

Full wwPDB X-ray Structure Validation Report (i)

Nov 8, 2023 – 06:08 PM JST

PDB ID : 8IR4

Title : Crystal structure of the SLF1 BRCT domain in complex with a Rad18 peptide

containing pS442

Authors : Xiang, S.; Huang, W.; Qiu, F.

Deposited on : 2023-03-17

Resolution : 1.62 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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:

Mol Probity : 4.02b-467

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.36

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

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

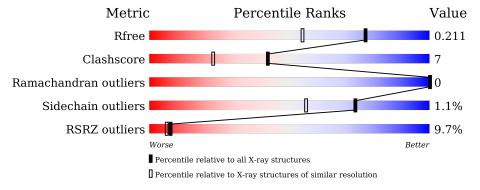
Validation Pipeline (wwPDB-VP) : 2.36

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 1.62 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}(\mathring{\rm A})) \end{array}$
R_{free}	130704	4693 (1.64-1.60)
Clashscore	141614	5002 (1.64-1.60)
Ramachandran outliers	138981	4888 (1.64-1.60)
Sidechain outliers	138945	4887 (1.64-1.60)
RSRZ outliers	127900	4609 (1.64-1.60)

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	207	4%	87%	8% 5%	%
1	В	207	12%	78%	16% 5%	6
2	С	17	18%	71%	24% 6	5%
2	D	17	35% 24%	59%	18%	_



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 4004 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 SMC5-SMC6 complex localization factor protein 1.

Mol	Chain	Residues	\mathbf{Atoms}					ZeroOcc	AltConf	Trace
1	A	196	Total 1594	C 1028	11	O 281	S 7	0	0	0
1	В	197		C 1041	N	О	S 7	0	2	0

There are 16 discrepancies between the modelled and reference sequences:

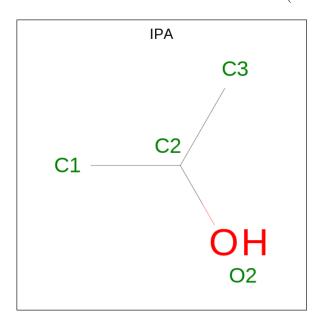
Chain	Residue	Modelled	Actual	Comment	Reference
A	200	LEU	-	expression tag	UNP Q9BQI6
A	201	GLU	-	expression tag	UNP Q9BQI6
A	202	HIS	-	expression tag	UNP Q9BQI6
A	203	HIS	_	expression tag	UNP Q9BQI6
A	204	HIS	-	expression tag	UNP Q9BQI6
A	205	HIS	-	expression tag	UNP Q9BQI6
A	206	HIS	-	expression tag	UNP Q9BQI6
A	207	HIS	-	expression tag	UNP Q9BQI6
В	200	LEU	-	expression tag	UNP Q9BQI6
В	201	GLU	-	expression tag	UNP Q9BQI6
В	202	HIS	-	expression tag	UNP Q9BQI6
В	203	HIS	-	expression tag	UNP Q9BQI6
В	204	HIS	-	expression tag	UNP Q9BQI6
В	205	HIS	-	expression tag	UNP Q9BQI6
В	206	HIS	-	expression tag	UNP Q9BQI6
В	207	HIS	-	expression tag	UNP Q9BQI6

• Molecule 2 is a protein called SER-ASP-SER-CYS-ASN-SER-SEP-SER-SER-ASP-ILE-ILE -ARG-ASP-LEU-LEU-GLU.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace			
2	C	16	Total	С	N	О	Р	S	0	0	0
2		10	124	69	20	33	1	1	U		
2	D	1.4	Total	С	N	О	Р	S	0	0	0
	ש	14	107	60	18	27	1	1	U	U	U



• Molecule 3 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C₃H₈O).



Mo	l Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 3 1	0	0
3	В	1	Total C O 4 3 1	0	0

• Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Cl 2 2	0	0
4	В	2	Total Cl 2 2	0	0

• Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Mg 2 2	0	0
5	В	1	Total Mg 1 1	0	0

• Molecule 6 is water.



