



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 25, 2024 – 07:02 PM EST

PDB ID : 5CJS  
Title : Crystal structure of a monomeric influenza hemagglutinin stem in complex with an broadly neutralizing antibody CR9114  
Authors : Zhu, X.; Wilson, I.A.  
Deposited on : 2015-07-15  
Resolution : 4.30 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:

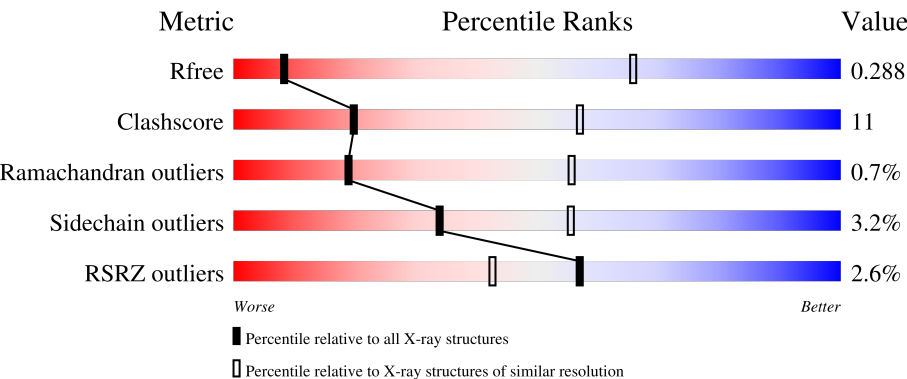
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

# 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 4.30 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>	164625	1028 (4.72-3.86)
Clashscore	180529	1030 (4.70-3.90)
Ramachandran outliers	177936	1014 (4.76-3.84)
Sidechain outliers	177891	1022 (4.76-3.82)
RSRZ outliers	164620	1026 (4.72-3.86)

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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	E	215	<div><div>2%</div><div>77%</div><div>18%</div><div>••</div></div>
1	L	215	<div><div>3%</div><div>77%</div><div>20%</div><div>••</div></div>
2	F	230	<div><div>73%</div><div>21%</div><div>6%</div></div>
2	H	230	<div><div>2%</div><div>73%</div><div>18%</div><div>•• 6%</div></div>
3	C	62	<div><div>3%</div><div>44%</div><div>37%</div><div>• 18%</div></div>
3	J	62	<div><div>56%</div><div>19%</div><div>8%</div><div>16%</div></div>

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Mol	Chain	Length	Quality of chain
4	D	191	<p>42% 29% 25% 4%</p>
4	K	191	<p>59% 19% 18% 3%</p>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9576 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 CR9114 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	211	Total	C	N	O	S	0	0	0
			1568	978	266	320	4			
1	E	211	Total	C	N	O	S	0	0	0
			1568	978	266	320	4			

- Molecule 2 is a protein called CR9114 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	217	Total	C	N	O	S	0	0	0
			1613	1017	269	320	7			
2	F	217	Total	C	N	O	S	0	0	0
			1613	1017	269	320	7			

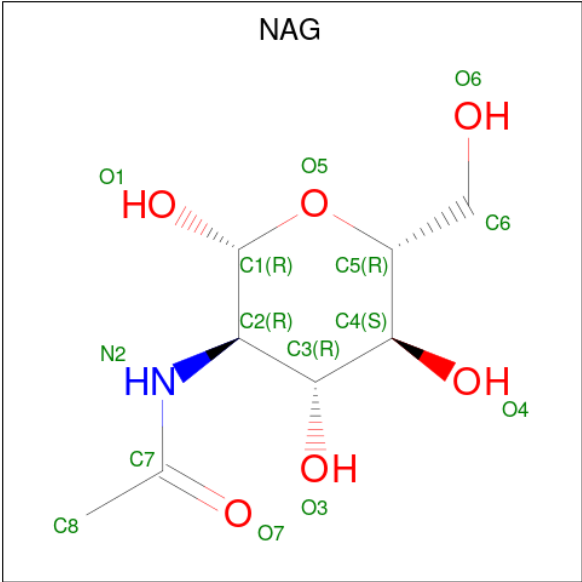
- Molecule 3 is a protein called Designed influenza hemagglutinin stem #4454, HA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	51	Total	C	N	O	S	0	0	0
			387	235	70	79	3			
3	J	52	Total	C	N	O	S	0	0	0
			397	242	72	80	3			

- Molecule 4 is a protein called Designed influenza hemagglutinin stem #4454, HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	143	Total	C	N	O	S	0	0	0
			1154	717	195	235	7			
4	K	156	Total	C	N	O	S	0	0	0
			1234	766	209	252	7			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

