



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 11, 2025 – 07:13 pm BST

PDB ID : 9R19 / pdb\_00009r19  
Title : Crystal structure of human ACE2 in complex with VHH B07 and VHH B10  
Authors : Blachier, S.; Vaney, M.C.; Fernandez, I.; Arbabian, A.; Rey, F.A.R.; Haouz, A.; BreLOT, A.  
Deposited on : 2025-04-25  
Resolution : 2.69 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 4-5-2 with Phenix2.0rc1  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

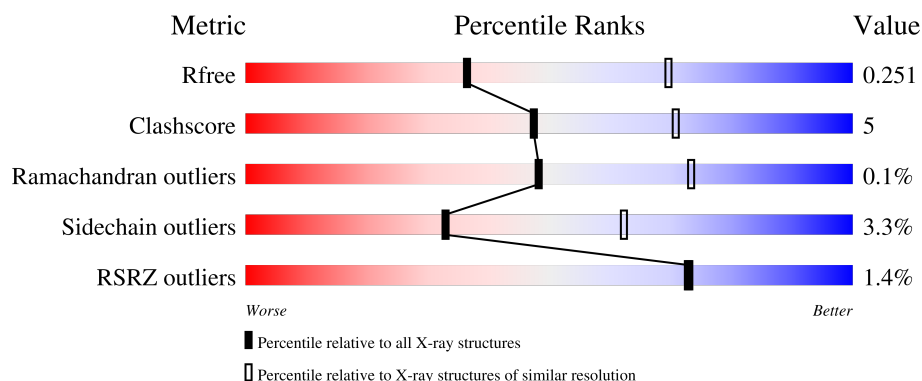
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.69 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))
$R_{free}$	164625	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (2.70-2.70)

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 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	604	<div> <div>85%</div> <div>13%</div> <div>..</div> </div>
1	B	604	<div> <div>%</div> <div>83%</div> <div>14%</div> <div>..</div> </div>
1	C	604	<div> <div>%</div> <div>81%</div> <div>17%</div> <div>..</div> </div>
2	D	153	<div> <div>75%</div> <div>7%</div> <div>..</div> <div>18%</div> </div>
2	E	153	<div> <div>3%</div> <div>74%</div> <div>6%</div> <div>•</div> <div>19%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	153	<div><div><div></div><div></div><div></div></div><div><div>5%</div><div>73%</div><div>6%</div><div>20%</div></div></div>
3	G	143	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>71%</div><div>13%</div><div>17%</div></div></div>
3	H	143	<div><div><div></div><div></div><div></div></div><div><div>5%</div><div>64%</div><div>16%</div><div>19%</div></div></div>
3	I	143	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>63%</div><div>17%</div><div>20%</div></div></div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 20408 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 Processed angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	597	Total	C	N	O	S	0	0	0
			4870	3115	806	920	29			
1	B	595	Total	C	N	O	S	0	0	0
			4856	3108	804	915	29			
1	C	596	Total	C	N	O	S	0	0	0
			4864	3112	805	918	29			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	616	GLY	-	expression tag	UNP Q9BYF1
A	617	SER	-	expression tag	UNP Q9BYF1
A	618	GLY	-	expression tag	UNP Q9BYF1
A	619	LEU	-	expression tag	UNP Q9BYF1
A	620	VAL	-	expression tag	UNP Q9BYF1
A	621	PRO	-	expression tag	UNP Q9BYF1
A	622	ARG	-	expression tag	UNP Q9BYF1
B	616	GLY	-	expression tag	UNP Q9BYF1
B	617	SER	-	expression tag	UNP Q9BYF1
B	618	GLY	-	expression tag	UNP Q9BYF1
B	619	LEU	-	expression tag	UNP Q9BYF1
B	620	VAL	-	expression tag	UNP Q9BYF1
B	621	PRO	-	expression tag	UNP Q9BYF1
B	622	ARG	-	expression tag	UNP Q9BYF1
C	616	GLY	-	expression tag	UNP Q9BYF1
C	617	SER	-	expression tag	UNP Q9BYF1
C	618	GLY	-	expression tag	UNP Q9BYF1
C	619	LEU	-	expression tag	UNP Q9BYF1
C	620	VAL	-	expression tag	UNP Q9BYF1
C	621	PRO	-	expression tag	UNP Q9BYF1
C	622	ARG	-	expression tag	UNP Q9BYF1

