



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 03:51 AM BST

PDB ID : 6Z2M  
Title : H11-D4, SARS-CoV-2 RBD, CR3022 ternary complex  
Authors : Naismith, J.H.; Ren, J.; Zhou, D.; Zhao, Y.; Stuart, D.I.  
Deposited on : 2020-05-17  
Resolution : 2.71 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.

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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)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

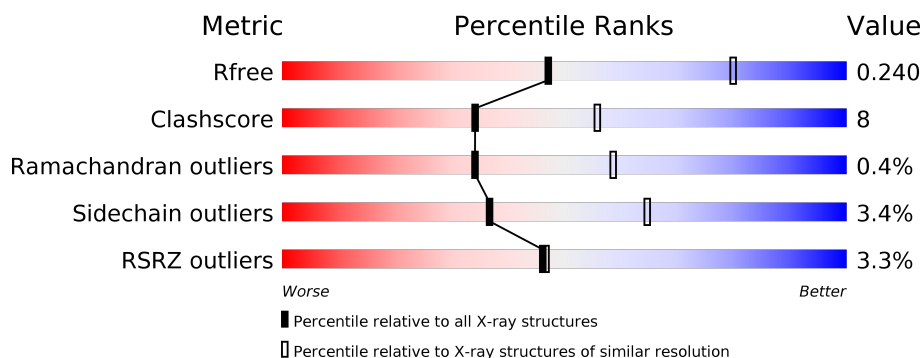
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.71 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	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	197	<div> <div>5%</div> <div> <div></div> <div>69%</div> <div>28%</div> <div>.</div> </div> </div>
1	E	197	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>17%</div> <div>..</div> </div> </div>
2	B	216	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>19%</div> <div>.</div> </div> </div>
2	H	216	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>16%</div> </div> </div>
3	C	219	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>21%</div> <div>.</div> </div> </div>
3	L	219	<div> <div></div> <div> <div></div> <div>80%</div> <div>19%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	D	127	<div><div></div><div>3%</div><div>84%</div><div>15%</div><div></div></div>
4	F	127	<div><div></div><div>10%</div><div>79%</div><div>20%</div><div></div></div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 11731 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	197	Total	C	N	O	S	0	0	0
			1560	1001	260	291	8			
1	E	195	Total	C	N	O	S	0	0	0
			1543	989	257	289	8			

- Molecule 2 is a protein called CR3022 antibody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	216	Total	C	N	O	S	0	1	0
			1609	1023	261	317	8			
2	H	216	Total	C	N	O	S	0	1	0
			1609	1023	261	317	8			

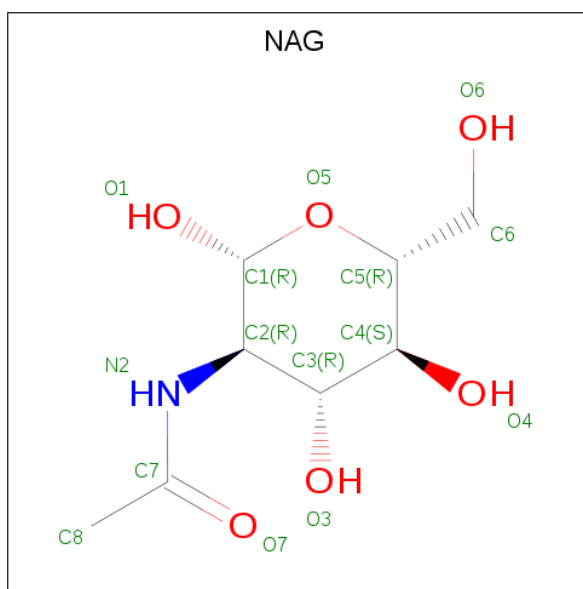
- Molecule 3 is a protein called CR3022 antibody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	219	Total	C	N	O	S	0	0	0
			1703	1070	282	347	4			
3	L	219	Total	C	N	O	S	0	0	0
			1703	1070	282	347	4			

- Molecule 4 is a protein called nanobody D4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	127	Total	C	N	O	S	0	0	0
			988	621	173	189	5			
4	D	127	Total	C	N	O	S	0	0	0
			988	621	173	189	5			

- Molecule 5 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>).

