



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 21, 2021 – 02:31 PM EDT

PDB ID : 7JIE  
Title : Structure of GII.4 P-domain in Complex with NORO-320 FAB  
Authors : Salmen, W.; Hu, L.; Prasad, B.  
Deposited on : 2020-07-23  
Resolution : 2.25 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.20
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)	:	2.20

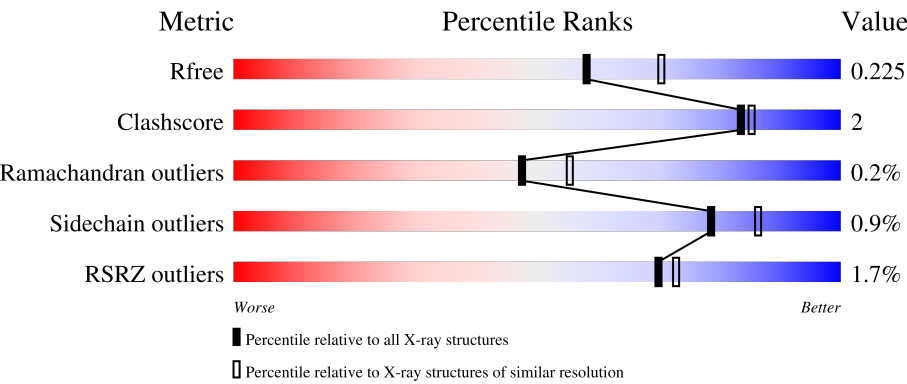
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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.



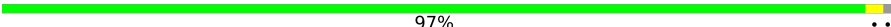
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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  $\geq 3$ , 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	A	307	<div><div>4%</div><div></div><div>92%</div><div>8%</div></div>
1	B	307	<div><div>3%</div><div></div><div>91%</div><div>9%</div></div>
2	C	238	<div><div>%</div><div></div><div>89%</div><div>5%</div><div>6%</div></div>
2	E	238	<div><div>%</div><div></div><div>87%</div><div>8%</div><div>..</div></div>
3	D	219	<div><div></div><div></div><div>95%</div><div>..</div></div>

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Mol	Chain	Length	Quality of chain
3	F	219	 97% ..

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 12523 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 VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2399	1520	411	458	10			
1	B	307	Total	C	N	O	S	0	0	0
			2399	1520	411	458	10			

- Molecule 2 is a protein called IgA Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	224	Total	C	N	O	S	0	0	0
			1660	1047	275	330	8			
2	E	228	Total	C	N	O	S	0	0	0
			1688	1063	280	337	8			

- Molecule 3 is a protein called IgA Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	217	Total	C	N	O	S	0	0	0
			1663	1041	280	336	6			
3	F	217	Total	C	N	O	S	0	0	0
			1663	1041	280	336	6			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	204	Total	O	0	0
			204	204		
4	B	190	Total	O	0	0
			190	190		
4	C	174	Total	O	0	0
			174	174		
4	D	154	Total	O	0	0
			154	154		

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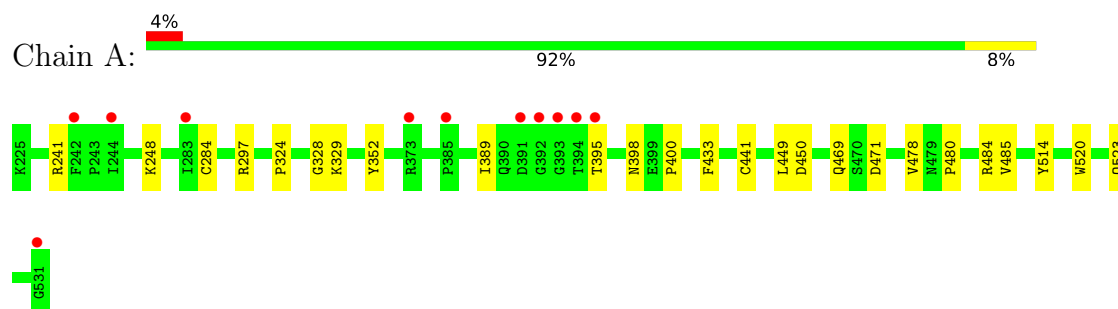
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	148	Total 148	O 148	0	0
4	F	181	Total 181	O 181	0	0

