



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 04:39 pm BST

PDB ID : 4Z5R  
Title : Rontalizumab Fab bound to Interferon- $\alpha$ 2  
Authors : Eigenbrot, C.; Maurer, B.; Bosanac, I.  
Deposited on : 2015-04-02  
Resolution : 3.00 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](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
Mogul	:	1.8.5 (274361), CSD as541be (2020)
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)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

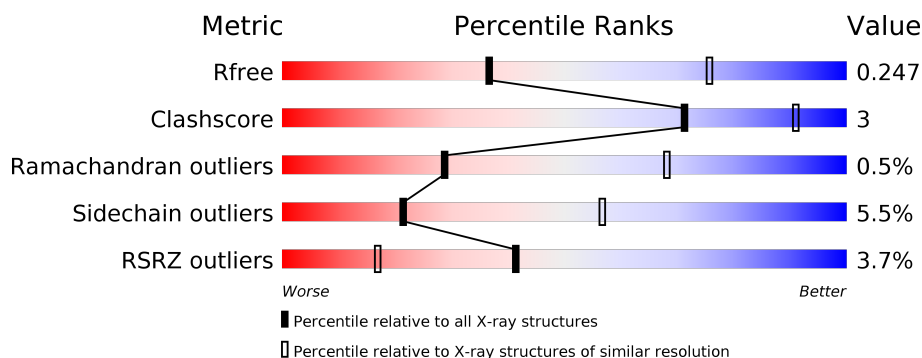
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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  $\geq 3$ , 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	D	165	<div> <div>2%</div> <div> <div></div> <div>69%</div> <div>13%</div> <div>•</div> <div>15%</div> </div> </div>
1	E	165	<div> <div>%</div> <div> <div></div> <div>70%</div> <div>12%</div> <div>•</div> <div>15%</div> </div> </div>
1	F	165	<div> <div>2%</div> <div> <div></div> <div>64%</div> <div>16%</div> <div>5%</div> <div>15%</div> </div> </div>
1	G	165	<div> <div>%</div> <div> <div></div> <div>68%</div> <div>13%</div> <div>•</div> <div>17%</div> </div> </div>
1	H	165	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>9%</div> <div>•</div> <div>16%</div> </div> </div>
1	I	165	<div> <div>2%</div> <div> <div></div> <div>67%</div> <div>13%</div> <div>•</div> <div>17%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	N	165	
1	X	165	
2	A	218	
2	J	218	
2	L	218	
2	P	218	
2	R	218	
2	T	218	
2	V	218	
2	Y	218	
3	B	225	
3	K	225	
3	M	225	
3	Q	225	
3	S	225	
3	U	225	
3	W	225	
3	Z	225	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 34056 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 Interferon alpha-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	141	Total	C	N	O	S	0	0	0
			1165	748	195	214	8			
1	E	141	Total	C	N	O	S	0	0	0
			1165	748	195	214	8			
1	F	140	Total	C	N	O	S	0	0	0
			1156	745	192	211	8			
1	G	137	Total	C	N	O	S	0	0	0
			1121	719	187	208	7			
1	H	139	Total	C	N	O	S	0	0	0
			1145	734	192	211	8			
1	I	137	Total	C	N	O	S	0	0	0
			1127	723	188	208	8			
1	X	137	Total	C	N	O	S	0	0	0
			1133	728	189	208	8			
1	N	145	Total	C	N	O	S	0	0	0
			1198	768	200	222	8			

- Molecule 2 is a protein called anti-IFN-a antibody rontalizumab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	217	Total	C	N	O	S	0	0	0
			1669	1041	282	340	6			
2	L	217	Total	C	N	O	S	0	0	0
			1669	1041	282	340	6			
2	V	217	Total	C	N	O	S	0	0	0
			1669	1041	282	340	6			
2	P	217	Total	C	N	O	S	0	0	0
			1669	1041	282	340	6			
2	R	217	Total	C	N	O	S	0	0	0
			1669	1041	282	340	6			
2	T	217	Total	C	N	O	S	0	0	0
			1669	1041	282	340	6			

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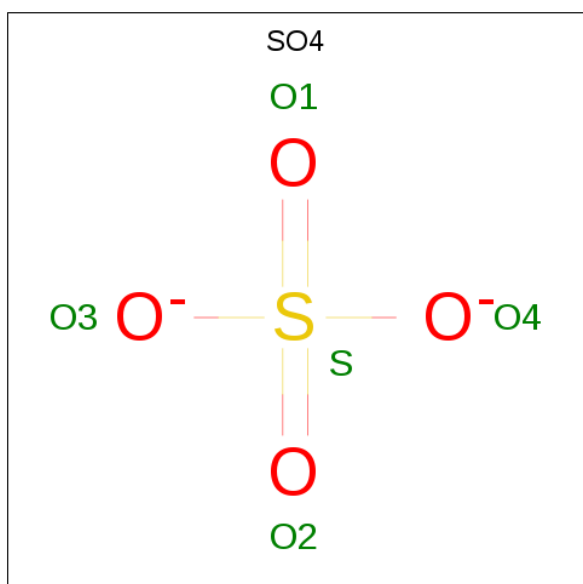
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	110	Total	C	N	O	S	0	0	0
			840	525	141	170	4			
2	A	217	Total	C	N	O	S	0	0	0
			1669	1041	282	340	6			

