



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 07:46 AM BST

PDB ID : 5I71  
Title : X-ray structure of the ts3 human serotonin transporter complexed with s-citalopram at the central site  
Authors : Coleman, J.A.; Green, E.M.; Gouaux, E.  
Deposited on : 2016-02-16  
Resolution : 3.15 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) 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 : 2.13.1  
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) : 2.13.1

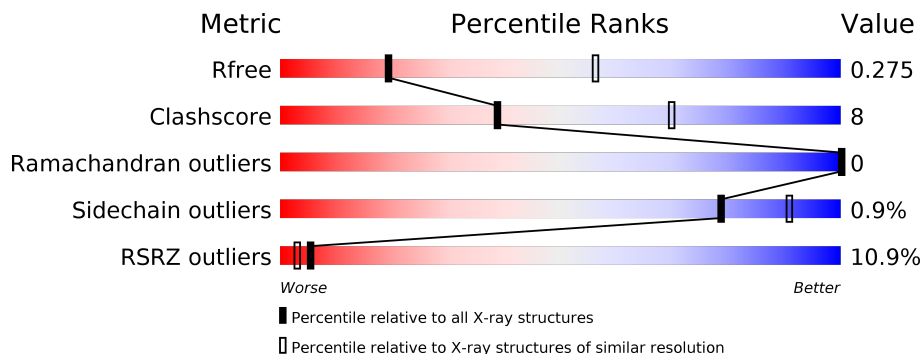
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.15 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	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	 3% 79% 19%
2	B	221	 21% 86% 13%
3	C	214	 19% 88% 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	CLR	A	703	-	-	-	X
8	HEX	A	705	-	-	-	X

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 7616 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
			Total	C	N	O	S			
1	A	542	4210	2810	652	724	24	0	0	0

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

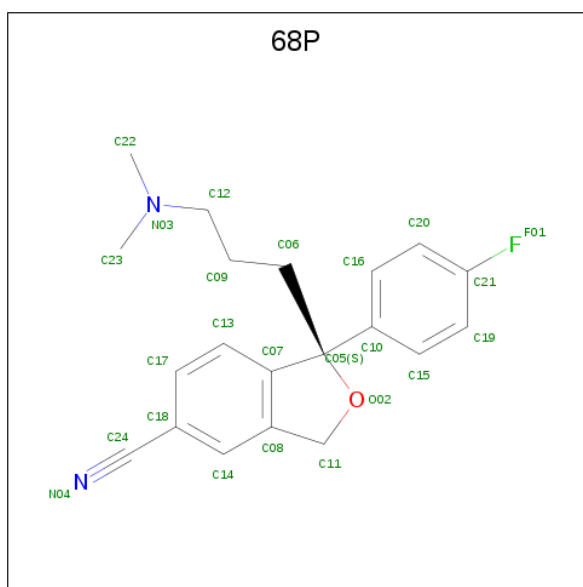
- Molecule 2 is a protein called 8B6 antibody, heavy chain.

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

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

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

- Molecule 4 is (1S)-1-[3-(dimethylamino)propyl]-1-(4-fluorophenyl)-1,3-dihydro-2-benzofuran-5-carbonitrile (three-letter code: 68P) (formula: C<sub>20</sub>H<sub>21</sub>FN<sub>2</sub>O).



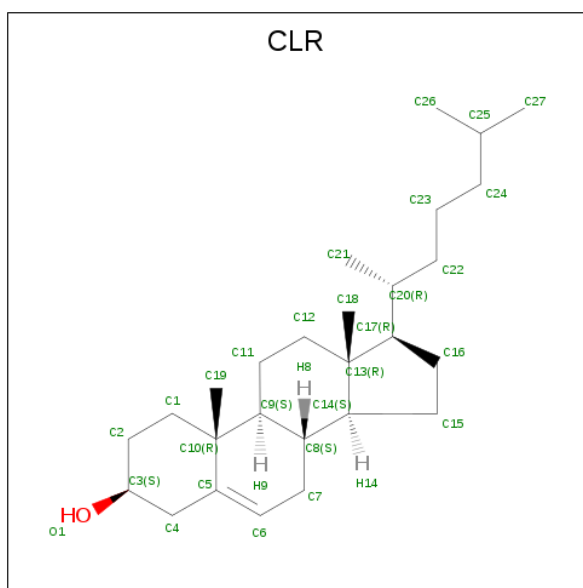
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
4	A	1	24	20	1	2	1	0	0

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



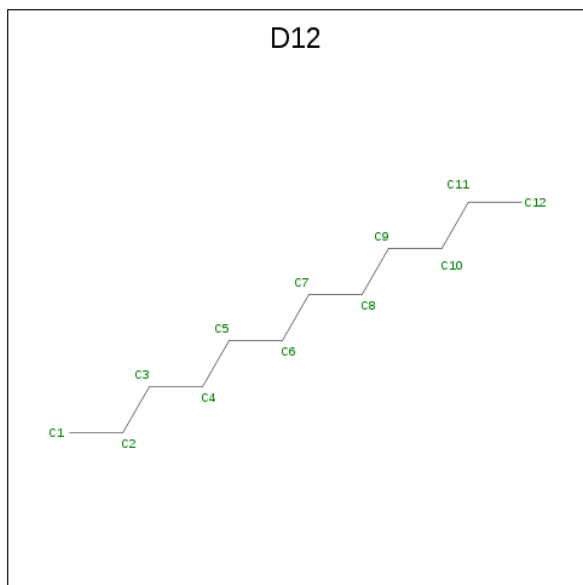
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O			
5	A	1	14	8	1	5	0	0	
5	A	1	14	8	1	5	0	0	

- Molecule 6 is CHOLESTEROL (three-letter code: CLR) (formula:  $C_{27}H_{46}O$ ).



