



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:40 PM UTC

PDB ID : 5I75 / pdb_00005i75
Title : X-ray structure of the ts3 human serotonin transporter complexed with s-citalopram at the central site and Br-citalopram at the allosteric site
Authors : Coleman, J.A.; Green, E.M.; Gouaux, E.
Deposited on : 2016-02-16
Resolution : 3.49 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

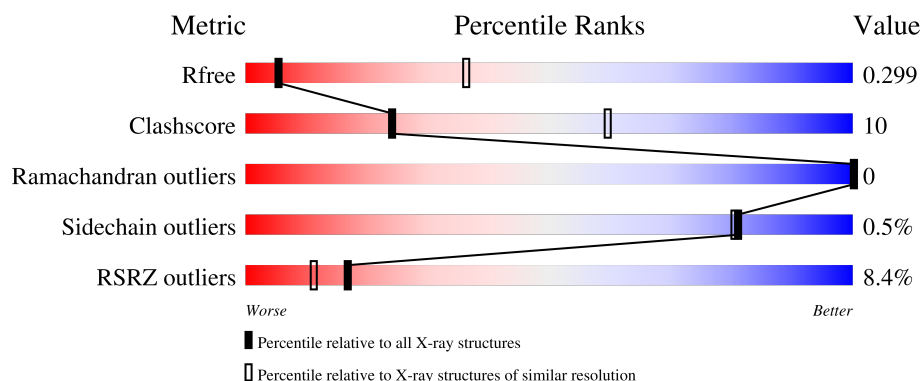
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.49 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	549	7% 74% 23% ..
2	B	221	12% 83% 16% .
3	C	214	7% 81% 19%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 7610 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 Sodium-dependent serotonin transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	540	Total	C	N	O	S	0	0	0
			4192	2801	647	720	24			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	74	GLY	-	cloning artifact	UNP P31645
A	75	SER	-	cloning artifact	UNP P31645
A	291	ALA	ILE	engineered mutation	UNP P31645
A	439	SER	THR	engineered mutation	UNP P31645
A	554	ALA	CYS	engineered mutation	UNP P31645
A	580	ALA	CYS	engineered mutation	UNP P31645
A	619	LEU	-	cloning artifact	UNP P31645
A	620	VAL	-	cloning artifact	UNP P31645
A	621	PRO	-	cloning artifact	UNP P31645
A	622	ARG	-	cloning artifact	UNP P31645

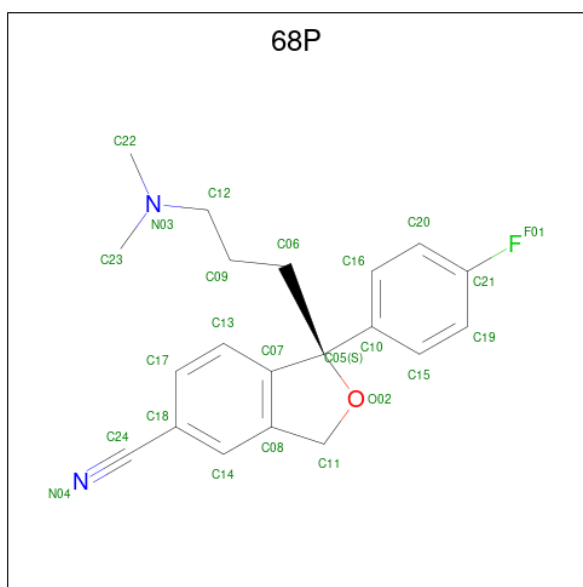
- Molecule 2 is a protein called 8B6 antibody, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	218	Total	C	N	O	S	0	0	0
			1643	1038	266	331	8			

- Molecule 3 is a protein called 8B6 antibody, light chain.

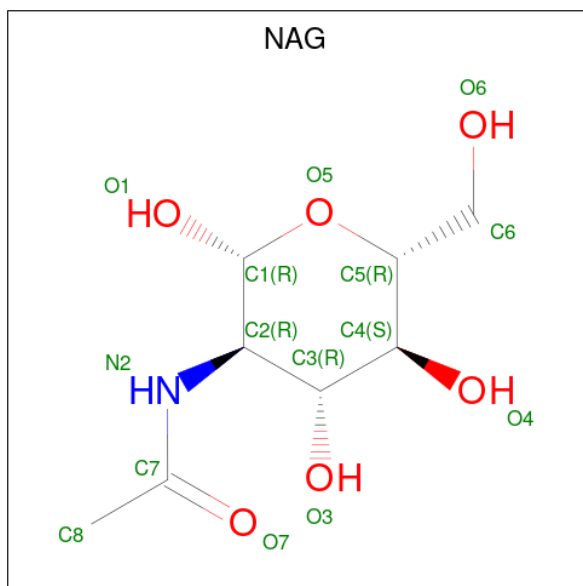
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	214	Total	C	N	O	S	0	0	0
			1662	1037	280	337	8			

- Molecule 4 is (1S)-1-[3-(dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-2-benzofuran-5-carbonitrile (CCD ID: 68P) (formula: C₂₀H₂₁FN₂O).



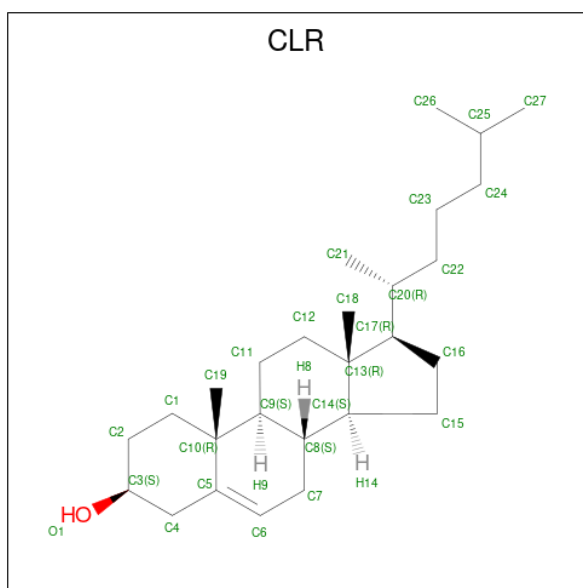
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0
			24	20	1	2	1	

