



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 02:51 PM EDT

PDB ID : 1BJ1  
Title : VASCULAR ENDOTHELIAL GROWTH FACTOR IN COMPLEX WITH A NEUTRALIZING ANTIBODY  
Authors : Muller, Y.A.; Christinger, H.W.; De Vos, A.M.  
Deposited on : 1998-06-30  
Resolution : 2.40 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	2.36.2
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)	:	2.36.2

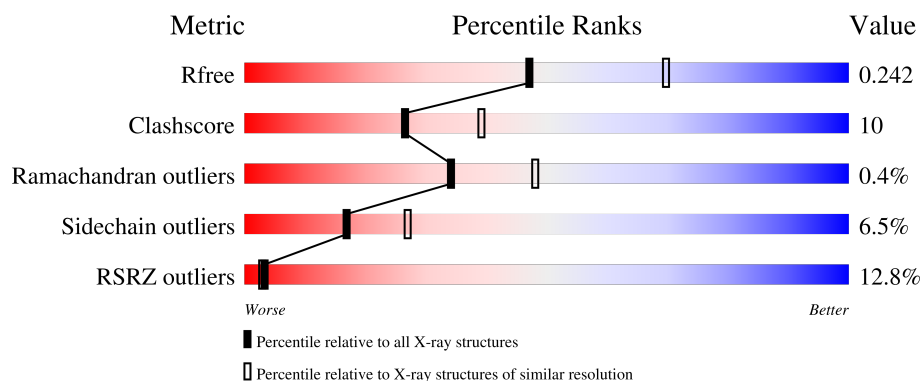
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	J	214	
1	L	214	
2	H	231	
2	K	231	
3	V	102	

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Mol	Chain	Length	Quality of chain
3	W	102	<div><div></div><div>2%</div><div>61%</div><div>30%</div><div>8%</div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8694 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 Fab fragment, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	213	Total	C	N	O	S	0	0	0
			1644	1031	272	336	5			
1	J	213	Total	C	N	O	S	0	0	0
			1644	1031	272	336	5			

- Molecule 2 is a protein called Fab fragment, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	218	Total	C	N	O	S	0	0	0
			1663	1064	273	320	6			
2	K	218	Total	C	N	O	S	0	0	0
			1663	1064	273	320	6			

- Molecule 3 is a protein called Vascular endothelial growth factor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	V	94	Total	C	N	O	S	0	0	0
			761	478	128	142	13			
3	W	94	Total	C	N	O	S	0	0	0
			761	478	128	142	13			

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	O	S	0	0
			5	4	1		
4	K	1	Total	O	S	0	0
			5	4	1		

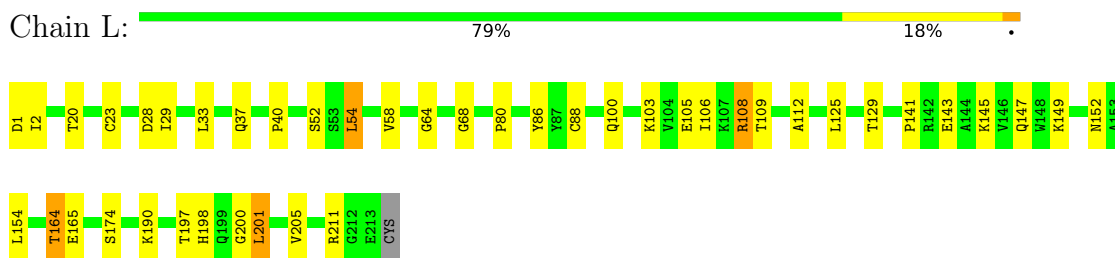
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	167	Total	O	0	0
			167	167		
5	H	190	Total	O	0	0
			190	190		
5	V	31	Total	O	0	0
			31	31		
5	W	34	Total	O	0	0
			34	34		
5	J	59	Total	O	0	0
			59	59		
5	K	67	Total	O	0	0
			67	67		