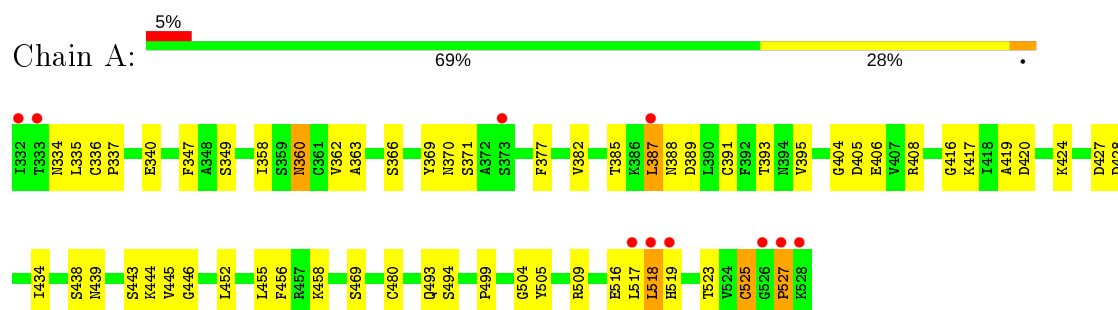


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		

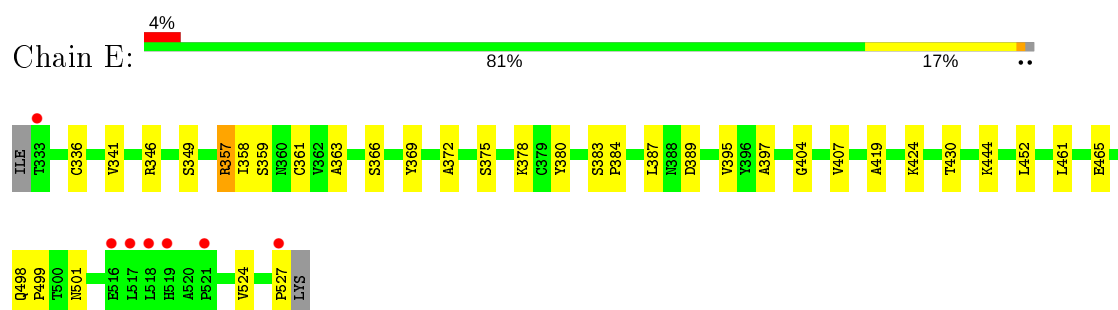
### 3 Residue-property plots [i](#)

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.

