



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:09 AM UTC

PDB ID : 7D2K / pdb_00007d2k
Title : Crystal structure of rat TRPV6 in complex with (4- phenylcyclohexyl)piperazine inhibitor Br-cis-22a
Authors : Singh, A.K.; Neuberger, A.; Nadezhdin, K.D.; Sobolevsky, A.I.
Deposited on : 2020-09-16
Resolution : 3.70 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 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

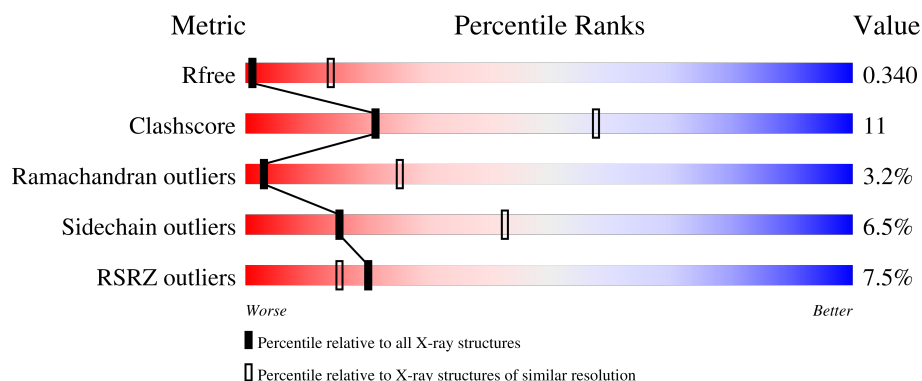
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

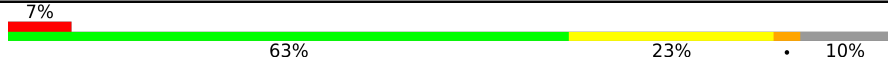
The reported resolution of this entry is 3.70 Å.

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}	180053	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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	672	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4872 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 Transient receptor potential cation channel subfamily V member 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	604	Total	C	N	O	S	0	0	0
			4819	3122	805	858	34			

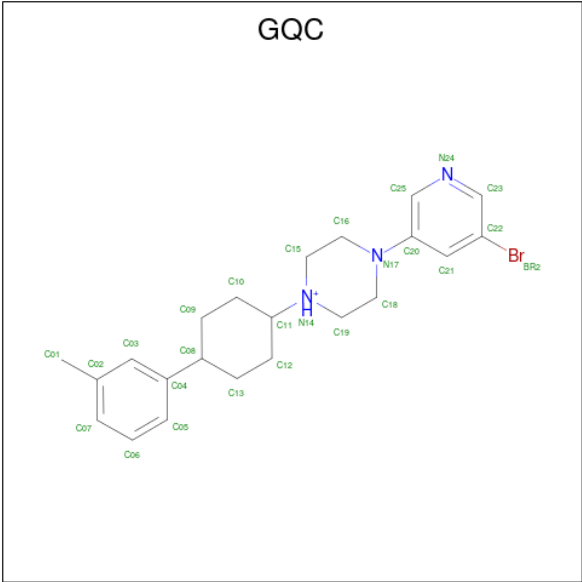
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	62	TYR	ILE	engineered mutation	UNP Q9R186
A	92	ASN	LEU	engineered mutation	UNP Q9R186
A	96	GLN	MET	engineered mutation	UNP Q9R186
A	670	VAL	-	expression tag	UNP Q9R186
A	671	PRO	-	expression tag	UNP Q9R186
A	672	ARG	-	expression tag	UNP Q9R186

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is 1-(5-bromanylpyridin-3-yl)-4-[4-(3-methylphenyl)cyclohexyl]piperazin-4-ium (CCD ID: GQC) (formula: C₂₂H₂₉BrN₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	Br	C	N	0	0
			26	1	22	3		
3	A	1	Total	Br	C	N	0	0
			26	1	22	3		

4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	146.23Å 146.23Å 114.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.12 – 3.70 47.12 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.12-3.70) 99.7 (47.12-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 3.66Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.316 , 0.327 0.328 , 0.340	Depositor DCC
R_{free} test set	690 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	172.0	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 111.1	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	0.86	EDS
Total number of atoms	4872	wwPDB-VP
Average B, all atoms (Å ²)	155.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, GQC

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	0.11	0/4930	0.30	0/6699

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4819	0	4853	106	0
2	A	1	0	0	0	0
3	A	52	0	0	0	0
All	All	4872	0	4853	106	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 11.

