wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 05:53 PM GMT

PDB ID	:	4JRA
Title	:	CRYSTAL STRUCTURE OF THE BOTULINUM NEUROTOXIN A RECEPTOR-BINDING DOMAIN IN COMPLEX WITH THE LUMINAL DOMAIN Of SV2C
Authors	:	Benoit, R.M.; Frey, D.; Wieser, M.M.; Jaussi, R.; Schertler, G.F.X.; Capitani, G.; Kammerer, R.A.
Deposited on	:	2013-03-21
Resolution	:	2.30 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

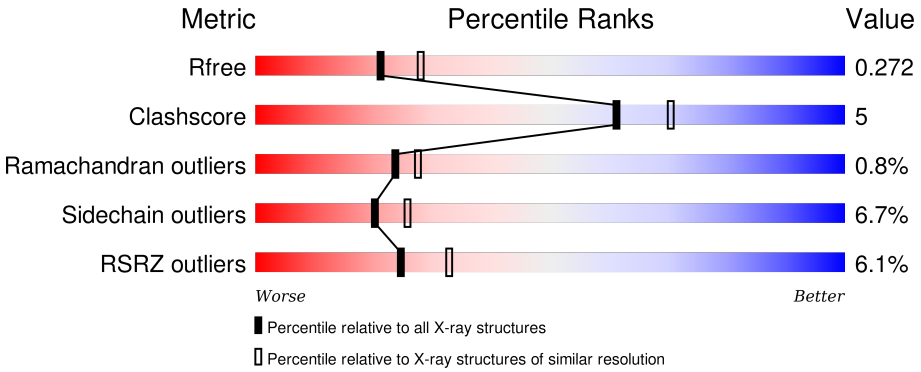
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 <=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	443	77% 16% • 6%
1	B	443	10% 72% 20% • 7%
2	C	136	11% 47% 12% • 39%
2	D	136	57% 11% • 32%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 16539 atoms, of which 8131 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 Botulinum neurotoxin type A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	416	Total	C	H	N	O	S	0	3	0
			6854	2195	3412	593	641	13			
1	B	413	Total	C	H	N	O	S	0	0	0
			6778	2176	3367	585	637	13			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	854	MET	-	EXPRESSION TAG	UNP P10845
A	855	LYS	-	EXPRESSION TAG	UNP P10845
A	856	LYS	-	EXPRESSION TAG	UNP P10845
A	857	HIS	-	EXPRESSION TAG	UNP P10845
A	858	HIS	-	EXPRESSION TAG	UNP P10845
A	859	HIS	-	EXPRESSION TAG	UNP P10845
A	860	HIS	-	EXPRESSION TAG	UNP P10845
A	861	HIS	-	EXPRESSION TAG	UNP P10845
A	862	HIS	-	EXPRESSION TAG	UNP P10845
A	863	GLY	-	EXPRESSION TAG	UNP P10845
A	864	SER	-	EXPRESSION TAG	UNP P10845
A	865	LEU	-	EXPRESSION TAG	UNP P10845
A	866	VAL	-	EXPRESSION TAG	UNP P10845
A	867	PRO	-	EXPRESSION TAG	UNP P10845
A	868	ARG	-	EXPRESSION TAG	UNP P10845
A	869	GLY	-	EXPRESSION TAG	UNP P10845
A	870	SER	-	EXPRESSION TAG	UNP P10845
B	854	MET	-	EXPRESSION TAG	UNP P10845
B	855	LYS	-	EXPRESSION TAG	UNP P10845
B	856	LYS	-	EXPRESSION TAG	UNP P10845
B	857	HIS	-	EXPRESSION TAG	UNP P10845
B	858	HIS	-	EXPRESSION TAG	UNP P10845
B	859	HIS	-	EXPRESSION TAG	UNP P10845
B	860	HIS	-	EXPRESSION TAG	UNP P10845
B	861	HIS	-	EXPRESSION TAG	UNP P10845

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Chain	Residue	Modelled	Actual	Comment	Reference
B	862	HIS	-	EXPRESSION TAG	UNP P10845
B	863	GLY	-	EXPRESSION TAG	UNP P10845
B	864	SER	-	EXPRESSION TAG	UNP P10845
B	865	LEU	-	EXPRESSION TAG	UNP P10845
B	866	VAL	-	EXPRESSION TAG	UNP P10845
B	867	PRO	-	EXPRESSION TAG	UNP P10845
B	868	ARG	-	EXPRESSION TAG	UNP P10845
B	869	GLY	-	EXPRESSION TAG	UNP P10845
B	870	SER	-	EXPRESSION TAG	UNP P10845