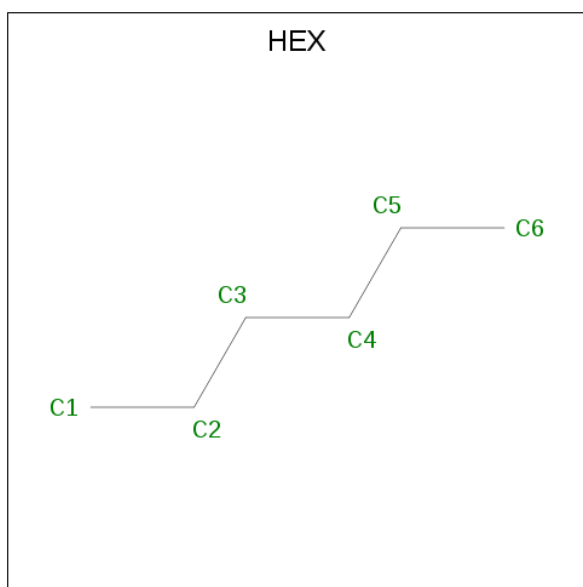
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
6	A	1	Total	C	O	0	0
			28	27	1		

- Molecule 7 is DODECANE (three-letter code: D12) (formula:  $C_{12}H_{26}$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
7	A	1	Total	C		0	0
			12	12			

- Molecule 8 is HEXANE (three-letter code: HEX) (formula:  $C_6H_{14}$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C 6 6	0	0

- Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

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

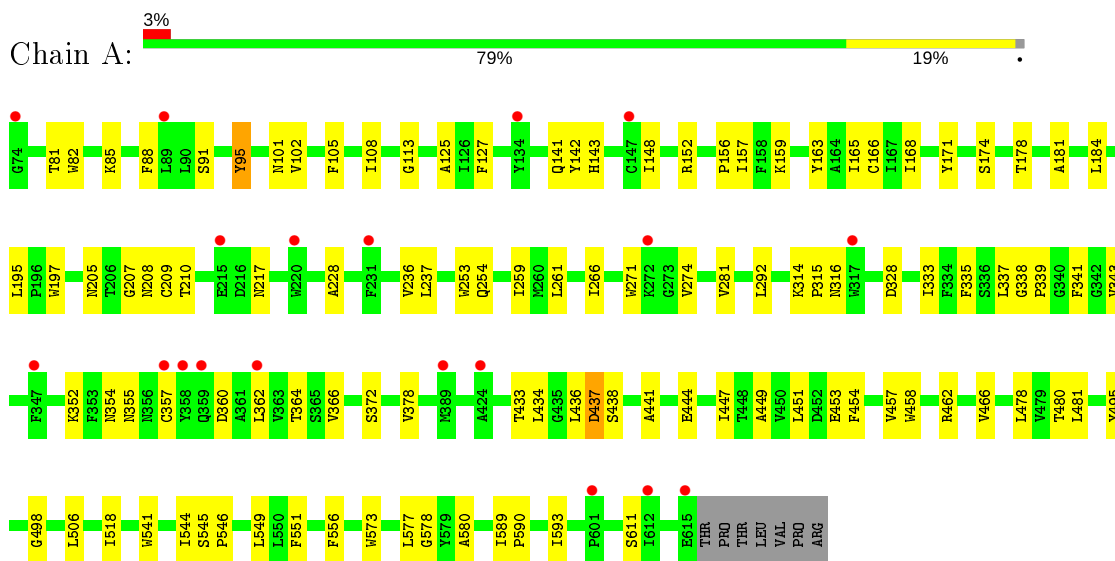
- Molecule 10 is water.

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

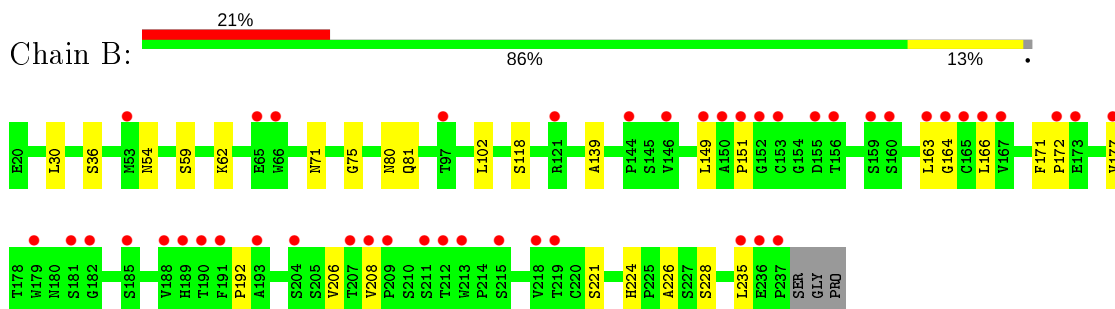
### 3 Residue-property plots [i](#)

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.

