



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:53 AM UTC

PDB ID : 7FJS / pdb_00007fjs
Title : Crystal structure of T6 Fab bound to the SARS-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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

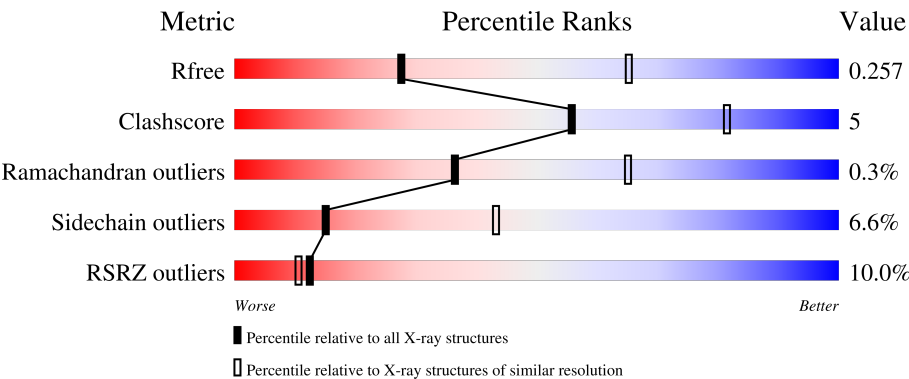
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 ≥ 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	2% 56% 10% • 33%
1	L	327	2% 56% 10% • 33%
2	B	195	18% 74% 18% • 6%
2	E	195	20% 82% 14% • •
3	C	216	9% 84% 13% •

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Mol	Chain	Length	Quality of chain
3	H	216	7% 82% 14%

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
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
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:

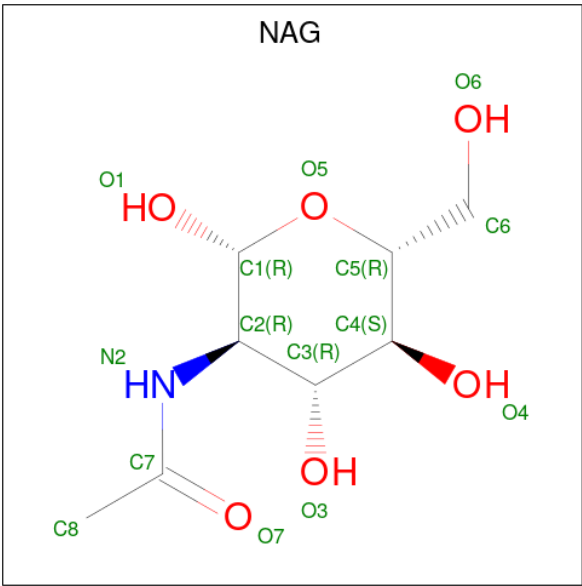
Chain	Residue	Modelled	Actual	Comment	Reference
E	417	ASN	LYS	variant	UNP P0DTC2
E	484	LYS	GLU	variant	UNP P0DTC2
E	501	TYR	ASN	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	484	LYS	GLU	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2

- Molecule 3 is a protein called T6 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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 (CCD ID: NAG) (formula:

C₈H₁₅NO₆).