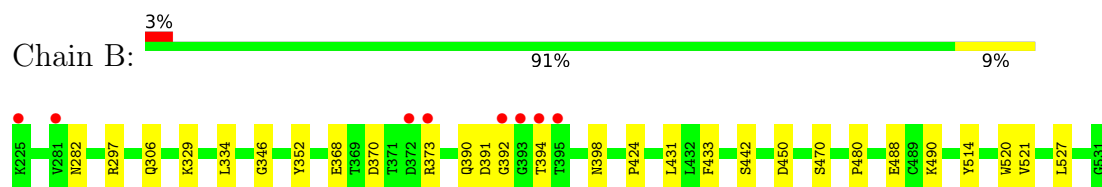
### 3 Residue-property plots

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.

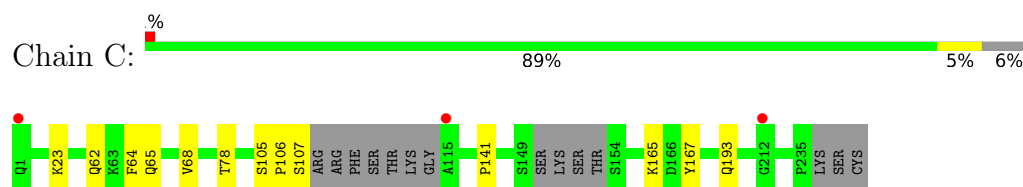
- Molecule 1: VP1



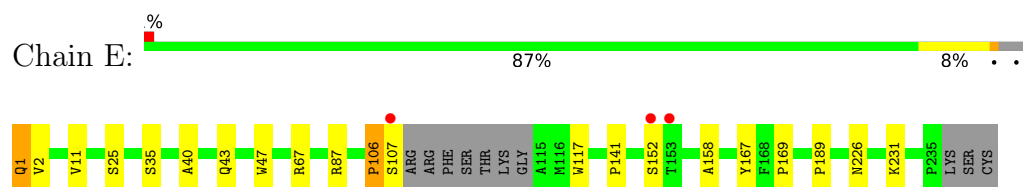
- Molecule 1: VP1



- Molecule 2: IgA Fab Heavy Chain



- Molecule 2: IgA Fab Heavy Chain



- Molecule 3: IgA Fab Light Chain





● Molecule 3: IgA Fab Light Chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.25Å 186.27Å 73.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.11 – 2.25 37.11 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.8 (37.11-2.25) 99.8 (37.11-2.25)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.48 (at 2.24Å)	Xtriage
Refinement program	PHENIX (dev_3386)	Depositor
R, $R_{free}$	0.181 , 0.225 0.181 , 0.225	Depositor DCC
$R_{free}$ test set	3926 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.6	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 47.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12523	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.46% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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	A	0.26	0/2469	0.49	0/3377
1	B	0.27	0/2469	0.49	0/3377
2	C	0.27	0/1699	0.48	0/2314
2	E	0.27	0/1728	0.48	0/2354
3	D	0.27	0/1699	0.46	0/2307
3	F	0.27	0/1699	0.47	0/2307
All	All	0.27	0/11763	0.48	0/16036

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	2399	0	2295	13	0
1	B	2399	0	2295	17	0
2	C	1660	0	1627	8	0
2	E	1688	0	1658	9	0
3	D	1663	0	1623	4	0
3	F	1663	0	1623	3	0
4	A	204	0	0	2	0
4	B	190	0	0	1	0
4	C	174	0	0	0	0
4	D	154	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	148	0	0	0	0
4	F	181	0	0	0	0
All	All	12523	0	11121	53	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 2.