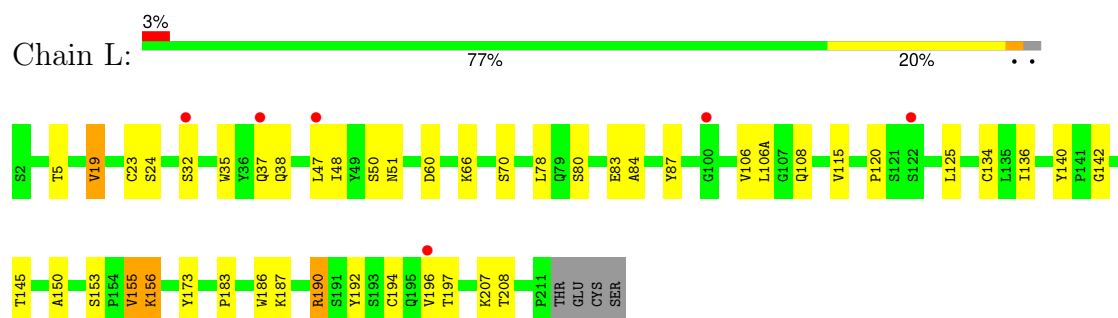


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	J	1	Total	C	N	O	0	0
			14	8	1	5		
5	K	1	Total	C	N	O	0	0
			14	8	1	5		

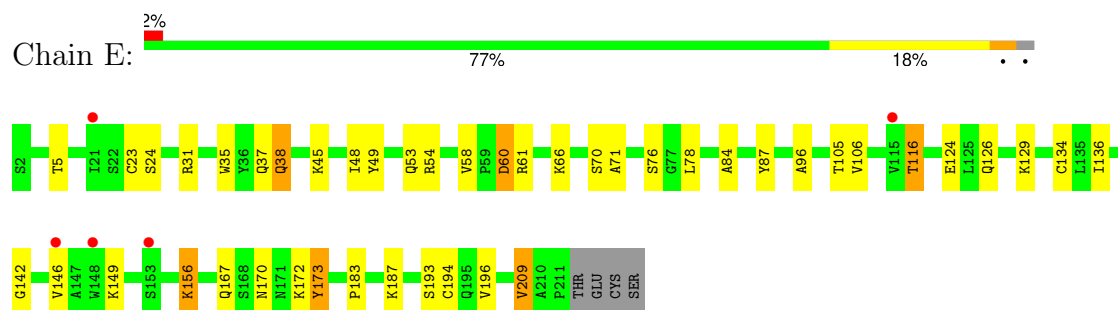
### 3 Residue-property plots

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. 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. 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.

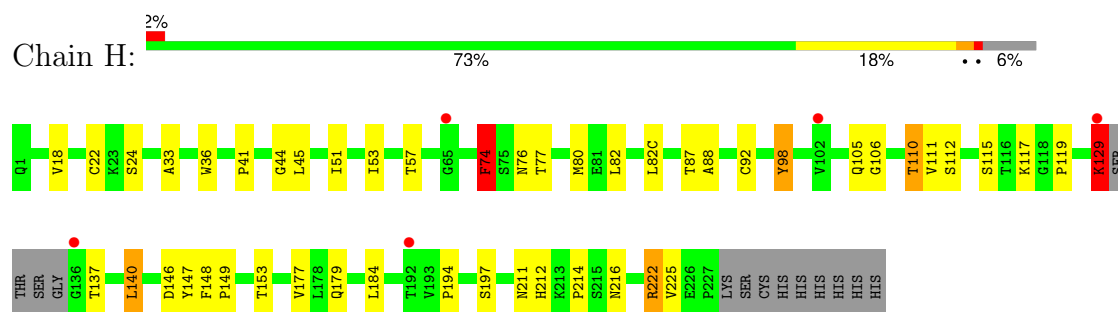
#### • Molecule 1: CR9114 light chain



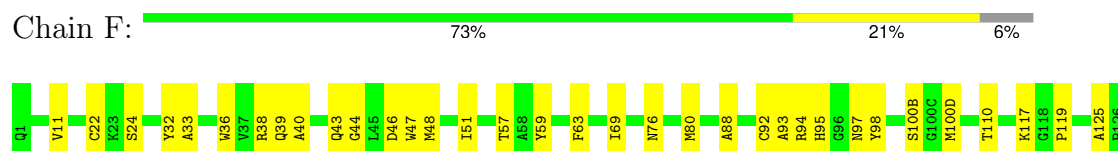
#### • Molecule 1: CR9114 light chain



#### • Molecule 2: CR9114 heavy chain

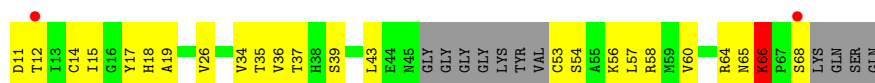
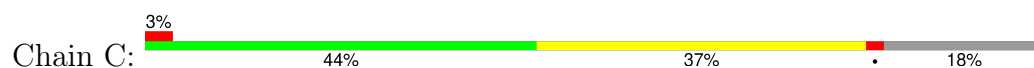