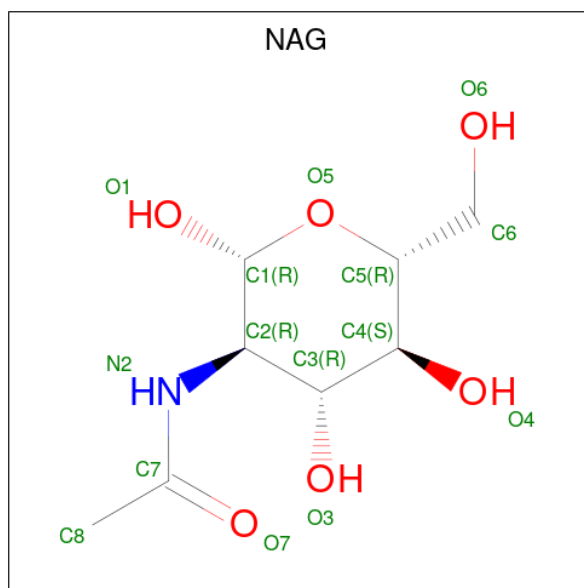
- Molecule 2 is a protein called VHH B10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	126	Total	C	N	O	S	0	0	0
			972	605	169	194	4			
2	E	124	Total	C	N	O	S	0	0	0
			957	597	166	190	4			
2	F	123	Total	C	N	O	S	0	0	0
			951	594	165	188	4			

- Molecule 3 is a protein called VHH B07.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	119	Total	C	N	O	S	0	0	0
			898	552	163	180	3			
3	H	116	Total	C	N	O	S	0	0	0
			883	543	160	177	3			
3	I	114	Total	C	N	O	S	0	0	0
			867	533	158	173	3			

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



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

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

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Cl	0	0
			2	2		
5	B	2	Total	Cl	0	0
			2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	47	Total	O	0	0
			47	47		
6	B	29	Total	O	0	0
			29	29		
6	C	9	Total	O	0	0
			9	9		
6	D	7	Total	O	0	0
			7	7		
6	E	1	Total	O	0	0
			1	1		

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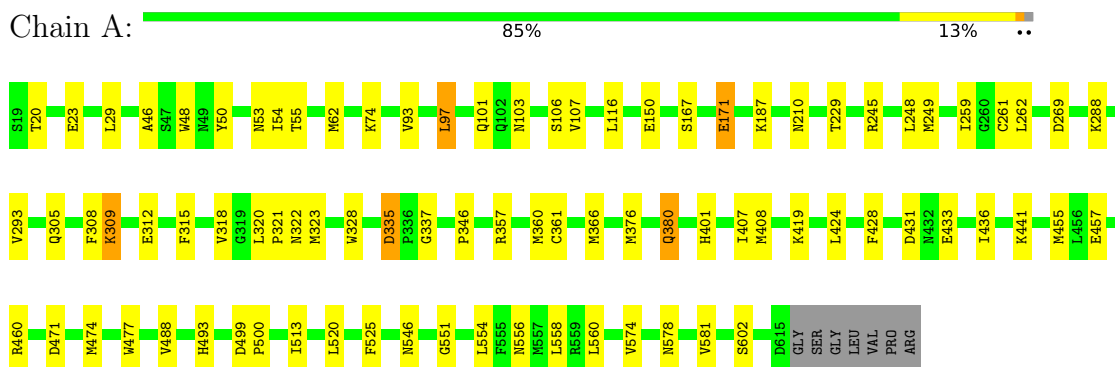
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total 1	O 1	0	0
6	G	8	Total 8	O 8	0	0
6	H	2	Total 2	O 2	0	0

