



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 10:17 PM EDT

PDB ID : 8E1G  
Title : SARS-CoV-2 RBD in complex with Omicron-neutralizing antibody 2A10  
Authors : Wasserman, H.; Hastie, K.M.; Buck, T.K.; Sapphire, E.O.  
Deposited on : 2022-08-10  
Resolution : 2.57 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)  
Xtrriage (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

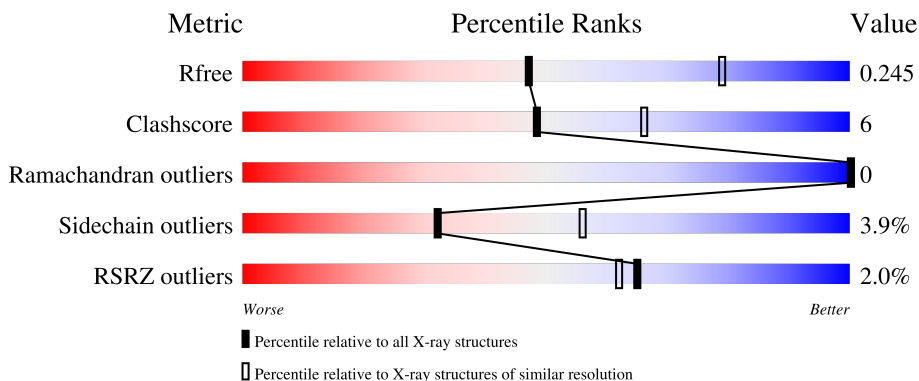
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.57 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.



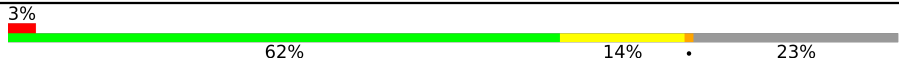
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

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	H	224	 88% 8% 5%
1	V	224	 75% 15% 7%
2	L	214	 84% 14%
2	T	214	 77% 21%
3	A	281	 76% 12% 11%

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Mol	Chain	Length	Quality of chain
3	B	281	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a small red segment (3%), a large green segment (62%), a yellow segment (14%), and a grey segment (23%).</p>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10185 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 2A10 Fab, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	H	213	Total 1608	C 1016	N 273	O 312	S 7	0	0	0
1	V	208	Total 1575	C 996	N 267	O 305	S 7	0	0	0

- Molecule 2 is a protein called 2A10 Fab, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	213	Total 1638	C 1023	N 272	O 337	S 6	0	0	0
2	T	213	Total 1638	C 1023	N 272	O 337	S 6	0	0	0

- Molecule 3 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	250	Total 1974	C 1263	N 332	O 369	S 10	0	0	0
3	B	217	Total 1724	C 1108	N 290	O 318	S 8	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

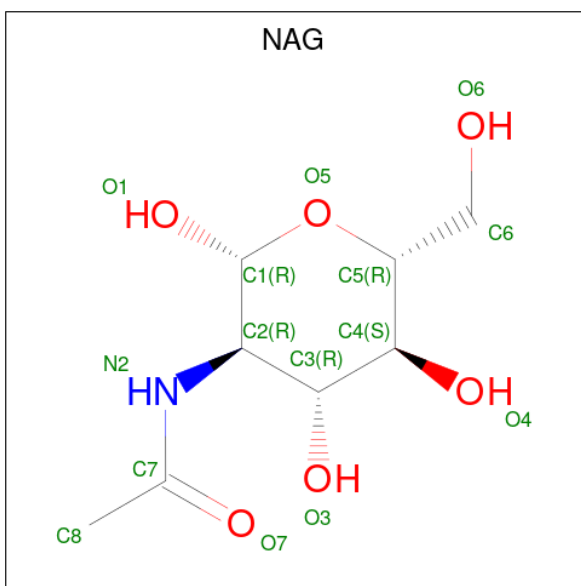
Chain	Residue	Modelled	Actual	Comment	Reference
A	592	LEU	-	expression tag	UNP P0DTC2
A	593	GLU	-	expression tag	UNP P0DTC2
A	594	VAL	-	expression tag	UNP P0DTC2
A	595	ASP	-	expression tag	UNP P0DTC2
A	596	ASP	-	expression tag	UNP P0DTC2
A	597	ASP	-	expression tag	UNP P0DTC2
A	598	ASP	-	expression tag	UNP P0DTC2
A	599	LYS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	592	LEU	-	expression tag	UNP P0DTC2
B	593	GLU	-	expression tag	UNP P0DTC2
B	594	VAL	-	expression tag	UNP P0DTC2
B	595	ASP	-	expression tag	UNP P0DTC2
B	596	ASP	-	expression tag	UNP P0DTC2
B	597	ASP	-	expression tag	UNP P0DTC2
B	598	ASP	-	expression tag	UNP P0DTC2
B	599	LYS	-	expression tag	UNP P0DTC2

