



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2026 – 05:09 PM UTC

PDB ID : 6C6Y / pdb_00006c6y
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

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>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

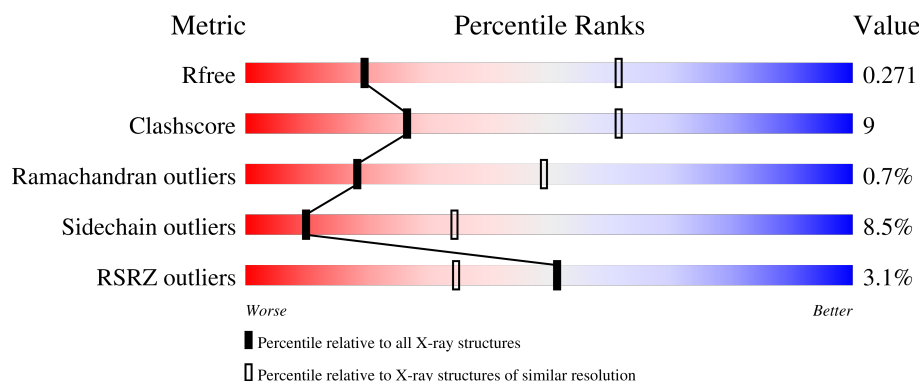
1 Overall quality at a glance

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}	180053	1153 (3.34-3.30)
Clashscore	190562	1193 (3.34-3.30)
Ramachandran outliers	187476	1172 (3.34-3.30)
Sidechain outliers	187428	1171 (3.34-3.30)
RSRZ outliers	180081	1153 (3.34-3.30)

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 ≥ 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	A	218	5% 72% 24% ..
1	H	218	4% 67% 25% 5% .
2	B	214	78% 21% .
2	L	214	2% 73% 24% .
3	R	208	4% 71% 25% .

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Mol	Chain	Length	Quality of chain
3	S	208	3% 76% 21%

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			

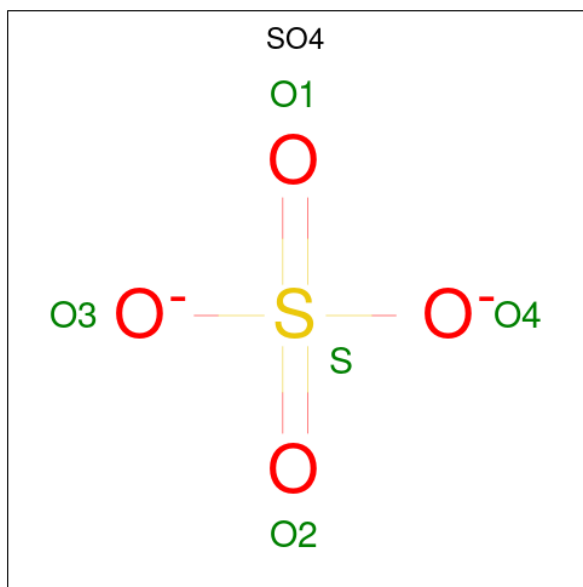
- Molecule 2 is a protein called JC57-14 Light chain.

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 (CCD ID: SO4) (formula: O₄S).