All (106) 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:360:ASN:H	1:A:361:PRO:HD2	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:MET:SD	1:A:445:ASN:ND2	2.68	0.66
1:A:631:ARG:NH2	1:A:633:GLU:OE2	2.31	0.64
1:A:352:LYS:HB2	1:A:371:LEU:HB3	1.79	0.63
1:A:516:PRO:HA	1:A:520:GLY:HA3	1.81	0.63
1:A:197:ASN:OD1	1:A:236:ASN:ND2	2.31	0.63
1:A:238:GLN:HG3	1:A:240:LEU:HD13	1.80	0.62
1:A:535:LEU:HD13	1:A:558:TYR:HE1	1.66	0.59
1:A:40:GLN:HB2	1:A:78:MET:HE2	1.84	0.59
1:A:409:LEU:HD13	1:A:410:GLY:H	1.67	0.58
1:A:256:GLN:NE2	1:A:309:GLN:OE1	2.37	0.58
1:A:264:HIS:HB3	1:A:276:LEU:HB3	1.86	0.58
1:A:236:ASN:OD1	1:A:237:ASN:N	2.37	0.57
1:A:36:GLN:HB3	1:A:78:MET:HE1	1.86	0.57
1:A:490:MET:HE3	1:A:494:TRP:HE1	1.69	0.57
1:A:352:LYS:HD2	1:A:371:LEU:HA	1.86	0.56
1:A:585:ALA:O	1:A:588:ARG:NH2	2.39	0.56
1:A:488:ASP:OD2	1:A:580:THR:OG1	2.23	0.56
1:A:36:GLN:O	1:A:40:GLN:N	2.37	0.55
1:A:188:ASP:HB3	1:A:191:ALA:HB2	1.88	0.55
1:A:161:TYR:OH	1:A:193:ASP:OD2	2.24	0.55
1:A:521:HIS:CG	1:A:543:PRO:HG3	2.42	0.54
1:A:619:GLY:N	1:A:627:ARG:O	2.35	0.54
1:A:198:THR:OG1	1:A:199:VAL:N	2.38	0.54
1:A:193:ASP:OD1	1:A:197:ASN:N	2.41	0.54
1:A:448:GLY:O	1:A:450:VAL:N	2.40	0.54
1:A:84:HIS:ND1	1:A:110:MET:SD	2.82	0.53
1:A:488:ASP:HA	1:A:491:ARG:HD2	1.91	0.53
1:A:485:ILE:HG13	1:A:489:LEU:HD23	1.90	0.52
1:A:592:TRP:HA	1:A:595:GLN:HG2	1.92	0.52
1:A:37:ASN:O	1:A:41:GLN:NE2	2.42	0.52
1:A:434:MET:HG2	1:A:455:PHE:HB2	1.92	0.52
1:A:310:THR:HG23	1:A:311:PRO:HD3	1.91	0.52
1:A:200:LEU:HB3	1:A:216:TYR:HE2	1.74	0.51
1:A:259:MET:HE2	1:A:311:PRO:HG3	1.93	0.51
1:A:314:GLU:OE1	1:A:314:GLU:N	2.43	0.51
1:A:190:ARG:HA	1:A:231:LEU:HD11	1.91	0.51
1:A:201:HIS:HE1	1:A:242:PRO:HD3	1.74	0.51
1:A:352:LYS:HD3	1:A:355:ILE:HD12	1.93	0.51
1:A:358:ARG:HG3	1:A:361:PRO:HG2	1.94	0.50
1:A:40:GLN:O	1:A:44:ILE:HG12	2.10	0.50
1:A:503:PHE:O	1:A:507:PHE:N	2.38	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:PHE:HD1	1:A:528:ALA:HA	1.75	0.50
1:A:441:MET:HB3	1:A:449:GLU:HG2	1.94	0.49
1:A:620:ARG:O	1:A:622:TYR:N	2.44	0.49
1:A:349:ARG:HD3	1:A:453:MET:HE2	1.95	0.48
1:A:350:PRO:HB2	1:A:371:LEU:HG	1.95	0.48
1:A:403:ILE:N	1:A:404:PRO:HD2	2.28	0.48
1:A:563:ILE:HA	1:A:567:LEU:HD21	1.95	0.48
1:A:398:ILE:HG21	1:A:428:ILE:HG22	1.96	0.48
1:A:424:PHE:O	1:A:428:ILE:HG13	2.13	0.48
1:A:301:ARG:HG3	1:A:304:ARG:NH2	2.29	0.47
1:A:379:PRO:HD2	1:A:381:ASP:H	1.79	0.47
