



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 11:23 am BST

PDB ID : 4U6V  
Title : Mechanisms of Neutralization of a Human Anti-Alpha Toxin Antibody  
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Deposited on : 2014-07-29  
Resolution : 2.56 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  
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

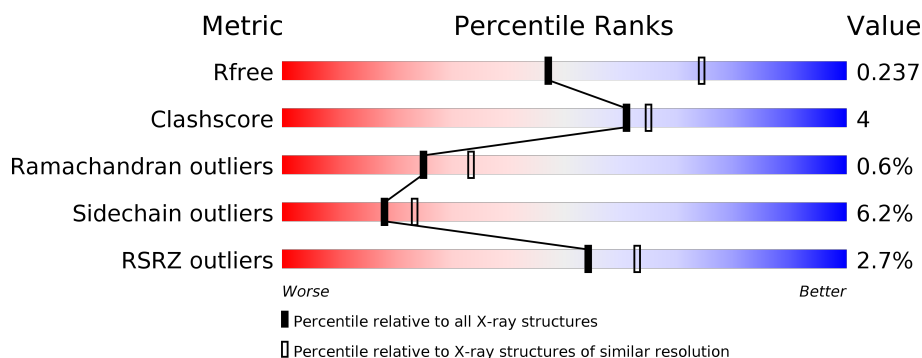
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.56 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	1279 (2.58-2.54)
Clashscore	141614	1327 (2.58-2.54)
Ramachandran outliers	138981	1312 (2.58-2.54)
Sidechain outliers	138945	1312 (2.58-2.54)
RSRZ outliers	127900	1269 (2.58-2.54)

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	H	225	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>12%</div> <div>•</div> </div> </div>
1	K	225	<div> <div>8%</div> <div> <div></div> <div>82%</div> <div>14%</div> <div>• •</div> </div> </div>
2	L	213	<div> <div>%</div> <div> <div></div> <div>87%</div> <div>11%</div> <div>•</div> </div> </div>
2	M	213	<div> <div>5%</div> <div> <div></div> <div>84%</div> <div>15%</div> <div>•</div> </div> </div>
3	A	293	<div> <div>%</div> <div> <div></div> <div>77%</div> <div>14%</div> <div>• 7%</div> </div> </div>
3	B	293	<div> <div></div> <div> <div></div> <div>79%</div> <div>12%</div> <div>• 7%</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11052 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, antigen binding fragment, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	218	Total	C	N	O	S	0	0	0
			1622	1017	278	320	7			
1	K	218	Total	C	N	O	S	0	0	0
			1622	1017	278	320	7			

- Molecule 2 is a protein called Fab, antigen binding fragment, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	213	Total	C	N	O	S	0	0	0
			1645	1033	273	333	6			
2	M	213	Total	C	N	O	S	0	0	0
			1645	1033	273	333	6			

- Molecule 3 is a protein called Alpha-hemolysin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	272	Total	C	N	O	S	0	0	0
			2200	1386	377	430	7			
3	B	272	Total	C	N	O	S	0	0	0
			2200	1386	377	430	7			

- 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	H	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	K	1	Total	O	S	0	0
			5	4	1		

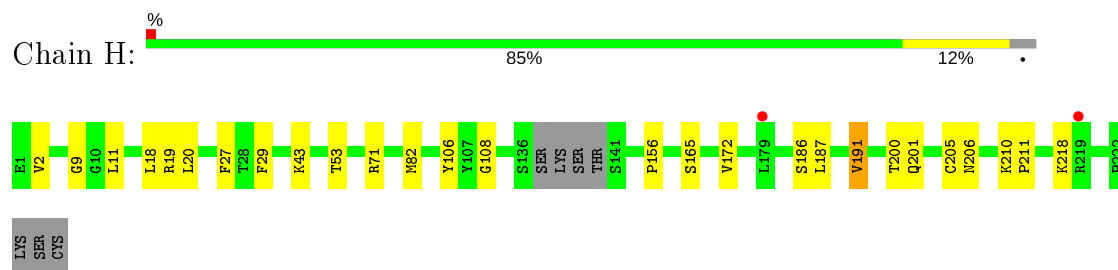
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	6	Total	O	0	0
			6	6		
5	L	15	Total	O	0	0
			15	15		
5	A	21	Total	O	0	0
			21	21		
5	K	5	Total	O	0	0
			5	5		
5	M	13	Total	O	0	0
			13	13		
5	B	28	Total	O	0	0
			28	28		

