



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2018 – 08:32 PM EDT

PDB ID : 6C6Y  
Title : Crystal structure of Middle-East Respiratory Syndrome (MERS) coronavirus neutralizing antibody JC57-14 isolated from a vaccinated rhesus macaque in complex with MERS Receptor Binding Domain  
Authors : Joyce, M.G.; Mascola, J.R.; Graham, B.S.; Kwong, P.D.  
Deposited on : 2018-01-19  
Resolution : 3.32 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030736  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030736

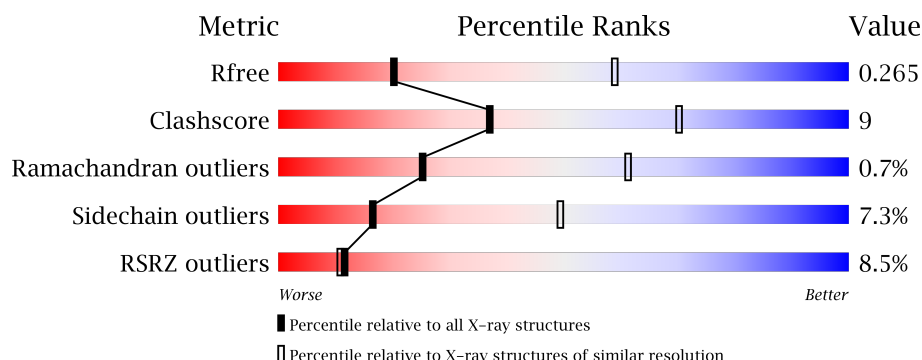
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.32 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))
$R_{free}$	100719	1002 (3.38-3.26)
Clashscore	112137	1066 (3.38-3.26)
Ramachandran outliers	110173	1048 (3.38-3.26)
Sidechain outliers	110143	1047 (3.38-3.26)
RSRZ outliers	101464	1007 (3.38-3.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	218	<div> <div>7%</div> <div>72%</div> <div>23%</div> <div>• •</div> </div>
1	H	218	<div> <div>10%</div> <div>69%</div> <div>23%</div> <div>• •</div> </div>
2	B	214	<div> <div>3%</div> <div>79%</div> <div>19%</div> <div>•</div> </div>
2	L	214	<div> <div>3%</div> <div>74%</div> <div>22%</div> <div>•</div> </div>
3	R	208	<div> <div>17%</div> <div>72%</div> <div>25%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
3	S	208	<div><div></div><div>11%</div><div>77%</div><div>21%</div><div></div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9703 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 JC57-14 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1596	1005	264	323	4			
1	H	210	Total	C	N	O	S	0	0	0
			1568	990	260	314	4			

- Molecule 2 is a protein called JC57-14 Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	0	0
			1656	1033	276	341	6			
2	L	214	Total	C	N	O	S	0	0	0
			1656	1033	276	341	6			

- Molecule 3 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	R	208	Total	C	N	O	S	0	0	0
			1611	1029	256	315	11			
3	S	208	Total	C	N	O	S	0	0	0
			1611	1029	256	315	11			

