



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:05 PM UTC

PDB ID : 7F7E / pdb_00007f7e
Title : SARS-CoV-2 S protein RBD in complex with A5-10 Fab
Authors : Dou, Y.; Wang, X.; Wang, K.; Liu, P.; Lu, B.
Deposited on : 2021-06-29
Resolution : 2.49 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

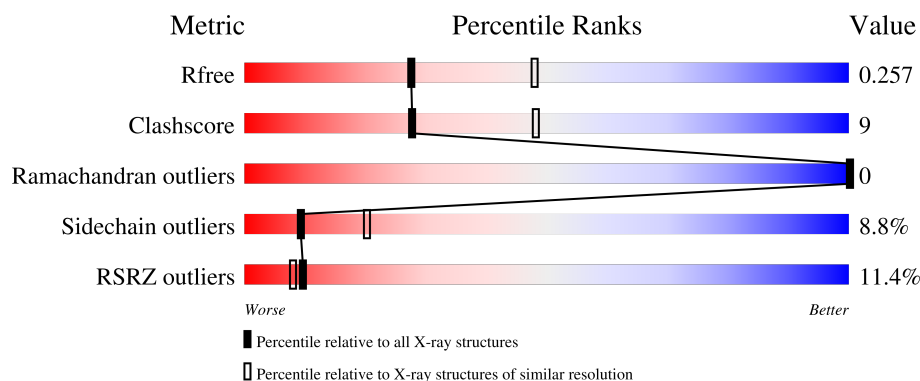
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	C	227	16% 76% 23% .
2	L	205	14% 74% 25% .
3	E	198	4% 72% 25% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4835 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 Heavy chain of A5-10 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	227	Total	C	N	O	S	0	0	0
			1691	1075	277	333	6			

- Molecule 2 is a protein called Light chain of A5-10 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	205	Total	C	N	O	S	0	0	0
			1560	978	264	313	5			

- Molecule 3 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	198	Total	C	N	O	S	0	0	0
			1570	1006	264	292	8			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	332	PRO	-	expression tag	UNP P0DTC2
E	528	HIS	-	expression tag	UNP P0DTC2
E	529	HIS	-	expression tag	UNP P0DTC2