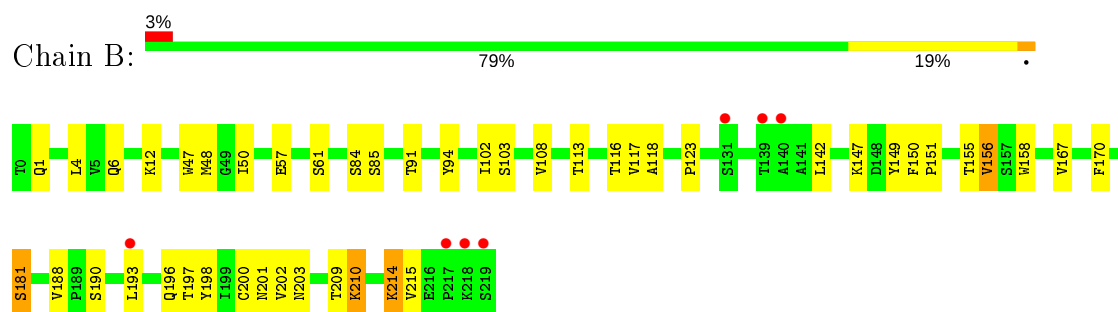
- Molecule 1: Spike glycoprotein



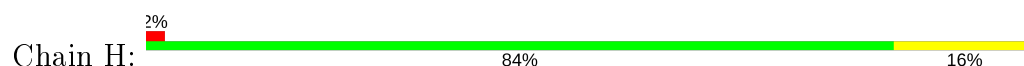
- Molecule 1: Spike glycoprotein

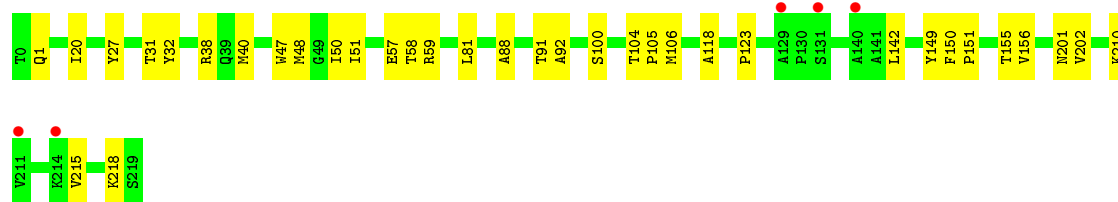


- Molecule 2: CR3022 antibody

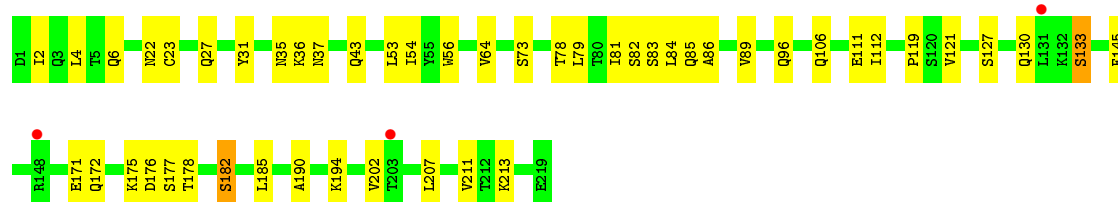
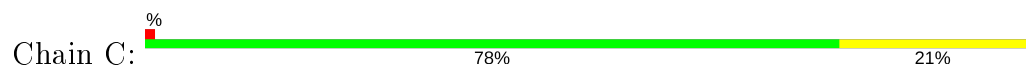


- Molecule 2: CR3022 antibody

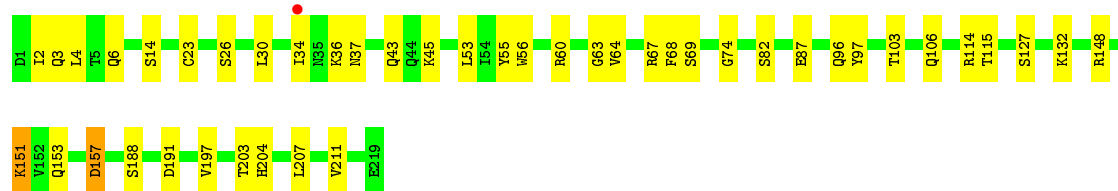
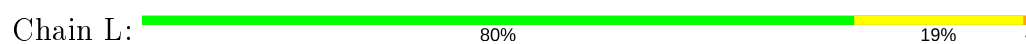




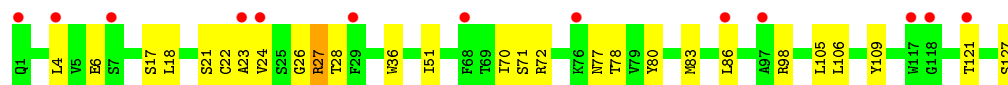
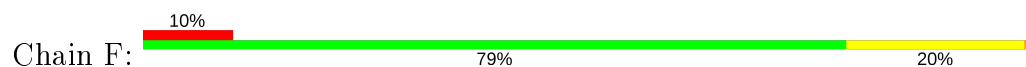
• Molecule 3: CR3022 antibody



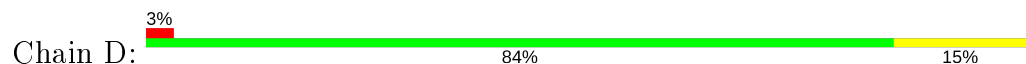
• Molecule 3: CR3022 antibody



• Molecule 4: nanobody D4



• Molecule 4: nanobody D4



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	149.72Å 150.40Å 119.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.86 – 2.71 74.86 – 2.71	Depositor EDS
% Data completeness (in resolution range)	64.3 (74.86-2.71) 64.3 (74.86-2.71)	Depositor EDS
$R_{merge}$	0.23	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.48 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.198 , 0.241 0.198 , 0.240	Depositor DCC
$R_{free}$ test set	2365 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.7	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 24.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.001 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	11731	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% 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	0.32	0/1604	0.54	1/2183 (0.0%)
1	E	0.32	0/1587	0.49	0/2161
2	B	0.30	0/1654	0.54	0/2253
2	H	0.30	0/1654	0.50	0/2253
3	C	0.31	0/1741	0.50	0/2367
3	L	0.30	0/1741	0.50	0/2367
4	D	0.29	0/1010	0.51	0/1366
4	F	0.28	0/1010	0.51	0/1366
All	All	0.30	0/12001	0.51	1/16316 (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	C	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	505	TYR	C-N-CA	6.02	136.76	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	171	GLU	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	A	1560	0	1483	43	0
1	E	1543	0	1459	22	0
2	B	1609	0	1585	36	0
2	H	1609	0	1585	23	0
3	C	1703	0	1649	37	0
3	L	1703	0	1649	26	1
4	D	988	0	951	10	0
4	F	988	0	951	17	1
5	A	14	0	13	0	0
5	E	14	0	13	0	0
All	All	11731	0	11338	194	1

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 8.