#### • Molecule 2: CR9114 heavy chain

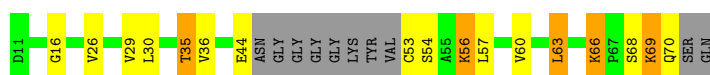




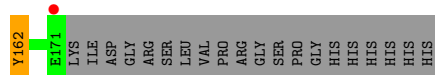
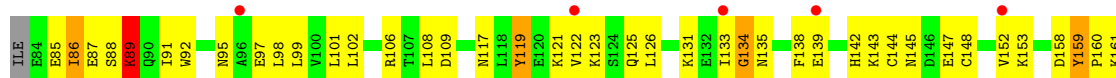
- Molecule 3: Designed influenza hemagglutinin stem #4454, HA1



- Molecule 3: Designed influenza hemagglutinin stem #4454, HA1



- Molecule 4: Designed influenza hemagglutinin stem #4454, HA2



- Molecule 4: Designed influenza hemagglutinin stem #4454, HA2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.87Å 110.87Å 359.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.01 – 4.30 48.01 – 4.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.01-4.30) 99.8 (48.01-4.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.21	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.96 (at 4.29Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.262 , 0.303 0.279 , 0.288	Depositor DCC
$R_{free}$ test set	927 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	147.6	Xtriage
Anisotropy	0.615	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 209.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.069 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	9576	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	179.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% 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: NAG

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	E	0.34	0/1606	0.71	2/2193 (0.1%)
1	L	0.39	0/1606	0.85	6/2193 (0.3%)
2	F	0.38	0/1652	0.69	0/2251
2	H	0.47	1/1652 (0.1%)	0.81	5/2251 (0.2%)
3	C	0.51	0/389	1.08	2/527 (0.4%)
3	J	0.47	0/399	0.98	2/539 (0.4%)
4	D	0.61	2/1176 (0.2%)	1.08	10/1581 (0.6%)
4	K	0.50	0/1257	0.92	3/1692 (0.2%)
All	All	0.45	3/9737 (0.0%)	0.85	30/13227 (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
4	D	0	1
4	K	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	129	LYS	CE-NZ	8.88	1.71	1.49
4	D	143	LYS	CE-NZ	6.59	1.65	1.49
4	D	11	GLU	CG-CD	5.08	1.59	1.51

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	190	ARG	NE-CZ-NH2	-11.53	114.53	120.30
4	K	83	ILE	CG1-CB-CG2	11.24	136.12	111.40
1	L	19	VAL	CG1-CB-CG2	8.04	123.76	110.90
4	D	131	LYS	CB-CA-C	-7.86	94.68	110.40
1	E	209	VAL	CG1-CB-CG2	7.55	122.97	110.90
1	L	156	LYS	CA-CB-CG	7.23	129.31	113.40
3	J	56	LYS	N-CA-CB	-6.92	98.15	110.60
4	D	131	LYS	CA-CB-CG	6.76	128.28	113.40
4	D	143	LYS	CD-CE-NZ	-6.52	96.70	111.70
1	L	155	VAL	CG1-CB-CG2	6.27	120.94	110.90
4	D	131	LYS	N-CA-CB	6.21	121.77	110.60
4	D	134	GLY	N-CA-C	-6.06	97.96	113.10
4	D	143	LYS	CG-CD-CE	6.05	130.05	111.90
2	H	222	ARG	CG-CD-NE	6.00	124.40	111.80
2	H	74	PHE	CB-CG-CD2	-6.00	116.60	120.80
2	H	74	PHE	CB-CG-CD1	5.98	124.99	120.80
4	D	119	TYR	CB-CA-C	-5.98	98.44	110.40
2	H	129	LYS	CB-CG-CD	5.87	126.87	111.60
1	L	190	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	E	156	LYS	CB-CG-CD	-5.52	97.25	111.60
4	D	89	LYS	CA-CB-CG	5.50	125.50	113.40
3	C	66	LYS	CA-CB-CG	5.45	125.38	113.40
1	L	19	VAL	CA-CB-CG2	5.39	118.98	110.90
4	D	11	GLU	CA-CB-CG	5.19	124.83	113.40
4	K	123	LYS	CD-CE-NZ	-5.18	99.78	111.70
3	C	66	LYS	CD-CE-NZ	-5.17	99.81	111.70
3	J	35	THR	OG1-CB-CG2	5.14	121.83	110.00
4	K	116	LYS	CG-CD-CE	-5.13	96.51	111.90
4	D	119	TYR	CB-CG-CD2	-5.13	117.92	121.00
2	H	110	THR	OG1-CB-CG2	5.04	121.60	110.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	159	TYR	Sidechain
4	K	59	MET	Peptide

## 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	E	1568	0	1521	29	1
1	L	1568	0	1521	26	0
2	F	1613	0	1572	32	0
2	H	1613	0	1572	34	1
3	C	387	0	386	20	0
3	J	397	0	401	11	0
4	D	1154	0	1073	52	0
4	K	1234	0	1134	33	0
5	C	14	0	13	0	0
5	J	14	0	13	0	0
5	K	14	0	13	0	0
All	All	9576	0	9219	212	1

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 11.

