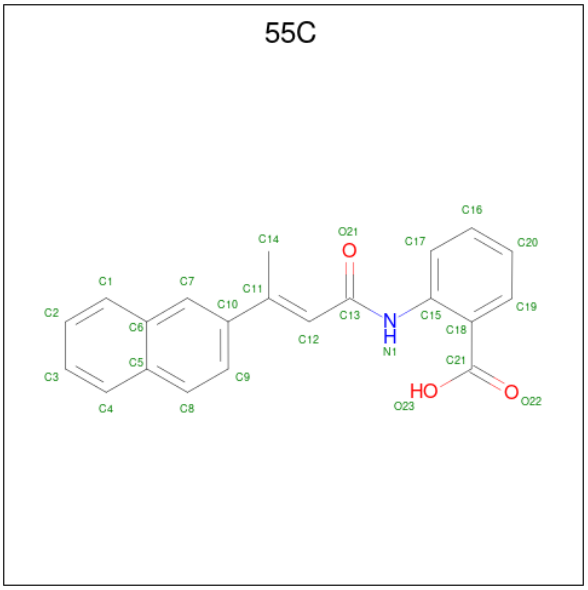
There are 3 unique types of molecules in this entry. The entry contains 10423 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	596	4982	3266	852	842	22	0	0	0
1	B	596	4982	3266	852	842	22	0	0	0

- Molecule 2 is 2-{[(2E)-3-(naphthalen-2-yl)but-2-enoyl]amino}benzoic acid (three-letter code: 55C) (formula: $C_{21}H_{17}NO_3$).



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

- Molecule 3 is water.

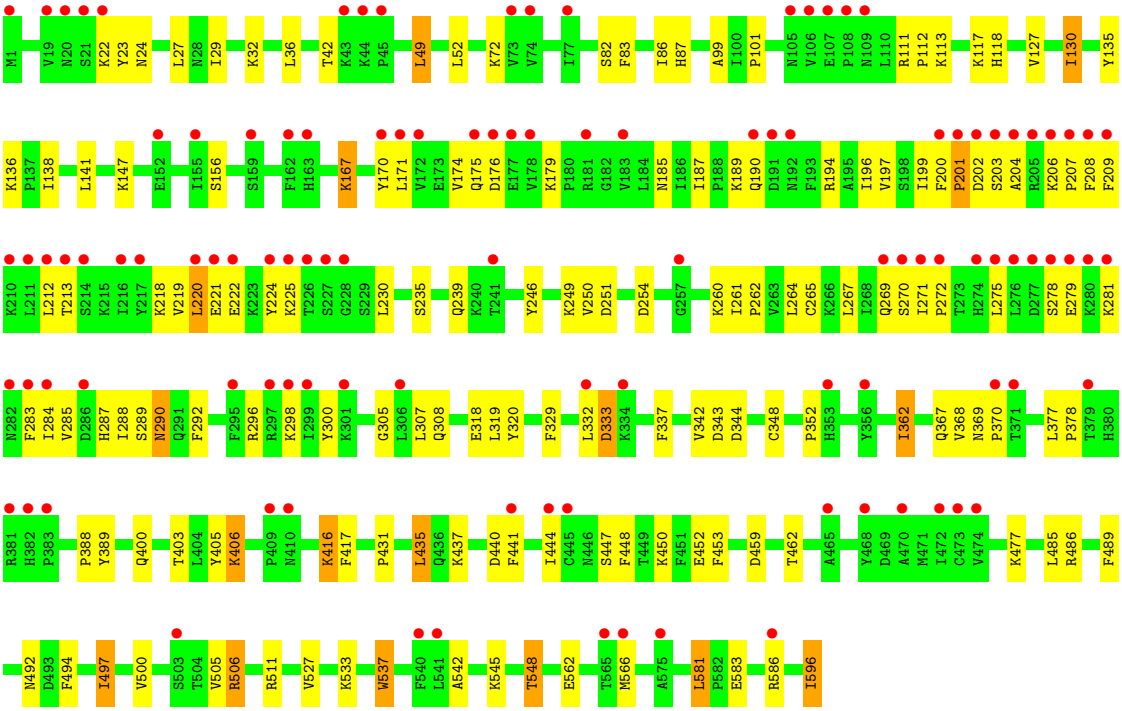
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	210	210	210	0	0
			Total	O		
3	B	199	199	199	0	0

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.