1:A:603:LEU:O	1:A:607:LEU:HB2	2.14	0.47
1:A:335:TYR:HE2	1:A:464:VAL:HG12	1.79	0.47
1:A:299:LYS:H	1:A:299:LYS:HD3	1.80	0.46
1:A:328:PHE:CZ	1:A:467:PHE:HA	2.50	0.46
1:A:382:ASP:OD1	1:A:382:ASP:N	2.39	0.46
1:A:372:LEU:HB3	1:A:374:GLU:OE1	2.16	0.46
1:A:492:PHE:CE1	1:A:569:MET:HG3	2.51	0.46
1:A:438:THR:HA	1:A:441:MET:HB2	1.98	0.46
1:A:534:GLU:HB3	1:A:540:ILE:HG12	1.98	0.45
1:A:302:GLU:N	1:A:302:GLU:OE1	2.50	0.45
1:A:328:PHE:HZ	1:A:467:PHE:HA	1.81	0.45
1:A:508:TYR:O	1:A:512:GLN:N	2.50	0.45
1:A:345:CYS:SG	1:A:387:GLY:HA3	2.56	0.45
1:A:535:LEU:HD13	1:A:558:TYR:CE1	2.49	0.45
1:A:284:SER:HA	1:A:290:SER:HB2	1.98	0.45
1:A:43:ARG:HA	1:A:46:GLU:HB2	1.99	0.45
1:A:480:MET:HE2	1:A:588:ARG:HD3	1.98	0.45
1:A:304:ARG:H	1:A:304:ARG:HG3	1.63	0.44
1:A:620:ARG:HG2	1:A:621:GLU:H	1.80	0.44
1:A:396:VAL:HG22	1:A:400:LEU:HD13	1.98	0.44
1:A:424:PHE:CD1	1:A:466:TYR:HB2	2.52	0.44
1:A:96:GLN:HA	1:A:99:MET:HE2	1.98	0.44
1:A:264:HIS:N	1:A:276:LEU:O	2.43	0.44
1:A:505:SER:HA	1:A:525:TYR:HE1	1.83	0.44
1:A:110:MET:HB2	1:A:115:TYR:O	2.18	0.44
1:A:200:LEU:HB3	1:A:216:TYR:CE2	2.52	0.44
1:A:519:LEU:HD11	1:A:543:PRO:HB3	2.00	0.44
1:A:197:ASN:HB3	1:A:201:HIS:HB2	1.99	0.43
1:A:469:ARG:HB3	1:A:470:GLY:H	1.63	0.43
1:A:289:GLN:H	1:A:289:GLN:HG2	1.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:ASN:N	1:A:364:ASN:OD1	2.50	0.43
1:A:620:ARG:NH1	1:A:626:ASP:OD1	2.49	0.43
1:A:73:HIS:HB3	1:A:75:LYS:NZ	2.34	0.43
1:A:300:LYS:HA	1:A:300:LYS:HD2	1.71	0.43
1:A:567:LEU:O	1:A:571:ASN:HB2	2.19	0.42
1:A:620:ARG:HB2	1:A:626:ASP:H	1.84	0.42
1:A:278:ASP:OD2	1:A:280:THR:OG1	2.31	0.42
1:A:424:PHE:CG	1:A:466:TYR:HB2	2.53	0.42
1:A:220:LEU:HD22	1:A:223:ASP:HB2	2.00	0.42
1:A:474:LEU:O	1:A:478:THR:OG1	2.34	0.42
1:A:71:GLU:O	1:A:74:GLN:HG3	2.19	0.42
1:A:313:LYS:HE2	1:A:313:LYS:HB3	1.83	0.42
1:A:218:LEU:O	1:A:221:SER:OG	2.26	0.41
1:A:523:TYR:CE1	1:A:527:MET:HG2	2.56	0.41
1:A:354:ARG:C	1:A:356:THR:H	2.27	0.41
1:A:393:VAL:HA	1:A:396:VAL:HG12	2.02	0.41
1:A:180:ARG:HE	1:A:180:ARG:HB3	1.73	0.41
1:A:335:TYR:CE2	1:A:464:VAL:HG12	2.56	0.41
1:A:479:ILE:HG23	1:A:588:ARG:HG3	2.02	0.41
1:A:608:PRO:HB2	1:A:609:ARG:H	1.73	0.41
1:A:299:LYS:O	1:A:301:ARG:NH2	2.55	0.40
1:A:450:VAL:HA	1:A:453:MET:HB2	2.03	0.40
1:A:535:LEU:HD22	1:A:558:TYR:OH	2.21	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	600/672 (89%)	513 (86%)	68 (11%)	19 (3%)	3 25