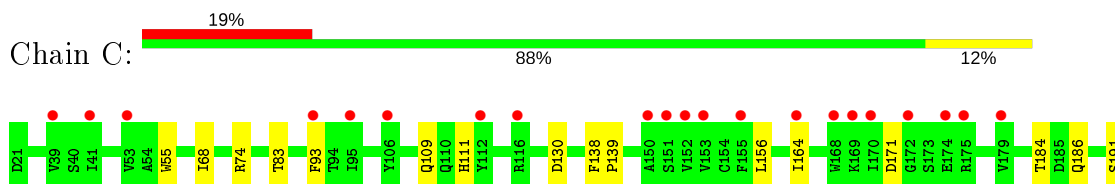
- Molecule 1: Sodium-dependent serotonin transporter



- Molecule 2: 8B6 antibody, heavy chain



- Molecule 3: 8B6 antibody, light chain





T192	•
Y193	
S194	
M195	
S196	•
S197	•
T198	•
L199	•
T200	•
L201	•
T202	•
K203	•
D204	•
E205	•
Y206	•
E207	•
R208	•
H209	•
N210	
S211	•
Y212	
T213	
C214	•
E215	
A216	•
T217	
H218	
K219	
T220	
I225	•
Y226	•
K227	•
S228	•
F229	•
N230	
R231	
M232	
E233	
C234	

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	129.72Å 163.74Å 140.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.33 – 3.15 53.33 – 3.15	Depositor EDS
% Data completeness (in resolution range)	97.0 (53.33-3.15) 96.9 (53.33-3.15)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.23 (at 3.13Å)	Xtrriage
Refinement program	PHENIX (DEV_2000: ???)	Depositor
R, $R_{free}$	0.240 , 0.276 0.239 , 0.275	Depositor DCC
$R_{free}$ test set	1277 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	115.5	Xtrriage
Anisotropy	0.125	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 99.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	7616	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	159.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NAG, D12, NA, HEX, 68P, CLR

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	0.31	0/4343	0.43	0/5938
2	B	0.21	0/1688	0.36	0/2309
3	C	0.21	0/1700	0.36	0/2307
All	All	0.27	0/7731	0.40	0/10554

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	4210	0	4101	82	0
2	B	1643	0	1589	16	0
3	C	1662	0	1585	15	0
4	A	24	0	0	2	0
5	A	28	0	26	1	0
6	A	28	0	46	5	0
7	A	12	0	26	2	0
8	A	6	0	14	0	0
9	A	2	0	0	0	0
10	A	1	0	0	0	0
All	All	7616	0	7387	113	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 8.