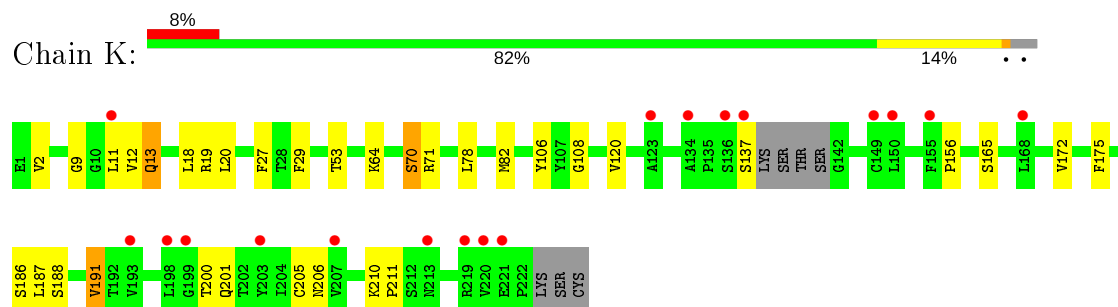
### 3 Residue-property plots [i](#)

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.

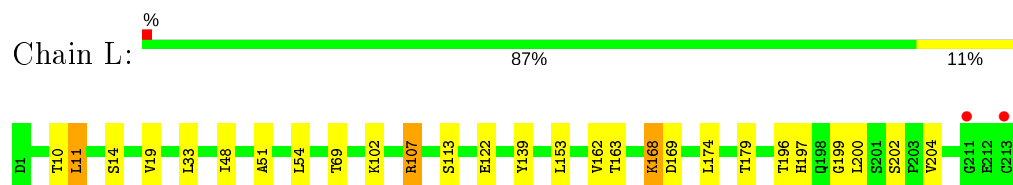
- Molecule 1: Fab, antigen binding fragment, heavy chain



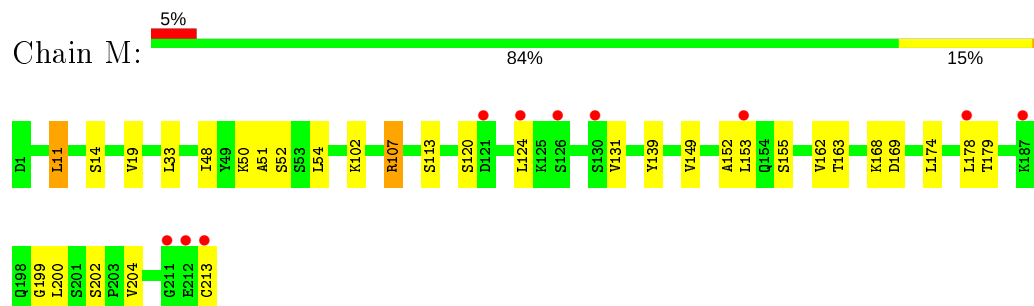
- Molecule 1: Fab, antigen binding fragment, heavy chain



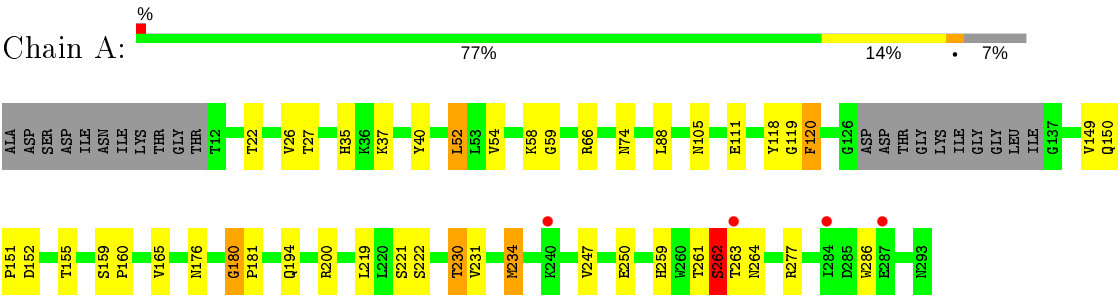
- Molecule 2: Fab, antigen binding fragment, light chain



