

wwPDB X-ray Structure Validation Summary Report (i)

May 13, 2024 – 12:18 PM EDT

PDB ID : 8SFZ

Title: High Affinity nanobodies against GFP

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Deposited on : 2023-04-11

Resolution : 1.90 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 (i) 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 (1)) 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 : 2.36.2

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)

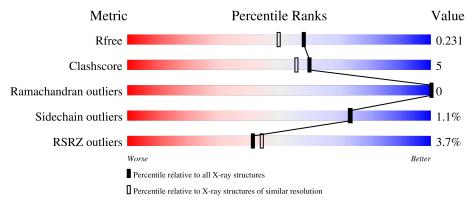
Validation Pipeline (wwPDB-VP) : 2.36.2

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 1.90 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},\ {\rm resolution\ range}(\mathring{\rm A})) \end{array}$		
R_{free}	130704	6207 (1.90-1.90)		
Clashscore	141614	6847 (1.90-1.90)		
Ramachandran outliers	138981	6760 (1.90-1.90)		
Sidechain outliers	138945	6760 (1.90-1.90)		
RSRZ outliers	127900	6082 (1.90-1.90)		

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 <=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	145	77%	7% • 15%
1	В	145	7%	9% • 12%
1	С	145	%	
			80%	9% 11%
2	D	253	81% 	9% 10%
2	F	253	80%	9% 11%



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Mol	Chain	Length	Quality of chain		
3	Е	253	81%	8%	10%



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 16608 atoms, of which 7856 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 LaG35.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	C	C 129	Total	С	Н	N	О	S	0	0	0
1			1941	629	942	172	194	4	0	U	
1	Λ	123	Total	С	Н	N	О	S	0	0	0
1	A	120	1845	596	893	166	186	4			
1	D	199	Total	С	Н	N	О	S	0	0	0
1	В	B 128	1910	617	924	172	192	5			

• Molecule 2 is a protein called Green fluorescent protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
2	2 D 228	Total	С	Н	N	О	S	0	0	0	
2		220	3534	1154	1724	306	344	6	0		
2	F 226	226	Total	С	Н	N	О	S	0	0	0
		220	3470	1145	1679	303	337	6	U	U	

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	ALA	-	insertion	UNP P42212
D	66	CR2	SER	chromophore	UNP P42212
D	66	CR2	TYR	chromophore	UNP P42212
D	66	CR2	GLY	chromophore	UNP P42212
D	72	ALA	SER	conflict	UNP P42212
D	177	HIS	GLN	conflict	UNP P42212
D	239	GLY	-	expression tag	UNP P42212
D	240	LEU	-	expression tag	UNP P42212
D	241	GLU	-	expression tag	UNP P42212
D	242	VAL	-	expression tag	UNP P42212
D	243	LEU	-	expression tag	UNP P42212
D	244	PHE	-	expression tag	UNP P42212
D	245	GLN	-	expression tag	UNP P42212
D	246	GLY	-	expression tag	UNP P42212



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Chain	Residue	Modelled Modelled	Actual	Comment	Reference
D	247	PRO	-	expression tag	UNP P42212
D	248	SER	-	expression tag	UNP P42212
D	249	HIS	-	expression tag	UNP P42212
D	250	HIS	-	expression tag	UNP P42212
D	251	HIS	-	expression tag	UNP P42212
D	252	HIS	-	expression tag	UNP P42212
D	253	HIS	-	expression tag	UNP P42212
D	254	HIS	-	expression tag	UNP P42212
F	1	ALA	-	insertion	UNP P42212
F	66	CR2	SER	chromophore	UNP P42212
F	66	CR2	TYR	chromophore	UNP P42212
F	66	CR2	GLY	chromophore	UNP P42212
F	72	ALA	SER	conflict	UNP P42212
F	177	HIS	GLN	conflict	UNP P42212
F	239	GLY	-	expression tag	UNP P42212
F	240	LEU	-	expression tag	UNP P42212
F	241	GLU	-	expression tag	UNP P42212
F	242	VAL	_	expression tag	UNP P42212
F	243	LEU	_	expression tag	UNP P42212
F	244	PHE	-	expression tag	UNP P42212
F	245	GLN	_	expression tag	UNP P42212
F	246	GLY	-	expression tag	UNP P42212
F	247	PRO	_	expression tag	UNP P42212
F	248	SER	-	expression tag	UNP P42212
F	249	HIS	-	expression tag	UNP P42212
F	250	HIS	-	expression tag	UNP P42212
F	251	HIS	-	expression tag	UNP P42212
F	252	HIS	-	expression tag	UNP P42212
F	253	HIS	-	expression tag	UNP P42212
F	254	HIS	-	expression tag	UNP P42212

