



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 15, 2025 – 10:08 AM EDT

PDB ID : 9CDS / pdb_00009cds
Title : Crystal structure of OspA ST1 from *B. burgdorferi* bound to monoclonal antibody LA-2
Authors : Laciak, A.R.; Lai, Y.-T.; Dhingra, Y.
Deposited on : 2024-06-25
Resolution : 1.85 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

<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 Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.45.1

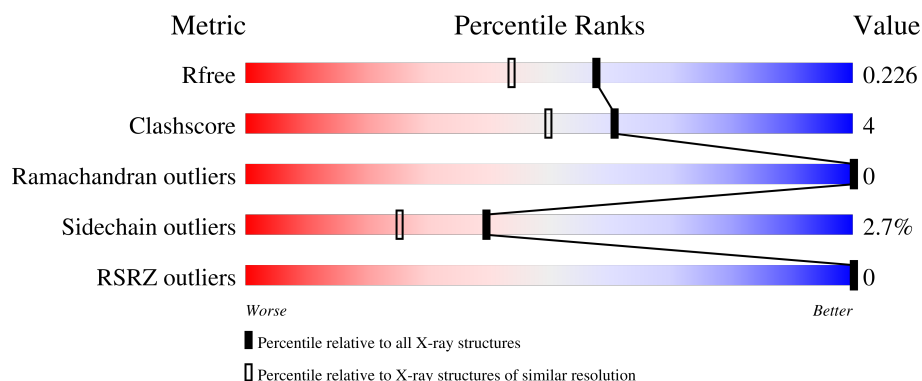
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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}	164625	3097 (1.86-1.86)
Clashscore	180529	3359 (1.86-1.86)
Ramachandran outliers	177936	3335 (1.86-1.86)
Sidechain outliers	177891	3335 (1.86-1.86)
RSRZ outliers	164620	3097 (1.86-1.86)

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	213	<div> <div>92%</div> <div>7%</div> </div>
1	D	213	<div> <div>86%</div> <div>13%</div> <div>.</div> </div>
2	B	213	<div> <div>84%</div> <div>13%</div> <div>..</div> </div>
2	E	213	<div> <div>81%</div> <div>17%</div> <div>.</div> </div>
3	C	290	<div> <div>77%</div> <div>8%</div> <div>14%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	290	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: a green segment representing 76%, a yellow segment representing 9%, and a grey segment representing 14%. The percentages are labeled below the bar.

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10807 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 Hybridoma Antibody LA2 (Light Chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	3	0
			1671	1040	284	341	6			
1	D	211	Total	C	N	O	S	0	2	0
			1648	1028	281	333	6			

- Molecule 2 is a protein called Hybridoma Antibody LA2 (Heavy Chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	210	Total	C	N	O	S	0	1	0
			1573	993	254	318	8			
2	E	211	Total	C	N	O	S	0	3	0
			1589	1003	256	322	8			

- Molecule 3 is a protein called Outer surface protein A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	248	Total	C	N	O	S	0	2	0
			1886	1171	313	401	1			
3	F	248	Total	C	N	O	S	0	0	0
			1877	1165	312	399	1			

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	9	MET	-	expression tag	UNP P0CL66
C	10	LYS	-	expression tag	UNP P0CL66
C	11	ALA	-	expression tag	UNP P0CL66
C	12	ILE	-	expression tag	UNP P0CL66
C	13	LEU	-	expression tag	UNP P0CL66
C	14	VAL	-	expression tag	UNP P0CL66
C	15	VAL	-	expression tag	UNP P0CL66
C	16	LEU	-	expression tag	UNP P0CL66