- Molecule 3 is a protein called anti-IFN-a antibody rontalizumab heavy chain modules VH and CH1 (Fab).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	213	Total	C	N	O	S	0	0	0
			1622	1033	268	316	5			
3	M	213	Total	C	N	O	S	0	0	0
			1622	1033	268	316	5			
3	W	213	Total	C	N	O	S	0	0	0
			1622	1033	268	316	5			
3	Q	213	Total	C	N	O	S	0	0	0
			1622	1033	268	316	5			
3	S	213	Total	C	N	O	S	0	0	0
			1622	1033	268	316	5			
3	U	213	Total	C	N	O	S	0	0	0
			1622	1033	268	316	5			
3	Z	117	Total	C	N	O	S	0	0	0
			929	593	155	178	3			
3	B	213	Total	C	N	O	S	0	0	0
			1622	1033	268	316	5			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

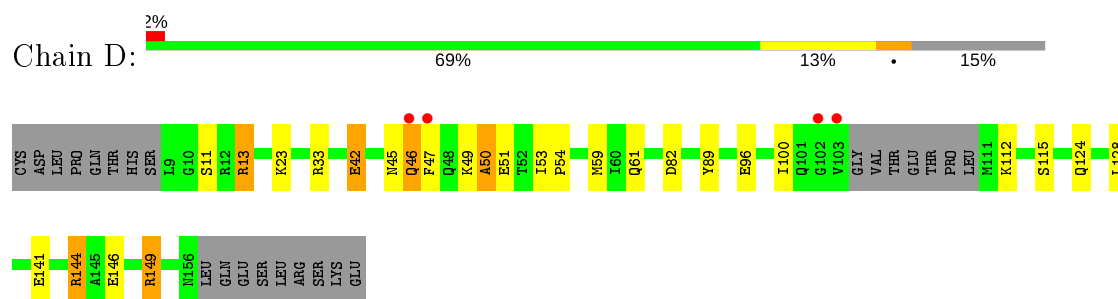


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	J	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	V	1	Total	O	S	0	0
			5	4	1		
4	V	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	P	1	Total	O	S	0	0
			5	4	1		

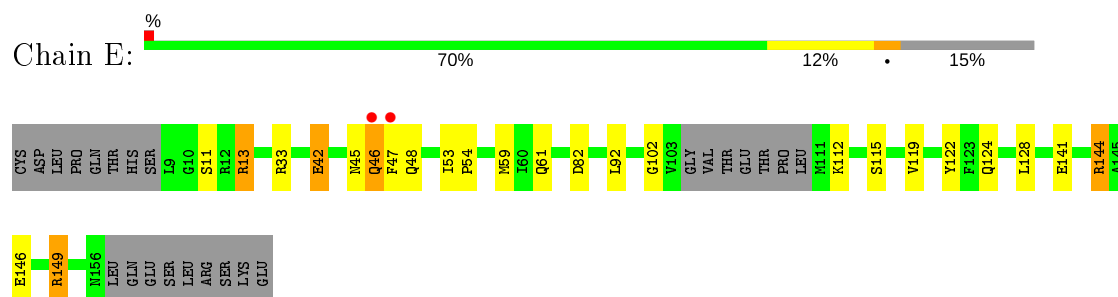
### 3 Residue-property plots [i](#)

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.