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




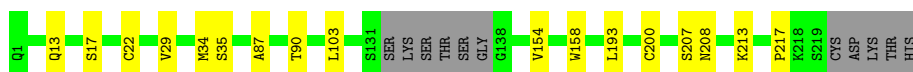
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	14	8	1	5	0	0
4	B	1	14	8	1	5	0	0

### 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.

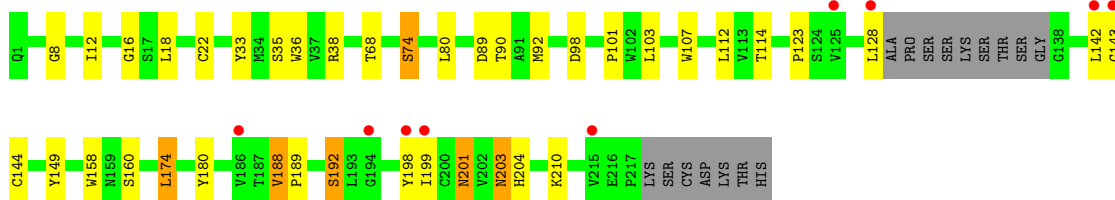
- Molecule 1: 2A10 Fab, heavy chain

Chain H: 




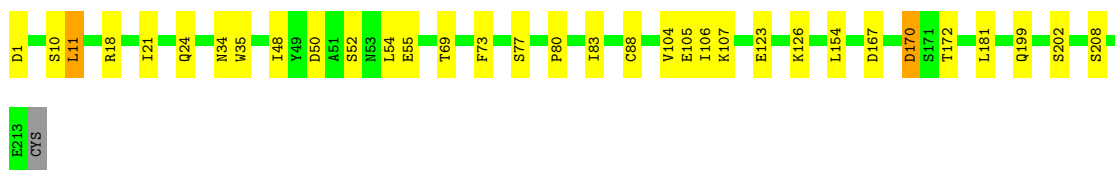
- Molecule 1: 2A10 Fab, heavy chain

Chain V: 




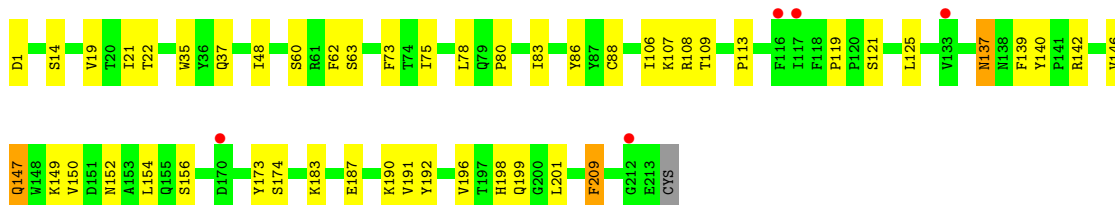
- Molecule 2: 2A10 Fab, light chain

Chain L: 

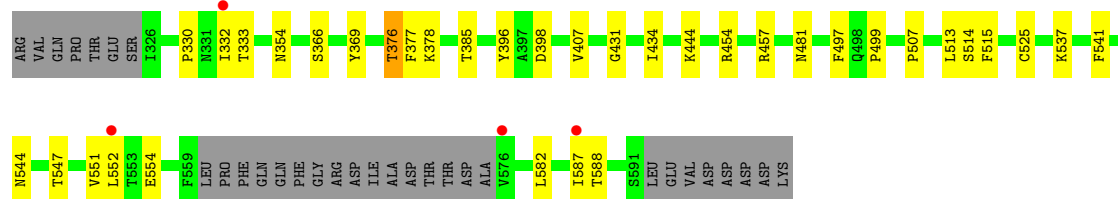
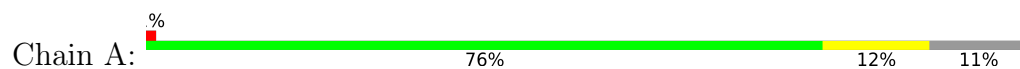


