



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 19, 2023 – 09:55 PM JST

PDB ID : 7C01  
Title : Molecular basis for a potent human neutralizing antibody targeting SARS-CoV-2 RBD  
Authors : Shi, R.; Qi, J.; Wang, Q.; Gao, F.G.; Yan, J.  
Deposited on : 2020-04-29  
Resolution : 2.88 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

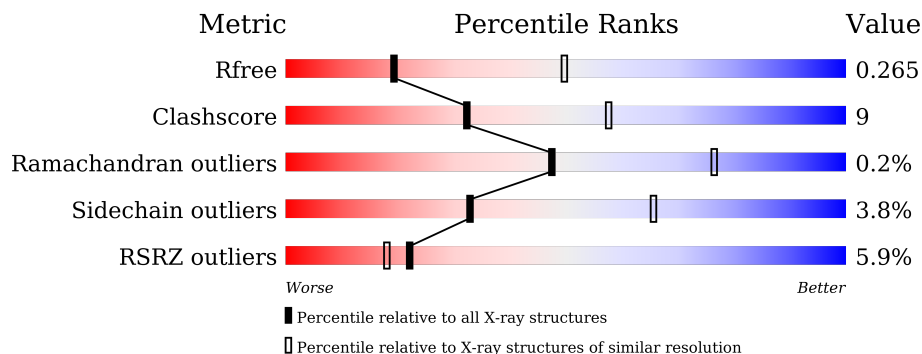
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.88 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	2691 (2.90-2.86)
Clashscore	141614	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)
RSRZ outliers	127900	2629 (2.90-2.86)

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  $\leq 5\%$ . 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	229	
1	B	229	
2	C	233	
2	H	233	
3	D	217	
3	L	217	

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 9670 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 Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	195	1543	989	257	289	8	0	0	0
1	B	195	1543	989	257	289	8	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	542	HIS	-	expression tag	UNP P0DTC2
A	543	HIS	-	expression tag	UNP P0DTC2
A	544	HIS	-	expression tag	UNP P0DTC2
A	545	HIS	-	expression tag	UNP P0DTC2
A	546	HIS	-	expression tag	UNP P0DTC2
A	547	HIS	-	expression tag	UNP P0DTC2
B	542	HIS	-	expression tag	UNP P0DTC2
B	543	HIS	-	expression tag	UNP P0DTC2
B	544	HIS	-	expression tag	UNP P0DTC2
B	545	HIS	-	expression tag	UNP P0DTC2
B	546	HIS	-	expression tag	UNP P0DTC2
B	547	HIS	-	expression tag	UNP P0DTC2

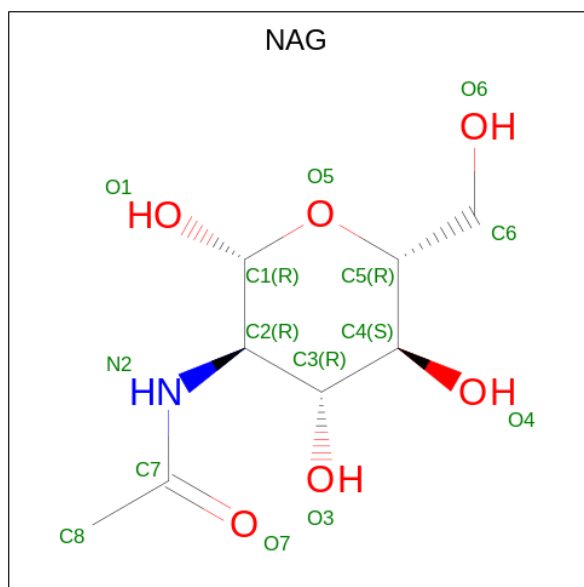
- Molecule 2 is a protein called CB6 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	218	1624	1025	270	321	8	0	0	0
2	C	218	1624	1025	270	321	8	0	0	0

