



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:51 PM GMT

PDB ID : 4FQR
Title : Crystal structure of broadly neutralizing antibody C05 bound to H3 influenza hemagglutinin
Authors : Ekiert, D.C.; Wilson, I.A.
Deposited on : 2012-06-25
Resolution : 4.10 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

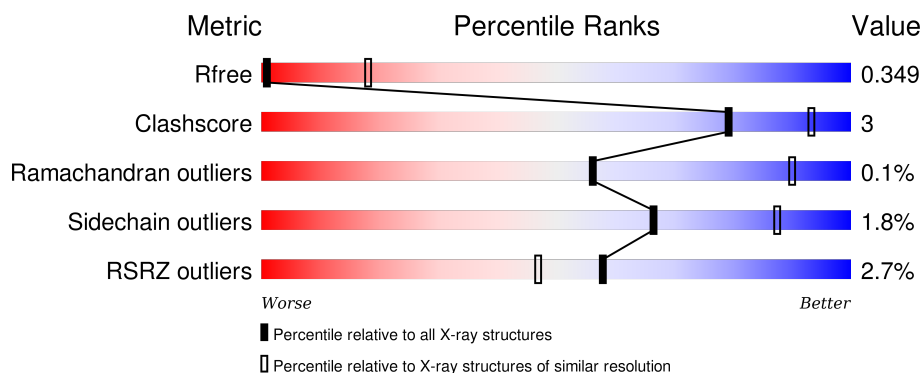
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.10 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}	91344	1018 (4.60-3.60)
Clashscore	102246	1117 (4.60-3.60)
Ramachandran outliers	100387	1063 (4.60-3.60)
Sidechain outliers	100360	1049 (4.60-3.60)
RSRZ outliers	91569	1022 (4.60-3.60)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	323	<div> <div>4%</div> <div>95%</div> <div>• •</div> </div>
1	C	323	<div> <div>2%</div> <div>95%</div> <div>• •</div> </div>
1	E	323	<div> <div>2%</div> <div>95%</div> <div>• •</div> </div>
1	G	323	<div> <div>2%</div> <div>95%</div> <div>• •</div> </div>
1	I	323	<div> <div>3%</div> <div>92%</div> <div>6% •</div> </div>

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Mol	Chain	Length	Quality of chain
1	K	323	
1	M	323	
1	O	323	
1	Q	323	
1	S	323	
1	U	323	
1	W	323	
2	B	174	
2	D	174	
2	F	174	
2	H	174	
2	J	174	
2	L	174	
2	N	174	
2	P	174	
2	R	174	
2	T	174	
2	V	174	
2	X	174	
3	a	241	
3	c	241	
3	e	241	
3	g	241	
3	i	241	
3	k	241	

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Mol	Chain	Length	Quality of chain
3	m	241	
3	o	241	
3	q	241	
3	s	241	
3	u	241	
3	w	241	
4	b	214	
4	d	214	
4	f	214	
4	h	214	
4	j	214	
4	l	214	
4	n	214	
4	p	214	
4	r	214	
4	t	214	
4	v	214	
4	x	214	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	A	601	-	-	-	X
5	NAG	C	501	-	-	-	X
5	NAG	D	201	-	-	-	X
5	NAG	G	502	-	-	-	X
5	NAG	I	501	-	-	-	X
5	NAG	L	201	-	-	-	X
5	NAG	N	201	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	O	501	-	-	-	X
5	NAG	S	501	-	-	-	X
5	NAG	T	201	-	-	-	X
6	NAG	K	603	-	-	-	X
6	NAG	O	504	-	-	-	X
7	NAG	I	506	-	-	-	X
7	NAG	M	507	-	-	-	X
7	NAG	U	507	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 90792 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 Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	12	0
			2553	1598	450	491	14			
1	C	318	Total	C	N	O	S	0	12	0
			2553	1598	450	491	14			
1	E	318	Total	C	N	O	S	0	12	0
			2553	1598	450	491	14			
1	G	318	Total	C	N	O	S	0	12	0
			2553	1598	450	491	14			
1	I	318	Total	C	N	O	S	0	12	0
			2553	1598	450	491	14			
1	K	318	Total	C	N	O	S	0	12	0
			2553	1598	450	491	14			
1	M	318	Total	C	N	O	S	0	12	0
			2553	1598	450	491	14			
1	O	318	Total	C	N	O	S	0	12	0
			2553	1598	450	491	14			
1	Q	318	Total	C	N	O	S	0	12	0
			2553	1598	450	491	14			
1	S	318	Total	C	N	O	S	0	12	0
			2553	1598	450	491	14			
1	U	318	Total	C	N	O	S	0	12	0
			2553	1598	450	491	14			
1	W	318	Total	C	N	O	S	0	12	0
			2553	1598	450	491	14			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	-	EXPRESSION TAG	UNP Q91MA7
A	8	ASP	-	EXPRESSION TAG	UNP Q91MA7
A	9	PRO	-	EXPRESSION TAG	UNP Q91MA7
A	10	GLY	-	EXPRESSION TAG	UNP Q91MA7
C	7	ALA	-	EXPRESSION TAG	UNP Q91MA7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	8	ASP	-	EXPRESSION TAG	UNP Q91MA7
C	9	PRO	-	EXPRESSION TAG	UNP Q91MA7
C	10	GLY	-	EXPRESSION TAG	UNP Q91MA7
E	7	ALA	-	EXPRESSION TAG	UNP Q91MA7
E	8	ASP	-	EXPRESSION TAG	UNP Q91MA7
E	9	PRO	-	EXPRESSION TAG	UNP Q91MA7
E	10	GLY	-	EXPRESSION TAG	UNP Q91MA7
G	7	ALA	-	EXPRESSION TAG	UNP Q91MA7
G	8	ASP	-	EXPRESSION TAG	UNP Q91MA7
G	9	PRO	-	EXPRESSION TAG	UNP Q91MA7
G	10	GLY	-	EXPRESSION TAG	UNP Q91MA7
I	7	ALA	-	EXPRESSION TAG	UNP Q91MA7
I	8	ASP	-	EXPRESSION TAG	UNP Q91MA7
I	9	PRO	-	EXPRESSION TAG	UNP Q91MA7
I	10	GLY	-	EXPRESSION TAG	UNP Q91MA7
K	7	ALA	-	EXPRESSION TAG	UNP Q91MA7
K	8	ASP	-	EXPRESSION TAG	UNP Q91MA7
K	9	PRO	-	EXPRESSION TAG	UNP Q91MA7
K	10	GLY	-	EXPRESSION TAG	UNP Q91MA7
M	7	ALA	-	EXPRESSION TAG	UNP Q91MA7
M	8	ASP	-	EXPRESSION TAG	UNP Q91MA7
M	9	PRO	-	EXPRESSION TAG	UNP Q91MA7
M	10	GLY	-	EXPRESSION TAG	UNP Q91MA7
O	7	ALA	-	EXPRESSION TAG	UNP Q91MA7
O	8	ASP	-	EXPRESSION TAG	UNP Q91MA7
O	9	PRO	-	EXPRESSION TAG	UNP Q91MA7
O	10	GLY	-	EXPRESSION TAG	UNP Q91MA7
Q	7	ALA	-	EXPRESSION TAG	UNP Q91MA7
Q	8	ASP	-	EXPRESSION TAG	UNP Q91MA7
Q	9	PRO	-	EXPRESSION TAG	UNP Q91MA7
Q	10	GLY	-	EXPRESSION TAG	UNP Q91MA7
S	7	ALA	-	EXPRESSION TAG	UNP Q91MA7
S	8	ASP	-	EXPRESSION TAG	UNP Q91MA7
S	9	PRO	-	EXPRESSION TAG	UNP Q91MA7
S	10	GLY	-	EXPRESSION TAG	UNP Q91MA7
U	7	ALA	-	EXPRESSION TAG	UNP Q91MA7
U	8	ASP	-	EXPRESSION TAG	UNP Q91MA7
U	9	PRO	-	EXPRESSION TAG	UNP Q91MA7
U	10	GLY	-	EXPRESSION TAG	UNP Q91MA7
W	7	ALA	-	EXPRESSION TAG	UNP Q91MA7
W	8	ASP	-	EXPRESSION TAG	UNP Q91MA7
W	9	PRO	-	EXPRESSION TAG	UNP Q91MA7

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Chain	Residue	Modelled	Actual	Comment	Reference
W	10	GLY	-	EXPRESSION TAG	UNP Q91MA7

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	7	0
			1446	901	251	287	7			
2	D	172	Total	C	N	O	S	0	7	0
			1446	901	251	287	7			
2	F	172	Total	C	N	O	S	0	7	0
			1446	901	251	287	7			
2	H	172	Total	C	N	O	S	0	7	0
			1446	901	251	287	7			
2	J	172	Total	C	N	O	S	0	7	0
			1446	901	251	287	7			
2	L	172	Total	C	N	O	S	0	7	0
			1446	901	251	287	7			
2	N	172	Total	C	N	O	S	0	7	0
			1446	901	251	287	7			
2	P	172	Total	C	N	O	S	0	7	0
			1446	901	251	287	7			
2	R	172	Total	C	N	O	S	0	7	0
			1446	901	251	287	7			
2	T	172	Total	C	N	O	S	0	7	0
			1446	901	251	287	7			
2	V	172	Total	C	N	O	S	0	7	0
			1446	901	251	287	7			
2	X	172	Total	C	N	O	S	0	7	0
			1446	901	251	287	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7
D	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7
F	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7
H	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7
J	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7
L	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7
N	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7
P	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7
R	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7

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Chain	Residue	Modelled	Actual	Comment	Reference
T	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7
V	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7
X	123	GLY	ARG	SEE REMARK 999	UNP Q91MA7

- Molecule 3 is a protein called Broadly neutralizing antibody C05, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	a	239	Total	C	N	O	S	0	4	0
			1806	1127	306	365	8			
3	c	239	Total	C	N	O	S	0	4	0
			1806	1127	306	365	8			
3	e	239	Total	C	N	O	S	0	4	0
			1806	1127	306	365	8			
3	g	239	Total	C	N	O	S	0	4	0
			1806	1127	306	365	8			
3	i	239	Total	C	N	O	S	0	4	0
			1806	1127	306	365	8			
3	k	239	Total	C	N	O	S	0	4	0
			1806	1127	306	365	8			
3	m	239	Total	C	N	O	S	0	4	0
			1806	1127	306	365	8			
3	o	239	Total	C	N	O	S	0	4	0
			1806	1127	306	365	8			
3	q	239	Total	C	N	O	S	0	4	0
			1806	1127	306	365	8			
3	s	239	Total	C	N	O	S	0	4	0
			1806	1127	306	365	8			
3	u	239	Total	C	N	O	S	0	4	0
			1806	1127	306	365	8			
3	w	239	Total	C	N	O	S	0	4	0
			1806	1127	306	365	8			

- Molecule 4 is a protein called Broadly neutralizing antibody C05, light chain.

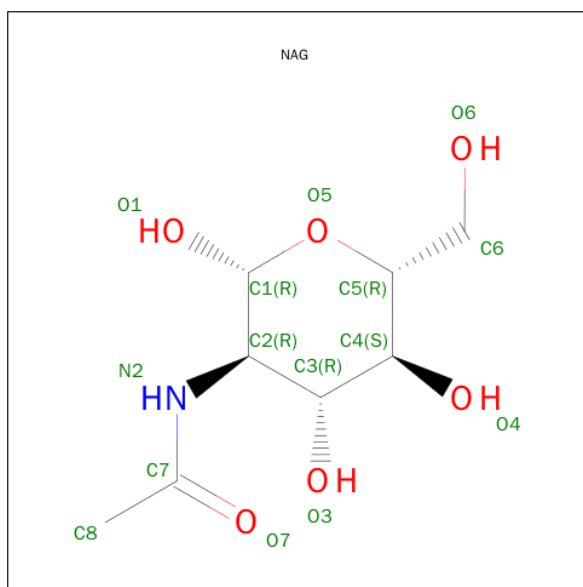
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	b	213	Total	C	N	O	S	0	1	0
			1648	1033	281	330	4			
4	d	213	Total	C	N	O	S	0	1	0
			1648	1033	281	330	4			
4	f	213	Total	C	N	O	S	0	1	0
			1648	1033	281	330	4			
4	h	213	Total	C	N	O	S	0	1	0
			1648	1033	281	330	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	j	213	Total	C	N	O	S	0	1	0
			1648	1033	281	330	4			
4	l	213	Total	C	N	O	S	0	1	0
			1648	1033	281	330	4			
4	n	213	Total	C	N	O	S	0	1	0
			1648	1033	281	330	4			
4	p	213	Total	C	N	O	S	0	1	0
			1648	1033	281	330	4			
4	r	213	Total	C	N	O	S	0	1	0
			1648	1033	281	330	4			
4	t	213	Total	C	N	O	S	0	1	0
			1648	1033	281	330	4			
4	v	213	Total	C	N	O	S	0	1	0
			1648	1033	281	330	4			
4	x	213	Total	C	N	O	S	0	1	0
			1648	1033	281	330	4			