- Molecule 2: 2A10 Fab, light chain

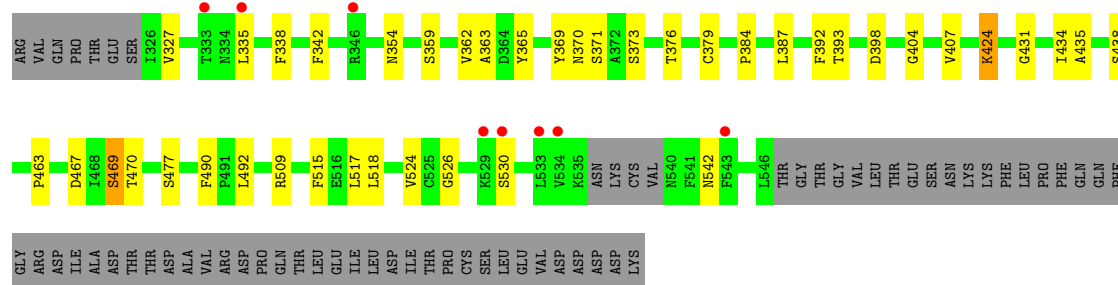
Chain T: 



- Molecule 3: Spike protein S1



- Molecule 3: Spike protein S1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.90Å 117.94Å 150.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	9.99 – 2.57 92.79 – 2.57	Depositor EDS
% Data completeness (in resolution range)	99.4 (9.99-2.57) 99.4 (92.79-2.57)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.39 (at 2.58Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.196 , 0.244 0.201 , 0.245	Depositor DCC
$R_{free}$ test set	2864 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	57.0	Xtrriage
Anisotropy	0.449	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 37.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10185	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% 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: 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	0.48	0/1647	0.66	0/2243
1	V	0.46	0/1613	0.66	0/2197
2	L	0.48	0/1673	0.63	0/2274
2	T	0.42	0/1673	0.62	0/2274
3	A	0.48	0/2024	0.60	0/2751
3	B	0.46	0/1771	0.59	0/2407
All	All	0.46	0/10401	0.63	0/14146

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	1608	0	1576	9	0
1	V	1575	0	1541	23	0
2	L	1638	0	1581	16	0
2	T	1638	0	1581	31	0
3	A	1974	0	1907	22	0
3	B	1724	0	1651	25	0
4	A	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	14	0	13	2	0
All	All	10185	0	9863	121	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 6.