- Molecule 3 is a protein called CB6 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	215	Total 1654	C 1035	N 276	O 338	S 5	0	0	0
3	D	215	Total 1654	C 1035	N 276	O 338	S 5	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

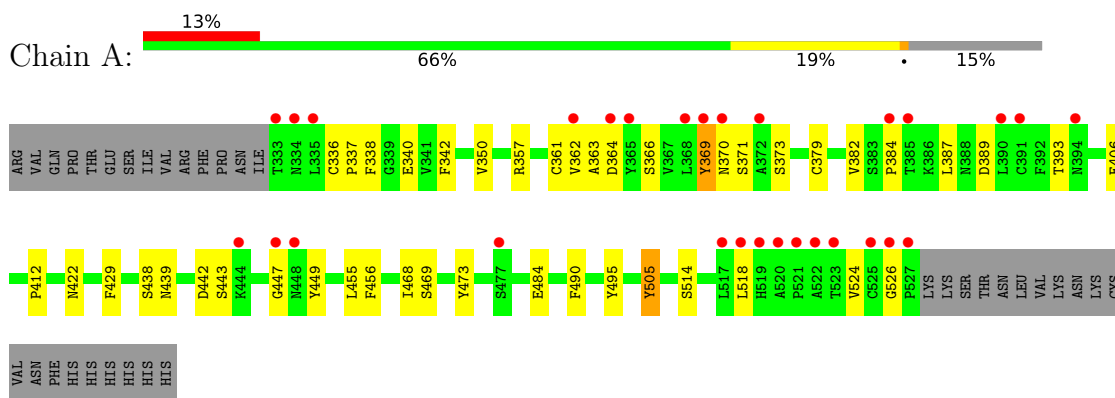


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	Total 14	C 8	N 1	O 5	0	0
4	B	1	Total 14	C 8	N 1	O 5	0	0

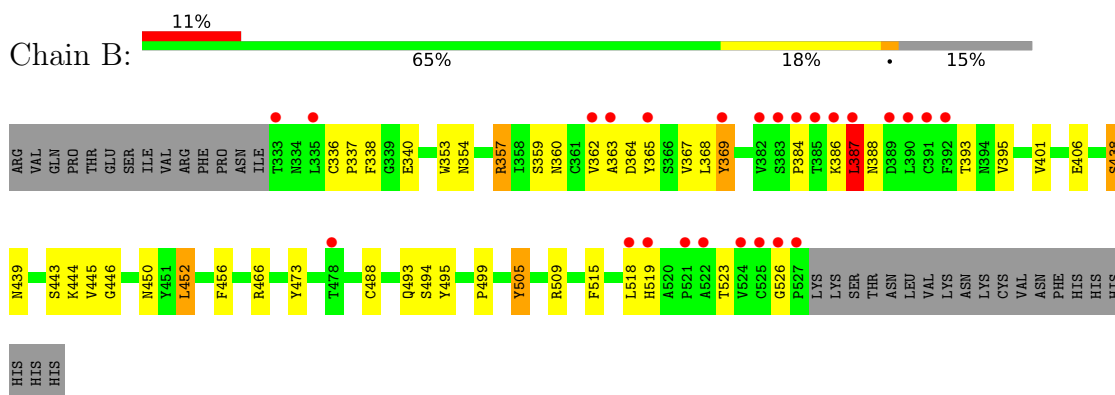
### 3 Residue-property plots [i](#)

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.