All (194) 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:198:TYR:H	2:B:214:LYS:HE2	1.09	1.08
2:B:214:LYS:NZ	2:B:215:VAL:O	2.01	0.91
2:B:198:TYR:N	2:B:214:LYS:HE2	1.87	0.88
4:D:13:GLN:HG2	4:D:126:SER:HB2	1.59	0.84
2:B:91:THR:HG23	2:B:116:THR:HA	1.67	0.77
1:A:388:ASN:HB3	1:A:527:PRO:O	1.86	0.74
1:A:391:CYS:HA	1:A:525:CYS:HB3	1.67	0.74
4:F:36:TRP:HD1	4:F:70:ILE:CD1	2.00	0.73
2:B:147:LYS:HA	2:B:181:SER:HB2	1.70	0.73
3:C:127:SER:HG	3:C:130:GLN:H	1.37	0.72
3:L:96:GLN:HE21	3:L:103:THR:HG22	1.55	0.71
3:C:22:ASN:OD1	3:C:78:THR:OG1	2.08	0.70
3:C:85:GLN:HG2	1:E:372:ALA:HB3	1.75	0.68
2:B:155:THR:OG1	2:B:203:ASN:N	2.26	0.68
1:A:404:GLY:HA3	1:A:504:GLY:HA2	1.75	0.67
2:B:142:LEU:HD13	2:B:215:VAL:HG21	1.77	0.67
4:F:83:MET:HE2	4:F:86:LEU:HD21	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:PRO:HB2	1:A:340:GLU:HG3	1.77	0.66
3:C:2:ILE:HG12	3:C:27:GLN:HB3	1.79	0.65
3:C:43:GLN:HB2	3:C:53:LEU:HD11	1.80	0.64
4:F:36:TRP:HD1	4:F:70:ILE:HD11	1.63	0.64
4:F:28:THR:HB	4:F:77:ASN:HD21	1.61	0.64
3:C:81:ILE:HG21	3:C:84:LEU:HD13	1.80	0.63
4:F:51:ILE:HD13	4:F:70:ILE:HG23	1.79	0.63
2:B:214:LYS:HD3	2:B:215:VAL:N	2.15	0.61
1:A:360:ASN:HA	1:A:523:THR:HB	1.83	0.61
3:L:43:GLN:HB2	3:L:53:LEU:HD11	1.83	0.61
3:L:6:GLN:O	3:L:106:GLN:NE2	2.32	0.61
2:H:142:LEU:HD13	2:H:215:VAL:HG21	1.83	0.60
1:A:455:LEU:HD11	1:A:493:GLN:HB2	1.82	0.60
2:H:32:TYR:HA	2:H:100:SER:HA	1.84	0.59
4:D:27:ARG:O	4:D:98:ARG:NH2	2.35	0.59
4:F:26:GLY:O	4:F:28:THR:HG23	2.03	0.59
3:L:188:SER:OG	3:L:191:ASP:OD2	2.20	0.59
3:L:151:LYS:HG3	3:L:203:THR:HB	1.83	0.58
3:C:6:GLN:O	3:C:106:GLN:NE2	2.31	0.58
2:H:51:ILE:HG13	2:H:58:THR:HG22	1.85	0.57
3:C:54:ILE:HD12	3:C:79:LEU:HD12	1.87	0.57
2:B:197:THR:HG22	2:B:214:LYS:HG3	1.87	0.56
1:A:349:SER:HB3	1:A:452:LEU:H	1.70	0.56
3:L:60:ARG:NH1	3:L:68:PHE:O	2.38	0.56
4:F:36:TRP:CD1	4:F:70:ILE:HD11	2.41	0.56
3:L:45:LYS:NZ	3:L:87:GLU:O	2.39	0.56
1:A:518:LEU:CD2	3:C:35:ASN:HB2	2.36	0.55
3:C:121:VAL:HG21	3:C:202:VAL:HG11	1.88	0.55
1:E:357:ARG:NH1	1:E:359:SER:OG	2.39	0.55
4:D:91:THR:HG23	4:D:124:THR:HA	1.88	0.55
1:A:518:LEU:CD2	3:C:35:ASN:CB	2.85	0.55
1:E:378:LYS:NZ	2:H:57:GLU:OE2	2.39	0.55
2:B:188:VAL:HG11	2:B:198:TYR:CE2	2.43	0.54
4:F:36:TRP:CD1	4:F:70:ILE:CD1	2.88	0.54
2:H:38:ARG:HD3	2:H:40:MET:HG3	1.89	0.54
3:L:157:ASP:HA	3:L:197:VAL:HG22	1.90	0.54
1:E:395:VAL:HG13	1:E:524:VAL:HG11	1.90	0.54
4:F:27:ARG:O	4:F:98:ARG:NH2	2.41	0.54
4:F:23:ALA:HA	4:F:78:THR:HG22	1.90	0.54
1:A:336:CYS:SG	1:A:363:ALA:HB2	2.48	0.54
1:A:371:SER:HA	3:L:67:ARG:HH12	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:THR:OG1	1:A:517:LEU:HA	2.07	0.53
1:E:384:PRO:HA	1:E:387:LEU:HG	1.91	0.53
4:F:71:SER:OG	4:F:80:TYR:HB2	2.09	0.53
3:C:207:LEU:HD13	3:C:211:VAL:HG23	1.90	0.53
2:H:88:ALA:O	2:H:91:THR:HG23	2.09	0.53