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



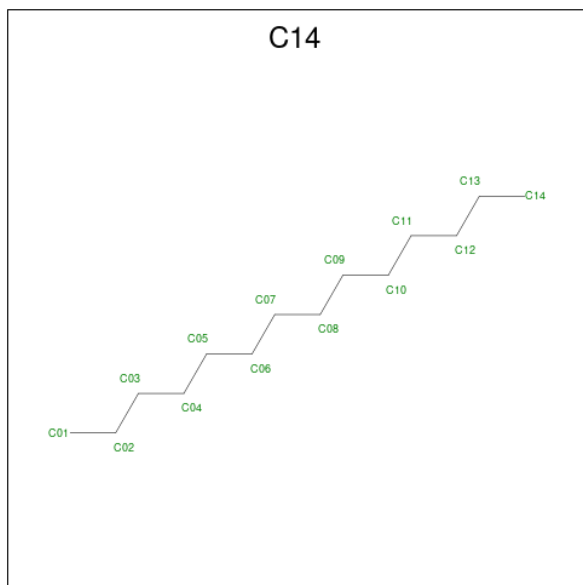
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	C	O	0
			28	27	1	

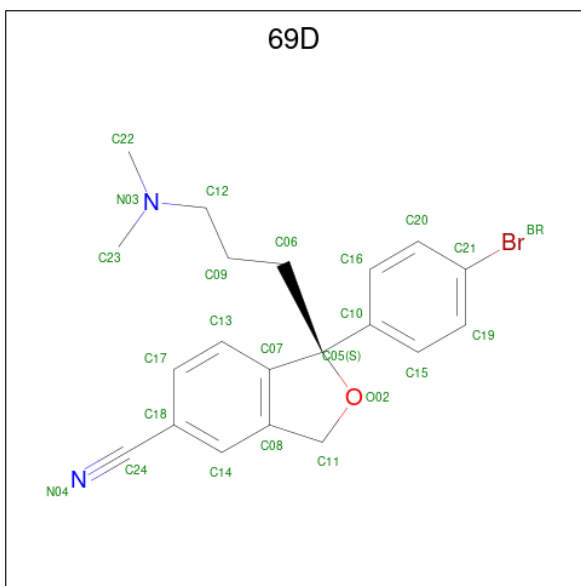
- Molecule 7 is TETRADECANE (CCD ID: C14) (formula: $C_{14}H_{30}$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	C		0
			14	14		

- Molecule 8 is (1S)-1-(4-bromophenyl)-1-[3-(dimethylamino)propyl]-1,3-dihydro-2-benzofura

n-5-carbonitrile (CCD ID: 69D) (formula: $C_{20}H_{21}BrN_2O$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	Br	C	N	O	0	0
			18	1	15	1	1		

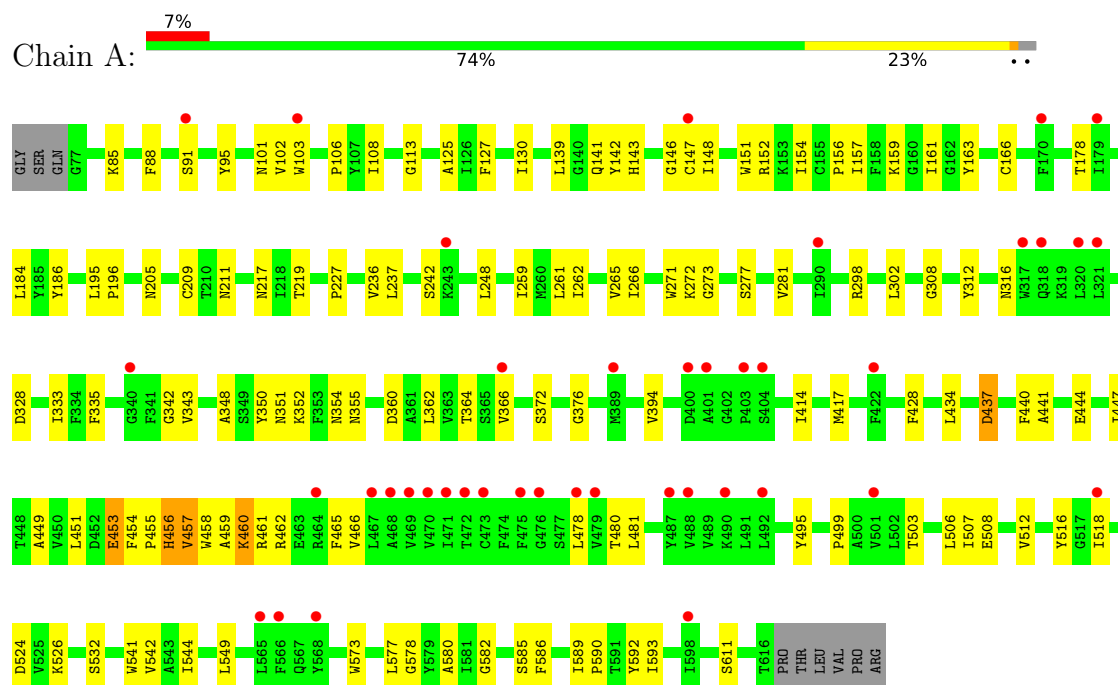
- Molecule 9 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Na	0	0
			1	1		

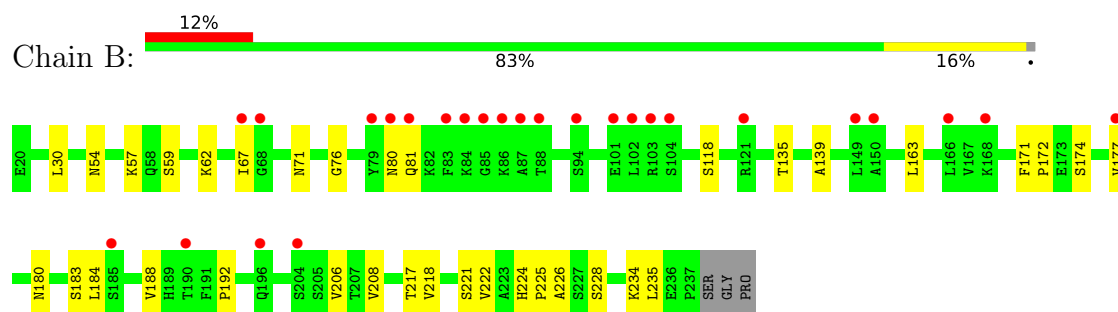
3 Residue-property plots

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.