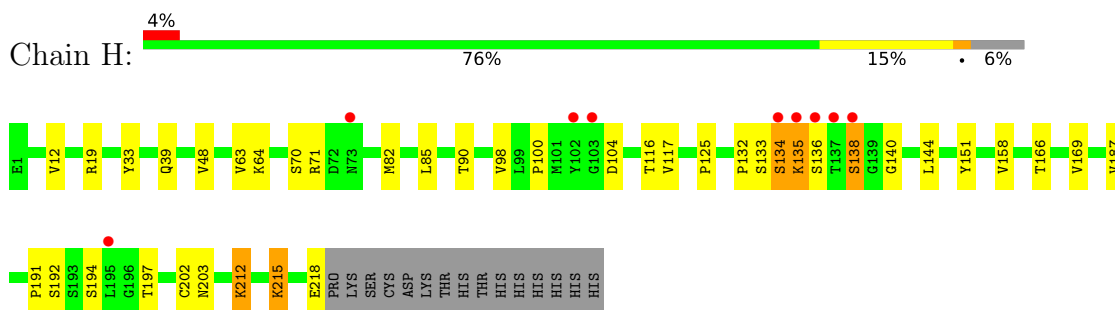
- Molecule 1: Spike protein S1



- Molecule 1: Spike protein S1



- Molecule 2: CB6 heavy chain



- Molecule 2: CB6 heavy chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.40Å 106.73Å 170.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.83 – 2.88 34.83 – 2.88	Depositor EDS
% Data completeness (in resolution range)	99.8 (34.83-2.88) 99.8 (34.83-2.88)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.54 (at 2.90Å)	Xtrriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, $R_{free}$	0.218 , 0.265 0.218 , 0.265	Depositor DCC
$R_{free}$ test set	1790 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	63.5	Xtrriage
Anisotropy	0.299	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 34.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	9670	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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	A	0.29	0/1587	0.48	0/2161
1	B	0.30	0/1587	0.53	2/2161 (0.1%)
2	C	0.30	0/1662	0.51	0/2265
2	H	0.28	0/1662	0.55	0/2265
3	D	0.30	0/1690	0.54	0/2295
3	L	0.26	0/1690	0.48	0/2295
All	All	0.29	0/9878	0.52	2/13442 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	H	0	1
3	D	0	1
3	L	0	1
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	387	LEU	CA-CB-CG	-5.85	101.84	115.30
1	B	357	ARG	NE-CZ-NH2	-5.71	117.44	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
3	D	29	ILE	Peptide
2	H	133	SER	Peptide
3	L	29	ILE	Peptide

## 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	1543	0	1459	33	0
1	B	1543	0	1459	30	1
2	C	1624	0	1588	32	0
2	H	1624	0	1588	23	0
3	D	1654	0	1609	30	1
3	L	1654	0	1609	33	0
4	A	14	0	13	1	0
4	B	14	0	13	0	0
All	All	9670	0	9338	167	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 9.