All (113) 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:362:LEU:O	1:A:366:VAL:HG23	1.41	1.16
1:A:360:ASP:O	1:A:364:THR:HG23	1.60	0.99
1:A:338:GLY:N	1:A:339:PRO:HD2	1.80	0.96
1:A:266:ILE:HG22	1:A:436:LEU:HD22	1.55	0.88
1:A:338:GLY:N	1:A:339:PRO:CD	2.37	0.86
1:A:141:GLN:NE2	1:A:357:CYS:SG	2.59	0.74
1:A:266:ILE:HG22	1:A:436:LEU:CD2	2.18	0.73
1:A:95:TYR:CE2	1:A:343:VAL:HG11	2.25	0.71
1:A:113:GLY:HA2	1:A:316:ASN:HB3	1.74	0.69
1:A:142:TYR:HD2	1:A:143:HIS:CE1	2.11	0.69
1:A:266:ILE:CG2	1:A:436:LEU:CD2	2.70	0.69
1:A:108:ILE:HD11	1:A:328:ASP:HB3	1.76	0.68
2:B:30:LEU:HD22	2:B:172:PRO:HD3	1.74	0.68
1:A:205:ASN:ND2	1:A:209:CYS:SG	2.66	0.68
1:A:337:LEU:C	1:A:339:PRO:CD	2.61	0.68
1:A:447:ILE:HD13	1:A:466:VAL:HG22	1.77	0.67
1:A:352:LYS:HB2	1:A:355:ASN:HB2	1.78	0.66
1:A:362:LEU:O	1:A:366:VAL:CG2	2.33	0.66
1:A:337:LEU:C	1:A:339:PRO:HD3	2.16	0.65
1:A:444:GLU:OE1	1:A:462:ARG:NH2	2.30	0.65
1:A:573:TRP:CE3	6:A:703:CLR:H71	2.32	0.65
1:A:253:TRP:CE2	1:A:254:GLN:NE2	2.66	0.64
1:A:437:ASP:N	1:A:437:ASP:OD1	2.28	0.64
1:A:101:ASN:ND2	1:A:372:SER:OG	2.30	0.63
1:A:142:TYR:HD2	1:A:143:HIS:ND1	1.98	0.62
2:B:192:PRO:HD3	3:C:184:THR:HG22	1.82	0.62
1:A:589:ILE:HG23	1:A:590:PRO:HD3	1.82	0.61
1:A:95:TYR:HD2	1:A:441:ALA:HB3	1.65	0.61
1:A:335:PHE:HE2	4:A:701:68P:N04	1.99	0.60
1:A:152:ARG:HE	1:A:159:LYS:HZ2	1.50	0.60
1:A:95:TYR:CD2	1:A:343:VAL:HG11	2.36	0.60
2:B:54:ASN:ND2	2:B:118:SER:OG	2.34	0.59
1:A:184:LEU:HD21	1:A:261:LEU:HD23	1.84	0.58
1:A:142:TYR:CD2	1:A:143:HIS:CE1	2.91	0.58
1:A:163:TYR:O	1:A:166:CYS:HB2	2.04	0.57
1:A:253:TRP:CZ2	1:A:254:GLN:NE2	2.72	0.57
1:A:266:ILE:CG2	1:A:436:LEU:HD22	2.31	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:ILE:HB	1:A:593:ILE:HG12	1.87	0.57
1:A:102:VAL:HG21	1:A:434:LEU:HD13	1.85	0.57
1:A:259:ILE:HG21	1:A:481:LEU:HD11	1.87	0.56
1:A:178:THR:O	1:A:181:ALA:HB3	2.06	0.56
3:C:186:GLN:HE21	3:C:191:SER:HB3	1.72	0.55
1:A:197:TRP:HB2	1:A:228:ALA:HA	1.87	0.55
1:A:178:THR:HG21	1:A:480:THR:HB	1.88	0.54
1:A:95:TYR:CD2	1:A:441:ALA:HB3	2.42	0.54
1:A:573:TRP:CZ3	6:A:703:CLR:H71	2.42	0.54
1:A:236:VAL:HG13	1:A:237:LEU:N	2.24	0.53
1:A:95:TYR:HA	1:A:438:SER:HA	1.91	0.53
1:A:498:GLY:HA2	4:A:701:68P:N04	2.23	0.53
1:A:454:PHE:HB3	1:A:457:VAL:CG1	2.38	0.52
2:B:59:SER:HB2	2:B:62:LYS:HB2	1.92	0.52
1:A:478:LEU:HD23	1:A:481:LEU:HD12	1.90	0.52
1:A:171:TYR:O	1:A:174:SER:HB2	2.09	0.52
1:A:207:GLY:HA3	5:A:702:NAG:H82	1.92	0.51
1:A:152:ARG:HH21	1:A:159:LYS:HZ1	1.59	0.51
1:A:81:THR:OG1	1:A:82:TRP:N	2.43	0.51
3:C:171:ASP:OD2	3:C:209:HIS:ND1	2.38	0.51
1:A:102:VAL:HG21	1:A:434:LEU:CD1	2.41	0.50
1:A:95:TYR:CD1	1:A:95:TYR:C	2.85	0.50
1:A:208:ASN:O	1:A:210:THR:HG23	2.12	0.50
3:C:74:ARG:HH21	3:C:83:THR:HG22	1.76	0.49
1:A:195:LEU:H	1:A:195:LEU:HD12	1.76	0.49
1:A:91:SER:HA	1:A:281:VAL:HG11	1.94	0.49
3:C:156:LEU:HD13	3:C:195:MET:HG3	1.96	0.48
1:A:580:ALA:HB1	6:A:703:CLR:H241	1.94	0.48
1:A:454:PHE:HB3	1:A:457:VAL:HG13	1.94	0.47
1:A:506:LEU:HD23	1:A:549:LEU:HB2	1.96	0.47
2:B:71:ASN:O	2:B:75:GLY:N	2.46	0.47
3:C:211:SER:HA	3:C:229:PHE:O	2.15	0.47
1:A:156:PRO:HG2	1:A:611:SER:HA	1.96	0.46
1:A:127:PHE:HB3	1:A:544:ILE:HG21	1.97	0.46
1:A:556:PHE:HB2	7:A:704:D12:H112	1.98	0.45
1:A:314:LYS:HA	1:A:315:PRO:HD3	1.84	0.45
2:B:163:LEU:HB3	2:B:235:LEU:HD22	1.99	0.45
3:C:130:ASP:HB3	3:C:220:THR:HG22	1.99	0.45
3:C:231:ARG:O	3:C:233:GLU:N	2.47	0.44
3:C:164:ILE:HB	3:C:218:HIS:HD2	1.82	0.44
1:A:148:ILE:HG13	1:A:449:ALA:HB1	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:TYR:HB3	1:A:578:GLY:HA3	1.99	0.44
2:B:151:PRO:HG3	3:C:138:PHE:HE2	1.82	0.44
1:A:165:ILE:O	1:A:168:ILE:HB	2.18	0.44
2:B:206:VAL:HG22	2:B:208:VAL:HG13	1.99	0.44
1:A:451:LEU:CD2	1:A:458:TRP:HB3	2.48	0.44
2:B:80:ASN:OD1	2:B:81:GLN:N	2.51	0.44
1:A:156:PRO:O	1:A:159:LYS:HB2	2.17	0.44
3:C:139:PRO:HB3	3:C:229:PHE:CE2	2.53	0.44
1:A:453:GLU:HG3	1:A:454:PHE:CD1	2.53	0.43
1:A:577:LEU:HD13	6:A:703:CLR:H151	2.00	0.43
3:C:55:TRP:HB2	3:C:68:ILE:HB	2.00	0.43
2:B:224:HIS:CE1	2:B:226:ALA:HB3	2.53	0.43
6:A:703:CLR:H162	6:A:703:CLR:H231	2.00	0.43
7:A:704:D12:H21	7:A:704:D12:H52	1.77	0.43
1:A:341:PHE:HD2	1:A:343:VAL:HG23	1.84	0.43
1:A:178:THR:HG22	1:A:259:ILE:HD12	2.00	0.42
2:B:139:ALA:HB3	2:B:171:PHE:CE2	2.55	0.42
1:A:338:GLY:H	1:A:339:PRO:HD2	1.77	0.42
3:C:215:GLU:HA	3:C:225:ILE:O	2.20	0.42
1:A:292:LEU:HD22	1:A:378:VAL:HG21	2.01	0.41
2:B:177:VAL:HA	2:B:221:SER:O	2.20	0.41
1:A:125:ALA:HB2	1:A:333:ILE:HG12	2.01	0.41
2:B:149:LEU:HD11	2:B:166:LEU:HB2	2.02	0.41
2:B:224:HIS:O	2:B:228:SER:N	2.53	0.41
3:C:55:TRP:CD2	3:C:93:PHE:HB2	2.55	0.41
1:A:518:ILE:HD11	1:A:541:TRP:CE3	2.55	0.41
1:A:433:THR:O	1:A:437:ASP:OD1	2.39	0.41
2:B:36:SER:HA	2:B:102:LEU:O	2.21	0.41
3:C:111:HIS:ND1	3:C:111:HIS:O	2.52	0.41
1:A:88:PHE:HZ	1:A:274:VAL:HB	1.85	0.41
1:A:545:SER:HB2	1:A:546:PRO:HD3	2.03	0.41
1:A:105:PHE:HA	1:A:108:ILE:HG22	2.03	0.40
1:A:343:VAL:HG13	1:A:441:ALA:HB1	2.04	0.40
1:A:85:LYS:NZ	1:A:360:ASP:OD2	2.47	0.40
2:B:149:LEU:HB2	2:B:164:GLY: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	540/549 (98%)	522 (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	968/984 (98%)	925 (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	429/462 (93%)	423 (99%)	6 (1%)	67	85
2	B	190/193 (98%)	190 (100%)	0	100	100
3	C	189/190 (100%)	188 (100%)	1 (0%)	88	95
All	All	808/845 (96%)	801 (99%)	7 (1%)	78	91