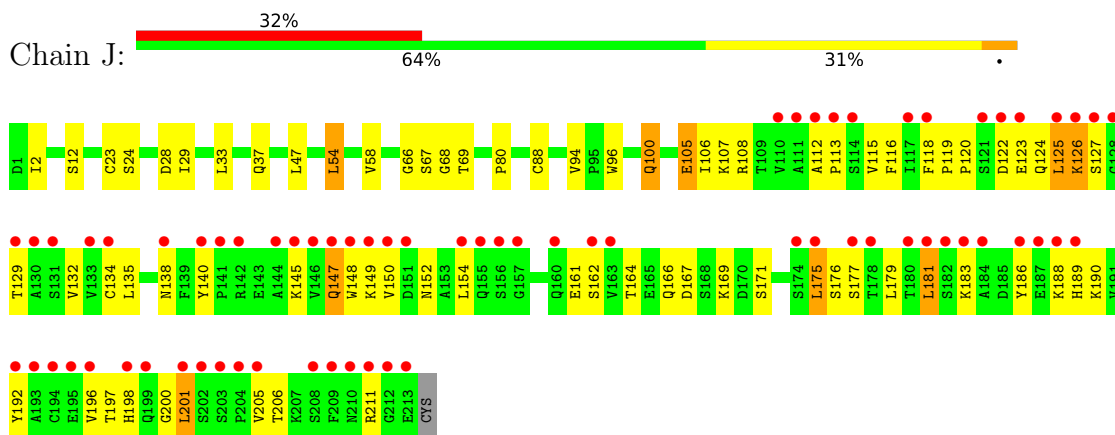
### 3 Residue-property plots

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.