 \bullet Molecule 3 is a protein called Green fluorescent protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
3	Е	227	Total 3497	C 1152	H 1694	N 307	O 338	S 6	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Е	1	ALA	-	insertion	UNP P42212
Е	66	CRO	SER	chromophore	UNP P42212



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Chain	Residue	Modelled	Actual	Comment	Reference
Е	66	CRO	TYR	chromophore	UNP P42212
Е	66	CRO	GLY	chromophore	UNP P42212
Е	72	ALA	SER	conflict	UNP P42212
Е	177	HIS	GLN	conflict	UNP P42212
Е	240	GLY	-	expression tag	UNP P42212
Е	241	LEU	-	expression tag	UNP P42212
Е	242	GLU	-	expression tag	UNP P42212
E	243	VAL	-	expression tag	UNP P42212
Е	244	LEU	-	expression tag	UNP P42212
Е	245	PHE	-	expression tag	UNP P42212
E	246	GLN	-	expression tag	UNP P42212
E	247	GLY	-	expression tag	UNP P42212
Е	248	PRO	-	expression tag	UNP P42212
E	249	SER	-	expression tag	UNP P42212
Е	250	HIS	-	expression tag	UNP P42212
E	251	HIS	-	expression tag	UNP P42212
Е	252	HIS	-	expression tag	UNP P42212
Е	253	HIS	-	expression tag	UNP P42212
Е	254	HIS	-	expression tag	UNP P42212
E	255	HIS	-	expression tag	UNP P42212

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	С	1	Total Na 1 1	0	0
4	A	1	Total Na 1 1	0	0

• Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	В	1	Total K 1 1	0	0
5	D	1	Total K 1 1	0	0
5	F	1	Total K 1 1	0	0

• Molecule 6 is water.

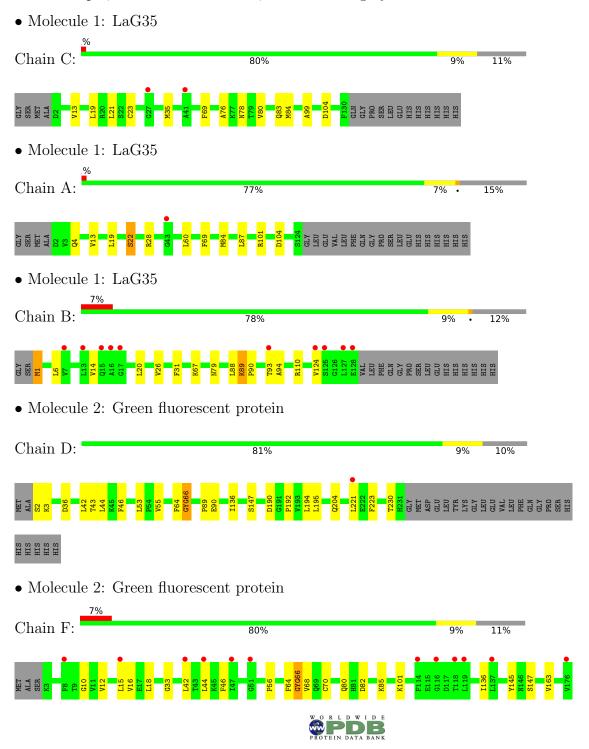


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	С	63	Total O 63 63	0	0
6	A	77	Total O 77 77	0	0
6	В	40	Total O 40 40	0	0
6	D	97	Total O 97 97	0	0
6	E	73	Total O 73 73	0	0
6	F	56	Total O 56 56	0	0