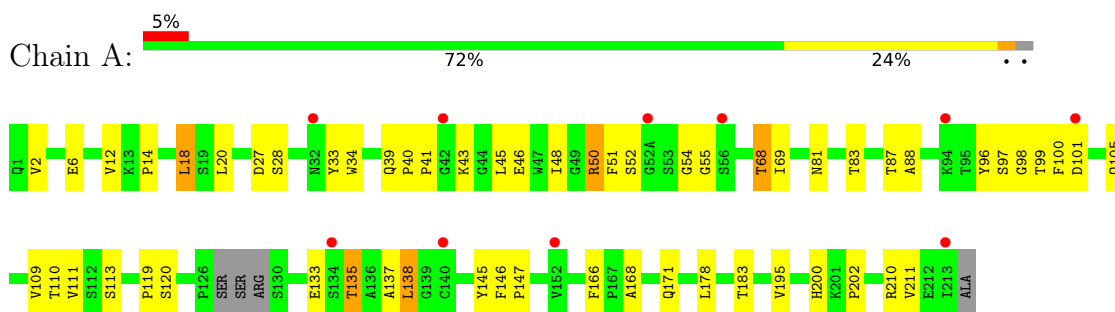


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		

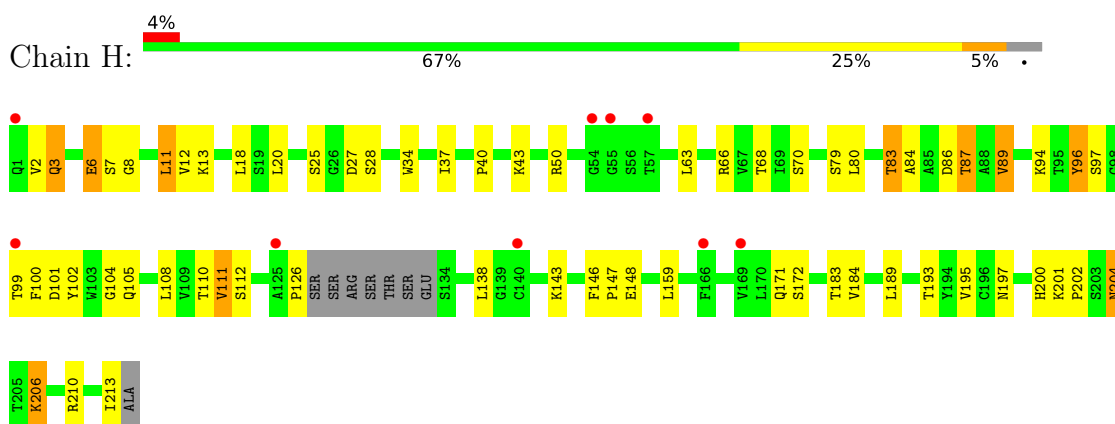
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

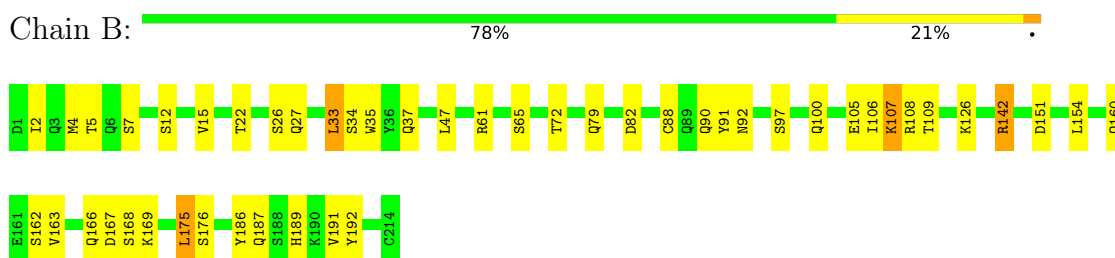
- Molecule 1: JC57-14 Heavy chain



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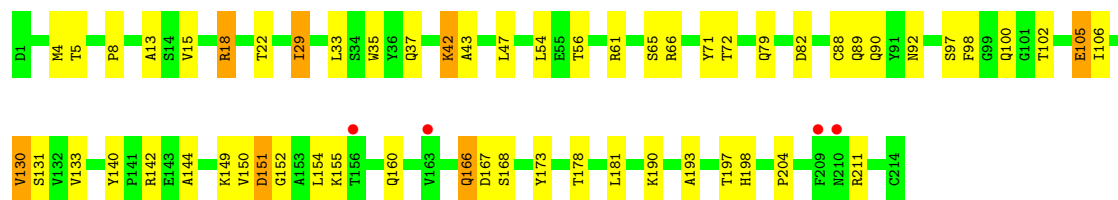


- Molecule 2: JC57-14 Light chain

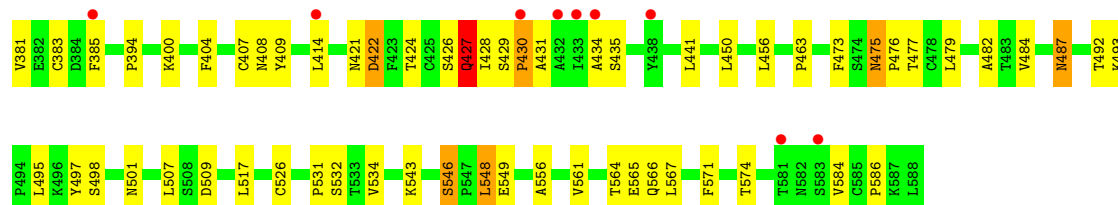
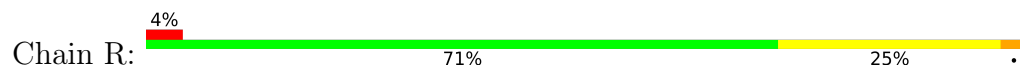