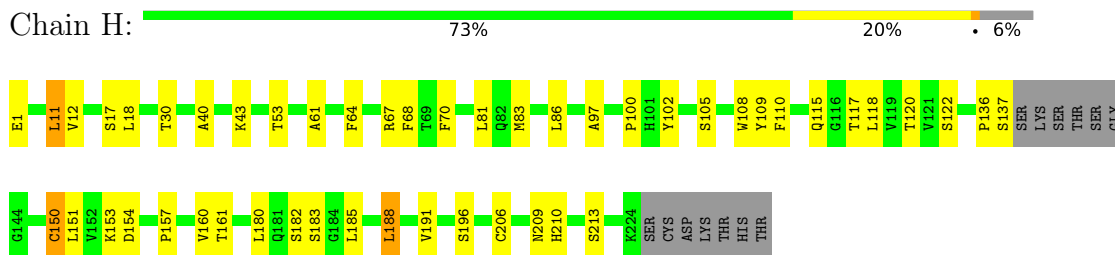
- Molecule 1: Fab fragment, light chain



- Molecule 1: Fab fragment, light chain

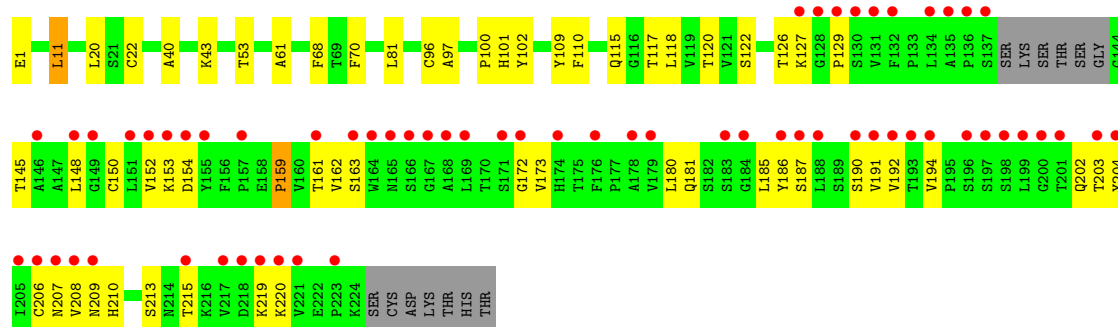


- Molecule 2: Fab fragment, heavy chain



- Molecule 2: Fab fragment, heavy chain





- Molecule 3: Vascular endothelial growth factor A

Chain V: 71% 21% 8%



- Molecule 3: Vascular endothelial growth factor A

Chain W: 2% 61% 30% 8%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.86Å 66.98Å 140.51Å 90.00° 94.27° 90.00°	Depositor
Resolution (Å)	8.00 – 2.40 78.18 – 2.39	Depositor EDS
% Data completeness (in resolution range)	94.8 (8.00-2.40) 94.0 (78.18-2.39)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.13 (at 2.40Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, $R_{free}$	0.196 , 0.266 0.185 , 0.242	Depositor DCC
$R_{free}$ test set	5908 reflections (9.51%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.0	Xtriage
Anisotropy	0.639	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 93.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8694	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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	J	0.54	0/1682	0.72	0/2287
1	L	0.62	0/1682	0.79	0/2287
2	H	0.65	1/1712 (0.1%)	0.84	1/2338 (0.0%)
2	K	0.54	0/1712	0.74	1/2338 (0.0%)
3	V	0.56	0/779	0.73	0/1050
3	W	0.58	0/779	0.74	0/1050
All	All	0.59	1/8346 (0.0%)	0.77	2/11350 (0.0%)

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
3	V	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	150	CYS	CB-SG	-5.18	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	188	LEU	CA-CB-CG	6.85	131.05	115.30
2	K	61	ALA	N-CA-C	-5.46	96.27	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	V	21	TYR	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	J	1644	0	1587	47	0
1	L	1644	0	1587	23	0
2	H	1663	0	1605	27	0
2	K	1663	0	1605	41	0
3	V	761	0	728	18	0
3	W	761	0	728	23	0
4	H	5	0	0	0	0
4	K	5	0	0	0	0
5	H	190	0	0	4	0
5	J	59	0	0	0	0
5	K	67	0	0	0	0
5	L	167	0	0	3	0
5	V	31	0	0	0	0
5	W	34	0	0	0	0
All	All	8694	0	7840	164	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 10.