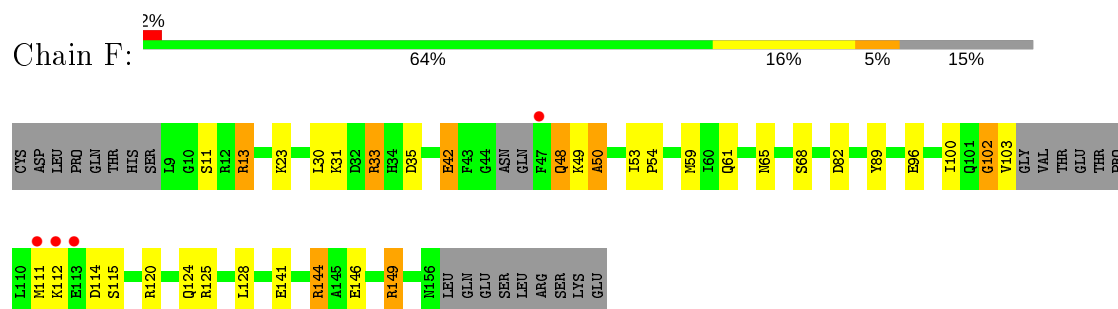
#### • Molecule 1: Interferon alpha-2



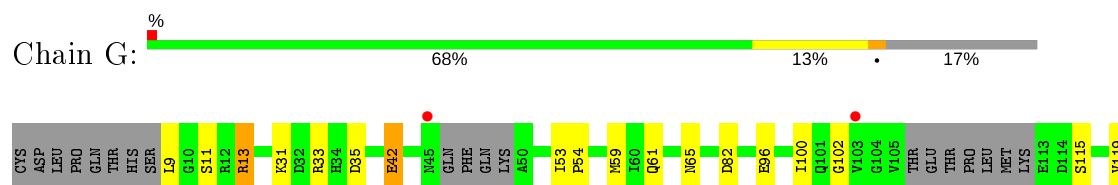
#### • Molecule 1: Interferon alpha-2



#### • Molecule 1: Interferon alpha-2

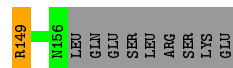
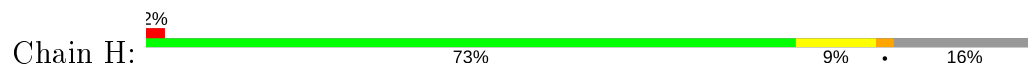


#### • Molecule 1: Interferon alpha-2

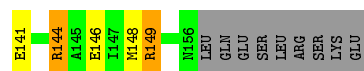




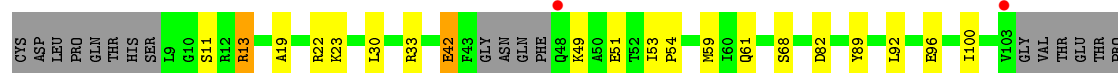
- Molecule 1: Interferon alpha-2



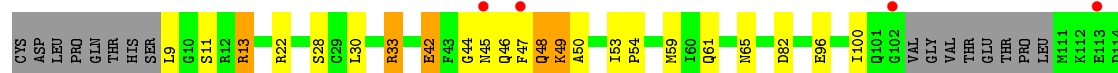
- Molecule 1: Interferon alpha-2



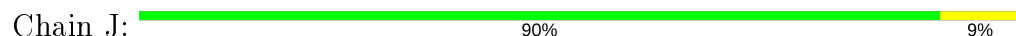
- Molecule 1: Interferon alpha-2



- Molecule 1: Interferon alpha-2



- Molecule 2: anti-IFN-a antibody rontalizumab light chain







- Molecule 2: anti-IFN- $\alpha$  antibody rontalizumab light chain

Chain L: 88% 11%



- Molecule 2: anti-IFN- $\alpha$  antibody rontalizumab light chain

Chain V: 89% 11%



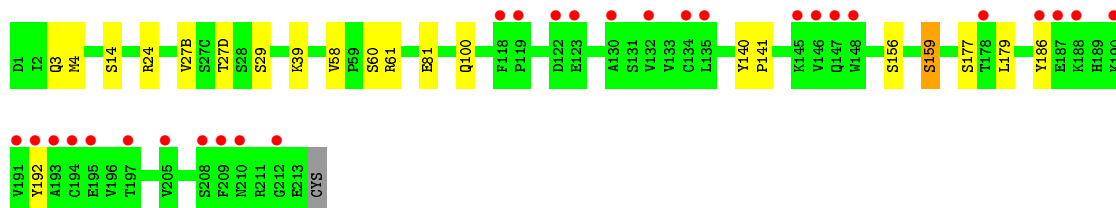
- Molecule 2: anti-IFN- $\alpha$  antibody rontalizumab light chain

Chain P: 89% 9%



- Molecule 2: anti-IFN- $\alpha$  antibody rontalizumab light chain

Chain R: 13% 90% 9%



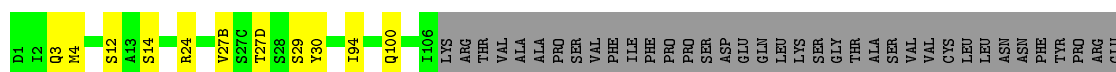
- Molecule 2: anti-IFN- $\alpha$  antibody rontalizumab light chain