2:H:1:GLN:NE2	2:H:27:TYR:O	2.42	0.53
2:B:158:TRP:CD1	2:B:167:VAL:HG21	2.45	0.52
3:L:53:LEU:HA	3:L:64:VAL:HG21	1.92	0.52
1:E:363:ALA:O	1:E:527:PRO:HD2	2.10	0.51
1:E:461:LEU:HD22	1:E:465:GLU:HB3	1.92	0.51
2:B:48:MET:HE1	2:B:94:TYR:HD1	1.74	0.51
1:E:358:ILE:HB	1:E:395:VAL:HG22	1.93	0.51
1:A:366:SER:HA	1:A:369:TYR:CZ	2.45	0.51
2:B:118:ALA:HB3	2:B:150:PHE:CE1	2.45	0.51
1:A:518:LEU:HD21	3:C:35:ASN:CB	2.41	0.50
2:B:117:VAL:HG23	2:B:117:VAL:O	2.12	0.50
1:E:404:GLY:O	1:E:407:VAL:HG12	2.12	0.50
1:A:391:CYS:CA	1:A:525:CYS:HB3	2.38	0.49
3:L:30:LEU:HD11	3:L:74:GLY:HA2	1.93	0.49
2:B:170:PHE:CE2	3:C:182:SER:HB3	2.47	0.49
2:H:38:ARG:HB2	2:H:48:MET:SD	2.52	0.49
1:E:336:CYS:SG	1:E:363:ALA:HB2	2.53	0.49
1:A:406:GLU:OE2	1:A:417:LYS:HE2	2.12	0.49
2:H:105:PRO:HG3	3:L:97:TYR:CZ	2.48	0.49
1:E:498:GLN:O	1:E:501:ASN:HB2	2.13	0.49
2:B:202:VAL:O	2:B:210:LYS:HA	2.12	0.49
2:B:196:GLN:HG3	2:B:197:THR:N	2.28	0.49
3:C:145:PHE:N	3:C:178:THR:OG1	2.47	0.48
2:H:118:ALA:HB3	2:H:150:PHE:CE1	2.48	0.48
2:B:150:PHE:CE1	2:B:151:PRO:HB3	2.49	0.48
3:L:204:HIS:HB3	3:L:207:LEU:HD12	1.95	0.48
3:L:67:ARG:HB2	3:L:82:SER:O	2.13	0.48
1:A:382:VAL:HG21	1:A:387:LEU:HD23	1.95	0.48
2:B:156:VAL:HA	2:B:201:ASN:O	2.14	0.48
1:E:366:SER:HA	1:E:369:TYR:CZ	2.49	0.48
1:A:518:LEU:HD21	3:C:35:ASN:HB2	1.96	0.48
1:A:347:PHE:CD2	1:A:509:ARG:HG2	2.48	0.47
3:C:86:ALA:O	3:C:89:VAL:HG23	2.14	0.47
4:F:106:LEU:HD12	4:F:109:TYR:HD2	1.78	0.47
3:C:89:VAL:HG13	3:C:111:GLU:HA	1.94	0.47
1:E:387:LEU:HA	1:E:389:ASP:OD2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:LEU:HD23	3:C:35:ASN:CB	2.43	0.47
2:H:47:TRP:HZ2	2:H:50:ILE:HB	1.78	0.47
2:B:123:PRO:HB3	2:B:149:TYR:HB3	1.96	0.47
2:B:190:SER:HA	2:B:193:LEU:HD13	1.96	0.47
2:H:156:VAL:HB	2:H:202:VAL:HG12	1.96	0.47
1:A:419:ALA:O	1:A:424:LYS:HD2	2.14	0.47
3:C:6:GLN:HA	3:C:23:CYS:HA	1.95	0.47
1:E:444:LYS:O	1:E:499:PRO:HD3	2.15	0.47
3:L:4:LEU:HD23	3:L:23:CYS:SG	2.55	0.47
4:D:5:VAL:O	4:D:22:CYS:HA	2.15	0.46
3:C:85:GLN:HG3	3:C:86:ALA:H	1.79	0.46
2:B:210:LYS:O	2:B:210:LYS:HG3	2.16	0.46
3:C:4:LEU:HD11	3:C:96:GLN:HG2	1.96	0.46
2:B:4:LEU:HG	2:B:108:VAL:HG12	1.98	0.46
3:L:151:LYS:HZ2	3:L:153:GLN:HG3	1.81	0.46
1:A:387:LEU:C	1:A:389:ASP:H	2.20	0.45
1:A:439:ASN:OD1	1:A:443:SER:OG	2.27	0.45
4:D:5:VAL:HG22	4:D:23:ALA:HB3	1.98	0.45
2:H:31:THR:HG22	2:H:100:SER:HB2	1.98	0.45
4:F:6:GLU:HB2	4:F:121:THR:HG23	1.98	0.45
3:C:172:GLN:HG2	3:C:177:SER:HA	1.98	0.45
1:E:383:SER:OG	2:H:104:THR:OG1	2.32	0.45
2:H:20:ILE:HD11	2:H:81:LEU:HD23	1.98	0.45
2:B:1:GLN:HA	3:L:63:GLY:HA3	1.97	0.45
1:A:335:LEU:HA	1:A:362:VAL:O	2.15	0.45
1:E:349:SER:HB3	1:E:452:LEU:H	1.82	0.45
2:B:6:GLN:NE2	2:B:113:THR:HG23	2.30	0.45
3:L:114:ARG:HG2	3:L:115:THR:N	2.32	0.45
2:B:203:ASN:ND2	2:B:210:LYS:HB2	2.32	0.45
4:F:105:LEU:HA	4:F:105:LEU:HD12	1.83	0.45