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	ASP
1	A	198	THR
1	A	355	ILE
1	A	379	PRO
1	A	449	GLU
1	A	468	ALA
1	A	69	GLY
1	A	636	GLN
1	A	472	GLN
1	A	608	PRO
1	A	88	LEU
1	A	360	ASN
1	A	46	GLU
1	A	362	ARG
1	A	519	LEU
1	A	67	PHE
1	A	353	PRO
1	A	311	PRO
1	A	406	ILE

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	520/584 (89%)	486 (94%)	34 (6%)	15	43

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	VAL
1	A	83	LEU
1	A	130	VAL
1	A	220	LEU
1	A	231	LEU
1	A	252	ILE
1	A	287	ASP
1	A	289	GLN

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Mol	Chain	Res	Type
1	A	294	LEU
1	A	310	THR
1	A	331	LEU
1	A	355	ILE
1	A	364	ASN
1	A	372	LEU
1	A	374	GLU
1	A	378	THR
1	A	403	ILE
1	A	409	LEU
1	A	420	LEU
1	A	438	THR
1	A	443	LEU
1	A	449	GLU
1	A	464	VAL
1	A	474	LEU
1	A	478	THR
1	A	515	ASP
1	A	539	ILE
1	A	548	VAL
1	A	553	MET
1	A	567	LEU
1	A	584	VAL
1	A	617	ILE
1	A	630	LEU
1	A	633	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	ASN
1	A	201	HIS
1	A	289	GLN
1	A	368	GLN

5.3.3 RNA ⓘ

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](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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	GQC	A	702	-	29,29,29	2.06	5 (17%)	40,40,40	1.82	9 (22%)
3	GQC	A	703	-	29,29,29	2.25	5 (17%)	40,40,40	1.83	10 (25%)

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	GQC	A	702	-	-	3/12/32/32	0/4/4/4
3	GQC	A	703	-	-	5/12/32/32	0/4/4/4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	703	GQC	C11-N14	-7.81	1.28	1.48
3	A	702	GQC	C11-N14	-7.19	1.30	1.48
3	A	703	GQC	C15-N14	-5.77	1.36	1.47
3	A	703	GQC	C19-N14	-5.25	1.37	1.47
3	A	702	GQC	C15-N14	-4.74	1.38	1.47
3	A	702	GQC	C19-N14	-4.30	1.39	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	GQC	C20-N17	3.70	1.49	1.38
3	A	703	GQC	C20-N17	3.18	1.47	1.38
3	A	703	GQC	BR2-C22	2.87	1.96	1.90
3	A	702	GQC	BR2-C22	2.53	1.95	1.90