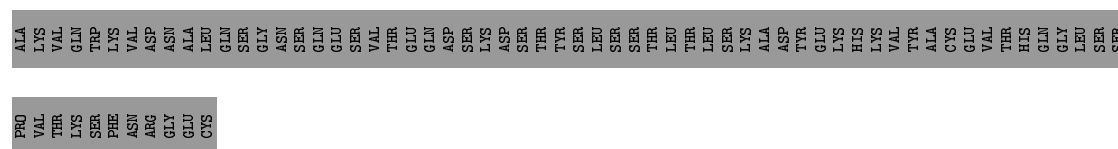
Chain T: 87% 11%



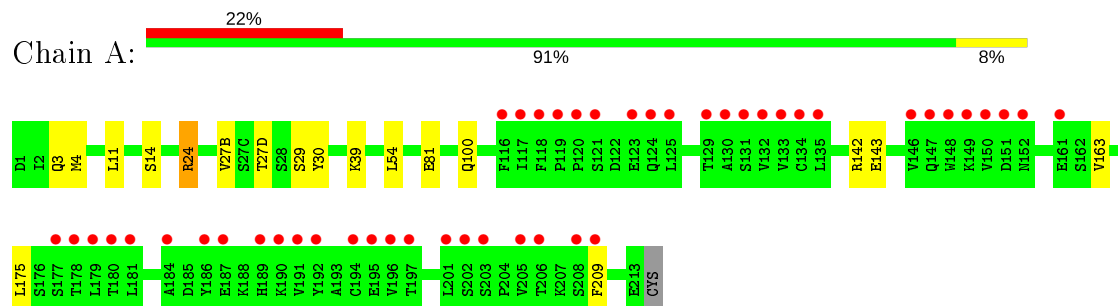
- Molecule 2: anti-IFN- $\alpha$  antibody rontalizumab light chain

Chain Y: 45% 5% 50%

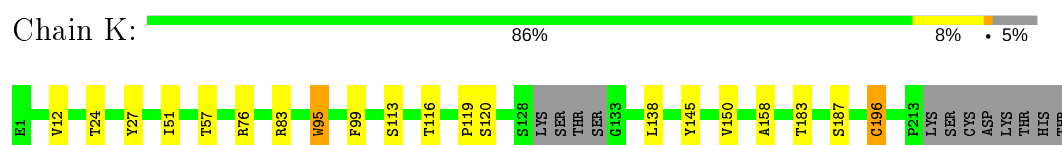




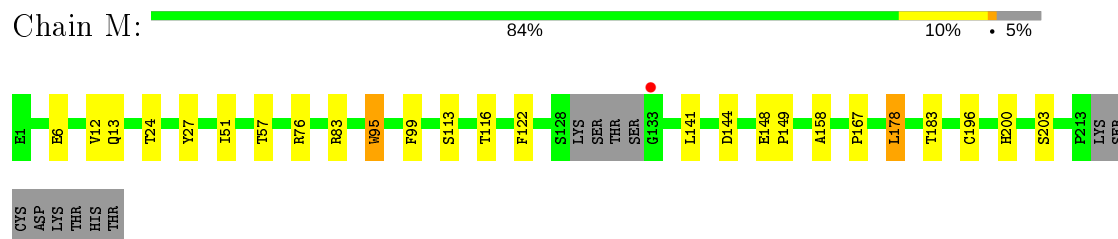
- Molecule 2: anti-IFN- $\alpha$  antibody rontalizumab light chain



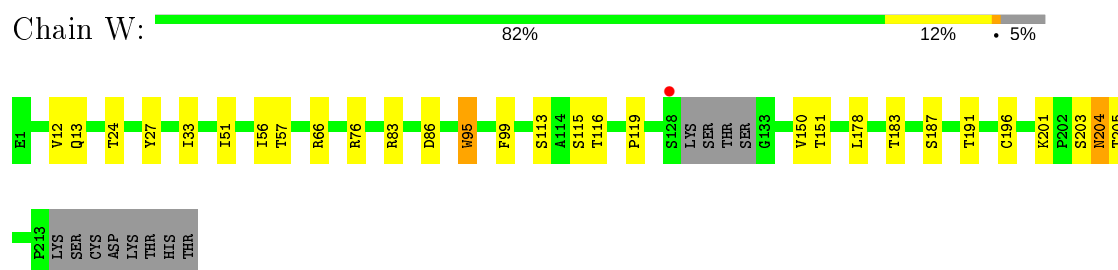
- Molecule 3: anti-IFN- $\alpha$  antibody rontalizumab heavy chain modules VH and CH1 (Fab)



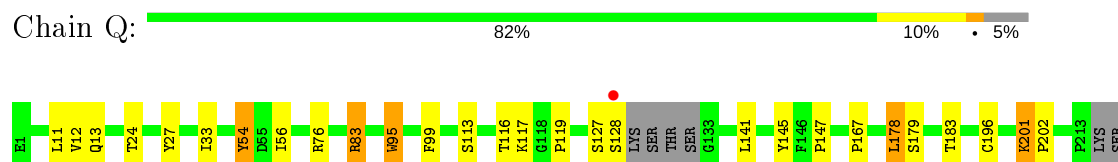
- Molecule 3: anti-IFN- $\alpha$  antibody rontalizumab heavy chain modules VH and CH1 (Fab)



