



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:37 AM UTC

PDB ID : 5I73 / pdb_00005i73
Title : X-ray structure of the ts3 human serotonin transporter complexed with s-citalopram at the central and allosteric sites
Authors : Coleman, J.A.; Green, E.M.; Gouaux, E.
Deposited on : 2016-02-16
Resolution : 3.24 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

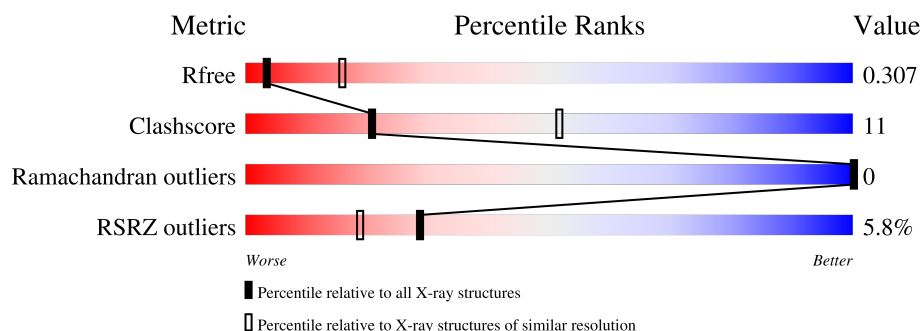
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.24 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	2153 (3.28-3.20)
Clashscore	190562	2275 (3.28-3.20)
Ramachandran outliers	187476	2233 (3.28-3.20)
RSRZ outliers	180081	2153 (3.28-3.20)

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	
2	B	221	
3	C	214	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 7633 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
			4198	2804	650	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

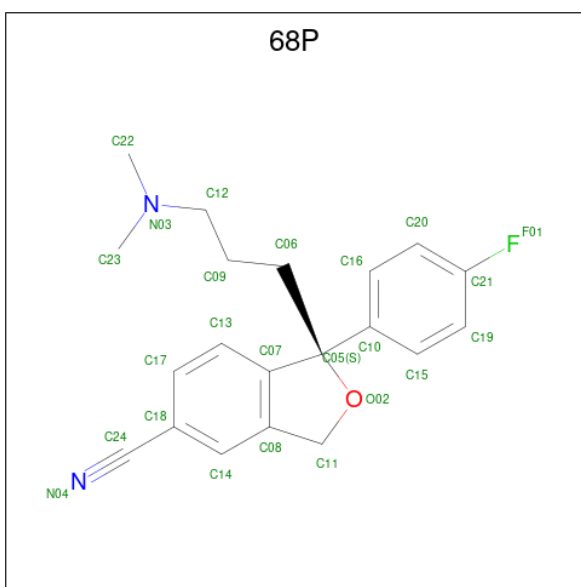
- Molecule 2 is a protein called 8B6 antibody, heavy chain.

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.

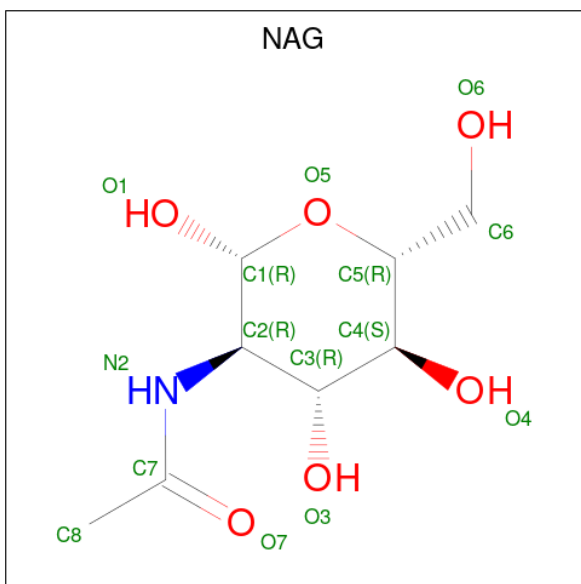
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	214	Total	C	N	O	S	0	0	0
			1662	1037	280	337	8			

- 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	0
			24	20	1	2	1		
4	A	1	Total	C	F	N	O	0	0
			24	20	1	2	1		

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



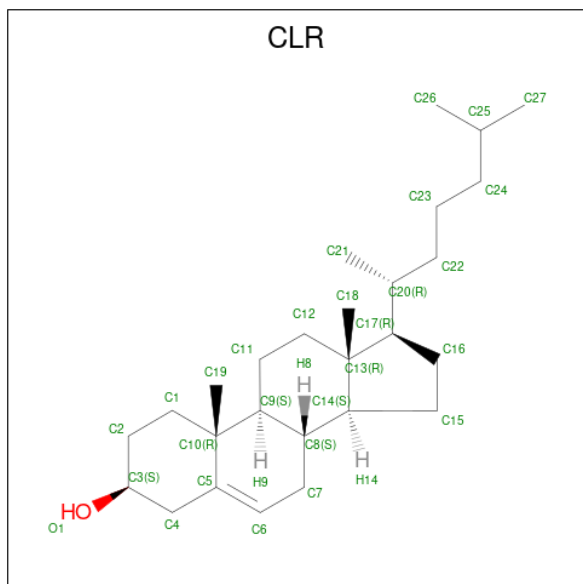
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

Continued on next page...

Continued from previous page...

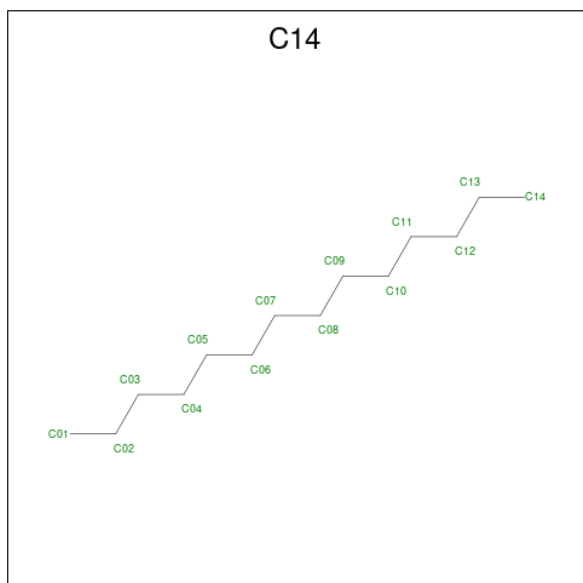
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