All (164) 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:183:SER:HA	5:H:331:HOH:O	1.53	1.08
2:K:150:CYS:HG	2:K:206:CYS:HG	0.93	0.85
2:K:22:CYS:HG	2:K:96:CYS:HG	1.02	0.85
2:H:150:CYS:SG	2:H:206:CYS:SG	2.50	0.84
2:K:22:CYS:SG	2:K:96:CYS:SG	2.65	0.79
2:K:150:CYS:SG	2:K:206:CYS:SG	2.69	0.78
1:J:113:PRO:HD2	1:J:201:LEU:HD13	1.65	0.77
1:L:80:PRO:HA	1:L:106:ILE:HD13	1.64	0.77
2:K:206:CYS:SG	2:K:219:LYS:HB3	2.26	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:198:HIS:CD2	1:L:200:GLY:H	2.08	0.71
1:J:145:LYS:HB3	1:J:197:THR:HB	1.71	0.71
2:K:150:CYS:HG	2:K:206:CYS:CB	2.04	0.71
2:K:129:PRO:HB2	2:K:152:VAL:HG12	1.73	0.70
2:H:210:HIS:HD2	2:H:213:SER:OG	1.77	0.67
2:K:203:THR:HG23	2:K:220:LYS:HE3	1.77	0.66
3:V:89:GLN:HE22	2:K:53:THR:H	1.44	0.66
2:H:157:PRO:O	2:H:210:HIS:HE1	1.78	0.66
1:J:198:HIS:CD2	1:J:200:GLY:H	2.13	0.65
1:J:161:GLU:HB2	1:J:175:LEU:HD21	1.78	0.65
3:W:34:ASP:O	3:W:37:GLN:HG2	1.96	0.65
2:K:40:ALA:HB3	2:K:43:LYS:HE3	1.78	0.64
1:J:190:LYS:HA	1:J:211:ARG:HB3	1.78	0.63
2:K:20:LEU:HD12	2:K:81:LEU:HD23	1.80	0.63
2:K:127:LYS:NZ	2:K:154:ASP:HB3	2.14	0.63
1:J:148:TRP:HE1	1:J:177:SER:HG	1.49	0.61
1:J:162:SER:HB2	1:J:176:SER:OG	2.00	0.61
1:J:123:GLU:O	1:J:126:LYS:HG3	2.00	0.61
3:V:60:CYS:HG	3:W:51:CYS:HG	1.49	0.60
1:L:28:ASP:OD1	1:L:68:GLY:HA2	2.00	0.60
3:V:92:GLY:HA2	2:K:101:HIS:CE1	2.37	0.59
2:K:161:THR:HB	2:K:209:ASN:HB3	1.84	0.59
2:K:127:LYS:HZ2	2:K:154:ASP:HB3	1.66	0.59
3:V:48:LYS:O	3:W:17:PHE:HE1	1.86	0.58
1:J:107:LYS:HA	1:J:140:TYR:OH	2.03	0.58
1:J:189:HIS:O	1:J:211:ARG:HD3	2.04	0.58
3:V:59:GLY:HA2	3:W:32:LEU:HD13	1.86	0.57
2:H:151:LEU:HG	2:H:153:LYS:HG3	1.85	0.57
1:J:113:PRO:HD3	1:J:198:HIS:CD2	2.38	0.57
1:J:115:VAL:CG2	1:J:196:VAL:HG21	2.35	0.57
1:L:54:LEU:HD22	1:L:58:VAL:HB	1.86	0.56
2:K:100:PRO:HD3	2:K:109:TYR:O	2.06	0.56
1:L:147:GLN:HG3	1:L:154:LEU:HD13	1.89	0.55
3:V:34:ASP:O	3:V:37:GLN:HG2	2.06	0.55
1:L:198:HIS:HD2	1:L:200:GLY:H	1.53	0.55
2:H:40:ALA:HB3	2:H:43:LYS:HE3	1.89	0.55
1:J:154:LEU:HD12	1:J:154:LEU:H	1.71	0.54
1:J:54:LEU:HD22	1:J:58:VAL:HB	1.90	0.54
1:J:205:VAL:HG12	1:J:206:THR:N	2.23	0.53
2:H:53:THR:H	3:W:89:GLN:HE22	1.56	0.53
3:W:44:GLU:H	3:W:44:GLU:CD	2.11	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:129:PRO:HA	2:K:154:ASP:O	2.08	0.53
2:K:153:LYS:HG2	2:K:187:SER:OG	2.09	0.53
2:K:173:VAL:HA	2:K:191:VAL:O	2.09	0.53