- Molecule 3: anti-IFN- $\alpha$  antibody rontalizumab heavy chain modules VH and CH1 (Fab)



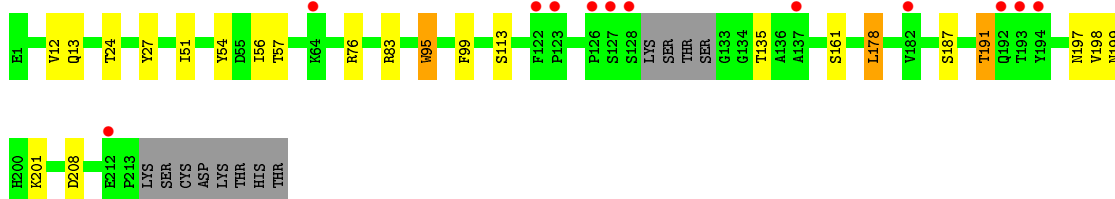
- Molecule 3: anti-IFN- $\alpha$  antibody rontalizumab heavy chain modules VH and CH1 (Fab)



CYS  
ASP  
LYS  
THR  
HIS  
THR

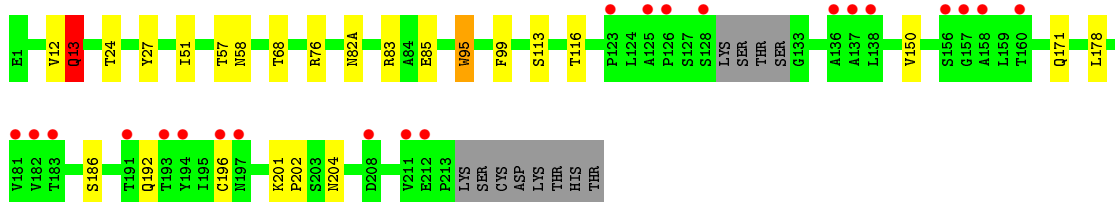
- Molecule 3: anti-IFN- $\alpha$  antibody rontalizumab heavy chain modules VH and CH1 (Fab)

Chain S: 5% 84% 9% 5%



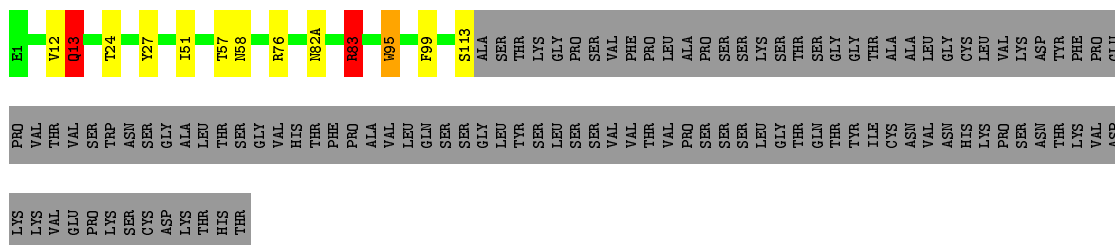
- Molecule 3: anti-IFN- $\alpha$  antibody rontalizumab heavy chain modules VH and CH1 (Fab)

Chain U: 10% 84% 10% 5%



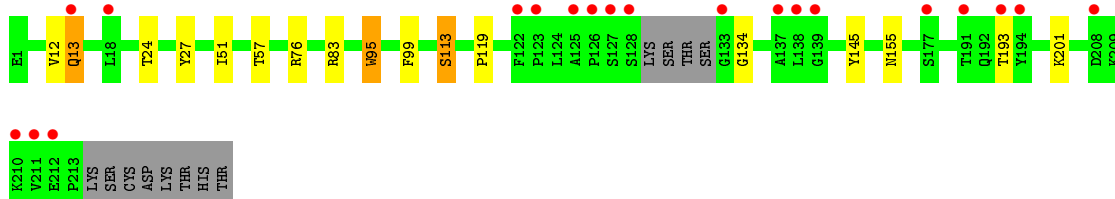
- Molecule 3: anti-IFN- $\alpha$  antibody rontalizumab heavy chain modules VH and CH1 (Fab)

Chain Z: 46% 48%



- Molecule 3: anti-IFN- $\alpha$  antibody rontalizumab heavy chain modules VH and CH1 (Fab)