All (212) 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:129:LYS:CE	2:H:129:LYS:NZ	1.71	1.52
4:D:133:ILE:HD11	4:D:139:GLU:HB2	1.45	0.94
3:J:26:VAL:HG21	3:J:60:VAL:HG22	1.54	0.87
1:E:142:GLY:HA3	1:E:173:TYR:CD2	2.17	0.80
3:C:26:VAL:HG21	3:C:60:VAL:HG22	1.65	0.78
2:H:117:LYS:NZ	2:H:146:ASP:O	2.17	0.78
4:D:159:TYR:HB3	4:D:160:PRO:HD3	1.66	0.77
1:L:142:GLY:HA3	1:L:173:TYR:CD2	2.22	0.75
1:E:116:THR:HG23	2:F:128:SER:HB2	1.68	0.75
4:K:17:MET:SD	4:K:23:GLY:HA3	2.27	0.74
4:D:123:LYS:HB2	4:D:138:PHE:HZ	1.52	0.73
4:K:9:PHE:HD1	4:K:10:THR:N	1.87	0.72
3:C:39:SER:OG	3:C:58:ARG:NH2	2.21	0.72
2:F:117:LYS:NZ	2:F:146:ASP:O	2.22	0.70
4:D:119:TYR:CE2	4:D:138:PHE:HE1	2.09	0.70
4:D:119:TYR:CE2	4:D:138:PHE:CE1	2.81	0.69
1:E:60:ASP:OD1	1:E:60:ASP:N	2.28	0.66
3:J:66:LYS:O	4:K:13:GLY:N	2.26	0.65
2:H:24:SER:HB3	2:H:76:ASN:HB3	1.77	0.65
4:D:133:ILE:HD11	4:D:139:GLU:CB	2.22	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:5:THR:HB	1:L:24:SER:HB2	1.80	0.64
4:K:62:GLN:HG3	4:K:63:TYR:N	2.14	0.63
2:F:166:LEU:HD21	2:F:191:VAL:HG21	1.80	0.63
3:C:17:TYR:OH	3:C:66:LYS:HB3	1.99	0.63
3:C:53:CYS:SG	3:C:54:SER:N	2.74	0.61
3:C:14:CYS:N	4:D:25:HIS:O	2.32	0.60
2:H:179:GLN:HG3	2:H:184:LEU:O	2.00	0.60
4:D:123:LYS:HB2	4:D:138:PHE:CZ	2.36	0.60
1:L:38:GLN:O	1:L:84:ALA:HB1	2.02	0.60
2:F:140:LEU:HD13	2:F:225:VAL:HG11	1.84	0.60
2:H:112:SER:HB3	2:H:148:PHE:HZ	1.65	0.60
4:D:126:LEU:HD12	4:D:138:PHE:CD2	2.37	0.59
1:L:108:GLN:HB2	1:L:140:TYR:CD1	2.38	0.59
1:L:108:GLN:HB2	1:L:140:TYR:CE1	2.38	0.59
1:L:32:SER:HB3	1:L:50:SER:HA	1.85	0.59
1:E:136:ILE:HG12	1:E:196:VAL:HG21	1.86	0.58
2:F:119:PRO:HD2	2:F:217:THR:HG21	1.84	0.58
1:L:145:THR:OG1	1:L:197:THR:HB	2.04	0.58
3:C:11:ASP:OD2	4:D:144:CYS:N	2.29	0.58
3:C:14:CYS:HB2	4:D:25:HIS:HB3	1.85	0.57
4:K:7:ALA:HB3	4:K:14:TRP:HE1	1.69	0.57
2:H:36:TRP:CE2	2:H:80:MET:HB2	2.38	0.57
3:C:26:VAL:HG21	3:C:60:VAL:CG2	2.34	0.57
2:H:129:LYS:HB2	2:H:137:THR:O	2.05	0.57
1:L:83:GLU:OE1	1:L:106:VAL:N	2.37	0.56
3:J:69:LYS:HG3	3:J:70:GLN:HG3	1.87	0.56
4:K:92:TRP:O	4:K:95:ASN:HB2	2.04	0.56
3:J:53:CYS:SG	3:J:54:SER:N	2.79	0.56
1:L:106(A):LEU:HA	1:L:140:TYR:OH	2.06	0.56
4:D:95:ASN:OD1	4:K:95:ASN:OD1	2.23	0.56
4:D:106:ARG:NH1	3:J:29:VAL:O	2.39	0.56
1:L:134:CYS:HG	1:L:194:CYS:HG	1.53	0.55
2:H:98:TYR:N	4:D:42:GLN:OE1	2.36	0.55
3:J:36:VAL:HG21	3:J:60:VAL:HG13	1.89	0.55
2:H:33:ALA:HB2	2:H:98:TYR:O	2.07	0.55
1:E:149:LYS:HB2	1:E:193:SER:HB2	1.89	0.55
2:F:51:ILE:HD12	2:F:57:THR:HG22	1.88	0.55
4:D:16:GLY:HA3	4:D:34:TYR:CE2	2.42	0.55
2:H:140:LEU:HD13	2:H:225:VAL:HG11	1.89	0.55
3:C:34:VAL:CG1	3:C:64:ARG:HG3	2.37	0.54
4:D:8:GLY:H	4:D:14:TRP:HE1	1.53	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:161:LYS:HG2	4:D:162:TYR:CE1	2.42	0.54
4:D:92:TRP:O	4:D:95:ASN:HB2	2.08	0.54
2:H:53:ILE:HG13	4:D:49:THR:OG1	2.08	0.54
3:C:19:ALA:HB2	4:D:13:GLY:HA3	1.90	0.54
1:E:183:PRO:O	1:E:187:LYS:HG3	2.08	0.53
3:C:60:VAL:HG11	4:D:108:LEU:HD21	1.90	0.53
4:K:128:ASN:ND2	4:K:170:ARG:HH12	2.07	0.53
3:C:36:VAL:HG21	3:C:60:VAL:HG13	1.90	0.53
