

wwPDB X-ray Structure Validation Summary Report (i)

Jun 11, 2024 – 07:23 pm BST

PDB ID : 8RP8

Title : Structure of K2 Fab in complex with human CD47 ECD

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Deposited on : 2024-01-12

Resolution : 2.00 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 : 1.8.4, 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) roteins) : Engh & Huber (2001)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

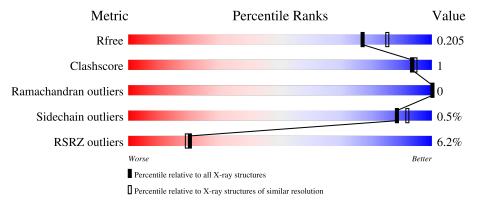
Validation Pipeline (wwPDB-VP) : 2.36.2

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 2.00 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\mathring{\rm A})}) \end{array}$
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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		
			9%		
1	A	223	91%	•	5%
			10%		
1	Н	223	93%		• 5%
			4%		
2	В	215	94%		5%
			4%		
2	L	215	95%		•
			3%		
3	\mathbf{C}	129	87%	5%	9%



Mol	Chain	Length	Quality of chain	- · · ·						
			3%							
3	D	129	84%	7%	9%					

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:

\mathbf{M}	ol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density	
6	<u>.</u> :	NAG	С	202	-	-	-	X	



2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 9297 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 K2 Fab heavy chain.

\mathbf{Mol}	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	A	212	Total 1580	C 998	- '	O 313	S 6	0	2	0
1	Н	211	Total 1568	C 991		O 310	S 6	0	1	0

• Molecule 2 is a protein called K2 Fab light chain.

Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace
2	В	214	Total 1663	C 1038	7.1	O 338	S 6	0	5	0
2	L	214	Total 1662	C 1035		O 339	S 6	0	4	0

• Molecule 3 is a protein called Leukocyte surface antigen CD47.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
3	С	118	Total	_		О	S	0	2	0	
		110	950	606	151	189	4				
9	D	118	Total	С	N	O	S	0	1	0	
3	D	110	946	602	151	189	4	U	1	U	

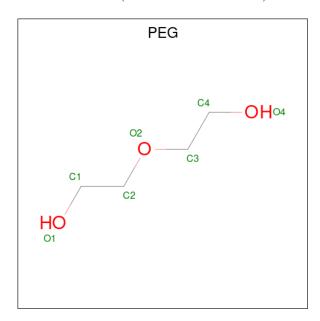
There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference	
С	15	GLY	CYS	conflict	UNP Q08722	
С	124	HIS	-	expression tag	UNP Q08722	
С	125	HIS	-	expression tag	UNP Q08722	
С	126	HIS	-	expression tag	UNP Q08722	
С	127	HIS	-	expression tag	UNP Q08722	
С	128	HIS	-	expression tag	UNP Q08722	
С	129	HIS	-	expression tag	UNP Q08722	
D	15	GLY	CYS	conflict	UNP Q08722	



Chain	Residue	Modelled	Actual	Comment	Reference
D	124	HIS	-	expression tag	UNP Q08722
D	125	HIS	-	expression tag	UNP Q08722
D	126	HIS	-	expression tag	UNP Q08722
D	127	HIS	-	expression tag	UNP Q08722
D	128	HIS	-	expression tag	UNP Q08722
D	129	HIS	-	expression tag	UNP Q08722

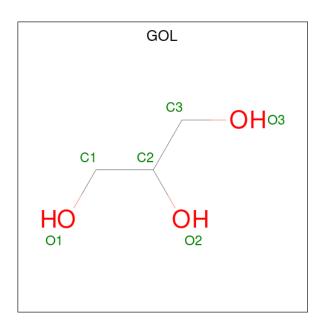
 $\bullet \ \ Molecule\ 4 \ is\ DI(HYDROXYETHYL)ETHER\ (three-letter\ code:\ PEG)\ (formula:\ C_4H_{10}O_3).$