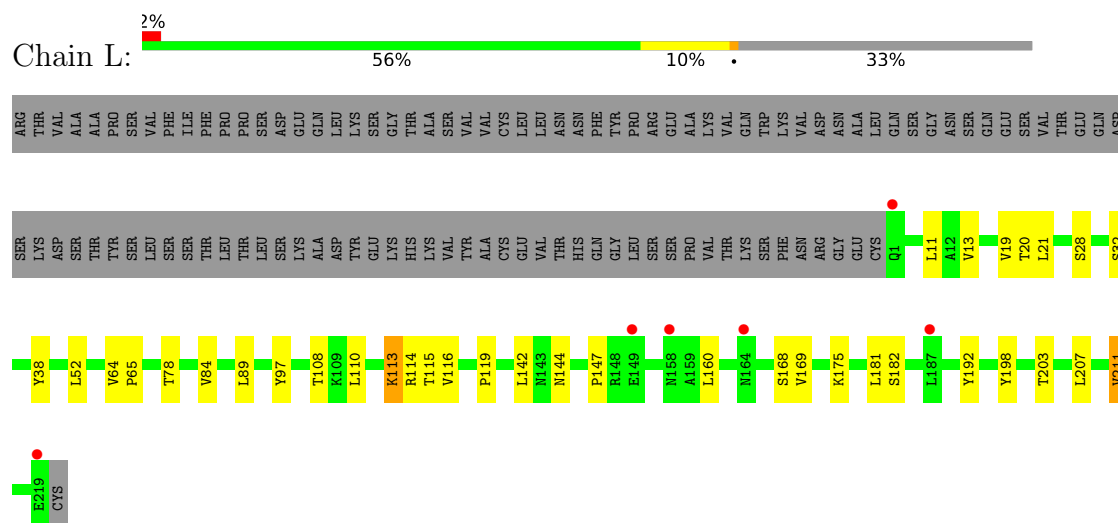


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

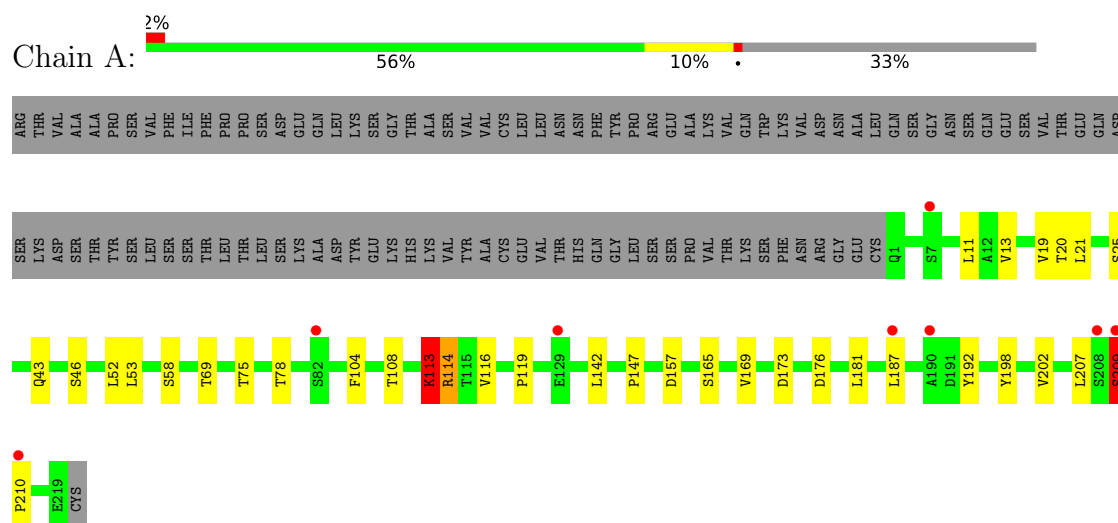
3 Residue-property plots

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.

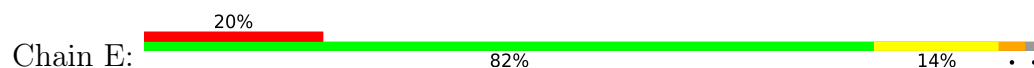
- Molecule 1: T6 light chain

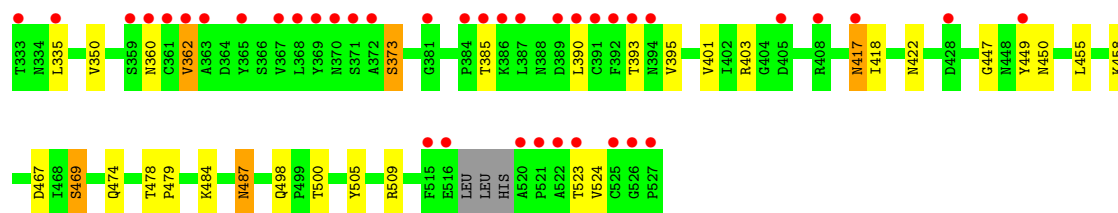


- Molecule 1: T6 light chain

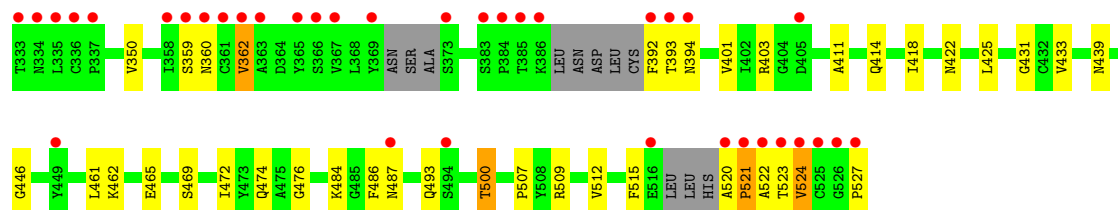
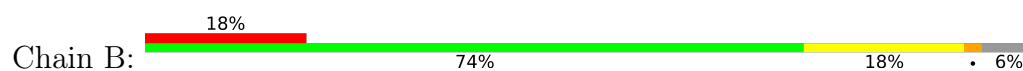