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

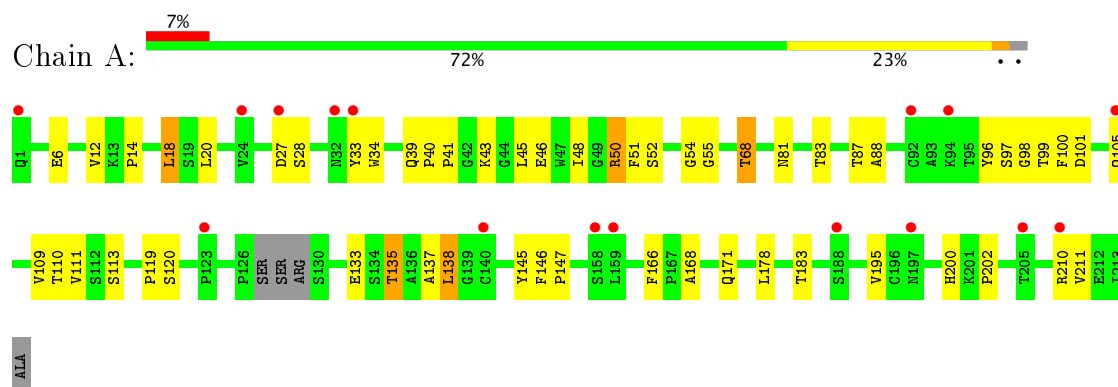


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		

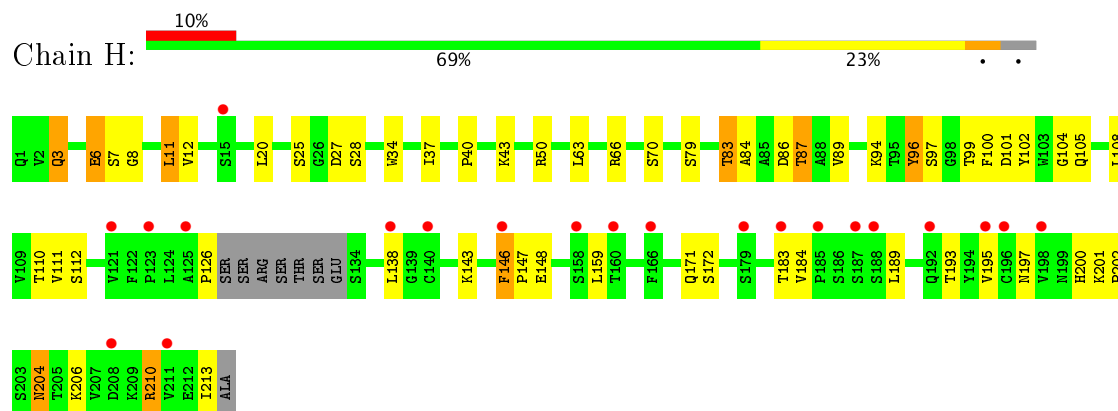
### 3 Residue-property plots [i](#)

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.