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	H	1	Total	C	N	O	0	0
			14	8	1	5		
5	I	1	Total	C	N	O	0	0
			14	8	1	5		
5	J	1	Total	C	N	O	0	0
			14	8	1	5		
5	K	1	Total	C	N	O	0	0
			14	8	1	5		
5	L	1	Total	C	N	O	0	0
			14	8	1	5		
5	M	1	Total	C	N	O	0	0
			14	8	1	5		
5	M	1	Total	C	N	O	0	0
			14	8	1	5		
5	N	1	Total	C	N	O	0	0
			14	8	1	5		
5	O	1	Total	C	N	O	0	0
			14	8	1	5		
5	O	1	Total	C	N	O	0	0
			14	8	1	5		
5	P	1	Total	C	N	O	0	0
			14	8	1	5		
5	Q	1	Total	C	N	O	0	0
			14	8	1	5		
5	Q	1	Total	C	N	O	0	0
			14	8	1	5		
5	R	1	Total	C	N	O	0	0
			14	8	1	5		
5	S	1	Total	C	N	O	0	0
			14	8	1	5		
5	S	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	T	1	Total	C	N	O	0	0
			14	8	1	5		
5	U	1	Total	C	N	O	0	0
			14	8	1	5		
5	U	1	Total	C	N	O	0	0
			14	8	1	5		
5	V	1	Total	C	N	O	0	0
			14	8	1	5		
5	W	1	Total	C	N	O	0	0
			14	8	1	5		
5	X	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	4	Total	C	N	O	0	0
			50	28	2	20		
6	C	4	Total	C	N	O	0	0
			50	28	2	20		
6	E	4	Total	C	N	O	0	0
			50	28	2	20		
6	G	4	Total	C	N	O	0	0
			50	28	2	20		
6	I	4	Total	C	N	O	0	0
			50	28	2	20		
6	K	4	Total	C	N	O	0	0
			50	28	2	20		
6	M	4	Total	C	N	O	0	0
			50	28	2	20		
6	O	4	Total	C	N	O	0	0
			50	28	2	20		
6	Q	4	Total	C	N	O	0	0
			50	28	2	20		
6	S	4	Total	C	N	O	0	0
			50	28	2	20		
6	U	4	Total	C	N	O	0	0
			50	28	2	20		
6	W	4	Total	C	N	O	0	0
			50	28	2	20		

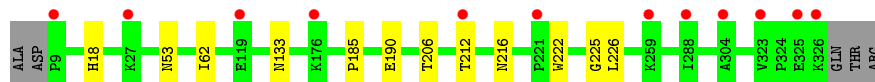
- Molecule 7 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	2	Total 28	C 16	N 2	O 10	0	0
7	C	2	Total 28	C 16	N 2	O 10	0	0
7	E	2	Total 28	C 16	N 2	O 10	0	0
7	G	2	Total 28	C 16	N 2	O 10	0	0
7	I	2	Total 28	C 16	N 2	O 10	0	0
7	K	2	Total 28	C 16	N 2	O 10	0	0
7	M	2	Total 28	C 16	N 2	O 10	0	0
7	O	2	Total 28	C 16	N 2	O 10	0	0
7	Q	2	Total 28	C 16	N 2	O 10	0	0
7	S	2	Total 28	C 16	N 2	O 10	0	0
7	U	2	Total 28	C 16	N 2	O 10	0	0
7	W	2	Total 28	C 16	N 2	O 10	0	0

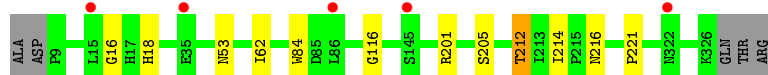
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Hemagglutinin HA1 chain



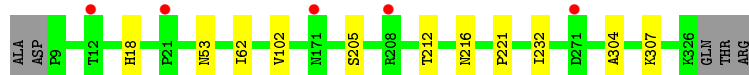
- Molecule 1: Hemagglutinin HA1 chain



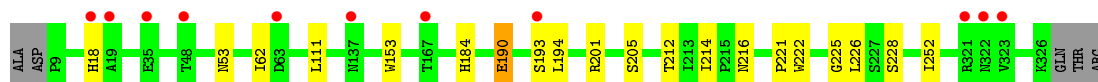
- Molecule 1: Hemagglutinin HA1 chain



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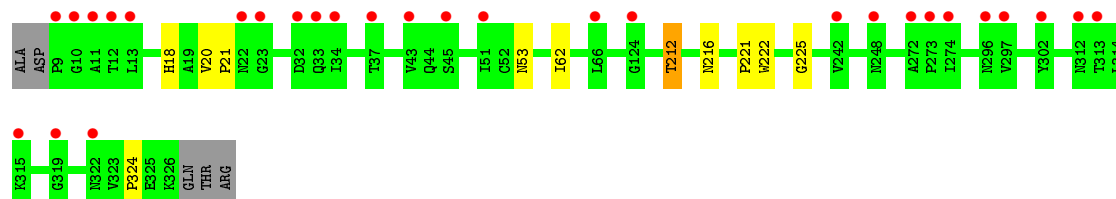
- Molecule 1: Hemagglutinin HA1 chain



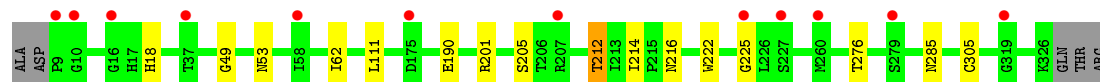
- Molecule 1: Hemagglutinin HA1 chain



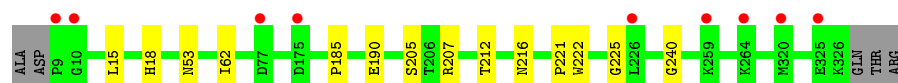
- Molecule 1: Hemagglutinin HA1 chain



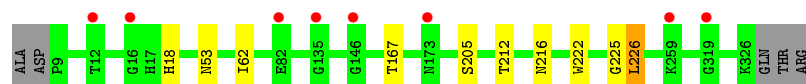
- Molecule 1: Hemagglutinin HA1 chain



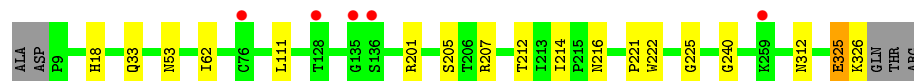
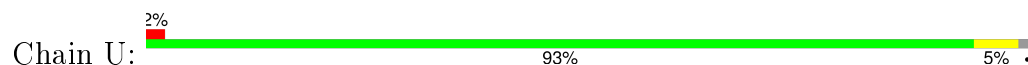
- Molecule 1: Hemagglutinin HA1 chain



- Molecule 1: Hemagglutinin HA1 chain

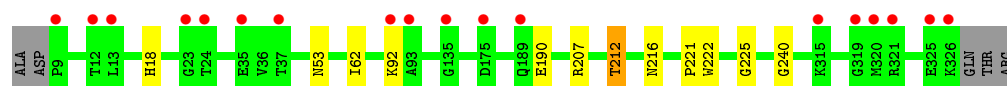


- Molecule 1: Hemagglutinin HA1 chain



- Molecule 1: Hemagglutinin HA1 chain

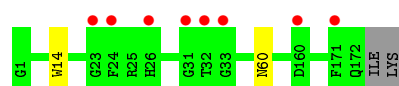




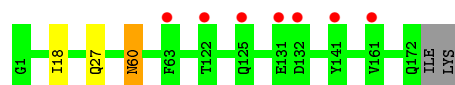
- Molecule 2: Hemagglutinin HA2 chain



- Molecule 2: Hemagglutinin HA2 chain



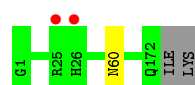
- Molecule 2: Hemagglutinin HA2 chain



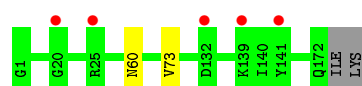
- Molecule 2: Hemagglutinin HA2 chain



- Molecule 2: Hemagglutinin HA2 chain

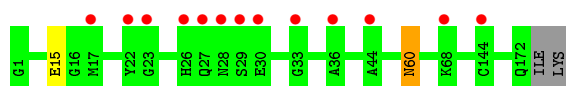


- Molecule 2: Hemagglutinin HA2 chain

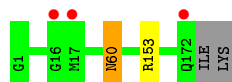


- Molecule 2: Hemagglutinin HA2 chain

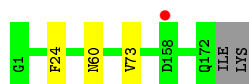




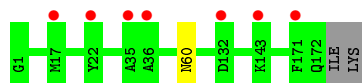
- Molecule 2: Hemagglutinin HA2 chain



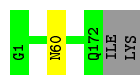
- Molecule 2: Hemagglutinin HA2 chain



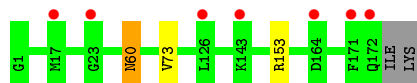
- Molecule 2: Hemagglutinin HA2 chain



- Molecule 2: Hemagglutinin HA2 chain



- Molecule 2: Hemagglutinin HA2 chain



- Molecule 3: Broadly neutralizing antibody C05, heavy chain

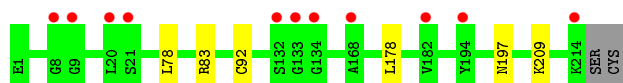


- Molecule 3: Broadly neutralizing antibody C05, heavy chain





- Molecule 3: Broadly neutralizing antibody C05, heavy chain



- Molecule 3: Broadly neutralizing antibody C05, heavy chain



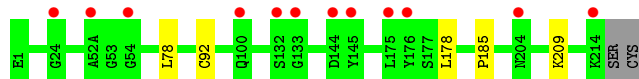
- Molecule 3: Broadly neutralizing antibody C05, heavy chain



- Molecule 3: Broadly neutralizing antibody C05, heavy chain



- Molecule 3: Broadly neutralizing antibody C05, heavy chain

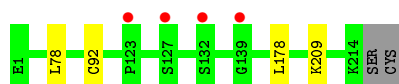


- Molecule 3: Broadly neutralizing antibody C05, heavy chain

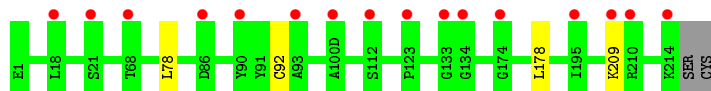


- Molecule 3: Broadly neutralizing antibody C05, heavy chain

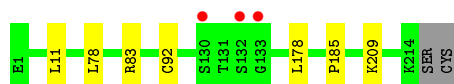




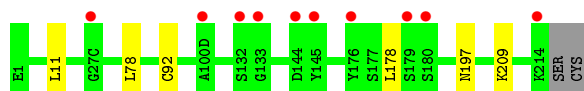
- Molecule 3: Broadly neutralizing antibody C05, heavy chain



- Molecule 3: Broadly neutralizing antibody C05, heavy chain



- Molecule 3: Broadly neutralizing antibody C05, heavy chain



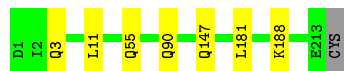
- Molecule 4: Broadly neutralizing antibody C05, light chain



- Molecule 4: Broadly neutralizing antibody C05, light chain

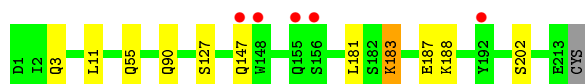


- Molecule 4: Broadly neutralizing antibody C05, light chain



- Molecule 4: Broadly neutralizing antibody C05, light chain

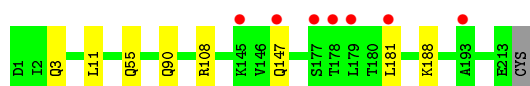




- Molecule 4: Broadly neutralizing antibody C05, light chain



- Molecule 4: Broadly neutralizing antibody C05, light chain



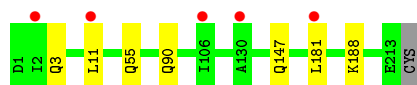
- Molecule 4: Broadly neutralizing antibody C05, light chain



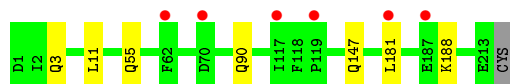
- Molecule 4: Broadly neutralizing antibody C05, light chain



- Molecule 4: Broadly neutralizing antibody C05, light chain

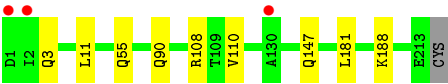


- Molecule 4: Broadly neutralizing antibody C05, light chain



- Molecule 4: Broadly neutralizing antibody C05, light chain





● Molecule 4: Broadly neutralizing antibody C05, light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	142.02Å 158.62Å 178.50Å 89.95° 85.44° 84.37°	Depositor
Resolution (Å)	49.07 – 4.10 49.07 – 4.10	Depositor EDS
% Data completeness (in resolution range)	73.9 (49.07-4.10) 73.8 (49.07-4.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 4.14Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.309 , 0.334 0.333 , 0.349	Depositor DCC
R_{free} test set	4527 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	77.6	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 26.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 89653 reflections	Xtriage
F_o, F_c correlation	0.75	EDS
Total number of atoms	90792	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.22 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.1185e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: BMA, PCA, NAG, MAN