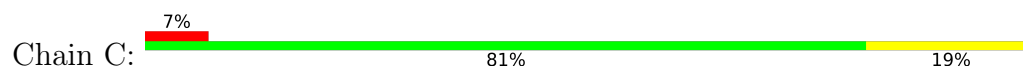
• Molecule 1: Sodium-dependent serotonin transporter

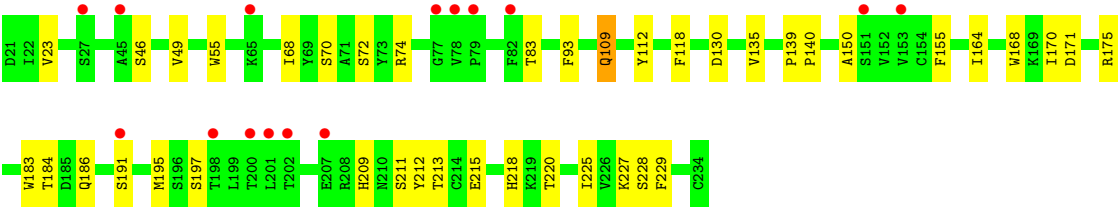


• Molecule 2: 8B6 antibody, heavy chain



• Molecule 3: 8B6 antibody, light chain





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	129.60Å 163.41Å 140.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	82.29 – 3.49 82.29 – 3.49	Depositor EDS
% Data completeness (in resolution range)	99.0 (82.29-3.49) 99.0 (82.29-3.49)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 3.49Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.244 , 0.286 0.251 , 0.299	Depositor DCC
R_{free} test set	959 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	124.3	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 191.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	7610	wwPDB-VP
Average B, all atoms (Å ²)	174.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% 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: NA, C14, CLR, NAG, 68P, 69D

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	0.21	0/4325	0.51	5/5915 (0.1%)
2	B	0.15	0/1688	0.40	0/2309
3	C	0.12	0/1700	0.38	0/2307
All	All	0.18	0/7713	0.46	5/10531 (0.0%)

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	A	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	457	VAL	N-CA-C	-5.78	104.88	110.72
1	A	460	LYS	N-CA-C	-5.40	105.29	111.07
1	A	453	GLU	CA-C-N	-5.13	116.72	123.34
1	A	453	GLU	C-N-CA	-5.13	116.72	123.34
1	A	455	PRO	CB-CA-C	-5.03	106.83	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	456	HIS	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	4192	0	4085	102	0
2	B	1643	0	1589	21	0
3	C	1662	0	1585	25	0
4	A	24	0	0	1	0
5	A	28	0	26	1	0
6	A	28	0	46	5	0
7	A	14	0	30	1	0
8	A	18	0	0	1	0
9	A	1	0	0	0	0
All	All	7610	0	7361	149	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 10.