- 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	0
			28	27	1		

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

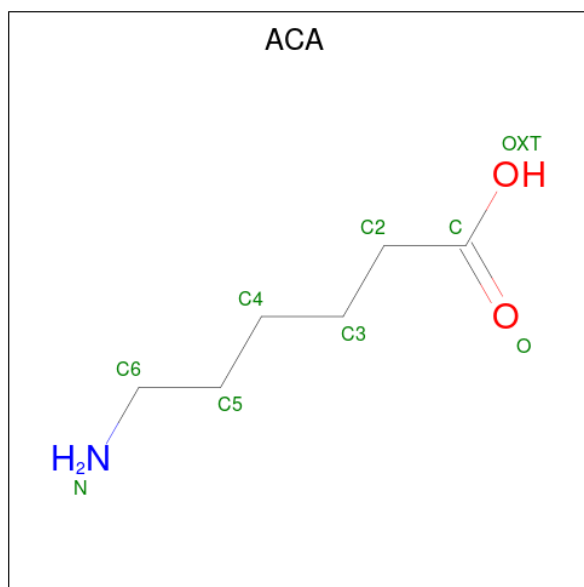


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	C	0	0
			14	14		

- Molecule 8 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	2	Total	Na	0	0
			2	2		

- Molecule 9 is 6-AMINOHEXANOIC ACID (CCD ID: ACA) (formula: C₆H₁₃NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			9	6	1	2		

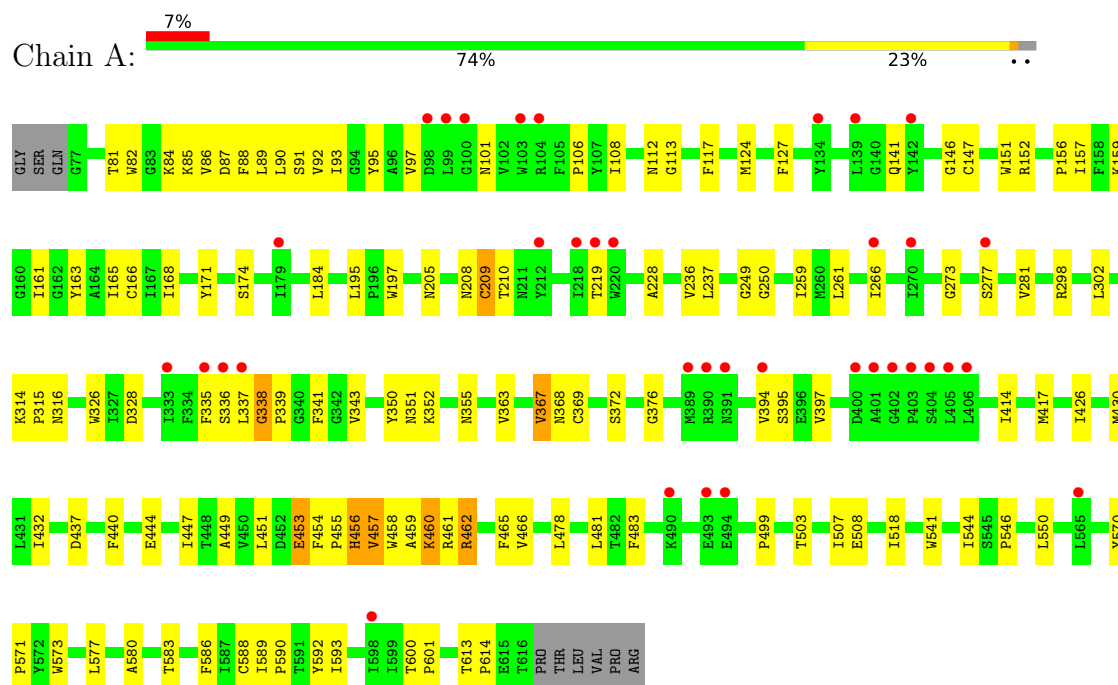
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1	Total	O	0	0
			1	1		

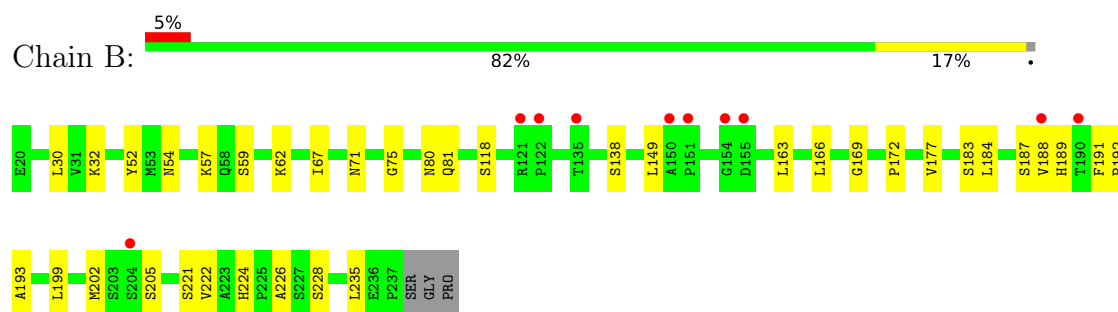
3 Residue-property plots

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.

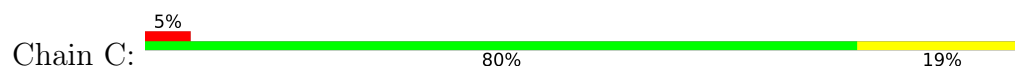
• Molecule 1: Sodium-dependent serotonin transporter

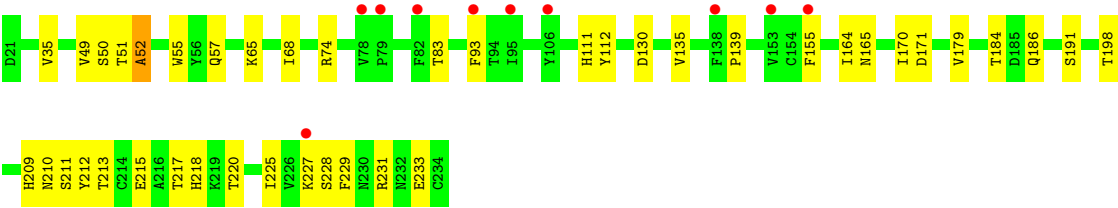


• Molecule 2: 8B6 antibody, heavy chain



• 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	129.85Å 163.21Å 140.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.18 – 3.24 50.18 – 3.24	Depositor EDS
% Data completeness (in resolution range)	98.3 (50.18-3.24) 98.4 (50.18-3.24)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 3.26Å)	Xtriage
Refinement program	PHENIX (DEV_2000: ???)	Depositor
R, R_{free}	0.233 , 0.275 0.262 , 0.307	Depositor DCC
R_{free} test set	1191 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	125.9	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 173.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7633	wwPDB-VP
Average B, all atoms (Å ²)	175.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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: ACA, CLR, NA, 68P, NAG, C14