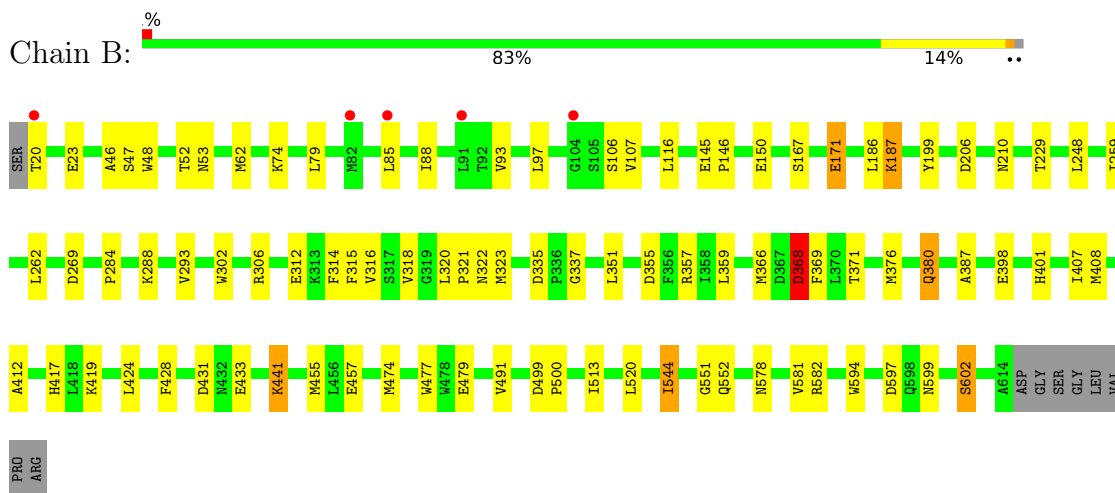
### 3 Residue-property plots [i](#)

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.

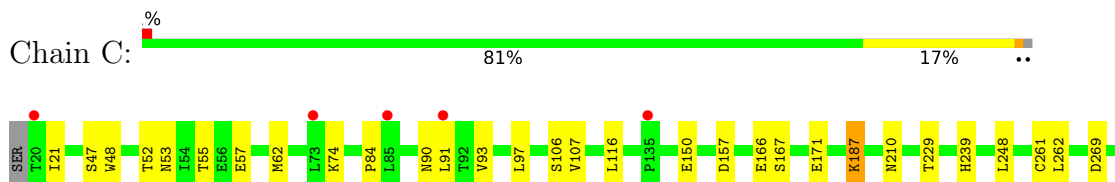
#### • Molecule 1: Processed angiotensin-converting enzyme 2



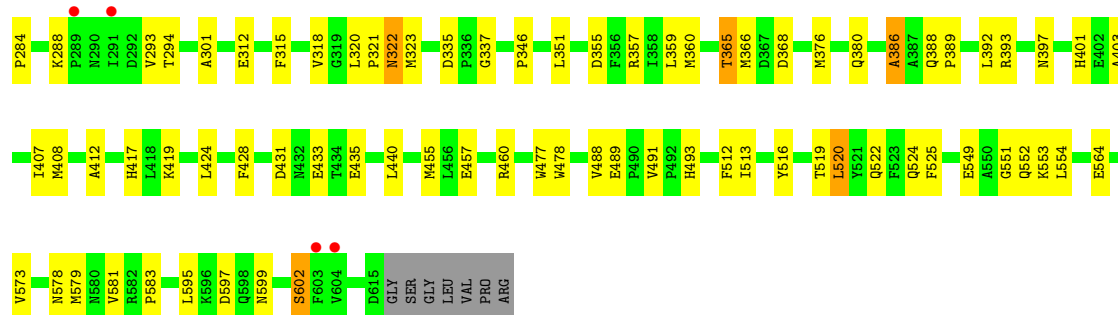
#### • Molecule 1: Processed angiotensin-converting enzyme 2



#### • Molecule 1: Processed angiotensin-converting enzyme 2



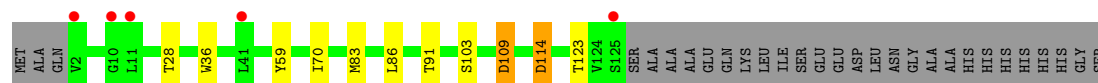
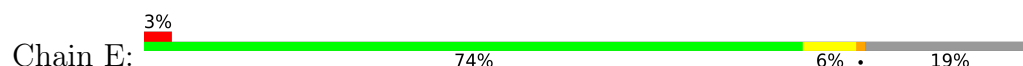