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	703	GQC	C10-C11-N14	-6.60	95.74	112.66
3	A	702	GQC	C10-C11-N14	-5.46	98.66	112.66
3	A	702	GQC	C09-C10-C11	4.41	118.49	109.98
3	A	703	GQC	C12-C11-N14	4.02	122.96	112.66
3	A	702	GQC	C12-C11-N14	3.62	121.94	112.66
3	A	703	GQC	C18-N17-C16	-3.48	103.73	111.57
3	A	702	GQC	C10-C09-C08	3.27	116.63	110.61
3	A	703	GQC	C25-N24-C23	3.06	121.67	117.51
3	A	702	GQC	C25-N24-C23	3.03	121.62	117.51
3	A	703	GQC	C09-C08-C04	-2.64	106.42	112.67
3	A	702	GQC	C18-N17-C16	-2.54	105.85	111.57
3	A	702	GQC	C13-C12-C11	2.37	114.56	109.98
3	A	703	GQC	C13-C08-C04	-2.36	107.09	112.67
3	A	702	GQC	C18-C19-N14	2.30	114.65	110.61
3	A	703	GQC	C15-N14-C11	-2.29	106.97	112.79
3	A	703	GQC	C05-C04-C03	2.17	121.25	118.74
3	A	703	GQC	C04-C03-C02	-2.16	119.26	121.37
3	A	702	GQC	C16-C15-N14	2.16	114.40	110.61
3	A	703	GQC	C20-C25-N24	-2.05	120.46	122.81

There are no chirality outliers.

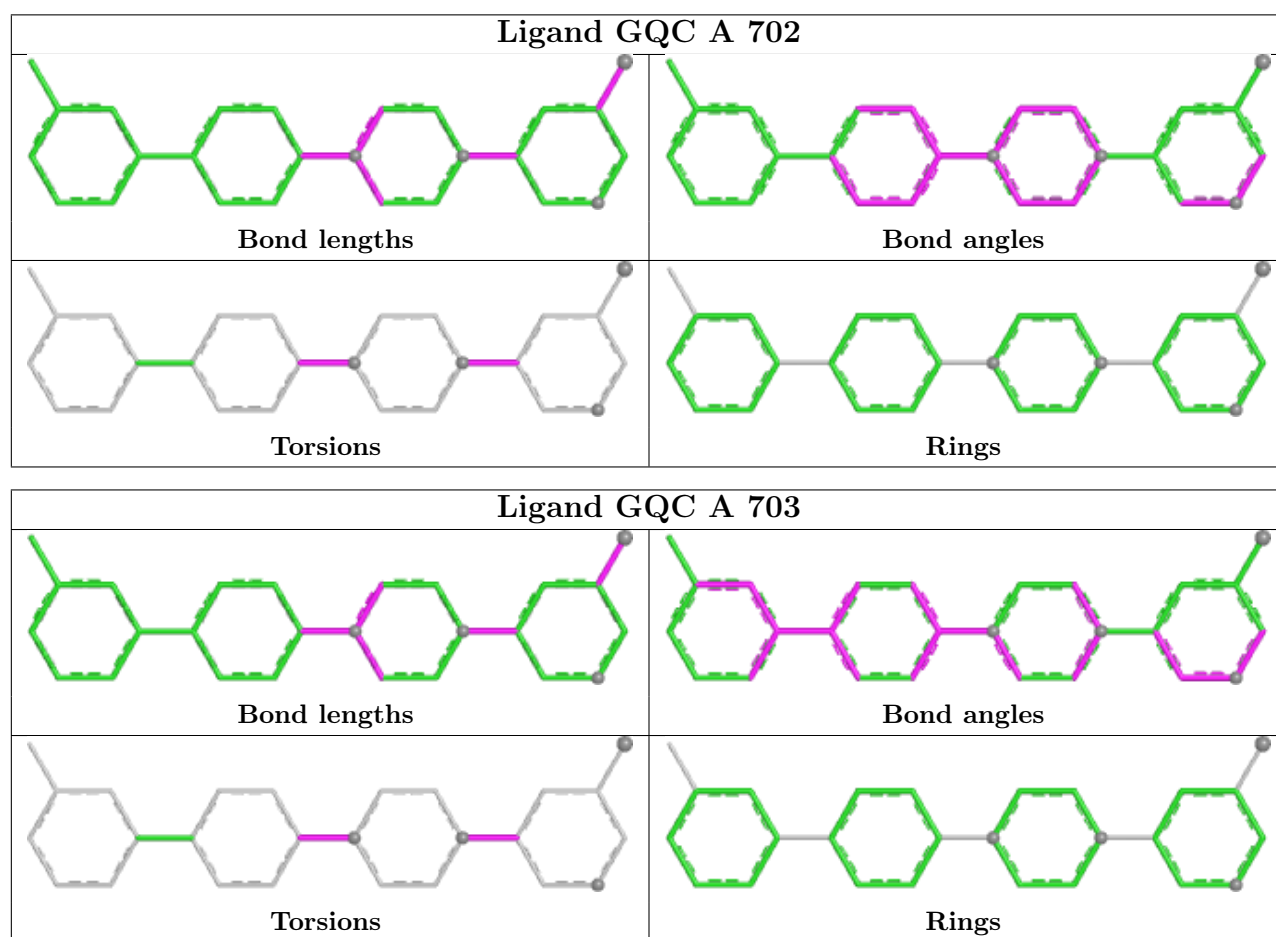
All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	703	GQC	C25-C20-N17-C16
3	A	703	GQC	C10-C11-N14-C15
3	A	703	GQC	C12-C11-N14-C19
3	A	703	GQC	C10-C11-N14-C19
3	A	703	GQC	C12-C11-N14-C15
3	A	702	GQC	C25-C20-N17-C18
3	A	702	GQC	C12-C11-N14-C19
3	A	702	GQC	C21-C20-N17-C18