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	0.40	2/4331 (0.0%)	0.79	12/5922 (0.2%)
2	B	0.28	0/1688	0.73	1/2309 (0.0%)
3	C	0.31	0/1700	0.72	4/2307 (0.2%)
All	All	0.36	2/7719 (0.0%)	0.76	17/10538 (0.2%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	209	CYS	C-N	-7.57	1.24	1.33
1	A	462	ARG	C-N	5.66	1.41	1.33

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	170	ILE	N-CA-C	7.76	117.82	110.53
2	B	187	SER	N-CA-C	7.47	121.98	111.30
1	A	338	GLY	CA-C-N	6.87	126.81	120.21
1	A	338	GLY	C-N-CA	6.87	126.81	120.21
1	A	249	GLY	N-CA-C	-6.85	103.31	112.14
3	C	52	ALA	N-CA-C	5.91	118.40	108.23
1	A	457	VAL	N-CA-C	-5.77	104.89	110.72
3	C	210	ASN	N-CA-C	5.76	120.02	112.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	460	LYS	N-CA-C	-5.42	105.27	111.07
1	A	369	CYS	N-CA-C	5.41	116.98	111.14
3	C	35	VAL	N-CA-C	-5.39	101.87	109.63
1	A	97	VAL	O-C-N	5.36	128.76	122.81
1	A	367	VAL	N-CA-C	5.27	115.48	110.53
1	A	453	GLU	CA-C-N	-5.12	116.74	123.34
1	A	453	GLU	C-N-CA	-5.12	116.74	123.34
1	A	395	SER	N-CA-C	-5.09	105.73	111.28
1	A	455	PRO	CB-CA-C	-5.02	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	4198	0	4094	117	0
2	B	1643	0	1589	22	0
3	C	1662	0	1585	27	0
4	A	48	0	0	1	0
5	A	28	0	26	1	0
6	A	28	0	46	5	0
7	A	14	0	30	2	0
8	A	2	0	0	0	0
9	A	9	0	6	0	0
10	A	1	0	0	0	0
All	All	7633	0	7376	166	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 (166) 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)
2:B:188:VAL:HG23	2:B:205:SER:O	1.50	1.12
1:A:86:VAL:CG1	1:A:90:LEU:HD13	1.92	0.98
1:A:277:SER:O	1:A:281:VAL:HG23	1.64	0.98
1:A:338:GLY:N	1:A:339:PRO:HD2	1.78	0.95
1:A:589:ILE:CG2	1:A:590:PRO:HD3	1.98	0.93
1:A:589:ILE:HG23	1:A:590:PRO:HD3	1.52	0.92
1:A:86:VAL:HG12	1:A:90:LEU:HD13	1.53	0.89
1:A:86:VAL:HG13	1:A:90:LEU:CD1	2.02	0.89
1:A:458:TRP:O	1:A:459:ALA:HB3	1.72	0.88
1:A:338:GLY:N	1:A:339:PRO:CD	2.39	0.86
1:A:161:ILE:HG13	1:A:589:ILE:HD12	1.57	0.85
1:A:454:PHE:HB3	1:A:457:VAL:HG11	1.59	0.85
1:A:444:GLU:OE1	1:A:462:ARG:NH2	2.10	0.84
1:A:277:SER:O	1:A:281:VAL:CG2	2.25	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	1.45	0.80
1:A:86:VAL:HG13	1:A:90:LEU:HD13	1.62	0.79
1:A:86:VAL:CG1	1:A:90:LEU:CD1	2.61	0.77
1:A:583:THR:HG21	7:A:704:C14:H081	1.68	0.76
1:A:205:ASN:ND2	1:A:209:CYS:SG	2.59	0.75
1:A:454:PHE:O	1:A:457:VAL:CG1	2.36	0.73
1:A:88:PHE:HE2	1:A:350:TYR:HB2	1.53	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	0.72
3:C:52:ALA:HB1	3:C:111:HIS:CE1	2.23	0.72
1:A:113:GLY:HA2	1:A:316:ASN:HB3	1.71	0.71
1:A:141:GLN:NE2	1:A:351:ASN:OD1	2.24	0.71
1:A:337:LEU:C	1:A:339:PRO:HD3	2.16	0.70
1:A:394:VAL:O	1:A:397:VAL:HG12	1.92	0.70
1:A:157:ILE:HB	1:A:593:ILE:HG12	1.71	0.70
1:A:337:LEU:C	1:A:339:PRO:CD	2.65	0.70
1:A:208:ASN:O	1:A:210:THR:HG23	1.91	0.69
1:A:91:SER:HA	1:A:281:VAL:HG11	1.73	0.69
1:A:589:ILE:HG23	1:A:590:PRO:CD	2.22	0.69
1:A:108:ILE:HD11	1:A:328:ASP:HB3	1.74	0.69
1:A:454:PHE:C	1:A:457:VAL:HG12	2.18	0.68
1:A:447:ILE:HD13	1:A:466:VAL:HG22	1.76	0.68
2:B:188:VAL:CG2	2:B:205:SER:O	2.37	0.67
1:A:88:PHE:CE2	1:A:350:TYR:HB2	2.28	0.67
1:A:152:ARG:HH21	1:A:159:LYS:HZ1	1.43	0.66
2:B:30:LEU:HD22	2:B:172:PRO:HD3	1.76	0.66
1:A:454:PHE:C	1:A:457:VAL:CG1	2.70	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:589:ILE:HG22	1:A:590:PRO:HD3	1.77	0.65
2:B:54:ASN:ND2	2:B:118:SER:OG	2.29	0.65
3:C:50:SER:OG	3:C:51:THR:N	2.27	0.65
3:C:211:SER:HA	3:C:229:PHE:O	1.97	0.65
1:A:414:ILE:HA	1:A:417:MET:HE2	1.78	0.64
3:C:52:ALA:CB	3:C:111:HIS:CE1	2.82	0.62
2:B:192:PRO:HD3	3:C:184:THR:HG22	1.81	0.62
1:A:437:ASP:N	1:A:437:ASP:OD1	2.32	0.62
1:A:161:ILE:CG1	1:A:589:ILE:HD12	2.29	0.62
1:A:147:CYS:H	1:A:449:ALA:CB	2.12	0.61
2:B:177:VAL:HA	2:B:221:SER:O	2.01	0.61
3:C:49:VAL:HG22	3:C:112:TYR:CE1	2.35	0.61
1:A:112:ASN:O	1:A:117:PHE:HB2	2.01	0.60
3:C:171:ASP:OD2	3:C:209:HIS:ND1	2.33	0.60
1:A:146:GLY:HA3	1:A:449:ALA:HA	1.82	0.59
1:A:588:CYS:O	1:A:592:TYR:HB2	2.02	0.59
1:A:273:GLY:HA2	1:A:462:ARG:CZ	2.31	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:101:ASN:ND2	1:A:372:SER:OG	2.34	0.59
1:A:458:TRP:CZ3	1:A:465:PHE:HB2	2.39	0.58
3:C:74:ARG:HH21	3:C:83:THR:HG22	1.67	0.58
1:A:586:PHE:O	1:A:589:ILE:HG22	2.02	0.58
1:A:86:VAL:HG13	1:A:90:LEU:HD11	1.85	0.57
2:B:224:HIS:O	2:B:228:SER:N	2.37	0.57
1:A:87:ASP:O	1:A:91:SER:HB2	2.03	0.56
1:A:236:VAL:HG13	1:A:237:LEU:N	2.20	0.55
1:A:85:LYS:HE2	1:A:355:ASN:HD21	1.71	0.55
1:A:456:HIS:N	1:A:458:TRP:O	2.35	0.55
3:C:49:VAL:HG13	3:C:112:TYR:CD1	2.41	0.55
1:A:454:PHE:CB	1:A:457:VAL:HG11	2.34	0.55
1:A:577:LEU:HD13	6:A:703:CLR:H151	1.89	0.55
1:A:352:LYS:HB2	1:A:355:ASN:HB2	1.90	0.53
1:A:440:PHE:O	1:A:444:GLU:HB2	2.08	0.53
2:B:32:LYS:HG2	2:B:138:SER:HA	1.90	0.52
1:A:573:TRP:CE3	6:A:703:CLR:H71	2.43	0.52
1:A:454:PHE:HB3	1:A:457:VAL:HG13	1.88	0.52