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	TYR
1	A	217	ASN
1	A	271	TRP
1	A	354	ASN
1	A	437	ASP

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Mol	Chain	Res	Type
1	A	551	PHE
3	C	109	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	26	GLN

### 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](#)

Of 8 ligands modelled in this entry, 2 are 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	$\# Z  > 2$
7	D12	A	704	-	11,11,11	0.30	0	10,10,10	0.84	0
8	HEX	A	705	-	5,5,5	0.31	0	4,4,4	0.57	0
4	68P	A	701	-	25,26,26	5.96	15 (60%)	30,37,37	1.52	5 (16%)
5	NAG	A	702	1	14,14,15	0.20	0	17,19,21	0.55	0
5	NAG	A	706	1	14,14,15	0.22	0	17,19,21	0.38	0
6	CLR	A	703	-	31,31,31	0.83	1 (3%)	48,48,48	1.31	4 (8%)



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
7	D12	A	704	-	-	3/9/9/9	-
8	HEX	A	705	-	-	0/3/3/3	-
4	68P	A	701	-	-	3/15/27/27	0/3/3/3
5	NAG	A	702	1	-	2/6/23/26	0/1/1/1
5	NAG	A	706	1	-	1/6/23/26	0/1/1/1
6	CLR	A	703	-	-	6/10/68/68	0/4/4/4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	701	68P	C13-C07	11.30	1.54	1.39
4	A	701	68P	C14-C08	9.57	1.55	1.39
4	A	701	68P	C15-C10	9.10	1.53	1.39
4	A	701	68P	C19-C15	8.65	1.54	1.38
4	A	701	68P	C16-C20	8.60	1.54	1.38
4	A	701	68P	C20-C21	8.42	1.53	1.37
4	A	701	68P	C16-C10	8.20	1.52	1.39
4	A	701	68P	C14-C18	7.86	1.53	1.39
4	A	701	68P	C19-C21	7.74	1.52	1.37
4	A	701	68P	C17-C13	7.64	1.52	1.38
4	A	701	68P	C08-C07	6.89	1.48	1.39
4	A	701	68P	C17-C18	5.02	1.50	1.39
4	A	701	68P	O02-C11	4.33	1.50	1.43
4	A	701	68P	C18-C24	4.03	1.53	1.44
4	A	701	68P	C11-C08	-2.02	1.47	1.50
6	A	703	CLR	C13-C14	-2.01	1.51	1.55

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	701	68P	C11-C08-C07	-4.14	106.76	108.80
4	A	701	68P	O02-C05-C07	3.15	107.08	102.54
6	A	703	CLR	C8-C7-C6	-3.08	108.31	112.73
6	A	703	CLR	C9-C10-C5	2.91	114.21	109.65
6	A	703	CLR	C13-C14-C8	-2.62	110.49	114.38
4	A	701	68P	C19-C21-C20	-2.51	119.48	122.83
4	A	701	68P	C11-C08-C14	2.36	133.66	129.29
4	A	701	68P	O02-C11-C08	2.33	108.00	105.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	703	CLR	C4-C5-C10	2.31	119.49	116.42

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	702	NAG	O5-C5-C6-O6
5	A	702	NAG	C4-C5-C6-O6
6	A	703	CLR	C17-C20-C22-C23
6	A	703	CLR	C21-C20-C22-C23
7	A	704	D12	C5-C6-C7-C8
5	A	706	NAG	O5-C5-C6-O6
7	A	704	D12	C7-C8-C9-C10
4	A	701	68P	C06-C05-C10-C16
6	A	703	CLR	C20-C22-C23-C24
7	A	704	D12	C4-C5-C6-C7
4	A	701	68P	C06-C05-C10-C15
4	A	701	68P	C09-C12-N03-C23
6	A	703	CLR	C23-C24-C25-C26
6	A	703	CLR	C23-C24-C25-C27
6	A	703	CLR	C22-C23-C24-C25