Chain B: 9% 87% 6% 5%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.83Å 331.86Å 98.14Å 90.00° 111.28° 90.00°	Depositor
Resolution (Å)	48.21 – 3.00 48.21 – 3.00	Depositor EDS
% Data completeness (in resolution range)	94.8 (48.21-3.00) 94.9 (48.21-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.70 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.223 , 0.251 0.215 , 0.247	Depositor DCC
$R_{free}$ test set	2285 reflections (2.24%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.6	Xtriage
Anisotropy	0.726	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 36.3	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	0.93	EDS
Total number of atoms	34056	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.73% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	D	0.48	0/1187	0.85	5/1594 (0.3%)
1	E	0.46	0/1187	0.87	5/1594 (0.3%)
1	F	0.47	0/1177	0.86	6/1579 (0.4%)
1	G	0.52	0/1141	0.90	5/1534 (0.3%)
1	H	0.43	0/1165	0.85	4/1563 (0.3%)
1	I	0.54	1/1147 (0.1%)	0.85	5/1540 (0.3%)
1	N	0.44	0/1220	0.88	7/1638 (0.4%)
1	X	0.42	0/1153	0.83	4/1547 (0.3%)
2	A	0.40	0/1707	0.65	1/2317 (0.0%)
2	J	0.54	0/1707	0.77	1/2317 (0.0%)
2	L	0.58	0/1707	0.80	1/2317 (0.0%)
2	P	0.55	0/1707	0.77	1/2317 (0.0%)
2	R	0.43	0/1707	0.68	1/2317 (0.0%)
2	T	0.49	1/1707 (0.1%)	0.70	1/2317 (0.0%)
2	V	0.54	0/1707	0.76	1/2317 (0.0%)
2	Y	0.45	0/861	0.76	1/1169 (0.1%)
3	B	0.42	0/1664	0.78	6/2270 (0.3%)
3	K	0.57	0/1664	0.82	3/2270 (0.1%)
3	M	0.62	1/1664 (0.1%)	0.84	3/2270 (0.1%)
3	Q	0.62	1/1664 (0.1%)	0.82	3/2270 (0.1%)
3	S	0.44	0/1664	0.74	3/2270 (0.1%)
3	U	0.46	0/1664	0.79	5/2270 (0.2%)
3	W	0.57	1/1664 (0.1%)	0.80	4/2270 (0.2%)
3	Z	0.47	0/953	0.81	5/1295 (0.4%)
All	All	0.51	5/34788 (0.0%)	0.79	81/47162 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	I	0	1
1	N	0	3
1	X	0	1
3	Q	0	1
3	Z	0	1
All	All	0	12

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	45	ASN	C-O	9.76	1.41	1.23
3	W	13	GLN	CD-OE1	-9.44	1.03	1.24
3	Q	13	GLN	CD-OE1	-8.69	1.04	1.24
3	M	13	GLN	CD-OE1	-7.85	1.06	1.24
2	T	27(B)	VAL	CB-CG1	-6.99	1.38	1.52

The worst 5 of 81 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	13	ARG	NE-CZ-NH2	-15.87	112.37	120.30
1	D	13	ARG	NE-CZ-NH2	-15.57	112.51	120.30
1	E	13	ARG	NE-CZ-NH2	-15.57	112.52	120.30
1	I	13	ARG	NE-CZ-NH2	-15.50	112.55	120.30
1	N	13	ARG	NE-CZ-NH2	-15.49	112.56	120.30

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	13	ARG	Sidechain
1	E	13	ARG	Sidechain
1	F	13	ARG	Sidechain
1	G	13	ARG	Sidechain
3	Q	83	ARG	Sidechain

## 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	D	1165	0	1163	11	1
1	E	1165	0	1163	8	0
1	F	1156	0	1159	24	0
1	G	1121	0	1114	10	2
1	H	1145	0	1145	10	0
1	I	1127	0	1124	9	2
1	N	1198	0	1195	18	1
1	X	1133	0	1136	24	1
2	A	1669	0	1611	10	0
2	J	1669	0	1611	5	1
2	L	1669	0	1611	8	0
2	P	1669	0	1611	9	0
2	R	1669	0	1611	12	0
2	T	1669	0	1611	16	0
2	V	1669	0	1611	11	0
2	Y	840	0	804	8	0
3	B	1622	0	1578	6	1
3	K	1622	0	1578	9	0
3	M	1622	0	1578	10	0
3	Q	1622	0	1578	13	0
3	S	1622	0	1578	13	1
3	U	1622	0	1578	18	0
3	W	1622	0	1578	11	0
3	Z	929	0	888	17	0
4	F	5	0	0	0	0
4	G	5	0	0	0	0
4	J	10	0	0	0	0
4	L	5	0	0	0	0
4	P	5	0	0	0	0
4	V	10	0	0	1	0
All	All	34056	0	33214	235	5

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.