1:A:452:LEU:HA	1:A:494:SER:HA	1.99	0.45
1:E:430:THR:OG1	1:E:430:THR:O	2.34	0.45
2:B:142:LEU:HD13	2:B:215:VAL:CG2	2.44	0.44
4:D:34:MET:HG3	4:D:53:TRP:CZ3	2.53	0.44
2:B:203:ASN:HA	2:B:209:THR:O	2.18	0.44
2:B:197:THR:HA	2:B:214:LYS:HE3	2.00	0.44
3:L:2:ILE:O	3:L:103:THR:HG21	2.18	0.44
2:B:12:LYS:HB2	2:B:117:VAL:HG12	1.99	0.44
1:A:334:ASN:N	1:A:334:ASN:OD1	2.50	0.43
1:E:341:VAL:HG11	1:E:397:ALA:HB1	1.99	0.43
2:H:105:PRO:HG2	3:L:55:TYR:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:23:ALA:HA	4:D:78:THR:HG22	1.99	0.43
1:E:361:CYS:SG	1:E:524:VAL:HG23	2.58	0.43
2:B:6:GLN:HE21	2:B:113:THR:HG23	1.83	0.43
4:F:28:THR:HG22	4:F:77:ASN:ND2	2.34	0.43
3:C:53:LEU:HA	3:C:64:VAL:HG21	1.99	0.43
3:L:207:LEU:HD13	3:L:211:VAL:HG12	2.01	0.43
1:E:378:LYS:HE3	1:E:380:TYR:OH	2.19	0.43
4:D:47:PHE:HE1	4:D:50:ALA:HB2	1.84	0.43
1:A:358:ILE:HB	1:A:395:VAL:HB	2.01	0.43
2:B:47:TRP:HZ2	2:B:50:ILE:HB	1.84	0.43
1:A:408:ARG:HH12	2:B:57:GLU:HB2	1.84	0.42
3:C:190:ALA:O	3:C:194:LYS:HG3	2.19	0.42
1:A:393:THR:N	1:A:516:GLU:O	2.49	0.42
1:A:369:TYR:CZ	1:A:385:THR:HG22	2.54	0.42
2:H:155:THR:O	2:H:202:VAL:HA	2.19	0.42
1:A:366:SER:O	1:A:370:ASN:HB2	2.19	0.42
3:C:119:PRO:HB3	3:C:145:PHE:HB3	2.01	0.42
2:B:170:PHE:CZ	3:C:182:SER:HB3	2.54	0.42
2:H:40:MET:HG2	2:H:92:ALA:HB2	2.00	0.42
3:L:37:ASN:O	3:L:56:TRP:HA	2.19	0.42
3:L:34:ILE:O	3:L:36:LYS:N	2.52	0.42
2:B:48:MET:HE1	2:B:94:TYR:CD1	2.54	0.42
3:C:121:VAL:O	3:C:213:LYS:HD2	2.20	0.42
3:C:36:LYS:HA	3:C:36:LYS:HD3	1.79	0.42
3:C:112:ILE:HB	3:C:172:GLN:OE1	2.19	0.42
1:E:419:ALA:O	1:E:424:LYS:HD2	2.20	0.42
1:A:518:LEU:CD2	3:C:35:ASN:HB3	2.49	0.42
3:C:130:GLN:O	3:C:133:SER:HB3	2.20	0.41
1:A:518:LEU:HD23	3:C:35:ASN:HB2	2.02	0.41
1:A:445:VAL:HG23	1:A:446:GLY:H	1.85	0.41
3:C:176:ASP:OD1	3:C:178:THR:HG22	2.20	0.41
3:L:151:LYS:HE3	3:L:203:THR:HB	2.02	0.41
4:F:4:LEU:HD13	4:F:24:VAL:HB	2.02	0.41
1:A:377:PHE:CE2	1:A:434:ILE:HG12	2.56	0.41
1:A:438:SER:HB3	1:A:509:ARG:HD2	2.02	0.41
2:H:123:PRO:HB3	2:H:149:TYR:HB3	2.02	0.41
3:L:3:GLN:H	3:L:26:SER:HB3	1.86	0.41
1:A:518:LEU:HD23	3:C:35:ASN:HB3	2.01	0.41
3:C:37:ASN:O	3:C:56:TRP:HA	2.20	0.41
1:A:416:GLY:N	1:A:420:ASP:OD2	2.47	0.41
1:A:444:LYS:O	1:A:499:PRO:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:102:ILE:HG13	2:B:103:SER:N	2.35	0.41
2:H:150:PHE:HA	2:H:151:PRO:HA	1.80	0.41
2:H:38:ARG:NH1	2:H:40:MET:SD	2.94	0.41
3:C:85:GLN:HG3	3:C:86:ALA:N	2.36	0.41
1:A:518:LEU:HD12	1:A:519:HIS:ND1	2.36	0.40
2:H:156:VAL:HA	2:H:201:ASN:O	2.21	0.40
4:F:18:LEU:HA	4:F:18:LEU:HD23	1.87	0.40
1:E:383:SER:HG	2:H:104:THR:HG1	1.65	0.40
1:A:493:GLN:HG3	4:D:104:SER:H	1.87	0.40
1:A:404:GLY:CA	1:A:504:GLY:HA2	2.48	0.40
1:A:455:LEU:CD1	1:A:493:GLN:HB2	2.50	0.40
4:D:18:LEU:HB2	4:D:86:LEU:HD11	2.04	0.40
3:L:30:LEU:CD1	3:L:74:GLY:HA2	2.52	0.40