- Molecule 2: Spike protein S1

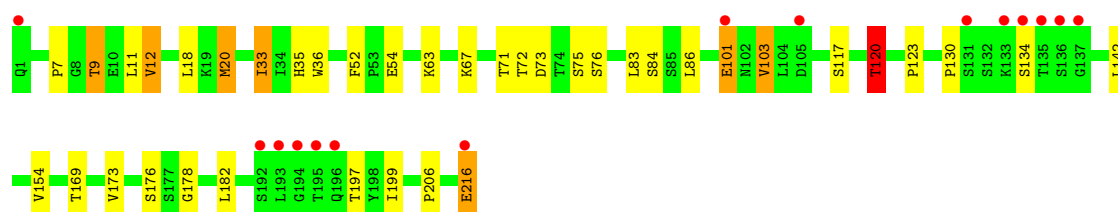
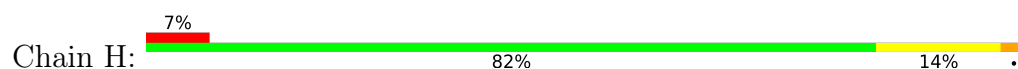




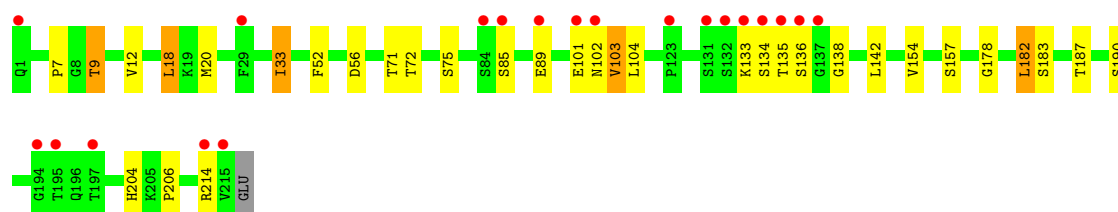
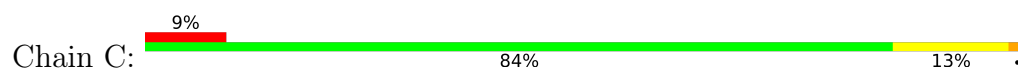
• Molecule 2: Spike protein S1



• 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.217 , 0.285 0.235 , 0.257	Depositor DCC
R_{free} test set	1882 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	38.4	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 33.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	9649	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

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	0.87	0/1744	1.26	5/2368 (0.2%)
1	L	0.87	0/1744	1.23	2/2368 (0.1%)
2	B	0.87	0/1504	1.26	2/2043 (0.1%)
2	E	0.88	0/1563	1.28	4/2127 (0.2%)
3	C	0.92	1/1646 (0.1%)	1.31	4/2246 (0.2%)
3	H	0.92	1/1656 (0.1%)	1.30	6/2258 (0.3%)
All	All	0.89	2/9857 (0.0%)	1.27	23/13410 (0.2%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	7	PRO	C-O	-6.35	1.16	1.23
3	C	7	PRO	C-O	-5.10	1.17	1.23

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	210	PRO	N-CA-C	-9.17	93.58	112.47
2	E	487	ASN	CB-CA-C	8.31	122.03	110.06
3	C	133	LYS	N-CA-C	-8.26	102.51	112.59
1	A	157	ASP	CB-CA-C	6.49	120.95	111.73
3	C	178	GLY	N-CA-C	-6.01	106.95	115.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	67	LYS	N-CA-C	-5.93	106.68	114.04
3	H	123	PRO	N-CA-C	5.90	120.76	111.38
2	E	373	SER	N-CA-C	-5.67	105.56	112.88
3	H	120	THR	CB-CA-C	5.58	118.93	109.84
3	C	138	GLY	N-CA-C	-5.41	107.85	115.32
3	H	178	GLY	N-CA-C	-5.39	107.83	115.43
3	C	56	ASP	CB-CA-C	5.34	120.18	111.26
1	L	142	LEU	N-CA-C	-5.34	99.82	108.52
1	A	104	PHE	CA-CB-CG	5.33	119.13	113.80
2	E	487	ASN	CA-CB-CG	5.29	117.89	112.60
2	E	450	ASN	CB-CA-C	5.28	119.83	110.85
1	A	114	ARG	N-CA-CB	-5.19	103.51	111.56
2	B	446	GLY	N-CA-C	-5.15	108.95	115.08
2	B	403	ARG	CB-CA-C	5.09	119.88	109.76
1	A	113	LYS	CB-CA-C	5.08	118.20	109.51
3	H	117	SER	N-CA-C	-5.07	106.87	113.16
1	L	144	ASN	CB-CA-C	5.06	120.48	110.42
3	H	169	THR	CB-CA-C	5.01	118.80	110.78