2:H:12:VAL:HG11	2:H:86:LEU:HD13	1.91	0.52
1:L:141:PRO:O	1:L:198:HIS:HE1	1.93	0.52
1:L:40:PRO:CG	1:L:165:GLU:HG2	2.40	0.52
1:J:28:ASP:OD1	1:J:68:GLY:HA2	2.09	0.52
2:H:161:THR:HG22	5:H:283:HOH:O	2.10	0.51
3:V:77:THR:CG2	3:W:14:VAL:HG22	2.40	0.51
1:L:103:LYS:HE2	5:L:379:HOH:O	2.11	0.51
1:L:112:ALA:HB1	1:L:201:LEU:HD13	1.92	0.51
3:W:73:GLU:HB3	3:W:97:LEU:HD11	1.92	0.51
1:J:2:ILE:HD13	1:J:29:ILE:HG22	1.92	0.50
1:J:80:PRO:HA	1:J:106:ILE:HD13	1.93	0.50
1:J:166:GLN:HE21	1:J:171:SER:HB3	1.75	0.50
2:K:145:THR:HG23	2:K:194:VAL:O	2.11	0.50
2:K:206:CYS:SG	2:K:206:CYS:O	2.71	0.49
2:K:11:LEU:HD21	2:K:122:SER:HB3	1.94	0.49
3:V:77:THR:HG22	3:W:14:VAL:HG22	1.95	0.49
3:V:71:THR:CG2	3:V:103:GLU:HB2	2.42	0.49
1:J:120:PRO:HD3	1:J:132:VAL:HG22	1.95	0.49
1:J:150:VAL:HG21	1:J:179:LEU:HD21	1.95	0.49
1:J:201:LEU:HG	1:J:205:VAL:HG23	1.95	0.49
2:K:180:LEU:HD23	2:K:186:TYR:CE1	2.48	0.49
1:J:24:SER:HA	1:J:69:THR:O	2.13	0.48
3:W:71:THR:CG2	3:W:103:GLU:HB2	2.42	0.48
3:V:44:GLU:H	3:V:44:GLU:CD	2.17	0.48
3:W:69:VAL:HG22	3:W:103:GLU:O	2.13	0.48
2:K:202:GLN:HG2	2:K:204:TYR:CZ	2.48	0.48
2:H:100:PRO:HD3	2:H:109:TYR:O	2.13	0.48
3:W:79:GLN:HA	3:W:92:GLY:O	2.14	0.48
1:J:161:GLU:HA	1:J:176:SER:O	2.14	0.47
3:W:71:THR:HG21	3:W:103:GLU:HB2	1.95	0.47
1:J:167:ASP:OD1	1:J:169:LYS:HB2	2.15	0.47
1:J:190:LYS:HG2	1:J:211:ARG:N	2.29	0.47
1:L:20:THR:HG21	5:L:323:HOH:O	2.13	0.47
2:H:67:ARG:C	2:H:68:PHE:HD1	2.18	0.47
2:H:68:PHE:N	2:H:68:PHE:CD1	2.83	0.47
1:J:12:SER:HA	1:J:105:GLU:O	2.15	0.47
1:L:52:SER:HB3	1:L:64:GLY:O	2.15	0.47
2:K:210:HIS:HB3	2:K:215:THR:HB	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:163:SER:OG	2:K:207:ASN:HB2	2.15	0.46
1:L:147:GLN:HE21	1:L:149:LYS:HG3	1.81	0.46
2:H:136:PRO:O	2:H:137:SER:HB2	2.15	0.46
2:K:97:ALA:HB1	2:K:110:PHE:HB3	1.97	0.46
2:H:30:THR:HG22	2:H:53:THR:O	2.16	0.46
1:J:120:PRO:HG3	1:J:186:TYR:CE1	2.51	0.46
3:V:71:THR:HG21	3:V:103:GLU:HB2	1.98	0.46
2:H:68:PHE:HD1	2:H:68:PHE:N	2.14	0.46
1:J:150:VAL:HG22	1:J:192:TYR:CD1	2.51	0.46
1:J:66:GLY:O	1:J:67:SER:HB3	2.16	0.45
1:J:181:LEU:HD13	1:J:186:TYR:HD1	1.82	0.45
2:K:210:HIS:HD2	2:K:213:SER:OG	1.98	0.45
2:H:11:LEU:HD21	2:H:122:SER:HB3	1.98	0.45
1:J:124:GLN:O	1:J:127:SER:HB2	2.17	0.45
1:J:23:CYS:SG	1:J:88:CYS:SG	3.10	0.45
1:L:23:CYS:HG	1:L:88:CYS:HG	1.62	0.45
1:L:145:LYS:HB3	1:L:197:THR:HB	1.99	0.45
3:V:39:TYR:HB3	3:V:42:GLU:HG2	1.99	0.45