4:D:134:GLY:O	4:D:135:ASN:OD1	2.27	0.52
2:H:146:ASP:HB3	2:H:184:LEU:HD13	1.89	0.52
2:F:24:SER:HB3	2:F:76:ASN:HB3	1.91	0.52
1:E:134:CYS:HG	1:E:194:CYS:HG	1.58	0.52
1:L:115:VAL:O	1:L:207:LYS:HE2	2.11	0.51
4:D:86:ILE:HA	4:D:89:LYS:HE2	1.93	0.51
1:L:80:SER:HA	1:L:106:VAL:HG11	1.92	0.51
2:H:112:SER:HB3	2:H:148:PHE:CZ	2.44	0.51
1:E:78:LEU:HD21	1:E:106:VAL:HG22	1.93	0.51
2:F:129:LYS:HD2	2:F:138:ALA:HB2	1.93	0.51
1:E:96:ALA:HB3	2:F:47:TRP:CG	2.46	0.51
4:K:119:TYR:CE2	4:K:136:GLY:HA2	2.46	0.51
3:C:68:SER:O	3:C:68:SER:OG	2.27	0.50
4:D:24:TYR:HB2	4:D:153:LYS:HE2	1.92	0.50
2:F:128:SER:O	2:F:129:LYS:HD3	2.11	0.50
4:K:128:ASN:O	4:K:170:ARG:NH2	2.44	0.50
1:E:37:GLN:O	1:E:45:LYS:N	2.42	0.50
4:K:119:TYR:CE1	4:K:138:PHE:CZ	3.00	0.50
1:E:38:GLN:O	1:E:84:ALA:HB1	2.12	0.49
2:H:51:ILE:HD12	2:H:57:THR:HG22	1.94	0.49
3:C:66:LYS:O	4:D:13:GLY:N	2.29	0.49
4:D:102:LEU:O	4:D:106:ARG:HG3	2.13	0.49
2:F:11:VAL:HG22	2:F:110:THR:HB	1.94	0.49
1:L:136:ILE:HG12	1:L:196:VAL:HG21	1.94	0.49
4:D:161:LYS:HB3	4:D:162:TYR:HD1	1.78	0.49
4:D:19:ASP:OD1	4:D:19:ASP:N	2.44	0.48
2:F:51:ILE:CD1	2:F:57:THR:HG22	2.42	0.48
1:E:49:TYR:CZ	1:E:53:GLN:HB3	2.48	0.48
4:K:164:GLU:O	4:K:168:LEU:HG	2.13	0.48
4:D:8:GLY:N	4:D:14:TRP:HE1	2.12	0.48
4:D:98:LEU:HD22	4:K:102:LEU:HD11	1.96	0.48
4:D:161:LYS:HB3	4:D:162:TYR:CD1	2.49	0.48
2:F:212:HIS:CD2	2:F:214:PRO:HD2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:18:HIS:HB2	4:D:20:GLY:O	2.13	0.48
4:D:148:CYS:HB2	4:D:162:TYR:OH	2.14	0.48
4:K:9:PHE:HD2	4:K:115:VAL:HG12	1.78	0.48
4:D:88:SER:O	4:D:91:ILE:HB	2.14	0.48
2:F:93:ALA:HB1	2:F:100(D):MET:HB3	1.96	0.48
2:H:87:THR:OG1	2:H:111:VAL:N	2.31	0.47
1:E:49:TYR:O	1:E:53:GLN:HB2	2.14	0.47
2:H:74:PHE:HD1	2:H:74:PHE:H	1.62	0.47
1:L:37:GLN:HB2	1:L:47:LEU:HD13	1.96	0.47
2:H:36:TRP:CD2	2:H:80:MET:HB2	2.50	0.47
2:H:146:ASP:HA	2:H:184:LEU:HB3	1.97	0.47
4:D:162:TYR:HD1	4:D:162:TYR:N	2.13	0.47
2:F:59:TYR:HE1	2:F:69:ILE:HG13	1.80	0.47
1:L:35:TRP:HB2	1:L:48:ILE:HB	1.97	0.46
2:F:95:HIS:HB3	2:F:100(B):SER:OG	2.15	0.46
3:C:56:LYS:O	3:C:57:LEU:HD23	2.14	0.46
4:K:61:THR:OG1	4:K:92:TRP:NE1	2.40	0.46
1:E:35:TRP:HB2	1:E:48:ILE:HB	1.98	0.46
2:H:22:CYS:O	2:H:77:THR:HA	2.15	0.46
2:F:129:LYS:HB3	2:F:137:THR:O	2.15	0.46
1:E:66:LYS:HA	1:E:71:ALA:HA	1.98	0.46
4:K:9:PHE:CD1	4:K:10:THR:N	2.76	0.46
4:K:20:GLY:HA3	4:K:36:ALA:HB1	1.98	0.46
4:K:42:GLN:NE2	4:K:46:ASN:OD1	2.48	0.46
2:H:129:LYS:NZ	2:H:129:LYS:CD	2.70	0.46
4:D:97:GLU:O	4:D:101:LEU:HG	2.16	0.46
1:E:146:VAL:HG22	1:E:196:VAL:HG22	1.96	0.46
1:E:38:GLN:HE22	2:F:39:GLN:HE22	1.64	0.46
4:D:145:ASN:ND2	4:D:147:GLU:HG2	2.31	0.45
1:L:78:LEU:HD21	1:L:106:VAL:HG22	1.98	0.45
1:L:150:ALA:N	1:L:153:SER:O	2.44	0.45
4:D:21:TRP:CZ3	4:D:45:ILE:HG13	2.51	0.45
1:E:87:TYR:CE1	2:F:44:GLY:HA2	2.50	0.45
4:K:19:ASP:OD1	4:K:19:ASP:N	2.46	0.45
4:D:44:ALA:O	4:D:48:ILE:HG12	2.16	0.45
2:F:39:GLN:O	2:F:88:ALA:HB1	2.17	0.45
2:F:125:ALA:O	2:F:127:SER:N	2.47	0.45
4:D:27:GLN:HG3	4:D:32:SER:HB3	1.98	0.45
4:D:86:ILE:HA	4:D:89:LYS:CE	2.46	0.45