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	17	2
2	B	1463	0	1379	27	2
2	E	1520	0	1432	16	1
3	C	1608	0	1565	10	2
3	H	1618	0	1571	10	3
4	B	14	0	13	0	0
4	E	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9649	0	9305	89	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 5.

All (89) 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
3:C:18:LEU:HD11	3:C:20:MET:HE2	1.75	0.67
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:182:LEU:C	3:C:182:LEU:HD12	2.43	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
1:L:115:THR:HB	3:C:102:ASN:CG	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:H:20:MET:HE2	3:H:36:TRP:HZ3	1.87	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%)	24 54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	217/327 (66%)	210 (97%)	7 (3%)	0	100	100
2	B	176/195 (90%)	170 (97%)	5 (3%)	1 (1%)	21	51
2	E	188/195 (96%)	181 (96%)	7 (4%)	0	100	100
3	C	213/216 (99%)	209 (98%)	3 (1%)	1 (0%)	24	54
3	H	214/216 (99%)	209 (98%)	4 (2%)	1 (0%)	24	54
All	All	1225/1476 (83%)	1190 (97%)	31 (2%)	4 (0%)	36	65

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 ⓘ

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%)	24	57
1	L	195/292 (67%)	182 (93%)	13 (7%)	15	43
2	B	158/168 (94%)	154 (98%)	4 (2%)	42	74
2	E	165/168 (98%)	156 (94%)	9 (6%)	19	50
3	C	185/186 (100%)	166 (90%)	19 (10%)	7	23
3	H	186/186 (100%)	168 (90%)	18 (10%)	8	25
All	All	1084/1292 (84%)	1012 (93%)	72 (7%)	15	43

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	20	THR
1	L	32	SER

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Mol	Chain	Res	Type
1	L	52	LEU
1	L	78	THR
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
1	L	211	VAL
2	E	362	VAL
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	9	THR
3	H	12	VAL
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	173	VAL
3	H	176	SER
3	H	197	THR
3	H	199	ILE
3	H	216	GLU
1	A	46	SER
1	A	52	LEU
1	A	58	SER
1	A	69	THR

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Mol	Chain	Res	Type
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	469	SER
2	B	500	THR
2	B	524	VAL
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	103	VAL
3	C	104	LEU
3	C	136	SER
3	C	142	LEU
3	C	157	SER
3	C	182	LEU
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 (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	35	GLN
1	L	44	GLN
1	L	205	GLN
2	E	474	GLN
3	H	5	GLN
3	H	39	GLN
3	H	102	ASN
1	A	44	GLN
1	A	205	GLN
2	B	487	ASN

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Mol	Chain	Res	Type
3	C	39	GLN
3	C	82	GLN
3	C	168	HIS

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 oligosaccharides 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	E	601	2	14,14,15	0.32	0	17,19,21	0.83	0
4	NAG	B	601	2	14,14,15	0.35	0	17,19,21	0.80	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	E	601	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	601	2	-	0/6/23/26	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	219/327 (66%)	0.43	8 (3%) 45 37	16, 29, 49, 66	0
1	L	219/327 (66%)	0.55	6 (2%) 56 47	18, 32, 56, 74	0
2	B	184/195 (94%)	1.10	36 (19%) 3 2	20, 32, 94, 111	0
2	E	192/195 (98%)	1.10	39 (20%) 3 2	18, 33, 99, 114	0
3	C	215/216 (99%)	0.71	20 (9%) 14 12	20, 32, 61, 99	0
3	H	216/216 (100%)	0.58	15 (6%) 23 18	18, 31, 64, 89	0
All	All	1245/1476 (84%)	0.73	124 (9%) 12 10	16, 31, 83, 114	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	134	SER	7.4
2	B	526	GLY	7.1
2	E	522	ALA	6.6
3	C	135	THR	6.6
2	E	527	PRO	6.2
2	B	522	ALA	6.1
3	C	102	ASN	5.9
2	E	521	PRO	5.9
3	C	136	SER	5.9
1	A	208	SER	5.7
2	B	392	PHE	5.5
2	E	390	LEU	5.2
2	B	362	VAL	5.1
2	B	524	VAL	5.0
2	E	520	ALA	5.0
2	B	337	PRO	5.0
2	B	335	LEU	4.8
2	E	391	CYS	4.8
2	B	336	CYS	4.8