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	0.42	0/2612	0.66	0/3558
1	C	0.39	0/2612	0.65	1/3558 (0.0%)
1	E	0.38	1/2612 (0.0%)	0.65	0/3558
1	G	0.39	0/2612	0.66	0/3558
1	I	0.48	2/2612 (0.1%)	0.69	2/3558 (0.1%)
1	K	0.39	0/2612	0.64	1/3558 (0.0%)
1	M	0.42	0/2612	0.68	2/3558 (0.1%)
1	O	0.41	1/2612 (0.0%)	0.65	1/3558 (0.0%)
1	Q	0.40	0/2612	0.66	0/3558
1	S	0.38	0/2612	0.66	1/3558 (0.0%)
1	U	0.44	1/2612 (0.0%)	0.68	1/3558 (0.0%)
1	W	0.42	1/2612 (0.0%)	0.65	1/3558 (0.0%)
2	B	0.37	0/1470	0.63	0/1975
2	D	0.36	0/1470	0.64	0/1975
2	F	0.41	0/1470	0.66	0/1975
2	H	0.37	0/1470	0.64	1/1975 (0.1%)
2	J	0.37	0/1470	0.63	0/1975
2	L	0.39	0/1470	0.64	0/1975
2	N	0.35	0/1470	0.63	0/1975
2	P	0.38	0/1470	0.63	1/1975 (0.1%)
2	R	0.36	0/1470	0.64	0/1975
2	T	0.36	0/1470	0.63	0/1975
2	V	0.37	0/1470	0.65	0/1975
2	X	0.36	0/1470	0.63	1/1975 (0.1%)
3	a	0.48	1/1837 (0.1%)	0.75	2/2500 (0.1%)
3	c	0.41	0/1837	0.68	0/2500
3	e	0.43	0/1837	0.71	0/2500
3	g	0.46	1/1837 (0.1%)	0.71	1/2500 (0.0%)
3	i	0.53	0/1837	0.79	1/2500 (0.0%)
3	k	0.42	0/1837	0.69	0/2500
3	m	0.41	0/1837	0.69	0/2500
3	o	0.43	0/1837	0.71	1/2500 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	q	0.43	0/1837	0.69	0/2500
3	s	0.42	0/1837	0.69	0/2500
3	u	0.41	0/1837	0.70	1/2500 (0.0%)
3	w	0.42	0/1837	0.69	1/2500 (0.0%)
4	b	0.45	0/1682	0.67	0/2280
4	d	0.50	1/1682 (0.1%)	0.72	0/2280
4	f	0.40	0/1682	0.66	0/2280
4	h	0.51	1/1682 (0.1%)	0.71	0/2280
4	j	0.44	0/1682	0.69	0/2280
4	l	0.44	0/1682	0.68	0/2280
4	n	0.48	1/1682 (0.1%)	0.69	0/2280
4	p	0.51	0/1682	0.78	4/2280 (0.2%)
4	r	0.39	0/1682	0.66	0/2280
4	t	0.37	0/1682	0.64	0/2280
4	v	0.48	1/1682 (0.1%)	0.70	0/2280
4	x	0.40	0/1682	0.66	0/2280
All	All	0.42	12/91212 (0.0%)	0.67	24/123756 (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
2	F	0	1
3	k	0	1
3	m	0	1
3	u	0	1
All	All	0	4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	190	GLU	CG-CD	-11.09	1.35	1.51
1	W	190	GLU	CB-CG	-7.77	1.37	1.52
3	a	100(D)	ALA	CA-CB	-7.11	1.37	1.52
3	g	116	THR	CB-CG2	-7.02	1.29	1.52
4	n	110	VAL	CB-CG2	-6.42	1.39	1.52
4	d	110	VAL	CB-CG2	-6.08	1.40	1.52
4	v	110	VAL	CB-CG2	-6.08	1.40	1.52
1	E	190	GLU	CB-CG	-6.05	1.40	1.52
1	U	325	GLU	CG-CD	-5.43	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	190	GLU	CB-CG	-5.37	1.42	1.52
1	I	190	GLU	CA-CB	-5.36	1.42	1.53
4	h	183	LYS	CE-NZ	-5.05	1.36	1.49

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	p	185	ASP	CB-CG-OD2	10.08	127.37	118.30
3	i	58	ASP	CB-CG-OD1	-8.49	110.66	118.30
1	M	20	VAL	N-CA-C	-8.49	88.08	111.00
4	p	185	ASP	CB-CG-OD1	-7.41	111.63	118.30
1	I	190	GLU	OE1-CD-OE2	7.20	131.93	123.30
3	a	58	ASP	CB-CG-OD1	-6.66	112.31	118.30
4	p	182	SER	CB-CA-C	-6.18	98.36	110.10
3	o	11	LEU	CB-CG-CD2	-6.07	100.68	111.00
3	u	11	LEU	CB-CG-CD2	-5.65	101.39	111.00
1	I	190	GLU	CA-CB-CG	-5.64	100.99	113.40
1	S	226	LEU	CB-CG-CD2	-5.53	101.60	111.00
1	K	212	THR	CA-CB-CG2	-5.45	104.77	112.40
3	g	189	LEU	CB-CG-CD2	-5.41	101.81	111.00
3	w	11	LEU	CB-CG-CD2	-5.29	102.01	111.00
3	a	66	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	O	212	THR	CA-CB-CG2	-5.19	105.13	112.40
4	p	185	ASP	N-CA-CB	5.13	119.84	110.60
1	W	212	THR	CA-CB-CG2	-5.12	105.23	112.40
2	P	153	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	M	212	THR	CA-CB-CG2	-5.05	105.33	112.40
1	U	325	GLU	N-CA-C	5.04	124.62	111.00
1	C	212	THR	CA-CB-CG2	-5.04	105.34	112.40
2	H	153	ARG	NE-CZ-NH1	5.04	122.82	120.30
2	X	153	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	18	ILE	Mainchain
3	k	185	PRO	Mainchain
3	m	185	PRO	Mainchain
3	u	185	PRO	Mainchain

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	2553	0	2491	11	1
1	C	2553	0	2491	11	0
1	E	2553	0	2491	11	0
1	G	2553	0	2490	10	0
1	I	2553	0	2491	18	0
1	K	2553	0	2491	13	0
1	M	2553	0	2490	11	0
1	O	2553	0	2490	15	0
1	Q	2553	0	2490	14	0
1	S	2553	0	2490	12	0
1	U	2553	0	2490	15	3
1	W	2553	0	2491	14	0
2	B	1446	0	1370	1	0
2	D	1446	0	1370	1	0
2	F	1446	0	1370	3	0
2	H	1446	0	1370	2	0
2	J	1446	0	1370	0	0
2	L	1446	0	1370	1	0
2	N	1446	0	1370	2	0
2	P	1446	0	1370	1	0
2	R	1446	0	1370	2	0
2	T	1446	0	1370	0	0
2	V	1446	0	1370	0	0
2	X	1446	0	1370	2	0
3	a	1806	0	1749	0	0
3	c	1806	0	1749	0	0
3	e	1806	0	1749	0	0
3	g	1806	0	1749	0	0
3	i	1806	0	1749	0	0
3	k	1806	0	1749	0	0
3	m	1806	0	1749	0	0
3	o	1806	0	1749	0	0
3	q	1806	0	1749	0	0
3	s	1806	0	1749	0	0
3	u	1806	0	1749	0	0
3	w	1806	0	1749	0	0
4	b	1648	0	1614	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	d	1648	0	1614	0	1
4	f	1648	0	1614	0	0
4	h	1648	0	1614	0	4
4	j	1648	0	1614	0	1
4	l	1648	0	1614	0	1
4	n	1648	0	1614	0	1
4	p	1648	0	1614	0	1
4	r	1648	0	1614	0	0
4	t	1648	0	1614	0	0
4	v	1648	0	1614	0	1
4	x	1648	0	1614	0	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
5	C	14	0	13	0	0
5	D	14	0	13	0	0
5	E	14	0	13	0	0
5	F	14	0	13	0	0
5	G	28	0	26	0	0
5	H	14	0	13	0	0
5	I	14	0	13	0	0
5	J	14	0	13	0	0
5	K	14	0	13	0	0
5	L	14	0	13	0	0
5	M	28	0	26	0	0
5	N	14	0	13	0	0
5	O	28	0	26	0	0
5	P	14	0	13	0	0
5	Q	28	0	26	0	0
5	R	14	0	13	0	0
5	S	28	0	26	0	0
5	T	14	0	13	0	0
5	U	28	0	26	0	0
5	V	14	0	13	0	0
5	W	14	0	13	0	0
5	X	14	0	13	0	0
6	A	50	0	43	0	0
6	C	50	0	43	0	0
6	E	50	0	43	0	0
6	G	50	0	43	0	0
6	I	50	0	43	0	0
6	K	50	0	43	0	0
6	M	50	0	43	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	O	50	0	43	0	0
6	Q	50	0	43	0	0
6	S	50	0	43	1	0
6	U	50	0	43	0	0
6	W	50	0	43	0	0
7	A	28	0	25	0	0
7	C	28	0	25	0	0
7	E	28	0	25	0	0
7	G	28	0	25	0	0
7	I	28	0	25	0	0
7	K	28	0	25	0	0
7	M	28	0	25	0	0
7	O	28	0	25	0	0
7	Q	28	0	25	0	0
7	S	28	0	25	0	0
7	U	28	0	25	0	0
7	W	28	0	25	0	0
All	All	90792	0	87888	105	7

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 3.

All (105) 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)
1:C:212:THR:HG21	1:E:216:ASN:ND2	1.99	0.78
1:I:212:THR:HG21	1:K:216:ASN:CG	2.07	0.75
1:O:212:THR:HG21	1:Q:216:ASN:CG	2.11	0.71
1:C:212:THR:HG21	1:E:216:ASN:CG	2.11	0.70
1:I:212:THR:HG21	1:K:216:ASN:ND2	2.09	0.68
1:U:212:THR:HG21	1:W:216:ASN:CG	2.15	0.67
1:A:216:ASN:CG	1:E:212:THR:HG21	2.14	0.67
1:O:212:THR:HG21	1:Q:216:ASN:ND2	2.10	0.66
1:I:214:ILE:HD11	1:K:216:ASN:HD21	1.60	0.65
1:S:216:ASN:CG	1:W:212:THR:HG21	2.19	0.64
1:A:216:ASN:ND2	1:E:212:THR:HG21	2.13	0.63
1:U:212:THR:HG21	1:W:216:ASN:ND2	2.14	0.62
1:A:222:TRP:CZ2	1:A:225:GLY:HA2	2.34	0.62
1:M:212:THR:HG21	1:O:216:ASN:CG	2.20	0.62
1:A:212:THR:HG21	1:C:216:ASN:CG	2.20	0.62
1:M:216:ASN:CG	1:Q:212:THR:HG21	2.19	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:216:ASN:ND2	1:Q:212:THR:HG21	2.15	0.61
1:S:216:ASN:ND2	1:W:212:THR:HG21	2.15	0.61
1:U:214:ILE:HD11	1:W:216:ASN:HD21	1.65	0.60
1:G:212:THR:HG21	1:I:216:ASN:CG	2.22	0.60
1:S:212:THR:HG21	1:U:216:ASN:CG	2.21	0.60
1:M:212:THR:HG21	1:O:216:ASN:ND2	2.17	0.60
1:O:214:ILE:HD11	1:Q:216:ASN:HD21	1.66	0.59
1:Q:222:TRP:CZ2	1:Q:225:GLY:HA2	2.37	0.59
1:G:216:ASN:ND2	1:K:212:THR:HG21	2.17	0.59
1:A:225:GLY:C	1:A:226:LEU:HD23	2.24	0.58
1:A:212:THR:HG21	1:C:216:ASN:ND2	2.17	0.58
1:I:222:TRP:CZ2	1:I:225:GLY:HA2	2.38	0.58
1:G:216:ASN:CG	1:K:212:THR:HG21	2.25	0.57
1:S:212:THR:HG21	1:U:216:ASN:ND2	2.19	0.57
1:A:222:TRP:CE2	1:A:225:GLY:HA2	2.40	0.56
1:G:212:THR:HG21	1:I:216:ASN:ND2	2.22	0.55
1:C:214:ILE:HD11	1:E:216:ASN:HD21	1.73	0.53
1:M:21:PRO:HA	2:N:15:GLU:OE2	2.10	0.52
1:Q:222:TRP:CE2	1:Q:225:GLY:HA2	2.44	0.52
1:E:222:TRP:CZ2	1:E:225:GLY:HA2	2.44	0.52
1:I:222:TRP:CE2	1:I:225:GLY:HA2	2.44	0.52
1:S:222:TRP:CZ2	1:S:225:GLY:HA2	2.46	0.51
1:U:205:SER:OG	1:W:221:PRO:HD3	2.10	0.51
1:O:222:TRP:CZ2	1:O:225:GLY:HA2	2.44	0.51
1:K:222:TRP:CZ2	1:K:225:GLY:HA2	2.46	0.50
1:I:201:ARG:HD2	1:K:216:ASN:OD1	2.12	0.49
1:O:205:SER:OG	1:Q:221:PRO:HD3	2.12	0.49
1:C:205:SER:OG	1:E:221:PRO:HD3	2.12	0.49
1:O:201:ARG:HD2	1:Q:216:ASN:OD1	2.13	0.48
1:I:205:SER:OG	1:K:221:PRO:HD3	2.14	0.48
1:U:325:GLU:O	1:U:326:LYS:C	2.53	0.47
1:E:222:TRP:CE2	1:E:225:GLY:HA2	2.50	0.47
1:Q:185:PRO:HB3	1:Q:190:GLU:CD	2.35	0.46
1:M:222:TRP:CZ2	1:M:225:GLY:HA2	2.50	0.46
1:K:222:TRP:CE2	1:K:225:GLY:HA2	2.50	0.46
1:Q:207[B]:ARG:NH1	1:Q:240:GLY:O	2.48	0.46
1:M:21:PRO:O	1:M:324:PRO:HG3	2.16	0.46
1:I:153:TRP:CD1	1:I:252:ILE:CD1	3.00	0.45
1:O:222:TRP:CE2	1:O:225:GLY:HA2	2.52	0.45
1:A:185:PRO:HB3	1:A:190:GLU:CD	2.38	0.44
1:G:304:ALA:HA	2:H:61:GLU:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:225:GLY:O	1:I:226:LEU:HD23	2.17	0.44
1:C:201:ARG:HD2	1:E:216:ASN:OD1	2.17	0.44
1:A:216:ASN:ND2	1:E:212:THR:CG2	2.80	0.44
1:G:216:ASN:OD1	1:K:212:THR:HG21	2.18	0.43
1:G:221:PRO:HD3	1:K:205:SER:OG	2.17	0.43
1:Q:15:LEU:HD11	2:R:24:PHE:CE2	2.54	0.43
1:G:102:VAL:HG22	1:G:232:ILE:HB	2.00	0.43
1:M:212:THR:HG21	1:O:216:ASN:OD1	2.19	0.43
1:I:111:LEU:HB2	2:L:73:VAL:HG11	2.00	0.43
1:M:212:THR:CG2	1:O:216:ASN:ND2	2.81	0.43
1:E:185:PRO:HB3	1:E:190:GLU:CD	2.39	0.42
1:I:214:ILE:HD11	1:K:216:ASN:ND2	2.32	0.42
1:M:216:ASN:ND2	1:Q:212:THR:CG2	2.82	0.42
1:W:207[B]:ARG:NH1	1:W:240:GLY:O	2.50	0.42
1:O:305:CYS:O	2:P:60:ASN:ND2	2.52	0.42
1:U:222:TRP:CZ2	1:U:225:GLY:HA2	2.54	0.42
1:I:184:HIS:O	1:I:228[B]:SER:HB3	2.20	0.42
1:O:49:GLY:HA2	1:O:285:ASN:O	2.19	0.42
1:S:212:THR:CG2	1:U:216:ASN:ND2	2.82	0.42
1:M:221:PRO:HD3	1:Q:205:SER:OG	2.20	0.42
1:I:225:GLY:C	1:I:226:LEU:HD23	2.40	0.42
1:O:111:LEU:HB2	2:R:73:VAL:HG11	2.01	0.41
1:S:216:ASN:ND2	1:W:212:THR:CG2	2.82	0.41
1:S:212:THR:HG21	1:U:216:ASN:OD1	2.20	0.41
2:X:60:ASN:ND2	2:X:60:ASN:O	2.54	0.41
1:S:167:THR:HB	6:S:503:NAG:H62	2.02	0.41
1:U:111:LEU:HB2	2:X:73:VAL:HG11	2.02	0.41
1:S:205:SER:OG	1:U:221:PRO:HD3	2.20	0.41
1:U:214:ILE:HD11	1:W:216:ASN:ND2	2.34	0.41
1:A:212:THR:CG2	1:C:216:ASN:ND2	2.83	0.41
1:U:207[B]:ARG:NH1	1:U:240:GLY:O	2.51	0.41
2:B:18:ILE:HB	1:K:275[B]:ASP:OD1	2.21	0.41
2:N:60:ASN:ND2	2:N:60:ASN:O	2.54	0.41
2:F:27:GLN:HB2	1:W:92:LYS:HD3	120.90	0.41
1:C:84:TRP:CE2	1:C:116:GLY:HA2	2.55	0.41
1:G:307:LYS:HD3	2:H:92:TRP:CE2	2.56	0.41
2:F:27:GLN:CB	1:W:92:LYS:HD3	121.55	0.41
1:A:206:THR:C	1:C:221:PRO:HG2	2.42	0.41
2:F:60:ASN:ND2	2:F:60:ASN:O	2.54	0.41
1:U:201:ARG:HD2	1:W:216:ASN:OD1	2.20	0.41
1:I:190:GLU:HA	1:I:193:SER:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:222:TRP:CZ2	1:W:225:GLY:HA2	2.56	0.40
1:S:226:LEU:HD23	1:S:226:LEU:HA	1.83	0.40
1:I:190:GLU:OE2	1:I:194:LEU:HD11	2.21	0.40
1:C:16:GLY:HA3	2:D:14:TRP:CH2	2.56	0.40
1:G:205:SER:OG	1:I:221:PRO:HD3	2.21	0.40
1:O:276:THR:O	1:O:276:THR:HG23	2.21	0.40
1:S:216:ASN:OD1	1:W:212:THR:HG21	2.20	0.40

