

Full wwPDB X-ray Structure Validation Report (i)

May 14, 2020 – 02:17 pm BST

PDB ID 6FLC

Title 2C8 Fab bound to EDIII of DenV 2 Authors : Flanagan, A.; Renner, M.; Grimes, J.M.

2018-01-25 Deposited on

2.00 Å(reported) Resolution

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

MolProbity 4.02b-467

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

Xtriage (Phenix) 1.13 EDS 2.11

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

> Refmac 5.8.0158

CCP4 7.0.044 (Gargrove) Engh & Huber (2001)

Ideal geometry (proteins) Ideal geometry (DNA, RNA) Parkinson et al. (1996)

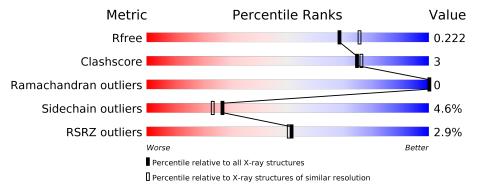
Validation Pipeline (wwPDB-VP) 2.11

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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
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 on 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	214	3% 87%	10% ••
1	L	214	90%	9% •
2	В	231	83%	10% • 6%
2	Н	231	% 8 7%	6% • 6%
3	G	98	88%	11% •
3	I	98	90%	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:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	301	-	-	X	-
4	GOL	В	301	-	X	-	-



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8758 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 Light chain of 2C8 Fab.

Mol	Chain	Residues	${f Atoms}$			ZeroOcc	AltConf	Trace		
1	Λ	A 211		С	N	О	S	0	0	0
1	A	211	1650	1030	284	330	6	U	U	U
1	Т	212	Total	С	N	О	S	0	0	0
	ь	212	1658	1034	286	332	6			

• Molecule 2 is a protein called Heavy chain of 2C8 Fab.

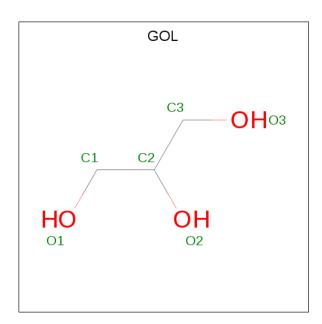
Mol	Chain	Residues	${f Atoms}$			ZeroOcc	AltConf	Trace		
2	В	216		C			S 7	0	0	0
			1645	1045	211	322	1			
9	П	216	Total	$^{\mathrm{C}}$	N	Ο	\mathbf{S}	0	0	
	11	210	1645	1045	271	322	7	0	0	

• Molecule 3 is a protein called Domain III of Dengue virus 2.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
3	G	98	Total 775		N 127			0	0	0
3	I	97	Total 766	C 494	N 125	O 142	S 5	0	0	0

• Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).





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

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	84	Total O 84 84	0	0
5	В	131	Total O 131 131	0	0
5	G	67	Total O 67 67	0	0
5	Н	143	Total O 143 143	0	0
5	I	40	Total O 40 40	0	0
5	L	130	Total O 130 130	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 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: Light chain of 2C8 Fab



 \bullet Molecule 3: Domain III of Dengue virus 2







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	42.56Å 61.42Å 104.59Å	Depositor
a, b, c, α , β , γ	77.54° 81.11° 85.53°	Depositor
Resolution (Å)	33.70 - 2.00	Depositor
resolution (A)	33.70 - 2.00	EDS
% Data completeness	97.0 (33.70-2.00)	Depositor
(in resolution range)	96.9 (33.70-2.00)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.89 (at 2.00Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
P. P.	0.180 , 0.216	Depositor
R, R_{free}	0.188 , 0.222	DCC
R_{free} test set	3395 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	27.9	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.35, 51.2	EDS
L-test for twinning ²	$ < L >=0.49, < 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	8758	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.22% 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: GOL