3:V:77:THR:O	3:W:14:VAL:HA	2.16	0.44
2:H:154:ASP:HB3	2:H:185:LEU:HD13	1.99	0.44
2:K:181:GLN:N	2:K:185:LEU:O	2.48	0.44
2:H:183:SER:CA	5:H:331:HOH:O	2.34	0.44
3:V:33:VAL:HG21	3:V:54:LEU:HD12	1.99	0.44
3:W:67:GLU:HG3	3:W:69:VAL:HG13	2.00	0.44
1:J:116:PHE:O	1:J:134:CYS:HA	2.18	0.44
1:J:149:LYS:HE2	1:J:154:LEU:HG	2.00	0.44
1:J:190:LYS:HG2	1:J:211:ARG:H	1.83	0.44
1:L:2:ILE:HD13	1:L:29:ILE:HG22	2.00	0.44
2:H:17:SER:HA	2:H:83:MET:O	2.18	0.44
2:K:129:PRO:HB2	2:K:152:VAL:CG1	2.44	0.44
3:W:33:VAL:HG21	3:W:54:LEU:HD12	2.00	0.44
1:L:147:GLN:NE2	1:L:149:LYS:HG3	2.33	0.43
2:H:102:TYR:HB2	2:H:105:SER:O	2.18	0.43
1:L:147:GLN:HG3	1:L:154:LEU:CD1	2.48	0.43
2:H:182:SER:O	5:H:331:HOH:O	2.20	0.43
3:W:39:TYR:HB3	3:W:42:GLU:HG2	2.00	0.43
1:J:37:GLN:HB2	1:J:47:LEU:HD11	2.00	0.43
1:L:108:ARG:HD3	1:L:109:THR:O	2.18	0.43
1:L:201:LEU:HG	1:L:205:VAL:HG23	2.01	0.43
3:W:75:ASN:HA	3:W:96:PHE:O	2.18	0.43
1:L:164:THR:CG2	5:L:244:HOH:O	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:97:ALA:HB1	2:H:110:PHE:HB3	2.01	0.43
1:L:37:GLN:HG3	1:L:86:TYR:CE2	2.54	0.43
1:J:135:LEU:HD22	2:K:191:VAL:HG11	2.01	0.43
1:J:147:GLN:NE2	1:J:149:LYS:HG3	2.34	0.43
2:K:191:VAL:CG1	2:K:192:VAL:N	2.82	0.42
1:J:115:VAL:HG21	1:J:196:VAL:HG21	2.01	0.42
3:V:82:ARG:HD2	2:K:102:TYR:CZ	2.55	0.42
2:K:70:PHE:CE1	2:K:81:LEU:HD13	2.55	0.42
1:J:183:LYS:O	1:J:186:TYR:HB3	2.21	0.41
3:V:101:LYS:HB2	3:V:101:LYS:HE2	1.83	0.41
1:J:115:VAL:HG22	1:J:196:VAL:HG21	2.03	0.41
2:K:172:GLY:O	2:K:192:VAL:HA	2.20	0.41
1:J:125:LEU:HD12	1:J:129:THR:O	2.21	0.41
2:K:68:PHE:N	2:K:68:PHE:CD1	2.89	0.41
2:K:70:PHE:HE1	2:K:81:LEU:HD13	1.85	0.41
3:V:24:SER:HB3	3:W:53:PRO:HD3	2.03	0.41
2:K:153:LYS:HA	2:K:187:SER:OG	2.21	0.41
2:K:162:VAL:HG11	2:K:190:SER:CB	2.51	0.41
1:L:164:THR:HG22	1:L:174:SER:H	1.86	0.41
2:H:102:TYR:CD1	3:W:92:GLY:HA3	2.56	0.40
2:H:108:TRP:CZ3	3:W:88:GLY:HA3	2.55	0.40
3:W:72:GLU:HB3	3:W:101:LYS:HB2	2.02	0.40
1:J:100:GLN:H	1:J:100:GLN:CD	2.25	0.40
2:H:61:ALA:HB3	2:H:64:PHE:HD2	1.86	0.40
2:H:210:HIS:CD2	2:H:213:SER:OG	2.66	0.40
3:W:66:LEU:O	3:W:107:LYS:HE3	2.21	0.40
1:J:112:ALA:HB1	1:J:201:LEU:CD1	2.50	0.40
2:K:208:VAL:HG12	2:K:209:ASN:N	2.36	0.40
2:H:70:PHE:CE1	2:H:81:LEU:HD13	2.57	0.40
3:V:89:GLN:HE21	3:V:89:GLN:HB3	1.74	0.40
1:J:118:PHE:HA	1:J:119:PRO:HD3	1.79	0.40
1:J:135:LEU:CD2	2:K:191:VAL:HG11	2.51	0.40

