



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 26, 2016 – 08:42 PM EDT

PDB ID : 5I75
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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027457
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

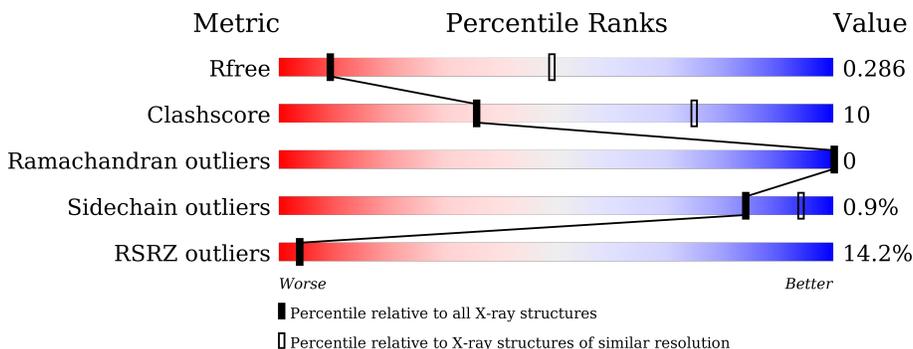
1 Overall quality at a glance

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}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	 10% 76% 22% ..
2	B	221	 14% 83% 16% .
3	C	214	 25% 81% 19%

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
4	68P	A	701	-	-	-	X
6	CLR	A	703	-	-	-	X

2 Entry composition [i](#)

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
			Total	C	N	O	S			
1	A	540	4192	2801	647	720	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

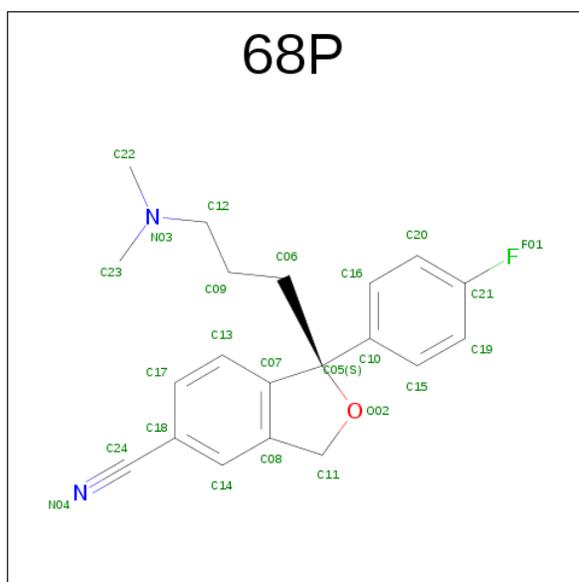
- Molecule 2 is a protein called 8B6 antibody, heavy chain.

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.

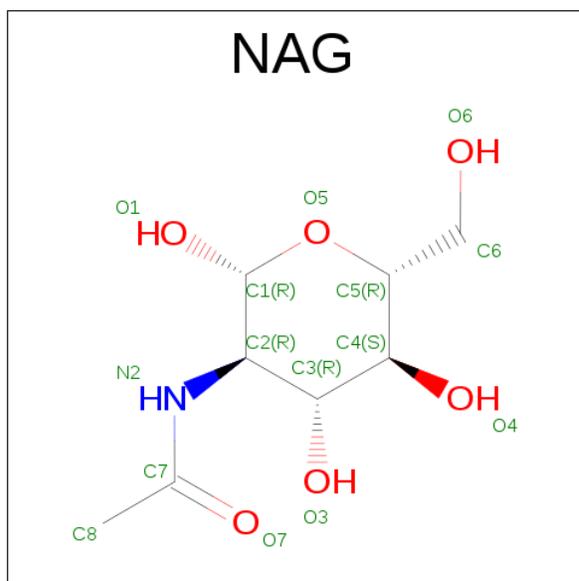
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	214	1662	1037	280	337	8	0	0	0