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	604/672 (89%)	0.57	45 (7%) 20 15	141, 153, 181, 192	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	560	ALA	6.4
1	A	159	LEU	5.7
1	A	563	ILE	4.7
1	A	360	ASN	4.5
1	A	566	THR	3.9
1	A	634	ASP	3.9
1	A	351	LEU	3.9
1	A	158	ASN	3.8
1	A	544	ALA	3.7
1	A	155	ARG	3.4
1	A	493	CYS	3.4
1	A	249	GLU	3.3
1	A	284	SER	3.3
1	A	157	HIS	3.2
1	A	359	THR	3.1
1	A	420	LEU	3.1
1	A	571	ASN	3.0
1	A	498	VAL	3.0
1	A	540	ILE	2.9
1	A	479	ILE	2.9
1	A	574	ILE	2.8
1	A	355	ILE	2.8
1	A	106	VAL	2.8
1	A	285	SER	2.8
1	A	570	LEU	2.7
1	A	633	GLU	2.7
1	A	497	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	273	THR	2.7
1	A	591	LEU	2.6
1	A	367	LEU	2.6
1	A	550	LEU	2.6
1	A	564	ILE	2.5
1	A	292	LEU	2.5
1	A	283	ASP	2.5
1	A	624	LEU	2.5
1	A	290	SER	2.3
1	A	390	VAL	2.3
1	A	243	PHE	2.3
1	A	602	MET	2.3
1	A	356	THR	2.2
1	A	156	PRO	2.2
1	A	341	CYS	2.1
1	A	470	GLY	2.1
1	A	483	LYS	2.0
1	A	543	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 oligosaccharides in this entry.