All (7) 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)
4:d:202:SER:OG	4:v:108:ARG:O[1_545]	1.78	0.42
4:h:202:SER:OG	4:n:108:ARG:O[1_564]	1.83	0.37
4:l:108:ARG:O	4:p:202:SER:OG[1_564]	1.87	0.33
1:U:312:ASN:ND2	4:h:187:GLU:OE2[1_646]	1.93	0.27
1:U:33:GLN:NE2	4:h:127:SER:O[1_646]	2.09	0.11
1:A:133:ASN:ND2	4:j:26:SER:O[1_545]	2.12	0.08
1:U:312:ASN:OD1	4:h:183:LYS:NZ[1_646]	2.16	0.04

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	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	46	82	
1	C	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	46	82	
1	E	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	46	82	
1	G	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	46	82	
1	I	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	46	82	
1	K	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	46	82	

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	46	82
1	O	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	46	82
1	Q	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	46	82
1	S	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	46	82
1	U	328/323 (102%)	323 (98%)	4 (1%)	1 (0%)	46	82
1	W	328/323 (102%)	322 (98%)	5 (2%)	1 (0%)	46	82
2	B	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
2	D	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
2	F	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
2	H	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
2	J	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
2	L	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
2	N	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
2	P	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
2	R	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
2	T	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
2	V	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
2	X	177/174 (102%)	172 (97%)	5 (3%)	0	100	100
3	a	241/241 (100%)	236 (98%)	5 (2%)	0	100	100
3	c	241/241 (100%)	236 (98%)	5 (2%)	0	100	100
3	e	241/241 (100%)	236 (98%)	5 (2%)	0	100	100
3	g	241/241 (100%)	236 (98%)	5 (2%)	0	100	100
3	i	241/241 (100%)	236 (98%)	5 (2%)	0	100	100
3	k	241/241 (100%)	235 (98%)	6 (2%)	0	100	100
3	m	241/241 (100%)	236 (98%)	5 (2%)	0	100	100
3	o	241/241 (100%)	236 (98%)	5 (2%)	0	100	100
3	q	241/241 (100%)	236 (98%)	5 (2%)	0	100	100
3	s	241/241 (100%)	236 (98%)	5 (2%)	0	100	100
3	u	241/241 (100%)	236 (98%)	5 (2%)	0	100	100
3	w	241/241 (100%)	236 (98%)	5 (2%)	0	100	100
4	b	212/214 (99%)	209 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	d	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
4	f	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
4	h	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
4	j	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
4	l	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
4	n	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
4	p	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
4	r	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
4	t	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
4	v	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
4	x	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
All	All	11496/11424 (101%)	11268 (98%)	216 (2%)	12 (0%)	56	90

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	ILE
1	C	62	ILE
1	E	62	ILE
1	G	62	ILE
1	I	62	ILE
1	K	62	ILE
1	M	62	ILE
1	O	62	ILE
1	Q	62	ILE
1	S	62	ILE
1	U	62	ILE
1	W	62	ILE

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	291/283 (103%)	289 (99%)	2 (1%)	88	94
1	C	291/283 (103%)	289 (99%)	2 (1%)	88	94
1	E	291/283 (103%)	289 (99%)	2 (1%)	88	94
1	G	291/283 (103%)	289 (99%)	2 (1%)	88	94
1	I	291/283 (103%)	289 (99%)	2 (1%)	88	94
1	K	291/283 (103%)	289 (99%)	2 (1%)	88	94
1	M	291/283 (103%)	289 (99%)	2 (1%)	88	94
1	O	291/283 (103%)	289 (99%)	2 (1%)	88	94
1	Q	291/283 (103%)	289 (99%)	2 (1%)	88	94
1	S	291/283 (103%)	289 (99%)	2 (1%)	88	94
1	U	291/283 (103%)	289 (99%)	2 (1%)	88	94
1	W	291/283 (103%)	289 (99%)	2 (1%)	88	94
2	B	153/148 (103%)	152 (99%)	1 (1%)	88	94
2	D	153/148 (103%)	152 (99%)	1 (1%)	88	94
2	F	153/148 (103%)	152 (99%)	1 (1%)	88	94
2	H	153/148 (103%)	152 (99%)	1 (1%)	88	94
2	J	153/148 (103%)	152 (99%)	1 (1%)	88	94
2	L	153/148 (103%)	152 (99%)	1 (1%)	88	94
2	N	153/148 (103%)	152 (99%)	1 (1%)	88	94
2	P	153/148 (103%)	152 (99%)	1 (1%)	88	94
2	R	153/148 (103%)	152 (99%)	1 (1%)	88	94
2	T	153/148 (103%)	152 (99%)	1 (1%)	88	94
2	V	153/148 (103%)	152 (99%)	1 (1%)	88	94
2	X	153/148 (103%)	152 (99%)	1 (1%)	88	94
3	a	202/200 (101%)	198 (98%)	4 (2%)	63	86
3	c	202/200 (101%)	197 (98%)	5 (2%)	55	82
3	e	202/200 (101%)	196 (97%)	6 (3%)	48	79
3	g	202/200 (101%)	198 (98%)	4 (2%)	63	86
3	i	202/200 (101%)	197 (98%)	5 (2%)	55	82
3	k	202/200 (101%)	196 (97%)	6 (3%)	48	79
3	m	202/200 (101%)	198 (98%)	4 (2%)	63	86
3	o	202/200 (101%)	196 (97%)	6 (3%)	48	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	q	202/200 (101%)	198 (98%)	4 (2%)	63	86
3	s	202/200 (101%)	198 (98%)	4 (2%)	63	86
3	u	202/200 (101%)	197 (98%)	5 (2%)	55	82
3	w	202/200 (101%)	197 (98%)	5 (2%)	55	82
4	b	187/187 (100%)	180 (96%)	7 (4%)	41	75
4	d	187/187 (100%)	180 (96%)	7 (4%)	41	75
4	f	187/187 (100%)	180 (96%)	7 (4%)	41	75
4	h	187/187 (100%)	180 (96%)	7 (4%)	41	75
4	j	187/187 (100%)	180 (96%)	7 (4%)	41	75
4	l	187/187 (100%)	180 (96%)	7 (4%)	41	75
4	n	187/187 (100%)	180 (96%)	7 (4%)	41	75
4	p	187/187 (100%)	180 (96%)	7 (4%)	41	75
4	r	187/187 (100%)	180 (96%)	7 (4%)	41	75
4	t	187/187 (100%)	180 (96%)	7 (4%)	41	75
4	v	187/187 (100%)	180 (96%)	7 (4%)	41	75
4	x	187/187 (100%)	180 (96%)	7 (4%)	41	75
All	All	9996/9816 (102%)	9818 (98%)	178 (2%)	66	87

All (178) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	53	ASN
2	B	60	ASN
1	C	18	HIS
1	C	53	ASN
2	D	60	ASN
1	E	18	HIS
1	E	53	ASN
2	F	60	ASN
1	G	18	HIS
1	G	53	ASN
2	H	60	ASN
1	I	18	HIS
1	I	53	ASN
2	J	60	ASN

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Mol	Chain	Res	Type
1	K	18	HIS
1	K	53	ASN
2	L	60	ASN
1	M	18	HIS
1	M	53	ASN
2	N	60	ASN
1	O	18	HIS
1	O	53	ASN
2	P	60	ASN
1	Q	18	HIS
1	Q	53	ASN
2	R	60	ASN
1	S	18	HIS
1	S	53	ASN
2	T	60	ASN
1	U	18	HIS
1	U	53	ASN
2	V	60	ASN
1	W	18	HIS
1	W	53	ASN
2	X	60	ASN
3	a	78	LEU
3	a	92	CYS
3	a	178	LEU
3	a	209	LYS
4	b	3	GLN
4	b	11	LEU
4	b	55	GLN
4	b	90	GLN
4	b	147	GLN
4	b	181	LEU
4	b	188	LYS
3	c	78	LEU
3	c	92	CYS
3	c	113	SER
3	c	178	LEU
3	c	209	LYS
4	d	3	GLN
4	d	11	LEU
4	d	55	GLN
4	d	90	GLN
4	d	147	GLN

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Mol	Chain	Res	Type
4	d	181	LEU
4	d	188	LYS
3	e	78	LEU
3	e	83	ARG
3	e	92	CYS
3	e	178	LEU
3	e	197	ASN
3	e	209	LYS
4	f	3	GLN
4	f	11	LEU
4	f	55	GLN
4	f	90	GLN
4	f	147	GLN
4	f	181	LEU
4	f	188	LYS
3	g	78	LEU
3	g	92	CYS
3	g	178	LEU
3	g	209	LYS
4	h	3	GLN
4	h	11	LEU
4	h	55	GLN
4	h	90	GLN
4	h	147	GLN
4	h	181	LEU
4	h	188	LYS
3	i	78	LEU
3	i	92	CYS
3	i	113	SER
3	i	178	LEU
3	i	209	LYS
4	j	3	GLN
4	j	11	LEU
4	j	55	GLN
4	j	90	GLN
4	j	147	GLN
4	j	181	LEU
4	j	188	LYS
3	k	78	LEU
3	k	83	ARG
3	k	92	CYS
3	k	178	LEU

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Mol	Chain	Res	Type
3	k	197	ASN
3	k	209	LYS
4	l	3	GLN
4	l	11	LEU
4	l	55	GLN
4	l	90	GLN
4	l	147	GLN
4	l	181	LEU
4	l	188	LYS
3	m	78	LEU
3	m	92	CYS
3	m	178	LEU
3	m	209	LYS
4	n	3	GLN
4	n	11	LEU
4	n	55	GLN
4	n	90	GLN
4	n	147	GLN
4	n	181	LEU
4	n	188	LYS
3	o	78	LEU
3	o	83	ARG
3	o	92	CYS
3	o	178	LEU
3	o	197	ASN
3	o	209	LYS
4	p	3	GLN
4	p	11	LEU
4	p	55	GLN
4	p	90	GLN
4	p	147	GLN
4	p	181	LEU
4	p	188	LYS
3	q	78	LEU
3	q	92	CYS
3	q	178	LEU
3	q	209	LYS
4	r	3	GLN
4	r	11	LEU
4	r	55	GLN
4	r	90	GLN
4	r	147	GLN

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Mol	Chain	Res	Type
4	r	181	LEU
4	r	188	LYS
3	s	78	LEU
3	s	92	CYS
3	s	178	LEU
3	s	209	LYS
4	t	3	GLN
4	t	11	LEU
4	t	55	GLN
4	t	90	GLN
4	t	147	GLN
4	t	181	LEU
4	t	188	LYS
3	u	78	LEU
3	u	83	ARG
3	u	92	CYS
3	u	178	LEU
3	u	209	LYS
4	v	3	GLN
4	v	11	LEU
4	v	55	GLN
4	v	90	GLN
4	v	147	GLN
4	v	181	LEU
4	v	188	LYS
3	w	78	LEU
3	w	92	CYS
3	w	178	LEU
3	w	197	ASN
3	w	209	LYS
4	x	3	GLN
4	x	11	LEU
4	x	55	GLN
4	x	90	GLN
4	x	147	GLN
4	x	181	LEU
4	x	188	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (107) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN

