



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2025 – 05:39 PM EDT

PDB ID : 1A7R / pdb_00001a7r
Title : FV FRAGMENT OF MOUSE MONOCLONAL ANTIBODY D1.3 (BALB/C, IGG1, K) VARIANT CHAIN L GLU81->ASP
Authors : Marks, C.; Henrick, K.; Winter, G.
Deposited on : 1998-03-16
Resolution : 2.01 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 ⓘ 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) : 2.43.1

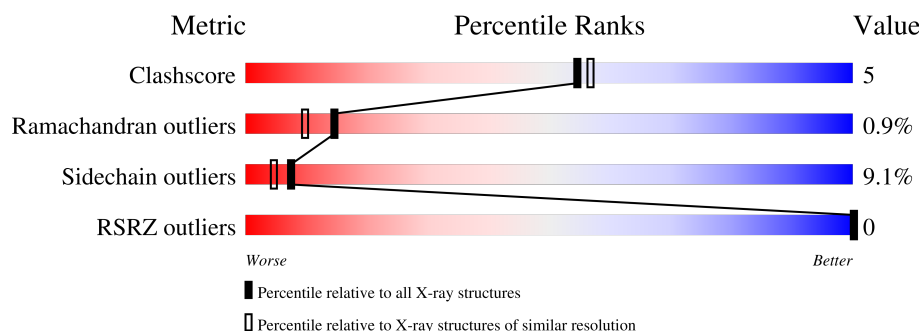
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 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))
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (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 $\leq 5\%$. 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	L	107	<div> <div>55%</div> <div>38%</div> <div>7%</div> </div>
2	H	116	<div> <div>55%</div> <div>39%</div> <div>• •</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1832 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 IGG1-KAPPA D1.3 FV (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	107	Total	C	N	O	S	0	0	0
			816	518	135	161	2			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	3	VAL	GLU	conflict	UNP P01635
L	50	TYR	LYS	conflict	UNP P01635
L	51	THR	ALA	conflict	UNP P01635
L	52	THR	GLN	conflict	UNP P01635
L	81	ASP	GLU	variant	UNP P01635
L	?	-	PRO	deletion	UNP P01635
L	96	ARG	TRP	conflict	UNP P01635

- Molecule 2 is a protein called IGG1-KAPPA D1.3 FV (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	116	Total	C	N	O	S	0	1	0
			905	566	160	175	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	312	LEU	VAL	conflict	UNP P01820

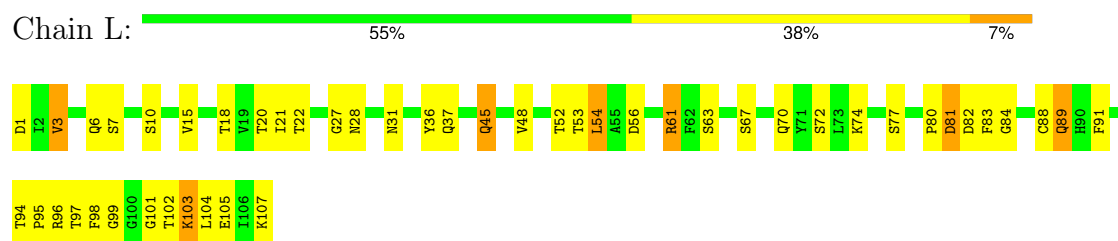
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	56	Total	O	0	0
			56	56		
3	H	55	Total	O	0	0
			55	55		

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: IGG1-KAPPA D1.3 FV (LIGHT CHAIN)