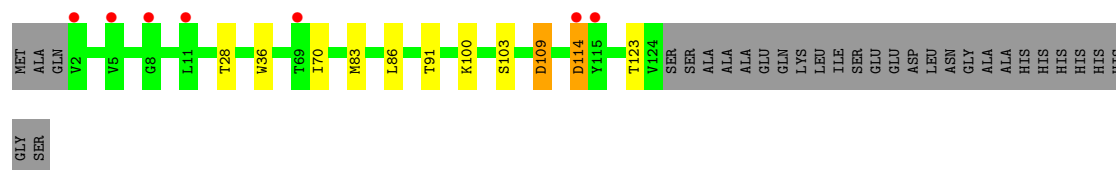
- Molecule 2: VHH B10



- Molecule 2: VHH B10



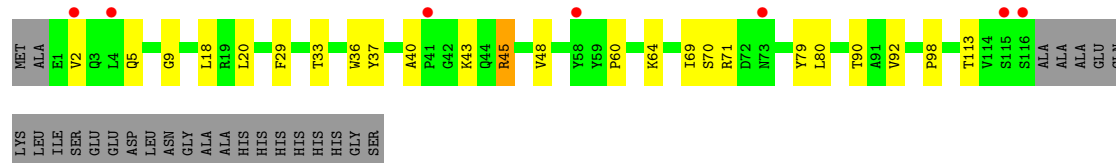
- Molecule 2: VHH B10



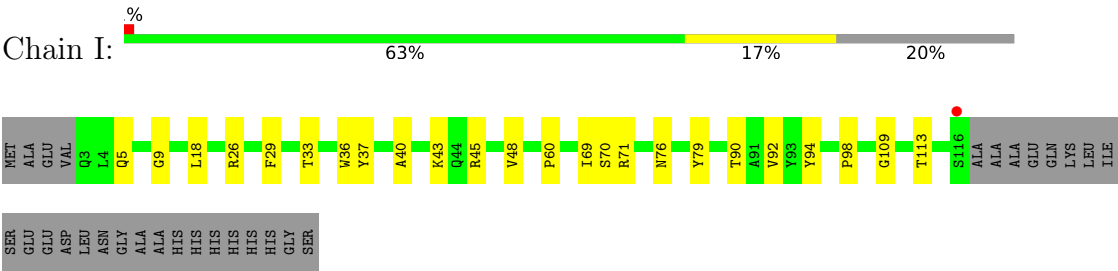
- Molecule 3: VHH B07



- Molecule 3: VHH B07



● Molecule 3: VHH B07



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.92Å 108.15Å 146.10Å 90.00° 98.89° 90.00°	Depositor
Resolution (Å)	48.30 – 2.69 48.30 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.30-2.69) 99.7 (48.30-2.69)	Depositor EDS
$R_{merge}$	0.22	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.74 (at 2.69Å)	Xtriage
Refinement program	BUSTER 2.10.4 (10-JUL-2024)	Depositor
R, $R_{free}$	0.220 , 0.255 0.214 , 0.251	Depositor DCC
$R_{free}$ test set	4180 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.6	Xtriage
Anisotropy	0.400	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 57.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	20408	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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: CL, 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	0.69	1/5007 (0.0%)	1.10	10/6803 (0.1%)
1	B	0.67	0/4993	1.09	8/6784 (0.1%)
1	C	0.65	0/5001	1.06	10/6795 (0.1%)
2	D	0.60	0/990	0.89	3/1336 (0.2%)
2	E	0.57	0/975	0.88	3/1316 (0.2%)
2	F	0.55	0/969	0.86	3/1308 (0.2%)
3	G	0.64	0/914	0.93	0/1240
3	H	0.58	0/899	0.87	0/1219
3	I	0.55	0/883	0.85	0/1197
All	All	0.65	1/20631 (0.0%)	1.03	37/27998 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	546	ASN	CG-ND2	-5.88	1.20	1.33

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	322	ASN	CA-CB-CG	11.97	124.57	112.60
1	C	322	ASN	OD1-CG-ND2	-8.10	114.50	122.60
1	A	103	ASN	OD1-CG-ND2	-7.97	114.63	122.60
1	C	397	ASN	CA-CB-CG	6.17	118.77	112.60
1	C	322	ASN	CB-CG-ND2	6.08	125.53	116.40

There are no chirality outliers.

There are no planarity outliers.