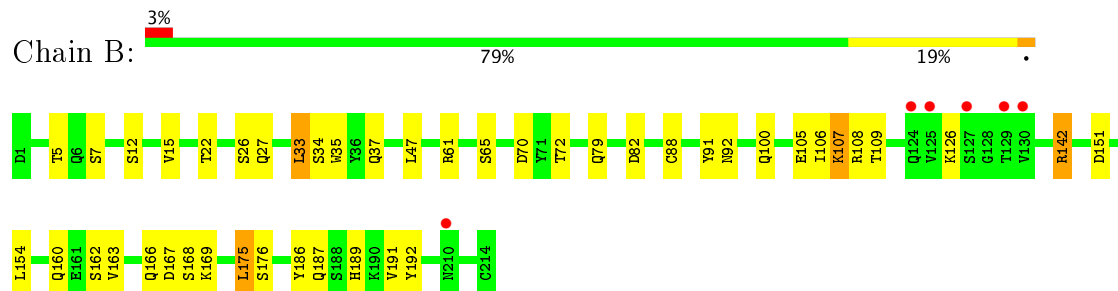
- Molecule 1: JC57-14 Heavy chain



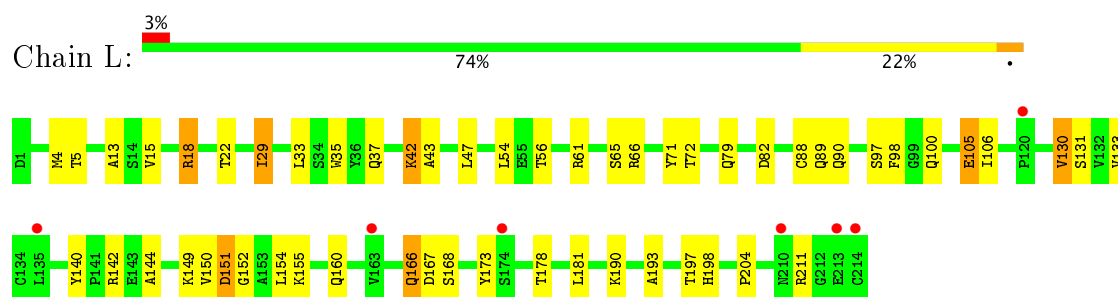
- Molecule 1: JC57-14 Heavy chain



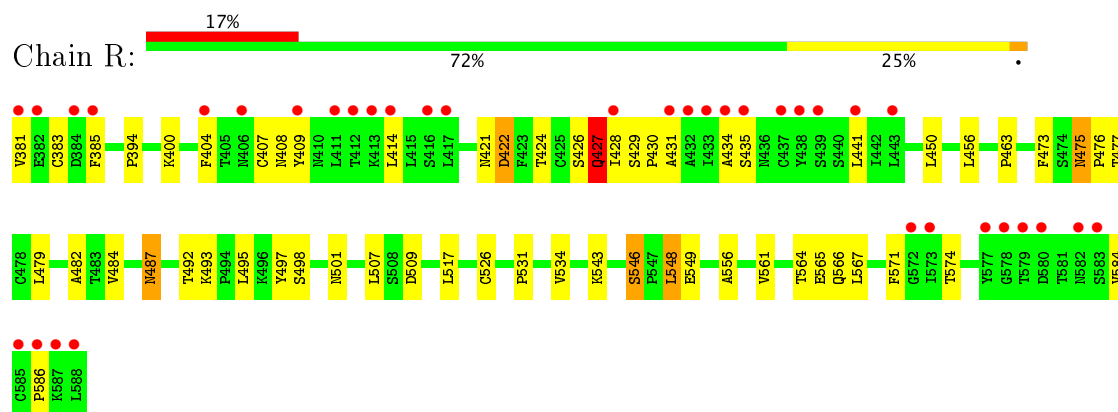
- Molecule 2: JC57-14 Light chain



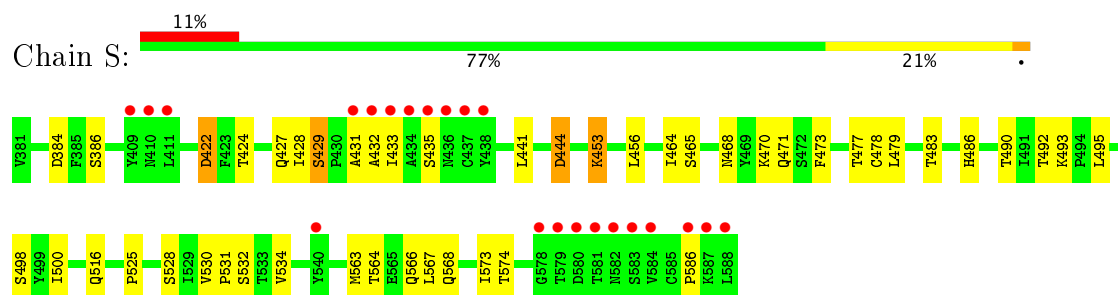
- Molecule 2: JC57-14 Light chain



• Molecule 3: Spike glycoprotein



• Molecule 3: Spike glycoprotein



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.58Å 148.07Å 259.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.44 – 3.32 48.74 – 3.32	Depositor EDS
% Data completeness (in resolution range)	80.5 (42.44-3.32) 80.5 (48.74-3.32)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.68 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, $R_{free}$	0.232 , 0.267 0.231 , 0.265	Depositor DCC
$R_{free}$ test set	970 reflections (5.08%)	DCC
Wilson B-factor (Å <sup>2</sup> )	71.7	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 64.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.026 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.035 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	9703	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% 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	A	0.26	0/1634	0.46	0/2232
1	H	0.25	0/1606	0.48	0/2194
2	B	0.25	0/1692	0.46	0/2300
2	L	0.26	0/1692	0.47	0/2300
3	R	0.25	0/1651	0.47	0/2254
3	S	0.24	0/1651	0.45	0/2254
All	All	0.25	0/9926	0.46	0/13534

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1596	0	1559	31	0
1	H	1568	0	1536	37	0
2	B	1656	0	1596	26	0
2	L	1656	0	1596	34	0
3	R	1611	0	1572	33	0
3	S	1611	0	1572	23	0
4	B	5	0	0	0	0
All	All	9703	0	9431	171	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 9.