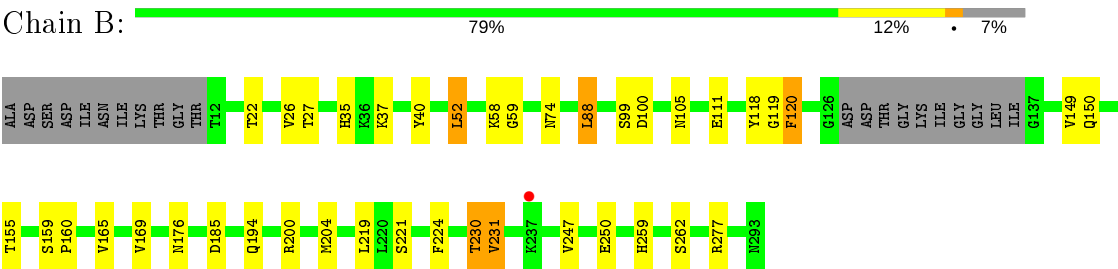
- Molecule 2: Fab, antigen binding fragment, light chain



● Molecule 3: Alpha-hemolysin



● Molecule 3: Alpha-hemolysin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.52Å 148.50Å 93.82Å 90.00° 99.82° 90.00°	Depositor
Resolution (Å)	92.45 – 2.56 74.25 – 2.56	Depositor EDS
% Data completeness (in resolution range)	99.3 (92.45-2.56) 99.5 (74.25-2.56)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 2.55Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.198 , 0.235 0.205 , 0.237	Depositor DCC
$R_{free}$ test set	3716 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	63.1	Xtriage
Anisotropy	0.381	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 47.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11052	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 6.69% 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](#)

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	H	0.48	0/1662	0.68	0/2264
1	K	0.47	0/1662	0.68	0/2264
2	L	0.49	0/1682	0.67	0/2283
2	M	0.49	0/1682	0.69	0/2283
3	A	0.46	0/2251	0.69	0/3044
3	B	0.45	0/2251	0.69	0/3044
All	All	0.47	0/11190	0.68	0/15182

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	H	1622	0	1565	10	0
1	K	1622	0	1565	17	0
2	L	1645	0	1598	9	0
2	M	1645	0	1598	14	0
3	A	2200	0	2124	27	0
3	B	2200	0	2124	20	0
4	A	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	10	0	0	0	0
4	K	5	0	0	1	0
5	A	21	0	0	0	0
5	B	28	0	0	0	0
5	H	6	0	0	0	0
5	K	5	0	0	0	0
5	L	15	0	0	0	0
5	M	13	0	0	0	0
All	All	11052	0	10574	96	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 4.