1:A:86:VAL:HA	1:A:89:LEU:HB3	1.92	0.52
2:B:71:ASN:O	2:B:75:GLY:N	2.43	0.52
1:A:197:TRP:HB2	1:A:228:ALA:HA	1.91	0.51
1:A:336:SER:OG	1:A:368:ASN:ND2	2.38	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:583:THR:CG2	7:A:704:C14:H081	2.38	0.51
1:A:184:LEU:HD21	1:A:261:LEU:HD23	1.92	0.51
3:C:49:VAL:HG12	3:C:49:VAL:O	2.11	0.51
1:A:161:ILE:HG13	1:A:589:ILE:CD1	2.34	0.51
1:A:460:LYS:HG3	1:A:461:ARG:N	2.25	0.50
1:A:478:LEU:HD23	1:A:481:LEU:HD12	1.94	0.50
2:B:59:SER:HB2	2:B:62:LYS:HB2	1.94	0.49
2:B:177:VAL:HG22	2:B:222:VAL:HG22	1.92	0.49
1:A:151:TRP:HZ2	1:A:508:GLU:HG2	1.77	0.49
3:C:55:TRP:HB2	3:C:68:ILE:HB	1.95	0.49
1:A:456:HIS:N	1:A:458:TRP:H	2.11	0.48
3:C:165:ASN:HB3	3:C:217:THR:HB	1.94	0.48
3:C:49:VAL:HG11	3:C:52:ALA:O	2.13	0.48
3:C:130:ASP:HB3	3:C:220:THR:HG22	1.96	0.48
1:A:457:VAL:HG13	1:A:458:TRP:N	2.28	0.48
1:A:163:TYR:O	1:A:166:CYS:HB2	2.14	0.48
1:A:580:ALA:HB1	6:A:703:CLR:H241	1.96	0.48
1:A:363:VAL:O	1:A:367:VAL:HG23	2.14	0.47
1:A:106:PRO:HG3	1:A:376:GLY:HA2	1.97	0.47
1:A:573:TRP:CZ3	6:A:703:CLR:H71	2.50	0.47
1:A:341:PHE:HD2	1:A:343:VAL:HG23	1.80	0.47
2:B:193:ALA:HA	2:B:202:MET:HB3	1.97	0.46
1:A:236:VAL:HG13	1:A:237:LEU:H	1.80	0.46
1:A:451:LEU:HD23	1:A:458:TRP:HB3	1.96	0.46
2:B:163:LEU:HB3	2:B:235:LEU:HD22	1.98	0.46
1:A:85:LYS:NZ	1:A:355:ASN:OD1	2.47	0.46
1:A:259:ILE:HG21	1:A:481:LEU:HD11	1.98	0.46
1:A:165:ILE:O	1:A:168:ILE:HB	2.16	0.46
3:C:164:ILE:HB	3:C:218:HIS:HD2	1.79	0.46
1:A:250:GLY:H	1:A:483:PHE:HE2	1.62	0.46
1:A:613:THR:HA	1:A:614:PRO:HD2	1.73	0.46
1:A:266:ILE:HA	1:A:440:PHE:HE1	1.80	0.45
3:C:186:GLN:HE21	3:C:191:SER:HB3	1.82	0.45
2:B:149:LEU:HD11	2:B:166:LEU:HB2	1.98	0.45
1:A:456:HIS:HA	1:A:458:TRP:O	2.17	0.45
1:A:156:PRO:O	1:A:159:LYS:HB2	2.16	0.45
2:B:57:LYS:HB2	2:B:67:ILE:HD11	1.98	0.45
2:B:224:HIS:CE1	2:B:226:ALA:HB3	2.51	0.44
1:A:81:THR:OG1	1:A:82:TRP:N	2.48	0.44
3:C:231:ARG:O	3:C:233:GLU:N	2.49	0.44
1:A:219:THR:OG1	5:A:706:NAG:H61	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:THR:O	1:A:507:ILE:HG12	2.17	0.44
1:A:195:LEU:HD12	1:A:195:LEU:H	1.83	0.43
1:A:453:GLU:HG3	1:A:454:PHE:CD1	2.53	0.43
1:A:447:ILE:HA	1:A:465:PHE:HE2	1.82	0.43
3:C:57:GLN:O	3:C:65:LYS:N	2.39	0.43
2:B:80:ASN:OD1	2:B:81:GLN:N	2.51	0.43
6:A:703:CLR:H162	6:A:703:CLR:H231	2.01	0.43
2:B:183:SER:HA	2:B:184:LEU:HA	1.51	0.43
3:C:215:GLU:HA	3:C:225:ILE:O	2.19	0.43
1:A:124:MET:HE2	1:A:326:TRP:HE3	1.82	0.43
1:A:171:TYR:O	1:A:174:SER:HB2	2.18	0.43
1:A:277:SER:O	1:A:281:VAL:HG21	2.12	0.42
1:A:451:LEU:CD2	1:A:458:TRP:HB3	2.49	0.42
2:B:52:TYR:HE1	2:B:71:ASN:HB2	1.84	0.42
3:C:55:TRP:CD2	3:C:93:PHE:HB2	2.54	0.42
3:C:212:TYR:HB2	3:C:229:PHE:CE1	2.54	0.42
1:A:394:VAL:O	1:A:397:VAL:CG1	2.63	0.41
1:A:600:THR:HA	1:A:601:PRO:HD3	1.89	0.41
1:A:426:ILE:O	1:A:430:MET:HB2	2.20	0.41
1:A:518:ILE:HD11	1:A:541:TRP:CE3	2.54	0.41
1:A:546:PRO:O	1:A:550:LEU:HB2	2.20	0.41
2:B:188:VAL:HG22	2:B:189:HIS:N	2.35	0.41
2:B:169:GLY:HA2	2:B:199:LEU:HB3	2.01	0.41
3:C:212:TYR:O	3:C:228:SER:HA	2.20	0.41
1:A:89:LEU:O	1:A:92:VAL:HG12	2.21	0.41
1:A:95:TYR:CD1	1:A:343:VAL:HG11	2.55	0.41
1:A:298:ARG:O	1:A:302:LEU:HG	2.20	0.41
1:A:335:PHE:HE2	4:A:701:68P:N04	2.18	0.41
1:A:437:ASP:HA	1:A:440:PHE:CD2	2.56	0.41
1:A:184:LEU:HA	1:A:432:ILE:HD11	2.01	0.41
1:A:570:TYR:HA	1:A:571:PRO:HD3	1.94	0.41
3:C:135:VAL:HA	3:C:155:PHE:O	2.21	0.41
3:C:179:VAL:HA	3:C:198:THR:O	2.21	0.41
3:C:139:PRO:HB3	3:C:229:PHE:CE2	2.56	0.41
1:A:84:LYS:O	1:A:85:LYS:C	2.63	0.40
2:B:191:PHE:HA	2:B:192:PRO:HD3	1.87	0.40
1:A:90:LEU:O	1:A:93:ILE:N	2.54	0.40
1:A:499:PRO:O	1:A:503:THR:OG1	2.29	0.40
3:C:50:SER:OG	3:C:51:THR:HG23	2.20	0.40
1:A:127:PHE:HB3	1:A:544:ILE:HG21	2.03	0.40
1:A:314:LYS:HA	1:A:315:PRO:HD3	1.88	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:213:THR:HA	3:C:227:LYS:O	2.22	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	456/549 (83%)	440 (96%)	16 (4%)	0	100	100
2	B	216/221 (98%)	207 (96%)	9 (4%)	0	100	100
3	C	212/214 (99%)	197 (93%)	15 (7%)	0	100	100
All	All	884/984 (90%)	844 (96%)	40 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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
4	68P	A	705	-	26,26,26	6.08	15 (57%)	29,37,37	1.26	5 (17%)
5	NAG	A	702	1	14,14,15	0.44	0	17,19,21	0.54	0
6	CLR	A	703	-	31,31,31	0.86	1 (3%)	48,48,48	1.36	6 (12%)
9	ACA	A	709	-	8,8,8	0.82	0	8,8,8	1.23	0
4	68P	A	701	-	26,26,26	6.07	15 (57%)	29,37,37	1.43	4 (13%)
7	C14	A	704	-	13,13,13	0.12	0	12,12,12	0.63	0
5	NAG	A	706	1	14,14,15	0.24	0	17,19,21	0.40	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
4	68P	A	705	-	-	7/15/27/27	0/3/3/3
5	NAG	A	702	1	-	2/6/23/26	0/1/1/1
6	CLR	A	703	-	-	6/10/68/68	0/4/4/4
9	ACA	A	709	-	-	4/6/6/6	-
4	68P	A	701	-	-	3/15/27/27	0/3/3/3
7	C14	A	704	-	-	7/11/11/11	-
5	NAG	A	706	1	-	1/6/23/26	0/1/1/1