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	17	LEU	-	expression tag	UNP P0CL66
C	18	TYR	-	expression tag	UNP P0CL66
C	19	THR	-	expression tag	UNP P0CL66
C	20	PHE	-	expression tag	UNP P0CL66
C	21	THR	-	expression tag	UNP P0CL66
C	22	THR	-	expression tag	UNP P0CL66
C	23	ALA	-	expression tag	UNP P0CL66
C	24	ASN	-	expression tag	UNP P0CL66
C	25	ALA	-	expression tag	UNP P0CL66
C	73	ALA	SER	conflict	UNP P0CL66
C	165	PHE	TYR	conflict	UNP P0CL66
C	166	ILE	VAL	conflict	UNP P0CL66
C	170	ARG	THR	conflict	UNP P0CL66
C	171	PHE	LEU	conflict	UNP P0CL66
C	190	ASP	ASN	conflict	UNP P0CL66
C	202	GLN	ASN	conflict	UNP P0CL66
C	253	VAL	THR	conflict	UNP P0CL66
C	274	LEU	-	expression tag	UNP P0CL66
C	275	VAL	-	expression tag	UNP P0CL66
C	276	PRO	-	expression tag	UNP P0CL66
C	277	ARG	-	expression tag	UNP P0CL66
C	278	GLY	-	expression tag	UNP P0CL66
C	279	SER	-	expression tag	UNP P0CL66
C	280	GLY	-	expression tag	UNP P0CL66
C	281	HIS	-	expression tag	UNP P0CL66
C	282	HIS	-	expression tag	UNP P0CL66
C	283	HIS	-	expression tag	UNP P0CL66
C	284	HIS	-	expression tag	UNP P0CL66
C	285	HIS	-	expression tag	UNP P0CL66
C	286	HIS	-	expression tag	UNP P0CL66
C	287	HIS	-	expression tag	UNP P0CL66
C	288	HIS	-	expression tag	UNP P0CL66
C	289	SER	-	expression tag	UNP P0CL66
C	290	ALA	-	expression tag	UNP P0CL66
C	291	TRP	-	expression tag	UNP P0CL66
C	292	SER	-	expression tag	UNP P0CL66
C	293	HIS	-	expression tag	UNP P0CL66
C	294	PRO	-	expression tag	UNP P0CL66
C	295	GLN	-	expression tag	UNP P0CL66
C	296	PHE	-	expression tag	UNP P0CL66
C	297	GLU	-	expression tag	UNP P0CL66
C	298	LYS	-	expression tag	UNP P0CL66

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	9	MET	-	expression tag	UNP P0CL66
F	10	LYS	-	expression tag	UNP P0CL66
F	11	ALA	-	expression tag	UNP P0CL66
F	12	ILE	-	expression tag	UNP P0CL66
F	13	LEU	-	expression tag	UNP P0CL66
F	14	VAL	-	expression tag	UNP P0CL66
F	15	VAL	-	expression tag	UNP P0CL66
F	16	LEU	-	expression tag	UNP P0CL66
F	17	LEU	-	expression tag	UNP P0CL66
F	18	TYR	-	expression tag	UNP P0CL66
F	19	THR	-	expression tag	UNP P0CL66
F	20	PHE	-	expression tag	UNP P0CL66
F	21	THR	-	expression tag	UNP P0CL66
F	22	THR	-	expression tag	UNP P0CL66
F	23	ALA	-	expression tag	UNP P0CL66
F	24	ASN	-	expression tag	UNP P0CL66
F	25	ALA	-	expression tag	UNP P0CL66
F	73	ALA	SER	conflict	UNP P0CL66
F	165	PHE	TYR	conflict	UNP P0CL66
F	166	ILE	VAL	conflict	UNP P0CL66
F	170	ARG	THR	conflict	UNP P0CL66
F	171	PHE	LEU	conflict	UNP P0CL66
F	190	ASP	ASN	conflict	UNP P0CL66
F	202	GLN	ASN	conflict	UNP P0CL66
F	253	VAL	THR	conflict	UNP P0CL66
F	274	LEU	-	expression tag	UNP P0CL66
F	275	VAL	-	expression tag	UNP P0CL66
F	276	PRO	-	expression tag	UNP P0CL66
F	277	ARG	-	expression tag	UNP P0CL66
F	278	GLY	-	expression tag	UNP P0CL66
F	279	SER	-	expression tag	UNP P0CL66
F	280	GLY	-	expression tag	UNP P0CL66
F	281	HIS	-	expression tag	UNP P0CL66
F	282	HIS	-	expression tag	UNP P0CL66
F	283	HIS	-	expression tag	UNP P0CL66
F	284	HIS	-	expression tag	UNP P0CL66
F	285	HIS	-	expression tag	UNP P0CL66
F	286	HIS	-	expression tag	UNP P0CL66
F	287	HIS	-	expression tag	UNP P0CL66
F	288	HIS	-	expression tag	UNP P0CL66
F	289	SER	-	expression tag	UNP P0CL66
F	290	ALA	-	expression tag	UNP P0CL66