There are no symmetry-related clashes.

## 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	J	211/214 (99%)	191 (90%)	19 (9%)	1 (0%)	29	41
1	L	211/214 (99%)	205 (97%)	6 (3%)	0	100	100
2	H	214/231 (93%)	209 (98%)	5 (2%)	0	100	100
2	K	214/231 (93%)	196 (92%)	17 (8%)	1 (0%)	29	41
3	V	92/102 (90%)	85 (92%)	6 (6%)	1 (1%)	14	20
3	W	92/102 (90%)	88 (96%)	3 (3%)	1 (1%)	14	20
All	All	1034/1094 (94%)	974 (94%)	56 (5%)	4 (0%)	34	48

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	138	ASN
3	V	26	CYS
3	W	26	CYS
2	K	159	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	J	190/191 (100%)	173 (91%)	17 (9%)	9	14
1	L	190/191 (100%)	176 (93%)	14 (7%)	13	22
2	H	182/194 (94%)	169 (93%)	13 (7%)	14	23
2	K	182/194 (94%)	173 (95%)	9 (5%)	25	40
3	V	89/96 (93%)	86 (97%)	3 (3%)	37	56
3	W	89/96 (93%)	85 (96%)	4 (4%)	27	44
All	All	922/962 (96%)	862 (94%)	60 (6%)	17	27

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1	ASP
1	L	33	LEU
1	L	54	LEU
1	L	100	GLN
1	L	105	GLU
1	L	108	ARG
1	L	125	LEU
1	L	129	THR
1	L	143	GLU
1	L	152	ASN
1	L	164	THR
1	L	190	LYS
1	L	201	LEU
1	L	211	ARG
2	H	1	GLU
2	H	11	LEU
2	H	18	LEU
2	H	115	GLN
2	H	117	THR
2	H	118	LEU
2	H	120	THR
2	H	160	VAL
2	H	180	LEU
2	H	188	LEU
2	H	191	VAL
2	H	196	SER
2	H	209	ASN
3	V	43	ILE
3	V	89	GLN
3	V	90	HIS
3	W	43	ILE
3	W	89	GLN
3	W	90	HIS
3	W	105	ARG
1	J	33	LEU
1	J	54	LEU
1	J	94	VAL
1	J	96	TRP
1	J	100	GLN
1	J	105	GLU
1	J	108	ARG
1	J	122	ASP

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Mol	Chain	Res	Type
1	J	125	LEU
1	J	126	LYS
1	J	147	GLN
1	J	152	ASN
1	J	164	THR
1	J	175	LEU
1	J	181	LEU
1	J	188	LYS
1	J	201	LEU
2	K	1	GLU
2	K	11	LEU
2	K	115	GLN
2	K	117	THR
2	K	118	LEU
2	K	120	THR
2	K	126	THR
2	K	148	LEU
2	K	159	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	147	GLN
1	L	160	GLN
1	L	198	HIS
2	H	101	HIS
2	H	202	GLN
2	H	209	ASN
2	H	210	HIS
3	V	22	GLN
3	V	89	GLN
3	V	98	GLN
3	W	22	GLN
3	W	89	GLN
1	J	3	GLN
1	J	137	ASN
1	J	147	GLN
1	J	152	ASN
1	J	160	GLN
1	J	198	HIS
2	K	101	HIS
2	K	174	HIS

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Mol	Chain	Res	Type
2	K	210	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 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	H	232	-	4,4,4	0.69	0	6,6,6	0.62	0
4	SO4	K	232	-	4,4,4	0.82	0	6,6,6	0.73	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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	J	213/214 (99%)	1.30	69 (32%) <b>0</b> <b>0</b>	13, 52, 120, 132	0
1	L	213/214 (99%)	-0.15	0 <b>100</b> <b>100</b>	7, 22, 43, 70	0
2	H	218/231 (94%)	-0.11	0 <b>100</b> <b>100</b>	9, 21, 43, 60	0
2	K	218/231 (94%)	1.07	63 (28%) <b>0</b> <b>0</b>	13, 41, 119, 140	0
3	V	94/102 (92%)	0.08	0 <b>100</b> <b>100</b>	11, 40, 68, 76	0
3	W	94/102 (92%)	0.10	2 (2%) 63 61	12, 38, 63, 76	0
All	All	1050/1094 (95%)	0.45	134 (12%) <b>3</b> <b>3</b>	7, 30, 114, 140	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	192	VAL	7.8
1	J	192	TYR	7.4
2	K	136	PRO	7.4
1	J	127	SER	6.7
2	K	148	LEU	6.6
2	K	187	SER	6.5
1	J	129	THR	6.0
2	K	198	SER	5.9
2	K	199	LEU	5.9
1	J	209	PHE	5.8
1	J	186	TYR	5.5
1	J	156	SER	5.5
2	K	155	TYR	5.4
2	K	188	LEU	5.4
1	J	117	ILE	5.3
2	K	193	THR	5.3
1	J	193	ALA	5.2
2	K	149	GLY	5.2
1	J	205	VAL	5.0