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	90.25Å 90.25Å 56.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.01 6.00 – 2.02	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-2.01) 92.9 (6.00-2.02)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.01Å)	Xtriage
Refinement program	CCP4	Depositor
R, R_{free}	0.170 , (Not available) 0.163 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	19.9	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 89.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	1832	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.73% 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	L	1.51	7/837 (0.8%)	2.64	52/1138 (4.6%)
2	H	1.34	0/930	2.43	54/1261 (4.3%)
All	All	1.42	7/1767 (0.4%)	2.53	106/2399 (4.4%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	70	GLN	CB-CG	-15.01	1.07	1.52
1	L	27	GLY	N-CA	6.24	1.51	1.45
1	L	61	ARG	NE-CZ	-5.91	1.26	1.33
1	L	52	THR	CA-CB	5.71	1.62	1.54
1	L	88	CYS	N-CA	5.68	1.52	1.45
1	L	53	THR	CA-CB	5.18	1.60	1.53
1	L	61	ARG	CD-NE	-5.06	1.39	1.46

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	61	ARG	CD-NE-CZ	38.90	178.86	124.40
1	L	63	SER	CA-C-N	-10.10	112.76	122.66
1	L	63	SER	C-N-CA	-10.10	112.76	122.66
1	L	70	GLN	N-CA-CB	-9.90	95.22	110.77
2	H	266	ARG	NE-CZ-NH2	-9.69	110.48	119.20
1	L	96	ARG	NH1-CZ-NH2	9.05	131.06	119.30
1	L	28	ASN	OD1-CG-ND2	-8.69	113.91	122.60
1	L	15	VAL	CA-C-O	-8.58	113.00	121.58
2	H	256	ASN	CA-CB-CG	-8.57	104.03	112.60
1	L	70	GLN	CA-CB-CG	8.53	131.15	114.10
2	H	228	SER	CA-CB-OG	-8.47	94.15	111.10
1	L	89	GLN	OE1-CD-NE2	-8.38	114.22	122.60
2	H	228	SER	CB-CA-C	-8.29	95.85	109.53
2	H	284	SER	CA-C-O	8.08	132.07	120.51
1	L	84	GLY	N-CA-C	-7.87	100.31	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	201	GLN	CA-C-O	7.85	134.15	120.80
2	H	240	PRO	N-CA-CB	7.78	107.27	103.22
2	H	201	GLN	OE1-CD-NE2	-7.74	114.86	122.60
1	L	99	GLY	N-CA-C	-7.67	100.49	112.85
1	L	67	SER	O-C-N	7.65	130.30	123.41
1	L	96	ARG	NE-CZ-NH2	-7.42	112.53	119.20
1	L	45	GLN	CB-CG-CD	7.33	125.06	112.60
1	L	37	GLN	OE1-CD-NE2	-7.31	115.29	122.60
2	H	240	PRO	O-C-N	7.22	124.55	121.15
2	H	277	GLN	OE1-CD-NE2	7.11	129.71	122.60
2	H	256	ASN	OD1-CG-ND2	-7.10	115.50	122.60
1	L	70	GLN	CB-CG-CD	7.05	124.59	112.60
2	H	273	ASN	OD1-CG-ND2	-6.97	115.63	122.60
1	L	102	THR	N-CA-CB	6.96	121.69	110.77
1	L	27	GLY	CA-C-O	-6.95	113.79	121.37
1	L	45	GLN	OE1-CD-NE2	-6.91	115.69	122.60
1	L	20	THR	CA-CB-OG1	-6.88	99.27	109.60
2	H	255	GLY	CA-C-O	-6.66	111.61	119.07
2	H	213	ALA	N-CA-CB	-6.63	102.00	110.03
2	H	226	GLY	CA-C-O	-6.62	111.65	119.06
2	H	283	ASN	OD1-CG-ND2	6.55	129.15	122.60
1	L	101	GLY	CA-C-O	6.50	126.95	121.88
2	H	266	ARG	NE-CZ-NH1	6.50	128.00	121.50
1	L	21	ILE	CB-CA-C	6.48	120.79	110.82