- Molecule 2: JC57-14 Light chain

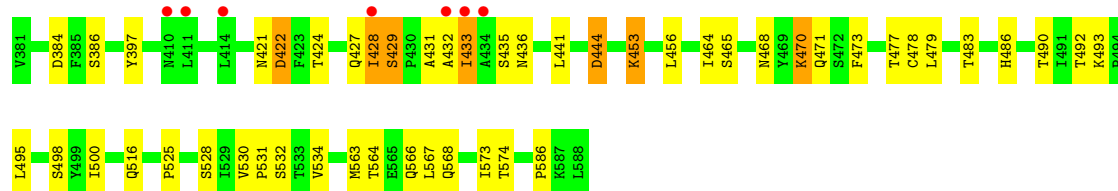
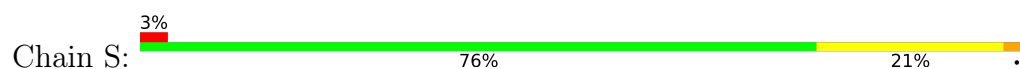




• Molecule 3: Spike glycoprotein



• Molecule 3: Spike glycoprotein



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	81.58Å 148.07Å 259.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.44 – 3.32 42.44 – 3.32	Depositor EDS
% Data completeness (in resolution range)	80.5 (42.44-3.32) 80.7 (42.44-3.32)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.68 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.232 , 0.267 0.234 , 0.271	Depositor DCC
R_{free} test set	972 reflections (4.10%)	wwPDB-VP
Wilson B-factor (Å ²)	71.7	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 83.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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	0.87	EDS
Total number of atoms	9703	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.17	0/1634	0.31	0/2232
1	H	0.12	0/1606	0.33	0/2194
2	B	0.10	0/1692	0.31	0/2300
2	L	0.11	0/1692	0.33	0/2300
3	R	0.12	0/1651	0.35	0/2254
3	S	0.10	0/1651	0.31	0/2254
All	All	0.12	0/9926	0.32	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	38	0
2	B	1656	0	1596	28	0
2	L	1656	0	1596	36	0
3	R	1611	0	1572	34	0
3	S	1611	0	1572	24	0
4	B	5	0	0	0	0
All	All	9703	0	9431	177	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 (177) 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:HD1	1:H:96:TYR:H	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:4:MET:HE2	2:B:90:GLN:HB3	1.80	0.62
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:N	3:R:422:ASP:OD1	2.35	0.60
3:R:487:ASN:N	3:R:487:ASN:OD1	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:CG	1:A:50:ARG:HH11	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:22:THR:HG22	2:B:72:THR:HG22	1.86	0.57
2:B:5:THR:HA	2:B:100:GLN:HE22	1.70	0.56
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
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:S:564:THR:OG1	3:S:566:GLN:O	2.24	0.56
3:R:475:ASN:OD1	3:R:475:ASN:N	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
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.89	0.53
2:L:92:ASN:O	3:R:532:SER:OG	2.21	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
2:B:186:TYR:O	2:B:192:TYR:OH	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:429:SER:C	3:S:431:ALA:HB2	2.38	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
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:B:100:GLN:H	2:B:100:GLN:CD	2.21	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
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:96:TYR:HE1	1:H:99:THR:HB	1.81	0.46
1:H:112:SER:HB2	1:H:146:PHE:HZ	1.80	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
3:R:507:LEU:C	3:R:509:ASP:H	2.24	0.46
3:S:397:TYR:OH	3:S:531:PRO:O	2.29	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:35:TRP:CZ3	2:B:88:CYS:HB3	2.51	0.46
2:B:163:VAL:HG22	2:B:175:LEU:HD12	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:96:TYR:CE2	3:R:543:LYS:HG2	2.51	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
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
2:B:2:ILE:O	2:B:97:SER:OG	2.30	0.44
1:A:54:GLY:HA3	1:A:55:GLY:HA2	1.84	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: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
2:L:105:GLU:OE1	2:L:140:TYR:OH	2.31	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:96:TYR:CD1	1:H:96:TYR:N	2.79	0.42
1:H:201:LYS:HB2	1:H:202:PRO:HD3	2.01	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
2:L:8:PRO:O	2:L:102:THR:OG1	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	2:L:18:ARG:HG3	2.19	0.41
2:L:89:GLN:HB2	2:L:98:PHE:CE1	2.55	0.41
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: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
1:H:66:ARG:HH12	1:H:86:ASP:CG	2.22	0.40
2:L:154:LEU:HD12	2:L:154:LEU:H	1.86	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	A	210/218 (96%)	194 (92%)	15 (7%)	1 (0%)	24	56
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%)	24	56
3	R	206/208 (99%)	190 (92%)	13 (6%)	3 (2%)	8	33
3	S	206/208 (99%)	195 (95%)	7 (3%)	4 (2%)	6	29
All	All	1252/1280 (98%)	1176 (94%)	67 (5%)	9 (1%)	18	49

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	R	429	SER
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%)	173 (93%)	13 (7%)	14	41
1	H	182/189 (96%)	153 (84%)	29 (16%)	2	12
2	B	192/192 (100%)	181 (94%)	11 (6%)	18	47
2	L	192/192 (100%)	180 (94%)	12 (6%)	16	44
3	R	190/190 (100%)	177 (93%)	13 (7%)	14	42
3	S	190/190 (100%)	172 (90%)	18 (10%)	8	30
All	All	1132/1142 (99%)	1036 (92%)	96 (8%)	10	34

