



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 10:01 AM BST

PDB ID : 2DD8  
Title : Crystal Structure of SARS-CoV Spike Receptor-Binding Domain Complexed with Neutralizing Antibody  
Authors : Prabakaran, P.; Gan, J.H.; Feng, Y.; Zhu, Z.Y.; Xiao, X.D.; Ji, X.; Dimitrov, D.S.  
Deposited on : 2006-01-24  
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

---

The 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 : 2.13.1  
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) : 2.13.1



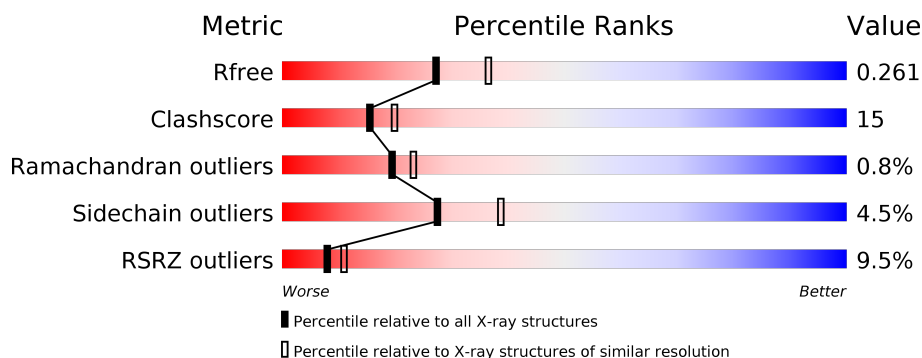
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 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	245	<div> <div>5%</div> <div> <div></div> <div>67%</div> <div>21%</div> <div>• 10%</div> </div> </div>
2	L	213	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>23%</div> <div>•</div> </div> </div>
3	S	202	<div> <div>20%</div> <div> <div></div> <div>61%</div> <div>30%</div> <div>• 5%</div> </div> </div>



## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5057 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 IGG Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	220	Total	C	N	O	S	0	0	0
			1612	1008	268	327	9			

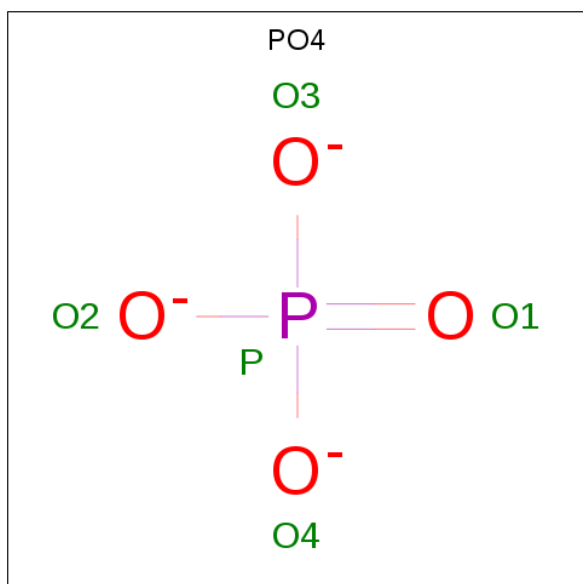
- Molecule 2 is a protein called IGG Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	212	Total	C	N	O	S	0	0	0
			1598	998	268	327	5			

- Molecule 3 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	S	192	Total	C	N	O	S	0	0	0
			1530	989	249	283	9			

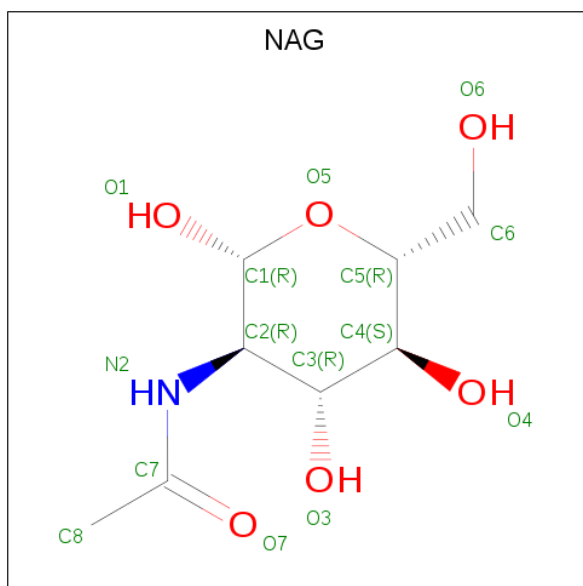
- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	O	P	0	0
			5	4	1		

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



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

- Molecule 6 is water.