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	705	68P	C13-C07	12.42	1.55	1.39
4	A	701	68P	C13-C07	11.67	1.54	1.39
4	A	701	68P	C14-C08	10.37	1.55	1.39
4	A	705	68P	C14-C08	10.14	1.55	1.39
4	A	701	68P	C19-C15	9.72	1.54	1.38
4	A	701	68P	C16-C20	9.67	1.54	1.38
4	A	705	68P	C19-C15	9.53	1.54	1.38
4	A	705	68P	C16-C20	9.46	1.54	1.38
4	A	701	68P	C15-C10	8.74	1.53	1.39
4	A	705	68P	C17-C13	8.69	1.52	1.38
4	A	705	68P	C15-C10	8.68	1.53	1.39
4	A	701	68P	C17-C13	8.55	1.52	1.38
4	A	701	68P	C20-C21	8.38	1.53	1.37
4	A	705	68P	C20-C21	8.21	1.53	1.37
4	A	701	68P	C16-C10	7.85	1.52	1.39
4	A	701	68P	C14-C18	7.83	1.53	1.39
4	A	705	68P	C16-C10	7.82	1.52	1.39
4	A	705	68P	C14-C18	7.79	1.53	1.39
4	A	705	68P	C19-C21	7.70	1.52	1.37
4	A	701	68P	C19-C21	7.68	1.52	1.37
4	A	701	68P	C08-C07	7.24	1.48	1.39
4	A	705	68P	C08-C07	7.24	1.48	1.39
4	A	705	68P	C17-C18	5.40	1.50	1.39
4	A	701	68P	C17-C18	5.18	1.50	1.39
4	A	705	68P	C18-C24	4.33	1.53	1.44
4	A	701	68P	C18-C24	4.22	1.53	1.44
4	A	701	68P	O02-C11	3.31	1.50	1.44
4	A	705	68P	O02-C11	3.01	1.49	1.44
4	A	705	68P	C11-C08	-2.11	1.47	1.50
6	A	703	CLR	C13-C14	-2.08	1.51	1.55
4	A	701	68P	C11-C08	-2.05	1.47	1.50

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	701	68P	C11-C08-C07	-3.95	106.76	108.83
6	A	703	CLR	C8-C7-C6	-3.20	108.33	112.76
6	A	703	CLR	C9-C10-C5	3.11	114.21	109.65
4	A	705	68P	O02-C11-C08	3.08	108.43	105.01
6	A	703	CLR	C13-C14-C8	-2.76	110.50	114.41
4	A	705	68P	C11-C08-C07	-2.75	107.39	108.83
4	A	701	68P	O02-C11-C08	2.68	107.99	105.01
4	A	701	68P	C19-C21-C20	-2.49	119.53	122.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	703	CLR	C4-C5-C10	2.42	119.52	116.42
4	A	701	68P	C11-C08-C14	2.40	133.64	129.35
4	A	705	68P	C13-C07-C05	2.38	133.68	130.29
4	A	705	68P	C19-C21-C20	-2.07	120.09	122.80
4	A	705	68P	C13-C07-C08	-2.03	118.86	120.76
6	A	703	CLR	C13-C17-C20	-2.03	116.36	119.50
6	A	703	CLR	C16-C17-C20	-2.02	109.12	112.18

There are no chirality outliers.