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

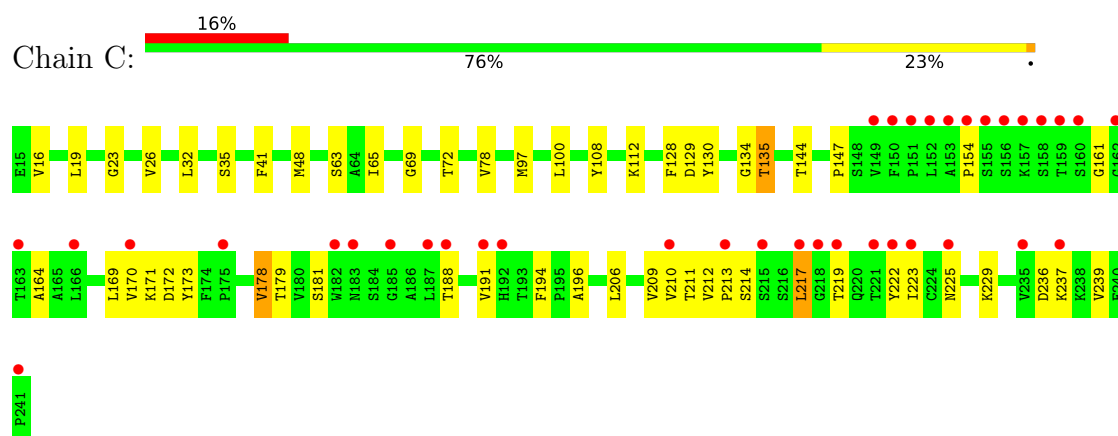


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	E	1	14	8	1	5	0	0

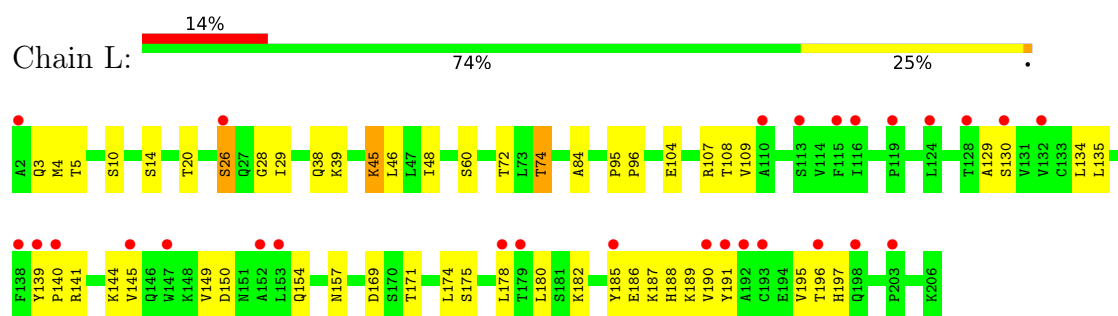
3 Residue-property plots [i](#)

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.

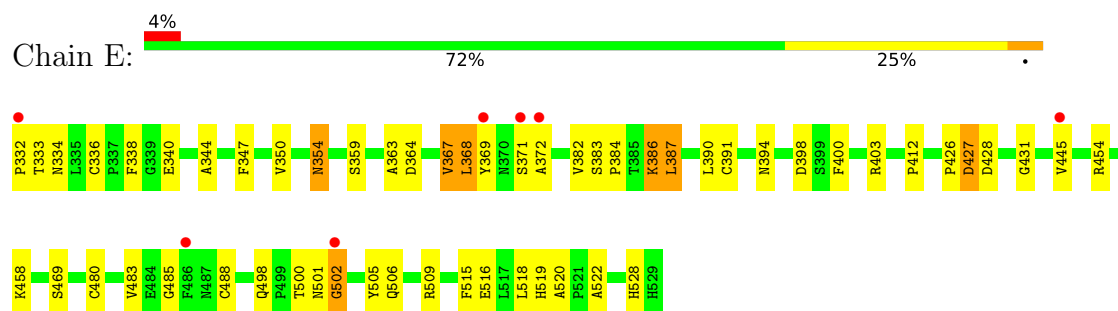
- Molecule 1: Heavy chain of A5-10 Fab



- Molecule 2: Light chain of A5-10 Fab



- Molecule 3: Spike protein S1



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	157.19Å 157.19Å 98.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.37 – 2.49 20.37 – 2.49	Depositor EDS
% Data completeness (in resolution range)	96.2 (20.37-2.49) 96.0 (20.37-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.50Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.214 , 0.256 0.215 , 0.257	Depositor DCC
R_{free} test set	1439 reflections (4.54%)	wwPDB-VP
Wilson B-factor (Å ²)	50.9	Xtriage
Anisotropy	0.718	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 53.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.002 for $-1/3^*h+1/3^*k+4/3^*l, -k, 2/3^*h+1/3^*k+1/3^*l$ 0.005 for $-2/3^*h-1/3^*k-4/3^*l, -1/3^*h-2/3^*k+4/3^*l, -1/3^*h+1/3^*k+1/3^*l$ 0.000 for $-h, 1/3^*h-1/3^*k-4/3^*l, -1/3^*h-2/3^*k+1/3^*l$ 0.012 for $-1/3^*h-2/3^*k+4/3^*l, -2/3^*h-1/3^*k-4/3^*l, 1/3^*h-1/3^*k-1/3^*l$ 0.000 for $-h, 2/3^*h+1/3^*k+4/3^*l, 1/3^*h+2/3^*k-1/3^*l$ 0.000 for $1/3^*h+2/3^*k-4/3^*l, -k, -2/3^*h-1/3^*k-1/3^*l$ 0.020 for $h, -h-k, -l$	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4835	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% 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	C	0.40	0/1733	0.61	0/2361
2	L	0.34	0/1596	0.53	0/2170
3	E	0.43	0/1617	0.68	2/2202 (0.1%)
All	All	0.39	0/4946	0.61	2/6733 (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	E	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	501	ASN	CA-C-N	-6.07	109.51	121.41
3	E	501	ASN	C-N-CA	-6.07	109.51	121.41

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	E	372	ALA	Peptide
3	E	502	GLY	Peptide

5.2 Too-close contacts ⓘ

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	C	1691	0	1651	27	0
2	L	1560	0	1517	33	0
3	E	1570	0	1481	29	0
4	E	14	0	13	1	0
All	All	4835	0	4662	85	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 9.