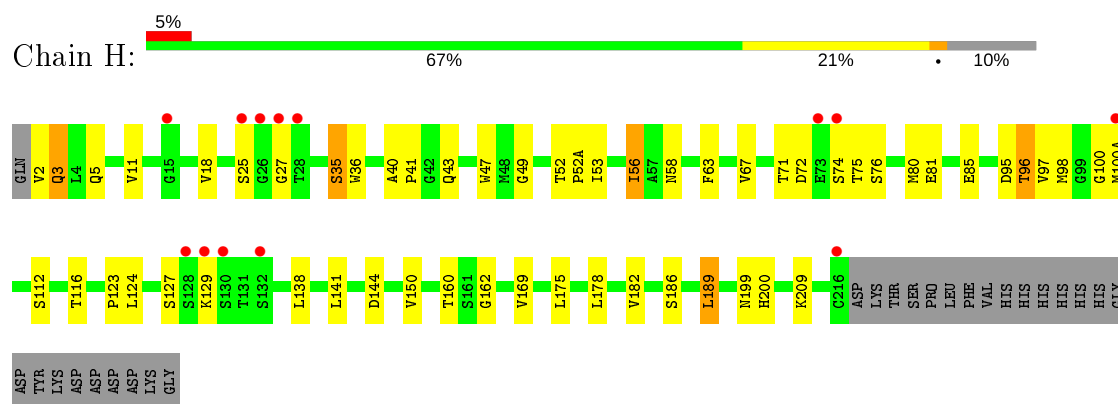
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	124	Total	O	0	0
			124	124		
6	L	110	Total	O	0	0
			110	110		
6	S	64	Total	O	0	0
			64	64		



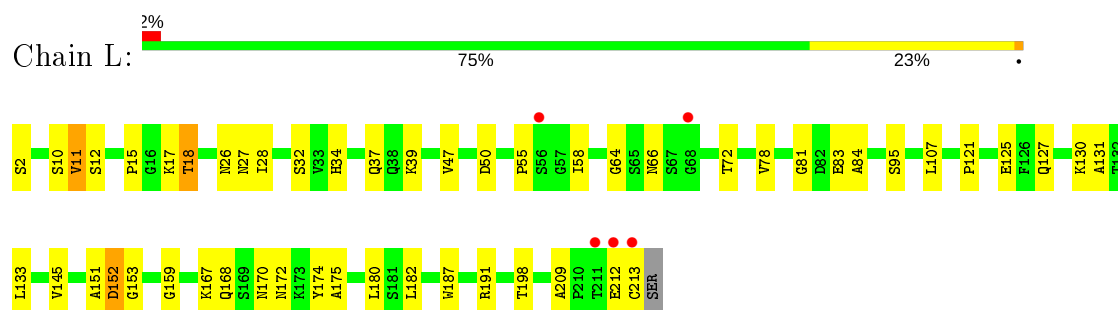
### 3 Residue-property plots [i](#)

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.