The worst 5 of 235 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:V:39:LYS:NZ	4:V:302:SO4:O3	2.03	0.92
1:G:125:ARG:CZ	3:Q:56:ILE:HD11	2.08	0.83
3:B:27:TYR:O	3:B:76:ARG:NH1	2.12	0.82
2:Y:27(D):THR:HG22	2:Y:29:SER:H	1.44	0.82
3:Q:27:TYR:O	3:Q:76:ARG:NH1	2.12	0.82

All (5) 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	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:13:GLN:NE2	1:I:27:PHE:CB[1_655]	2.05	0.15
2:J:202:SER:OG	1:G:132:GLU:OE2[1_556]	2.07	0.13
1:D:89:TYR:OH	1:N:65:ASN:O[2_645]	2.15	0.05
1:G:65:ASN:O	1:I:89:TYR:OH[1_554]	2.16	0.04
1:X:23:LYS:O	3:B:113:SER:CB[1_455]	2.18	0.02

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	D	137/165 (83%)	131 (96%)	4 (3%)	2 (2%)	10	42
1	E	137/165 (83%)	131 (96%)	3 (2%)	3 (2%)	6	31
1	F	134/165 (81%)	127 (95%)	4 (3%)	3 (2%)	6	31
1	G	131/165 (79%)	126 (96%)	4 (3%)	1 (1%)	19	57
1	H	133/165 (81%)	128 (96%)	4 (3%)	1 (1%)	19	57
1	I	131/165 (79%)	126 (96%)	5 (4%)	0	100	100
1	N	141/165 (86%)	129 (92%)	8 (6%)	4 (3%)	5	25
1	X	131/165 (79%)	126 (96%)	5 (4%)	0	100	100
2	A	215/218 (99%)	200 (93%)	14 (6%)	1 (0%)	29	68
2	J	215/218 (99%)	207 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	215/218 (99%)	204 (95%)	10 (5%)	1 (0%)	29	68
2	P	215/218 (99%)	207 (96%)	8 (4%)	0	100	100
2	R	215/218 (99%)	203 (94%)	11 (5%)	1 (0%)	29	68
2	T	215/218 (99%)	207 (96%)	8 (4%)	0	100	100
2	V	215/218 (99%)	207 (96%)	8 (4%)	0	100	100
2	Y	108/218 (50%)	103 (95%)	5 (5%)	0	100	100
3	B	209/225 (93%)	198 (95%)	9 (4%)	2 (1%)	15	53
3	K	209/225 (93%)	201 (96%)	8 (4%)	0	100	100
3	M	209/225 (93%)	199 (95%)	9 (4%)	1 (0%)	29	68
3	Q	209/225 (93%)	200 (96%)	8 (4%)	1 (0%)	29	68
3	S	209/225 (93%)	198 (95%)	11 (5%)	0	100	100
3	U	209/225 (93%)	198 (95%)	10 (5%)	1 (0%)	29	68
3	W	209/225 (93%)	200 (96%)	8 (4%)	1 (0%)	29	68
3	Z	115/225 (51%)	112 (97%)	3 (3%)	0	100	100
All	All	4266/4864 (88%)	4068 (95%)	175 (4%)	23 (0%)	29	68

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	46	GLN
3	U	204	ASN
1	N	47	PHE
1	N	48	GLN
1	D	50	ALA

### 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	D	129/152 (85%)	121 (94%)	8 (6%)	18	52
1	E	129/152 (85%)	120 (93%)	9 (7%)	15	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	128/152 (84%)	120 (94%)	8 (6%)	18	51
1	G	124/152 (82%)	116 (94%)	8 (6%)	17	50
1	H	127/152 (84%)	119 (94%)	8 (6%)	18	51
1	I	125/152 (82%)	115 (92%)	10 (8%)	12	40
1	N	133/152 (88%)	121 (91%)	12 (9%)	9	35
1	X	126/152 (83%)	117 (93%)	9 (7%)	14	46
2	A	192/193 (100%)	187 (97%)	5 (3%)	46	78
2	J	192/193 (100%)	182 (95%)	10 (5%)	23	59
2	L	192/193 (100%)	182 (95%)	10 (5%)	23	59
2	P	192/193 (100%)	181 (94%)	11 (6%)	20	56
2	R	192/193 (100%)	185 (96%)	7 (4%)	35	70
2	T	192/193 (100%)	183 (95%)	9 (5%)	26	63
2	V	192/193 (100%)	183 (95%)	9 (5%)	26	63
2	Y	96/193 (50%)	90 (94%)	6 (6%)	18	51
3	B	181/193 (94%)	175 (97%)	6 (3%)	38	73
3	K	181/193 (94%)	172 (95%)	9 (5%)	24	60
3	M	181/193 (94%)	172 (95%)	9 (5%)	24	60
3	Q	181/193 (94%)	170 (94%)	11 (6%)	18	53
3	S	181/193 (94%)	173 (96%)	8 (4%)	28	65
3	U	181/193 (94%)	171 (94%)	10 (6%)	21	57
3	W	181/193 (94%)	169 (93%)	12 (7%)	16	49
3	Z	99/193 (51%)	94 (95%)	5 (5%)	24	60
All	All	3827/4304 (89%)	3618 (94%)	209 (6%)	21	57