All (30) torsion outliers are listed below:

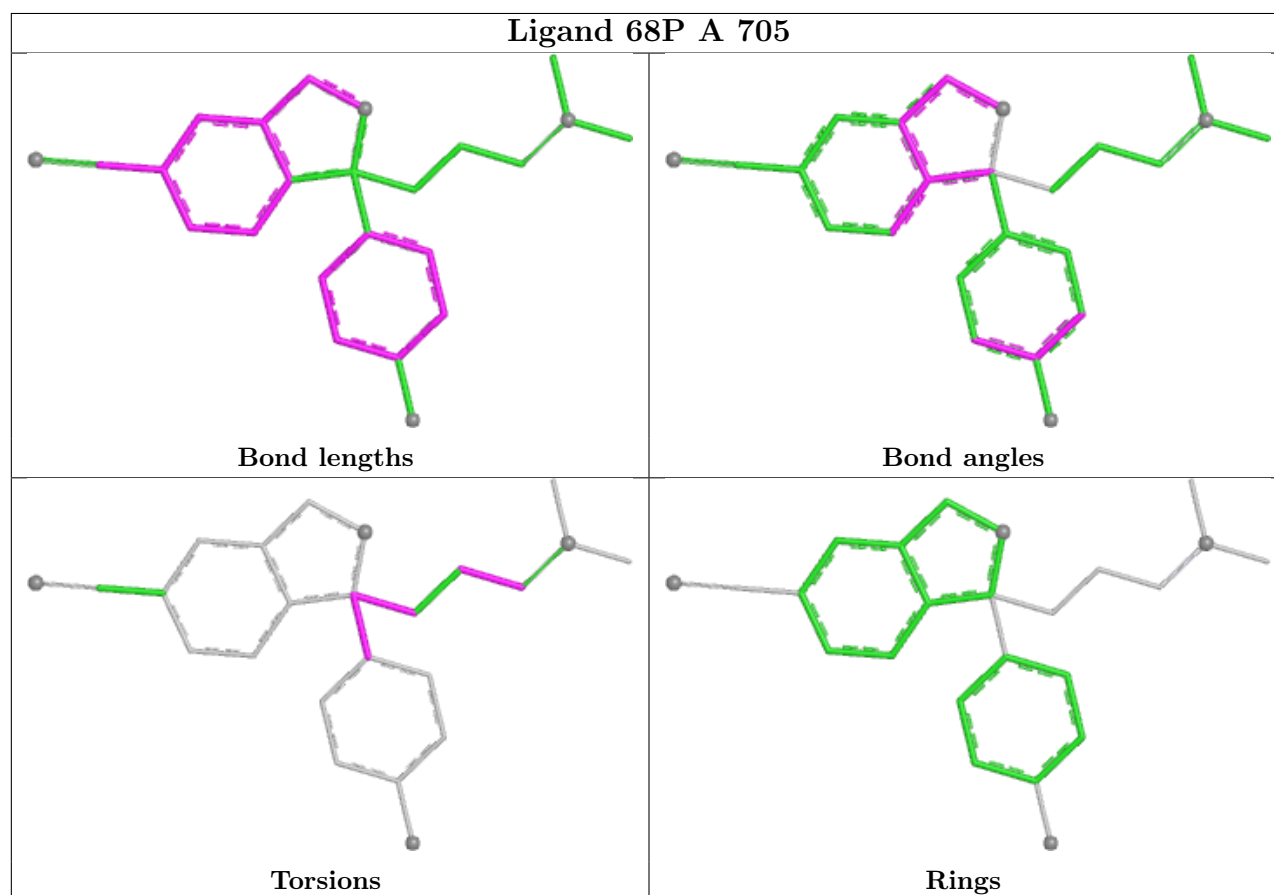
Mol	Chain	Res	Type	Atoms
4	A	705	68P	C10-C05-C06-C09
4	A	705	68P	O02-C05-C06-C09
4	A	705	68P	C07-C05-C06-C09
5	A	702	NAG	O5-C5-C6-O6
5	A	702	NAG	C4-C5-C6-O6
4	A	705	68P	C06-C09-C12-N03
6	A	703	CLR	C17-C20-C22-C23
6	A	703	CLR	C21-C20-C22-C23
9	A	709	ACA	C2-C3-C4-C5
7	A	704	C14	C03-C04-C05-C06
7	A	704	C14	C09-C10-C11-C12
9	A	709	ACA	C-C2-C3-C4
5	A	706	NAG	O5-C5-C6-O6
7	A	704	C14	C11-C12-C13-C14
7	A	704	C14	C01-C02-C03-C04
7	A	704	C14	C08-C09-C10-C11
7	A	704	C14	C04-C05-C06-C07
6	A	703	CLR	C20-C22-C23-C24
4	A	705	68P	C07-C05-C10-C15
6	A	703	CLR	C23-C24-C25-C26
7	A	704	C14	C06-C07-C08-C09
4	A	701	68P	C06-C05-C10-C15
4	A	701	68P	C09-C12-N03-C23
4	A	705	68P	C07-C05-C10-C16
4	A	701	68P	C06-C05-C10-C16
9	A	709	ACA	O-C-C2-C3
6	A	703	CLR	C23-C24-C25-C27
9	A	709	ACA	OXT-C-C2-C3
6	A	703	CLR	C22-C23-C24-C25
4	A	705	68P	C06-C05-C10-C15