## 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	4870	0	4638	52	0
1	B	4856	0	4630	52	0
1	C	4864	0	4633	60	0
2	D	972	0	929	4	0
2	E	957	0	913	5	0
2	F	951	0	908	4	0
3	G	898	0	869	14	0
3	H	883	0	854	12	0
3	I	867	0	836	18	0
4	A	56	0	52	1	0
4	B	56	0	52	5	0
4	C	70	0	65	2	0
5	A	2	0	0	0	0
5	B	2	0	0	1	0
6	A	47	0	0	0	0
6	B	29	0	0	0	0
6	C	9	0	0	0	0
6	D	7	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
6	G	8	0	0	0	0
6	H	2	0	0	0	0
All	All	20408	0	19379	217	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 5.

The worst 5 of 217 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)
4:B:704:NAG:H61	1:C:393:ARG:HH12	1.23	1.02
3:I:36:TRP:HD1	3:I:69:ILE:HD12	1.33	0.93
3:G:36:TRP:HD1	3:G:69:ILE:HD12	1.34	0.91
1:A:312:GLU:HA	1:A:376:MET:HE1	1.53	0.89
1:B:323:MET:HE3	1:B:376:MET:HE3	1.54	0.89

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	A	595/604 (98%)	580 (98%)	14 (2%)	1 (0%)	44	68
1	B	593/604 (98%)	575 (97%)	17 (3%)	1 (0%)	44	68
1	C	594/604 (98%)	572 (96%)	21 (4%)	1 (0%)	44	68
2	D	124/153 (81%)	121 (98%)	3 (2%)	0	100	100
2	E	122/153 (80%)	118 (97%)	4 (3%)	0	100	100
2	F	121/153 (79%)	117 (97%)	4 (3%)	0	100	100
3	G	117/143 (82%)	114 (97%)	3 (3%)	0	100	100
3	H	114/143 (80%)	110 (96%)	4 (4%)	0	100	100
3	I	112/143 (78%)	110 (98%)	2 (2%)	0	100	100
All	All	2492/2700 (92%)	2417 (97%)	72 (3%)	3 (0%)	48	73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	337	GLY
1	C	337	GLY
1	B	337	GLY

### 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	527/532 (99%)	510 (97%)	17 (3%)	34	63
1	B	525/532 (99%)	504 (96%)	21 (4%)	27	55
1	C	526/532 (99%)	511 (97%)	15 (3%)	37	67
2	D	102/121 (84%)	97 (95%)	5 (5%)	21	47
2	E	100/121 (83%)	97 (97%)	3 (3%)	36	65
2	F	99/121 (82%)	96 (97%)	3 (3%)	36	65
3	G	96/115 (84%)	93 (97%)	3 (3%)	35	64
3	H	96/115 (84%)	93 (97%)	3 (3%)	35	64
3	I	94/115 (82%)	93 (99%)	1 (1%)	70	87
All	All	2165/2304 (94%)	2094 (97%)	71 (3%)	33	62

5 of 71 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	126	SER
2	E	109	ASP
3	G	70	SER
1	B	210	ASN
1	B	187	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	601	ASN
3	H	5	GLN
2	D	84	ASN
3	G	5	GLN
3	H	76	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

Of 17 ligands modelled in this entry, 4 are monoatomic - leaving 13 for Mogul analysis.

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	C	701	1	14,14,15	0.42	0	17,19,21	1.97	2 (11%)
4	NAG	A	702	1	14,14,15	0.59	0	17,19,21	1.19	1 (5%)
4	NAG	C	704	1	14,14,15	0.24	0	17,19,21	0.50	0
4	NAG	B	702	1	14,14,15	0.31	0	17,19,21	0.52	0
4	NAG	C	703	1	14,14,15	0.36	0	17,19,21	0.96	1 (5%)
4	NAG	C	705	1	14,14,15	0.32	0	17,19,21	0.53	0
4	NAG	A	703	1	14,14,15	0.31	0	17,19,21	0.74	0
4	NAG	A	704	1	14,14,15	0.33	0	17,19,21	0.79	1 (5%)
4	NAG	A	701	1	14,14,15	0.59	0	17,19,21	1.53	1 (5%)
4	NAG	B	704	1	14,14,15	0.32	0	17,19,21	1.08	1 (5%)
4	NAG	B	701	1	14,14,15	0.28	0	17,19,21	0.87	1 (5%)
4	NAG	C	702	1	14,14,15	0.26	0	17,19,21	0.51	0
4	NAG	B	703	1	14,14,15	0.28	0	17,19,21	0.51	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	C	701	1	-	5/6/23/26	0/1/1/1
4	NAG	A	702	1	-	0/6/23/26	0/1/1/1
4	NAG	C	704	1	-	0/6/23/26	0/1/1/1
4	NAG	B	702	1	-	2/6/23/26	0/1/1/1
4	NAG	C	703	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	705	1	-	1/6/23/26	0/1/1/1
4	NAG	A	703	1	-	2/6/23/26	0/1/1/1
4	NAG	A	704	1	-	2/6/23/26	0/1/1/1
4	NAG	A	701	1	-	3/6/23/26	0/1/1/1
4	NAG	B	704	1	-	4/6/23/26	0/1/1/1
4	NAG	B	701	1	-	2/6/23/26	0/1/1/1
4	NAG	C	702	1	-	2/6/23/26	0/1/1/1
4	NAG	B	703	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	701	NAG	C1-O5-C5	5.97	120.28	112.19
4	C	701	NAG	C1-O5-C5	5.92	120.21	112.19
4	C	701	NAG	C2-N2-C7	4.77	129.69	122.90
4	A	702	NAG	C1-O5-C5	4.55	118.36	112.19
4	B	704	NAG	C2-N2-C7	3.36	127.69	122.90