All (171) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:189:LEU:HD13	1:H:213:ILE:CD1	1.48	1.43
1:H:189:LEU:HD13	1:H:213:ILE:HD11	1.30	1.13
1:H:189:LEU:HD13	1:H:213:ILE:HD12	1.40	1.00
1:H:189:LEU:CD1	1:H:213:ILE:CD1	2.39	0.99
1:H:189:LEU:CD1	1:H:213:ILE:HD11	1.97	0.95
1:H:66:ARG:NH1	1:H:86:ASP:OD2	2.12	0.82
3:S:422:ASP:OD2	3:S:453:LYS:NZ	2.14	0.80
2:L:105:GLU:HG3	2:L:166:GLN:HE22	1.45	0.79
1:H:96:TYR:H	1:H:96:TYR:HD1	1.30	0.79
2:B:151:ASP:HB2	2:B:189:HIS:HB3	1.67	0.75
1:A:97:SER:HA	3:S:531:PRO:HG3	1.70	0.72
1:H:97:SER:HA	3:R:531:PRO:HG3	1.70	0.72
3:R:381:VAL:O	3:R:408:ASN:N	2.21	0.71
1:H:204:ASN:O	1:H:206:LYS:NZ	2.24	0.71
1:A:68:THR:HG23	1:A:81:ASN:HB3	1.72	0.70
1:H:195:VAL:HG22	1:H:210:ARG:HG3	1.74	0.68
3:S:516:GLN:HB3	3:S:525:PRO:HG2	1.74	0.67
3:S:483:THR:HG22	3:S:568:GLN:HG2	1.75	0.67
3:R:435:SER:HA	3:R:586:PRO:HG3	1.78	0.66
1:H:8:GLY:HA3	1:H:20:LEU:HD23	1.78	0.64
3:R:394:PRO:HG3	3:R:400:LYS:HG3	1.80	0.63
2:B:65:SER:OG	2:B:72:THR:OG1	2.18	0.62
2:B:5:THR:OG1	2:L:151:ASP:O	2.19	0.61
2:L:166:GLN:NE2	2:L:173:TYR:OH	2.33	0.60
3:R:422:ASP:OD1	3:R:422:ASP:N	2.35	0.60
3:R:487:ASN:OD1	3:R:487:ASN:N	2.34	0.60
1:A:87:THR:HG22	1:A:111:VAL:H	1.67	0.60
1:A:18:LEU:HD11	1:A:20:LEU:HG	1.84	0.59
2:L:56:THR:HG23	3:R:546:SER:HB3	1.83	0.59
2:B:15:VAL:HG13	2:B:79:GLN:HA	1.83	0.59
3:R:426:SER:OG	3:R:427:GLN:OE1	2.19	0.59
1:A:12:VAL:HG21	1:A:18:LEU:HB2	1.85	0.59
3:S:444:ASP:OD1	3:S:444:ASP:N	2.35	0.58
2:B:142:ARG:HD2	2:B:163:VAL:HG11	1.85	0.58
2:L:4:MET:O	2:L:100:GLN:NE2	2.37	0.58
1:A:50:ARG:HH11	1:A:50:ARG:CG	2.17	0.57
2:B:22:THR:HG22	2:B:72:THR:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:37:ILE:HD11	1:H:100:PHE:CZ	2.41	0.56
1:H:40:PRO:HB2	1:H:43:LYS:HD2	1.87	0.56
2:B:5:THR:HA	2:B:100:GLN:HE22	1.70	0.56
3:S:422:ASP:N	3:S:422:ASP:OD1	2.35	0.56
2:L:22:THR:HG22	2:L:72:THR:HG22	1.87	0.56
3:R:475:ASN:N	3:R:475:ASN:OD1	2.39	0.55
2:L:37:GLN:HB2	2:L:47:LEU:HD11	1.88	0.55
3:S:465:SER:O	3:S:470:LYS:NZ	2.39	0.55
1:A:18:LEU:HD22	1:A:109:VAL:HG11	1.88	0.54
1:H:171:GLN:NE2	2:L:160:GLN:OE1	2.40	0.54
3:S:456:LEU:HB3	3:S:479:LEU:HD21	1.90	0.54
1:A:39:GLN:HB2	1:A:45:LEU:HD23	1.91	0.53
1:H:204:ASN:O	1:H:204:ASN:ND2	2.40	0.53
3:R:381:VAL:HG22	3:R:408:ASN:HB2	1.91	0.53
3:S:564:THR:OG1	3:S:566:GLN:O	2.24	0.53
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.89	0.53
3:S:493:LYS:HG2	3:S:567:LEU:HB2	1.91	0.52
1:H:70:SER:HB2	1:H:79:SER:HB2	1.92	0.52
3:R:409:TYR:HE1	3:R:434:ALA:HA	1.75	0.52
3:R:484:VAL:O	3:R:566:GLN:NE2	2.42	0.52
3:S:435:SER:HA	3:S:586:PRO:HG3	1.91	0.52
3:S:428:ILE:HB	3:S:431:ALA:HB1	1.92	0.51