All (121) 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)
2:L:11:LEU:HD22	2:L:104:VAL:HG22	1.73	0.70
1:V:160:SER:H	1:V:201:ASN:HD21	1.42	0.67
3:A:332:ILE:HD11	3:A:525:CYS:HB2	1.80	0.63
3:A:378:LYS:HG2	3:B:379:CYS:O	1.99	0.62
2:T:198:HIS:CG	2:T:199:GLN:H	2.21	0.59
2:T:108:ARG:NH1	2:T:109:THR:O	2.31	0.57
1:V:123:PRO:HB3	1:V:149:TYR:HB3	1.86	0.57
2:T:147:GLN:HG2	2:T:154:LEU:HD11	1.87	0.57
3:A:330:PRO:HD3	3:A:544:ASN:OD1	2.05	0.57
2:T:113:PRO:HD3	2:T:198:HIS:ND1	2.21	0.56
2:T:198:HIS:CG	2:T:199:GLN:N	2.75	0.55
2:T:119:PRO:HB3	2:T:209:PHE:CE1	2.42	0.54
2:T:142:ARG:HD3	2:T:173:TYR:CD1	2.43	0.54
2:T:198:HIS:CD2	2:T:199:GLN:H	2.25	0.54
2:T:62:PHE:CE1	2:T:75:ILE:HG12	2.43	0.54
2:T:146:VAL:HG22	2:T:196:VAL:HG22	1.89	0.53
2:L:35:TRP:CE2	2:L:73:PHE:HB2	2.43	0.53
3:B:424:LYS:HB3	3:B:463:PRO:HA	1.91	0.53
2:L:154:LEU:H	2:L:154:LEU:HD12	1.74	0.52
1:H:87:ALA:O	1:H:90:THR:HG22	2.09	0.52
3:A:551:VAL:HG13	3:A:588:THR:HB	1.93	0.51
1:V:174:LEU:HG	1:V:180:TYR:CE1	2.45	0.51
3:A:444:LYS:O	3:A:499:PRO:HD3	2.11	0.50
3:A:541:PHE:CZ	3:A:587:ILE:HD13	2.47	0.49
1:V:8:GLY:O	1:V:18:LEU:HD11	2.12	0.49
1:H:13:GLN:H	1:H:13:GLN:CD	2.16	0.49
1:H:29:VAL:HG13	1:H:34:MET:HG3	1.95	0.48
2:L:80:PRO:O	2:L:83:ILE:HG13	2.13	0.48
1:V:38:ARG:NH1	1:V:89:ASP:OD2	2.40	0.48
2:T:139:PHE:HE1	2:T:174:SER:HA	1.78	0.48
2:T:35:TRP:HB2	2:T:48:ILE:HB	1.96	0.48
1:V:188:VAL:HG21	1:V:198:TYR:CE2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:404:GLY:O	3:B:407:VAL:HG23	2.12	0.48
1:V:188:VAL:HG21	1:V:198:TYR:CZ	2.49	0.48
2:T:80:PRO:O	2:T:83:ILE:HG12	2.13	0.48
1:V:160:SER:N	1:V:201:ASN:HD21	2.10	0.47
1:V:128:LEU:HD12	1:V:144:CYS:N	2.29	0.47
2:T:108:ARG:HG2	2:T:109:THR:N	2.29	0.47
3:A:369:TYR:HB2	3:B:369:TYR:OH	2.15	0.47
1:H:17:SER:HB2	1:V:74:SER:HB2	1.95	0.47
2:T:108:ARG:HG2	2:T:109:THR:H	1.79	0.47
3:A:366:SER:HA	3:A:369:TYR:CZ	2.49	0.47
1:V:189:PRO:O	1:V:192:SER:OG	2.33	0.47
3:B:467:ASP:OD1	3:B:469:SER:HB3	2.14	0.47
3:B:393:THR:HG21	3:B:518:LEU:HB2	1.96	0.47
1:H:213:LYS:HD3	1:H:213:LYS:HA	1.70	0.46
3:A:396:TYR:HB2	3:A:514:SER:HB3	1.96	0.46
2:L:35:TRP:CZ3	2:L:88:CYS:HB3	2.51	0.46
2:L:48:ILE:HD13	2:L:54:LEU:HD12	1.98	0.46
2:T:35:TRP:CE2	2:T:73:PHE:HB2	2.50	0.46
3:B:354:ASN:O	3:B:398:ASP:HA	2.16	0.46
2:T:149:LYS:HD3	2:T:152:ASN:OD1	2.16	0.45
2:T:107:LYS:HA	2:T:140:TYR:OH	2.17	0.45
3:A:541:PHE:CD2	3:A:552:LEU:HD21	2.52	0.45
1:V:92:MET:HE2	1:V:112:LEU:HD13	1.99	0.45
3:B:338:PHE:HB3	4:B:601:NAG:H81	1.99	0.45
2:L:21:ILE:HD12	2:L:73:PHE:HD2	1.82	0.45
3:A:376:THR:HG21	3:A:407:VAL:HG11	1.98	0.45
2:L:154:LEU:HD12	2:L:154:LEU:N	2.32	0.45
3:B:371:SER:HG	3:B:373:SER:HG	1.65	0.45
3:A:354:ASN:O	3:A:398:ASP:HA	2.17	0.44
3:B:342:PHE:HB2	4:B:601:NAG:H82	1.99	0.44
2:T:150:VAL:HG13	2:T:192:TYR:CE1	2.53	0.44
3:A:330:PRO:HB2	3:A:332:ILE:HG12	1.99	0.44
2:T:150:VAL:HA	2:T:191:VAL:O	2.17	0.44
3:B:327:VAL:HG23	3:B:530:SER:HA	2.00	0.44
3:B:365:TYR:CD2	3:B:387:LEU:HB3	2.51	0.44
1:H:193:LEU:HD22	1:H:217:PRO:HG3	1.98	0.44
1:V:90:THR:HG23	1:V:114:THR:HA	1.99	0.44