All (167) 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:A:384:PRO:HA	1:A:387:LEU:HD23	1.53	0.88
1:B:386:LYS:O	1:B:388:ASN:N	2.10	0.84
3:L:7:SER:HB2	3:L:24:ARG:HH22	1.42	0.83
3:D:40:PRO:HG2	3:D:167:GLU:HG2	1.59	0.82
2:C:30:SER:CB	2:C:73:ASN:HD22	1.92	0.82
1:B:337:PRO:HB2	1:B:340:GLU:HG3	1.60	0.81
3:L:187:ASP:HA	3:L:190:LYS:HE2	1.62	0.81
1:A:337:PRO:HB2	1:A:340:GLU:HG3	1.66	0.77
2:C:192:SER:HA	2:C:195:LEU:HD13	1.65	0.76
3:D:157:GLN:OE1	3:D:160:ASN:ND2	2.18	0.76
2:C:96:ALA:HB3	2:C:106:LEU:HD23	1.67	0.75
3:D:153:ASP:OD2	3:D:191:HIS:HB3	1.86	0.74
2:C:30:SER:HB3	2:C:73:ASN:HD22	1.52	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:48:VAL:HG23	2:H:63:VAL:HG21	1.71	0.73
1:B:362:VAL:HG13	1:B:526:GLY:HA2	1.72	0.71
3:L:18:ARG:O	1:B:450:ASN:ND2	2.24	0.71
1:A:384:PRO:HA	1:A:387:LEU:CD2	2.21	0.71
2:C:30:SER:HB2	2:C:73:ASN:HD22	1.60	0.67
2:C:30:SER:HB3	2:C:73:ASN:ND2	2.10	0.67
2:H:132:PRO:HG3	2:H:144:LEU:HB3	1.79	0.65
2:H:132:PRO:HD2	2:H:218:GLU:HB2	1.77	0.65
1:B:353:TRP:O	1:B:466:ARG:NH2	2.29	0.65
3:D:37:GLN:HB2	3:D:47:LEU:HD11	1.80	0.64
3:L:115:PRO:HB3	3:L:141:PHE:HB3	1.81	0.62
2:C:171:THR:HG23	2:C:184:LEU:HD21	1.81	0.62
1:A:495:TYR:O	1:A:505:TYR:OH	2.16	0.62
3:L:83:PHE:HB3	3:L:108:ILE:HG12	1.81	0.61
2:H:90:THR:HG23	2:H:116:THR:HA	1.81	0.61
2:H:134:SER:HB2	2:H:135:LYS:HD2	1.81	0.61
1:A:439:ASN:O	1:A:443:SER:OG	2.14	0.60
2:C:11:LEU:HB2	2:C:153:PRO:HG3	1.84	0.60
2:C:27:PHE:O	2:C:76:ASN:ND2	2.28	0.60
2:C:136:SER:HA	3:D:118:PHE:CD2	2.36	0.60
1:B:365:TYR:HD1	1:B:388:ASN:HB2	1.67	0.59
1:B:363:ALA:O	1:B:526:GLY:HA3	2.02	0.59
2:H:215:LYS:HE2	3:L:125:GLU:OE2	2.03	0.59
2:C:125:PRO:HB3	2:C:151:TYR:HB3	1.85	0.58
3:L:8:PRO:HB3	1:B:446:GLY:HA3	1.86	0.58
3:L:79:GLN:HG3	3:L:80:PRO:HD2	1.85	0.58
2:H:33:TYR:HB2	2:H:98:VAL:HB	1.86	0.58
2:H:104:ASP:H	3:L:91:SER:HB2	1.69	0.57
3:D:169:ASP:HB3	3:D:172:ASP:OD2	2.03	0.57
1:A:371:SER:OG	1:A:373:SER:OG	2.21	0.57
1:B:359:SER:HB3	1:B:360:ASN:ND2	2.20	0.56
3:D:163:GLU:HB2	3:D:177:LEU:HD21	1.87	0.56
3:D:152:VAL:HG12	3:D:157:GLN:HG2	1.87	0.56
1:B:406:GLU:OE1	1:B:495:TYR:OH	2.19	0.56
2:H:125:PRO:HB3	2:H:151:TYR:HB3	1.87	0.56
3:L:108:ILE:O	3:L:168:GLN:NE2	2.39	0.55
3:L:11:LEU:HD21	3:L:19:VAL:HG13	1.89	0.55
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.89	0.55
3:D:115:PRO:HB3	3:D:141:PHE:HB3	1.89	0.54
2:C:179:SER:HB3	2:C:181:LEU:HD12	1.88	0.54
3:D:21:ILE:HD13	3:D:104:THR:OG1	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:63:SER:OG	3:D:74:THR:OG1	2.25	0.54