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)
3:E:403:ARG:HG2	3:E:505:TYR:HA	1.64	0.79
2:L:3:GLN:HA	2:L:96:PRO:HD2	1.65	0.78
3:E:485:GLY:H	3:E:488:CYS:HB2	1.49	0.76
1:C:213:PRO:HD2	1:C:217:LEU:HD22	1.71	0.72
2:L:144:LYS:HB2	2:L:196:THR:HB	1.74	0.68
2:L:107:ARG:NH1	2:L:108:THR:O	2.26	0.68
1:C:164:ALA:HB2	1:C:214:SER:HB3	1.78	0.66
2:L:182:LYS:HA	2:L:185:TYR:HB3	1.81	0.62
1:C:196:ALA:HB2	1:C:206:LEU:HD23	1.83	0.61
1:C:23:GLY:H	1:C:135:THR:HG21	1.67	0.60
2:L:145:VAL:HG12	2:L:195:VAL:HG22	1.84	0.59
1:C:196:ALA:HA	1:C:206:LEU:HB3	1.84	0.59
3:E:502:GLY:H	3:E:506:GLN:HE21	1.53	0.57
2:L:20:THR:HG22	2:L:74:THR:HB	1.86	0.56
2:L:154:GLN:HE21	2:L:157:ASN:HD21	1.51	0.56
3:E:485:GLY:N	3:E:488:CYS:HB2	2.20	0.56
2:L:4:MET:HG2	2:L:95:PRO:HB3	1.87	0.56
2:L:28:GLY:HA2	3:E:500:THR:HG21	1.88	0.54
1:C:65:ILE:HG13	1:C:72:THR:HG22	1.89	0.54
3:E:371:SER:OG	4:E:601:NAG:H83	2.07	0.54
2:L:107:ARG:HD3	2:L:139:TYR:HB2	1.89	0.54
2:L:39:LYS:HD3	2:L:84:ALA:HB2	1.90	0.53
1:C:223:ILE:HD12	1:C:236:ASP:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:135:LEU:HD11	2:L:145:VAL:HG11	1.90	0.52
3:E:340:GLU:O	3:E:344:ALA:HB2	2.08	0.52
1:C:154:PRO:HG3	1:C:239:VAL:HG12	1.89	0.52
3:E:391:CYS:HB3	3:E:522:ALA:HB1	1.91	0.52
1:C:170:VAL:HG11	1:C:178:VAL:HG11	1.91	0.52
1:C:108:TYR:O	1:C:134:GLY:HA2	2.11	0.51
1:C:181:SER:HB2	1:C:225:ASN:HB2	1.93	0.50
3:E:364:ASP:O	3:E:367:VAL:HG22	2.12	0.49
3:E:480:CYS:O	3:E:483:VAL:HG22	2.13	0.49
2:L:130:SER:HA	2:L:178:LEU:O	2.13	0.49
1:C:147:PRO:HB3	1:C:173:TYR:HB3	1.94	0.48
1:C:41:PHE:CE2	1:C:112:LYS:HD2	2.48	0.48
2:L:150:ASP:HA	2:L:190:VAL:HB	1.95	0.48
3:E:383:SER:HB3	3:E:386:LYS:HD3	1.94	0.48
1:C:161:GLY:O	1:C:214:SER:OG	2.30	0.48
1:C:169:LEU:HD23	1:C:171:LYS:HB2	1.96	0.47
3:E:336:CYS:SG	3:E:363:ALA:HB2	2.54	0.47
2:L:144:LYS:O	2:L:195:VAL:HA	2.14	0.47
2:L:149:VAL:HG13	2:L:191:TYR:HE1	1.80	0.47
2:L:45:LYS:HA	2:L:45:LYS:HD2	1.34	0.46
3:E:518:LEU:O	3:E:520:ALA:N	2.49	0.46
1:C:97:MET:HE2	1:C:100:LEU:HD21	1.97	0.46
2:L:129:ALA:N	2:L:180:LEU:O	2.41	0.46
1:C:194:PHE:CZ	2:L:175:SER:HB3	2.52	0.45