2:B:167:ASP:OD1	2:B:168:SER:N	2.44	0.51
1:H:27:ASP:OD1	1:H:28:SER:N	2.43	0.51
3:S:500:ILE:HD11	3:S:530:VAL:HG11	1.91	0.51
3:R:564:THR:OG1	3:R:566:GLN:O	2.22	0.51
1:A:119:PRO:HB3	1:A:145:TYR:HB3	1.92	0.51
1:H:200:HIS:CD2	1:H:202:PRO:HD2	2.46	0.51
1:H:89:VAL:HA	1:H:108:LEU:HA	1.90	0.51
2:B:108:ARG:HG2	2:B:109:THR:H	1.75	0.51
1:A:195:VAL:HG12	1:A:210:ARG:HG3	1.93	0.50
2:L:42:LYS:HE2	2:L:43:ALA:H	1.75	0.50
2:B:26:SER:HB2	2:L:190:LYS:HD2	1.93	0.50
1:A:50:ARG:CG	1:A:50:ARG:NH1	2.73	0.50
2:B:12:SER:HB3	2:B:107:LYS:HB3	1.94	0.50
3:S:464:ILE:HA	3:S:468:ASN:HB2	1.94	0.50
1:A:33:TYR:CE2	1:A:52:SER:HB2	2.48	0.49
1:A:138:LEU:HB2	1:A:211:VAL:HG11	1.94	0.49
1:A:27:ASP:OD1	1:A:28:SER:N	2.46	0.49
3:R:385:PHE:CG	3:R:414:LEU:HD21	2.48	0.49
1:H:11:LEU:HD23	1:H:147:PRO:HG3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ARG:HH11	1:A:50:ARG:HG3	1.77	0.49
3:R:546:SER:OG	3:R:549:GLU:OE2	2.30	0.49
2:L:29:ILE:HD11	2:L:90:GLN:HB3	1.95	0.48
1:H:34:TRP:CZ3	1:H:94:LYS:HB2	2.48	0.48
2:L:133:VAL:HG22	2:L:178:THR:HG22	1.95	0.48
3:R:477:THR:HG22	3:R:574:THR:HG23	1.95	0.48
2:L:150:VAL:HG11	2:L:155:LYS:HG2	1.94	0.48
1:H:3:GLN:HB2	1:H:25:SER:HB2	1.94	0.48
2:B:61:ARG:NH2	2:B:82:ASP:OD1	2.45	0.47
3:S:456:LEU:HD12	3:S:464:ILE:HG21	1.96	0.47
1:H:147:PRO:HD2	1:H:202:PRO:HG2	1.95	0.47
3:S:384:ASP:OD2	3:S:386:SER:OG	2.28	0.47
2:L:5:THR:HA	2:L:100:GLN:HE22	1.79	0.47
1:A:137:ALA:HB2	1:A:183:THR:HG22	1.96	0.47
2:B:186:TYR:O	2:B:192:TYR:OH	2.28	0.47
1:A:200:HIS:CD2	1:A:202:PRO:HD2	2.50	0.47
1:H:189:LEU:HD13	1:H:213:ILE:HD13	1.72	0.47
3:R:493:LYS:HG2	3:R:567:LEU:HB2	1.95	0.47
2:B:105:GLU:HB2	2:B:166:GLN:OE1	2.14	0.47
1:A:166:PHE:CE2	2:B:176:SER:HB3	2.50	0.46
2:L:144:ALA:HB2	2:L:198:HIS:HD2	1.80	0.46
1:A:14:PRO:HG2	1:A:113:SER:HB3	1.97	0.46
1:H:3:GLN:N	1:H:25:SER:O	2.39	0.46
1:H:112:SER:HB2	1:H:146:PHE:HZ	1.80	0.46
1:H:96:TYR:HE1	1:H:99:THR:HB	1.81	0.46
2:L:61:ARG:NH2	2:L:82:ASP:OD1	2.48	0.46
1:H:87:THR:HG23	1:H:111:VAL:H	1.81	0.46
3:R:548:LEU:HD13	3:R:548:LEU:H	1.80	0.46
3:S:456:LEU:HD23	3:S:479:LEU:HD21	1.98	0.46
1:A:133:GLU:O	1:A:135:THR:N	2.47	0.46
2:L:89:GLN:HG2	2:L:90:GLN:N	2.30	0.46
2:B:163:VAL:HG22	2:B:175:LEU:HD12	1.97	0.46
2:B:35:TRP:CZ3	2:B:88:CYS:HB3	2.51	0.46
1:A:41:PRO:HD3	1:A:88:ALA:HA	1.98	0.45
1:H:6:GLU:OE2	1:H:104:GLY:HA3	2.17	0.45
1:H:96:TYR:CE2	3:R:543:LYS:HG2	2.51	0.45
3:S:429:SER:C	3:S:431:ALA:HB2	2.38	0.45
3:R:427:GLN:O	3:R:476:PRO:HB3	2.16	0.45
3:R:497:TYR:HB2	3:R:561:VAL:HB	1.99	0.45
1:H:83:THR:OG1	1:H:84:ALA:N	2.50	0.45
1:A:14:PRO:HA	1:A:111:VAL:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:90:GLN:HE21	2:L:97:SER:H	1.63	0.44