1:A:484:GLU:OE2	1:A:490:PHE:HB2	2.08	0.54
1:A:362:VAL:HB	1:A:526:GLY:HA2	1.88	0.53
3:L:18:ARG:HH22	1:B:452:LEU:HD11	1.74	0.53
2:H:166:THR:O	2:H:169:VAL:HG12	2.08	0.53
1:B:495:TYR:O	1:B:505:TYR:OH	2.20	0.53
2:H:140:GLY:O	2:H:192:SER:N	2.37	0.52
1:A:350:VAL:HG22	1:A:422:ASN:HB3	1.91	0.52
1:A:468:ILE:HG13	1:A:468:ILE:O	2.10	0.52
1:B:493:GLN:HE21	1:B:494:SER:H	1.58	0.52
2:H:136:SER:O	2:H:138:SER:N	2.39	0.52
1:A:384:PRO:CA	1:A:387:LEU:HD23	2.33	0.52
2:C:12:VAL:HG11	2:C:85:LEU:HD13	1.92	0.52
1:B:359:SER:HB3	1:B:360:ASN:HD22	1.74	0.52
1:A:369:TYR:CE1	1:A:384:PRO:HB2	2.45	0.52
1:A:393:THR:HG21	1:A:518:LEU:HD12	1.92	0.52
3:L:45:LYS:HD2	3:L:46:LEU:N	2.24	0.52
1:B:445:VAL:HG22	1:B:499:PRO:HG3	1.92	0.52
2:C:132:PRO:HG3	2:C:144:LEU:HB3	1.92	0.52
2:C:104:ASP:H	3:D:91:SER:HB2	1.74	0.51
1:B:439:ASN:O	1:B:443:SER:HB2	2.11	0.51
2:C:136:SER:HA	3:D:118:PHE:HD2	1.74	0.51
1:A:364:ASP:OD1	1:A:366:SER:OG	2.28	0.51
1:A:389:ASP:OD2	1:A:389:ASP:N	2.39	0.50
3:D:160:ASN:OD1	3:D:160:ASN:N	2.45	0.50
1:B:395:VAL:HG22	1:B:515:PHE:HD1	1.77	0.50
3:L:165:VAL:HG22	3:L:177:LEU:HD12	1.94	0.50
3:L:7:SER:HB2	3:L:24:ARG:NH2	2.21	0.49
1:A:379:CYS:HB3	1:A:382:VAL:HG13	1.95	0.49
2:C:194:SER:OG	2:C:200:TYR:OH	2.31	0.49
1:A:379:CYS:SG	1:A:384:PRO:HB3	2.53	0.48
1:A:338:PHE:HE2	1:A:363:ALA:HB1	1.78	0.48
3:D:165:VAL:HG22	3:D:177:LEU:HG	1.96	0.48
3:D:152:VAL:O	3:D:155:ALA:HB3	2.14	0.48
1:B:369:TYR:CE2	1:B:384:PRO:HB2	2.49	0.48
2:H:187:VAL:HG21	3:L:137:LEU:HD22	1.95	0.48
3:L:185:LYS:O	3:L:189:GLU:HG3	2.14	0.48
1:A:338:PHE:CE2	1:A:363:ALA:HB1	2.49	0.47
1:A:370:ASN:O	1:A:370:ASN:ND2	2.47	0.47
1:A:505:TYR:CE2	3:L:32:TYR:HE1	2.32	0.47
3:D:142:TYR:CG	3:D:143:PRO:HA	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:140:GLY:O	2:H:191:PRO:HA	2.15	0.47
2:C:98:VAL:HG22	2:C:106:LEU:HG	1.95	0.47
2:H:158:VAL:HA	2:H:203:ASN:O	2.14	0.46
3:L:168:GLN:HG3	3:L:175:TYR:CZ	2.50	0.46
3:D:39:LYS:HE3	3:D:81:GLU:O	2.14	0.46
1:A:387:LEU:HA	1:A:389:ASP:OD2	2.15	0.46
3:L:192:LYS:HE2	3:L:212:ASN:HD22	1.81	0.46
1:B:364:ASP:O	1:B:367:VAL:HG22	2.16	0.46
3:D:96:PRO:HB3	3:D:98:TYR:CE1	2.51	0.46
3:L:209:LYS:HD3	3:L:209:LYS:HA	1.79	0.46
2:C:6:GLU:OE2	2:C:110:GLY:HA3	2.16	0.46
2:C:192:SER:HA	2:C:195:LEU:CD1	2.40	0.46
1:A:447:GLY:HA3	1:A:449:TYR:CE2	2.50	0.46
2:C:190:VAL:HG21	2:C:200:TYR:CZ	2.51	0.46
1:B:338:PHE:HE2	1:B:363:ALA:HB1	1.81	0.46
1:B:456:PHE:HB3	1:B:473:TYR:CD1	2.52	0.45
3:D:177:LEU:HD23	3:D:178:SER:N	2.31	0.45