All (53) 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)
1:B:390:GLN:NE2	1:B:394:THR:OG1	2.32	0.62
1:B:470:SER:HB3	1:B:520:TRP:HB3	1.82	0.61
1:B:391:ASP:O	1:B:394:THR:OG1	2.15	0.59
1:B:394:THR:HB	1:B:398:ASN:HD21	1.67	0.59
1:B:282:ASN:ND2	1:B:306:GLN:OE1	2.38	0.57
2:E:1:GLN:CD	2:E:2:VAL:H	2.08	0.57
2:E:11:VAL:HG21	2:E:169:PRO:HG3	1.87	0.56
3:D:168:VAL:HG22	3:D:180:LEU:HD12	1.88	0.56
2:C:62:GLN:CD	2:C:62:GLN:H	2.10	0.55
2:E:106:PRO:O	2:E:107:SER:HB2	2.06	0.55
1:A:248:LYS:NZ	4:A:605:HOH:O	2.40	0.55
1:A:480:PRO:HB3	1:A:514:TYR:HE1	1.72	0.55
1:B:480:PRO:HB3	1:B:514:TYR:HE1	1.71	0.54
3:F:113:ARG:HH11	3:F:113:ARG:HG3	1.72	0.54
3:D:24:ARG:NH2	4:D:308:HOH:O	2.42	0.52
1:A:284:CYS:HA	1:A:324:PRO:HD3	1.91	0.51
1:B:490:LYS:HG3	1:B:527:LEU:HD21	1.92	0.50
1:B:329:LYS:HG2	1:B:352:TYR:CD2	2.47	0.49
1:B:306:GLN:NE2	4:B:611:HOH:O	2.44	0.49
1:B:470:SER:OG	1:B:521:VAL:O	2.29	0.49
1:B:394:THR:CB	1:B:398:ASN:HD21	2.26	0.49
2:C:62:GLN:H	2:C:62:GLN:NE2	2.10	0.48
1:A:471:ASP:OD2	1:A:523:GLN:NE2	2.46	0.48
1:A:297:ARG:NE	4:A:607:HOH:O	2.40	0.48
1:B:297:ARG:NH1	1:B:368:GLU:OE2	2.46	0.48
2:C:141:PRO:HB3	2:C:167:TYR:HB3	1.97	0.47
2:E:117:TRP:HB3	3:F:99:THR:HG21	1.95	0.47
2:C:23:LYS:HA	2:C:78:THR:HG23	1.97	0.47
1:A:328:GLY:HA3	1:A:400:PRO:HB3	1.96	0.46
2:E:40:ALA:HB3	2:E:43:GLN:HG3	1.97	0.46
1:A:433:PHE:HB3	1:A:450:ASP:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:62:GLN:HA	2:C:65:GLN:HG2	1.98	0.46
1:A:241:ARG:HB2	1:A:449:LEU:HD21	1.97	0.45
1:B:488:GLU:HG3	1:B:527:LEU:HD22	1.99	0.45
2:C:64:PHE:O	2:C:68:VAL:HG12	2.15	0.45
1:A:395:THR:O	1:A:398:ASN:ND2	2.50	0.45
1:A:469:GLN:HB2	1:A:520:TRP:CD1	2.53	0.44
1:B:433:PHE:HB3	1:B:450:ASP:HB3	2.00	0.44
1:A:478:VAL:HG22	1:A:485:VAL:HG22	2.00	0.44
2:C:106:PRO:O	2:C:107:SER:HB3	2.18	0.43
3:D:42:LEU:HD13	3:D:91:TYR:CZ	2.53	0.43
2:E:152:SER:HB3	2:E:158:ALA:HB2	2.01	0.43
1:A:389:ILE:HG22	1:A:441:CYS:HB2	2.02	0.42
3:D:31:HIS:HB3	3:D:33:ASN:OD1	2.19	0.42
2:E:35:SER:HB3	2:E:47:TRP:NE1	2.35	0.42
1:B:424:PRO:HD3	1:B:431:LEU:HG	2.02	0.42
3:F:150:LYS:HB3	3:F:202:THR:HB	2.00	0.41
2:C:165:LYS:NZ	2:C:193:GLN:OE1	2.54	0.41
2:E:231:LYS:HD2	2:E:231:LYS:HA	1.73	0.41
1:B:394:THR:HB	1:B:398:ASN:ND2	2.34	0.40
1:B:334:LEU:O	1:B:346:GLY:HA2	2.22	0.40
1:A:329:LYS:HG2	1:A:352:TYR:CD2	2.56	0.40
2:E:141:PRO:HB3	2:E:167:TYR:HB3	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	Percentiles	
1	A	305/307 (99%)	301 (99%)	4 (1%)	0	100	100
1	B	305/307 (99%)	300 (98%)	3 (1%)	2 (1%)	22	21
2	C	218/238 (92%)	212 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	224/238 (94%)	219 (98%)	4 (2%)	1 (0%)	34	37
3	D	215/219 (98%)	213 (99%)	2 (1%)	0	100	100
3	F	215/219 (98%)	213 (99%)	2 (1%)	0	100	100
All	All	1482/1528 (97%)	1458 (98%)	21 (1%)	3 (0%)	47	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	392	GLY
1	B	373	ARG
2	E	106	PRO