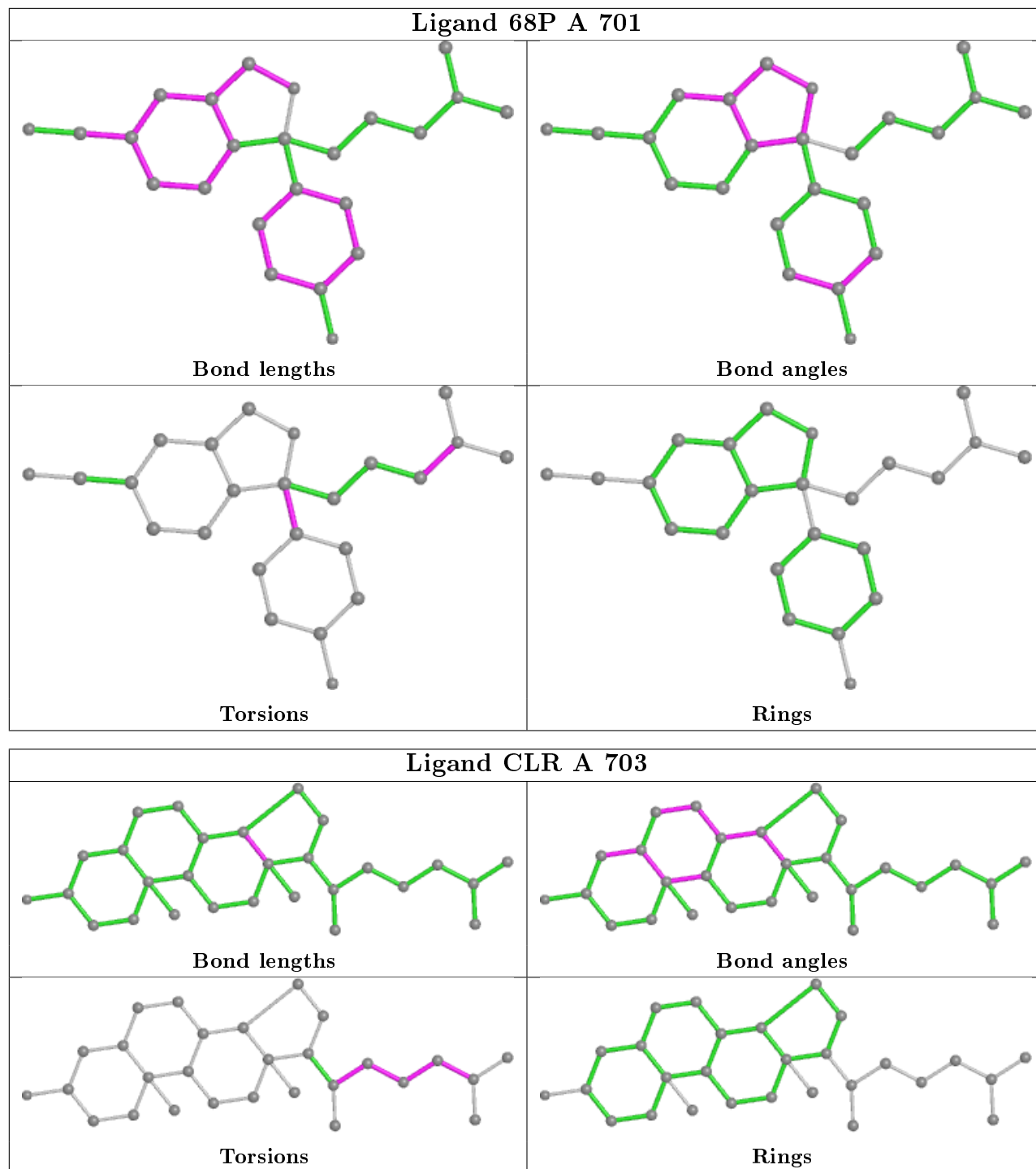
There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	704	D12	2	0
4	A	701	68P	2	0
5	A	702	NAG	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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	542/549 (98%)	0.22	19 (3%) 44 27	77, 133, 204, 309	0
2	B	218/221 (98%)	0.89	46 (21%) 1 0	81, 164, 318, 362	0
3	C	214/214 (100%)	0.83	41 (19%) 1 0	92, 186, 333, 444	0
All	All	974/984 (98%)	0.51	106 (10%) 5 3	77, 144, 297, 444	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	151	PRO	10.4
3	C	203	LYS	7.1
3	C	201	LEU	6.7
3	C	170	ILE	6.1
2	B	190	THR	5.6
2	B	150	ALA	5.4
2	B	204	SER	5.4
2	B	211	SER	5.4
3	C	151	SER	5.3
2	B	152	GLY	5.2
3	C	225	ILE	5.0
2	B	167	VAL	5.0
2	B	149	LEU	4.9
3	C	200	THR	4.8
2	B	172	PRO	4.8
1	A	134	TYR	4.7
2	B	155	ASP	4.7
2	B	179	TRP	4.6
2	B	182	GLY	4.5
3	C	153	VAL	4.5
2	B	166	LEU	4.4
1	A	615	GLU	4.4
2	B	212	THR	4.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	C	152	VAL	4.4
1	A	357	CYS	4.3
2	B	208	VAL	4.2
3	C	199	LEU	4.2
3	C	206	TYR	4.2
2	B	209	PRO	4.1
3	C	198	THR	4.1
2	B	185	SER	4.1
1	A	74	GLY	4.0
2	B	188	VAL	4.0
3	C	226	VAL	3.8
3	C	202	THR	3.7
2	B	218	VAL	3.7
3	C	169	LYS	3.6
3	C	155	PHE	3.6
3	C	216	ALA	3.5
1	A	359	GLN	3.5
2	B	165	CYS	3.4
1	A	389	MET	3.4
3	C	95	ILE	3.4
2	B	181	SER	3.3
1	A	272	LYS	3.3
3	C	207	GLU	3.3
1	A	147	CYS	3.2
3	C	106	TYR	3.2
2	B	213	TRP	3.2
2	B	153	CYS	3.1
2	B	219	THR	3.1
3	C	212	TYR	3.1
2	B	191	PHE	3.1
3	C	172	GLY	3.1
1	A	317	TRP	3.0
1	A	215	GLU	3.0
2	B	164	GLY	3.0
3	C	227	LYS	3.0
3	C	204	ASP	2.9
2	B	144	PRO	2.9
2	B	163	LEU	2.9
2	B	146	VAL	2.9
2	B	160	SER	2.9
1	A	601	PRO	2.9
3	C	168	TRP	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	C	228	SER	2.8
2	B	236	GLU	2.7
3	C	229	PHE	2.7
3	C	174	GLU	2.6
2	B	207	THR	2.6
3	C	179	VAL	2.6
2	B	121	ARG	2.6
2	B	177	VAL	2.6
3	C	112	TYR	2.5
2	B	173	GLU	2.5
3	C	41	ILE	2.5
2	B	53	MET	2.5
1	A	358	TYR	2.5
1	A	612	ILE	2.5
1	A	220	TRP	2.4
3	C	116	ARG	2.4
3	C	197	SER	2.4
2	B	156	THR	2.4
1	A	231	PHE	2.4
3	C	164	ILE	2.4
1	A	424	ALA	2.4
2	B	97	THR	2.4
2	B	66	TRP	2.3
2	B	193	ALA	2.3
3	C	150	ALA	2.2
2	B	65	GLU	2.2
3	C	93	PHE	2.2
3	C	209	HIS	2.2
3	C	175	ARG	2.1
1	A	89	LEU	2.1
2	B	189	HIS	2.1
3	C	193	TYR	2.1
1	A	347	PHE	2.1
3	C	214	CYS	2.1
2	B	215	SER	2.1
2	B	235	LEU	2.0
3	C	53	VAL	2.0
1	A	362	LEU	2.0
2	B	237	PRO	2.0
2	B	159	SER	2.0
3	C	39	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.