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	291	TRP	-	expression tag	UNP P0CL66
F	292	SER	-	expression tag	UNP P0CL66
F	293	HIS	-	expression tag	UNP P0CL66
F	294	PRO	-	expression tag	UNP P0CL66
F	295	GLN	-	expression tag	UNP P0CL66
F	296	PHE	-	expression tag	UNP P0CL66
F	297	GLU	-	expression tag	UNP P0CL66
F	298	LYS	-	expression tag	UNP P0CL66

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	123	Total	O	0	0
			123	123		
4	B	93	Total	O	0	0
			93	93		
4	C	78	Total	O	0	0
			78	78		
4	D	130	Total	O	0	0
			130	130		
4	E	70	Total	O	0	0
			70	70		
4	F	69	Total	O	0	0
			69	69		

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.

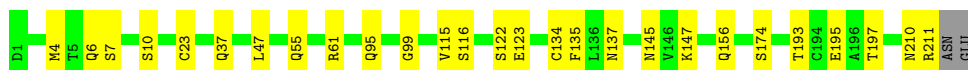
- Molecule 1: Hybridoma Antibody LA2 (Light Chain)

Chain A: 




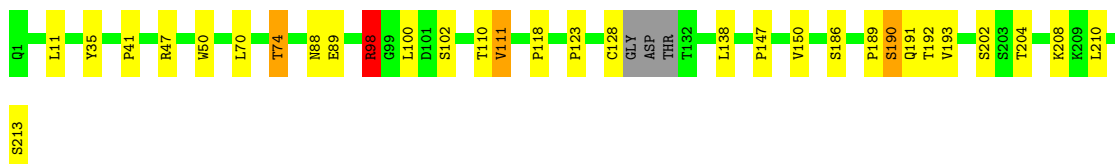
- Molecule 1: Hybridoma Antibody LA2 (Light Chain)

Chain D: 




- Molecule 2: Hybridoma Antibody LA2 (Heavy Chain)

Chain B: 



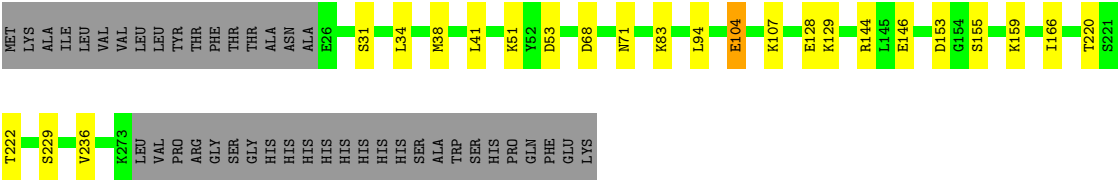
- Molecule 2: Hybridoma Antibody LA2 (Heavy Chain)

Chain E: 

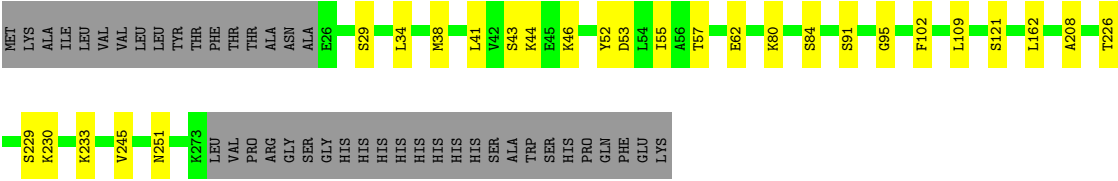


- Molecule 3: Outer surface protein A

Chain C: 