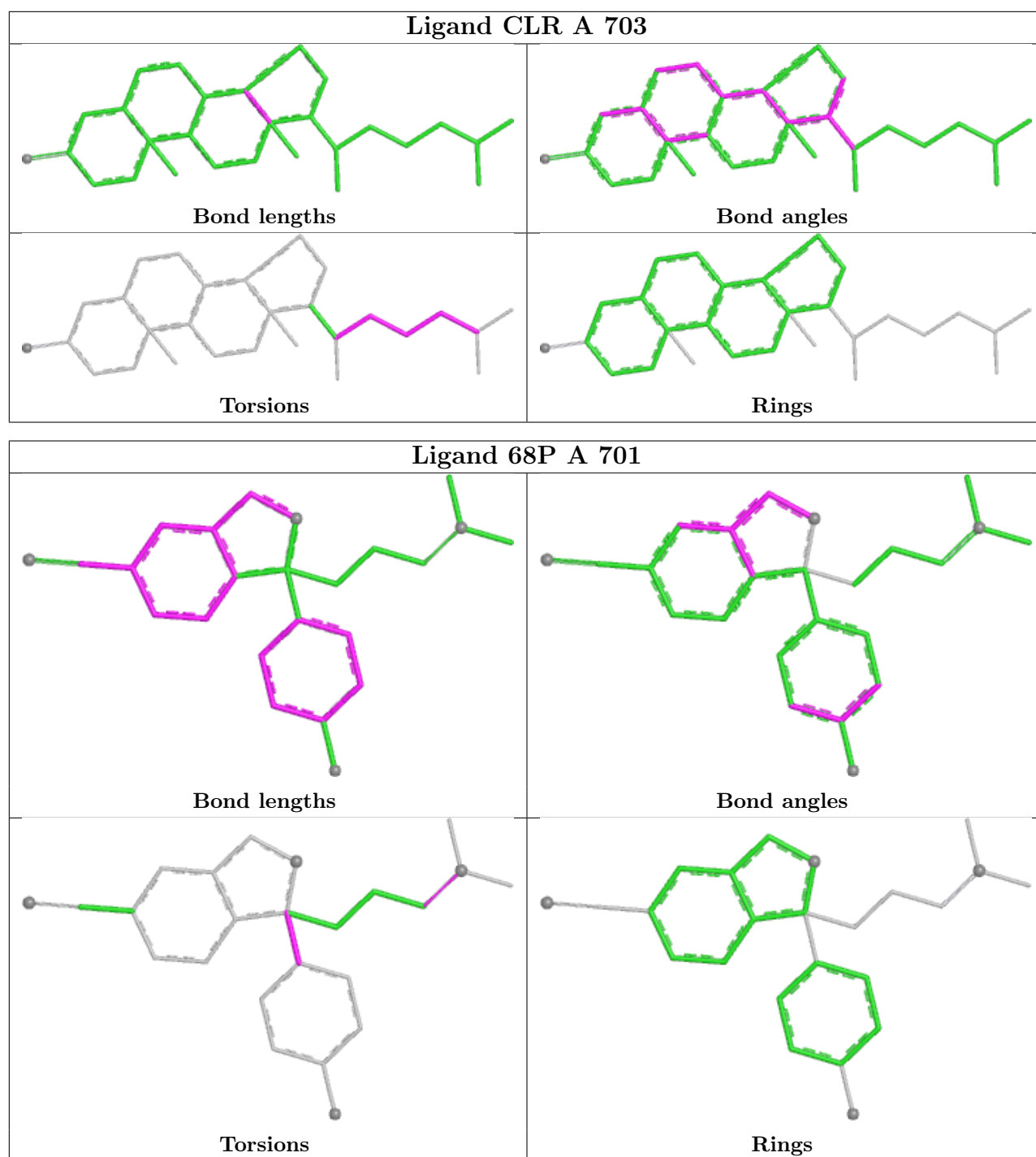
There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	703	CLR	5	0
4	A	701	68P	1	0
7	A	704	C14	2	0
5	A	706	NAG	1	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%)	0.15	36 (6%)	24 16	83, 146, 214, 351	0
2	B	218/221 (98%)	-0.00	10 (4%)	37 24	93, 173, 323, 427	0
3	C	214/214 (100%)	-0.04	10 (4%)	36 23	100, 206, 375, 496	0
All	All	972/984 (98%)	0.07	56 (5%)	29 19	83, 158, 313, 496	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	401	ALA	7.2
1	A	103	TRP	7.1
1	A	403	PRO	7.0
1	A	490	LYS	7.0
1	A	494	GLU	6.7
1	A	104	ARG	6.3
1	A	390	ARG	5.3
2	B	121	ARG	5.2
2	B	204	SER	5.1
1	A	493	GLU	5.0
1	A	389	MET	5.0
1	A	402	GLY	4.9
2	B	190	THR	4.9
1	A	218	ILE	4.4
1	A	337	LEU	4.4
1	A	99	LEU	4.4
2	B	155	ASP	4.3
1	A	404	SER	4.1
1	A	100	GLY	3.7
3	C	106	TYR	3.4
1	A	400	ASP	3.4
3	C	79	PRO	3.4
3	C	78	VAL	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	220	TRP	3.3
3	C	153	VAL	3.2
3	C	82	PHE	3.1
1	A	212	TYR	3.0
1	A	336	SER	3.0
1	A	219	THR	3.0
1	A	142	TYR	3.0
3	C	227	LYS	2.9
1	A	134	TYR	2.9
1	A	598	ILE	2.7
1	A	335	PHE	2.7
2	B	135	THR	2.7
2	B	188	VAL	2.7
1	A	565	LEU	2.6
1	A	270	ILE	2.6
1	A	139	LEU	2.6
1	A	405	LEU	2.5
1	A	98	ASP	2.4
1	A	179	ILE	2.4
3	C	93	PHE	2.4
1	A	277	SER	2.4
2	B	122	PRO	2.4
1	A	391	ASN	2.3
1	A	406	LEU	2.2
2	B	151	PRO	2.2
3	C	95	ILE	2.2
1	A	333	ILE	2.1
3	C	138	PHE	2.1
2	B	150	ALA	2.1
1	A	266	ILE	2.1
2	B	154	GLY	2.1
3	C	155	PHE	2.1
1	A	394	VAL	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 ⓘ