- Molecule 2 is a protein called Synaptic vesicle glycoprotein 2C.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	83	Total	C	H	N	O	S	0	0	0
			1320	444	634	103	134	5			
2	D	93	Total	C	H	N	O	S	0	0	0
			1497	502	718	121	151	5			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	439	MET	-	EXPRESSION TAG	UNP Q496J9
C	440	LYS	-	EXPRESSION TAG	UNP Q496J9
C	441	LYS	-	EXPRESSION TAG	UNP Q496J9
C	442	HIS	-	EXPRESSION TAG	UNP Q496J9
C	443	HIS	-	EXPRESSION TAG	UNP Q496J9
C	444	HIS	-	EXPRESSION TAG	UNP Q496J9
C	445	HIS	-	EXPRESSION TAG	UNP Q496J9
C	446	HIS	-	EXPRESSION TAG	UNP Q496J9
C	447	HIS	-	EXPRESSION TAG	UNP Q496J9
C	448	GLY	-	EXPRESSION TAG	UNP Q496J9
C	449	SER	-	EXPRESSION TAG	UNP Q496J9
C	450	LEU	-	EXPRESSION TAG	UNP Q496J9
C	451	VAL	-	EXPRESSION TAG	UNP Q496J9
C	452	PRO	-	EXPRESSION TAG	UNP Q496J9
C	453	ARG	-	EXPRESSION TAG	UNP Q496J9
C	454	GLY	-	EXPRESSION TAG	UNP Q496J9
C	455	SER	-	EXPRESSION TAG	UNP Q496J9
D	439	MET	-	EXPRESSION TAG	UNP Q496J9
D	440	LYS	-	EXPRESSION TAG	UNP Q496J9
D	441	LYS	-	EXPRESSION TAG	UNP Q496J9
D	442	HIS	-	EXPRESSION TAG	UNP Q496J9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	443	HIS	-	EXPRESSION TAG	UNP Q496J9
D	444	HIS	-	EXPRESSION TAG	UNP Q496J9
D	445	HIS	-	EXPRESSION TAG	UNP Q496J9
D	446	HIS	-	EXPRESSION TAG	UNP Q496J9
D	447	HIS	-	EXPRESSION TAG	UNP Q496J9
D	448	GLY	-	EXPRESSION TAG	UNP Q496J9
D	449	SER	-	EXPRESSION TAG	UNP Q496J9
D	450	LEU	-	EXPRESSION TAG	UNP Q496J9
D	451	VAL	-	EXPRESSION TAG	UNP Q496J9
D	452	PRO	-	EXPRESSION TAG	UNP Q496J9
D	453	ARG	-	EXPRESSION TAG	UNP Q496J9
D	454	GLY	-	EXPRESSION TAG	UNP Q496J9
D	455	SER	-	EXPRESSION TAG	UNP Q496J9

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	6	Total Cl 6 6	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 5 is water.

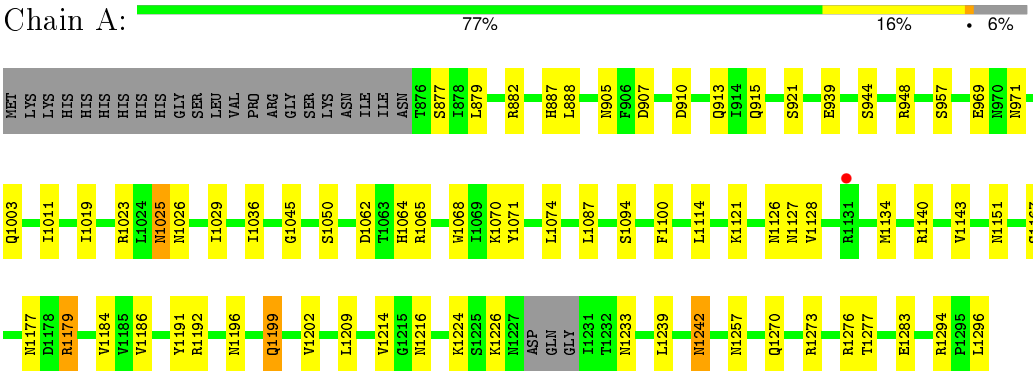
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	50	Total O 50 50	0	0
5	B	18	Total O 18 18	0	0
5	C	6	Total O 6 6	0	0
5	D	8	Total O 8 8	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