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 4 3	0	0
4	Н	1	Total C O 7 4 3	0	0

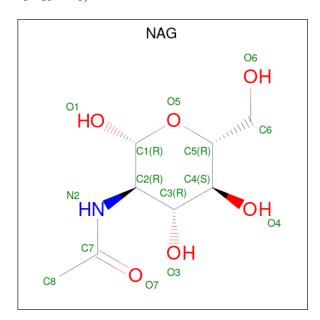
 \bullet Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $\mathrm{C_3H_8O_3}).$





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	В	1	Total C O 6 3 3	0	0
5	L	1	Total C O 6 3 3	0	0

• Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



\mathbf{Mol}	Chain	Residues	Atoms				ZeroOcc	AltConf
6	С	1	Total 14	C 8	N 1	O 5	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	
6	С	1	Total C N O	0	0	
0		1	14 8 1 5	0	0	
6	\mathbf{C}	1	Total C N O	0	0	
		1	14 8 1 5		0	
6	D	1	Total C N O	0	0	
0	D	1	14 8 1 5	0		
6	D	1	Total C N O	0	0	
0	D	1	14 8 1 5	0		
6	D	1	Total C N O	0	0	
	ש	1	14 8 1 5			

• Molecule 7 is water.

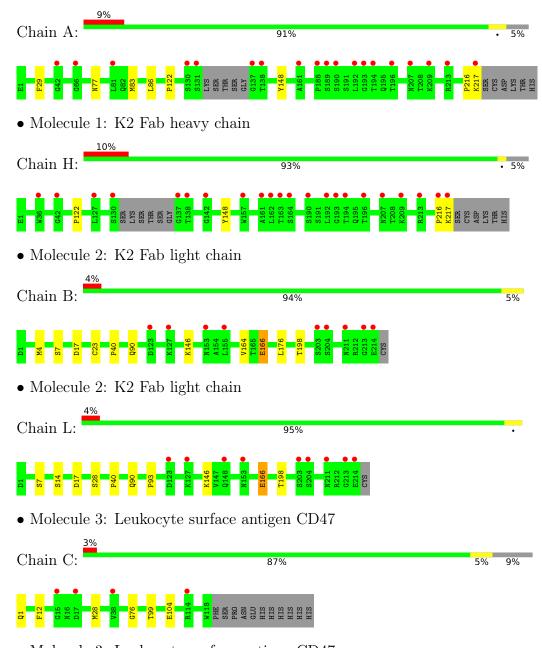
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	108	Total O 108 108	0	0
7	В	185	Total O 185 185	0	2
7	С	96	Total O 96 96	0	0
7	D	115	Total O 115 115	0	0
7	Н	127	Total O 127 127	0	0
7	L	187	Total O 187 187	0	0



3 Residue-property plots (i)

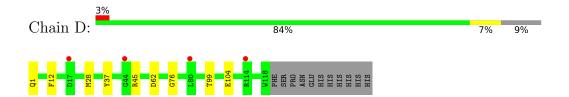
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: K2 Fab heavy chain



• Molecule 3: Leukocyte surface antigen CD47







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	69.42Å 71.81Å 78.38Å	Depositor
a, b, c, α , β , γ	109.45° 95.55° 118.90°	Depositor
Resolution (Å)	20.06 - 2.00	Depositor
rtesolution (A)	20.06 - 2.00	EDS
% Data completeness	97.4 (20.06-2.00)	Depositor
(in resolution range)	97.4 (20.06-2.00)	EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	7.25 (at 2.01Å)	Xtriage
Refinement program	BUSTER 2.11.8, REFMAC 5.8.0419	Depositor
R, R_{free}	0.180 , 0.214	Depositor
It, It free	0.174 , 0.205	DCC
R_{free} test set	3862 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	29.2	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.34, 46.5	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	9297	wwPDB-VP
Average B, all atoms (\mathring{A}^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.78% 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: PCA, GOL, NAG, PEG

