



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 01:31 PM JST

PDB ID : 7FJS  
Title : Crystal structure of T6 Fab bound to theSARS-CoV-2 RBD of B.1.351  
Authors : Wang, X.; Zhang, L.; Zhang, S.; Liang, Q.  
Deposited on : 2021-08-04  
Resolution : 2.90 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

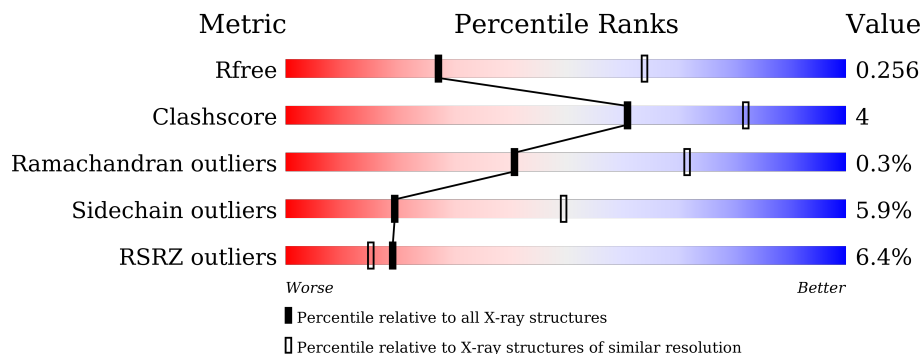
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	327	
1	L	327	
2	B	195	
2	E	195	
3	C	216	
3	H	216	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
4	NAG	E	601	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9649 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 T6 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	219	Total	C	N	O	S	0	0	0
			1706	1074	285	343	4			
1	A	219	Total	C	N	O	S	0	0	0
			1706	1074	285	343	4			

- Molecule 2 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	E	192	Total	C	N	O	S	0	0	0
			1520	975	252	285	8			
2	B	184	Total	C	N	O	S	0	0	0
			1463	942	242	272	7			

There are 6 discrepancies between the modelled and reference sequences:

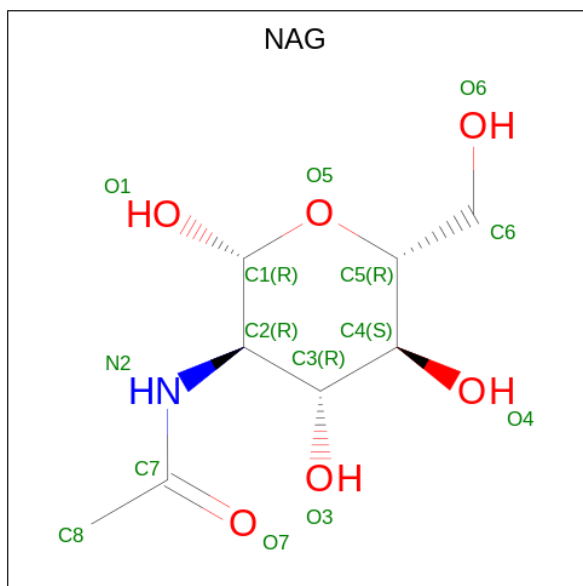
Chain	Residue	Modelled	Actual	Comment	Reference
E	417	ASN	LYS	variant	UNP P0DTC2
E	484	LYS	GLU	variant	UNP P0DTC2
E	501	TYR	ASN	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	484	LYS	GLU	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2

- Molecule 3 is a protein called T6 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	216	Total	C	N	O	S	0	0	0
			1618	1015	265	332	6			
3	C	215	Total	C	N	O	S	0	0	0
			1608	1010	264	328	6			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:

C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

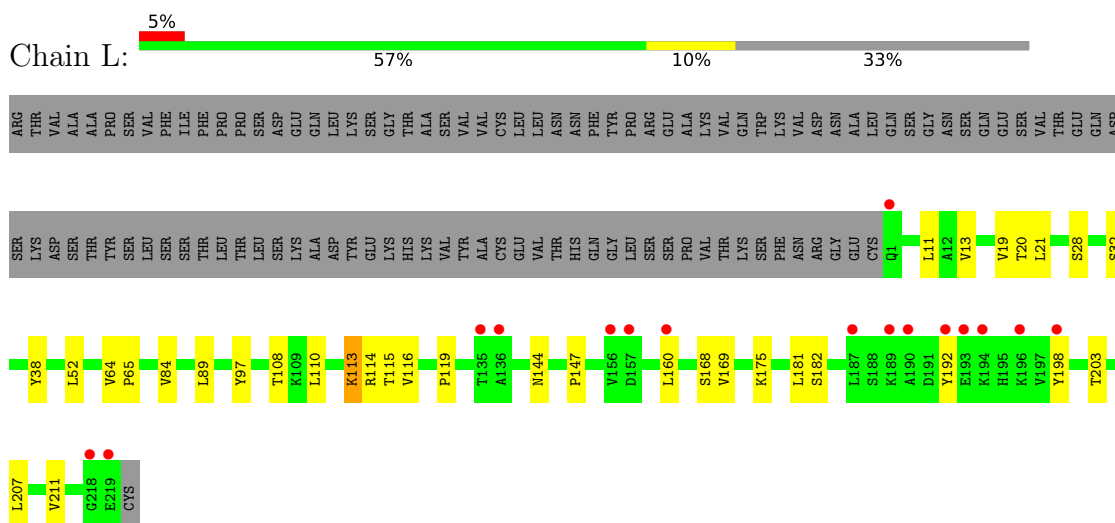


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	E	1	14	8	1	5	0	0
4	B	1	14	8	1	5	0	0

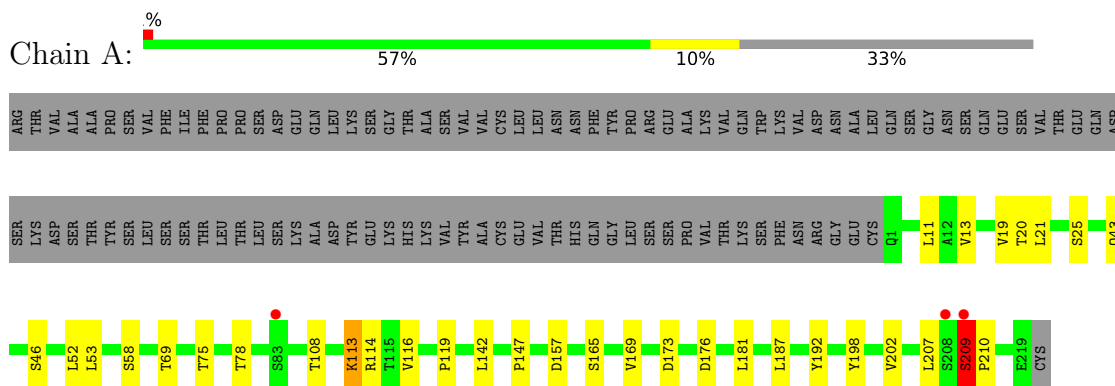
### 3 Residue-property plots [i](#)

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.

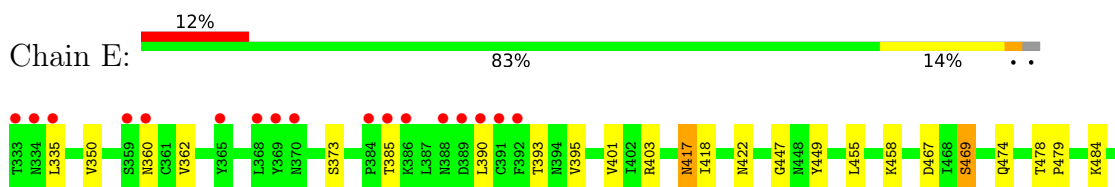
- Molecule 1: T6 light chain

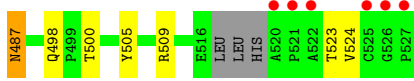


- Molecule 1: T6 light chain

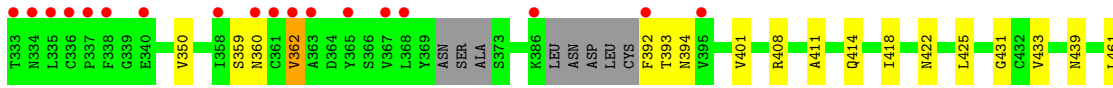
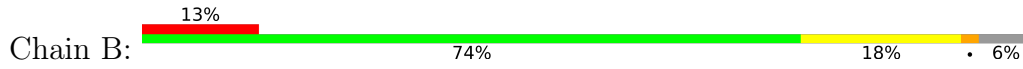