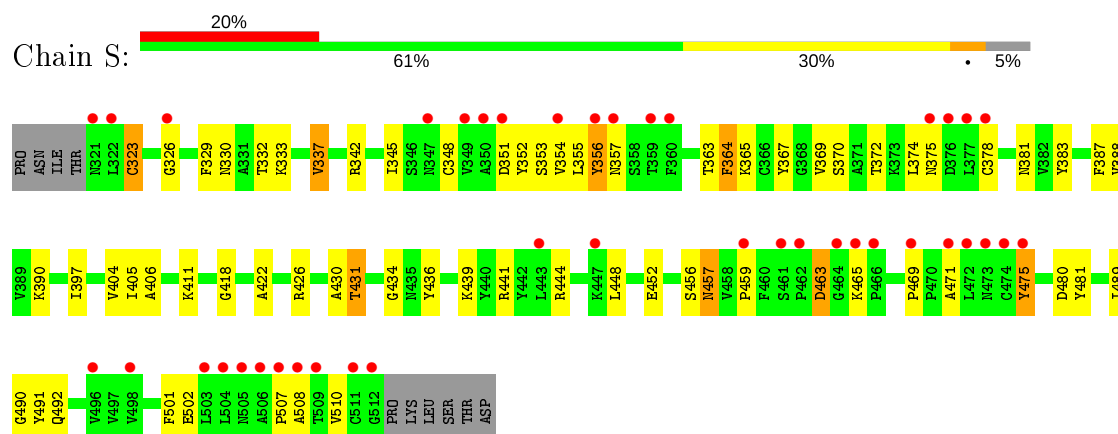
#### • Molecule 1: IGG Heavy Chain



#### • Molecule 2: IGG Light Chain



#### • Molecule 3: Spike glycoprotein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.69Å 68.61Å 80.08Å 90.00° 98.08° 90.00°	Depositor
Resolution (Å)	29.02 – 2.30 29.02 – 2.29	Depositor EDS
% Data completeness (in resolution range)	89.3 (29.02-2.30) 88.8 (29.02-2.29)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.29 (at 2.29Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.199 , 0.261 0.199 , 0.261	Depositor DCC
$R_{free}$ test set	1377 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.9	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 61.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5057	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% 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: PO4, 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	H	0.37	0/1646	0.64	0/2241
2	L	0.36	0/1639	0.63	0/2240
3	S	0.35	0/1578	0.59	0/2154
All	All	0.36	0/4863	0.62	0/6635

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	1612	0	1590	50	0
2	L	1598	0	1528	38	0
3	S	1530	0	1451	54	0
4	H	5	0	0	0	0
5	S	14	0	13	3	0
6	H	124	0	0	3	0
6	L	110	0	0	4	0
6	S	64	0	0	2	0
All	All	5057	0	4582	138	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 15.

All (138) 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:96:THR:HG22	1:H:100:GLY:H	1.28	0.98
1:H:2:VAL:O	1:H:25:SER:HB3	1.71	0.90
1:H:96:THR:HG23	1:H:98:MET:H	1.38	0.88
1:H:11:VAL:HG11	1:H:116:THR:HG21	1.57	0.87
3:S:329:PHE:HB2	5:S:1330:NAG:H82	1.62	0.80
3:S:406:ALA:O	3:S:411:LYS:HE3	1.84	0.77
3:S:469:PRO:HA	3:S:471:ALA:N	2.02	0.75
1:H:75:THR:O	1:H:75:THR:HG22	1.89	0.73
1:H:71:THR:CG2	1:H:75:THR:HA	2.19	0.72
3:S:431:THR:HG22	3:S:434:GLY:H	1.55	0.71
1:H:96:THR:HG22	1:H:100:GLY:N	2.03	0.71
3:S:352:TYR:CD2	3:S:374:LEU:HB3	2.25	0.70
1:H:96:THR:HG23	1:H:98:MET:N	2.06	0.70
2:L:131:ALA:HB3	2:L:182:LEU:HD12	1.74	0.69
1:H:36:TRP:CE2	1:H:80:MET:HB2	2.28	0.68
3:S:469:PRO:HA	3:S:471:ALA:H	1.57	0.68
3:S:342:ARG:HD3	3:S:383:TYR:HD2	1.58	0.67
1:H:40:ALA:HB3	1:H:43:GLN:HG3	1.76	0.67
3:S:426:ARG:O	3:S:430:ALA:HB3	1.97	0.65
3:S:378:CYS:HB3	3:S:508:ALA:CB	2.27	0.65
2:L:10:SER:O	2:L:11:VAL:HG23	1.97	0.65
1:H:5:GLN:NE2	1:H:25:SER:HA	2.13	0.64
2:L:121:PRO:HG3	2:L:133:LEU:HD12	1.79	0.64
3:S:390:LYS:HB2	3:S:481:TYR:CE1	2.34	0.63
3:S:356:TYR:HA	3:S:364:PHE:HE2	1.65	0.62
3:S:439:LYS:HG2	3:S:480:ASP:OD1	2.01	0.61
3:S:356:TYR:HD1	3:S:357:ASN:HD22	1.49	0.61
1:H:169:VAL:HA	6:H:563:HOH:O	2.00	0.61
1:H:123:PRO:HD3	1:H:209:LYS:HE2	1.83	0.60
1:H:11:VAL:HG21	1:H:116:THR:HG22	1.83	0.59
2:L:151:ALA:C	2:L:153:GLY:H	2.06	0.59
1:H:85:GLU:H	1:H:85:GLU:CD	2.05	0.59
3:S:355:LEU:HD12	3:S:356:TYR:N	2.18	0.58
1:H:178:LEU:HD12	1:H:178:LEU:C	2.23	0.58
1:H:71:THR:HG21	1:H:75:THR:HA	1.83	0.58
3:S:351:ASP:OD2	3:S:354:VAL:HG23	2.03	0.58
3:S:356:TYR:HE2	3:S:372:THR:HG22	1.68	0.58
3:S:352:TYR:HD2	3:S:374:LEU:HB3	1.67	0.58