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	
IVIOI		RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	0.36	0/1623	0.58	0/2208
1	Н	0.37	0/1608	0.59	0/2188
2	В	0.44	0/1707	0.62	0/2316
2	L	0.44	0/1700	0.63	0/2306
3	С	0.39	0/963	0.60	0/1305
3	D	0.40	0/956	0.61	0/1295
All	All	0.40	0/8557	0.60	0/11618

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	1580	0	1546	4	0
1	Н	1568	0	1533	2	0
2	В	1663	0	1631	6	0
2	L	1662	0	1621	6	0
3	С	950	0	936	3	0
3	D	946	0	927	5	0
4	A	7	0	10	0	0



n previous	paae
	n previous

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Н	7	0	10	0	0
5	В	6	0	8	0	0
5	L	6	0	8	0	0
6	С	42	0	39	1	0
6	D	42	0	39	1	0
7	A	108	0	0	0	0
7	В	185	0	0	0	0
7	С	96	0	0	0	0
7	D	115	0	0	0	0
7	Н	127	0	0	0	0
7	L	187	0	0	0	0
All	All	9297	0	8308	23	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 1.

The worst 5 of 23 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned} \operatorname{Clash} \ \operatorname{overlap}\ (\begin{subarray}{c} \begin{subarray}{c} \begi$
2:B:40:PRO:HG2	2:B:166:GLU:HG3	1.76	0.68
3:D:12:PHE:HB3	6:D:201:NAG:H82	1.79	0.65
3:C:12:PHE:HB3	6:C:201:NAG:H82	1.80	0.64
2:L:40:PRO:HG2	2:L:166:GLU:HG3	1.80	0.63
2:B:164[A]:VAL:HG22	2:B:176:LEU:HD12	1.91	0.52

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	210/223 (94%)	203 (97%)	7 (3%)	0	100 100



I 'omtamalod	trom	mmonia	maaa
Continued	11 0116	DICUIUUS	Daue
	.,	10	1

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	Н	208/223 (93%)	202 (97%)	6 (3%)	0	100	100
2	В	217/215 (101%)	210 (97%)	7 (3%)	0	100	100
2	L	216/215 (100%)	210 (97%)	6 (3%)	0	100	100
3	\mathbf{C}	118/129 (92%)	116 (98%)	2 (2%)	0	100	100
3	D	117/129 (91%)	115 (98%)	2 (2%)	0	100	100
All	All	1086/1134 (96%)	1056 (97%)	30 (3%)	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	176/184 (96%)	176 (100%)	0	100 100
1	Н	174/184 (95%)	174 (100%)	0	100 100
2	В	193/189 (102%)	191 (99%)	2 (1%)	76 81
2	L	192/189 (102%)	188 (98%)	4 (2%)	53 57
3	С	108/117 (92%)	108 (100%)	0	100 100
3	D	107/117 (92%)	107 (100%)	0	100 100
All	All	950/980 (97%)	944 (99%)	6 (1%)	88 90

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	28[B]	SER
2	L	90	GLN
2	L	166	GLU
2	В	166	GLU
2	В	90	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	77	ASN
2	В	211	ASN
2	L	79	GLN
2	L	211	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

2 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	Trmo	Chain	Chain Res	Res Link	В	Bond lengths			Bond angles		
MIOI	Type	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2	
3	PCA	С	1	3	7,8,9	0.77	0	9,10,12	1.27	1 (11%)	
3	PCA	D	1	3	7,8,9	0.81	0	9,10,12	1.67	2 (22%)	

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.

\mathbf{Mol}	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PCA	С	1	3	-	0/0/11/13	0/1/1/1
3	PCA	D	1	3	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
3	D	1	PCA	CB-CA-C	-3.26	108.22	112.70
3	С	1	PCA	CB-CA-C	-2.77	108.89	112.70
3	D	1	PCA	OE-CD-CG	-2.20	122.92	126.76



There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

10 ligands 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).