- Molecule 2: Spike protein S1

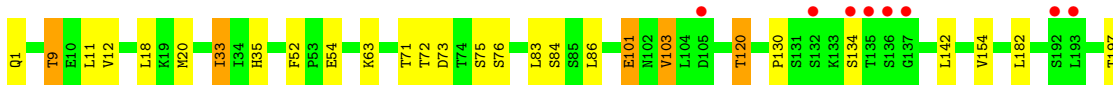
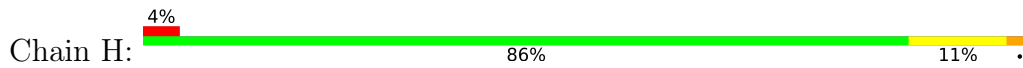




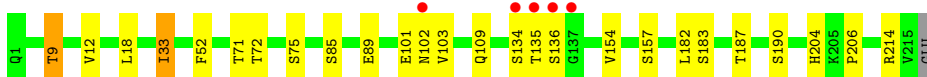
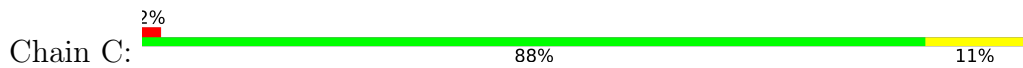
- Molecule 2: Spike protein S1



- Molecule 3: T6 heavy chain



- Molecule 3: T6 heavy chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.10Å 109.61Å 162.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.73 – 2.90 47.73 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (47.73-2.90) 99.6 (47.73-2.90)	Depositor EDS
$R_{merge}$	0.23	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.33 (at 2.91Å)	Xtrriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.217 , 0.285 0.236 , 0.256	Depositor DCC
$R_{free}$ test set	1882 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.4	Xtrriage
Anisotropy	0.326	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 35.2	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	0.88	EDS
Total number of atoms	9649	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% 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	A	0.59	0/1744	0.82	2/2368 (0.1%)
1	L	0.58	0/1744	0.79	1/2368 (0.0%)
2	B	0.57	0/1504	0.80	0/2043
2	E	0.57	0/1563	0.79	1/2127 (0.0%)
3	C	0.62	0/1646	0.84	0/2246
3	H	0.62	0/1656	0.83	0/2258
All	All	0.59	0/9857	0.81	4/13410 (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
3	H	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	210	PRO	N-CA-C	-7.12	93.58	112.10
2	E	487	ASN	CB-CA-C	5.81	122.03	110.40
1	A	157	ASP	CB-CA-C	5.27	120.95	110.40
1	L	144	ASN	CB-CA-C	5.04	120.48	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	134	SER	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	1706	0	1666	14	2
1	L	1706	0	1666	16	2
2	B	1463	0	1379	27	2
2	E	1520	0	1432	16	1
3	C	1608	0	1565	7	2
3	H	1618	0	1571	9	3
4	B	14	0	13	0	0
4	E	14	0	13	0	0
All	All	9649	0	9305	85	6

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 4.