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:96:THR:HG21	2:L:34:HIS:NE2	2.19	0.57
1:H:100:GLY:HA3	2:L:34:HIS:CD2	2.38	0.57
1:H:71:THR:HG22	1:H:75:THR:HA	1.87	0.57
3:S:367:TYR:O	3:S:369:VAL:HG23	2.06	0.56
3:S:356:TYR:HA	3:S:364:PHE:CE2	2.40	0.56
1:H:58:ASN:HB3	6:L:284:HOH:O	2.06	0.55
1:H:162:GLY:O	1:H:182:VAL:HA	2.06	0.55
3:S:329:PHE:HB2	5:S:1330:NAG:C8	2.34	0.55
3:S:323:CYS:SG	3:S:345:ILE:HG23	2.47	0.55
1:H:186:SER:O	1:H:189:LEU:HB2	2.07	0.54
1:H:63:PHE:HB3	1:H:67:VAL:HG23	1.88	0.54
2:L:209:ALA:O	2:L:212:GLU:HB3	2.07	0.54
2:L:131:ALA:HB3	2:L:182:LEU:CD1	2.36	0.54
1:H:35:SER:HB2	1:H:95:ASP:OD1	2.08	0.54
2:L:55:PRO:HG2	2:L:58:ILE:HG12	1.90	0.54
1:H:127:SER:HB2	1:H:129:LYS:HG3	1.89	0.54
2:L:159:GLY:O	2:L:180:LEU:HD12	2.09	0.53
1:H:199:ASN:ND2	6:H:527:HOH:O	2.41	0.53
1:H:47:TRP:CZ2	1:H:49:GLY:HA2	2.44	0.53
3:S:337:VAL:HG22	3:S:388:VAL:O	2.09	0.52
2:L:167:LYS:HG2	2:L:174:TYR:CZ	2.45	0.51
3:S:353:SER:O	3:S:357:ASN:ND2	2.44	0.51
2:L:151:ALA:O	2:L:153:GLY:N	2.42	0.51
1:H:27:GLY:O	1:H:76:SER:HB2	2.11	0.51
3:S:342:ARG:HD3	3:S:383:TYR:CD2	2.43	0.51
1:H:75:THR:O	1:H:75:THR:CG2	2.58	0.49
2:L:17:LYS:O	2:L:78:VAL:HG23	2.11	0.49
3:S:332:THR:HG22	3:S:333:LYS:HG3	1.93	0.49
3:S:378:CYS:HB3	3:S:508:ALA:HB2	1.94	0.49
2:L:170:ASN:O	2:L:172:ASN:HB2	2.13	0.48
3:S:475:TYR:N	3:S:475:TYR:CD1	2.81	0.48
2:L:39:LYS:HE3	2:L:81:GLY:O	2.13	0.48
1:H:47:TRP:CH2	1:H:49:GLY:HA2	2.49	0.48
3:S:326:GLY:HA2	5:S:1330:NAG:C8	2.44	0.48
2:L:18:THR:HG22	6:L:287:HOH:O	2.13	0.48
3:S:448:LEU:HA	3:S:452:GLU:OE1	2.14	0.48
2:L:121:PRO:HG3	2:L:133:LEU:CD1	2.42	0.48
3:S:353:SER:HA	3:S:356:TYR:HB3	1.96	0.48
1:H:5:GLN:HE21	1:H:25:SER:HA	1.80	0.47
2:L:168:GLN:OE1	2:L:175:ALA:HB2	2.14	0.47
1:H:71:THR:HG22	1:H:72:ASP:N	2.30	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:3:GLN:HA	6:H:621:HOH:O	2.15	0.47
2:L:125:GLU:HG2	2:L:130:LYS:O	2.14	0.47
2:L:133:LEU:HD12	2:L:133:LEU:N	2.29	0.47
1:H:52:THR:HG22	1:H:53:ILE:HG22	1.96	0.46
3:S:354:VAL:O	3:S:354:VAL:HG12	2.13	0.46
2:L:32:SER:OG	2:L:50:ASP:HA	2.15	0.46
3:S:463:ASP:O	3:S:465:LYS:HG2	2.15	0.46
2:L:55:PRO:HG2	2:L:58:ILE:CG1	2.45	0.46
2:L:2:SER:HA	6:L:218:HOH:O	2.16	0.46
3:S:397:ILE:O	3:S:397:ILE:HG22	2.15	0.46
2:L:212:GLU:O	2:L:213:CYS:HB3	2.15	0.46
3:S:381:ASN:HB2	3:S:502:GLU:OE1	2.15	0.46
3:S:418:GLY:HA2	3:S:501:PHE:CD2	2.51	0.45
1:H:127:SER:C	1:H:129:LYS:H	2.19	0.45
2:L:83:GLU:O	2:L:84:ALA:HB2	2.16	0.45
3:S:469:PRO:CA	3:S:471:ALA:H	2.28	0.45
3:S:337:VAL:HG13	3:S:387:PHE:CD1	2.51	0.45
1:H:150:VAL:HG22	1:H:178:LEU:HD21	1.98	0.45
1:H:144:ASP:HB3	1:H:175:LEU:HD13	1.99	0.45
2:L:151:ALA:C	2:L:153:GLY:N	2.70	0.45
1:H:63:PHE:HB3	1:H:67:VAL:CG2	2.47	0.44
3:S:431:THR:HG22	3:S:434:GLY:N	2.28	0.44
3:S:348:CYS:O	3:S:510:VAL:HA	2.18	0.44
3:S:326:GLY:O	3:S:330:ASN:HB2	2.18	0.44
3:S:441:ARG:HD2	3:S:444:ARG:HD2	2.00	0.44
1:H:11:VAL:HG11	1:H:116:THR:CG2	2.38	0.44
1:H:52(A):PRO:HB3	1:H:75:THR:HG23	2.00	0.44
2:L:167:LYS:HG2	2:L:174:TYR:CE2	2.53	0.43
2:L:145:VAL:HG23	2:L:198:THR:O	2.18	0.43
2:L:64:GLY:HA2	2:L:72:THR:O	2.18	0.43
1:H:18:VAL:O	1:H:81:GLU:HA	2.19	0.43
1:H:85:GLU:N	1:H:85:GLU:CD	2.71	0.43
3:S:436:TYR:HA	3:S:481:TYR:O	2.19	0.43
2:L:15:PRO:HD3	2:L:107:LEU:O	2.18	0.43
2:L:37:GLN:HB2	2:L:47:VAL:HG11	2.01	0.43
3:S:404:VAL:HG23	3:S:405:ILE:N	2.33	0.42
1:H:56:ILE:HG12	3:S:491:TYR:HE2	1.84	0.42
1:H:11:VAL:CG1	1:H:116:THR:HG21	2.38	0.42
1:H:41:PRO:O	1:H:43:GLN:HG2	2.19	0.42
3:S:418:GLY:HA2	3:S:501:PHE:HD2	1.84	0.42
3:S:489:ILE:HA	3:S:492:GLN:NE2	2.34	0.42