2:L:166:GLN:HE21	2:L:166:GLN:HB2	1.46	0.44
2:L:197:THR:HG22	2:L:204:PRO:HB3	2.00	0.44
1:H:87:THR:HG23	1:H:111:VAL:HG12	1.99	0.44
1:A:54:GLY:HA3	1:A:55:GLY:HA2	1.84	0.43
2:B:100:GLN:H	2:B:100:GLN:CD	2.21	0.43
2:B:100:GLN:NE2	2:L:152:GLY:O	2.51	0.43
3:S:470:LYS:NZ	3:S:470:LYS:HB2	2.33	0.43
1:A:96:TYR:HE2	1:A:101:ASP:OD2	2.01	0.43
2:L:105:GLU:OE1	2:L:140:TYR:OH	2.31	0.43
2:B:27:GLN:HG2	2:L:190:LYS:NZ	2.34	0.43
2:L:15:VAL:HG13	2:L:79:GLN:HA	2.01	0.43
2:L:167:ASP:OD1	2:L:168:SER:N	2.50	0.43
3:R:441:LEU:HB2	3:R:584:VAL:HG11	2.00	0.43
1:H:126:PRO:HD2	1:H:213:ILE:HG12	1.99	0.43
2:L:66:ARG:NE	2:L:71:TYR:OH	2.52	0.43
3:R:463:PRO:HB3	3:R:501:ASN:HA	2.01	0.43
3:R:482:ALA:HB3	3:R:571:PHE:HE2	1.84	0.43
1:H:171:GLN:OE1	1:H:172:SER:N	2.47	0.43
1:H:201:LYS:HB2	1:H:202:PRO:HD3	2.01	0.42
1:H:96:TYR:CD1	1:H:96:TYR:N	2.79	0.42
3:R:383:CYS:HB3	3:R:404:PHE:CD1	2.53	0.42
3:R:456:LEU:HD13	3:R:479:LEU:HD21	2.01	0.42
1:H:101:ASP:HB3	1:H:102:TYR:CD2	2.54	0.42
3:R:428:ILE:HG22	3:R:430:PRO:O	2.20	0.42
2:L:149:LYS:HB2	2:L:193:ALA:HB3	2.01	0.42
3:R:498:SER:HB3	3:R:534:VAL:HG23	2.01	0.42
1:A:40:PRO:HG2	1:A:43:LYS:HB2	2.02	0.42
3:R:409:TYR:CE1	3:R:434:ALA:HA	2.54	0.42
3:S:478:CYS:HB2	3:S:573:ILE:HB	2.00	0.42
1:A:168:ALA:HA	1:A:178:LEU:HB3	2.00	0.42
2:B:92:ASN:O	3:S:532:SER:OG	2.26	0.42
3:R:421:ASN:HD22	3:R:450:LEU:HD21	1.84	0.42
3:R:526:CYS:SG	3:R:556:ALA:HB2	2.60	0.42
1:A:34:TRP:HB2	1:A:51:PHE:CZ	2.55	0.41
2:L:105:GLU:CG	2:L:166:GLN:HE22	2.26	0.41
3:R:404:PHE:HB3	3:R:407:CYS:SG	2.60	0.41
1:A:99:THR:OG1	1:A:100:PHE:N	2.53	0.41
1:A:146:PHE:HA	1:A:147:PRO:HA	1.84	0.41
2:L:18:ARG:HG3	2:L:18:ARG:O	2.19	0.41
2:L:89:GLN:HB2	2:L:98:PHE:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:498:SER:HB3	3:S:534:VAL:HG23	2.02	0.41
2:L:130:VAL:HG23	2:L:181:LEU:O	2.21	0.41
3:R:507:LEU:C	3:R:509:ASP:H	2.24	0.41
3:S:477:THR:HG22	3:S:574:THR:HG23	2.01	0.41
2:L:35:TRP:CZ3	2:L:88:CYS:HB3	2.56	0.41
2:B:33:LEU:HG	2:B:34:SER:N	2.36	0.41
1:A:98:GLY:HA3	2:B:91:TYR:HB2	2.03	0.41
1:A:171:GLN:HG3	2:B:160:GLN:HE22	1.85	0.41
2:B:151:ASP:HA	2:B:191:VAL:HG23	2.02	0.41
2:L:13:ALA:O	2:L:106:ILE:HA	2.21	0.41
2:L:154:LEU:HD12	2:L:154:LEU:H	1.86	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	210/218 (96%)	194 (92%)	15 (7%)	1 (0%)	32	67
1	H	206/218 (94%)	187 (91%)	19 (9%)	0	100	100
2	B	212/214 (99%)	206 (97%)	6 (3%)	0	100	100
2	L	212/214 (99%)	204 (96%)	7 (3%)	1 (0%)	32	67
3	R	206/208 (99%)	190 (92%)	13 (6%)	3 (2%)	12	45
3	S	206/208 (99%)	195 (95%)	7 (3%)	4 (2%)	9	41
All	All	1252/1280 (98%)	1176 (94%)	67 (5%)	9 (1%)	25	61