All (85) 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:B:520:ALA:HB1	2:B:521:PRO:HD2	1.49	0.92
2:B:487:ASN:HD21	3:C:33:ILE:HD13	1.44	0.81
1:L:116:VAL:HG22	1:L:147:PRO:HD3	1.64	0.78
2:E:360:ASN:H	2:E:523:THR:HB	1.50	0.77
3:C:9:THR:HG21	3:C:206:PRO:HG3	1.67	0.75
1:L:13:VAL:HG11	1:L:19:VAL:HG22	1.67	0.74
2:B:520:ALA:HB1	2:B:521:PRO:CD	2.22	0.70
1:A:13:VAL:HG11	1:A:19:VAL:HG22	1.80	0.63
2:B:393:THR:O	2:B:394:ASN:OD1	2.17	0.62
3:H:9:THR:HG21	3:H:206:PRO:HG3	1.84	0.60
2:B:431:GLY:HA2	2:B:515:PHE:CD2	2.37	0.60
2:E:350:VAL:HG22	2:E:422:ASN:HB3	1.86	0.57
3:H:83:LEU:HB3	3:H:86:LEU:HD21	1.84	0.57
1:A:43:GLN:HB2	1:A:53:LEU:HD11	1.86	0.57
2:B:350:VAL:HG22	2:B:422:ASN:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:175:LYS:HD2	2:B:462:LYS:HE3	1.88	0.56
2:B:359:SER:HA	2:B:524:VAL:HG22	1.87	0.56
2:E:417:ASN:OD1	2:E:455:LEU:HA	2.06	0.55
1:L:207:LEU:HD13	1:L:211:VAL:HG12	1.89	0.55
1:L:21:LEU:HD22	1:L:108:THR:HG21	1.89	0.53
2:E:403:ARG:HD2	2:E:505:TYR:HA	1.89	0.53
1:A:192:TYR:HA	1:A:198:TYR:OH	2.09	0.53
3:H:12:VAL:HG22	3:H:18:LEU:HD13	1.92	0.51
2:E:395:VAL:HG23	2:E:524:VAL:HG11	1.92	0.51
1:A:116:VAL:HG22	1:A:147:PRO:HD3	1.91	0.51
1:A:11:LEU:HD11	1:A:19:VAL:HG13	1.93	0.51
2:B:433:VAL:HG22	2:B:512:VAL:HG13	1.92	0.50
2:B:392:PHE:CD1	2:B:515:PHE:HB3	2.45	0.50
2:B:425:LEU:HD21	2:B:512:VAL:HG11	1.94	0.50
2:B:360:ASN:N	2:B:523:THR:O	2.44	0.50
1:L:11:LEU:HD11	1:L:19:VAL:HG13	1.94	0.49
2:E:350:VAL:HG21	2:E:418:ILE:HG23	1.94	0.49
3:C:154:VAL:HG12	3:C:204:HIS:HB2	1.94	0.49
1:A:169:VAL:HG22	1:A:181:LEU:HD12	1.95	0.48
2:E:401:VAL:HG22	2:E:509:ARG:HG2	1.95	0.48
1:L:192:TYR:HA	1:L:198:TYR:OH	2.14	0.48
1:A:119:PRO:HD2	1:A:207:LEU:HG	1.96	0.47
1:L:19:VAL:HG23	1:L:84:VAL:HG21	1.96	0.47
2:B:431:GLY:HA2	2:B:515:PHE:CE2	2.49	0.47
1:A:113:LYS:HB2	1:A:113:LYS:HE2	1.54	0.47
2:B:486:PHE:O	2:B:487:ASN:HB2	2.15	0.47
3:H:33:ILE:HG22	3:H:52:PHE:CD1	2.51	0.46
1:A:173:ASP:HB3	1:A:176:ASP:OD1	2.15	0.46
2:B:472:ILE:HD12	2:B:484:LYS:HG3	1.96	0.46
1:A:25:SER:OG	1:A:75:THR:HA	2.15	0.46
2:E:335:LEU:HD23	2:E:362:VAL:HG13	1.97	0.46
2:B:401:VAL:HG22	2:B:509:ARG:HG2	1.97	0.46
3:C:33:ILE:HG22	3:C:52:PHE:CD1	2.50	0.46
3:C:134:SER:HA	3:C:135:THR:HA	1.45	0.46
3:H:154:VAL:CG2	3:H:182:LEU:HD21	2.47	0.45
2:B:362:VAL:HG13	2:B:527:PRO:HG3	1.98	0.45
1:L:169:VAL:HG22	1:L:181:LEU:HD12	1.98	0.45
2:B:393:THR:OG1	2:B:394:ASN:N	2.48	0.45
1:L:113:LYS:HB2	1:L:113:LYS:HE2	1.73	0.45
2:B:484:LYS:HB2	2:B:484:LYS:HE2	1.67	0.45
2:B:360:ASN:H	2:B:523:THR:HB	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:119:PRO:HG2	1:L:207:LEU:HD11	1.99	0.45
1:L:38:TYR:CZ	2:E:479:PRO:HG3	2.53	0.44
2:E:467:ASP:OD1	2:E:469:SER:HB3	2.18	0.44
2:E:447:GLY:HA2	2:E:498:GLN:HG2	1.99	0.44
1:A:21:LEU:HD22	1:A:108:THR:HG21	1.99	0.43
1:L:19:VAL:HG21	1:L:110:LEU:HD11	2.00	0.43
1:A:142:LEU:HD21	1:A:202:VAL:HG13	1.99	0.43
2:B:411:ALA:HB3	2:B:414:GLN:HG3	1.99	0.43
3:H:101:GLU:H	3:H:101:GLU:HG2	1.49	0.43
3:H:73:ASP:HB3	3:H:76:SER:OG	2.18	0.43
2:E:484:LYS:HE3	2:E:484:LYS:HB2	1.81	0.43
1:A:20:THR:HG23	1:A:78:THR:HG23	2.01	0.42
1:L:19:VAL:CG2	1:L:84:VAL:HG21	2.48	0.42
1:L:115:THR:HB	3:C:102:ASN:OD1	2.19	0.42
2:B:350:VAL:HG21	2:B:418:ILE:HG23	2.01	0.42
2:B:474:GLN:HG2	2:B:476:GLY:O	2.20	0.42
1:L:64:VAL:HA	1:L:65:PRO:HD3	1.94	0.42
3:H:33:ILE:HD11	3:H:35:HIS:HE2	1.85	0.42
2:B:461:LEU:HD22	2:B:465:GLU:HB3	2.01	0.42
2:E:395:VAL:CG2	2:E:524:VAL:HG11	2.50	0.42
1:A:20:THR:HG23	1:A:78:THR:CG2	2.49	0.41
2:B:439:ASN:HA	2:B:507:PRO:HG2	2.02	0.41
2:E:478:THR:HA	2:E:479:PRO:HD3	1.86	0.41
3:C:154:VAL:HG23	3:C:182:LEU:HD21	2.01	0.41
3:H:130:PRO:HD2	3:H:216:GLU:HG3	2.03	0.41
2:B:425:LEU:HD23	2:B:425:LEU:HA	1.92	0.41
2:B:521:PRO:HB2	2:B:522:ALA:H	1.76	0.41
2:E:458:LYS:NZ	2:E:474:GLN:O	2.54	0.40
2:E:418:ILE:HA	2:E:422:ASN:HB2	2.03	0.40