3:A:537:LYS:N	3:A:551:VAL:HG23	2.33	0.44
2:T:192:TYR:HB2	2:T:209:PHE:CE2	2.54	0.43
3:B:335:LEU:HD23	3:B:362:VAL:HG13	2.00	0.43
2:T:121:SER:O	2:T:125:LEU:HD12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:190:LYS:HG2	2:T:191:VAL:N	2.33	0.43
3:A:497:PHE:CE2	3:A:507:PRO:HB3	2.54	0.43
2:L:105:GLU:HG2	2:L:106:ILE:N	2.31	0.43
3:B:517:LEU:HD12	3:B:517:LEU:HA	1.82	0.43
2:T:19:VAL:HG21	2:T:78:LEU:HD22	2.01	0.43
2:T:137:ASN:HD22	2:T:137:ASN:HA	1.64	0.43
1:H:207:SER:OG	1:H:208:ASN:N	2.52	0.43
3:B:431:GLY:HA2	3:B:515:PHE:CD2	2.54	0.43
1:V:36:TRP:CE2	1:V:80:LEU:HB2	2.53	0.43
1:V:188:VAL:HG22	1:V:189:PRO:HD2	2.00	0.42
1:V:203:ASN:HD22	1:V:204:HIS:N	2.17	0.42
1:V:203:ASN:OD1	1:V:210:LYS:HE3	2.19	0.42
3:B:438:SER:HB3	3:B:509:ARG:HG3	2.01	0.42
1:H:158:TRP:CH2	1:H:200:CYS:HB3	2.54	0.42
2:T:21:ILE:HD12	2:T:73:PHE:HD2	1.84	0.42
1:V:107:TRP:CD1	1:V:107:TRP:N	2.88	0.42
1:V:142:LEU:HD21	1:V:198:TYR:CD2	2.55	0.42
2:L:170:ASP:HB3	2:L:172:THR:OG1	2.20	0.42
3:B:359:SER:HA	3:B:524:VAL:HG22	2.01	0.42
1:V:33:TYR:HB2	1:V:98:ASP:HB2	2.02	0.42
1:V:143:GLY:HA2	1:V:158:TRP:CH2	2.55	0.42
2:T:37:GLN:HB2	2:T:86:TYR:CE2	2.54	0.42
3:A:454:ARG:HD2	3:A:457:ARG:HD2	2.02	0.42
2:T:113:PRO:HD2	2:T:201:LEU:HD21	2.00	0.42
2:L:24:GLN:HA	2:L:69:THR:O	2.20	0.41
3:A:385:THR:HG21	3:B:370:ASN:HA	2.02	0.41
3:B:490:PHE:HE2	3:B:492:LEU:HB2	1.85	0.41
2:L:167:ASP:OD2	2:L:170:ASP:N	2.41	0.41
2:T:183:LYS:O	2:T:187:GLU:HG2	2.21	0.41
3:B:376:THR:O	3:B:434:ILE:HA	2.19	0.41
3:B:392:PHE:CE1	3:B:515:PHE:HB3	2.55	0.41
2:L:50:ASP:O	2:L:52:SER:N	2.52	0.41
3:A:431:GLY:HA2	3:A:515:PHE:CD2	2.56	0.41
2:L:55:GLU:OE1	2:L:55:GLU:HA	2.21	0.41
3:B:327:VAL:HA	3:B:542:ASN:HB3	2.01	0.41
3:B:363:ALA:O	3:B:526:GLY:HA2	2.21	0.41
3:B:369:TYR:CD1	3:B:384:PRO:HB2	2.56	0.41
1:H:103:LEU:HD13	2:L:34:ASN:ND2	2.36	0.41
3:A:551:VAL:CG1	3:A:588:THR:HB	2.50	0.41
1:V:33:TYR:CZ	1:V:101:PRO:HD3	2.56	0.40
2:T:78:LEU:HG	2:T:106:ILE:HD11	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:366:SER:HA	3:A:369:TYR:CE2	2.56	0.40
3:B:435:ALA:HA	3:B:509:ARG:O	2.21	0.40
2:T:35:TRP:CH2	2:T:88:CYS:HB3	2.56	0.40
1:V:12:ILE:HD11	1:V:16:GLY:HA3	2.04	0.40
2:L:123:GLU:O	2:L:126:LYS:HB2	2.21	0.40
3:A:377:PHE:CE2	3:A:434:ILE:HD13	2.57	0.40
3:A:431:GLY:HA3	3:A:513:LEU:O	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	209/224 (93%)	199 (95%)	10 (5%)	0	100	100
1	V	204/224 (91%)	198 (97%)	6 (3%)	0	100	100
2	L	211/214 (99%)	202 (96%)	9 (4%)	0	100	100
2	T	211/214 (99%)	201 (95%)	10 (5%)	0	100	100
3	A	246/281 (88%)	234 (95%)	12 (5%)	0	100	100
3	B	213/281 (76%)	202 (95%)	11 (5%)	0	100	100
All	All	1294/1438 (90%)	1236 (96%)	58 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	H	180/190 (95%)	177 (98%)	3 (2%)	60	79
1	V	176/190 (93%)	165 (94%)	11 (6%)	18	35
2	L	188/189 (100%)	177 (94%)	11 (6%)	19	37
2	T	188/189 (100%)	179 (95%)	9 (5%)	25	47
3	A	220/248 (89%)	214 (97%)	6 (3%)	44	68
3	B	189/248 (76%)	185 (98%)	4 (2%)	53	75
All	All	1141/1254 (91%)	1097 (96%)	44 (4%)	32	56