3:L:125:GLU:O	3:L:128:LYS:HB3	2.16	0.45
3:L:149:GLN:HB3	3:L:197:GLU:HB3	1.97	0.45
2:H:82:MET:HB3	2:H:85:LEU:HD21	1.98	0.45
3:D:19:VAL:HG21	3:D:78:LEU:HD22	1.98	0.45
2:H:33:TYR:CB	2:H:98:VAL:HB	2.45	0.45
2:C:120:ALA:HB3	2:C:152:PHE:CE1	2.52	0.45
3:D:189:GLU:HA	3:D:213:ARG:CZ	2.47	0.45
1:B:387:LEU:HD12	1:B:387:LEU:HA	1.76	0.45
3:L:188:TYR:O	3:L:194:TYR:OH	2.31	0.45
2:C:30:SER:CB	2:C:73:ASN:ND2	2.68	0.45
3:L:66:GLY:HA3	3:L:71:PHE:HA	1.99	0.44
1:B:368:LEU:HD23	1:B:368:LEU:HA	1.83	0.44
2:H:12:VAL:O	2:H:117:VAL:HA	2.18	0.44
2:C:192:SER:CA	2:C:195:LEU:HD13	2.40	0.44
1:A:456:PHE:HB3	1:A:473:TYR:CD1	2.52	0.44
2:H:194:SER:HA	2:H:197:THR:OG1	2.18	0.44
3:L:153:ASP:OD2	3:L:191:HIS:HB3	2.18	0.44
1:B:401:VAL:HG22	1:B:509:ARG:HG2	1.99	0.44
1:A:455:LEU:HD22	2:H:100:PRO:HB2	1.99	0.44
3:D:185:LYS:HE2	3:D:189:GLU:OE2	2.18	0.43
3:L:67:SER:HA	3:L:71:PHE:CE2	2.54	0.43
3:D:119:ILE:HD12	3:D:196:CYS:SG	2.59	0.43
3:D:149:GLN:HB3	3:D:197:GLU:HB3	1.99	0.43
3:L:24:ARG:HA	3:L:69:THR:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:14:SER:HB3	3:D:109:LYS:HG2	1.99	0.43
3:L:45:LYS:HD2	3:L:46:LEU:H	1.82	0.43
2:C:132:PRO:HD2	2:C:218:GLU:HB2	2.00	0.43
3:D:122:PRO:HD3	3:D:134:VAL:HG22	2.01	0.43
2:C:145:GLY:HA2	2:C:160:TRP:CH2	2.54	0.43
3:L:142:TYR:CG	3:L:143:PRO:HA	2.54	0.43
2:C:3:GLN:HG2	2:C:25:SER:OG	2.19	0.42
1:A:379:CYS:HB2	1:A:384:PRO:HD3	2.01	0.42
1:B:393:THR:HG21	1:B:518:LEU:HD12	2.01	0.42
3:D:63:SER:HG	3:D:74:THR:HG1	1.66	0.42
1:A:387:LEU:CA	1:A:389:ASP:OD2	2.68	0.42
1:B:336:CYS:SG	1:B:363:ALA:HB2	2.58	0.42
2:H:39:GLN:NE2	3:L:38:GLN:OE1	2.48	0.42
1:B:393:THR:O	1:B:523:THR:OG1	2.38	0.42
1:B:438:SER:O	1:B:438:SER:OG	2.36	0.42
1:A:342:PHE:HB2	4:A:601:NAG:H82	2.02	0.41
3:D:152:VAL:HG12	3:D:157:GLN:CG	2.48	0.41
1:A:412:PRO:HG3	1:A:429:PHE:HB3	2.03	0.41
1:A:438:SER:OG	1:A:442:ASP:OD2	2.30	0.41
2:H:70:SER:OG	2:H:71:ARG:N	2.53	0.41
2:H:212:LYS:HD2	2:H:212:LYS:C	2.41	0.41
2:C:194:SER:HG	2:C:200:TYR:HH	1.63	0.41
2:C:175:VAL:HG21	3:D:162:GLN:HB3	2.03	0.41
1:A:336:CYS:SG	1:A:363:ALA:HB2	2.61	0.41
1:A:361:CYS:H	1:A:524:VAL:HG12	1.85	0.40
1:A:406:GLU:OE1	1:A:495:TYR:OH	2.26	0.40
2:C:133:SER:OG	2:C:134:SER:N	2.54	0.40
2:C:190:VAL:HG22	2:C:191:PRO:HD2	2.02	0.40
3:L:11:LEU:HD12	1:B:444:LYS:HD3	2.02	0.40
1:B:473:TYR:O	1:B:488:CYS:HA	2.22	0.40
2:C:90:THR:HG23	2:C:116:THR:HA	2.04	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)
1:B:357:ARG:NH2	3:D:153:ASP:OD1[3_544]	2.12	0.08