3:C:35:THR:HG22	3:C:65:ASN:HB3	1.98	0.45
2:F:97:ASN:ND2	4:K:38:GLN:OE1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:87:TYR:CE2	2:H:44:GLY:HA2	2.51	0.45
4:D:159:TYR:HB3	4:D:160:PRO:CD	2.43	0.45
4:K:119:TYR:HD1	4:K:119:TYR:O	1.99	0.45
1:L:183:PRO:O	1:L:187:LYS:HG3	2.16	0.45
2:H:119:PRO:HB3	2:H:147:TYR:HB3	1.99	0.45
1:E:23:CYS:O	1:E:70:SER:HA	2.17	0.45
4:K:62:GLN:CG	4:K:63:TYR:N	2.71	0.44
1:L:192:TYR:O	1:L:208:THR:HG23	2.17	0.44
4:D:7:ALA:HB1	4:D:8:GLY:HA3	1.99	0.44
1:L:51:ASN:OD1	1:L:66:LYS:HD3	2.17	0.44
4:D:109:ASP:OD2	3:J:30:LEU:HD11	2.17	0.44
1:L:60:ASP:OD1	1:L:60:ASP:N	2.48	0.44
2:F:33:ALA:HB2	2:F:98:TYR:O	2.18	0.44
3:C:43:LEU:HD12	3:C:43:LEU:HA	1.78	0.44
2:H:22:CYS:SG	2:H:92:CYS:SG	3.11	0.44
4:D:142:HIS:ND1	4:D:162:TYR:CD2	2.85	0.44
1:E:61:ARG:HB2	1:E:76:SER:O	2.18	0.44
2:F:40:ALA:HB3	2:F:43:GLN:HG3	2.00	0.44
4:D:99:LEU:HD23	4:D:99:LEU:HA	1.79	0.43
4:D:162:TYR:CD1	4:D:162:TYR:N	2.85	0.43
1:E:124:GLU:HG2	1:E:129:LYS:O	2.18	0.43
3:J:63:LEU:HB3	4:K:111:HIS:CG	2.54	0.43
1:L:142:GLY:HA3	1:L:173:TYR:CG	2.53	0.43
2:H:148:PHE:HA	2:H:149:PRO:HA	1.81	0.43
2:H:194:PRO:HG2	2:H:197:SER:HB3	2.00	0.43
4:K:41:THR:HG22	4:K:45:ILE:HD12	2.00	0.43
1:L:186:TRP:HA	1:L:192:TYR:HE2	1.84	0.43
3:C:18:HIS:HD2	3:C:37:THR:HG21	1.83	0.43
2:F:153:THR:CG2	2:F:211:ASN:HB3	2.48	0.43
4:D:117:ASN:O	4:D:121:LYS:HB2	2.19	0.42
1:E:87:TYR:HE1	2:F:44:GLY:HA2	1.84	0.42
1:E:142:GLY:HA3	1:E:173:TYR:CE2	2.53	0.42
4:K:9:PHE:HD1	4:K:10:THR:H	1.66	0.42
2:H:105:GLN:HG2	2:H:106:GLY:O	2.19	0.42
1:E:31:ARG:HA	1:E:31:ARG:HD3	1.84	0.42
3:J:26:VAL:HG21	3:J:60:VAL:CG2	2.37	0.42
1:E:167:GLN:NE2	1:E:172:LYS:HB2	2.35	0.42
4:K:44:ALA:O	4:K:48:ILE:HG12	2.19	0.42
2:H:153:THR:CG2	2:H:211:ASN:HB3	2.50	0.42
2:F:38:ARG:HG2	2:F:46:ASP:HB3	2.01	0.42
2:H:18:VAL:HG12	2:H:82(C):LEU:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:45:LEU:HA	2:H:45:LEU:HD23	1.80	0.42
1:L:120:PRO:HB2	1:L:125:LEU:HD21	2.01	0.42
1:E:38:GLN:HE22	2:F:39:GLN:NE2	2.18	0.42
2:H:212:HIS:CD2	2:H:214:PRO:HD2	2.55	0.41
4:K:120:GLU:HA	4:K:123:LYS:HB3	2.02	0.41
4:D:142:HIS:CE1	4:D:162:TYR:CD2	3.07	0.41
2:H:41:PRO:HD3	2:H:88:ALA:HA	2.01	0.41
2:H:222:ARG:HH11	2:H:222:ARG:HD3	1.69	0.41
2:H:82:LEU:HD12	2:H:82:LEU:HA	1.82	0.41
4:D:158:ASP:OD1	4:D:160:PRO:HD2	2.20	0.41
1:E:5:THR:HB	1:E:24:SER:HB2	2.02	0.41
2:F:32:TYR:HB2	2:F:94:ARG:HD2	2.02	0.41
3:J:56:LYS:O	3:J:57:LEU:HD23	2.20	0.41
4:K:21:TRP:CZ3	4:K:45:ILE:HG13	2.55	0.41
4:K:7:ALA:HB3	4:K:14:TRP:NE1	2.34	0.41
3:C:15:ILE:CD1	4:D:122:VAL:HG21	2.50	0.41
4:D:125:GLN:NE2	4:D:152:VAL:O	2.42	0.41
4:K:111:HIS:O	4:K:115:VAL:HG23	2.21	0.41
1:E:167:GLN:NE2	1:E:170:ASN:OD1	2.51	0.41
1:L:23:CYS:O	1:L:70:SER:HA	2.21	0.41
2:F:36:TRP:CE2	2:F:80:MET:HB2	2.56	0.41
4:K:94:TYR:HA	4:K:97:GLU:HG2	2.03	0.41
2:H:74:PHE:CD1	2:H:74:PHE:N	2.89	0.41
3:J:16:GLY:HA3	4:K:14:TRP:CZ2	2.56	0.41
2:F:22:CYS:SG	2:F:92:CYS:SG	3.13	0.40
2:F:48:MET:HA	2:F:63:PHE:CD2	2.56	0.40
4:K:7:ALA:CB	4:K:14:TRP:HE1	2.34	0.40
1:E:54:ARG:NH1	1:E:58:VAL:O	2.48	0.40