All (149) 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)
8:A:705:69D:C11	8:A:705:69D:O02	1.69	1.34
1:A:458:TRP:O	1:A:459:ALA:HB3	1.72	0.88
1:A:454:PHE:HB3	1:A:457:VAL:HG11	1.59	0.85
1:A:205:ASN:ND2	1:A:209:CYS:SG	2.51	0.84
1:A:454:PHE:HB3	1:A:457:VAL:CG1	2.08	0.83
1:A:147:CYS:H	1:A:449:ALA:HB2	1.43	0.82
1:A:444:GLU:OE1	1:A:462:ARG:NH2	2.13	0.81
2:B:30:LEU:HD22	2:B:172:PRO:HD3	1.64	0.80
1:A:447:ILE:HD13	1:A:466:VAL:HG22	1.65	0.78
1:A:101:ASN:ND2	1:A:372:SER:OG	2.19	0.76
1:A:454:PHE:O	1:A:457:VAL:CG1	2.36	0.73
1:A:141:GLN:NE2	1:A:351:ASN:OD1	2.21	0.73
1:A:454:PHE:O	1:A:458:TRP:HB2	1.89	0.73
1:A:458:TRP:O	1:A:459:ALA:CB	2.36	0.73
1:A:437:ASP:OD1	1:A:437:ASP:N	2.21	0.69
1:A:152:ARG:HH21	1:A:159:LYS:HZ1	1.40	0.69
1:A:85:LYS:NZ	1:A:360:ASP:OD2	2.26	0.69
1:A:108:ILE:HD11	1:A:328:ASP:HB3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:PHE:C	1:A:457:VAL:HG12	2.18	0.68
2:B:192:PRO:HD3	3:C:184:THR:HG22	1.74	0.67
1:A:414:ILE:HA	1:A:417:MET:HE2	1.74	0.67
1:A:362:LEU:O	1:A:366:VAL:HG23	1.95	0.67
1:A:157:ILE:HB	1:A:593:ILE:HG12	1.76	0.66
3:C:211:SER:HA	3:C:229:PHE:O	1.95	0.66
1:A:454:PHE:C	1:A:457:VAL:CG1	2.70	0.65
1:A:88:PHE:HE2	1:A:350:TYR:HB2	1.61	0.64
2:B:54:ASN:ND2	2:B:118:SER:OG	2.28	0.64
1:A:589:ILE:HG23	1:A:590:PRO:HD3	1.82	0.62
3:C:74:ARG:HH21	3:C:83:THR:HG22	1.65	0.61
1:A:147:CYS:H	1:A:449:ALA:CB	2.13	0.61
3:C:171:ASP:OD2	3:C:209:HIS:ND1	2.33	0.61
1:A:146:GLY:HA3	1:A:449:ALA:HA	1.83	0.60
1:A:360:ASP:O	1:A:364:THR:HG23	2.01	0.60
3:C:186:GLN:HE21	3:C:191:SER:HB3	1.66	0.60
2:B:59:SER:HB2	2:B:62:LYS:HB2	1.85	0.59
1:A:91:SER:HA	1:A:281:VAL:HG11	1.84	0.59
1:A:454:PHE:O	1:A:457:VAL:HG13	2.02	0.59
1:A:454:PHE:O	1:A:457:VAL:HG12	2.02	0.59
1:A:113:GLY:HA2	1:A:316:ASN:HB3	1.85	0.58
1:A:277:SER:O	1:A:281:VAL:HG23	2.04	0.58
1:A:454:PHE:CB	1:A:457:VAL:HG11	2.34	0.56
1:A:151:TRP:HZ2	1:A:508:GLU:HG2	1.70	0.56
1:A:573:TRP:CZ3	6:A:703:CLR:H71	2.41	0.56
1:A:352:LYS:HB2	1:A:355:ASN:HB2	1.88	0.56
1:A:456:HIS:N	1:A:458:TRP:O	2.36	0.55
1:A:161:ILE:HD11	1:A:507:ILE:HG22	1.87	0.55
1:A:516:TYR:OH	1:A:524:ASP:OD2	2.21	0.55
3:C:130:ASP:HB3	3:C:220:THR:HG22	1.89	0.54
2:B:177:VAL:HA	2:B:221:SER:O	2.07	0.54
1:A:184:LEU:HD21	1:A:261:LEU:HD23	1.91	0.53
3:C:215:GLU:HA	3:C:225:ILE:O	2.08	0.53
1:A:106:PRO:HG3	1:A:376:GLY:HA2	1.92	0.52
1:A:454:PHE:HB3	1:A:457:VAL:HG13	1.88	0.52
1:A:273:GLY:HA2	1:A:462:ARG:CZ	2.40	0.52
1:A:266:ILE:HA	1:A:440:PHE:HE1	1.76	0.51
1:A:195:LEU:HD12	1:A:195:LEU:H	1.75	0.51
2:B:163:LEU:HB3	2:B:235:LEU:HD22	1.92	0.51
1:A:460:LYS:HG3	1:A:461:ARG:N	2.25	0.50
1:A:447:ILE:HA	1:A:465:PHE:HE2	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:THR:HG21	1:A:480:THR:HB	1.93	0.49
2:B:57:LYS:HB2	2:B:67:ILE:HD11	1.93	0.49
3:C:164:ILE:HB	3:C:218:HIS:HD2	1.76	0.49
3:C:139:PRO:HB3	3:C:229:PHE:CE2	2.47	0.49
1:A:458:TRP:CZ3	1:A:465:PHE:HB2	2.48	0.49
1:A:259:ILE:HG21	1:A:481:LEU:HD11	1.95	0.49
2:B:188:VAL:HG22	2:B:206:VAL:HB	1.93	0.49
1:A:573:TRP:CE3	6:A:703:CLR:H71	2.47	0.49
1:A:456:HIS:N	1:A:458:TRP:H	2.11	0.48
1:A:582:GLY:O	1:A:585:SER:OG	2.27	0.48
1:A:163:TYR:O	1:A:166:CYS:HB2	2.13	0.48
3:C:49:VAL:HG13	3:C:112:TYR:CE1	2.48	0.48
2:B:206:VAL:HG22	2:B:208:VAL:HG13	1.95	0.48
3:C:49:VAL:HG13	3:C:112:TYR:CD1	2.48	0.48
1:A:457:VAL:HG13	1:A:458:TRP:N	2.28	0.48
1:A:102:VAL:HG21	1:A:434:LEU:HD13	1.95	0.48
3:C:213:THR:HA	3:C:227:LYS:O	2.14	0.48
2:B:183:SER:HA	2:B:184:LEU:HA	1.56	0.48
2:B:80:ASN:OD1	2:B:81:GLN:N	2.47	0.47
3:C:23:VAL:H	3:C:46:SER:HB3	1.79	0.47
1:A:127:PHE:HB3	1:A:544:ILE:HG21	1.96	0.47
1:A:580:ALA:HB1	6:A:703:CLR:H241	1.95	0.47
3:C:135:VAL:HA	3:C:155:PHE:O	2.15	0.47
2:B:224:HIS:CE1	2:B:226:ALA:HB3	2.49	0.47
1:A:478:LEU:HD23	1:A:481:LEU:HD12	1.97	0.47
3:C:212:TYR:O	3:C:228:SER:HA	2.15	0.47
2:B:180:ASN:HD21	2:B:218:VAL:HA	1.78	0.47
1:A:186:TYR:HB3	1:A:428:PHE:CE2	2.50	0.46
1:A:451:LEU:HD23	1:A:458:TRP:HB3	1.96	0.46
1:A:277:SER:O	1:A:281:VAL:CG2	2.64	0.46
2:B:71:ASN:HB3	2:B:76:GLY:H	1.81	0.46
3:C:140:PRO:HG2	3:C:150:ALA:HB1	1.97	0.46
2:B:224:HIS:O	2:B:228:SER:N	2.48	0.46
1:A:335:PHE:HE2	4:A:701:68P:N04	2.14	0.46
1:A:154:ILE:HG23	1:A:516:TYR:HB2	1.98	0.45
1:A:156:PRO:HG2	1:A:611:SER:HA	1.99	0.45
1:A:518:ILE:HD11	1:A:541:TRP:CE3	2.51	0.45
3:C:55:TRP:CD2	3:C:93:PHE:HB2	2.51	0.45
1:A:456:HIS:HA	1:A:458:TRP:O	2.17	0.45
2:B:174:SER:HB3	2:B:225:PRO:HG2	1.99	0.45
1:A:95:TYR:HB2	1:A:441:ALA:CB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:177:VAL:HG22	2:B:222:VAL:HG22	1.98	0.44
3:C:55:TRP:HB2	3:C:68:ILE:HB	1.99	0.44
1:A:148:ILE:HG13	1:A:449:ALA:HB1	2.00	0.44
1:A:186:TYR:HB3	1:A:428:PHE:CD2	2.53	0.44
1:A:503:THR:O	1:A:507:ILE:HG12	2.17	0.44
1:A:219:THR:OG1	5:A:706:NAG:H61	2.18	0.44
1:A:526:LYS:HD3	1:A:532:SER:HB2	1.99	0.44
1:A:577:LEU:HD13	6:A:703:CLR:H151	2.00	0.44
1:A:453:GLU:HG3	1:A:454:PHE:CD1	2.53	0.43
2:B:174:SER:O	2:B:225:PRO:HD2	2.17	0.43
1:A:103:TRP:C	1:A:106:PRO:HD2	2.43	0.43
1:A:242:SER:HB2	1:A:248:LEU:HA	2.00	0.43
1:A:506:LEU:HD23	1:A:549:LEU:HB2	2.00	0.43
1:A:308:GLY:HA2	1:A:394:VAL:HG21	2.01	0.43
6:A:703:CLR:H162	6:A:703:CLR:H231	2.00	0.43
1:A:142:TYR:HD2	1:A:143:HIS:CE1	2.36	0.43
1:A:312:TYR:CZ	1:A:376:GLY:HA3	2.53	0.42
1:A:495:TYR:HB3	1:A:578:GLY:HA3	2.01	0.42
1:A:451:LEU:CD2	1:A:458:TRP:HB3	2.49	0.42
1:A:147:CYS:SG	1:A:342:GLY:HA3	2.60	0.42
1:A:151:TRP:CZ2	1:A:508:GLU:HG2	2.53	0.42
1:A:499:PRO:O	1:A:503:THR:OG1	2.31	0.42
2:B:217:THR:HG23	2:B:234:LYS:HE3	2.02	0.42
2:B:139:ALA:HB3	2:B:171:PHE:CE2	2.55	0.42
1:A:125:ALA:O	1:A:130:ILE:HG12	2.20	0.41
1:A:236:VAL:HG13	1:A:237:LEU:N	2.35	0.41
3:C:170:ILE:HG13	3:C:175:ARG:HB2	2.02	0.41
1:A:141:GLN:NE2	1:A:355:ASN:HB3	2.35	0.41
1:A:156:PRO:O	1:A:592:TYR:HE2	2.03	0.41
1:A:271:TRP:NE1	1:A:272:LYS:HG3	2.35	0.41
3:C:183:TRP:CD1	3:C:195:MET:HB3	2.56	0.41
1:A:125:ALA:HB2	1:A:333:ILE:HG12	2.03	0.41
1:A:139:LEU:HD11	1:A:512:VAL:HG11	2.01	0.41
1:A:211:ASN:HB3	1:A:227:PRO:HG3	2.02	0.41
3:C:139:PRO:HA	3:C:140:PRO:HD3	1.97	0.41
1:A:262:ILE:O	1:A:265:VAL:HG12	2.21	0.41
1:A:586:PHE:CZ	7:A:704:C14:H032	2.55	0.41
2:B:135:THR:HG21	2:B:172:PRO:HB3	2.01	0.41
1:A:518:ILE:HG21	1:A:542:VAL:HG22	2.03	0.41
1:A:95:TYR:HB2	1:A:441:ALA:HB3	2.03	0.41
1:A:95:TYR:CD1	1:A:343:VAL:HG11	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:LEU:HA	1:A:196:PRO:HD3	1.98	0.41
3:C:109:GLN:HB2	3:C:118:PHE:CD2	2.56	0.41
1:A:141:GLN:HB2	1:A:348:ALA:HB1	2.02	0.40
3:C:70:SER:O	3:C:72:SER:N	2.51	0.40
3:C:212:TYR:HB2	3:C:229:PHE:CE1	2.55	0.40
1:A:161:ILE:HD11	1:A:507:ILE:CG2	2.51	0.40
1:A:298:ARG:O	1:A:302:LEU:HG	2.22	0.40
3:C:168:TRP:NE1	3:C:197:SER:OG	2.34	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	538/549 (98%)	520 (97%)	18 (3%)	0	100	100
2	B	216/221 (98%)	204 (94%)	12 (6%)	0	100	100
3	C	212/214 (99%)	199 (94%)	13 (6%)	0	100	100
All	All	966/984 (98%)	923 (96%)	43 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	427/462 (92%)	424 (99%)	3 (1%)	76	78
2	B	190/193 (98%)	190 (100%)	0	100	100
3	C	189/190 (100%)	188 (100%)	1 (0%)	81	80
All	All	806/845 (95%)	802 (100%)	4 (0%)	81	80