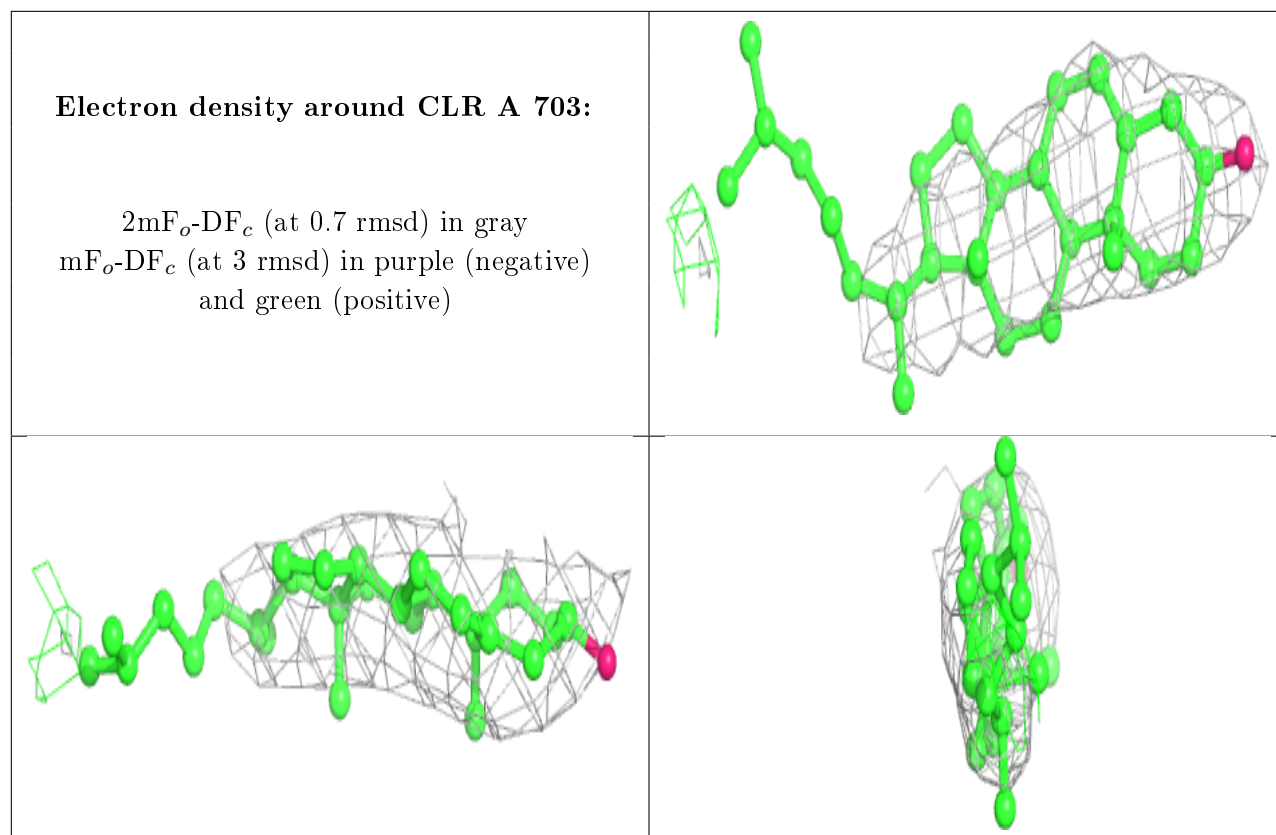
## 6.4 Ligands [i](#)