All (96) 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)
3:A:88:LEU:CD1	3:A:230:THR:HG21	1.56	1.35
1:K:175:PHE:O	1:K:187:LEU:CD1	1.96	1.14
3:A:88:LEU:HD12	3:A:230:THR:HG21	1.01	1.01
3:A:88:LEU:CD1	3:A:230:THR:CG2	2.42	0.97
3:A:88:LEU:HD12	3:A:230:THR:CG2	1.97	0.94
3:A:88:LEU:CD2	3:A:247:VAL:HG22	1.98	0.93
3:A:261:THR:O	3:A:262:SER:HB2	1.76	0.83
1:K:175:PHE:O	1:K:187:LEU:HD12	1.79	0.82
3:A:88:LEU:HD22	3:A:247:VAL:HG22	1.60	0.81
3:B:88:LEU:HD13	3:B:247:VAL:HG22	1.63	0.80
1:K:175:PHE:O	1:K:187:LEU:HD11	1.84	0.77
3:A:88:LEU:HD11	3:A:230:THR:HG21	1.62	0.76
3:B:100:ASP:HB3	3:B:231:VAL:HG13	1.68	0.75
3:A:234:MET:HG3	3:A:286:TRP:CE2	2.22	0.74
3:B:100:ASP:HB3	3:B:231:VAL:CG1	2.22	0.70
2:M:50:LYS:O	2:M:51:ALA:HB3	1.92	0.70
1:H:218:LYS:NZ	2:L:122:GLU:OE1	2.26	0.68
1:K:9:GLY:HA2	1:K:18:LEU:HD21	1.76	0.66
3:B:88:LEU:HG	3:B:230:THR:HG21	1.77	0.65
1:H:9:GLY:HA2	1:H:18:LEU:HD21	1.77	0.65
1:K:165:SER:H	1:K:206:ASN:HD21	1.48	0.61
1:K:175:PHE:O	1:K:187:LEU:HD13	1.99	0.60
1:H:165:SER:H	1:H:206:ASN:HD21	1.49	0.59
3:B:118:TYR:CE2	3:B:120:PHE:HA	2.40	0.56
2:M:50:LYS:CG	2:M:50:LYS:O	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:119:GLY:O	3:B:120:PHE:HB2	2.05	0.56
3:A:119:GLY:O	3:A:120:PHE:HB2	2.06	0.55
2:M:200:LEU:HD13	2:M:204:VAL:HG23	1.89	0.55
3:A:118:TYR:CE2	3:A:120:PHE:HA	2.41	0.55
3:A:88:LEU:HD11	3:A:230:THR:CG2	2.25	0.55
1:H:172:VAL:HG22	1:H:191:VAL:HG13	1.89	0.55
3:A:111:GLU:HG2	3:A:149:VAL:HG12	1.89	0.54
2:L:200:LEU:HD13	2:L:204:VAL:HG23	1.88	0.54
1:K:172:VAL:HG22	1:K:191:VAL:HG13	1.89	0.54
3:B:111:GLU:HG2	3:B:149:VAL:HG12	1.90	0.53
3:A:26:VAL:HG22	3:A:37:LYS:HG3	1.90	0.53
3:B:26:VAL:HG22	3:B:37:LYS:HG3	1.91	0.53
2:M:162:VAL:HG12	2:M:163:THR:O	2.11	0.50
1:K:11:LEU:HD21	1:K:156:PRO:HG3	1.93	0.50
2:L:162:VAL:HG12	2:L:163:THR:O	2.11	0.50
3:B:52:LEU:HD23	3:B:52:LEU:N	2.26	0.50
3:A:52:LEU:HD23	3:A:52:LEU:N	2.27	0.49
2:M:50:LYS:O	2:M:51:ALA:CB	2.58	0.49
3:B:74:ASN:O	3:B:259:HIS:HA	2.13	0.49
1:H:29:PHE:O	1:H:71:ARG:NH2	2.45	0.49
2:L:197:HIS:CD2	2:L:199:GLY:H	2.31	0.48
1:K:187:LEU:HG	1:K:188:SER:N	2.28	0.48
2:M:197:HIS:CD2	2:M:199:GLY:H	2.30	0.48
3:B:250:GLU:OE1	3:B:277:ARG:NH2	2.46	0.48
3:A:151:PRO:O	3:A:152:ASP:HB2	2.14	0.48
2:M:131:VAL:HG13	2:M:178:LEU:HB3	1.96	0.48
3:B:194:GLN:HE22	3:B:200:ARG:HH21	1.62	0.47
3:A:194:GLN:HE22	3:A:200:ARG:HH21	1.62	0.47
3:A:74:ASN:O	3:A:259:HIS:HA	2.14	0.47
3:B:88:LEU:CD1	3:B:247:VAL:HG22	2.39	0.47
3:A:150:GLN:NE2	3:A:155:THR:OG1	2.49	0.46
2:M:50:LYS:HG2	2:M:50:LYS:O	2.15	0.46
3:A:250:GLU:OE1	3:A:277:ARG:NH2	2.47	0.46
3:B:99:SER:OG	3:B:231:VAL:HG22	2.17	0.45
1:K:64:LYS:NZ	4:K:301:SO4:O2	2.32	0.45
2:M:149:VAL:O	2:M:152:ALA:HB3	2.17	0.45
1:H:2:VAL:HG13	1:H:27:PHE:CD2	2.52	0.45
1:H:210:LYS:HB2	1:H:211:PRO:HD3	1.99	0.45
2:M:168:LYS:HG3	2:M:169:ASP:N	2.31	0.45
3:B:150:GLN:NE2	3:B:155:THR:OG1	2.49	0.44
1:K:20:LEU:HG	1:K:82:MET:HE2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:106:TYR:CZ	1:H:108:GLY:HA2	2.53	0.44
1:K:13:GLN:HE21	1:K:13:GLN:N	2.15	0.44
1:K:2:VAL:HG13	1:K:27:PHE:CD2	2.53	0.44
3:A:160:PRO:HB3	3:A:165:VAL:HG23	1.98	0.44
3:A:180:GLY:O	3:A:181:PRO:C	2.56	0.43
1:K:29:PHE:O	1:K:71:ARG:NH2	2.51	0.43
3:B:160:PRO:HB3	3:B:165:VAL:HG23	1.99	0.43
1:K:70:SER:O	1:K:78:LEU:HD12	2.18	0.43
2:L:11:LEU:C	2:L:11:LEU:HD12	2.38	0.43
3:B:176:ASN:OD1	3:B:176:ASN:C	2.57	0.43
1:K:210:LYS:HB2	1:K:211:PRO:HD3	2.00	0.43
2:L:168:LYS:HG3	2:L:169:ASP:N	2.34	0.43
3:B:35:HIS:O	3:B:59:GLY:HA3	2.18	0.43
3:A:35:HIS:O	3:A:59:GLY:HA3	2.19	0.42
3:A:176:ASN:C	3:A:176:ASN:OD1	2.57	0.42
3:A:263:THR:O	3:A:264:ASN:HB3	2.19	0.42
1:H:20:LEU:HG	1:H:82:MET:HE2	2.01	0.42
1:K:106:TYR:CZ	1:K:108:GLY:HA2	2.55	0.42
1:H:11:LEU:HD21	1:H:156:PRO:HG3	2.01	0.41
2:M:11:LEU:C	2:M:11:LEU:HD12	2.40	0.41
2:L:168:LYS:HE2	2:L:169:ASP:HB3	2.02	0.41
3:B:169:VAL:HG21	3:B:224:PHE:CZ	2.55	0.41
3:B:22:THR:HA	3:B:40:TYR:O	2.20	0.41
2:L:162:VAL:HG22	2:L:174:LEU:HD12	2.03	0.41
3:A:22:THR:HA	3:A:40:TYR:O	2.21	0.41
2:M:107:ARG:HD2	2:M:139:TYR:CG	2.56	0.41
2:M:120:SER:O	2:M:124:LEU:HG	2.20	0.41
2:L:107:ARG:HD2	2:L:139:TYR:CG	2.56	0.41
2:M:162:VAL:HG22	2:M:174:LEU:HD12	2.03	0.40
3:A:54:VAL:HG22	3:A:231:VAL:HG22	2.02	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	H	214/225 (95%)	208 (97%)	6 (3%)	0	100	100
1	K	214/225 (95%)	207 (97%)	7 (3%)	0	100	100
2	L	211/213 (99%)	192 (91%)	18 (8%)	1 (0%)	29	39
2	M	211/213 (99%)	196 (93%)	15 (7%)	0	100	100
3	A	268/293 (92%)	252 (94%)	12 (4%)	4 (2%)	10	13
3	B	268/293 (92%)	253 (94%)	12 (4%)	3 (1%)	14	19
All	All	1386/1462 (95%)	1308 (94%)	70 (5%)	8 (1%)	25	33