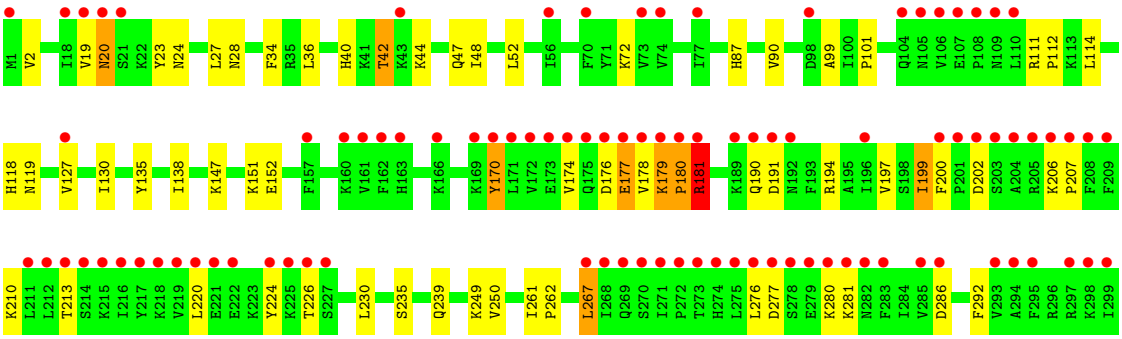
• Molecule 1: Telomerase reverse transcriptase

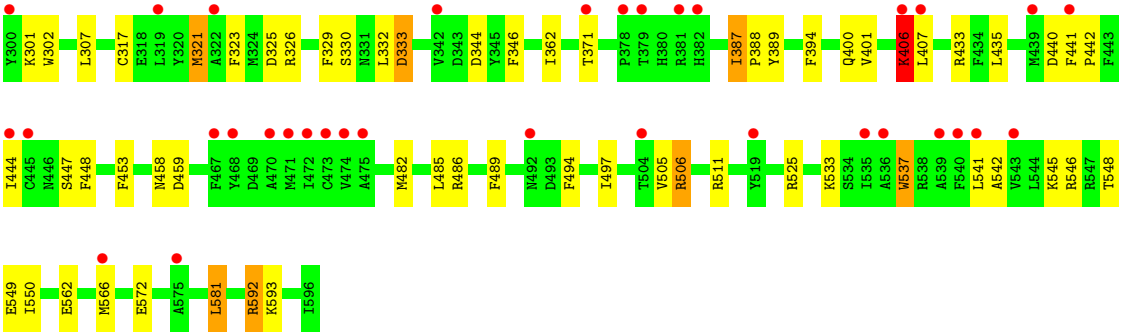
Chain A:



• Molecule 1: Telomerase reverse transcriptase

Chain B:




Y300 K301 W302 L307 C317 E318 L319 Y320 M321 A322 F323 M324 D325 R326 F329 S330 N331 L332 D333 V342 D343 D344 Y345 F346 I362 T371 P378 T379 H380 R381 H382 I387 P388 Y389 F394 Q400 V401 K406 L407 R433 F434 L435 M439 D440 F441 P442 F443
I444 C445 M446 S447 F448 F453 N458 D459 F467 Y468 D469 A470 M471 I472 C473 V474 A475 M482 L485 R486 F489 N492 D493 F494 I497 T504 V505 R506 R511 Y519 R525 K533 S534 I535 A536 W537 R538 A539 F540 L541 A542 V543 L544 K545 R546 R547 T548
E549 I550 E562 M566 E572 A575 L581 R592 K593 I596

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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 (5.03%)	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)	0.34 , 45.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	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.*

[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: 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 (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	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: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
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: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: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: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: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: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: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: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: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: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: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
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

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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: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:152:GLU:H	1:B:152:GLU:CD	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: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: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: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:296:ARG:C	1:A:298:LYS:H	2.22	0.42
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
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:290:ASN:OD1	1:A:290:ASN:N	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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%)	7 6
1	B	594/596 (100%)	547 (92%)	40 (7%)	7 (1%)	13 14
All	All	1188/1192 (100%)	1089 (92%)	80 (7%)	19 (2%)	9 9

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 (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	552/552 (100%)	514 (93%)	38 (7%)	15 20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	552/552 (100%)	514 (93%)	38 (7%)	15	20
All	All	1104/1104 (100%)	1028 (93%)	76 (7%)	15	20

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

Sometimes 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 monosaccharides 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	0.93	0	34,37,37	0.94	1 (2%)
2	55C	A	601	-	27,27,27	0.93	0	34,37,37	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 (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601	55C	O21-C13-N1	2.77	126.23	123.05

There are no chirality outliers.

There are no torsion outliers.