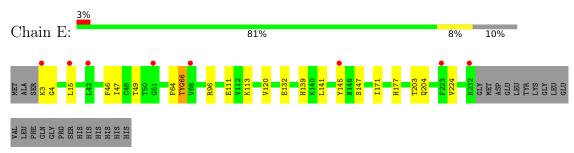
3 Residue-property plots (i)

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 3: Green fluorescent protein





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants	69.65Å 101.73Å 184.48Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.10 - 1.90	Depositor
resolution (A)	46.10 - 1.90	EDS
% Data completeness	99.3 (46.10-1.90)	Depositor
(in resolution range)	99.3 (46.10-1.90)	EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.51 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.19.2-4158	Depositor
P.P.	0.207 , 0.231	Depositor
R, R_{free}	0.206 , 0.231	DCC
R_{free} test set	1999 reflections (1.94%)	wwPDB-VP
Wilson B-factor (Å ²)	35.9	Xtriage
Anisotropy	0.420	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.39, 43.4	EDS
L-test for twinning ²	$ < L > = 0.50, < L^2> = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16608	wwPDB-VP
Average B, all atoms $(Å^2)$	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.36% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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: K, NA, CR2, CRO

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).

Mal	Mol Chain		Bond lengths		ond angles
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	0.69	1/973 (0.1%)	0.75	1/1317 (0.1%)
1	В	0.55	0/1007	0.73	0/1362
1	С	0.65	0/1021	0.74	0/1382
2	D	0.60	0/1833	0.70	0/2479
2	F	0.50	0/1814	0.62	0/2453
3	Е	0.54	0/1827	0.66	0/2470
All	All	0.58	1/8475 (0.0%)	0.69	1/11463 (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 maintenain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	Е	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\text{\AA})$	Ideal(Å)
1	A	22	SER	CA-CB	5.43	1.61	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	60	LEU	CA-CB-CG	5.21	127.29	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
3	Е	96	ARG	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	952	893	893	7	0
1	В	986	924	932	12	0
1	С	999	942	942	9	0
2	D	1810	1724	1737	19	0
2	F	1791	1679	1719	19	0
3	Е	1803	1694	1735	15	0
4	A	1	0	0	0	0
4	С	1	0	0	0	0
5	В	1	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
6	A	77	0	0	1	0
6	В	40	0	0	0	0
6	С	63	0	0	1	0
6	D	97	0	0	1	0
6	E	73	0	0	3	0
6	F	56	0	0	1	0
All	All	8752	7856	7958	75	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 75 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
2:F:70:CYS:O	2:F:85:LYS:NZ	2.01	0.93
1:A:101:ARG:NH1	1:B:1:MET:O	2.10	0.84
2:F:82:ASP:OD2	2:F:85:LYS:HD2	1.88	0.74
1:B:6:LEU:HD22	1:B:26:VAL:HG22	1.71	0.73
3:E:111:GLU:OE1	3:E:113:LYS:NZ	2.23	0.72



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	Percei	ntiles
1	A	121/145 (83%)	120 (99%)	1 (1%)	0	100	100
1	В	126/145 (87%)	119 (94%)	7 (6%)	0	100	100
1	С	127/145 (88%)	125 (98%)	2 (2%)	0	100	100
2	D	223/253 (88%)	221 (99%)	2 (1%)	0	100	100
2	F	221/253 (87%)	211 (96%)	10 (4%)	0	100	100
3	E	222/253 (88%)	218 (98%)	4 (2%)	0	100	100
All	All	1040/1194 (87%)	1014 (98%)	26 (2%)	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	Perce	ntiles
1	A	97/116 (84%)	94 (97%)	3 (3%)	40	32
1	В	100/116 (86%)	97 (97%)	3 (3%)	41	33
1	\mathbf{C}	102/116 (88%)	102 (100%)	0	100	100
2	D	194/219 (89%)	193 (100%)	1 (0%)	88	89
2	F	189/219 (86%)	187 (99%)	2 (1%)	73	73
3	E	192/219 (88%)	191 (100%)	1 (0%)	88	89