All (1) 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)
3:L:14:SER:OG	4:F:127:SER:OG[1_556]	2.07	0.13

## 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	195/197 (99%)	175 (90%)	17 (9%)	3 (2%)	10	24
1	E	193/197 (98%)	176 (91%)	17 (9%)	0	100	100
2	B	213/216 (99%)	203 (95%)	9 (4%)	1 (0%)	29	53
2	H	213/216 (99%)	204 (96%)	9 (4%)	0	100	100
3	C	217/219 (99%)	207 (95%)	10 (5%)	0	100	100
3	L	217/219 (99%)	207 (95%)	10 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	125/127 (98%)	123 (98%)	1 (1%)	1 (1%)	19	41
4	F	125/127 (98%)	123 (98%)	1 (1%)	1 (1%)	19	41
All	All	1498/1518 (99%)	1418 (95%)	74 (5%)	6 (0%)	34	58

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	27	ARG
1	A	360	ASN
1	A	518	LEU
4	F	27	ARG
1	A	527	PRO
2	B	156	VAL

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	170/170 (100%)	161 (95%)	9 (5%)	22	46
1	E	168/170 (99%)	165 (98%)	3 (2%)	59	82
2	B	182/181 (101%)	175 (96%)	7 (4%)	33	60
2	H	182/181 (101%)	178 (98%)	4 (2%)	52	78
3	C	194/194 (100%)	186 (96%)	8 (4%)	30	57
3	L	194/194 (100%)	188 (97%)	6 (3%)	40	68
4	D	101/101 (100%)	98 (97%)	3 (3%)	41	69
4	F	101/101 (100%)	97 (96%)	4 (4%)	31	58
All	All	1292/1292 (100%)	1248 (97%)	44 (3%)	37	65