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	Bo	ond angles
MIOI		RMSZ	# Z >5	RMSZ	# Z > 5
1	A	0.45	0/1690	0.68	0/2297
1	L	0.42	0/1698	0.67	0/2308
2	В	0.47	0/1688	0.71	0/2305
2	Н	0.44	0/1688	0.70	1/2305~(0.0%)
3	G	0.40	0/792	0.67	0/1070
3	I	0.40	0/783	0.66	0/1059
All	All	0.44	0/8339	0.69	1/11344 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	${f Atoms}$	Z	$\operatorname{Observed}(^{o})$	$\operatorname{Ideal}({}^o)$
2	Н	185	LEU	CA-CB-CG	6.69	130.69	115.30

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	1650	0	1573	14	0
1	L	1658	0	1579	9	0
2	В	1645	0	1607	18	0
2	Н	1645	0	1605	6	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	775	0	789	5	0
3	I	766	0	776	3	0
4	A	6	0	8	5	0
4	В	12	0	16	0	0
4	L	6	0	8	0	0
5	A	84	0	0	0	0
5	В	131	0	0	0	0
5	G	67	0	0	1	0
5	Н	143	0	0	0	0
5	I	40	0	0	0	0
5	L	130	0	0	0	0
All	All	8758	0	7961	50	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 3.

All (50) 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)
4:A:301:GOL:O1	2:B:102:LYS:HE3	1.50	1.09
4:A:301:GOL:HO1	2:B:102:LYS:HE3	1.30	0.96
2:B:148:CYS:SG	2:B:203:CYS:CB	2.54	0.95
4:A:301:GOL:O1	2:B:102:LYS:CE	2.24	0.84
3:G:325:GLN:NE2	5:G:401:HOH:O	2.11	0.81
2:B:148:CYS:SG	2:B:203:CYS:HB2	2.22	0.79
2:B:136:CYS:HB2	2:B:221:ARG:HB2	1.67	0.76
1:A:78:LEU:HD12	1:A:82:ASP:HB2	1.70	0.73
1:A:83:PHE:CD2	1:A:106:ILE:HG12	2.27	0.70
2:H:99:THR:HG21	2:H:108:PHE:CG	2.30	0.66
1:L:150:ILE:HD11	1:L:179:LEU:HD21	1.78	0.66
1:A:150:ILE:HD11	1:A:179:LEU:HD21	1.80	0.64
1:L:13:VAL:HG11	1:L:19:VAL:HG21	1.83	0.61
1:A:195:GLU:HG2	1:A:206:VAL:HG22	1.84	0.59
2:H:127:PRO:HB3	2:H:153:TYR:HB3	1.85	0.59
1:L:195:GLU:HG2	1:L:206:VAL:HG22	1.85	0.59
2:B:127:PRO:HB3	2:B:153:TYR:HB3	1.86	0.58
1:L:37:GLN:HB2	1:L:47:LEU:HD11	1.87	0.56
1:A:37:GLN:HB2	1:A:47:LEU:HD11	1.88	0.55
3:G:387:LEU:HD22	3:G:389:LEU:HD21	1.88	0.54
2:B:148:CYS:HG	2:B:203:CYS:CB	2.16	0.53
2:H:11:LEU:HD11	2:H:155:PRO:HB3	1.92	0.52