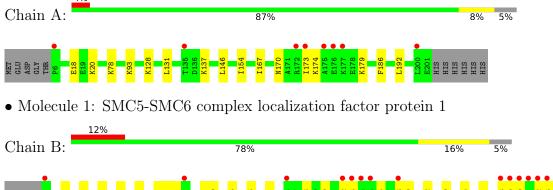
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	279	Total O 279 279	0	0
6	В	234	Total O 234 234	0	0
6	С	15	Total O 15 15	0	0
6	D	21	Total O 21 21	0	0



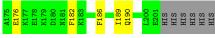
3 Residue-property plots (i)

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: SMC5-SMC6 complex localization factor protein 1







 \bullet Molecule 2: SER-ASP-SER-CYS-ASN-SER-SEP-SER-SER-ASP-ILE-ILE-ARG-ASP-LEU-LE U-GLU



 \bullet Molecule 2: SER-ASP-SER-CYS-ASN-SER-SEP-SER-SER-ASP-ILE-ILE-ARG-ASP-LEU-LE U-GLU





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	40.42Å 76.10Å 141.37Å	Donositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.60 - 1.62	Depositor
Resolution (A)	35.34 - 1.62	EDS
% Data completeness	97.6 (29.60-1.62)	Depositor
(in resolution range)	97.6 (35.34-1.62)	EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.32 (at 1.62Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
D D.	0.181 , 0.213	Depositor
R, R_{free}	0.180 , 0.211	DCC
R_{free} test set	2828 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	18.5	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.34, 50.3	EDS
L-test for twinning ²	$ < L >=0.48, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4004	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.21% 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: IPA, MG, CL, SEP

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	Chain	$\mid \text{RMSZ} \mid \# Z > 5$		RMSZ	# Z > 5	
1	A	0.29	0/1630	0.54	0/2189	
1	В	0.29	0/1654	0.55	0/2222	
2	С	0.25	0/112	0.51	0/148	
2	D	0.27	0/95	0.63	0/125	
All	All	0.29	0/3491	0.55	0/4684	

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	1594	0	1651	11	0
1	В	1615	0	1675	31	0
2	С	124	0	109	2	0
2	D	107	0	99	13	0
3	A	4	0	8	0	0
3	В	4	0	8	0	0
4	A	2	0	0	1	0
4	В	2	0	0	0	0
5	A	2	0	0	0	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	В	1	0	0	0	0
6	A	279	0	0	1	0
6	В	234	0	0	6	1
6	С	15	0	0	0	0
6	D	21	0	0	1	0
All	All	4004	0	3550	48	1

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 7.

All (48) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

A + 1	A4 a 2	Interatomic	Clash
Atom-1	Atom-2	${\rm distance}({\rm \AA})$	overlap (Å)
1:B:133:VAL:HG21	1:B:189:ILE:HD11	1.41	1.02
1:B:190:GLN:HE21	2:D:451:LEU:HD11	1.42	0.82
1:B:138:ARG:NH1	2:D:449:ASP:OD2	2.13	0.81
1:A:18:GLU:OE1	6:A:1101:HOH:O	1.97	0.81
1:B:133:VAL:HG13	6:B:403:HOH:O	1.84	0.76
1:B:42[B]:ASN:ND2	6:B:404:HOH:O	2.24	0.71
1:B:138:ARG:HB3	2:D:450:LEU:HD21	1.73	0.70
1:B:133:VAL:HG22	1:B:168:ALA:HA	1.72	0.70
1:B:173:ILE:HG12	1:B:186:PHE:HB3	1.74	0.69
1:A:128:LYS:HE3	1:A:154:ILE:HD11	1.75	0.68
2:D:445:ASP:HB3	2:D:448:ARG:NH1	2.08	0.67
1:B:190:GLN:NE2	2:D:451:LEU:HD11	2.12	0.64
2:D:445:ASP:HB3	2:D:448:ARG:HH11	1.61	0.64
1:B:128[B]:LYS:HE2	1:B:154:ILE:HD11	1.86	0.58
2:D:448:ARG:HH11	2:D:448:ARG:HG2	1.71	0.56
1:A:78:LYS:HD3	6:B:532:HOH:O	2.06	0.55
1:B:121:PRO:HB2	1:B:150:LYS:HG3	1.88	0.54
2:D:447:ILE:O	2:D:451:LEU:HD13	2.09	0.53
1:B:132:LEU:HD11	1:B:182:PHE:CE2	2.43	0.53
1:B:168:ALA:HB1	1:B:172:ARG:HG2	1.90	0.52
1:A:179:LYS:HE3	1:A:186:PHE:HB2	1.91	0.52
1:B:25:LYS:NZ	6:B:402:HOH:O	2.17	0.52
1:B:94:ILE:HD11	1:B:106:SER:HB3	1.92	0.51
1:B:169:SER:OG	6:B:403:HOH:O	2.19	0.51
1:A:174:LYS:HB2	1:A:179:LYS:NZ	2.28	0.49
1:B:136:ASP:H	1:B:139:SER:HB3	1.77	0.49
1:B:130:VAL:HG22	1:B:154:ILE:HG13	1.94	0.48
1:B:128[B]:LYS:NZ	1:B:161:SER:O	2.35	0.46