1	L	82	ASP	CA-C-O	-6.25	111.74	119.18
2	H	227	PHE	CA-C-O	-6.22	114.61	121.33
2	H	228	SER	O-C-N	6.18	130.33	123.16
2	H	263	LEU	N-CA-CB	-6.16	101.60	110.65
2	H	267	LEU	CB-CA-C	-6.05	98.30	109.37
2	H	206	GLU	CA-C-O	-6.03	114.17	121.28
2	H	290	THR	CA-CB-OG1	-6.01	100.59	109.60
1	L	22	THR	O-C-N	6.00	130.99	123.19
1	L	22	THR	CA-CB-OG1	-6.00	100.61	109.60
1	L	1	ASP	CB-CG-OD2	-5.98	104.64	118.40
2	H	202	VAL	N-CA-C	-5.97	99.87	108.53
2	H	312	LEU	CA-C-O	-5.96	113.92	120.36
1	L	105	GLU	OE1-CD-OE2	5.87	136.98	122.90
1	L	98	PHE	CA-CB-CG	5.86	119.66	113.80
2	H	201	GLN	CA-C-N	5.86	130.66	123.10
2	H	201	GLN	C-N-CA	5.86	130.66	123.10
1	L	31	ASN	CA-CB-CG	-5.85	106.75	112.60
1	L	67	SER	CA-C-O	-5.84	114.58	121.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	314	VAL	O-C-N	5.83	129.44	122.62
2	H	221	THR	CB-CA-C	5.83	120.50	109.37
2	H	304	ASP	CA-C-O	-5.79	112.83	119.60
1	L	83	PHE	CB-CA-C	5.77	120.08	109.46
2	H	311	THR	CA-CB-OG1	-5.74	100.99	109.60
2	H	240	PRO	N-CA-C	-5.72	104.45	110.58
1	L	89	GLN	CG-CD-NE2	5.68	124.92	116.40
2	H	286	HIS	O-C-N	5.67	130.71	123.11
2	H	235	ASN	CB-CG-ND2	5.62	124.83	116.40
2	H	286	HIS	CA-CB-CG	-5.61	108.19	113.80
2	H	306	TRP	CA-C-O	-5.60	114.83	121.16
1	L	105	GLU	CG-CD-OE2	-5.58	105.56	118.40
1	L	70	GLN	CB-CA-C	5.56	119.03	110.14
1	L	54	LEU	CA-C-O	-5.54	114.73	121.05
2	H	281	LYS	CA-CB-CG	-5.53	103.03	114.10
2	H	239	GLN	CA-C-N	5.53	123.64	119.66
2	H	239	GLN	C-N-CA	5.53	123.64	119.66
1	L	6	GLN	CA-C-N	-5.51	111.27	122.45
1	L	6	GLN	C-N-CA	-5.51	111.27	122.45
1	L	88	CYS	N-CA-C	-5.47	101.66	110.14
1	L	80	PRO	CA-C-N	5.44	129.30	120.60
1	L	80	PRO	C-N-CA	5.44	129.30	120.60
2	H	218	LEU	N-CA-CB	-5.43	103.15	111.56
1	L	37	GLN	CB-CG-CD	-5.42	103.39	112.60
2	H	228	SER	N-CA-CB	5.39	118.97	110.23
2	H	237	VAL	CA-C-N	-5.38	114.14	122.59
2	H	237	VAL	C-N-CA	-5.38	114.14	122.59
2	H	311	THR	CA-C-O	-5.38	114.47	120.54
1	L	91	PHE	CA-CB-CG	5.38	119.17	113.80
2	H	216	GLN	N-CA-C	-5.37	103.60	110.53
2	H	203	GLN	N-CA-CB	-5.35	101.55	111.13
1	L	10	SER	N-CA-CB	5.32	120.76	111.13
2	H	218	LEU	CB-CA-C	5.30	120.49	110.62
1	L	81	ASP	CA-CB-CG	5.30	117.90	112.60
1	L	72	SER	CA-CB-OG	-5.28	100.53	111.10
2	H	267	LEU	N-CA-C	5.24	118.28	109.95
1	L	18	THR	CA-CB-OG1	-5.22	101.77	109.60
1	L	7	SER	CA-CB-OG	-5.21	100.67	111.10
1	L	97	THR	OG1-CB-CG2	-5.18	98.95	109.30
2	H	201	GLN	CA-CB-CG	5.16	124.42	114.10
2	H	308	GLN	CB-CG-CD	5.16	121.37	112.60
1	L	56	ASP	N-CA-CB	5.15	117.61	109.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	103	LYS	CA-CB-CG	-5.14	103.82	114.10
1	L	96	ARG	NE-CZ-NH1	-5.09	116.41	121.50
2	H	295	CYS	N-CA-C	-5.08	101.87	109.95
2	H	227	PHE	CA-CB-CG	5.06	118.86	113.80
2	H	260	ASN	CB-CG-ND2	-5.06	108.81	116.40
1	L	97	THR	CA-CB-CG2	5.05	119.09	110.50
2	H	214	PRO	N-CA-CB	5.01	108.10	103.39