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	217	ASN
1	A	354	ASN
1	A	437	ASP
3	C	109	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	141	GLN
1	A	177	ASN
1	A	223	HIS
1	A	416	ASN
3	C	28	HIS
3	C	158	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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
5	NAG	A	706	1	14,14,15	0.24	0	17,19,21	0.40	0
5	NAG	A	702	1	14,14,15	0.29	0	17,19,21	0.44	0
4	68P	A	701	-	26,26,26	6.03	15 (57%)	29,37,37	1.33	4 (13%)
8	69D	A	705	-	19,20,26	6.63	11 (57%)	25,28,37	5.03	10 (40%)
7	C14	A	704	-	13,13,13	0.31	0	12,12,12	0.82	0
6	CLR	A	703	-	31,31,31	0.86	1 (3%)	48,48,48	1.36	6 (12%)

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
5	NAG	A	706	1	-	1/6/23/26	0/1/1/1
5	NAG	A	702	1	-	1/6/23/26	0/1/1/1
4	68P	A	701	-	-	2/15/27/27	0/3/3/3
8	69D	A	705	-	-	0/6/15/27	0/3/3/3
7	C14	A	704	-	-	4/11/11/11	-
6	CLR	A	703	-	-	6/10/68/68	0/4/4/4

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	705	69D	O02-C11	14.78	1.69	1.43
8	A	705	69D	C17-C13	-12.61	1.18	1.38
8	A	705	69D	C14-C08	12.34	1.58	1.39
8	A	705	69D	C17-C18	-12.07	1.14	1.39
4	A	701	68P	C13-C07	11.79	1.55	1.39
4	A	701	68P	C14-C08	10.21	1.55	1.39
4	A	701	68P	C16-C20	9.61	1.54	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	701	68P	C19-C15	9.52	1.54	1.38
4	A	701	68P	C15-C10	8.68	1.53	1.39
4	A	701	68P	C17-C13	8.54	1.52	1.38
4	A	701	68P	C20-C21	8.42	1.53	1.37
4	A	701	68P	C14-C18	7.81	1.53	1.39
4	A	701	68P	C16-C10	7.81	1.52	1.39
4	A	701	68P	C19-C21	7.71	1.52	1.37
8	A	705	69D	C07-C05	-7.50	1.32	1.52
4	A	701	68P	C08-C07	6.87	1.47	1.39
8	A	705	69D	C11-C08	6.62	1.59	1.50
4	A	701	68P	C17-C18	5.29	1.50	1.39
4	A	701	68P	C18-C24	4.24	1.53	1.44
8	A	705	69D	C18-C24	3.94	1.52	1.44
8	A	705	69D	C10-C05	3.92	1.57	1.52
8	A	705	69D	C14-C18	-3.43	1.33	1.39
4	A	701	68P	O02-C11	3.23	1.49	1.44
8	A	705	69D	C13-C07	-2.77	1.36	1.39
8	A	705	69D	C08-C07	-2.35	1.35	1.39
4	A	701	68P	C05-C10	-2.15	1.50	1.53
6	A	703	CLR	C13-C14	-2.05	1.51	1.55

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	705	69D	C11-C08-C07	-16.52	100.11	108.85
8	A	705	69D	C13-C07-C08	-9.69	109.55	120.80
8	A	705	69D	C08-C07-C05	8.04	127.86	106.39
8	A	705	69D	C11-C08-C14	7.55	142.87	129.35
8	A	705	69D	C13-C17-C18	7.53	129.95	120.35
8	A	705	69D	C17-C13-C07	5.28	129.85	121.12
8	A	705	69D	C14-C08-C07	-3.87	117.01	120.80
4	A	701	68P	C11-C08-C07	-3.65	106.92	108.83
8	A	705	69D	C18-C14-C08	-3.55	116.34	120.77
6	A	703	CLR	C8-C7-C6	-3.20	108.33	112.76
6	A	703	CLR	C9-C10-C5	3.12	114.22	109.65
8	A	705	69D	C13-C07-C05	-3.07	122.57	128.97
8	A	705	69D	O02-C11-C08	-3.02	101.79	104.70
6	A	703	CLR	C13-C14-C8	-2.77	110.48	114.41
4	A	701	68P	O02-C11-C08	2.66	107.97	105.01
6	A	703	CLR	C4-C5-C10	2.47	119.59	116.42
4	A	701	68P	C11-C08-C14	2.23	133.35	129.35
4	A	701	68P	C19-C21-C20	-2.09	120.06	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	703	CLR	C16-C17-C20	-2.02	109.11	112.18
6	A	703	CLR	C13-C17-C20	-2.02	116.37	119.50