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:74:SER:O	1:H:75:THR:HB	2.20	0.42
3:S:375:ASN:HB2	6:S:270:HOH:O	2.20	0.42
3:S:363:THR:HB	3:S:422:ALA:HB3	2.01	0.42
2:L:12:SER:HB3	2:L:107:LEU:HD11	2.01	0.42
3:S:390:LYS:HG2	3:S:490:GLY:O	2.20	0.41
3:S:383:TYR:HE1	3:S:502:GLU:OE1	2.03	0.41
1:H:150:VAL:CG2	1:H:178:LEU:HD21	2.50	0.41
2:L:182:LEU:HD11	2:L:187:TRP:HB2	2.02	0.41
1:H:150:VAL:HG12	1:H:200:HIS:CD2	2.56	0.41
3:S:456:SER:O	3:S:457:ASN:HB3	2.21	0.41
2:L:182:LEU:CD1	2:L:187:TRP:HB2	2.50	0.41
6:L:258:HOH:O	3:S:365:LYS:HE3	2.21	0.41
2:L:152:ASP:OD1	2:L:191:ARG:N	2.46	0.41
2:L:159:GLY:O	2:L:180:LEU:HA	2.20	0.41
1:H:56:ILE:HD11	3:S:390:LYS:NZ	2.35	0.41
3:S:459:PRO:HG2	6:S:242:HOH:O	2.21	0.41
2:L:212:GLU:HG2	2:L:212:GLU:O	2.20	0.40
2:L:28:ILE:HG23	2:L:66:ASN:OD1	2.21	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	H	218/245 (89%)	206 (94%)	11 (5%)	1 (0%)	29	35
2	L	210/213 (99%)	197 (94%)	11 (5%)	2 (1%)	15	17
3	S	190/202 (94%)	166 (87%)	22 (12%)	2 (1%)	14	15
All	All	618/660 (94%)	569 (92%)	44 (7%)	5 (1%)	19	23