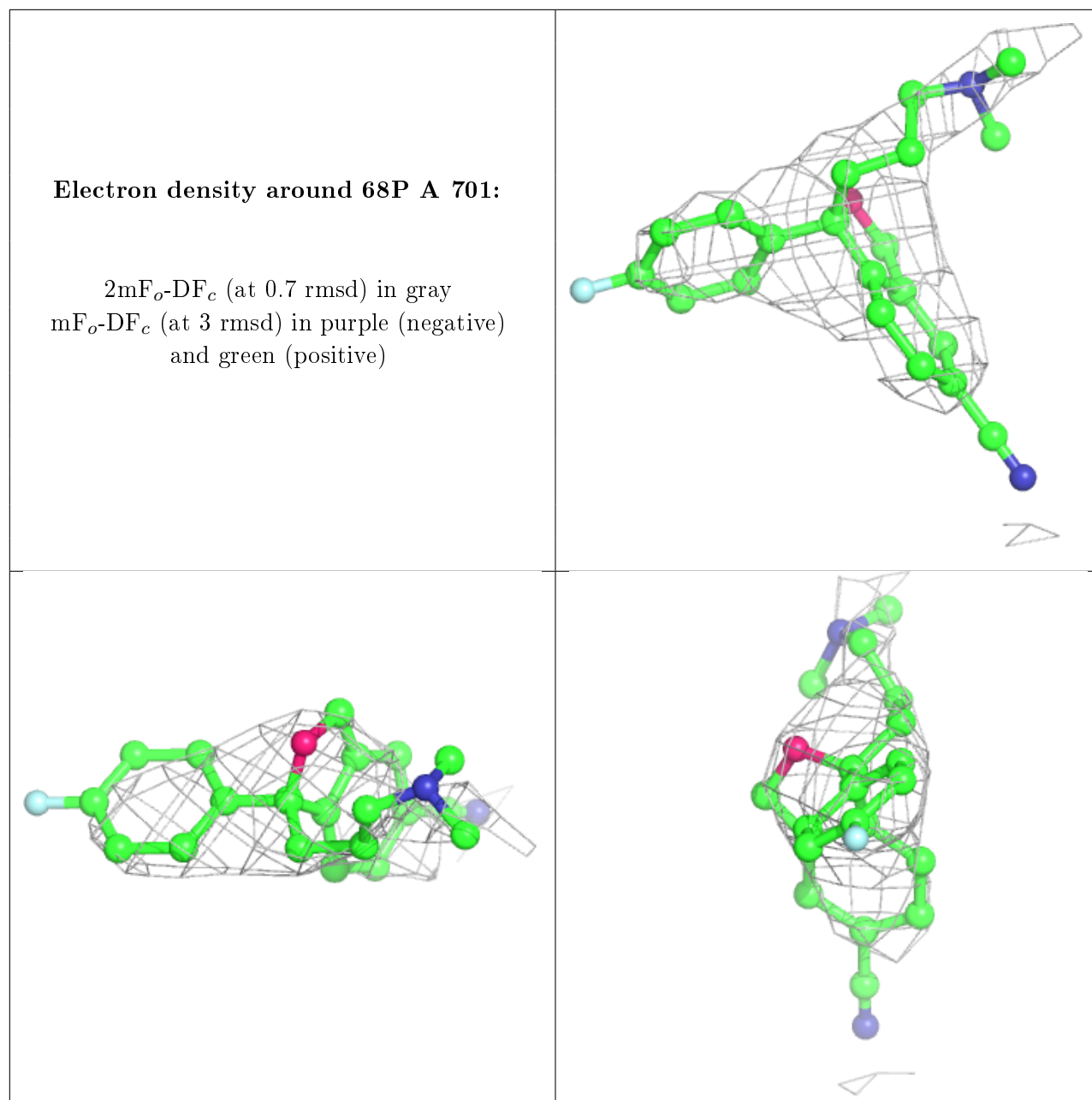
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
8	HEX	A	705	6/6	0.73	0.75	87,100,105,108	0
5	NAG	A	706	14/15	0.76	0.37	302,304,306,307	0
7	D12	A	704	12/12	0.79	0.36	85,97,104,105	0
6	CLR	A	703	28/28	0.79	0.42	159,175,199,210	0
9	NA	A	707	1/1	0.83	0.06	123,123,123,123	0
4	68P	A	701	24/24	0.91	0.49	95,123,143,154	0
5	NAG	A	702	14/15	0.93	0.17	66,85,156,158	0
9	NA	A	708	1/1	0.95	0.19	115,115,115,115	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.







## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.