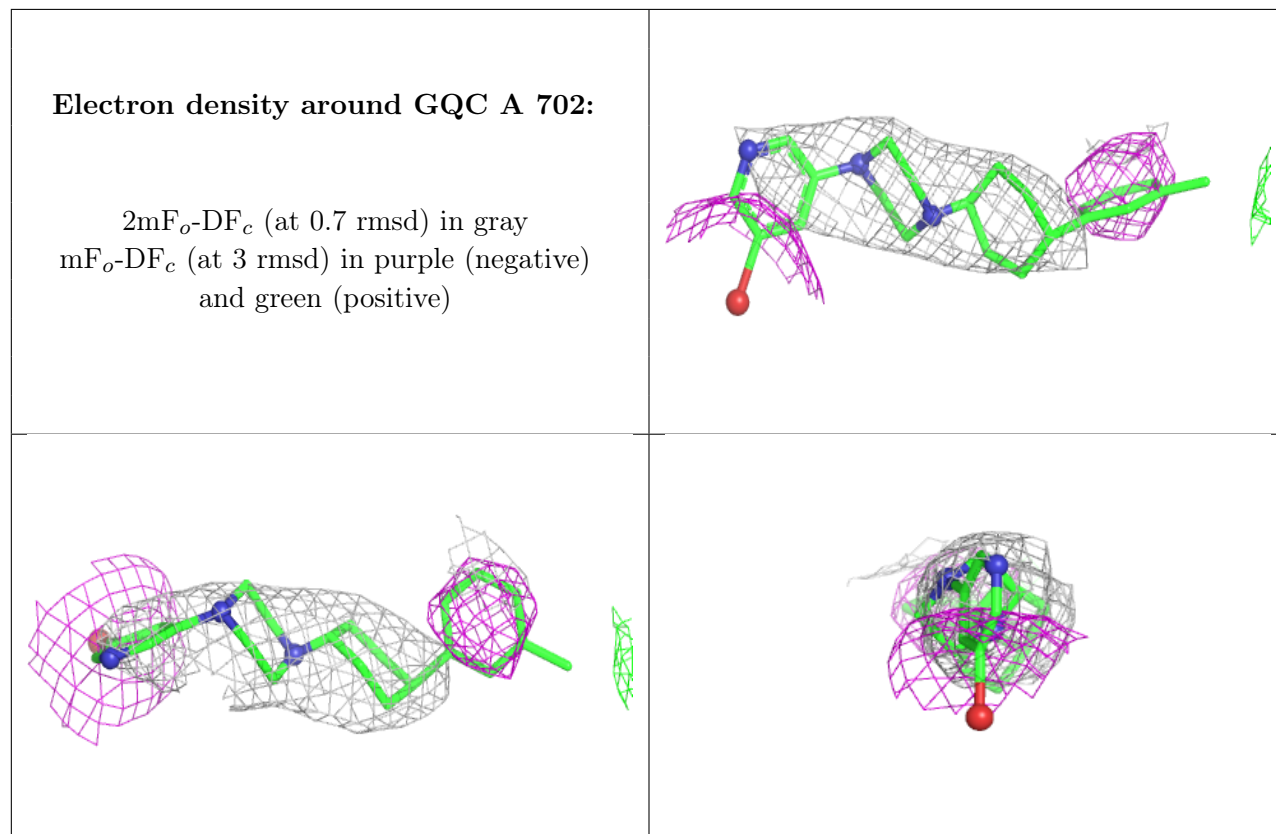
6.4 Ligands [i](#)

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(Å ²)	Q<0.9
3	GQC	A	702	26/26	0.25	0.32	144,148,159,163	0
3	GQC	A	703	26/26	0.93	0.15	20,20,20,20	26
2	CA	A	701	1/1	0.96	0.13	154,154,154,154	1

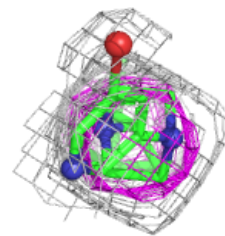
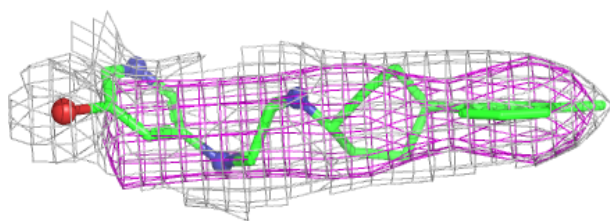
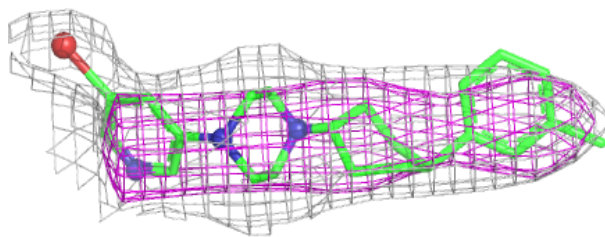
The following is a graphical depiction of the model fit to experimental electron density of all

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 GQC A 703:

$2mF_o-DF_c$ (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.