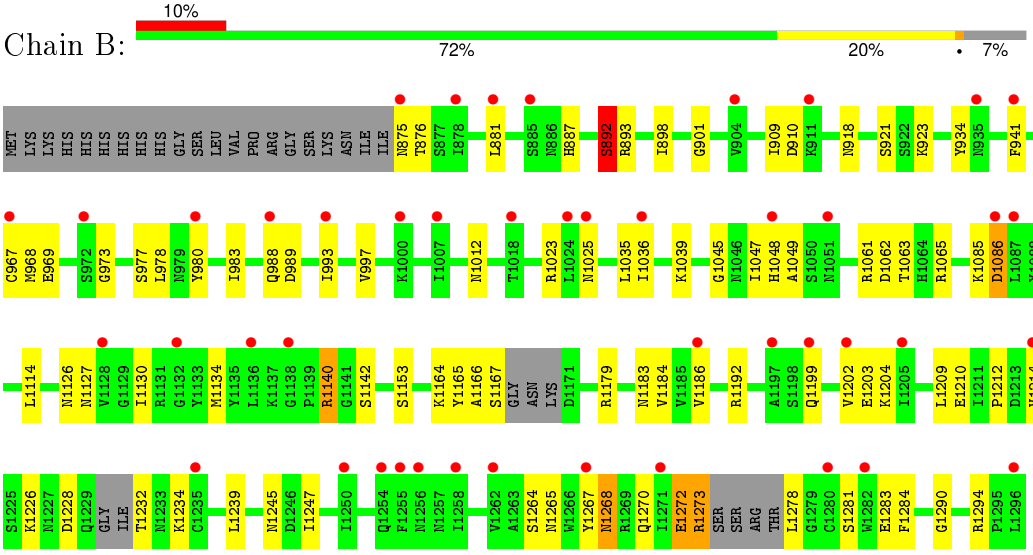
- Molecule 1: Botulinum neurotoxin type A

Chain A:



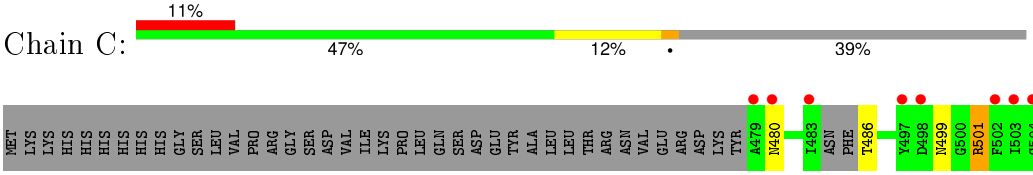
- Molecule 1: Botulinum neurotoxin type A

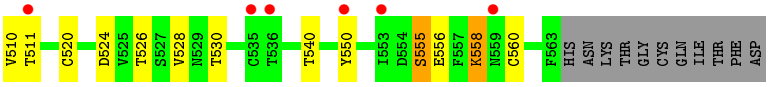
Chain B:



- Molecule 2: Synaptic vesicle glycoprotein 2C

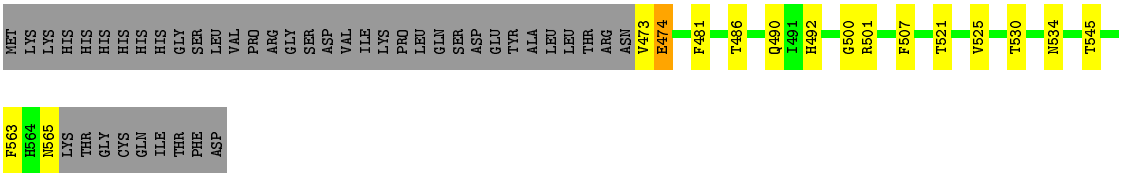
Chain C:





- Molecule 2: Synaptic vesicle glycoprotein 2C

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	115.44Å 105.26Å 127.96Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	19.93 – 2.30 19.93 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.93-2.30) 99.9 (19.93-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 2.30Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1389)	Depositor
R, R_{free}	0.235 , 0.269 0.237 , 0.272	Depositor DCC
R_{free} test set	2035 reflections (3.00%)	DCC
Wilson B-factor (Å^2)	29.6	Xtriage
Anisotropy	0.519	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.44 , 32.5	EDS
Estimated twinning fraction	0.430 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Outliers	0 of 67843 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	16539	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.29% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, CL

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	0.44	0/3524	0.60	0/4761
1	B	0.33	0/3481	0.52	0/4703
2	C	0.31	0/703	0.48	0/945
2	D	0.46	0/800	0.58	0/1077
All	All	0.39	0/8508	0.56	0/11486

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
2	D	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
2	D	563	PHE	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	3442	3412	3401	35	0
1	B	3411	3367	3363	38	0
2	C	686	634	633	12	0
2	D	779	718	716	6	0
3	A	6	0	0	0	0
4	A	2	0	0	0	0
5	A	50	0	0	7	0
5	B	18	0	0	0	0
5	C	6	0	0	1	0
5	D	8	0	0	1	0
All	All	8408	8131	8113	90	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 5.

The worst 5 of 90 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:1216:ASN:ND2	5:A:1432:HOH:O	2.14	0.78
1:A:1186:VAL:O	5:A:1425:HOH:O	2.07	0.71
1:B:1265:ASN:OD1	1:B:1268:ASN:ND2	2.23	0.71
2:D:565:ASN:OD1	5:D:608:HOH:O	2.09	0.70
1:A:1179:ARG:NH2	5:A:1413:HOH:O	2.25	0.68

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	413/443 (93%)	385 (93%)	28 (7%)	0	100 100
1	B	405/443 (91%)	349 (86%)	49 (12%)	7 (2%)	11 10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	C	79/136 (58%)	71 (90%)	8 (10%)	0	100 100
2	D	91/136 (67%)	87 (96%)	3 (3%)	1 (1%)	17 18
All	All	988/1158 (85%)	892 (90%)	88 (9%)	8 (1%)	24 27

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1166	ALA
2	D	474	GLU
1	B	1140	ARG
1	B	892	SER
1	B	980	TYR

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	387/408 (95%)	364 (94%)	23 (6%)	24 32
1	B	382/408 (94%)	351 (92%)	31 (8%)	15 18
2	C	79/128 (62%)	74 (94%)	5 (6%)	22 29
2	D	89/128 (70%)	85 (96%)	4 (4%)	34 46
All	All	937/1072 (87%)	874 (93%)	63 (7%)	20 26

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	969	GLU
1	B	1048	HIS
2	C	558	LYS
1	B	977	SER
1	B	997	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	988	GLN
2	C	480	ASN
2	C	499	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	416/443 (93%)	0.05	1 (0%) 95 97	12, 22, 43, 59	0
1	B	413/443 (93%)	0.81	45 (10%) 7 11	26, 51, 75, 103	0
2	C	83/136 (61%)	1.08	15 (18%) 2 3	26, 56, 73, 78	0
2	D	93/136 (68%)	0.04	0 100 100	14, 27, 44, 66	0
All	All	1005/1158 (86%)	0.44	61 (6%) 25 33	12, 37, 71, 103	0

The worst 5 of 61 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	483	ILE	6.5
1	B	875	ASN	6.1
1	B	1202	VAL	5.2
1	B	1087	LEU	5.1
1	B	1138	GLY	5.1

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 carbohydrates 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. 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, 95^{th} 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
3	CL	A	1308	1/1	0.99	0.15	0.37	24,24,24,24	0
3	CL	A	1301	1/1	0.93	0.14	0.36	37,37,37,37	0
4	NA	A	1306	1/1	0.99	0.13	-0.87	22,22,22,22	0
3	CL	A	1305	1/1	0.97	0.12	-1.15	32,32,32,32	0
3	CL	A	1303	1/1	0.99	0.08	-2.44	30,30,30,30	0
3	CL	A	1304	1/1	0.99	0.08	-3.45	24,24,24,24	0
4	NA	A	1307	1/1	0.98	0.10	-5.66	15,15,15,15	0
3	CL	A	1302	1/1	0.94	0.07	-	45,45,45,45	0

6.5 Other polymers (i)

There are no such residues in this entry.