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	R	429	SER

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Mol	Chain	Res	Type
3	R	431	ALA
3	S	429	SER
3	R	427	GLN
2	L	151	ASP
3	S	427	GLN
3	S	432	ALA
3	S	433	ILE
1	A	48	ILE

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	186/189 (98%)	175 (94%)	11 (6%)	23	59
1	H	182/189 (96%)	159 (87%)	23 (13%)	5	23
2	B	192/192 (100%)	180 (94%)	12 (6%)	21	56
2	L	192/192 (100%)	180 (94%)	12 (6%)	21	56
3	R	190/190 (100%)	178 (94%)	12 (6%)	21	56
3	S	190/190 (100%)	177 (93%)	13 (7%)	18	53
All	All	1132/1142 (99%)	1049 (93%)	83 (7%)	16	49

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	18	LEU
1	A	46	GLU
1	A	50	ARG
1	A	68	THR
1	A	83	THR
1	A	105	GLN
1	A	110	THR
1	A	120	SER
1	A	135	THR

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Mol	Chain	Res	Type
1	A	138	LEU
2	B	7	SER
2	B	33	LEU
2	B	70	ASP
2	B	106	ILE
2	B	107	LYS
2	B	126	LYS
2	B	142	ARG
2	B	154	LEU
2	B	162	SER
2	B	169	LYS
2	B	175	LEU
2	B	187	GLN
1	H	3	GLN
1	H	6	GLU
1	H	7	SER
1	H	11	LEU
1	H	12	VAL
1	H	50	ARG
1	H	63	LEU
1	H	83	THR
1	H	87	THR
1	H	96	TYR
1	H	105	GLN
1	H	110	THR
1	H	138	LEU
1	H	143	LYS
1	H	146	PHE
1	H	148	GLU
1	H	159	LEU
1	H	183	THR
1	H	184	VAL
1	H	193	THR
1	H	197	ASN
1	H	204	ASN
1	H	210	ARG
2	L	18	ARG
2	L	29	ILE
2	L	33	LEU
2	L	42	LYS
2	L	54	LEU
2	L	65	SER

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Mol	Chain	Res	Type
2	L	105	GLU
2	L	130	VAL
2	L	131	SER
2	L	142	ARG
2	L	166	GLN
2	L	211	ARG
3	R	422	ASP
3	R	424	THR
3	R	427	GLN
3	R	473	PHE
3	R	475	ASN
3	R	487	ASN
3	R	492	THR
3	R	495	LEU
3	R	517	LEU
3	R	546	SER
3	R	548	LEU
3	R	565	GLU
3	S	422	ASP
3	S	424	THR
3	S	441	LEU
3	S	444	ASP
3	S	453	LYS
3	S	471	GLN
3	S	473	PHE
3	S	486	HIS
3	S	490	THR
3	S	492	THR
3	S	495	LEU
3	S	528	SER
3	S	563	MET

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

Mol	Chain	Res	Type
2	L	166	GLN

### 5.3.3 RNA ⓘ

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](#)

1 ligand is 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	B	301	-	4,4,4	0.14	0	6,6,6	0.05	0

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
4	SO4	B	301	-	-	0/0/0/0	0/0/0/0