1:C:171:LYS:HG2	1:C:172:ASP:OD2	2.17	0.45
3:E:364:ASP:OD1	3:E:367:VAL:HG13	2.17	0.45
1:C:65:ILE:HD11	1:C:69:GLY:HA2	2.00	0.44
1:C:112:LYS:O	1:C:128:PHE:HA	2.18	0.44
1:C:212:VAL:HG21	1:C:222:TYR:OH	2.18	0.44
3:E:350:VAL:HA	3:E:400:PHE:HB2	1.99	0.44
2:L:169:ASP:OD1	2:L:171:THR:OG1	2.23	0.44
3:E:431:GLY:HA2	3:E:515:PHE:CD2	2.53	0.44
2:L:187:LYS:HB3	2:L:187:LYS:HE3	1.72	0.44
3:E:354:ASN:O	3:E:398:ASP:HA	2.18	0.44
1:C:48:MET:HE3	1:C:48:MET:HB3	1.91	0.44
1:C:209:VAL:HG21	2:L:134:LEU:HD13	1.99	0.44
2:L:45:LYS:HE2	2:L:46:LEU:H	1.83	0.43
3:E:427:ASP:OD1	3:E:427:ASP:N	2.51	0.43
1:C:129:ASP:OD1	1:C:130:TYR:N	2.50	0.43
1:C:188:THR:O	1:C:191:VAL:HG22	2.19	0.43
2:L:139:TYR:HB3	2:L:140:PRO:HD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:189:LYS:HD3	2:L:189:LYS:HA	1.86	0.42
1:C:16:VAL:HB	1:C:130:TYR:CE2	2.54	0.42
2:L:4:MET:HE3	2:L:26:SER:HB3	2.02	0.42
3:E:332:PRO:HB2	3:E:333:THR:H	1.68	0.42
3:E:412:PRO:HB3	3:E:426:PRO:O	2.20	0.42
1:C:171:LYS:NZ	2:L:130:SER:HB3	2.34	0.42
2:L:38:GLN:O	2:L:84:ALA:HB1	2.19	0.42
2:L:135:LEU:HD13	2:L:174:LEU:HD22	2.02	0.42
3:E:458:LYS:HA	3:E:458:LYS:HD2	1.89	0.42
2:L:140:PRO:HD2	2:L:197:HIS:HE1	1.85	0.41
3:E:347:PHE:CD2	3:E:509:ARG:HG2	2.54	0.41
2:L:169:ASP:O	2:L:171:THR:HG23	2.21	0.41
3:E:454:ARG:NH2	3:E:469:SER:O	2.51	0.41
3:E:502:GLY:N	3:E:506:GLN:HE21	2.17	0.41
3:E:368:LEU:HA	3:E:368:LEU:HD23	1.77	0.41
2:L:135:LEU:HB2	2:L:174:LEU:HB3	2.03	0.41
3:E:338:PHE:HE2	3:E:363:ALA:HB1	1.86	0.41
3:E:394:ASN:HB2	3:E:516:GLU:OE1	2.20	0.41
3:E:384:PRO:HA	3:E:387:LEU:CD2	2.51	0.40
2:L:140:PRO:HD2	2:L:197:HIS:CE1	2.57	0.40
3:E:364:ASP:CG	3:E:367:VAL:HG13	2.46	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	C	225/227 (99%)	211 (94%)	14 (6%)	0	100	100
2	L	203/205 (99%)	190 (94%)	13 (6%)	0	100	100
3	E	196/198 (99%)	180 (92%)	16 (8%)	0	100	100
All	All	624/630 (99%)	581 (93%)	43 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	C	187/187 (100%)	171 (91%)	16 (9%)	10	21
2	L	176/176 (100%)	161 (92%)	15 (8%)	10	22
3	E	171/171 (100%)	155 (91%)	16 (9%)	8	18
All	All	534/534 (100%)	487 (91%)	47 (9%)	9	20