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A		Interatomic	Clash
Atom-1	Atom-2	${\rm distance} \; (\mathring{\rm A})$	${ m overlap}({ m \AA})$
1:A:25:ALA:O	1:A:69:THR:OG1	2.28	0.52
1:A:83:PHE:CG	1:A:106:ILE:HG12	2.46	0.51
2:B:203:CYS:SG	2:B:203:CYS:O	2.69	0.50
4:A:301:GOL:H31	2:B:109:ASP:HB2	1.95	0.49
2:B:203:CYS:SG	2:B:216:LYS:HB2	2.53	0.48
1:A:2:ILE:HG12	1:A:27:LYS:HB2	1.95	0.48
2:H:107:TYR:CG	1:L:49:TYR:HB2	2.49	0.48
4:A:301:GOL:HO1	2:B:102:LYS:CE	2.14	0.47
2:B:148:CYS:HG	2:B:203:CYS:HB2	1.79	0.47
1:L:150:ILE:HD12	1:L:155:ARG:HG3	1.96	0.47
1:L:2:ILE:HG12	1:L:27:LYS:HB2	1.97	0.46
3:G:332:PRO:HA	3:G:358:VAL:O	2.16	0.46
3:I:332:PRO:HA	3:I:358:VAL:O	2.16	0.45
3:G:332:PRO:HD2	2:H:103:TRP:CG	2.52	0.44
1:A:83:PHE:CE2	1:A:106:ILE:HG12	2.53	0.44
1:A:155:ARG:HG2	1:A:179:LEU:HD11	2.00	0.44
2:H:11:LEU:HD12	2:H:118:THR:HB	2.00	0.43
1:A:78:LEU:HD12	1:A:82:ASP:CB	2.44	0.42
1:A:49:TYR:HB2	2:B:107:TYR:CG	2.54	0.42
2:B:27:PHE:CE2	2:B:29:PHE:HA	2.55	0.41
2:B:103:TRP:CG	3:I:332:PRO:HD2	2.55	0.41
3:G:316:GLN:HG2	3:G:316:GLN:H	1.50	0.41
2:B:62:TYR:HB2	2:B:67:LYS:HG3	2.03	0.41
3:I:352:ILE:HD11	3:I:370:GLU:HB2	2.02	0.41
1:A:164:THR:HG23	2:B:174:PHE:CD2	2.55	0.41
1:L:13:VAL:HG11	1:L:19:VAL:CG2	2.48	0.40
1:L:19:VAL:HG11	1:L:104:LEU:HD11	2.03	0.40
1:A:46:LEU:HD13	1:A:55:ALA:HB2	2.03	0.40

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	Perce	\mathbf{ntiles}
1	A	$209/214\ (98\%)$	203 (97%)	6 (3%)	0	100	100
1	L	210/214~(98%)	204 (97%)	6 (3%)	0	100	100
2	В	$212/231 \; (92\%)$	208 (98%)	4 (2%)	0	100	100
2	Н	$212/231 \; (92\%)$	208 (98%)	4 (2%)	0	100	100
3	G	96/98~(98%)	95 (99%)	1 (1%)	0	100	100
3	I	95/98 (97%)	94 (99%)	1 (1%)	0	100	100
All	All	1034/1086~(95%)	1012 (98%)	22 (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	Percer	$_{ m tiles}$
1	A	186/189 (98%)	179 (96%)	7 (4%)	33	31
1	L	187/189 (99%)	181 (97%)	6 (3%)	39	38
2	В	184/196 (94%)	174 (95%)	10 (5%)	22	18
2	Н	184/196 (94%)	177 (96%)	7 (4%)	33	31
3	G	88/88 (100%)	81 (92%)	7 (8%)	12	7
3	I	87/88 (99%)	82 (94%)	5 (6%)	20	16
All	All	916/946 (97%)	874 (95%)	42 (5%)	27	23

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ARG
1	A	46	LEU
1	A	70	GLN
1	A	78	LEU
1	A	80	SER
1	A	168	SER
1	A	205	ILE



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Mol	Chain	${f Res}$	$egin{array}{c} Tus \ page \end{array}$
2	В	13	GLN
2	В	35	THR
2	В	83	LEU
2	В	98	CYS
2	В	99	CYS THR
2	В	135	VAL
2	В	148	CYS
2	В	185	LEU
2	В	191	VAL
2	В	203	CYS
3	G	297	MET
3	G	298	SER
3	G	316	GLN
3	G	338	GLU
3	G	345	ARG
3	G	377	TYR
3	G	394	LYS
2	Н	35	THR
2	Н	43	LYS
2	Н	83	LEU
2	Н	98	CYS
2	Н	99	THR
2	Н	178	LEU
2	Н	185	LEU
3	I	298	SER
3	I	307	LYS
3	I	338	GLU
3	I	377	TYR
3	I	387	LEU
1	L	24	ARG
1	L	46	LEU
1	L	78	LEU
1	L	147	LYS
1	L	181	LEU
1	L	194	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	Н	84	GLN
2	Н	106	HIS



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 carbohydrates in this entry.

5.6 Ligand geometry (i)

4 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).