## 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	193/229 (84%)	186 (96%)	7 (4%)	0	100	100
1	B	193/229 (84%)	182 (94%)	10 (5%)	1 (0%)	29	59
2	C	216/233 (93%)	213 (99%)	3 (1%)	0	100	100
2	H	216/233 (93%)	205 (95%)	10 (5%)	1 (0%)	29	59
3	D	213/217 (98%)	205 (96%)	8 (4%)	0	100	100
3	L	213/217 (98%)	207 (97%)	6 (3%)	0	100	100
All	All	1244/1358 (92%)	1198 (96%)	44 (4%)	2 (0%)	47	76

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	387	LEU
2	H	134	SER

### 5.3.2 Protein sidechains [i](#)

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	168/202 (83%)	163 (97%)	5 (3%)	41	73
1	B	168/202 (83%)	162 (96%)	6 (4%)	35	67
2	C	183/198 (92%)	178 (97%)	5 (3%)	44	75
2	H	183/198 (92%)	176 (96%)	7 (4%)	33	65
3	D	190/192 (99%)	182 (96%)	8 (4%)	30	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	L	190/192 (99%)	180 (95%)	10 (5%)	22	52
All	All	1082/1184 (91%)	1041 (96%)	41 (4%)	33	65

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	357	ARG
1	A	369	TYR
1	A	469	SER
1	A	505	TYR
1	A	514	SER
2	H	19	ARG
2	H	64	LYS
2	H	135	LYS
2	H	138	SER
2	H	202	CYS
2	H	212	LYS
2	H	215	LYS
3	L	7	SER
3	L	18	ARG
3	L	33	LEU
3	L	63	SER
3	L	79	GLN
3	L	90	GLN
3	L	107	GLU
3	L	171	LYS
3	L	178	SER
3	L	209	LYS
1	B	354	ASN
1	B	369	TYR
1	B	438	SER
1	B	452	LEU
1	B	505	TYR
1	B	519	HIS
2	C	6	GLU
2	C	119	SER
2	C	138	SER
2	C	205	ASN
2	C	207	LYS
3	D	33	LEU
3	D	77	SER
3	D	79	GLN