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	703	CLR	C17-C20-C22-C23
4	A	701	68P	C09-C12-N03-C23
6	A	703	CLR	C21-C20-C22-C23
7	A	704	C14	C09-C10-C11-C12
7	A	704	C14	C03-C04-C05-C06
5	A	706	NAG	O5-C5-C6-O6
7	A	704	C14	C05-C06-C07-C08
4	A	701	68P	C05-C06-C09-C12
7	A	704	C14	C07-C08-C09-C10
6	A	703	CLR	C20-C22-C23-C24
5	A	702	NAG	O5-C5-C6-O6
6	A	703	CLR	C23-C24-C25-C26
6	A	703	CLR	C23-C24-C25-C27
6	A	703	CLR	C22-C23-C24-C25

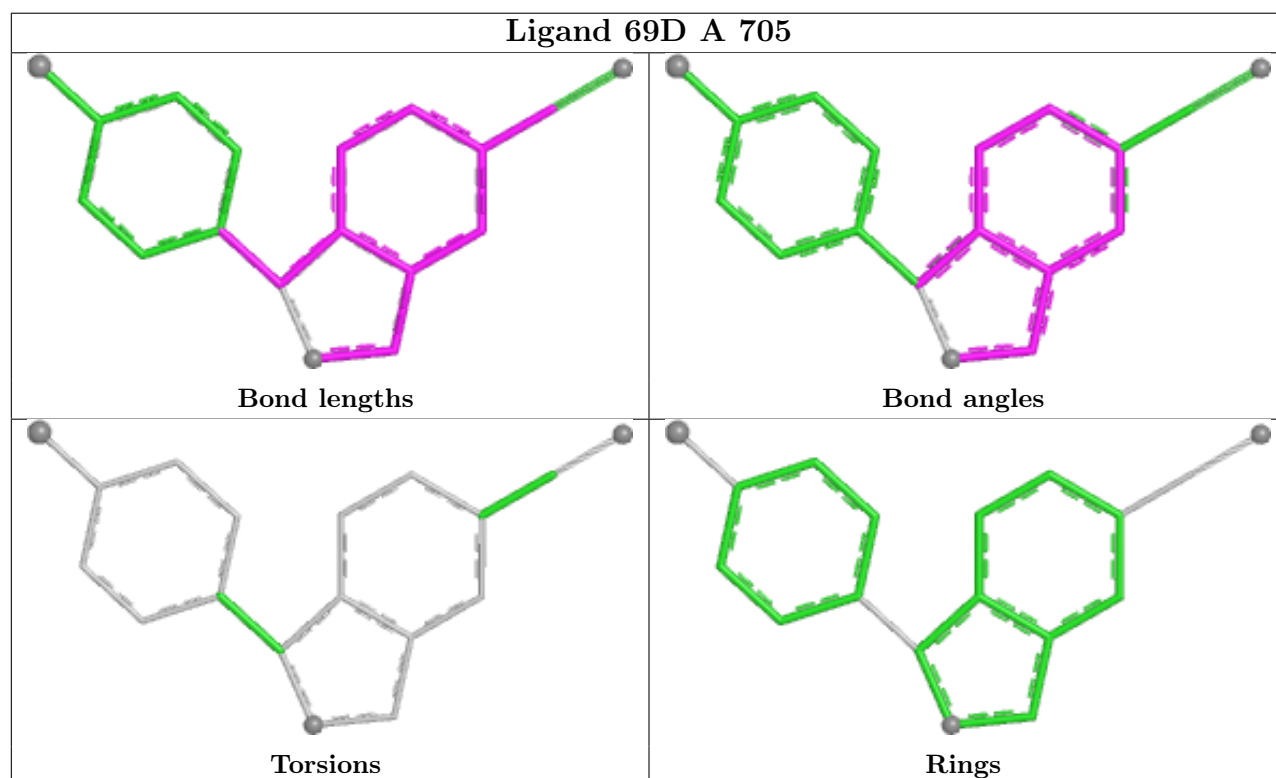
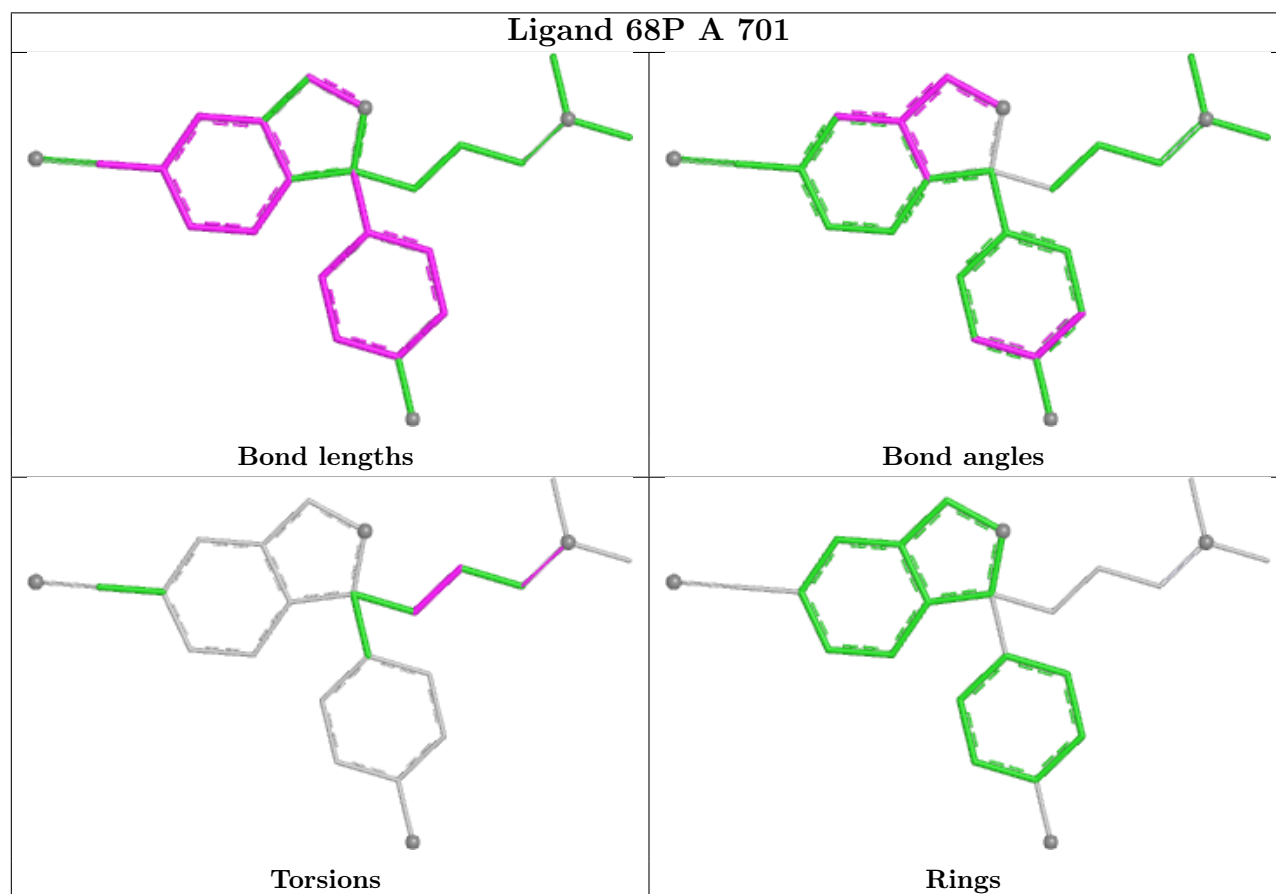
There are no ring outliers.