5 of 209 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	P	14	SER
1	H	59	MET
1	N	144	ARG
2	P	100	GLN
3	Q	116	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
2	V	147	GLN
3	Q	199	ASN
1	X	124	GLN
2	L	199	GLN
2	R	124	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

8 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	SO4	J	302	-	4,4,4	0.62	0	6,6,6	0.32	0
4	SO4	L	301	-	4,4,4	0.57	0	6,6,6	0.34	0
4	SO4	F	201	-	4,4,4	0.43	0	6,6,6	0.20	0
4	SO4	V	302	-	4,4,4	0.53	0	6,6,6	0.41	0
4	SO4	G	501	-	4,4,4	0.52	0	6,6,6	0.26	0
4	SO4	P	301	-	4,4,4	0.70	0	6,6,6	0.63	0
4	SO4	V	301	-	4,4,4	0.67	0	6,6,6	0.71	0
4	SO4	J	301	-	4,4,4	0.54	0	6,6,6	0.33	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	V	302	SO4	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 ⓘ

### 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	D	141/165 (85%)	-0.01	4 (2%) 53 25	48, 70, 120, 167	0
1	E	141/165 (85%)	-0.08	2 (1%) 75 49	50, 71, 122, 180	0
1	F	140/165 (84%)	-0.06	4 (2%) 51 23	49, 70, 121, 152	0
1	G	137/165 (83%)	-0.03	2 (1%) 73 46	41, 61, 103, 133	1 (0%)
1	H	139/165 (84%)	-0.05	4 (2%) 51 23	61, 80, 121, 161	0
1	I	137/165 (83%)	0.01	4 (2%) 51 23	57, 74, 104, 140	0
1	N	145/165 (87%)	0.07	7 (4%) 30 11	59, 83, 144, 186	0
1	X	137/165 (83%)	0.06	3 (2%) 62 33	64, 82, 115, 139	0
2	A	217/218 (99%)	0.85	47 (21%) 0 0	65, 96, 158, 172	3 (1%)
2	J	217/218 (99%)	-0.30	0 100 100	41, 54, 74, 104	1 (0%)
2	L	217/218 (99%)	-0.36	0 100 100	41, 52, 71, 94	0
2	P	217/218 (99%)	-0.36	0 100 100	37, 53, 73, 96	0
2	R	217/218 (99%)	0.44	28 (12%) 3 1	57, 84, 136, 149	0
2	T	217/218 (99%)	0.05	1 (0%) 91 75	70, 86, 110, 125	0
2	V	217/218 (99%)	-0.30	0 100 100	45, 57, 78, 98	0
2	Y	110/218 (50%)	-0.03	0 100 100	65, 80, 102, 113	0
3	B	213/225 (94%)	0.49	20 (9%) 8 3	64, 100, 159, 167	0
3	K	213/225 (94%)	-0.36	0 100 100	40, 54, 79, 101	0
3	M	213/225 (94%)	-0.32	1 (0%) 91 75	40, 57, 84, 101	0
3	Q	213/225 (94%)	-0.20	1 (0%) 91 75	38, 54, 81, 110	0
3	S	213/225 (94%)	0.21	12 (5%) 24 8	60, 85, 136, 155	0
3	U	213/225 (94%)	0.45	22 (10%) 6 2	65, 85, 134, 152	0
3	W	213/225 (94%)	-0.29	1 (0%) 91 75	43, 58, 85, 114	0
3	Z	117/225 (52%)	0.00	0 100 100	66, 82, 105, 116	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	4354/4864 (89%)	-0.00	163 (3%) 41 17	37, 71, 131, 186	5 (0%)

The worst 5 of 163 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	128	SER	6.1
2	A	194	CYS	6.1
2	A	195	GLU	5.6
3	U	128	SER	5.4
2	R	194	CYS	5.3

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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<sup>th</sup> 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	B-factors(Å <sup>2</sup> )	Q<0.9
4	SO4	J	302	5/5	0.86	0.36	74,86,93,97	0
4	SO4	P	301	5/5	0.89	0.26	66,70,78,81	0
4	SO4	J	301	5/5	0.90	0.28	74,76,85,87	0
4	SO4	F	201	5/5	0.91	0.28	96,97,109,111	0
4	SO4	V	301	5/5	0.92	0.24	69,74,85,96	0
4	SO4	G	501	5/5	0.93	0.24	79,86,97,103	0
4	SO4	L	301	5/5	0.94	0.41	68,69,81,84	0
4	SO4	V	302	5/5	0.94	0.14	78,80,93,94	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.