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Mol	Chain	Res	Type	RSRZ
3	C	133	LYS	4.7
2	B	520	ALA	4.7
2	B	527	PRO	4.6
2	B	365	TYR	4.6
1	A	209	SER	4.5
3	H	135	THR	4.4
2	B	369	TYR	4.4
2	B	525	CYS	4.4
2	E	525	CYS	4.3
2	B	373	SER	4.3
2	B	333	THR	4.3
2	B	386	LYS	4.3
2	E	516	GLU	4.3
3	C	197	THR	4.0
2	B	393	THR	4.0
3	H	105	ASP	3.9
2	E	392	PHE	3.9
3	C	137	GLY	3.9
2	B	360	ASN	3.9
3	H	196	GLN	3.9
2	E	393	THR	3.9
2	B	523	THR	3.9
3	C	89	GLU	3.8
2	B	384	PRO	3.8
2	B	363	ALA	3.8
3	C	131	SER	3.8
2	E	333	THR	3.8
2	B	521	PRO	3.7
2	E	387	LEU	3.7
2	B	334	ASN	3.7
2	B	367	VAL	3.7
2	E	384	PRO	3.6
2	B	487	ASN	3.6
2	B	383	SER	3.5
3	H	136	SER	3.5
2	E	526	GLY	3.5
2	E	386	LYS	3.4
2	E	363	ALA	3.4
2	E	385	THR	3.4
2	E	449	TYR	3.4
2	E	394	ASN	3.4
2	B	385	THR	3.4

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Mol	Chain	Res	Type	RSRZ
3	H	137	GLY	3.4
2	E	367	VAL	3.3
3	C	195	THR	3.3
2	E	335	LEU	3.3
2	B	358	ILE	3.2
2	E	365	TYR	3.2
1	A	190	ALA	3.2
2	E	370	ASN	3.1
3	C	101	GLU	3.1
2	E	359	SER	3.1
2	E	389	ASP	3.1
3	H	1	GLN	3.1
2	B	366	SER	3.0
1	L	187	LEU	3.0
1	L	219	GLU	3.0
2	E	369	TYR	3.0
2	E	360	ASN	3.0
3	H	216	GLU	2.9
3	H	193	LEU	2.9
2	E	371	SER	2.9
2	B	516	GLU	2.9
3	H	134	SER	2.9
2	E	362	VAL	2.8
2	E	372	ALA	2.8
1	A	82	SER	2.8
3	C	194	GLY	2.7
3	C	1	GLN	2.7
2	E	515	PHE	2.7
2	B	361	CYS	2.7
1	L	1	GLN	2.7
2	E	417	ASN	2.7
1	A	210	PRO	2.6
3	H	194	GLY	2.6
2	E	523	THR	2.6
3	C	132	SER	2.6
3	C	215	VAL	2.6
3	C	84	SER	2.5
2	B	394	ASN	2.4
2	B	494	SER	2.4
3	H	101	GLU	2.4
2	E	368	LEU	2.4
2	E	361	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	405	ASP	2.4
3	C	85	SER	2.4
2	B	359	SER	2.3
3	H	195	THR	2.3
3	H	192	SER	2.3
2	B	449	TYR	2.3
1	A	129	GLU	2.2
2	E	381	GLY	2.2
3	C	214	ARG	2.2
1	A	7	SER	2.2
3	H	133	LYS	2.2
2	E	428	ASP	2.2
3	C	29	PHE	2.2
1	L	149	GLU	2.2
1	L	158	ASN	2.1
3	H	131	SER	2.1
1	A	187	LEU	2.1
3	C	123	PRO	2.0
2	E	405	ASP	2.0
1	L	164	ASN	2.0
2	E	408	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	B	601	14/15	0.58	0.22	30,30,30,30	0
4	NAG	E	601	14/15	0.63	0.28	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.