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Mol	Chain	Res	Type
3	D	90	GLN
3	D	109	LYS
3	D	139	ASN
3	D	176	SER
3	D	178	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	498	GLN
1	B	360	ASN
2	C	73	ASN
2	C	205	ASN
2	C	210	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	A	601	1	14,14,15	0.26	0	17,19,21	0.49	0
4	NAG	B	601	1	14,14,15	0.27	0	17,19,21	0.45	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	NAG	A	601	1	-	2/6/23/26	0/1/1/1
4	NAG	B	601	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	NAG	O5-C5-C6-O6
4	B	601	NAG	O5-C5-C6-O6
4	A	601	NAG	C4-C5-C6-O6
4	B	601	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	601	NAG	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	A	195/229 (85%)	0.68	29 (14%) 2 1	34, 56, 133, 185	0
1	B	195/229 (85%)	0.62	25 (12%) 3 2	35, 58, 130, 161	0
2	C	218/233 (93%)	0.11	5 (2%) 60 59	33, 55, 85, 136	0
2	H	218/233 (93%)	0.35	9 (4%) 37 32	41, 62, 112, 212	0
3	D	215/217 (99%)	0.40	3 (1%) 75 75	36, 62, 88, 126	0
3	L	215/217 (99%)	0.14	3 (1%) 75 75	37, 55, 78, 130	0
All	All	1256/1358 (92%)	0.37	74 (5%) 22 18	33, 58, 112, 212	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	138	SER	8.0
1	A	333	THR	7.9
1	B	385	THR	6.9
2	H	136	SER	6.7
1	B	333	THR	6.6
1	A	519	HIS	6.5
2	H	137	THR	6.2
1	A	447	GLY	5.7
1	B	522	ALA	5.4
1	B	384	PRO	5.1
1	B	521	PRO	4.6
1	A	369	TYR	4.5
1	B	519	HIS	4.4
1	A	448	ASN	4.4
1	A	385	THR	4.1
1	B	369	TYR	4.1
1	A	523	THR	4.1
1	A	365	TYR	4.0
1	B	365	TYR	4.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	521	PRO	4.0
1	A	334	ASN	3.9
1	B	518	LEU	3.9
1	A	517	LEU	3.8
1	A	364	ASP	3.8
1	A	525	CYS	3.7
1	B	525	CYS	3.6
1	A	391	CYS	3.5
1	B	386	LYS	3.5
2	H	195	LEU	3.3
1	B	527	PRO	3.3
1	B	391	CYS	3.2
3	L	215	GLU	3.1
1	A	372	ALA	3.1
1	B	387	LEU	3.1
1	A	335	LEU	3.0
1	A	394	ASN	3.0
1	A	520	ALA	3.0
1	A	362	VAL	2.9
1	B	362	VAL	2.9
3	D	78	LEU	2.9
2	C	103	GLY	2.8
1	A	384	PRO	2.8
1	A	522	ALA	2.8
1	B	524	VAL	2.8
1	B	363	ALA	2.7
1	B	382	VAL	2.7
1	B	526	GLY	2.7
1	B	392	PHE	2.7
1	B	389	ASP	2.6
2	C	136	SER	2.6
1	B	390	LEU	2.4
2	H	135	LYS	2.4
1	A	370	ASN	2.4
1	A	518	LEU	2.3
2	H	102	TYR	2.3
3	D	108	ILE	2.3
3	L	83	PHE	2.3
1	A	444	LYS	2.3
2	H	73	ASN	2.3
1	A	368	LEU	2.2
1	A	390	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	35	SER	2.2
1	B	383	SER	2.2
1	B	478	THR	2.2
3	D	21	ILE	2.2
1	A	527	PRO	2.1
2	H	134	SER	2.1
3	L	214	GLY	2.1
2	H	103	GLY	2.1
1	A	477	SER	2.1
1	A	526	GLY	2.1
2	C	104	ASP	2.1
1	B	335	LEU	2.0
2	C	195	LEU	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
4	NAG	B	601	14/15	0.81	0.18	76,91,98,102	0
4	NAG	A	601	14/15	0.85	0.21	75,85,93,96	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.