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A + 1	A 4 0	Interatomic	Clash
Atom-1	Atom-2	${\rm distance}(\mathring{\rm A})$	overlap (Å)
1:A:137:LYS:NZ	2:C:450:LEU:HA	2.31	0.46
1:B:142:LEU:HD11	2:D:450:LEU:HG	1.97	0.46
1:A:170:ASN:HB3	1:A:173:ILE:HD11	1.97	0.46
1:B:176:GLU:HB2	1:B:186:PHE:CE2	2.51	0.45
1:B:150:LYS:NZ	6:B:405:HOH:O	2.36	0.45
1:B:99:ARG:NH2	1:B:100:TYR:OH	2.50	0.44
1:B:170:ASN:O	1:B:174:LYS:HD3	2.18	0.44
1:A:131:LEU:HD23	1:A:167:ILE:HB	2.00	0.44
1:B:17:MET:CE	2:D:440:ASN:HB2	2.48	0.43
1:B:47:ILE:HG13	1:B:73:ILE:HD11	2.00	0.43
2:D:438:SER:N	6:D:502:HOH:O	2.51	0.43
1:B:138:ARG:HB3	2:D:450:LEU:CD2	2.45	0.43
1:A:137:LYS:NZ	2:C:449:ASP:O	2.37	0.43
1:B:93:LYS:HE3	1:B:95:GLU:OE2	2.19	0.42
1:B:169:SER:O	1:B:173:ILE:HG13	2.20	0.41
1:B:138:ARG:HD3	1:B:138:ARG:HA	1.77	0.41
1:B:170:ASN:O	1:B:173:ILE:HB	2.21	0.41
1:A:20:LYS:NZ	4:A:1002:CL:CL	2.77	0.41
2:D:446:ILE:O	2:D:450:LEU:HD23	2.21	0.41
1:A:146:LEU:HD21	1:A:192:LEU:HD21	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	1100111 1		$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
6:B:549:HOH:O	6:B:607:HOH:O[1_655]	2.12	0.08

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	Percent	iles
1	A	194/207 (94%)	192 (99%)	2 (1%)	0	100 1	.00



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	В	197/207 (95%)	194 (98%)	3 (2%)	0	100	100
2	С	13/17 (76%)	11 (85%)	2 (15%)	0	100	100
2	D	11/17 (65%)	9 (82%)	2 (18%)	0	100	100
All	All	415/448 (93%)	406 (98%)	9 (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	Percentiles		
1	A	171/181 (94%)	170 (99%)	1 (1%)	86 76		
1	В	174/181~(96%)	172 (99%)	2 (1%)	73 56		
2	С	15/16 (94%)	14 (93%)	1 (7%)	16 3		
2	D	13/16 (81%)	13 (100%)	0	100 100		
All	All	373/394~(95%)	369 (99%)	4 (1%)	73 56		

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93	LYS
1	В	116	LYS
1	В	174	LYS
2	С	439	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	В	190	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)