All (6) 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:L:28:SER:OG	3:C:89:GLU:OE2[4_544]	1.16	1.04
1:L:28:SER:CB	3:C:89:GLU:OE2[4_544]	1.57	0.63
3:H:120:THR:CG2	1:A:209:SER:CB[2_455]	1.83	0.37
3:H:54:GLU:OE2	2:B:500:THR:O[3_554]	2.04	0.16
3:H:11:LEU:CD2	1:A:209:SER:OG[2_455]	2.08	0.12
2:E:500:THR:OG1	2:B:493:GLN:NE2[3_554]	2.10	0.10

## 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	217/327 (66%)	211 (97%)	5 (2%)	1 (0%)	29	61
1	L	217/327 (66%)	210 (97%)	7 (3%)	0	100	100
2	B	176/195 (90%)	170 (97%)	5 (3%)	1 (1%)	25	58
2	E	188/195 (96%)	181 (96%)	7 (4%)	0	100	100
3	C	213/216 (99%)	209 (98%)	3 (1%)	1 (0%)	29	61
3	H	214/216 (99%)	209 (98%)	4 (2%)	1 (0%)	29	61
All	All	1225/1476 (83%)	1190 (97%)	31 (2%)	4 (0%)	41	71

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	103	VAL
3	C	103	VAL
2	B	521	PRO
1	A	209	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	195/292 (67%)	186 (95%)	9 (5%)	27	60
1	L	195/292 (67%)	184 (94%)	11 (6%)	21	52
2	B	158/168 (94%)	153 (97%)	5 (3%)	39	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	165/168 (98%)	157 (95%)	8 (5%)	25	58
3	C	185/186 (100%)	169 (91%)	16 (9%)	10	30
3	H	186/186 (100%)	171 (92%)	15 (8%)	11	33
All	All	1084/1292 (84%)	1020 (94%)	64 (6%)	19	49

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	20	THR
1	L	32	SER
1	L	52	LEU
1	L	89	LEU
1	L	97	TYR
1	L	113	LYS
1	L	114	ARG
1	L	160	LEU
1	L	168	SER
1	L	182	SER
1	L	203	THR
2	E	373	SER
2	E	385	THR
2	E	390	LEU
2	E	393	THR
2	E	417	ASN
2	E	449	TYR
2	E	469	SER
2	E	487	ASN
3	H	1	GLN
3	H	9	THR
3	H	20	MET
3	H	33	ILE
3	H	63	LYS
3	H	71	THR
3	H	72	THR
3	H	75	SER
3	H	84	SER
3	H	101	GLU
3	H	103	VAL
3	H	120	THR
3	H	142	LEU
3	H	197	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	H	216	GLU
1	A	46	SER
1	A	52	LEU
1	A	58	SER
1	A	69	THR
1	A	113	LYS
1	A	114	ARG
1	A	165	SER
1	A	187	LEU
1	A	209	SER
2	B	362	VAL
2	B	408	ARG
2	B	469	SER
2	B	493	GLN
2	B	500	THR
3	C	9	THR
3	C	12	VAL
3	C	18	LEU
3	C	33	ILE
3	C	71	THR
3	C	72	THR
3	C	75	SER
3	C	85	SER
3	C	101	GLU
3	C	109	GLN
3	C	136	SER
3	C	157	SER
3	C	183	SER
3	C	187	THR
3	C	190	SER
3	C	214	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	L	35	GLN
1	L	44	GLN
1	L	205	GLN
3	H	5	GLN
3	H	39	GLN
1	A	44	GLN
1	A	205	GLN