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	6	GLU
1	A	18	LEU
1	A	46	GLU
1	A	50	ARG
1	A	68	THR
1	A	69	ILE
1	A	83	THR

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Mol	Chain	Res	Type
1	A	105	GLN
1	A	110	THR
1	A	120	SER
1	A	135	THR
1	A	138	LEU
2	B	7	SER
2	B	33	LEU
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	2	VAL
1	H	3	GLN
1	H	6	GLU
1	H	7	SER
1	H	11	LEU
1	H	12	VAL
1	H	13	LYS
1	H	18	LEU
1	H	50	ARG
1	H	63	LEU
1	H	68	THR
1	H	80	LEU
1	H	83	THR
1	H	87	THR
1	H	89	VAL
1	H	96	TYR
1	H	105	GLN
1	H	110	THR
1	H	111	VAL
1	H	138	LEU
1	H	143	LYS
1	H	148	GLU
1	H	159	LEU
1	H	183	THR
1	H	184	VAL
1	H	193	THR

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Mol	Chain	Res	Type
1	H	197	ASN
1	H	204	ASN
1	H	206	LYS
2	L	18	ARG
2	L	29	ILE
2	L	33	LEU
2	L	42	LYS
2	L	54	LEU
2	L	65	SER
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	430	PRO
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	421	ASN
3	S	422	ASP
3	S	424	THR
3	S	428	ILE
3	S	433	ILE
3	S	436	ASN
3	S	441	LEU
3	S	444	ASP
3	S	453	LYS
3	S	470	LYS
3	S	471	GLN
3	S	473	PHE
3	S	486	HIS
3	S	490	THR

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Mol	Chain	Res	Type
3	S	492	THR
3	S	495	LEU
3	S	528	SER
3	S	563	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	164	HIS
2	B	37	GLN
2	B	137	ASN
2	B	160	GLN
2	B	171	ASN
2	B	199	GLN
1	H	32	ASN
1	H	39	GLN
1	H	76	ASN
1	H	200	HIS
2	L	3	GLN
2	L	31	ASN
2	L	38	GLN
2	L	166	GLN
3	R	421	ASN
3	R	436	ASN
3	S	475	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides 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	0.24	0	6,6,6	0.07	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, 95th 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 ²)	Q<0.9
1	A	214/218 (98%)	0.48	10 (4%) 36 24	56, 100, 143, 179	0
1	H	210/218 (96%)	0.39	9 (4%) 40 26	31, 85, 151, 178	0
2	B	214/214 (100%)	-0.01	0 100 100	32, 63, 148, 171	0
2	L	214/214 (100%)	0.16	4 (1%) 66 47	29, 58, 134, 208	0
3	R	208/208 (100%)	0.34	9 (4%) 40 26	23, 66, 270, 353	0
3	S	208/208 (100%)	0.31	7 (3%) 48 32	41, 82, 246, 390	0
All	All	1268/1280 (99%)	0.28	39 (3%) 51 35	23, 77, 172, 390	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	R	433	ILE	12.0
3	S	433	ILE	8.7
3	S	432	ALA	3.7
2	L	210	ASN	3.5
1	A	140	CYS	3.4
3	R	432	ALA	3.1
3	R	414	LEU	3.1
3	R	430	PRO	3.1
3	R	438	TYR	3.0
1	A	94	LYS	2.9
3	R	385	PHE	2.8
1	H	55	GLY	2.7
3	S	414	LEU	2.7
1	A	213	ILE	2.7
1	H	169	VAL	2.6
2	L	163	VAL	2.5
1	A	32	ASN	2.5
1	H	54	GLY	2.5
1	H	140	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	134	SER	2.4
3	R	434	ALA	2.4
2	L	156	THR	2.3
3	S	434	ALA	2.3
1	H	125	ALA	2.3
1	H	1	GLN	2.3
1	H	99	THR	2.2
3	S	410	ASN	2.2
1	A	52(A)	GLY	2.1
1	H	57	THR	2.1
3	R	581	THR	2.1
1	A	152	VAL	2.1
1	A	42	GLY	2.1
1	A	101	ASP	2.1
1	H	166	PHE	2.1
3	R	583	SER	2.1
2	L	209	PHE	2.1
3	S	411	LEU	2.0
1	A	56	SER	2.0
3	S	428	ILE	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 oligosaccharides 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, 95th 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	B	301	5/5	0.79	0.12	115,115,116,116	0

6.5 Other polymers [i](#)

There are no such residues in this entry.