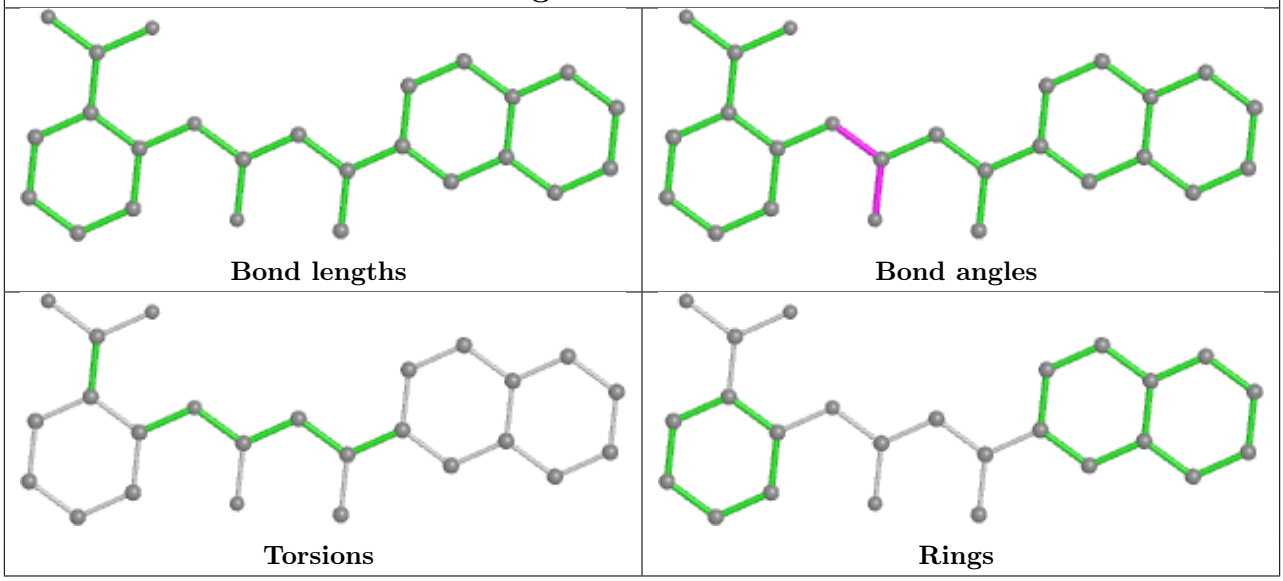
There are no ring outliers.

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 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 55C B 601