### 5.3.2 Protein sidechains ⓘ

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	266/266 (100%)	265 (100%)	1 (0%)	91	94
1	B	266/266 (100%)	264 (99%)	2 (1%)	81	88
2	C	188/201 (94%)	187 (100%)	1 (0%)	88	92
2	E	192/201 (96%)	186 (97%)	6 (3%)	40	49
3	D	190/192 (99%)	189 (100%)	1 (0%)	88	92
3	F	190/192 (99%)	190 (100%)	0	100	100
All	All	1292/1318 (98%)	1281 (99%)	11 (1%)	78	86

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	484	ARG
1	B	370	ASP
1	B	442	SER
2	C	105	SER
3	D	193	LYS

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Mol	Chain	Res	Type
2	E	1	GLN
2	E	25	SER
2	E	67	ARG
2	E	87	ARG
2	E	189	PRO
2	E	226	ASN

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

Mol	Chain	Res	Type
2	C	62	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](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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

### 6.1 Protein, DNA and RNA chains

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	307/307 (100%)	-0.07	11 (3%) 42 44	21, 31, 48, 66	0
1	B	307/307 (100%)	-0.08	8 (2%) 56 59	22, 33, 56, 70	0
2	C	224/238 (94%)	-0.51	3 (1%) 77 79	22, 31, 50, 62	0
2	E	228/238 (95%)	-0.36	3 (1%) 77 79	22, 30, 54, 64	0
3	D	217/219 (99%)	-0.56	0 100 100	19, 31, 43, 50	0
3	F	217/219 (99%)	-0.59	0 100 100	21, 28, 41, 54	0
All	All	1500/1528 (98%)	-0.33	25 (1%) 70 73	19, 31, 49, 70	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	393	GLY	5.4
2	E	153	THR	4.6
1	B	393	GLY	4.4
2	C	115	ALA	4.2
1	B	392	GLY	4.0
1	A	392	GLY	3.6
1	B	373	ARG	3.4
1	A	531	GLY	3.3
1	B	394	THR	3.1
1	A	244	ILE	3.0
1	A	394	THR	2.8
1	B	281	VAL	2.6
1	B	225	LYS	2.6
2	C	1	GLN	2.5
1	A	391	ASP	2.5
1	B	395	THR	2.5
2	E	152	SER	2.4
1	A	283	ILE	2.3
1	A	373	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	395	THR	2.2
1	B	372	ASP	2.2
1	A	385	PRO	2.2
1	A	242	PHE	2.2
2	E	107	SER	2.1
2	C	212	GLY	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 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.