All (1) 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)
2:H:115:SER:O	1:E:126:GLN:NE2[2_454]	2.05	0.15



## 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	E	209/215 (97%)	203 (97%)	6 (3%)	0	100	100
1	L	209/215 (97%)	203 (97%)	6 (3%)	0	100	100
2	F	213/230 (93%)	208 (98%)	4 (2%)	1 (0%)	25	63
2	H	213/230 (93%)	207 (97%)	5 (2%)	1 (0%)	25	63
3	C	47/62 (76%)	42 (89%)	5 (11%)	0	100	100
3	J	48/62 (77%)	45 (94%)	1 (2%)	2 (4%)	2	18
4	D	139/191 (73%)	138 (99%)	1 (1%)	0	100	100
4	K	152/191 (80%)	142 (93%)	6 (4%)	4 (3%)	4	26
All	All	1230/1396 (88%)	1188 (97%)	34 (3%)	8 (1%)	19	56

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	K	6	ILE
4	K	7	ALA
4	K	174	ASP
4	K	176	ARG
3	J	69	LYS
3	J	68	SER
2	H	216	ASN
2	F	151	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	E	175/179 (98%)	168 (96%)	7 (4%)	27	49
1	L	175/179 (98%)	171 (98%)	4 (2%)	45	65
2	F	181/193 (94%)	180 (99%)	1 (1%)	84	88
2	H	181/193 (94%)	175 (97%)	6 (3%)	33	55
3	C	47/54 (87%)	45 (96%)	2 (4%)	25	48
3	J	48/54 (89%)	44 (92%)	4 (8%)	9	28
4	D	125/165 (76%)	119 (95%)	6 (5%)	21	44
4	K	130/165 (79%)	126 (97%)	4 (3%)	35	56
All	All	1062/1182 (90%)	1028 (97%)	34 (3%)	34	55