Mal	Trimo	Chain	Dag	Link	Во	ond leng	ths	Bond angles		
Mol	Type	Chain	Res	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	D	202	3	14,14,15	0.27	0	17,19,21	0.56	0
4	PEG	A	301	-	6,6,6	0.11	0	5,5,5	0.14	0
6	NAG	D	201	3	14,14,15	0.30	0	17,19,21	0.57	0
5	GOL	В	301	-	5,5,5	0.07	0	5,5,5	0.33	0
6	NAG	С	202	3	14,14,15	0.26	0	17,19,21	0.54	0
6	NAG	С	203	3	14,14,15	0.27	0	17,19,21	0.51	0
6	NAG	D	203	3	14,14,15	0.27	0	17,19,21	0.50	0
6	NAG	С	201	3	14,14,15	0.30	0	17,19,21	0.51	0
5	GOL	L	301	-	5,5,5	0.04	0	5,5,5	0.27	0
4	PEG	Н	301	-	6,6,6	0.14	0	5,5,5	0.12	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
6	NAG	D	202	3	-	0/6/23/26	0/1/1/1
4	PEG	A	301	-	-	2/4/4/4	-



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	D	201	3	-	0/6/23/26	0/1/1/1
5	GOL	В	301	-	-	1/4/4/4	-
6	NAG	С	202	3	-	0/6/23/26	0/1/1/1
6	NAG	С	203	3	-	0/6/23/26	0/1/1/1
6	NAG	D	203	3	-	0/6/23/26	0/1/1/1
6	NAG	С	201	3	-	0/6/23/26	0/1/1/1
5	GOL	L	301	-	-	1/4/4/4	-
4	PEG	Н	301	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	Н	301	PEG	O1-C1-C2-O2
4	A	301	PEG	O1-C1-C2-O2
5	В	301	GOL	C1-C2-C3-O3
4	Н	301	PEG	C4-C3-O2-C2
4	A	301	PEG	O2-C3-C4-O4

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	201	NAG	1	0
6	С	201	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, 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>	$\#\mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q < 0.9
1	A	212/223~(95%)	0.34	19 (8%) 9 8	21, 38, 65, 76	0
1	Н	211/223 (94%)	0.29	22 (10%) 6 5	21, 37, 67, 79	0
2	В	214/215 (99%)	0.06	9 (4%) 36 35	18, 30, 54, 75	0
2	L	214/215 (99%)	-0.00	9 (4%) 36 35	18, 30, 55, 81	0
3	С	117/129 (90%)	-0.03	4 (3%) 45 44	23, 35, 46, 52	0
3	D	117/129 (90%)	-0.12	4 (3%) 45 44	22, 32, 44, 50	0
All	All	1085/1134 (95%)	0.12	67 (6%) 20 19	18, 34, 59, 81	0

The worst 5 of 67 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	В	213	GLY	6.2
1	Н	193	GLY	5.9
1	Н	194	THR	5.6
1	A	131	SER	5.2
2	L	213	GLY	4.6

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
3	PCA	С	1	8/9	0.81	0.25	35,39,43,51	0
3	PCA	D	1	8/9	0.92	0.15	33,37,40,48	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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
6	NAG	С	202	14/15	0.68	0.42	66,69,69,70	0
5	GOL	В	301	6/6	0.73	0.35	60,60,60,60	0
6	NAG	С	201	14/15	0.78	0.22	40,46,50,51	0
5	GOL	L	301	6/6	0.79	0.38	63,63,64,64	0
4	PEG	Н	301	7/7	0.81	0.18	55,56,58,58	0
6	NAG	С	203	14/15	0.82	0.31	60,63,63,64	0
6	NAG	D	202	14/15	0.83	0.45	59,61,62,63	0
6	NAG	D	203	14/15	0.84	0.30	55,57,59,59	0
6	NAG	D	201	14/15	0.86	0.17	35,41,45,46	0
4	PEG	A	301	7/7	0.90	0.13	48,50,51,52	0

6.5 Other polymers (i)

There are no such residues in this entry.