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Mol	Chain	Res	Type
1	A	137	ASN
1	A	189	GLN
2	B	53	ASN
2	B	60	ASN
2	B	125	GLN
1	C	53	ASN
2	D	53	ASN
2	D	60	ASN
2	D	125	GLN
1	E	53	ASN
1	E	189	GLN
1	E	211	GLN
2	F	53	ASN
2	F	60	ASN
2	F	125	GLN
1	G	53	ASN
2	H	53	ASN
2	H	60	ASN
2	H	125	GLN
1	I	53	ASN
1	I	189	GLN
2	J	53	ASN
2	J	60	ASN
2	J	125	GLN
1	K	18	HIS
1	K	53	ASN
1	K	189	GLN
2	L	53	ASN
2	L	60	ASN
2	L	125	GLN
1	M	18	HIS
1	M	53	ASN
2	N	53	ASN
2	N	60	ASN
2	N	125	GLN
1	O	53	ASN
2	P	53	ASN
2	P	60	ASN
2	P	125	GLN
1	Q	53	ASN
1	Q	189	GLN
1	Q	211	GLN

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Mol	Chain	Res	Type
2	R	53	ASN
2	R	60	ASN
2	R	125	GLN
1	S	53	ASN
1	S	189	GLN
2	T	53	ASN
2	T	60	ASN
2	T	125	GLN
1	U	18	HIS
1	U	53	ASN
2	V	53	ASN
2	V	60	ASN
2	V	125	GLN
1	W	53	ASN
2	X	53	ASN
2	X	60	ASN
2	X	125	GLN
3	a	192	GLN
4	b	55	GLN
4	b	189	HIS
4	b	199	GLN
3	c	192	GLN
4	d	55	GLN
4	d	189	HIS
4	d	199	GLN
3	e	192	GLN
4	f	55	GLN
4	f	189	HIS
4	f	199	GLN
3	g	192	GLN
4	h	55	GLN
4	h	189	HIS
4	h	199	GLN
3	i	192	GLN
4	j	55	GLN
4	j	189	HIS
4	j	199	GLN
3	k	192	GLN
4	l	55	GLN
4	l	189	HIS
3	m	192	GLN
4	n	55	GLN

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Mol	Chain	Res	Type
4	n	189	HIS
4	n	199	GLN
3	o	192	GLN
4	p	55	GLN
4	p	189	HIS
4	p	199	GLN
3	q	192	GLN
4	r	55	GLN
4	r	189	HIS
4	r	199	GLN
3	s	192	GLN
4	t	55	GLN
4	t	189	HIS
4	t	199	GLN
3	u	192	GLN
4	v	55	GLN
4	v	189	HIS
4	v	199	GLN
3	w	192	GLN
4	x	55	GLN
4	x	189	HIS
4	x	199	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues 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
3	PCA	a	1	3	7,8,9	2.03	2 (28%)	9,10,12	2.19	4 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PCA	c	1	3	7,8,9	1.94	2 (28%)	9,10,12	2.21	4 (44%)
3	PCA	e	1	3	7,8,9	1.92	2 (28%)	9,10,12	2.22	4 (44%)
3	PCA	g	1	3	7,8,9	1.83	2 (28%)	9,10,12	2.22	4 (44%)
3	PCA	i	1	3	7,8,9	1.98	2 (28%)	9,10,12	2.12	4 (44%)
3	PCA	k	1	3	7,8,9	1.89	2 (28%)	9,10,12	2.23	5 (55%)
3	PCA	m	1	3	7,8,9	1.89	2 (28%)	9,10,12	2.04	4 (44%)
3	PCA	o	1	3	7,8,9	1.93	2 (28%)	9,10,12	2.15	4 (44%)
3	PCA	q	1	3	7,8,9	1.86	2 (28%)	9,10,12	2.14	4 (44%)
3	PCA	s	1	3	7,8,9	2.04	2 (28%)	9,10,12	2.21	4 (44%)
3	PCA	u	1	3	7,8,9	1.93	2 (28%)	9,10,12	2.19	4 (44%)
3	PCA	w	1	3	7,8,9	1.93	2 (28%)	9,10,12	2.17	4 (44%)

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
3	PCA	a	1	3	-	0/0/11/13	0/1/1/1
3	PCA	c	1	3	-	0/0/11/13	0/1/1/1
3	PCA	e	1	3	-	0/0/11/13	0/1/1/1
3	PCA	g	1	3	-	0/0/11/13	0/1/1/1
3	PCA	i	1	3	-	0/0/11/13	0/1/1/1
3	PCA	k	1	3	-	0/0/11/13	0/1/1/1
3	PCA	m	1	3	-	0/0/11/13	0/1/1/1
3	PCA	o	1	3	-	0/0/11/13	0/1/1/1
3	PCA	q	1	3	-	0/0/11/13	0/1/1/1
3	PCA	s	1	3	-	0/0/11/13	0/1/1/1
3	PCA	u	1	3	-	0/0/11/13	0/1/1/1
3	PCA	w	1	3	-	0/0/11/13	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	g	1	PCA	CA-N	2.67	1.49	1.46
3	q	1	PCA	CA-N	2.83	1.50	1.46
3	k	1	PCA	CA-N	2.85	1.50	1.46
3	m	1	PCA	CA-N	2.97	1.50	1.46
3	u	1	PCA	CA-N	3.01	1.50	1.46
3	c	1	PCA	CA-N	3.02	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	e	1	PCA	CA-N	3.06	1.50	1.46
3	o	1	PCA	CA-N	3.10	1.50	1.46
3	w	1	PCA	CA-N	3.11	1.50	1.46
3	i	1	PCA	CA-N	3.15	1.50	1.46
3	a	1	PCA	CA-N	3.37	1.50	1.46
3	s	1	PCA	CA-N	3.43	1.50	1.46
3	q	1	PCA	CD-N	3.88	1.46	1.33
3	m	1	PCA	CD-N	3.90	1.46	1.33
3	g	1	PCA	CD-N	3.91	1.46	1.33
3	w	1	PCA	CD-N	3.93	1.46	1.33
3	o	1	PCA	CD-N	3.95	1.46	1.33
3	e	1	PCA	CD-N	3.95	1.46	1.33
3	k	1	PCA	CD-N	3.96	1.46	1.33
3	u	1	PCA	CD-N	4.01	1.47	1.33
3	c	1	PCA	CD-N	4.02	1.47	1.33
3	i	1	PCA	CD-N	4.04	1.47	1.33
3	s	1	PCA	CD-N	4.06	1.47	1.33
3	a	1	PCA	CD-N	4.07	1.47	1.33

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	e	1	PCA	CB-CA-C	-3.98	107.32	112.76
3	s	1	PCA	CB-CA-C	-3.98	107.32	112.76
3	o	1	PCA	CB-CA-C	-3.66	107.76	112.76
3	a	1	PCA	CB-CA-C	-3.65	107.77	112.76
3	w	1	PCA	CB-CA-C	-3.62	107.81	112.76
3	g	1	PCA	CB-CA-C	-3.50	107.97	112.76
3	c	1	PCA	CB-CA-C	-3.48	108.01	112.76
3	q	1	PCA	CB-CA-C	-3.41	108.09	112.76
3	u	1	PCA	CB-CA-C	-3.41	108.11	112.76
3	k	1	PCA	CA-N-CD	-3.38	102.48	113.81
3	i	1	PCA	CA-N-CD	-3.33	102.66	113.81
3	g	1	PCA	CA-N-CD	-3.29	102.77	113.81
3	c	1	PCA	CA-N-CD	-3.26	102.90	113.81
3	u	1	PCA	CA-N-CD	-3.21	103.06	113.81
3	w	1	PCA	CA-N-CD	-3.16	103.21	113.81
3	q	1	PCA	CA-N-CD	-3.15	103.26	113.81
3	m	1	PCA	CB-CA-C	-3.15	108.46	112.76
3	e	1	PCA	CA-N-CD	-3.09	103.45	113.81
3	o	1	PCA	CA-N-CD	-3.09	103.45	113.81
3	a	1	PCA	CA-N-CD	-3.07	103.53	113.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	m	1	PCA	CA-N-CD	-3.07	103.53	113.81
3	k	1	PCA	CB-CA-C	-3.04	108.61	112.76
3	s	1	PCA	CA-N-CD	-3.03	103.67	113.81
3	i	1	PCA	CB-CA-C	-2.90	108.80	112.76
3	k	1	PCA	OE-CD-CG	-2.69	120.80	126.81
3	u	1	PCA	OE-CD-CG	-2.65	120.89	126.81
3	c	1	PCA	OE-CD-CG	-2.61	120.98	126.81
3	a	1	PCA	OE-CD-CG	-2.58	121.04	126.81
3	s	1	PCA	OE-CD-CG	-2.50	121.23	126.81
3	g	1	PCA	OE-CD-CG	-2.50	121.24	126.81
3	i	1	PCA	OE-CD-CG	-2.44	121.36	126.81
3	w	1	PCA	OE-CD-CG	-2.36	121.54	126.81
3	o	1	PCA	OE-CD-CG	-2.35	121.57	126.81
3	e	1	PCA	OE-CD-CG	-2.31	121.64	126.81
3	q	1	PCA	OE-CD-CG	-2.28	121.71	126.81
3	m	1	PCA	OE-CD-CG	-2.02	122.30	126.81
3	k	1	PCA	CG-CD-N	2.00	115.25	108.04
3	s	1	PCA	CB-CA-N	2.47	110.41	103.20
3	a	1	PCA	CB-CA-N	2.54	110.62	103.20
3	o	1	PCA	CB-CA-N	2.62	110.86	103.20
3	e	1	PCA	CB-CA-N	2.66	110.97	103.20
3	w	1	PCA	CB-CA-N	2.71	111.11	103.20
3	u	1	PCA	CB-CA-N	2.72	111.12	103.20
3	q	1	PCA	CB-CA-N	2.73	111.17	103.20
3	m	1	PCA	CB-CA-N	2.74	111.18	103.20
3	c	1	PCA	CB-CA-N	2.80	111.38	103.20
3	g	1	PCA	CB-CA-N	2.83	111.47	103.20
3	k	1	PCA	CB-CA-N	2.93	111.75	103.20
3	i	1	PCA	CB-CA-N	2.94	111.79	103.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

72 carbohydrates 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
6	NAG	A	602	1,6	14,14,15	0.47	0	15,19,21	0.86	0
6	NAG	A	603	6	14,14,15	0.63	0	15,19,21	1.10	2 (13%)
6	BMA	A	604	6	11,11,12	0.71	0	14,15,17	1.35	2 (14%)
6	MAN	A	605	6	11,11,12	0.59	0	14,15,17	0.70	0
7	NAG	A	606	1,7	14,14,15	0.52	0	15,19,21	0.50	0
7	NAG	A	607	7	14,14,15	0.46	0	15,19,21	0.72	0
6	NAG	C	502	1,6	14,14,15	0.50	0	15,19,21	0.76	0
6	NAG	C	503	6	14,14,15	0.52	0	15,19,21	0.65	0
6	BMA	C	504	6	11,11,12	0.68	0	14,15,17	1.22	1 (7%)
6	MAN	C	505	6	11,11,12	0.59	0	14,15,17	0.71	0
7	NAG	C	506	1,7	14,14,15	0.59	0	15,19,21	0.73	0
7	NAG	C	507	7	14,14,15	0.42	0	15,19,21	0.98	1 (6%)
6	NAG	E	602	1,6	14,14,15	0.50	0	15,19,21	0.82	0
6	NAG	E	603	6	14,14,15	0.56	0	15,19,21	0.73	0
6	BMA	E	604	6	11,11,12	0.71	0	14,15,17	0.98	1 (7%)
6	MAN	E	605	6	11,11,12	0.64	0	14,15,17	0.85	1 (7%)
7	NAG	E	606	1,7	14,14,15	0.56	0	15,19,21	0.59	0
7	NAG	E	607	7	14,14,15	0.45	0	15,19,21	0.96	1 (6%)
6	NAG	G	503	1,6	14,14,15	0.59	0	15,19,21	0.90	0
6	NAG	G	504	6	14,14,15	0.53	0	15,19,21	0.80	0
6	BMA	G	505	6	11,11,12	0.73	0	14,15,17	1.20	1 (7%)
6	MAN	G	506	6	11,11,12	0.57	0	14,15,17	0.83	1 (7%)
7	NAG	G	507	1,7	14,14,15	0.49	0	15,19,21	0.85	0
7	NAG	G	508	7	14,14,15	0.45	0	15,19,21	1.16	1 (6%)
6	NAG	I	502	1,6	14,14,15	0.49	0	15,19,21	0.75	0
6	NAG	I	503	6	14,14,15	0.52	0	15,19,21	0.69	0
6	BMA	I	504	6	11,11,12	0.69	0	14,15,17	1.00	1 (7%)
6	MAN	I	505	6	11,11,12	0.61	0	14,15,17	0.91	1 (7%)
7	NAG	I	506	1,7	14,14,15	0.56	0	15,19,21	0.61	0
7	NAG	I	507	7	14,14,15	0.49	0	15,19,21	0.86	1 (6%)
6	NAG	K	602	1,6	14,14,15	0.48	0	15,19,21	0.71	0
6	NAG	K	603	6	14,14,15	0.51	0	15,19,21	0.73	0
6	BMA	K	604	6	11,11,12	0.73	0	14,15,17	0.98	1 (7%)
6	MAN	K	605	6	11,11,12	0.59	0	14,15,17	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	K	606	1,7	14,14,15	0.54	0	15,19,21	0.47	0
7	NAG	K	607	7	14,14,15	0.44	0	15,19,21	0.96	1 (6%)
6	NAG	M	503	1,6	14,14,15	0.43	0	15,19,21	1.21	1 (6%)
6	NAG	M	504	6	14,14,15	0.49	0	15,19,21	0.79	0
6	BMA	M	505	6	11,11,12	0.66	0	14,15,17	1.01	1 (7%)
6	MAN	M	506	6	11,11,12	0.61	0	14,15,17	1.00	1 (7%)
7	NAG	M	507	1,7	14,14,15	0.55	0	15,19,21	0.66	0
7	NAG	M	508	7	14,14,15	0.51	0	15,19,21	0.95	1 (6%)
6	NAG	O	503	1,6	14,14,15	0.57	0	15,19,21	0.80	0
6	NAG	O	504	6	14,14,15	0.54	0	15,19,21	0.78	0
6	BMA	O	505	6	11,11,12	0.79	0	14,15,17	0.96	1 (7%)
6	MAN	O	506	6	11,11,12	0.60	0	14,15,17	0.98	1 (7%)
7	NAG	O	507	1,7	14,14,15	0.53	0	15,19,21	0.61	0
7	NAG	O	508	7	14,14,15	0.49	0	15,19,21	0.86	1 (6%)
6	NAG	Q	503	1,6	14,14,15	0.49	0	15,19,21	0.79	0
6	NAG	Q	504	6	14,14,15	0.52	0	15,19,21	0.94	0
6	BMA	Q	505	6	11,11,12	0.75	0	14,15,17	1.01	1 (7%)
6	MAN	Q	506	6	11,11,12	0.60	0	14,15,17	0.82	1 (7%)
7	NAG	Q	507	1,7	14,14,15	0.57	0	15,19,21	0.77	0
7	NAG	Q	508	7	14,14,15	0.50	0	15,19,21	0.89	1 (6%)
6	NAG	S	503	1,6	14,14,15	0.44	0	15,19,21	0.94	1 (6%)
6	NAG	S	504	6	14,14,15	0.51	0	15,19,21	1.03	1 (6%)
6	BMA	S	505	6	11,11,12	0.72	0	14,15,17	1.11	1 (7%)
6	MAN	S	506	6	11,11,12	0.60	0	14,15,17	0.76	1 (7%)
7	NAG	S	507	1,7	14,14,15	0.56	0	15,19,21	0.63	0
7	NAG	S	508	7	14,14,15	0.53	0	15,19,21	0.83	1 (6%)
6	NAG	U	503	1,6	14,14,15	0.52	0	15,19,21	1.05	0
6	NAG	U	504	6	14,14,15	0.53	0	15,19,21	0.98	0
6	BMA	U	505	6	11,11,12	0.75	0	14,15,17	0.93	1 (7%)
6	MAN	U	506	6	11,11,12	0.59	0	14,15,17	0.76	0
7	NAG	U	507	1,7	14,14,15	0.51	0	15,19,21	0.68	0
7	NAG	U	508	7	14,14,15	0.50	0	15,19,21	0.91	1 (6%)
6	NAG	W	602	1,6	14,14,15	0.46	0	15,19,21	0.88	0
6	NAG	W	603	6	14,14,15	0.54	0	15,19,21	0.62	0
6	BMA	W	604	6	11,11,12	0.72	0	14,15,17	0.98	1 (7%)
6	MAN	W	605	6	11,11,12	0.57	0	14,15,17	0.82	1 (7%)
7	NAG	W	606	1,7	14,14,15	0.55	0	15,19,21	0.55	0
7	NAG	W	607	7	14,14,15	0.52	0	15,19,21	0.96	1 (6%)