There are no chirality outliers.

There are no planarity outliers.

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	L	816	0	783	4	0
2	H	905	0	873	12	0
3	H	55	0	0	0	0
3	L	56	0	0	1	0
All	All	1832	0	1656	16	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.

All (16) 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)
2:H:299[A]:ARG:NH1	2:H:302:ARG:NH2	2.24	0.85
2:H:218:LEU:HD12	2:H:282:MET:HB2	1.80	0.64
2:H:267:LEU:HD23	2:H:282:MET:HG2	1.88	0.56
1:L:3:VAL:HG12	3:L:424:HOH:O	2.08	0.53
2:H:299[A]:ARG:NH1	2:H:302:ARG:HH22	2.06	0.47
2:H:211:LEU:HD11	2:H:315:SER:CB	2.46	0.46
1:L:36:TYR:HE2	1:L:89:GLN:HE21	1.62	0.46
1:L:48:VAL:HG22	1:L:54:LEU:HD23	1.97	0.45
2:H:267:LEU:HD22	2:H:280:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:94:THR:HB	1:L:95:PRO:HA	1.99	0.44
2:H:201:GLN:N	2:H:201:GLN:OE1	2.51	0.43
2:H:222:CYS:HB2	2:H:236:TRP:CH2	2.54	0.43
2:H:218:LEU:HB3	2:H:285:LEU:HD11	2.02	0.41
2:H:211:LEU:HD11	2:H:315:SER:HB2	2.02	0.41
2:H:209:PRO:CG	2:H:218:LEU:HD23	2.50	0.41
2:H:297:ARG:O	2:H:303:LEU:HA	2.20	0.41

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	L	105/107 (98%)	102 (97%)	2 (2%)	1 (1%)	13	8
2	H	115/116 (99%)	110 (96%)	4 (4%)	1 (1%)	14	10
All	All	220/223 (99%)	212 (96%)	6 (3%)	2 (1%)	14	10

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	284	SER
1	L	77	SER

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	L	89/91 (98%)	81 (91%)	8 (9%)	8	5
2	H	99/100 (99%)	90 (91%)	9 (9%)	7	5
All	All	188/191 (98%)	171 (91%)	17 (9%)	7	5

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	3	VAL
1	L	45	GLN
1	L	61	ARG
1	L	74	LYS
1	L	81	ASP
1	L	103	LYS
1	L	104	LEU
1	L	107	LYS
2	H	201	GLN
2	H	207	SER
2	H	218	LEU
2	H	221	THR
2	H	235	ASN
2	H	261	SER
2	H	275	LYS
2	H	276	SER
2	H	315	SER

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

Mol	Chain	Res	Type
1	L	30	HIS
1	L	89	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	L	107/107 (100%)	-1.15	0 100 100	9, 16, 29, 42	6 (5%)
2	H	116/116 (100%)	-1.16	0 100 100	7, 16, 30, 37	4 (3%)
All	All	223/223 (100%)	-1.15	0 100 100	7, 16, 29, 42	10 (4%)

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 monosaccharides 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.