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Mol	Chain	Res	Type	RSRZ
1	J	131	SER	5.0
1	J	178	THR	5.0
2	K	153	LYS	4.9
1	J	150	VAL	4.9
2	K	221	VAL	4.8
1	J	194	CYS	4.8
1	J	195	GLU	4.7
1	J	148	TRP	4.7
1	J	189	HIS	4.7
1	J	203	SER	4.7
1	J	196	VAL	4.6
1	J	181	LEU	4.6
1	J	126	LYS	4.5
1	J	154	LEU	4.5
1	J	144	ALA	4.4
1	J	130	ALA	4.3
1	J	210	ASN	4.3
2	K	215	THR	4.2
2	K	218	ASP	4.2
2	K	208	VAL	4.1
1	J	151	ASP	4.1
2	K	167	GLY	4.1
2	K	146	ALA	4.0
2	K	204	TYR	3.9
2	K	131	VAL	3.9
1	J	110	VAL	3.9
1	J	212	GLY	3.8
1	J	198	HIS	3.8
1	J	111	ALA	3.8
1	J	146	VAL	3.8
2	K	194	VAL	3.8
1	J	147	GLN	3.8
2	K	217	VAL	3.8
1	J	125	LEU	3.7
2	K	209	ASN	3.7
1	J	180	THR	3.7
1	J	213	GLU	3.7
2	K	203	THR	3.7
2	K	223	PRO	3.6
2	K	137	SER	3.6
2	K	220	LYS	3.6
2	K	206	CYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	J	208	SER	3.5
2	K	200	GLY	3.4
2	K	169	LEU	3.4
1	J	140	TYR	3.4
1	J	145	LYS	3.4
2	K	151	LEU	3.3
2	K	176	PHE	3.3
1	J	128	GLY	3.3
1	J	123	GLU	3.3
2	K	171	SER	3.2
1	J	199	GLN	3.2
2	K	161	THR	3.2
2	K	179	VAL	3.2
1	J	114	SER	3.2
1	J	174	SER	3.1
2	K	165	ASN	3.1
1	J	121	SER	3.1
1	J	182	SER	3.0
2	K	201	THR	3.0
1	J	157	GLY	3.0
1	J	112	ALA	3.0
2	K	205	ILE	3.0
1	J	149	LYS	2.9
1	J	183	LYS	2.9
1	J	138	ASN	2.9
1	J	113	PRO	2.9
1	J	142	ARG	2.9
1	J	202	SER	2.8
2	K	163	SER	2.8
2	K	191	VAL	2.8
2	K	219	LYS	2.8
2	K	129	PRO	2.8
1	J	211	ARG	2.8
2	K	178	ALA	2.8
2	K	174	HIS	2.8
2	K	184	GLY	2.7
2	K	197	SER	2.7
1	J	122	ASP	2.7
2	K	130	SER	2.7
2	K	190	SER	2.7
1	J	134	CYS	2.6
2	K	207	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
2	K	164	TRP	2.6
1	J	175	LEU	2.6
1	J	162	SER	2.6
1	J	133	VAL	2.6
2	K	168	ALA	2.6
2	K	132	PHE	2.6
2	K	134	LEU	2.5
1	J	160	GLN	2.5
1	J	187	GLU	2.5
2	K	166	SER	2.4
2	K	183	SER	2.4
1	J	141	PRO	2.3
1	J	163	VAL	2.3
2	K	128	GLY	2.3
2	K	196	SER	2.3
1	J	155	GLN	2.3
2	K	135	ALA	2.3
1	J	188	LYS	2.2
1	J	184	ALA	2.2
2	K	152	VAL	2.2
1	J	204	PRO	2.1
2	K	157	PRO	2.1
3	W	43	ILE	2.1
1	J	118	PHE	2.1
2	K	172	GLY	2.1
3	W	72	GLU	2.1
1	J	177	SER	2.1
2	K	127	LYS	2.1
1	J	201	LEU	2.1
2	K	154	ASP	2.0
2	K	186	TYR	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](#)

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( $\text{\AA}^2$ )	Q<0.9
4	SO4	K	232	5/5	0.96	0.22	58,61,64,66	0
4	SO4	H	232	5/5	0.98	0.16	37,42,48,50	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.