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	19	VAL
1	L	155	VAL
1	L	156	LYS
1	L	190	ARG
2	H	74	PHE
2	H	98	TYR
2	H	110	THR
2	H	129	LYS
2	H	140	LEU
2	H	177	VAL
3	C	12	THR
3	C	66	LYS
4	D	60	ASN
4	D	85	GLU
4	D	86	ILE
4	D	87	GLU
4	D	89	LYS
4	D	162	TYR
1	E	38	GLN
1	E	60	ASP
1	E	105	THR
1	E	116	THR
1	E	156	LYS
1	E	173	TYR
1	E	209	VAL
2	F	140	LEU
3	J	35	THR

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Mol	Chain	Res	Type
3	J	44	GLU
3	J	63	LEU
3	J	66	LYS
4	K	9	PHE
4	K	61	THR
4	K	83	ILE
4	K	119	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	189	HIS
4	D	95	ASN
1	E	38	GLN
2	F	216	ASN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

3 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
5	NAG	C	101	3	14,14,15	0.56	0	17,19,21	0.95	1 (5%)
5	NAG	J	501	3	14,14,15	0.39	0	17,19,21	0.68	0
5	NAG	K	201	4	14,14,15	0.72	1 (7%)	17,19,21	0.83	1 (5%)

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
5	NAG	C	101	3	-	0/6/23/26	0/1/1/1
5	NAG	J	501	3	-	2/6/23/26	0/1/1/1
5	NAG	K	201	4	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	201	NAG	C1-C2	2.41	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	101	NAG	C1-O5-C5	3.36	116.68	112.19
5	K	201	NAG	C1-O5-C5	2.69	115.79	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	J	501	NAG	O5-C5-C6-O6
5	J	501	NAG	C4-C5-C6-O6

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 ⓘ

**Warning:** The R factor obtained from EDS is 0.3235, which does not match the depositor's R factor of 0.262. Please interpret the results in this section carefully.

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	E	211/215 (98%)	0.30	5 (2%) 59 45	170, 185, 198, 204	0
1	L	211/215 (98%)	0.27	6 (2%) 55 41	121, 183, 201, 203	0
2	F	217/230 (94%)	0.08	1 (0%) 87 76	103, 170, 190, 196	0
2	H	217/230 (94%)	0.32	5 (2%) 61 46	98, 174, 185, 194	0
3	C	51/62 (82%)	0.40	2 (3%) 44 34	180, 190, 208, 216	0
3	J	52/62 (83%)	0.34	0 100 100	155, 172, 199, 206	0
4	D	143/191 (74%)	0.49	8 (5%) 31 26	121, 204, 218, 220	0
4	K	156/191 (81%)	0.33	6 (3%) 44 34	150, 160, 212, 218	0
All	All	1258/1396 (90%)	0.29	33 (2%) 57 42	98, 180, 211, 220	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	68	SER	3.8
4	D	6	ILE	3.7
2	H	192	THR	3.6
1	E	148	TRP	3.5
4	D	152	VAL	3.3
4	D	96	ALA	3.1
1	L	37	GLN	3.0
1	L	196	VAL	2.9
3	C	12	THR	2.9
4	K	98	LEU	2.9
2	H	129	LYS	2.8
1	L	47	LEU	2.8
4	K	96	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
4	K	18	VAL	2.6
4	K	102	LEU	2.4
2	H	136	GLY	2.4
4	K	64	THR	2.3
1	L	122	SER	2.3
1	E	21	ILE	2.3
4	D	171	GLU	2.3
2	H	65	GLY	2.3
4	D	122	VAL	2.2
1	L	100	GLY	2.2
1	E	146	VAL	2.2
1	L	32	SER	2.2
4	K	19	ASP	2.2
4	D	139	GLU	2.1
1	E	115	VAL	2.1
1	E	153	SER	2.1
4	D	60	ASN	2.1
4	D	133	ILE	2.1
2	F	213	LYS	2.1
2	H	102	VAL	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(Å <sup>2</sup> )	Q<0.9
5	NAG	J	501	14/15	0.04	0.19	190,190,190,190	0
5	NAG	K	201	14/15	0.35	0.24	173,173,173,173	0
5	NAG	C	101	14/15	0.64	0.15	192,192,192,192	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.