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



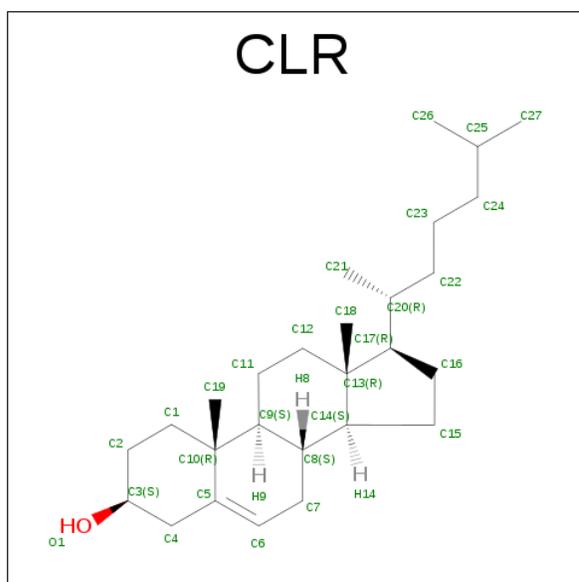
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
4	A	1	24	20	1	2	1	0	0

- Molecule 5 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



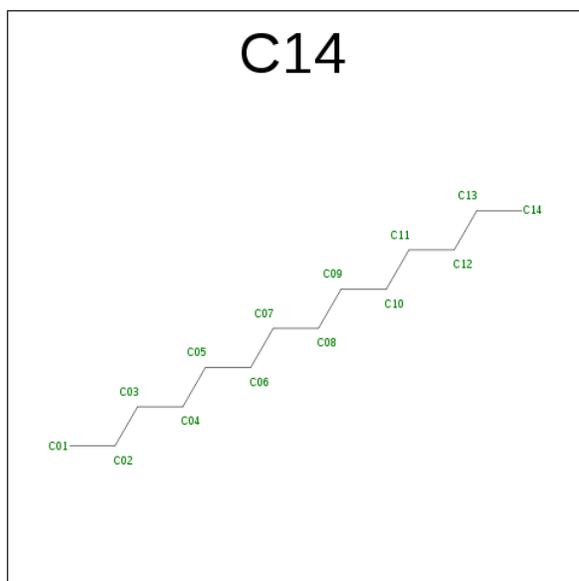
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O			
5	A	1	14	8	1	5	0	0	
5	A	1	14	8	1	5	0	0	

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



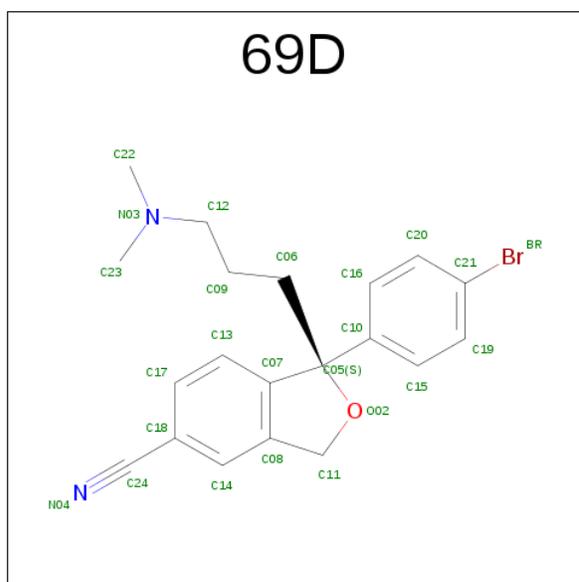
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	C O	0	0
			28	27 1		

- Molecule 7 is TETRADECANE (three-letter code: C14) (formula: $C_{14}H_{30}$).



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

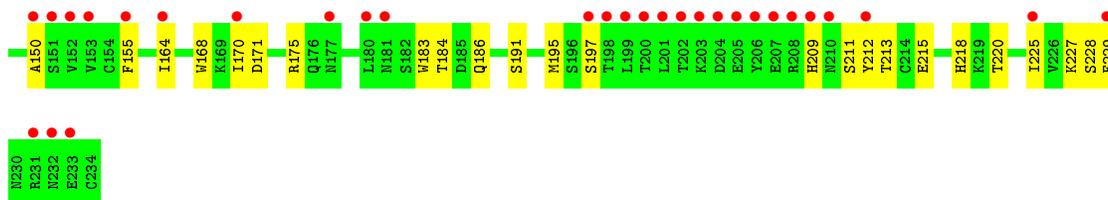
- Molecule 8 is (1S)-1-(4-bromophenyl)-1-[3-(dimethylamino)propyl]-1,3-dihydro-2-benzofuran-5-carbonitrile (three-letter code: 69D) (formula: $C_{20}H_{21}BrN_2O$).