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
6	NAG	A	602	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	603	6	-	0/6/23/26	0/1/1/1
6	BMA	A	604	6	-	0/2/19/22	0/1/1/1
6	MAN	A	605	6	-	0/2/19/22	0/1/1/1
7	NAG	A	606	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	607	7	-	0/6/23/26	0/1/1/1
6	NAG	C	502	1,6	-	0/6/23/26	0/1/1/1
6	NAG	C	503	6	-	0/6/23/26	0/1/1/1
6	BMA	C	504	6	-	0/2/19/22	0/1/1/1
6	MAN	C	505	6	-	0/2/19/22	0/1/1/1
7	NAG	C	506	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	507	7	-	0/6/23/26	0/1/1/1
6	NAG	E	602	1,6	-	0/6/23/26	0/1/1/1
6	NAG	E	603	6	-	0/6/23/26	0/1/1/1
6	BMA	E	604	6	-	0/2/19/22	0/1/1/1
6	MAN	E	605	6	-	0/2/19/22	0/1/1/1
7	NAG	E	606	1,7	-	0/6/23/26	0/1/1/1
7	NAG	E	607	7	-	0/6/23/26	0/1/1/1
6	NAG	G	503	1,6	-	0/6/23/26	0/1/1/1
6	NAG	G	504	6	-	0/6/23/26	0/1/1/1
6	BMA	G	505	6	-	0/2/19/22	0/1/1/1
6	MAN	G	506	6	-	0/2/19/22	0/1/1/1
7	NAG	G	507	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	508	7	-	0/6/23/26	0/1/1/1
6	NAG	I	502	1,6	-	0/6/23/26	0/1/1/1
6	NAG	I	503	6	-	0/6/23/26	0/1/1/1
6	BMA	I	504	6	-	0/2/19/22	0/1/1/1
6	MAN	I	505	6	-	0/2/19/22	0/1/1/1
7	NAG	I	506	1,7	-	0/6/23/26	0/1/1/1
7	NAG	I	507	7	-	0/6/23/26	0/1/1/1
6	NAG	K	602	1,6	-	0/6/23/26	0/1/1/1
6	NAG	K	603	6	-	0/6/23/26	0/1/1/1
6	BMA	K	604	6	-	0/2/19/22	0/1/1/1
6	MAN	K	605	6	-	0/2/19/22	0/1/1/1
7	NAG	K	606	1,7	-	0/6/23/26	0/1/1/1
7	NAG	K	607	7	-	0/6/23/26	0/1/1/1
6	NAG	M	503	1,6	-	0/6/23/26	0/1/1/1
6	NAG	M	504	6	-	0/6/23/26	0/1/1/1
6	BMA	M	505	6	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	M	506	6	-	0/2/19/22	0/1/1/1
7	NAG	M	507	1,7	-	0/6/23/26	0/1/1/1
7	NAG	M	508	7	-	0/6/23/26	0/1/1/1
6	NAG	O	503	1,6	-	0/6/23/26	0/1/1/1
6	NAG	O	504	6	-	0/6/23/26	0/1/1/1
6	BMA	O	505	6	-	0/2/19/22	0/1/1/1
6	MAN	O	506	6	-	0/2/19/22	0/1/1/1
7	NAG	O	507	1,7	-	0/6/23/26	0/1/1/1
7	NAG	O	508	7	-	0/6/23/26	0/1/1/1
6	NAG	Q	503	1,6	-	0/6/23/26	0/1/1/1
6	NAG	Q	504	6	-	0/6/23/26	0/1/1/1
6	BMA	Q	505	6	-	0/2/19/22	0/1/1/1
6	MAN	Q	506	6	-	0/2/19/22	0/1/1/1
7	NAG	Q	507	1,7	-	0/6/23/26	0/1/1/1
7	NAG	Q	508	7	-	0/6/23/26	0/1/1/1
6	NAG	S	503	1,6	-	0/6/23/26	0/1/1/1
6	NAG	S	504	6	-	0/6/23/26	0/1/1/1
6	BMA	S	505	6	-	0/2/19/22	0/1/1/1
6	MAN	S	506	6	-	0/2/19/22	0/1/1/1
7	NAG	S	507	1,7	-	0/6/23/26	0/1/1/1
7	NAG	S	508	7	-	0/6/23/26	0/1/1/1
6	NAG	U	503	1,6	-	0/6/23/26	0/1/1/1
6	NAG	U	504	6	-	0/6/23/26	0/1/1/1
6	BMA	U	505	6	-	0/2/19/22	0/1/1/1
6	MAN	U	506	6	-	0/2/19/22	0/1/1/1
7	NAG	U	507	1,7	-	0/6/23/26	0/1/1/1
7	NAG	U	508	7	-	0/6/23/26	0/1/1/1
6	NAG	W	602	1,6	-	0/6/23/26	0/1/1/1
6	NAG	W	603	6	-	0/6/23/26	0/1/1/1
6	BMA	W	604	6	-	0/2/19/22	0/1/1/1
6	MAN	W	605	6	-	0/2/19/22	0/1/1/1
7	NAG	W	606	1,7	-	0/6/23/26	0/1/1/1
7	NAG	W	607	7	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	506	MAN	O5-C1-C2	-2.57	106.68	110.86
6	I	505	MAN	O5-C1-C2	-2.53	106.75	110.86
6	O	506	MAN	O5-C1-C2	-2.34	107.06	110.86
6	A	603	NAG	C1-O5-C5	-2.33	109.29	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	W	605	MAN	O5-C1-C2	-2.19	107.31	110.86
6	G	506	MAN	O5-C1-C2	-2.18	107.33	110.86
6	E	605	MAN	O5-C1-C2	-2.15	107.38	110.86
6	Q	506	MAN	O5-C1-C2	-2.13	107.40	110.86
6	S	506	MAN	O5-C1-C2	-2.11	107.44	110.86
7	S	508	NAG	C1-O5-C5	2.06	114.87	112.25
6	S	504	NAG	O6-C6-C5	2.07	118.16	111.33
6	S	503	NAG	C1-O5-C5	2.21	115.05	112.25
6	A	604	BMA	C1-O5-C5	2.23	115.08	112.25
7	O	508	NAG	C1-O5-C5	2.25	115.11	112.25
6	A	603	NAG	O5-C5-C6	2.35	112.43	107.35
7	Q	508	NAG	C1-O5-C5	2.53	115.46	112.25
7	I	507	NAG	C1-O5-C5	2.53	115.46	112.25
7	U	508	NAG	C1-O5-C5	2.59	115.53	112.25
7	W	607	NAG	C1-O5-C5	2.74	115.73	112.25
7	M	508	NAG	C1-O5-C5	2.77	115.76	112.25
7	K	607	NAG	C1-O5-C5	2.94	115.98	112.25
7	C	507	NAG	C1-O5-C5	2.96	116.01	112.25
6	M	505	BMA	C1-C2-C3	3.03	113.13	109.54
6	E	604	BMA	C1-C2-C3	3.05	113.15	109.54
6	K	604	BMA	C1-C2-C3	3.07	113.17	109.54
7	E	607	NAG	C1-O5-C5	3.08	116.16	112.25
6	O	505	BMA	C1-C2-C3	3.08	113.18	109.54
6	U	505	BMA	C1-C2-C3	3.09	113.19	109.54
6	Q	505	BMA	C1-C2-C3	3.23	113.36	109.54
6	W	604	BMA	C1-C2-C3	3.24	113.37	109.54
6	C	504	BMA	C1-C2-C3	3.28	113.42	109.54
6	I	504	BMA	C1-C2-C3	3.32	113.46	109.54
6	M	503	NAG	C1-O5-C5	3.39	116.55	112.25
7	G	508	NAG	C1-O5-C5	3.48	116.67	112.25
6	S	505	BMA	C1-C2-C3	3.54	113.73	109.54
6	G	505	BMA	C1-C2-C3	3.76	113.99	109.54
6	A	604	BMA	C1-C2-C3	3.93	114.19	109.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	S	503	NAG	1	0

5.6 Ligand geometry ⓘ

30 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	1.53	2 (14%)	15,19,21	3.95	7 (46%)
5	NAG	B	201	2	14,14,15	0.60	0	15,19,21	0.86	1 (6%)
5	NAG	C	501	1	14,14,15	0.44	0	15,19,21	1.18	2 (13%)
5	NAG	D	201	2	14,14,15	0.52	0	15,19,21	1.31	1 (6%)
5	NAG	E	601	1	14,14,15	0.47	0	15,19,21	1.34	2 (13%)
5	NAG	F	201	2	14,14,15	0.49	0	15,19,21	1.10	1 (6%)
5	NAG	G	501	1	14,14,15	0.38	0	15,19,21	1.09	1 (6%)
5	NAG	G	502	1	14,14,15	0.48	0	15,19,21	1.22	2 (13%)
5	NAG	H	201	2	14,14,15	0.56	0	15,19,21	0.89	1 (6%)
5	NAG	I	501	1	14,14,15	0.44	0	15,19,21	0.98	1 (6%)
5	NAG	J	201	2	14,14,15	0.51	0	15,19,21	1.34	1 (6%)
5	NAG	K	601	1	14,14,15	0.47	0	15,19,21	1.47	2 (13%)
5	NAG	L	201	2	14,14,15	0.54	0	15,19,21	0.83	0
5	NAG	M	501	1	14,14,15	0.42	0	15,19,21	1.21	2 (13%)
5	NAG	M	502	1	14,14,15	0.45	0	15,19,21	1.22	2 (13%)
5	NAG	N	201	2	14,14,15	0.54	0	15,19,21	1.15	2 (13%)
5	NAG	O	501	1	14,14,15	0.49	0	15,19,21	0.86	0
5	NAG	O	502	1	14,14,15	0.49	0	15,19,21	1.36	3 (20%)
5	NAG	P	201	2	14,14,15	0.55	0	15,19,21	0.93	0
5	NAG	Q	501	1	14,14,15	0.42	0	15,19,21	0.98	0
5	NAG	Q	502	1	14,14,15	0.57	0	15,19,21	1.31	2 (13%)
5	NAG	R	201	2	14,14,15	0.51	0	15,19,21	1.08	1 (6%)
5	NAG	S	501	1	14,14,15	0.45	0	15,19,21	1.06	1 (6%)
5	NAG	S	502	1	14,14,15	0.51	0	15,19,21	1.46	3 (20%)
5	NAG	T	201	2	14,14,15	0.57	0	15,19,21	1.04	1 (6%)
5	NAG	U	501	1	14,14,15	0.46	0	15,19,21	0.99	1 (6%)
5	NAG	U	502	1	14,14,15	0.46	0	15,19,21	1.34	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	V	201	2	14,14,15	0.53	0	15,19,21	0.93	1 (6%)
5	NAG	W	601	1	14,14,15	0.53	0	15,19,21	1.54	4 (26%)
5	NAG	X	201	2	14,14,15	0.52	0	15,19,21	0.95	1 (6%)