Mol	Tuno	Chain	Res	Link	В	ond leng	gths	Е	ond ang	gles
WIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	В	302	-	5,5,5	0.43	0	5,5,5	0.56	0
4	GOL	A	301	-	5,5,5	1.04	0	5,5,5	0.71	0
4	GOL	L	301	-	5,5,5	0.71	0	5,5,5	0.62	0
4	GOL	В	301	-	5,5,5	0.79	0	5,5,5	1.78	2 (40%)

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
4	GOL	В	302	_	-	1/4/4/4	-
4	GOL	A	301	-	-	4/4/4/4	-
4	GOL	L	301	-	-	4/4/4/4	-
4	GOL	В	301	-	-	4/4/4/4	-



There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
4	В	301	GOL	O1-C1-C2	-2.54	98.02	110.20
4	В	301	GOL	O2-C2-C3	2.38	119.61	109.12

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	301	GOL	C1-C2-C3-O3
4	В	301	GOL	O1-C1-C2-C3
4	В	301	GOL	C1-C2-C3-O3
4	В	302	GOL	C1-C2-C3-O3
4	A	301	GOL	O1-C1-C2-C3
4	L	301	GOL	O1-C1-C2-C3
4	L	301	GOL	C1-C2-C3-O3
4	A	301	GOL	O1-C1-C2-O2
4	A	301	GOL	O2-C2-C3-O3
4	L	301	GOL	O2-C2-C3-O3
4	В	301	GOL	O2-C2-C3-O3
4	В	301	GOL	O1-C1-C2-O2
4	L	301	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	301	GOL	5	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	$\langle { m RSRZ} \rangle$	$\# \mathrm{RSRZ} {>} 2$	$OWAB(\AA^2)$	Q < 0.9
1	A	211/214 (98%)	0.01	6 (2%) 53 51	25, 39, 64, 79	0
1	L	212/214 (99%)	-0.05	2 (0%) 84 83	18, 30, 53, 70	0
2	В	$216/231 \ (93\%)$	-0.00	6 (2%) 53 51	21, 31, 54, 92	0
2	Н	$216/231 \ (93\%)$	-0.15	2 (0%) 84 83	17, 27, 45, 71	0
3	G	98/98 (100%)	0.08	2 (2%) 65 63	22, 37, 58, 71	0
3	I	97/98 (98%)	0.51	12 (12%) 4 3	31, 43, 68, 91	0
All	All	1050/1086~(96%)	0.02	30 (2%) 51 50	17, 34, 59, 92	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	В	136	CYS	5.0
1	L	202	THR	4.9
3	I	346	HIS	4.9
3	I	345	ARG	4.3
2	В	195	THR	4.2
1	A	83	PHE	4.2
3	I	373	PHE	4.0
2	В	135	VAL	3.5
3	G	354	VAL	3.3
3	I	342	LEU	3.2
3	G	316	GLN	3.1
3	I	392	PHE	3.0
3	I	377	TYR	2.9
3	I	375	ASP	2.9
3	I	343	GLU	2.8
3	I	372	PRO	2.7
2	В	143	SER	2.7
2	Н	1	GLU	2.7
3	I	348	LEU	2.5



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Mol	Chain	Res	Type	RSRZ
1	L	201	SER	2.4
3	I	313	ALA	2.4
2	В	193	SER	2.4
1	A	152	GLY	2.4
3	I	347	VAL	2.3
2	В	1	GLU	2.3
1	A	157	ASN	2.3
2	Н	136	CYS	2.2
1	A	153	SER	2.1
1	A	3	GLN	2.1
1	A	40	GLN	2.0

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 carbohydrates 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	${f B\text{-factors}}({f \AA}^2)$	Q < 0.9
4	GOL	В	302	6/6	0.73	0.23	49,50,50,50	0
4	GOL	A	301	6/6	0.79	0.18	46,47,47,47	0
4	GOL	L	301	6/6	0.84	0.19	40,41,42,43	0
4	GOL	В	301	6/6	0.92	0.14	35,37,37,38	0

6.5 Other polymers (i)

There are no such residues in this entry.