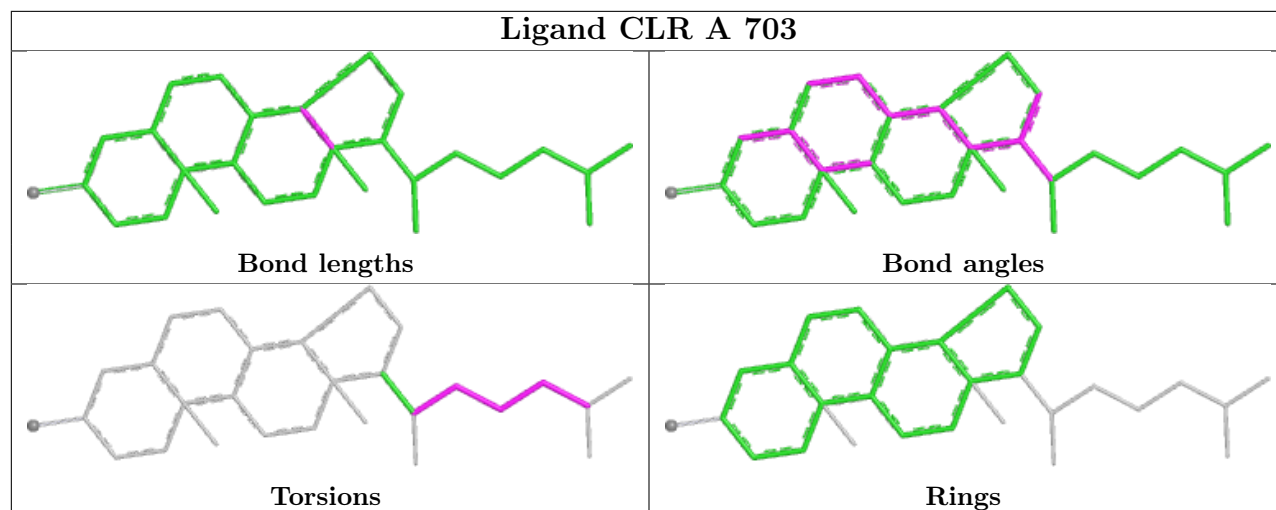
5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	706	NAG	1	0
4	A	701	68P	1	0
8	A	705	69D	1	0
7	A	704	C14	1	0
6	A	703	CLR	5	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	540/549 (98%)	0.01	41 (7%)	20 13	85, 146, 212, 284	0
2	B	218/221 (98%)	0.43	26 (11%)	9 6	78, 176, 313, 473	0
3	C	214/214 (100%)	0.16	15 (7%)	22 14	105, 201, 403, 703	0
All	All	972/984 (98%)	0.14	82 (8%)	17 11	78, 158, 323, 703	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	190	THR	8.1
2	B	81	GLN	6.9
1	A	479	VAL	6.1
3	C	200	THR	5.6
2	B	85	GLY	5.2
1	A	403	PRO	5.2
1	A	468	ALA	5.1
3	C	78	VAL	5.0
2	B	88	THR	4.8
1	A	469	VAL	4.7
1	A	476	GLY	4.6
2	B	103	ARG	4.6
1	A	401	ALA	4.5
1	A	565	LEU	4.5
2	B	84	LYS	4.5
2	B	83	PHE	4.4
3	C	153	VAL	4.4
1	A	475	PHE	4.3
2	B	87	ALA	4.3
2	B	196	GLN	4.3
3	C	79	PRO	4.2
1	A	472	THR	4.2
1	A	317	TRP	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	170	PHE	4.1
1	A	490	LYS	4.0
1	A	467	LEU	4.0
2	B	80	ASN	3.9
1	A	473	CYS	3.8
3	C	202	THR	3.8
3	C	151	SER	3.7
2	B	104	SER	3.6
1	A	422	PHE	3.6
1	A	488	VAL	3.6
1	A	566	PHE	3.5
3	C	198	THR	3.3
3	C	27	SER	3.2
1	A	321	LEU	3.2
1	A	179	ILE	3.2
3	C	77	GLY	3.2
2	B	149	LEU	3.1
2	B	166	LEU	3.1
1	A	487	TYR	3.1
1	A	478	LEU	3.1
1	A	290	ILE	3.0
2	B	204	SER	3.0
1	A	243	LYS	3.0
1	A	400	ASP	3.0
2	B	177	VAL	3.0
3	C	82	PHE	2.9
2	B	79	TYR	2.8
1	A	320	LEU	2.8
2	B	68	GLY	2.8
2	B	101	GLU	2.7
2	B	150	ALA	2.7
1	A	471	ILE	2.6
1	A	598	ILE	2.6
1	A	568	TYR	2.6
1	A	389	MET	2.6
1	A	404	SER	2.6
2	B	102	LEU	2.5
1	A	147	CYS	2.5
2	B	86	LYS	2.5
1	A	492	LEU	2.5
1	A	501	VAL	2.4
2	B	94	SER	2.4

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Mol	Chain	Res	Type	RSRZ
3	C	45	ALA	2.3
1	A	103	TRP	2.3
1	A	340	GLY	2.3
2	B	185	SER	2.3
1	A	470	VAL	2.3
2	B	121	ARG	2.3
3	C	207	GLU	2.3
1	A	91	SER	2.3
3	C	65	LYS	2.3
1	A	518	ILE	2.2
2	B	67	ILE	2.2
1	A	318	GLN	2.2
3	C	191	SER	2.2
1	A	464	ARG	2.2
2	B	168	LYS	2.1
3	C	201	LEU	2.1
1	A	366	VAL	2.1

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.