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	-	0/6/23/26	0/1/1/1
5	NAG	B	201	2	-	0/6/23/26	0/1/1/1
5	NAG	C	501	1	-	0/6/23/26	0/1/1/1
5	NAG	D	201	2	-	0/6/23/26	0/1/1/1
5	NAG	E	601	1	-	0/6/23/26	0/1/1/1
5	NAG	F	201	2	-	0/6/23/26	0/1/1/1
5	NAG	G	501	1	-	0/6/23/26	0/1/1/1
5	NAG	G	502	1	-	0/6/23/26	0/1/1/1
5	NAG	H	201	2	-	0/6/23/26	0/1/1/1
5	NAG	I	501	1	-	0/6/23/26	0/1/1/1
5	NAG	J	201	2	-	0/6/23/26	0/1/1/1
5	NAG	K	601	1	-	0/6/23/26	0/1/1/1
5	NAG	L	201	2	-	0/6/23/26	0/1/1/1
5	NAG	M	501	1	-	0/6/23/26	0/1/1/1
5	NAG	M	502	1	-	0/6/23/26	0/1/1/1
5	NAG	N	201	2	-	0/6/23/26	0/1/1/1
5	NAG	O	501	1	-	0/6/23/26	0/1/1/1
5	NAG	O	502	1	-	0/6/23/26	0/1/1/1
5	NAG	P	201	2	-	0/6/23/26	0/1/1/1
5	NAG	Q	501	1	-	0/6/23/26	0/1/1/1
5	NAG	Q	502	1	-	0/6/23/26	0/1/1/1
5	NAG	R	201	2	-	0/6/23/26	0/1/1/1
5	NAG	S	501	1	-	0/6/23/26	0/1/1/1
5	NAG	S	502	1	-	0/6/23/26	0/1/1/1
5	NAG	T	201	2	-	0/6/23/26	0/1/1/1
5	NAG	U	501	1	-	0/6/23/26	0/1/1/1
5	NAG	U	502	1	-	0/6/23/26	0/1/1/1
5	NAG	V	201	2	-	0/6/23/26	0/1/1/1
5	NAG	W	601	1	-	0/6/23/26	0/1/1/1
5	NAG	X	201	2	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	NAG	C2-N2	-3.84	1.39	1.46
5	A	601	NAG	C8-C7	-3.61	1.43	1.50

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	NAG	C2-N2-C7	-8.85	111.67	123.04
5	A	601	NAG	C4-C3-C2	-7.40	99.72	111.23
5	A	601	NAG	C8-C7-N2	-5.19	106.18	116.11
5	A	601	NAG	C3-C4-C5	-4.98	101.51	110.20
5	S	502	NAG	C4-C3-C2	-2.69	107.05	111.23
5	K	601	NAG	C4-C3-C2	-2.67	107.08	111.23
5	S	501	NAG	C4-C3-C2	-2.59	107.20	111.23
5	W	601	NAG	C4-C3-C2	-2.50	107.34	111.23
5	M	501	NAG	C4-C3-C2	-2.48	107.37	111.23
5	C	501	NAG	C4-C3-C2	-2.42	107.47	111.23
5	A	601	NAG	C1-O5-C5	-2.39	109.21	112.25
5	U	501	NAG	C4-C3-C2	-2.33	107.60	111.23
5	O	502	NAG	C4-C3-C2	-2.31	107.64	111.23
5	S	502	NAG	O7-C7-C8	-2.27	117.89	122.06
5	W	601	NAG	O7-C7-C8	-2.26	117.92	122.06
5	G	502	NAG	C4-C3-C2	-2.26	107.72	111.23
5	E	601	NAG	C4-C3-C2	-2.24	107.74	111.23
5	U	502	NAG	C4-C3-C2	-2.15	107.88	111.23
5	M	502	NAG	C4-C3-C2	-2.15	107.88	111.23
5	I	501	NAG	C4-C3-C2	-2.13	107.92	111.23
5	Q	502	NAG	O7-C7-C8	-2.11	118.19	122.06
5	N	201	NAG	O3-C3-C4	-2.02	105.79	110.34
5	B	201	NAG	C1-O5-C5	2.11	114.93	112.25
5	H	201	NAG	C1-O5-C5	2.18	115.02	112.25
5	V	201	NAG	C1-O5-C5	2.22	115.07	112.25
5	O	502	NAG	C1-O5-C5	2.33	115.21	112.25
5	X	201	NAG	C1-O5-C5	2.36	115.24	112.25
5	W	601	NAG	O5-C5-C6	2.37	112.48	107.35
5	T	201	NAG	C1-O5-C5	2.40	115.29	112.25
5	G	502	NAG	O5-C5-C6	2.43	112.60	107.35
5	E	601	NAG	O5-C5-C6	2.45	112.65	107.35
5	G	501	NAG	C1-O5-C5	2.55	115.49	112.25
5	O	502	NAG	O5-C5-C6	2.61	113.00	107.35
5	M	502	NAG	O5-C5-C6	2.68	113.14	107.35
5	S	502	NAG	O5-C5-C6	2.70	113.19	107.35
5	M	501	NAG	C1-O5-C5	2.76	115.75	112.25
5	N	201	NAG	C1-O5-C5	2.84	115.85	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	NAG	C1-O5-C5	2.86	115.88	112.25
5	R	201	NAG	C1-O5-C5	2.91	115.95	112.25
5	W	601	NAG	C1-O5-C5	3.05	116.12	112.25
5	U	502	NAG	O5-C5-C6	3.09	114.04	107.35
5	K	601	NAG	O5-C5-C6	3.11	114.08	107.35
5	F	201	NAG	C1-O5-C5	3.15	116.24	112.25
5	Q	502	NAG	O5-C5-C6	3.15	114.17	107.35
5	A	601	NAG	O7-C7-N2	3.64	129.29	121.86
5	D	201	NAG	C1-O5-C5	3.88	117.17	112.25
5	J	201	NAG	C1-O5-C5	4.45	117.90	112.25
5	A	601	NAG	O3-C3-C2	4.62	118.27	109.11

There are no chirality outliers.

There are no torsion outliers.

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	318/323 (98%)	0.25	12 (3%) 44 34	33, 40, 68, 127	0
1	C	318/323 (98%)	0.14	5 (1%) 74 64	24, 43, 70, 106	0
1	E	318/323 (98%)	0.17	6 (1%) 70 60	30, 41, 77, 116	0
1	G	318/323 (98%)	0.05	5 (1%) 74 64	21, 33, 78, 132	0
1	I	318/323 (98%)	0.24	11 (3%) 48 37	25, 42, 64, 102	0
1	K	318/323 (98%)	0.06	2 (0%) 90 86	29, 42, 61, 112	0
1	M	318/323 (98%)	0.57	29 (9%) 11 9	58, 70, 100, 141	0
1	O	318/323 (98%)	0.24	12 (3%) 44 34	38, 61, 90, 116	0
1	Q	318/323 (98%)	0.11	9 (2%) 56 45	40, 49, 72, 115	0
1	S	318/323 (98%)	0.34	8 (2%) 61 49	43, 60, 76, 109	0
1	U	318/323 (98%)	0.03	5 (1%) 74 64	33, 42, 74, 121	0
1	W	318/323 (98%)	0.19	18 (5%) 27 20	31, 38, 91, 159	0
2	B	172/174 (98%)	0.01	3 (1%) 73 63	34, 61, 97, 111	0
2	D	172/174 (98%)	0.29	8 (4%) 35 27	40, 58, 81, 85	0
2	F	172/174 (98%)	0.19	7 (4%) 41 31	46, 61, 92, 97	0
2	H	172/174 (98%)	0.16	3 (1%) 73 63	15, 74, 123, 133	0
2	J	172/174 (98%)	0.11	2 (1%) 81 73	39, 61, 89, 96	0
2	L	172/174 (98%)	0.12	5 (2%) 55 43	23, 54, 94, 102	0
2	N	172/174 (98%)	0.32	13 (7%) 17 12	40, 87, 125, 133	0
2	P	172/174 (98%)	0.21	3 (1%) 73 63	40, 81, 115, 128	0
2	R	172/174 (98%)	0.02	1 (0%) 90 86	33, 61, 100, 111	0
2	T	172/174 (98%)	0.20	7 (4%) 41 31	43, 70, 121, 136	0
2	V	172/174 (98%)	-0.03	0 100 100	35, 57, 102, 115	0
2	X	172/174 (98%)	0.18	7 (4%) 41 31	36, 76, 130, 139	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
3	a	238/241 (98%)	-0.10	1 (0%) 93 90	23, 37, 62, 74	0
3	c	238/241 (98%)	0.07	1 (0%) 93 90	26, 36, 54, 59	0
3	e	238/241 (98%)	0.28	11 (4%) 36 27	45, 66, 75, 83	0
3	g	238/241 (98%)	0.03	0 100 100	18, 39, 95, 107	0
3	i	238/241 (98%)	0.03	2 (0%) 87 82	23, 30, 59, 70	0
3	k	238/241 (98%)	0.20	5 (2%) 67 56	50, 65, 91, 107	0
3	m	238/241 (98%)	0.18	12 (5%) 32 25	39, 47, 73, 86	0
3	o	238/241 (98%)	0.60	21 (8%) 12 9	70, 85, 107, 124	0
3	q	238/241 (98%)	0.19	4 (1%) 73 63	38, 54, 81, 91	0
3	s	238/241 (98%)	0.51	16 (6%) 21 14	63, 81, 100, 126	0
3	u	238/241 (98%)	0.03	3 (1%) 79 71	42, 57, 74, 86	0
3	w	238/241 (98%)	0.20	10 (4%) 40 31	28, 47, 83, 97	0
4	b	213/214 (99%)	-0.08	0 100 100	17, 28, 62, 66	0
4	d	213/214 (99%)	-0.03	0 100 100	23, 39, 67, 73	0
4	f	213/214 (99%)	-0.09	0 100 100	44, 54, 86, 97	0
4	h	213/214 (99%)	0.07	5 (2%) 64 53	20, 33, 85, 91	0
4	j	213/214 (99%)	-0.05	0 100 100	23, 31, 66, 80	0
4	l	213/214 (99%)	0.22	7 (3%) 50 38	54, 79, 103, 107	0
4	n	213/214 (99%)	0.16	3 (1%) 78 69	33, 44, 55, 62	0
4	p	213/214 (99%)	0.29	7 (3%) 50 38	70, 79, 105, 111	0
4	r	213/214 (99%)	0.19	5 (2%) 64 53	33, 53, 68, 73	0
4	t	213/214 (99%)	0.24	6 (2%) 56 45	47, 68, 105, 115	0
4	v	213/214 (99%)	0.11	3 (1%) 78 69	34, 48, 84, 93	0
4	x	213/214 (99%)	0.08	4 (1%) 70 60	25, 41, 54, 59	0
All	All	11292/11424 (98%)	0.16	307 (2%) 58 47	15, 51, 98, 159	0

All (307) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	o	133	GLY	7.2
1	M	37	THR	6.5
4	l	177	SER	6.5
2	N	27	GLN	6.0
3	w	132	SER	5.7