All (5) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
3	S	370	SER
1	H	3	GLN
2	L	152	ASP
3	S	507	PRO
2	L	11	VAL

### 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	185/208 (89%)	174 (94%)	11 (6%)	19	27
2	L	180/181 (99%)	175 (97%)	5 (3%)	43	60
3	S	167/177 (94%)	159 (95%)	8 (5%)	25	36
All	All	532/566 (94%)	508 (96%)	24 (4%)	27	39

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	35	SER
1	H	56	ILE
1	H	96	THR
1	H	97	VAL
1	H	100(A)	MET
1	H	112	SER
1	H	124	LEU
1	H	138	LEU
1	H	141	LEU
1	H	160	THR
1	H	189	LEU
2	L	18	THR
2	L	26	ASN
2	L	27	ASN
2	L	95	SER
2	L	127	GLN
3	S	323	CYS
3	S	337	VAL

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
3	S	356	TYR
3	S	364	PHE
3	S	431	THR
3	S	457	ASN
3	S	463	ASP
3	S	475	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	5	GLN
1	H	43	GLN
1	H	171	GLN
1	H	192	GLN
1	H	199	ASN
2	L	27	ASN
3	S	357	ASN
3	S	381	ASN
3	S	457	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	PO4	H	501	-	4,4,4	1.61	0	6,6,6	0.43	0
5	NAG	S	1330	3	14,14,15	0.51	0	17,19,21	0.74	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	S	1330	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	S	1330	NAG	C2-N2-C7	-2.22	119.74	122.90

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	S	1330	NAG	C8-C7-N2-C2
5	S	1330	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	S	1330	NAG	3	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.



## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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	220/245 (89%)	0.18	13 (5%) 22 28	24, 40, 77, 100	0
2	L	212/213 (99%)	-0.03	5 (2%) 59 66	22, 41, 69, 101	0
3	S	192/202 (95%)	1.08	41 (21%) 0 1	31, 60, 97, 100	0
All	All	624/660 (94%)	0.38	59 (9%) 8 11	22, 44, 91, 101	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	213	CYS	9.1
3	S	356	TYR	8.6
3	S	508	ALA	8.1
3	S	507	PRO	7.6
1	H	216	CYS	6.7
3	S	322	LEU	6.4
3	S	504	LEU	5.8
3	S	465	LYS	5.4
3	S	472	LEU	5.3
3	S	506	ALA	4.8
3	S	509	THR	4.7
3	S	354	VAL	4.7
3	S	377	LEU	4.5
3	S	378	CYS	4.4
1	H	128	SER	4.3
1	H	73	GLU	4.2
3	S	375	ASN	4.1
1	H	132	SER	3.9
3	S	350	ALA	3.8
3	S	464	GLY	3.7
3	S	461	SER	3.7
3	S	321	ASN	3.5
3	S	505	ASN	3.5

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	L	56	SER	3.5
3	S	474	CYS	3.5
3	S	376	ASP	3.4
3	S	357	ASN	3.4
3	S	349	VAL	3.3
3	S	512	GLY	3.3
3	S	471	ALA	3.1
3	S	475	TYR	3.0
2	L	211	THR	2.9
3	S	466	PRO	2.9
2	L	212	GLU	2.8
3	S	359	THR	2.8
3	S	496	VAL	2.8
3	S	498	VAL	2.7
3	S	443	LEU	2.6
1	H	130	SER	2.6
3	S	511	CYS	2.6
2	L	68	GLY	2.6
3	S	347	ASN	2.5
3	S	447	LYS	2.5
1	H	100(A)	MET	2.4
1	H	129	LYS	2.4
3	S	459	PRO	2.4
3	S	351	ASP	2.4
1	H	27	GLY	2.4
1	H	25	SER	2.3
1	H	15	GLY	2.3
3	S	469	PRO	2.3
3	S	473	ASN	2.3
1	H	28	THR	2.2
3	S	462	PRO	2.2
1	H	74	SER	2.2
3	S	326	GLY	2.2
3	S	503	LEU	2.1
3	S	360	PHE	2.0
1	H	26	GLY	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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( $\text{\AA}^2$ )	Q<0.9
5	NAG	S	1330	14/15	0.71	0.29	86,91,98,98	0
4	PO4	H	501	5/5	0.97	0.11	67,67,72,74	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.