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Mol	Chain	Res	Type
2	B	487	ASN
3	C	39	GLN
3	C	82	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 [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	B	601	2	14,14,15	0.35	0	17,19,21	0.81	0
4	NAG	E	601	2	14,14,15	0.32	0	17,19,21	0.84	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	601	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	E	601	2	-	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 (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	601	NAG	C8-C7-N2-C2
4	E	601	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	219/327 (66%)	0.21	3 (1%) 75 75	16, 29, 49, 66	0
1	L	219/327 (66%)	0.45	16 (7%) 15 11	18, 32, 56, 74	0
2	B	184/195 (94%)	0.75	25 (13%) 3 2	20, 32, 94, 111	0
2	E	192/195 (98%)	0.69	23 (11%) 4 3	18, 33, 99, 114	0
3	C	215/216 (99%)	0.28	5 (2%) 60 58	20, 32, 61, 99	0
3	H	216/216 (100%)	0.23	8 (3%) 41 37	18, 31, 64, 89	0
All	All	1245/1476 (84%)	0.42	80 (6%) 19 15	16, 31, 83, 114	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	135	THR	10.1
2	B	525	CYS	8.7
3	C	134	SER	8.1
2	E	391	CYS	8.0
2	E	525	CYS	7.2
2	E	333	THR	6.1
2	B	333	THR	6.1
2	B	335	LEU	5.7
2	B	526	GLY	5.6
2	B	527	PRO	5.2
2	E	526	GLY	5.1
2	E	521	PRO	5.0
2	B	524	VAL	5.0
2	B	334	ASN	5.0
2	E	527	PRO	4.9
2	B	360	ASN	4.9
2	E	522	ALA	4.7
2	E	335	LEU	4.5
2	E	370	ASN	4.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	B	336	CYS	4.3
2	B	365	TYR	4.3
3	H	136	SER	4.0
2	B	363	ALA	3.9
2	B	337	PRO	3.9
2	E	334	ASN	3.9
2	E	520	ALA	3.8
3	H	132	SER	3.7
1	A	208	SER	3.7
2	E	389	ASP	3.6
2	B	522	ALA	3.6
2	B	367	VAL	3.6
2	B	362	VAL	3.6
2	E	369	TYR	3.4
2	E	390	LEU	3.3
2	E	392	PHE	3.3
2	B	523	THR	3.3
1	L	157	ASP	3.2
2	E	365	TYR	3.2
2	E	360	ASN	3.2
2	B	358	ILE	3.1
2	E	385	THR	3.0
3	C	102	ASN	3.0
3	C	136	SER	3.0
2	E	386	LYS	3.0
1	A	209	SER	3.0
2	B	386	LYS	3.0
3	H	135	THR	2.9
3	H	193	LEU	2.9
1	L	187	LEU	2.9
1	L	194	LYS	2.8
2	B	395	VAL	2.8
1	L	135	THR	2.7
2	B	340	GLU	2.7
3	H	192	SER	2.7
2	B	338	PHE	2.6
2	E	359	SER	2.6
1	L	192	TYR	2.5
2	E	368	LEU	2.5
1	L	193	GLU	2.5
3	H	137	GLY	2.5
2	E	384	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	392	PHE	2.4
2	B	361	CYS	2.4
3	C	137	GLY	2.4
1	L	156	VAL	2.4
1	A	83	SER	2.3
1	L	218	GLY	2.3
1	L	190	ALA	2.3
3	H	134	SER	2.2
2	B	368	LEU	2.2
3	H	105	ASP	2.2
1	L	1	GLN	2.2
1	L	189	LYS	2.2
1	L	219	GLU	2.2
1	L	136	ALA	2.1
1	L	196	LYS	2.1
1	L	160	LEU	2.1
2	E	388	ASN	2.1
2	B	520	ALA	2.1
1	L	198	TYR	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	E	601	14/15	0.69	0.50	30,30,30,30	0
4	NAG	B	601	14/15	0.69	0.35	30,30,30,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.