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 (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	596/596 (100%)	1.08	110 (18%)	1	1	24, 50, 126, 192	0
1	B	596/596 (100%)	1.30	129 (21%)	0	1	25, 51, 144, 187	0
All	All	1192/1192 (100%)	1.19	239 (20%)	1	1	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	16.2
1	A	204	ALA	12.4
1	B	211	LEU	11.6
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	6.9
1	B	225	LYS	6.7
1	A	200	PHE	6.6
1	B	190	GLN	6.6
1	B	279	GLU	6.5
1	B	221	GLU	6.5
1	B	226	THR	6.4
1	B	219	VAL	6.4
1	B	218	LYS	6.3
1	A	190	GLN	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	A	203	SER	5.8
1	B	203	SER	5.8
1	A	163	HIS	5.8
1	A	271	ILE	5.7
1	B	172	VAL	5.7
1	B	176	ASP	5.6
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	5.0
1	B	201	PRO	5.0
1	B	281	LYS	5.0
1	A	170	TYR	5.0
1	B	282	ASN	4.9
1	B	382	HIS	4.8
1	B	189	LYS	4.8
1	B	212	LEU	4.8
1	A	279	GLU	4.8
1	B	277	ASP	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	4.6
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	444	ILE	4.4
1	B	163	HIS	4.4
1	A	275	LEU	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	A	106	VAL	4.3
1	B	181	ARG	4.2
1	B	273	THR	4.2
1	A	206	LYS	4.2
1	B	342	VAL	4.2
1	B	180	PRO	4.2
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	370	PRO	4.0
1	A	283	PHE	4.0
1	A	105	ASN	4.0
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	444	ILE	3.9
1	B	379	THR	3.8
1	B	213	THR	3.8
1	B	208	PHE	3.8
1	B	20	ASN	3.8
1	A	276	LEU	3.7
1	A	214	SER	3.7
1	A	202	ASP	3.7
1	B	74	VAL	3.7
1	A	332	LEU	3.6
1	A	192	ASN	3.6
1	A	299	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	356	TYR	3.6
1	A	213	THR	3.5
1	B	470	ALA	3.5
1	A	381	ARG	3.5
1	A	278	SER	3.5
1	B	468	TYR	3.5
1	B	105	ASN	3.5
1	B	173	GLU	3.5
1	B	169	LYS	3.5
1	B	1	MET	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	A	172	VAL	3.3
1	B	298	LYS	3.3
1	B	294	ALA	3.3
1	B	540	PHE	3.3
1	A	282	ASN	3.2
1	A	107	GLU	3.2
1	A	306	LEU	3.2
1	A	474	VAL	3.2
1	A	410	ASN	3.2
1	A	280	LYS	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	A	109	ASN	3.1
1	B	179	LYS	3.1
1	B	319	LEU	3.1
1	B	473	CYS	3.1
1	B	322	ALA	3.1
1	B	519	TYR	3.1
1	A	371	THR	3.1
1	A	221	GLU	3.1
1	B	19	VAL	3.0
1	B	293	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	472	ILE	2.9
1	B	170	TYR	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	2.8
1	B	104	GLN	2.7
1	A	301	LYS	2.7
1	B	160	LYS	2.7
1	A	209	PHE	2.7
1	B	541	LEU	2.7
1	A	44	LYS	2.7
1	B	475	ALA	2.6
1	B	575	ALA	2.6
1	A	217	TYR	2.6
1	A	269	GLN	2.6
1	B	162	PHE	2.6
1	B	406	LYS	2.6
1	B	268	ILE	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	A	565	THR	2.5
1	B	492	ASN	2.4
1	A	541	LEU	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	441	PHE	2.4
1	B	98	ASP	2.4
1	A	108	PRO	2.4
1	A	183	VAL	2.4
1	A	274	HIS	2.3
1	A	575	ALA	2.3
1	B	215	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	162	PHE	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	2.3
1	A	226	THR	2.2
1	A	152	GLU	2.2
1	B	224	TYR	2.2
1	B	161	VAL	2.2
1	B	77	ILE	2.2
1	A	210	LYS	2.2
1	B	504	THR	2.2
1	B	471	MET	2.2
1	B	441	PHE	2.1
1	A	465	ALA	2.1
1	B	18	ILE	2.1
1	A	586	ARG	2.1
1	A	353	HIS	2.1
1	A	286	ASP	2.1
1	A	472	ILE	2.1
1	B	407	LEU	2.1
1	A	503	SER	2.1
1	B	280	LYS	2.1
1	A	468	TYR	2.1
1	A	216	ILE	2.1
1	B	439	MET	2.1
1	B	381	ARG	2.1
1	A	159	SER	2.1
1	A	334	LYS	2.1
1	B	196	ILE	2.1
1	A	297	ARG	2.1
1	A	22	LYS	2.1
1	A	284	ILE	2.0
1	A	409	PRO	2.0
1	B	295	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	77	ILE	2.0
1	B	566	MET	2.0
1	A	181	ARG	2.0
1	A	383	PRO	2.0
1	B	127	VAL	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 monosaccharides in this entry.

6.4 Ligands (i)

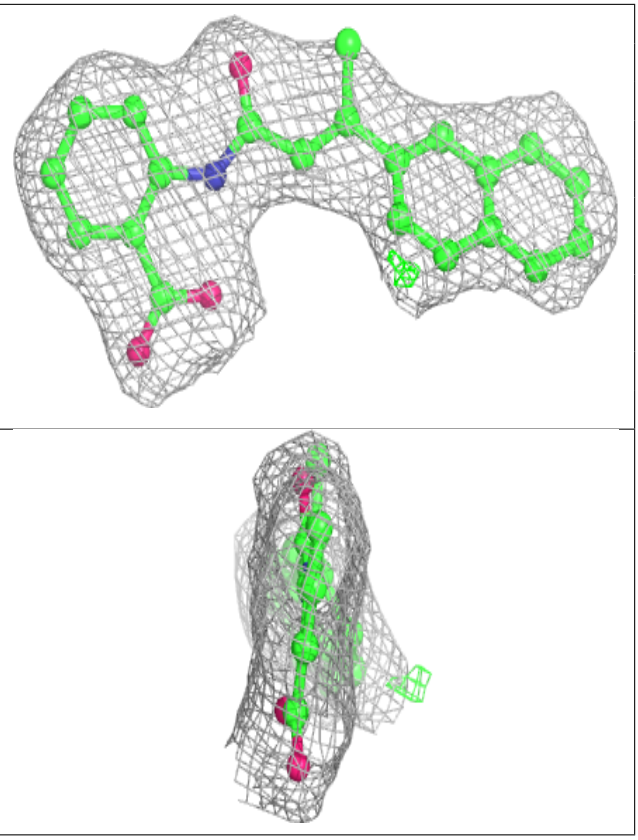
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	55C	B	601	25/25	0.86	0.14	44,49,58,63	0
2	55C	A	601	25/25	0.88	0.13	42,48,60,67	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 55C B 601:

$2mF_o$-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.