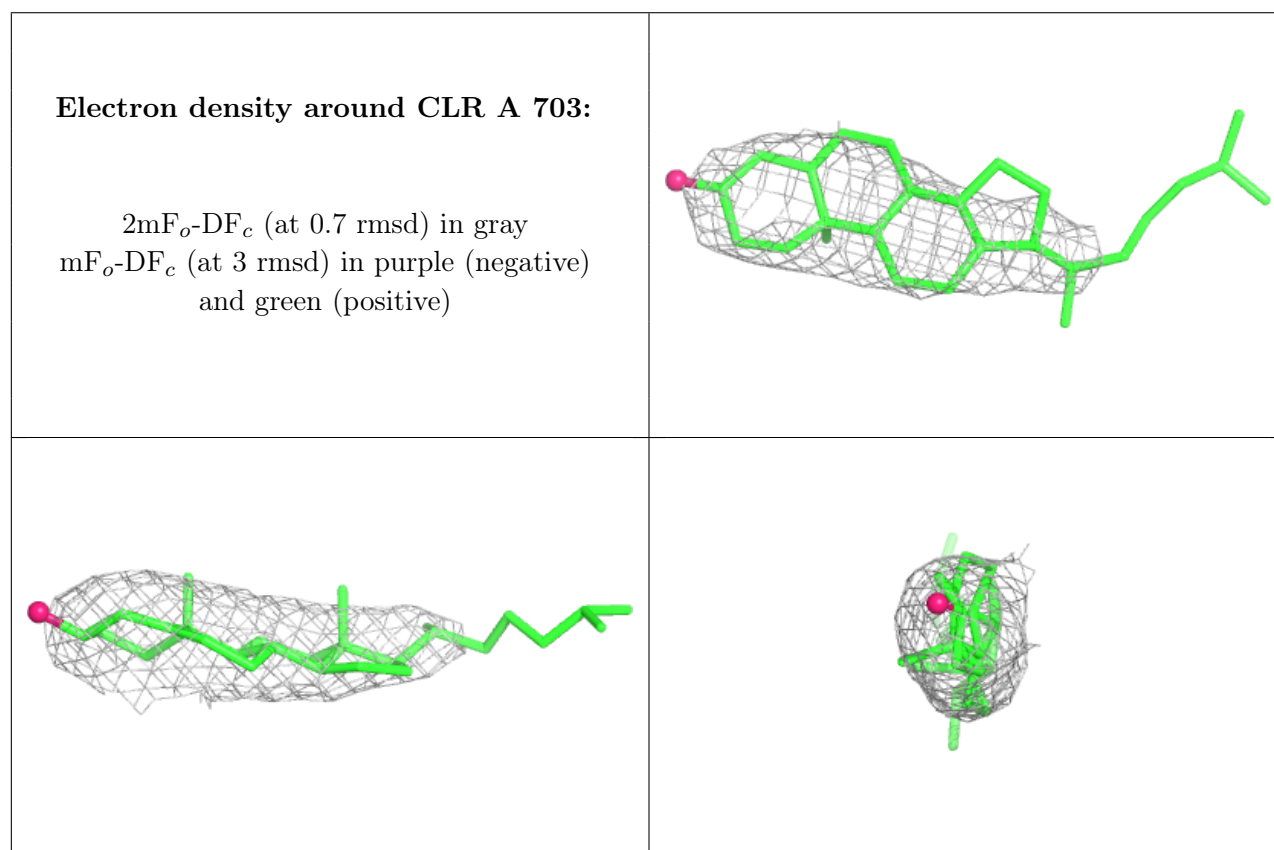
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	A	706	14/15	0.64	0.11	221,236,244,249	0
7	C14	A	704	14/14	0.86	0.20	69,72,77,79	14
5	NAG	A	702	14/15	0.89	0.09	82,101,167,180	0
6	CLR	A	703	28/28	0.90	0.16	154,168,182,200	0
8	69D	A	705	18/24	0.90	0.11	147,164,195,198	0
4	68P	A	701	24/24	0.92	0.10	108,135,151,171	0

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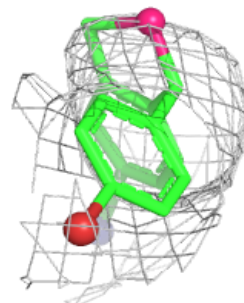
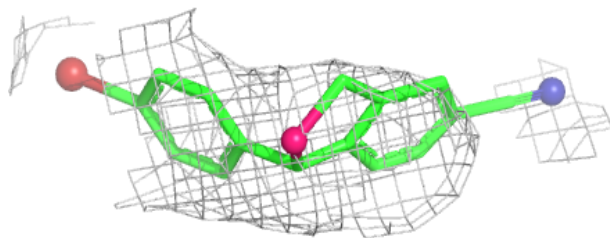
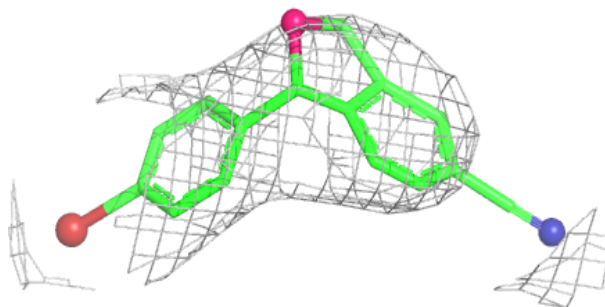
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	NA	A	707	1/1	0.98	0.03	98,98,98,98	0

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.



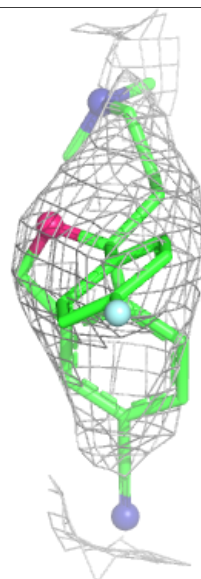
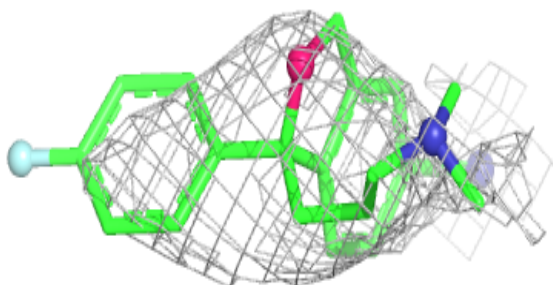
Electron density around 69D A 705:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 68P A 701:

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 ⓘ

There are no such residues in this entry.