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

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

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



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)	Xtrriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.244 , 0.286 0.242 , 0.286	Depositor DCC
R_{free} test set	1814 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	124.3	Xtrriage
Anisotropy	0.110	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 103.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.18$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	7610	wwPDB-VP
Average B, all atoms (Å ²)	174.0	wwPDB-VP

Xtrriage'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, 0.375 respectively for untwinned datasets, and 0.333, 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, NA, 69D, 68P, CLR, 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	0.28	0/4325	0.43	0/5915
2	B	0.25	0/1688	0.43	0/2309
3	C	0.25	0/1700	0.42	0/2307
All	All	0.27	0/7713	0.43	0/10531

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.

There are no bond angle outliers.

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 [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	4192	0	4085	98	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	145	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.

The worst 5 of 145 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

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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	421 (99%)	6 (1%)	74	91
2	B	190/193 (98%)	190 (100%)	0	100	100
3	C	189/190 (100%)	188 (100%)	1 (0%)	92	97
All	All	806/845 (95%)	799 (99%)	7 (1%)	84	94

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	354	ASN
3	C	109	GLN
1	A	437	ASP
1	A	217	ASN
1	A	551	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	141	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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
4	68P	A	701	-	24,26,26	5.82	14 (58%)	31,37,37	1.35	4 (12%)
5	NAG	A	702	1	14,14,15	0.27	0	15,19,21	0.35	0
6	CLR	A	703	-	31,31,31	0.81	0	48,48,48	1.24	4 (8%)
7	C14	A	704	-	13,13,13	0.31	0	12,12,12	0.81	0
8	69D	A	705	-	19,20,26	6.87	11 (57%)	23,28,37	3.38	8 (34%)
5	NAG	A	706	1	14,14,15	0.22	0	15,19,21	0.28	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	701	-	-	0/15/27/27	0/3/3/3
5	NAG	A	702	1	-	0/6/23/26	0/1/1/1
6	CLR	A	703	-	-	0/10/68/68	0/4/4/4
7	C14	A	704	-	-	0/11/11/11	0/0/0/0
8	69D	A	705	-	-	0/6/15/27	0/3/3/3
5	NAG	A	706	1	-	0/6/23/26	0/1/1/1

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	705	69D	C07-C05	-14.07	1.32	1.51
8	A	705	69D	C17-C18	-11.35	1.14	1.39
8	A	705	69D	C17-C13	-10.29	1.18	1.38
8	A	705	69D	C14-C18	-3.29	1.33	1.39
8	A	705	69D	C13-C07	-2.43	1.36	1.39

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	705	69D	C13-C07-C08	-8.99	109.55	120.80
8	A	705	69D	O02-C11-C08	-3.89	101.79	105.03
4	A	701	68P	C09-C06-C05	-3.62	108.76	115.23
8	A	705	69D	C18-C14-C08	-3.22	116.34	120.70
8	A	705	69D	C14-C08-C07	-3.08	117.01	120.93

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	701	68P	1	0
6	A	703	CLR	5	0
7	A	704	C14	1	0
8	A	705	69D	1	0
5	A	706	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	540/549 (98%)	0.53	53 (9%) 10 9	85, 146, 212, 284	0
2	B	218/221 (98%)	0.64	31 (14%) 4 4	78, 176, 313, 473	0
3	C	214/214 (100%)	1.08	54 (25%) 1 1	105, 201, 403, 703	0
All	All	972/984 (98%)	0.67	138 (14%) 4 4	78, 158, 323, 703	0

The worst 5 of 138 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	151	PRO	21.0
2	B	150	ALA	10.9
3	C	202	THR	10.7
3	C	206	TYR	9.4
3	C	201	LEU	8.9

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
6	CLR	A	703	28/28	0.80	0.78	5.21	154,168,182,200	0
4	68P	A	701	24/24	0.88	0.45	2.02	108,135,151,171	0
5	NAG	A	706	14/15	0.83	0.33	1.38	221,236,244,249	0
7	C14	A	704	14/14	0.90	0.37	0.79	69,72,77,79	14
5	NAG	A	702	14/15	0.94	0.26	0.44	82,101,167,180	0
8	69D	A	705	18/24	0.84	0.29	0.20	147,164,195,198	0
9	NA	A	707	1/1	0.93	0.12	-1.19	98,98,98,98	0

6.5 Other polymers [i](#)

There are no such residues in this entry.