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

Mol	Chain	Res	Type
1	A	387	LEU

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Mol	Chain	Res	Type
1	A	405	ASP
1	A	427	ASP
1	A	428	ASP
1	A	456	PHE
1	A	458	LYS
1	A	469	SER
1	A	480	CYS
1	A	525	CYS
2	B	61	SER
2	B	84	SER
2	B	85	SER
2	B	181	SER
2	B	200	CYS
2	B	210	LYS
2	B	214	LYS
3	C	31	TYR
3	C	73	SER
3	C	82	SER
3	C	83	SER
3	C	133	SER
3	C	175	LYS
3	C	182	SER
3	C	185	LEU
1	E	346	ARG
1	E	357	ARG
1	E	375	SER
2	H	59	ARG
2	H	106	MET
2	H	210	LYS
2	H	218	LYS
3	L	69	SER
3	L	127	SER
3	L	132	LYS
3	L	148	ARG
3	L	151	LYS
3	L	157	ASP
4	F	17	SER
4	F	21	SER
4	F	22	CYS
4	F	72	ARG
4	D	17	SER
4	D	72	ARG

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Mol	Chain	Res	Type
4	D	88	TYR

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

Mol	Chain	Res	Type
1	A	360	ASN
2	B	203	ASN
3	L	3	GLN
4	F	77	ASN
4	D	1	GLN
4	D	13	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	$\# Z  > 2$
5	NAG	A	601	1	14,14,15	0.64	0	17,19,21	0.74	1 (5%)
5	NAG	E	601	1	14,14,15	0.34	0	17,19,21	0.91	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	601	1	-	1/6/23/26	0/1/1/1
5	NAG	E	601	1	-	2/6/23/26	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(°)
5	E	601	NAG	C1-O5-C5	3.35	116.73	112.19
5	A	601	NAG	C1-O5-C5	2.25	115.25	112.19

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	H	1
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	132:SER	C	137:GLY	N	7.85
1	H	132:SER	C	137:GLY	N	6.87

## 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	197/197 (100%)	0.20	10 (5%)	28 27	27, 51, 127, 207	0
1	E	195/197 (98%)	0.30	7 (3%)	42 42	23, 48, 106, 149	0
2	B	216/216 (100%)	0.16	7 (3%)	47 48	19, 49, 99, 112	0
2	H	216/216 (100%)	0.26	5 (2%)	60 62	19, 40, 87, 118	0
3	C	219/219 (100%)	0.11	3 (1%)	75 77	26, 50, 79, 106	0
3	L	219/219 (100%)	0.07	1 (0%)	91 92	21, 45, 72, 108	0
4	D	127/127 (100%)	0.08	4 (3%)	49 50	32, 63, 108, 137	0
4	F	127/127 (100%)	0.69	13 (10%)	6 5	37, 65, 97, 154	0
All	All	1516/1518 (99%)	0.21	50 (3%)	46 47	19, 49, 98, 207	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	519	HIS	7.9
1	A	528	LYS	7.7
1	A	333	THR	7.3
1	E	518	LEU	5.6
1	A	332	ILE	4.9
2	B	131[A]	SER	4.2
4	D	1	GLN	4.1
1	A	527	PRO	4.0
4	F	4	LEU	3.7
4	F	1	GLN	3.6
2	B	139	THR	3.6
2	H	140	ALA	3.6
1	A	517	LEU	3.5
3	L	34	ILE	3.4
2	H	214	LYS	3.3
1	E	521	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	193	LEU	3.1
1	E	516	GLU	3.1
1	A	526	GLY	3.0
3	C	148	ARG	3.0
2	B	218	LYS	2.9
2	B	140	ALA	2.9
1	A	387	LEU	2.9
4	F	76	LYS	2.9
4	F	121	THR	2.9
4	F	7	SER	2.8
1	E	333	THR	2.8
4	F	118	GLY	2.7
4	F	24	VAL	2.7
4	D	88	TYR	2.7
1	E	517	LEU	2.7
2	B	217	PRO	2.6
4	F	97	ALA	2.6
2	H	131[A]	SER	2.6
2	H	129	ALA	2.5
4	D	26	GLY	2.4
4	D	29	PHE	2.4
1	A	373	SER	2.4
4	F	117	TRP	2.4
1	A	518	LEU	2.4
4	F	29	PHE	2.3
4	F	86	LEU	2.3
2	H	211	VAL	2.2
2	B	219	SER	2.2
1	E	527	PRO	2.2
1	A	519	HIS	2.1
3	C	131	LEU	2.1
4	F	68	PHE	2.1
3	C	203	THR	2.0
4	F	23	ALA	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	A	601	14/15	0.92	0.17	57,76,87,91	0
5	NAG	E	601	14/15	0.94	0.20	54,64,68,69	0

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

There are no such residues in this entry.