• Molecule 3: Outer surface protein A



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	68.56Å 68.56Å 619.74Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	59.10 – 1.85 59.10 – 1.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (59.10-1.85) 100.0 (59.10-1.85)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.202 , 0.233 0.193 , 0.226	Depositor DCC
R_{free} test set	6937 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	36.3	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 24.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.480 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.495 for H, K, L 0.505 for -K, -H, -L	Depositor
Outliers	0 of 139280 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10807	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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

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	0.52	0/1717	0.95	0/2327
1	D	0.51	0/1691	0.96	0/2292
2	B	0.53	0/1616	0.97	1/2204 (0.0%)
2	E	0.53	0/1638	0.94	0/2234
3	C	0.49	0/1902	0.95	2/2549 (0.1%)
3	F	0.50	0/1887	0.94	0/2528
All	All	0.51	0/10451	0.95	3/14134 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
2	B	0	1
2	E	0	1
All	All	0	3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	74	THR	CA-CB-OG1	-5.78	100.94	109.60
3	C	53	ASP	CA-CB-CG	5.45	118.05	112.60
3	C	68	ASP	CA-CB-CG	5.10	117.70	112.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	98	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	D	61	ARG	Sidechain
2	E	98	ARG	Sidechain

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	1671	0	1611	11	0
1	D	1648	0	1595	13	0
2	B	1573	0	1538	21	0
2	E	1589	0	1558	19	0
3	C	1886	0	1966	15	0
3	F	1877	0	1953	12	0
4	A	123	0	0	2	0
4	B	93	0	0	3	0
4	C	78	0	0	2	0
4	D	130	0	0	2	0
4	E	70	0	0	0	0
4	F	69	0	0	0	0
All	All	10807	0	10221	83	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 4.

The worst 5 of 83 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)
3:C:31:SER:HB3	3:C:41:LEU:HG	1.66	0.76
2:B:41:PRO:HD2	4:B:323:HOH:O	1.91	0.70
3:C:159:LYS:HD3	3:C:166:ILE:HD11	1.74	0.69
3:C:144:ARG:NH1	3:C:146:GLU:OE2	2.26	0.68
3:F:43:SER:HB3	3:F:53:ASP:OD1	1.93	0.68

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	214/213 (100%)	209 (98%)	5 (2%)	0	100	100
1	D	211/213 (99%)	208 (99%)	3 (1%)	0	100	100
2	B	207/213 (97%)	205 (99%)	2 (1%)	0	100	100
2	E	210/213 (99%)	205 (98%)	5 (2%)	0	100	100
3	C	248/290 (86%)	244 (98%)	4 (2%)	0	100	100
3	F	246/290 (85%)	239 (97%)	7 (3%)	0	100	100
All	All	1336/1432 (93%)	1310 (98%)	26 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	191/188 (102%)	188 (98%)	3 (2%)	58	46
1	D	188/188 (100%)	184 (98%)	4 (2%)	48	34
2	B	181/182 (100%)	171 (94%)	10 (6%)	18	6
2	E	184/182 (101%)	178 (97%)	6 (3%)	33	18
3	C	218/252 (86%)	215 (99%)	3 (1%)	62	53
3	F	216/252 (86%)	210 (97%)	6 (3%)	38	24
All	All	1178/1244 (95%)	1146 (97%)	32 (3%)	40	25

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	162	LEU
3	F	233	LYS
2	B	213	SER
2	B	193	VAL
3	F	245	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	137	ASN
1	D	145	ASN
2	E	199	HIS
2	E	39	GLN
2	B	171	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	213/213 (100%)	-1.14	0 100 100	21, 36, 49, 65	3 (1%)
1	D	211/213 (99%)	-1.13	0 100 100	24, 36, 52, 60	2 (0%)
2	B	210/213 (98%)	-1.05	0 100 100	20, 40, 59, 67	1 (0%)
2	E	211/213 (99%)	-1.03	0 100 100	22, 41, 61, 67	3 (1%)
3	C	248/290 (85%)	-0.88	0 100 100	23, 52, 76, 83	2 (0%)
3	F	248/290 (85%)	-0.97	0 100 100	29, 49, 69, 83	0
All	All	1341/1432 (93%)	-1.03	0 100 100	20, 42, 67, 83	11 (0%)

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.