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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	214/218 (98%)	0.67	16 (7%) 15 14	56, 100, 143, 179	0
1	H	210/218 (96%)	0.61	21 (10%) 8 7	31, 85, 151, 178	0
2	B	214/214 (100%)	-0.01	6 (2%) 53 52	32, 63, 148, 171	0
2	L	214/214 (100%)	0.26	7 (3%) 47 44	29, 58, 134, 208	0
3	R	208/208 (100%)	0.90	36 (17%) 2 1	23, 66, 270, 353	0
3	S	208/208 (100%)	0.64	22 (10%) 7 5	41, 82, 246, 390	0
All	All	1268/1280 (99%)	0.51	108 (8%) 11 11	23, 77, 172, 390	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	R	432	ALA	16.1
3	S	432	ALA	14.7
3	S	433	ILE	11.3
3	S	434	ALA	11.0
3	R	433	ILE	9.9
3	R	583	SER	8.8
3	R	434	ALA	8.3
3	R	580	ASP	8.3
3	S	588	LEU	7.5
3	S	435	SER	7.3
2	L	210	ASN	7.3
3	R	586	PRO	7.0
3	S	587	LYS	6.6
3	R	588	LEU	6.0
3	R	438	TYR	5.7
3	S	580	ASP	5.5
3	R	582	ASN	5.0
2	L	214	CYS	5.0
3	R	435	SER	4.8

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Mol	Chain	Res	Type	RSRZ
3	R	439	SER	4.7
3	S	410	ASN	4.6
1	A	140	CYS	4.5
3	R	587	LYS	4.5
3	S	581	THR	4.4
1	H	183	THR	4.4
3	S	584	VAL	4.3
3	R	385	PHE	4.3
3	R	577	TYR	4.2
3	R	437	CYS	4.1
1	A	27	ASP	4.1
1	A	1	GLN	4.0
3	S	579	THR	3.7
3	R	414	LEU	3.6
3	R	431	ALA	3.6
3	R	413	LYS	3.6
3	S	578	GLY	3.6
3	R	382	GLU	3.5
1	A	32	ASN	3.4
1	A	33	TYR	3.3
1	H	123	PRO	3.3
2	B	129	THR	3.2
1	H	125	ALA	3.2
3	S	540	TYR	3.1
1	H	160	THR	3.1
3	S	409	TYR	3.0
3	R	381	VAL	3.0
3	R	585	CYS	3.0
1	A	197	ASN	2.9
1	H	121	VAL	2.9
1	H	140	CYS	2.9
3	S	431	ALA	2.9
3	S	582	ASN	2.8
3	R	406	ASN	2.7
3	R	443	LEU	2.7
3	R	412	THR	2.7
1	A	94	LYS	2.6
1	A	188	SER	2.5
3	S	586	PRO	2.5
3	S	411	LEU	2.5
1	H	15	SER	2.5
1	H	196	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
3	R	404	PHE	2.5
2	B	130	VAL	2.5
2	L	213	GLU	2.5
3	S	583	SER	2.5
3	S	436	ASN	2.4
1	H	146	PHE	2.4
2	B	210	ASN	2.4
3	R	573	ILE	2.4
1	A	105	GLN	2.4
3	R	578	GLY	2.4
1	H	208	ASP	2.4
1	H	166	PHE	2.4
1	H	195	VAL	2.4
2	L	163	VAL	2.4
3	R	572	GLY	2.3
1	H	179	SER	2.3
3	R	416	SER	2.3
1	H	188	SER	2.3
1	H	185	PRO	2.3
2	B	124	GLN	2.3
1	H	158	SER	2.2
1	H	187	SER	2.2
3	R	411	LEU	2.2
1	A	210	ARG	2.2
2	B	125	VAL	2.2
2	L	120	PRO	2.2
3	R	409	TYR	2.2
3	R	579	THR	2.2
1	A	123	PRO	2.2
3	R	384	ASP	2.2
1	H	138	LEU	2.2
3	R	417	LEU	2.2
2	L	174	SER	2.2
1	A	24	VAL	2.1
1	H	211	VAL	2.1
1	A	92	CYS	2.1
2	B	127	SER	2.1
3	R	441	LEU	2.1
3	R	428	ILE	2.1
1	H	192	GLN	2.1
2	L	135	LEU	2.1
1	H	198	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	159	LEU	2.1
3	S	437	CYS	2.0
3	S	438	TYR	2.0
1	A	205	THR	2.0
1	A	158	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q < 0.9
4	SO4	B	301	5/5	0.93	0.13	-	115,115,116,116	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.