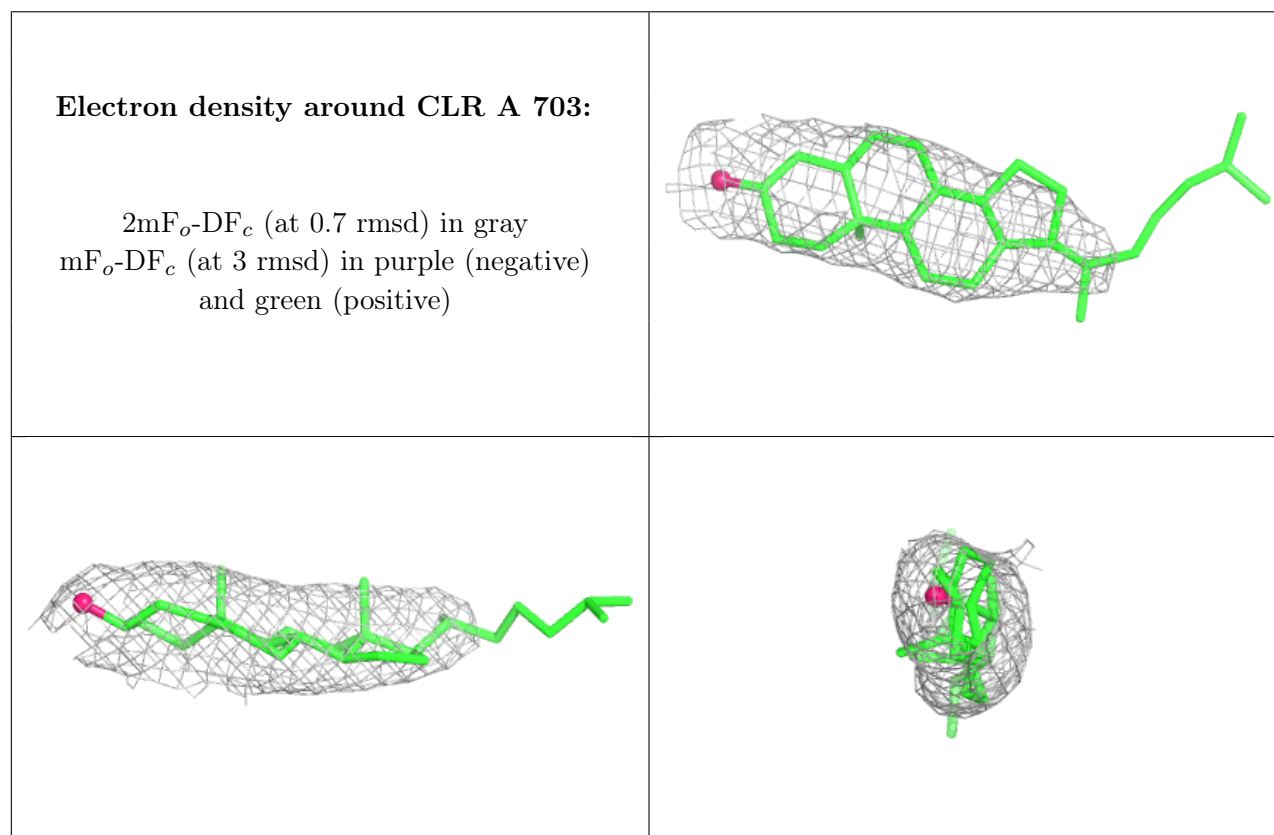
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

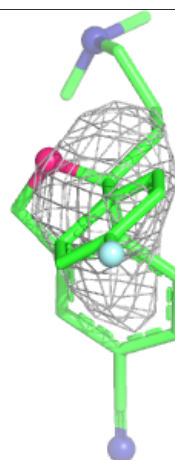
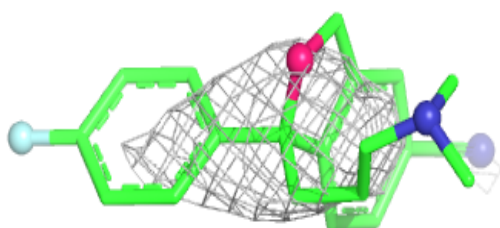
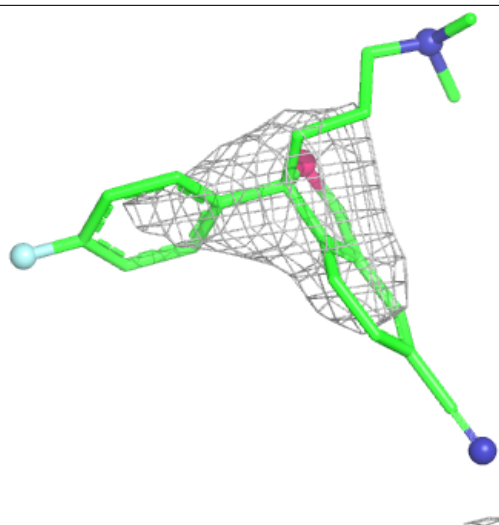
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	ACA	A	709	9/9	0.50	0.12	118,144,199,204	0
5	NAG	A	706	14/15	0.75	0.14	266,279,291,294	0
6	CLR	A	703	28/28	0.90	0.16	165,196,215,233	0
5	NAG	A	702	14/15	0.92	0.09	82,111,149,154	0
4	68P	A	701	24/24	0.93	0.13	134,148,167,180	0
7	C14	A	704	14/14	0.93	0.18	103,104,109,109	14
8	NA	A	707	1/1	0.93	0.19	260,260,260,260	0
4	68P	A	705	24/24	0.93	0.15	134,173,213,222	0
8	NA	A	708	1/1	0.99	0.02	130,130,130,130	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.



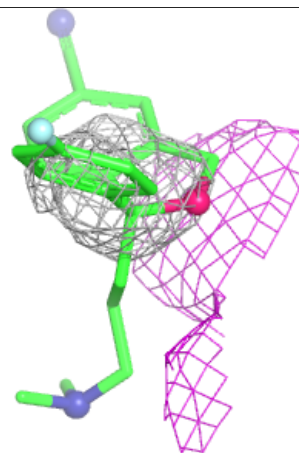
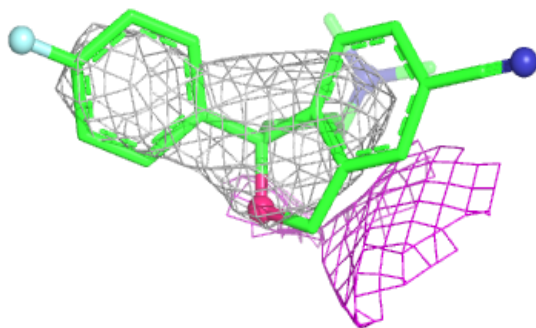
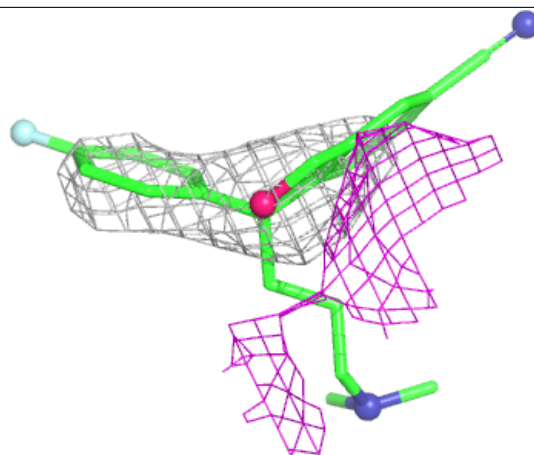
Electron density around 68P A 701:

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



Electron density around 68P 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.