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	19	LEU
1	C	26	VAL
1	C	32	LEU
1	C	35	SER
1	C	63	SER
1	C	78	VAL
1	C	135	THR
1	C	144	THR
1	C	178	VAL
1	C	179	THR
1	C	210	VAL
1	C	211	THR
1	C	217	LEU
1	C	219	THR
1	C	229	LYS
1	C	237	LYS
2	L	5	THR
2	L	10	SER
2	L	14	SER
2	L	26	SER
2	L	29	ILE
2	L	45	LYS
2	L	48	ILE

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Mol	Chain	Res	Type
2	L	60	SER
2	L	72	THR
2	L	74	THR
2	L	104	GLU
2	L	109	VAL
2	L	141	ARG
2	L	186	GLU
2	L	188	HIS
3	E	334	ASN
3	E	354	ASN
3	E	359	SER
3	E	367	VAL
3	E	368	LEU
3	E	369	TYR
3	E	382	VAL
3	E	386	LYS
3	E	387	LEU
3	E	390	LEU
3	E	427	ASP
3	E	428	ASP
3	E	445	VAL
3	E	498	GLN
3	E	519	HIS
3	E	528	HIS

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

Mol	Chain	Res	Type
1	C	98	ASN
2	L	154	GLN
3	E	409	GLN
3	E	414	GLN
3	E	498	GLN

5.3.3 RNA ⓘ

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](#)

1 ligand is 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	3	14,14,15	1.18	1 (7%)	17,19,21	1.50	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	E	601	3	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	601	NAG	O5-C1	4.15	1.50	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	601	NAG	C1-O5-C5	5.39	119.41	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	601	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	C	227/227 (100%)	0.49	37 (16%) 4 3	38, 53, 189, 234	0
2	L	205/205 (100%)	0.77	28 (13%) 6 5	43, 91, 158, 187	0
3	E	198/198 (100%)	0.21	7 (3%) 47 42	39, 60, 105, 132	0
All	All	630/630 (100%)	0.49	72 (11%) 10 8	38, 68, 161, 234	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	217	LEU	5.4
3	E	372	ALA	4.6
1	C	154	PRO	4.1
2	L	192	ALA	4.1
2	L	153	LEU	3.8
1	C	153	ALA	3.7
2	L	139	TYR	3.5
1	C	155	SER	3.4
2	L	130	SER	3.1
1	C	222	TYR	3.0
3	E	371	SER	3.0
1	C	166	LEU	3.0
2	L	116	ILE	2.9
1	C	160	SER	2.8
1	C	150	PHE	2.8
1	C	162	GLY	2.8
2	L	132	VAL	2.8
2	L	178	LEU	2.8
2	L	140	PRO	2.7
2	L	203	PRO	2.7
2	L	115	PHE	2.6
3	E	369	TYR	2.6
1	C	187	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
2	L	191	TYR	2.6
1	C	223	ILE	2.5
1	C	221	THR	2.5
2	L	193	CYS	2.5
1	C	235	VAL	2.5
1	C	156	SER	2.5
1	C	185	GLY	2.4
1	C	151	PRO	2.4
2	L	2	ALA	2.4
1	C	241	PRO	2.3
1	C	159	THR	2.3
2	L	119	PRO	2.3
2	L	185	TYR	2.2
1	C	192	HIS	2.2
1	C	219	THR	2.2
1	C	152	LEU	2.2
3	E	486	PHE	2.2
2	L	152	ALA	2.2
2	L	179	THR	2.2
2	L	26	SER	2.2
2	L	190	VAL	2.1
1	C	215	SER	2.1
1	C	237	LYS	2.1
2	L	145	VAL	2.1
1	C	225	ASN	2.1
1	C	163	THR	2.1
1	C	170	VAL	2.1
2	L	110	ALA	2.1
2	L	147	TRP	2.1
1	C	157	LYS	2.1
3	E	332	PRO	2.1
1	C	210	VAL	2.1
2	L	138	PHE	2.1
1	C	182	TRP	2.1
2	L	128	THR	2.1
1	C	149	VAL	2.0
1	C	191	VAL	2.0
1	C	183	ASN	2.0
2	L	124	LEU	2.0
3	E	502	GLY	2.0
1	C	188	THR	2.0
2	L	196	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	158	SER	2.0
1	C	175	PRO	2.0
1	C	213	PRO	2.0
2	L	198	GLN	2.0
3	E	445	VAL	2.0
1	C	218	GLY	2.0
2	L	113	SER	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	E	601	14/15	0.67	0.14	71,74,84,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.