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	True	Type Chain		Tiple	Bond lengths			Bond angles		
MIOI	ol Type Chain Res	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2		
2	SEP	D	442	2	8,9,10	1.42	1 (12%)	8,12,14	0.73	0
2	SEP	С	442	2	8,9,10	1.47	1 (12%)	8,12,14	0.85	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
2	SEP	D	442	2	-	1/5/8/10	-
2	SEP	С	442	2	-	0/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(A)	$\operatorname{Ideal}(\text{\AA})$
2	С	442	SEP	P-O1P	3.37	1.61	1.50
2	D	442	SEP	P-O1P	3.10	1.60	1.50

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

	Mol	Chain	Res	Type	Atoms
Γ	2	D	442	SEP	CB-OG-P-O1P



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)

Of 9 ligands modelled in this entry, 7 are monoatomic - leaving 2 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	Trino	Type Chain	hain Res	Res Link	Bond lengths			Bond angles		
MOI	туре			Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
3	IPA	A	1001	-	3,3,3	0.53	0	3,3,3	0.35	0
3	IPA	В	301	-	3,3,3	0.53	0	3,3,3	0.32	0

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 > 2		$OWAB(Å^2)$	Q < 0.9
1	A	196/207 (94%)	-0.06	8 (4%) 37	33	12, 20, 40, 59	0
1	В	197/207 (95%)	0.55	24 (12%) 4	3	12, 22, 81, 133	0
2	С	15/17 (88%)	1.31	3 (20%) 1	1	21, 34, 83, 95	0
2	D	13/17 (76%)	1.53	6 (46%) 0	0	24, 40, 64, 84	0
All	All	421/448 (93%)	0.32	41 (9%) 7	6	12, 21, 69, 133	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	171	ALA	18.5
1	В	133	VAL	12.1
1	В	173	ILE	11.9
1	В	174	LYS	6.6
2	С	440	ASN	6.6
1	В	178	GLU	6.1
1	В	170	ASN	6.1
1	В	5	THR	5.2
1	В	135	THR	5.1
1	В	180	ASP	4.9
1	В	132	LEU	4.7
2	С	439	CYS	4.5
1	В	134	ARG	4.4
2	D	451	LEU	4.3
1	A	177	LYS	4.2
2	D	450	LEU	4.2
1	В	183	LYS	4.1
2	С	437	ASP	3.9
1	A	6	PRO	3.9
2	D	439	CYS	3.8
1	A	135	THR	3.7



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Mol	Chain	Res	Type	RSRZ
1	A	176	GLU	3.4
1	В	138	ARG	3.4
1	В	172	ARG	3.3
1	В	177	LYS	3.2
1	В	169	SER	3.2
2	D	438	SER	3.0
1	В	181	ASN	3.0
1	В	175	ALA	3.0
1	A	175	ALA	2.9
1	В	186	PHE	2.8
1	В	168	ALA	2.7
1	A	172	ARG	2.5
1	В	126	ARG	2.4
1	В	96	LYS	2.4
1	В	182	PHE	2.3
1	A	200	LEU	2.2
1	A	173	ILE	2.2
2	D	449	ASP	2.1
2	D	440	ASN	2.0
1	В	200	LEU	2.0

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	SEP	С	442	10/11	0.97	0.09	15,18,22,28	0
2	SEP	D	442	10/11	0.97	0.11	18,20,25,32	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	${f B-factors}({f \AA}^2)$	Q < 0.9
5	MG	A	1005	1/1	0.89	0.23	38,38,38,38	0
3	IPA	В	301	4/4	0.91	0.15	20,26,27,32	0
4	CL	A	1003	1/1	0.97	0.08	34,34,34,34	0
3	IPA	A	1001	4/4	0.97	0.07	19,20,24,29	0
5	MG	A	1004	1/1	0.98	0.26	36,36,36,36	0
4	CL	В	303	1/1	0.98	0.09	27,27,27,27	0
5	MG	В	304	1/1	0.98	0.09	24,24,24,24	0
4	CL	A	1002	1/1	0.99	0.07	19,19,19,19	0
4	CL	В	302	1/1	1.00	0.12	17,17,17,17	0

6.5 Other polymers (i)

There are no such residues in this entry.