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	262	SER
3	A	180	GLY
3	A	262	SER
2	L	51	ALA
3	A	120	PHE
3	B	120	PHE
3	B	159	SER
3	A	159	SER

### 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	H	179/186 (96%)	170 (95%)	9 (5%)	24	33
1	K	179/186 (96%)	167 (93%)	12 (7%)	16	21
2	L	187/187 (100%)	171 (91%)	16 (9%)	10	13
2	M	187/187 (100%)	171 (91%)	16 (9%)	10	13
3	A	243/259 (94%)	232 (96%)	11 (4%)	27	37
3	B	243/259 (94%)	232 (96%)	11 (4%)	27	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1218/1264 (96%)	1143 (94%)	75 (6%)	18	23

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	19	ARG
1	H	43	LYS
1	H	53	THR
1	H	186	SER
1	H	187	LEU
1	H	191	VAL
1	H	200	THR
1	H	201	GLN
1	H	205	CYS
2	L	10	THR
2	L	11	LEU
2	L	14	SER
2	L	19	VAL
2	L	33	LEU
2	L	48	ILE
2	L	54	LEU
2	L	69	THR
2	L	102	LYS
2	L	107	ARG
2	L	113	SER
2	L	153	LEU
2	L	168	LYS
2	L	179	THR
2	L	196	THR
2	L	202	SER
3	A	27	THR
3	A	52	LEU
3	A	58	LYS
3	A	66	ARG
3	A	105	ASN
3	A	219	LEU
3	A	221	SER
3	A	222	SER
3	A	230	THR
3	A	234	MET
3	A	262	SER
1	K	12	VAL