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	704	NAG	C3-C2-N2-C7
4	B	704	NAG	C8-C7-N2-C2
4	B	704	NAG	O7-C7-N2-C2
4	C	701	NAG	C3-C2-N2-C7
4	C	701	NAG	C8-C7-N2-C2

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	701	NAG	2	0
4	A	701	NAG	1	0
4	B	704	NAG	5	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	597/604 (98%)	-0.41	0 <span>100</span> <span>100</span>	32, 47, 69, 84	0
1	B	595/604 (98%)	-0.19	5 (0%) <span>82</span> <span>82</span>	34, 57, 92, 122	0
1	C	596/604 (98%)	0.09	9 (1%) <span>71</span> <span>71</span>	48, 69, 111, 138	0
2	D	126/153 (82%)	-0.17	0 <span>100</span> <span>100</span>	42, 65, 81, 88	0
2	E	124/153 (81%)	0.42	5 (4%) <span>43</span> <span>41</span>	49, 91, 136, 147	0
2	F	123/153 (80%)	0.53	7 (5%) <span>30</span> <span>28</span>	68, 107, 142, 153	0
3	G	119/143 (83%)	-0.17	1 (0%) <span>82</span> <span>82</span>	46, 62, 83, 124	0
3	H	116/143 (81%)	0.78	7 (6%) <span>29</span> <span>27</span>	83, 114, 141, 153	0
3	I	114/143 (79%)	0.73	1 (0%) <span>81</span> <span>80</span>	99, 132, 160, 167	0
All	All	2510/2700 (92%)	-0.02	35 (1%) <span>73</span> <span>73</span>	32, 63, 131, 167	0

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	119	ALA	4.5
1	C	291	ILE	3.7
3	H	116	SER	3.5
1	C	91	LEU	2.9
2	E	2	VAL	2.9

### 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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	B	703	14/15	0.51	0.14	108,109,109,109	0
4	NAG	B	702	14/15	0.59	0.18	113,114,114,114	0
4	NAG	A	704	14/15	0.62	0.19	89,90,91,91	0
4	NAG	C	704	14/15	0.68	0.14	134,134,135,135	0
4	NAG	C	705	14/15	0.69	0.13	86,87,87,88	0
4	NAG	C	703	14/15	0.73	0.15	77,78,79,80	0
4	NAG	C	702	14/15	0.80	0.11	94,94,95,95	0
4	NAG	B	704	14/15	0.82	0.15	77,79,79,79	0
4	NAG	A	702	14/15	0.84	0.13	71,72,73,73	0
4	NAG	C	701	14/15	0.84	0.17	70,71,72,73	0
4	NAG	B	701	14/15	0.84	0.09	72,73,73,74	0
4	NAG	A	701	14/15	0.86	0.12	68,69,71,71	0
4	NAG	A	703	14/15	0.88	0.10	75,77,77,77	0
5	CL	B	705	1/1	0.88	0.13	71,71,71,71	0
5	CL	A	705	1/1	0.96	0.08	51,51,51,51	0
5	CL	A	706	1/1	0.99	0.09	32,32,32,32	0
5	CL	B	706	1/1	0.99	0.03	42,42,42,42	0

## 6.5 Other polymers

There are no such residues in this entry.