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	22	CYS
1	H	35	SER
1	H	154	VAL
1	V	22	CYS
1	V	35	SER
1	V	68	THR
1	V	74	SER
1	V	103	LEU
1	V	174	LEU
1	V	188	VAL
1	V	192	SER
1	V	199	ILE
1	V	201	ASN
1	V	203	ASN
2	L	1	ASP
2	L	10	SER
2	L	11	LEU
2	L	18	ARG
2	L	77	SER
2	L	107	LYS
2	L	170	ASP
2	L	181	LEU
2	L	199	GLN
2	L	202	SER
2	L	208	SER
2	T	1	ASP
2	T	14	SER
2	T	22	THR

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Mol	Chain	Res	Type
2	T	60	SER
2	T	63	SER
2	T	137	ASN
2	T	147	GLN
2	T	156	SER
2	T	209	PHE
3	A	333	THR
3	A	376	THR
3	A	481	ASN
3	A	547	THR
3	A	554	GLU
3	A	582	LEU
3	B	424	LYS
3	B	469	SER
3	B	470	THR
3	B	477	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	V	13	GLN
1	V	159	ASN
1	V	175	GLN
1	V	201	ASN
1	V	203	ASN
2	T	160	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

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	B	601	3	14,14,15	0.47	0	17,19,21	0.61	1 (5%)
4	NAG	A	601	3	14,14,15	0.45	0	17,19,21	0.71	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
4	NAG	B	601	3	-	2/6/23/26	0/1/1/1
4	NAG	A	601	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	NAG	C1-O5-C5	2.23	115.21	112.19
4	B	601	NAG	C1-O5-C5	2.10	115.04	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 2 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	601	NAG	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	H	213/224 (95%)	0.18	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	40, 54, 82, 94	0
1	V	208/224 (92%)	0.39	9 (4%) <span style="border: 1px solid red; padding: 2px;">35</span> <span style="border: 1px solid red; padding: 2px;">31</span>	41, 55, 100, 114	0
2	L	213/214 (99%)	0.20	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	44, 53, 65, 85	0
2	T	213/214 (99%)	0.23	5 (2%) <span style="border: 1px solid blue; padding: 2px;">60</span> <span style="border: 1px solid blue; padding: 2px;">57</span>	46, 73, 93, 109	0
3	A	250/281 (88%)	0.24	4 (1%) <span style="border: 1px solid blue; padding: 2px;">72</span> <span style="border: 1px solid blue; padding: 2px;">69</span>	41, 58, 89, 109	0
3	B	217/281 (77%)	0.44	8 (3%) <span style="border: 1px solid red; padding: 2px;">41</span> <span style="border: 1px solid red; padding: 2px;">37</span>	44, 65, 105, 115	0
All	All	1314/1438 (91%)	0.28	26 (1%) <span style="border: 1px solid blue; padding: 2px;">65</span> <span style="border: 1px solid blue; padding: 2px;">62</span>	40, 58, 93, 115	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	V	215	VAL	4.4
3	B	534	VAL	4.3
3	B	533	LEU	4.0
3	B	333	THR	3.8
3	A	576	VAL	3.8
1	V	142	LEU	3.8
3	B	529	LYS	3.7
1	V	199	ILE	3.6
3	A	332	ILE	3.3
1	V	125	VAL	3.2
3	B	530	SER	3.1
1	V	143	GLY	3.0
3	B	543	PHE	2.9
3	B	335	LEU	2.9
1	V	198	TYR	2.8
1	V	128	LEU	2.7
2	T	212	GLY	2.6
2	T	133	VAL	2.5
3	A	552	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	T	170	ASP	2.4
2	T	117	ILE	2.3
1	V	186	VAL	2.3
3	B	346	ARG	2.2
3	A	587	ILE	2.1
1	V	194	GLY	2.0
2	T	116	PHE	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	0.84	0.14	78,85,95,95	0
4	NAG	A	601	14/15	0.87	0.15	63,76,80,83	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.