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Mol	Chain	Res	Type
1	K	13	GLN
1	K	19	ARG
1	K	53	THR
1	K	70	SER
1	K	120	VAL
1	K	137	SER
1	K	186	SER
1	K	191	VAL
1	K	200	THR
1	K	201	GLN
1	K	205	CYS
2	M	11	LEU
2	M	14	SER
2	M	19	VAL
2	M	33	LEU
2	M	48	ILE
2	M	52	SER
2	M	54	LEU
2	M	102	LYS
2	M	107	ARG
2	M	113	SER
2	M	153	LEU
2	M	155	SER
2	M	179	THR
2	M	196	THR
2	M	202	SER
2	M	213	CYS
3	B	27	THR
3	B	52	LEU
3	B	58	LYS
3	B	88	LEU
3	B	105	ASN
3	B	185	ASP
3	B	204	MET
3	B	219	LEU
3	B	221	SER
3	B	230	THR
3	B	231	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	105	HIS
1	H	206	ASN
2	L	123	GLN
2	L	197	HIS
2	L	198	GLN
3	A	74	ASN
3	A	150	GLN
3	A	178	ASN
3	A	194	GLN
3	A	209	ASN
3	A	257	GLN
1	K	13	GLN
1	K	206	ASN
2	M	197	HIS
2	M	198	GLN
3	B	74	ASN
3	B	97	GLN
3	B	150	GLN
3	B	172	ASN
3	B	194	GLN
3	B	209	ASN
3	B	257	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](#)

6 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	301	-	4,4,4	0.37	0	6,6,6	0.20	0
4	SO4	H	302	-	4,4,4	0.41	0	6,6,6	0.32	0
4	SO4	A	301	-	4,4,4	0.40	0	6,6,6	0.16	0
4	SO4	A	302	-	4,4,4	0.41	0	6,6,6	0.20	0
4	SO4	A	303	-	4,4,4	0.43	0	6,6,6	0.31	0
4	SO4	K	301	-	4,4,4	0.32	0	6,6,6	0.46	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	K	301	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	H	218/225 (96%)	0.50	2 (0%) 84 89	48, 72, 96, 119	0
1	K	218/225 (96%)	0.74	18 (8%) 11 15	46, 74, 128, 151	0
2	L	213/213 (100%)	0.50	2 (0%) 84 89	39, 66, 123, 143	0
2	M	213/213 (100%)	0.69	11 (5%) 27 34	43, 74, 138, 162	0
3	A	272/293 (92%)	0.57	4 (1%) 73 80	45, 69, 109, 138	0
3	B	272/293 (92%)	0.56	1 (0%) 92 96	45, 70, 106, 132	0
All	All	1406/1462 (96%)	0.59	38 (2%) 54 63	39, 71, 119, 162	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	213	CYS	9.8
2	L	213	CYS	5.4
2	M	153	LEU	4.8
1	K	134	ALA	4.0
1	K	220	VAL	3.7
1	K	219	ARG	3.6
3	A	240	LYS	3.4
1	K	198	LEU	3.3
1	K	221	GLU	3.2
2	M	212	GLU	3.2
1	K	137	SER	2.9
1	K	155	PHE	2.8
3	A	263	THR	2.8
2	M	121	ASP	2.7
3	B	237	LYS	2.6
1	K	150	LEU	2.6
1	K	207	VAL	2.6
1	H	179	LEU	2.5
1	K	136	SER	2.4

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Mol	Chain	Res	Type	RSRZ
3	A	287	GLU	2.4
2	L	211	GLY	2.3
2	M	211	GLY	2.3
1	K	11	LEU	2.3
2	M	178	LEU	2.3
1	K	123	ALA	2.2
1	K	203	TYR	2.2
1	K	193	VAL	2.2
3	A	284	ILE	2.2
1	K	199	GLY	2.1
2	M	124	LEU	2.1
2	M	187	LYS	2.1
1	K	213	ASN	2.1
1	H	219	ARG	2.1
1	K	168	LEU	2.0
1	K	149	CYS	2.0
2	M	193	CYS	2.0
2	M	126	SER	2.0
2	M	130	SER	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 carbohydrates 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
4	SO4	A	303	5/5	0.65	0.23	122,129,140,140	0
4	SO4	H	302	5/5	0.71	0.28	98,114,129,134	0
4	SO4	A	301	5/5	0.75	0.34	118,123,136,139	0
4	SO4	A	302	5/5	0.82	0.26	107,119,127,132	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	H	301	5/5	0.90	0.31	90,109,118,122	0
4	SO4	K	301	5/5	0.92	0.23	85,96,96,109	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.