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Mol	Chain	Analysed Rotameric Outliers		Percentiles	
All	All	874/1005 (87%)	864 (99%)	10 (1%)	73 73

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	Е	145	TYR
2	F	145	TYR
2	F	147	SER
1	В	1	MET
1	В	20	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	В	59	HIS
2	D	157	GLN
2	F	77	HIS
2	F	184	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)

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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	Bo	Bond lengths			Bond angles		
			nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
3	CRO	Е	66	3	20,20,24	2.71	8 (40%)	25,27,34	3.60	7 (28%)	
2	CR2	F	66	2	20,20,21	2.75	8 (40%)	25,27,29	2.59	8 (32%)	



	Mol	Type	Chain	Res	s Link	Bond lengths			Bond angles		
				nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
	2	CR2	D	66	2	20,20,21	2.71	6 (30%)	25,27,29	3.16	9 (36%)

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
3	CRO	Е	66	3	-	1/6/25/32	0/2/2/2
2	CR2	F	66	2	-	0/6/25/26	0/2/2/2
2	CR2	D	66	2	-	1/6/25/26	0/2/2/2

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(A)
3	Е	66	CRO	C1-N3	6.28	1.47	1.37
2	D	66	CR2	C1-N3	5.79	1.46	1.37
2	F	66	CR2	CA2-C2	5.75	1.54	1.48
2	D	66	CR2	CA2-C2	5.63	1.54	1.48
2	F	66	CR2	C1-N3	5.07	1.45	1.37

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
3	Е	66	CRO	O2-C2-CA2	-12.07	124.18	130.96
3	Е	66	CRO	CA2-C2-N3	8.95	107.61	103.37
2	D	66	CR2	CA2-C2-N3	8.87	107.56	103.37
2	D	66	CR2	C2-N3-C1	-8.51	103.83	107.99
2	F	66	CR2	O2-C2-CA2	-6.93	127.07	130.96

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	66	CR2	C3-CA3-N3-C2
3	Е	66	CRO	C3-CA3-N3-C2

There are no ring outliers.

3 monomers are involved in 3 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Е	66	CRO	1	0
2	F	66	CR2	1	0
2	D	66	CR2	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 5 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 (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, 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>	# RSRZ > 2	$OWAB(\AA^2)$	Q < 0.9
1	A	123/145 (84%)	-0.06	1 (0%) 86 87	29, 37, 58, 77	0
1	В	128/145 (88%)	0.59	10 (7%) 13 14	29, 49, 79, 90	0
1	С	129/145 (88%)	0.11	2 (1%) 72 74	29, 40, 61, 89	0
2	D	227/253 (89%)	0.18	1 (0%) 92 93	29, 39, 62, 80	0
2	F	225/253~(88%)	0.65	17 (7%) 13 15	34, 56, 76, 115	0
3	Е	226/253 (89%)	0.48	8 (3%) 44 47	28, 45, 65, 123	0
All	All	1058/1194 (88%)	0.36	39 (3%) 41 44	28, 43, 71, 123	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	127	LEU	4.1
2	F	51	GLY	4.0
1	С	27	GLY	3.9
1	В	13	LEU	3.9
3	Е	15	LEU	3.8

6.2 Non-standard residues in protein, DNA, RNA chains (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^{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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
2	CR2	F	66	19/20	0.89	0.14	45,56,63,68	0
3	CRO	E	66	19/23	0.93	0.17	32,40,50,54	0
2	CR2	D	66	19/20	0.94	0.12	32,37,45,46	0



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^{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	$\mathbf{B} ext{-}\mathbf{factors}(\mathring{\mathbf{A}}^2)$	Q < 0.9
4	NA	A	201	1/1	0.92	0.11	48,48,48,48	0
5	K	В	201	1/1	0.92	0.10	58,58,58,58	0
4	NA	С	201	1/1	0.93	0.10	39,39,39,39	0
5	K	D	301	1/1	0.99	0.11	40,40,40,40	0
5	K	F	301	1/1	0.99	0.13	38,38,38,38	1

6.5 Other polymers (i)

There are no such residues in this entry.