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Mol	Chain	Res	Type	RSRZ
4	v	1	ASP	5.6
2	N	29	SER	5.0
3	s	133	GLY	4.9
1	M	242	VAL	4.9
1	A	9	PRO	4.6
3	m	144	ASP	4.6
2	D	23	GLY	4.5
1	W	326	LYS	4.5
2	X	23	GLY	4.3
1	M	9	PRO	4.2
1	W	9	PRO	4.1
3	e	20	LEU	4.1
1	M	12	THR	4.1
3	m	132	SER	4.0
2	N	33	GLY	4.0
2	F	161	VAL	3.8
3	e	9	GLY	3.8
2	N	26	HIS	3.8
3	s	209	LYS	3.7
1	W	319	GLY	3.7
1	S	16	GLY	3.7
3	u	132	SER	3.6
2	T	36	ALA	3.6
1	C	35	GLU	3.6
3	m	204	ASN	3.6
4	v	2	ILE	3.6
1	A	326	LYS	3.5
4	t	117	ILE	3.5
2	J	26	HIS	3.5
2	D	32	THR	3.4
1	E	9	PRO	3.4
1	M	10	GLY	3.4
3	e	132	SER	3.4
1	Q	259	LYS	3.4
3	w	144	ASP	3.4
3	o	132	SER	3.4
3	w	133	GLY	3.3
3	w	145	TYR	3.3
1	W	37	THR	3.3
1	U	135	GLY	3.3
2	X	17[A]	MET	3.3
1	M	22	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	S	146	GLY	3.2
2	J	25	ARG	3.2
1	I	323	VAL	3.2
1	M	11	ALA	3.2
4	r	2	ILE	3.2
3	o	129	LYS	3.2
4	h	148	TRP	3.2
3	o	27(C)	GLY	3.2
1	W	320	MET	3.2
3	o	134	GLY	3.2
1	O	9	PRO	3.2
3	m	133	GLY	3.2
3	e	8	GLY	3.1
1	A	288	ILE	3.1
3	s	21[A]	SER	3.1
3	e	21[A]	SER	3.1
3	s	195	ILE	3.1
3	q	123	PRO	3.1
1	E	175	ASP	3.0
2	X	126	LEU	3.0
4	p	64	GLY	3.0
1	O	37	THR	3.0
2	D	26	HIS	3.0
1	A	119	GLU	3.0
4	n	1	ASP	3.0
2	F	122	THR	2.9
1	O	225	GLY	2.9
3	s	214	LYS	2.9
1	M	302	TYR	2.9
1	W	23	GLY	2.9
3	e	133	GLY	2.9
3	m	145	TYR	2.9
2	X	164	ASP	2.9
1	O	319	GLY	2.9
2	L	25	ARG	2.8
1	M	23	GLY	2.8
4	p	65	GLY	2.8
3	o	209	LYS	2.8
4	n	151	ASP	2.8
4	r	106	ILE	2.8
1	C	86	LEU	2.8
1	I	19	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
3	s	18	LEU	2.8
3	e	194	TYR	2.8
3	k	21[A]	SER	2.7
3	w	180	SER	2.7
3	s	134	GLY	2.7
1	W	12	THR	2.7
3	w	27(C)	GLY	2.7
1	A	176	LYS	2.7
4	l	178	THR	2.7
3	s	86	ASP	2.7
1	K	12	THR	2.7
2	D	171	PHE	2.7
3	k	214	LYS	2.7
1	Q	10	GLY	2.7
1	O	175	ASP	2.7
2	F	141	TYR	2.7
3	o	20	LEU	2.7
3	q	139	GLY	2.7
3	m	100	GLN	2.6
4	t	181	LEU	2.6
2	L	132	ASP	2.6
4	r	181	LEU	2.6
1	S	135	GLY	2.6
3	e	134	GLY	2.6
2	N	36	ALA	2.6
2	P	16	GLY	2.6
1	M	43	VAL	2.6
3	k	168	ALA	2.6
4	h	156	SER	2.6
1	M	313	THR	2.6
4	t	119	PRO	2.6
2	T	35	ALA	2.6
1	M	312	ASN	2.6
1	E	12	THR	2.6
1	I	322	ASN	2.6
1	M	322	ASN	2.6
4	p	187	GLU	2.6
3	s	100(D)	ALA	2.6
3	w	179	SER	2.5
1	Q	9	PRO	2.5
4	p	199	GLN	2.5
4	t	62	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
3	o	21[A]	SER	2.5
3	s	123	PRO	2.5
1	O	58	ILE	2.5
2	D	160	ASP	2.5
1	W	35	GLU	2.5
1	O	227[A]	SER	2.5
3	o	58	ASP	2.5
1	W	135	GLY	2.5
3	a	27	SER	2.5
1	W	321[A]	ARG	2.5
1	O	10	GLY	2.5
4	l	181	LEU	2.5
4	t	70	ASP	2.5
4	l	193	ALA	2.5
3	s	210	ARG	2.5
2	L	20	GLY	2.5
1	E	58	ILE	2.4
1	S	82	GLU	2.4
3	w	100(D)	ALA	2.4
2	N	23	GLY	2.4
1	A	325	GLU	2.4
2	P	172	GLN	2.4
3	m	214	LYS	2.4
1	M	45	SER	2.4
1	W	189	GLN	2.4
1	M	315	LYS	2.4
2	T	22	TYR	2.4
3	e	214	LYS	2.4
1	O	260[A]	MET	2.4
1	Q	264	LYS	2.4
1	M	274[A]	ILE	2.4
3	k	211	VAL	2.4
2	X	143	LYS	2.4
1	M	272	ALA	2.4
1	U	259	LYS	2.4
3	k	182	VAL	2.4
2	H	34	GLN	2.4
1	Q	77	ASP	2.4
2	N	28	ASN	2.4
2	T	143	LYS	2.4
3	s	90	TYR	2.4
3	e	168	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	M	32[A]	ASP	2.3
3	i	133	GLY	2.3
1	M	319	GLY	2.3
2	R	158	ASP	2.3
1	M	273	PRO	2.3
1	M	297	VAL	2.3
1	I	35	GLU	2.3
3	o	8	GLY	2.3
4	v	130	ALA	2.3
1	Q	175	ASP	2.3
1	E	10	GLY	2.3
1	G	208	ARG	2.3
1	E	306	PRO	2.3
1	W	92	LYS	2.3
1	I	137	ASN	2.3
4	h	155	GLN	2.3
2	L	141	TYR	2.3
1	M	13	LEU	2.3
2	D	24	PHE	2.3
1	A	27	LYS	2.3
1	S	319	GLY	2.3
3	w	214	LYS	2.2
4	l	145	LYS	2.2
1	Q	320	MET	2.2
4	t	187	GLU	2.2
4	p	77	SER	2.2
2	P	17[A]	MET	2.2
2	X	172	GLN	2.2
1	Q	226	LEU	2.2
1	W	325	GLU	2.2
3	s	68	THR	2.2
1	I	321[A]	ARG	2.2
4	h	147	GLN	2.2
3	o	175	LEU	2.2
3	o	196	CYS	2.2
2	N	44	ALA	2.2
4	x	29	ILE	2.2
3	m	52(A)	ALA	2.2
1	O	279	SER	2.2
1	K	175	ASP	2.2
1	G	12	THR	2.2
1	S	259	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	W	175	ASP	2.2
2	X	171	PHE	2.2
2	D	33	GLY	2.2
2	N	17[A]	MET	2.2
3	u	130	SER	2.2
4	r	130	ALA	2.2
1	O	16	GLY	2.2
2	B	11	GLU	2.2
4	p	66	GLY	2.2
1	I	18	HIS	2.2
1	W	13	LEU	2.2
1	G	271	ASP	2.2
2	F	132	ASP	2.2
3	q	127	SER	2.2
4	x	33	LEU	2.2
1	I	167	THR	2.1
2	N	30	GLU	2.1
3	o	19[A]	ARG	2.1
3	m	176	TYR	2.1
1	U	128	THR	2.1
1	W	24[A]	THR	2.1
4	r	11	LEU	2.1
1	M	51	ILE	2.1
3	m	54	GLY	2.1
2	F	63	PHE	2.1
4	l	179	LEU	2.1
1	U	76	CYS	2.1
1	A	221	PRO	2.1
2	F	131	GLU	2.1
4	n	2	ILE	2.1
4	h	192	TYR	2.1
3	s	112	SER	2.1
1	A	304	ALA	2.1
3	o	174	GLY	2.1
1	M	33	GLN	2.1
2	B	171	PHE	2.1
4	p	76	SER	2.1
2	T	17[A]	MET	2.1
1	A	259	LYS	2.1
2	B	157	TYR	2.1
2	T	171	PHE	2.1
2	N	22	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
2	L	139	LYS	2.1
3	e	182	VAL	2.1
3	o	24	GLY	2.1
3	u	133	GLY	2.1
4	l	147	GLN	2.1
1	M	124	GLY	2.1
3	m	24	GLY	2.1
3	o	29	LEU	2.1
3	s	93	ALA	2.1
1	C	15	LEU	2.1
3	m	175	LEU	2.1
3	q	132	SER	2.1
1	S	173	ASN	2.1
3	o	135	THR	2.1
2	F	125	GLN	2.1
3	o	78	LEU	2.1
1	W	315	LYS	2.1
3	c	7	SER	2.1
1	U	136	SER	2.1
1	A	212	THR	2.1
2	H	24	PHE	2.1
2	T	132	ASP	2.1
1	G	21	PRO	2.0
3	o	4	LEU	2.0
1	M	248	ASN	2.0
4	x	151	ASP	2.0
1	C	145	SER	2.0
1	M	66	LEU	2.0
1	O	207[A]	ARG	2.0
2	D	31	GLY	2.0
1	I	193	SER	2.0
1	W	93	ALA	2.0
3	o	68	THR	2.0
1	G	171	ASN	2.0
1	I	63	ASP	2.0
2	N	68	LYS	2.0
2	H	157	TYR	2.0
1	Q	325	GLU	2.0
3	s	174	GLY	2.0
1	M	34	ILE	2.0
1	S	12	THR	2.0
1	A	323	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
3	o	128	SER	2.0
3	w	176	TYR	2.0
1	I	48	THR	2.0
2	N	144	CYS	2.0
1	M	296	ASN	2.0
3	i	98	MET	2.0
1	C	322	ASN	2.0
4	x	28	ASP	2.0

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	PCA	e	1	8/9	0.83	0.29	-	54,56,59,62	0
3	PCA	g	1	8/9	0.95	0.22	-	35,36,38,38	0
3	PCA	a	1	8/9	0.89	0.36	-	36,36,37,38	0
3	PCA	c	1	8/9	0.86	0.31	-	36,37,38,39	0
3	PCA	m	1	8/9	0.86	0.21	-	40,41,41,41	0
3	PCA	o	1	8/9	0.89	0.15	-	77,78,79,79	0
3	PCA	i	1	8/9	0.80	0.36	-	32,32,33,33	0
3	PCA	k	1	8/9	0.89	0.18	-	50,52,54,57	0
3	PCA	u	1	8/9	0.80	0.37	-	54,55,56,56	0
3	PCA	w	1	8/9	0.89	0.36	-	27,27,27,29	0
3	PCA	q	1	8/9	0.85	0.29	-	57,57,58,58	0
3	PCA	s	1	8/9	0.82	0.29	-	63,64,64,64	0

6.3 Carbohydrates ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
7	NAG	U	507	14/15	0.73	0.48	4.11	42,44,47,47	0
7	NAG	Q	507	14/15	0.82	0.30	1.19	46,50,54,57	0
7	NAG	C	506	14/15	0.76	0.39	1.05	43,45,49,50	0
6	NAG	K	603	14/15	0.84	0.51	0.98	51,60,69,71	0
6	NAG	A	602	14/15	0.70	0.38	0.93	45,48,60,61	0
6	NAG	O	504	14/15	0.82	0.41	0.71	47,52,59,62	0
7	NAG	A	606	14/15	0.80	0.39	0.62	37,40,44,49	0
7	NAG	S	507	14/15	0.80	0.33	0.43	59,63,67,70	0
7	NAG	I	506	14/15	0.77	0.44	0.21	50,57,61,63	0
7	NAG	W	606	14/15	0.76	0.34	0.10	53,60,66,68	0
7	NAG	K	606	14/15	0.79	0.33	-0.22	40,47,50,53	0
7	NAG	M	507	14/15	0.75	0.45	-0.28	70,73,76,76	0
7	NAG	G	507	14/15	0.76	0.28	-0.59	37,42,47,49	0
6	NAG	Q	503	14/15	0.82	0.25	-0.63	54,60,70,71	0
7	NAG	O	507	14/15	0.81	0.30	-0.66	71,77,82,84	0
6	NAG	E	602	14/15	0.85	0.27	-0.72	40,46,56,56	0
6	NAG	K	602	14/15	0.76	0.29	-0.94	49,56,67,67	0
7	NAG	E	606	14/15	0.77	0.26	-1.06	60,66,70,74	0
6	NAG	O	503	14/15	0.89	0.22	-1.31	43,49,57,58	0
6	NAG	I	503	14/15	0.91	0.21	-1.34	42,50,60,62	0
6	NAG	C	503	14/15	0.90	0.19	-1.35	32,34,37,40	0
6	NAG	M	503	14/15	0.85	0.20	-1.46	66,67,68,68	0
6	NAG	I	502	14/15	0.94	0.18	-1.47	40,47,57,58	0
6	NAG	U	503	14/15	0.93	0.17	-1.48	41,43,48,48	0
6	NAG	C	502	14/15	0.92	0.15	-1.65	30,32,34,34	0
6	MAN	U	506	11/12	0.89	0.24	-	74,78,81,82	0
6	MAN	C	505	11/12	0.84	0.24	-	56,59,60,61	0
6	BMA	M	505	11/12	0.53	0.32	-	78,82,85,86	0
6	MAN	M	506	11/12	0.69	0.46	-	88,92,93,93	0
6	MAN	E	605	11/12	0.85	0.17	-	76,78,80,81	0
6	NAG	U	504	14/15	0.86	0.37	-	44,46,55,58	0
6	NAG	G	504	14/15	0.91	0.20	-	30,37,45,47	0
6	NAG	A	603	14/15	0.72	0.29	-	45,54,65,65	0
7	NAG	I	507	14/15	0.81	0.24	-	62,74,81,82	0
7	NAG	S	508	14/15	0.72	0.34	-	70,80,86,87	0
6	NAG	S	503	14/15	0.85	0.24	-	53,58,69,69	0
6	NAG	W	602	14/15	0.73	0.30	-	39,46,56,57	0
7	NAG	O	508	14/15	0.86	0.34	-	82,93,102,102	0
7	NAG	W	607	14/15	0.79	0.34	-	67,78,86,87	0
7	NAG	E	607	14/15	0.73	0.35	-	75,83,89,90	0
7	NAG	A	607	14/15	0.77	0.59	-	51,59,65,65	0
6	MAN	W	605	11/12	0.57	0.45	-	78,81,84,84	0
6	BMA	E	604	11/12	0.79	0.25	-	64,68,72,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MAN	I	505	11/12	0.76	0.25	-	75,78,80,80	0
6	MAN	S	506	11/12	0.81	0.33	-	81,83,84,84	0
6	BMA	Q	505	11/12	0.68	0.32	-	82,87,91,92	0
6	BMA	C	504	11/12	0.75	0.28	-	44,48,51,53	0
6	BMA	G	505	11/12	0.76	0.21	-	51,55,58,60	0
7	NAG	U	508	14/15	0.82	0.40	-	48,56,62,63	0
6	MAN	K	605	11/12	0.59	0.30	-	84,87,89,90	0
6	MAN	O	506	11/12	0.49	0.49	-	78,81,81,82	0
6	BMA	O	505	11/12	0.56	0.42	-	66,70,72,75	0
6	BMA	W	604	11/12	0.73	0.29	-	68,73,76,76	0
6	BMA	K	604	11/12	0.82	0.23	-	75,79,82,83	0
6	MAN	G	506	11/12	0.80	0.30	-	62,65,66,67	0
6	NAG	M	504	14/15	0.73	0.34	-	66,69,71,74	0
6	NAG	S	504	14/15	0.88	0.32	-	52,58,68,69	0
6	BMA	S	505	11/12	0.80	0.16	-	72,75,77,79	0
6	NAG	Q	504	14/15	0.85	0.48	-	57,66,77,78	0
6	NAG	G	503	14/15	0.93	0.18	-	26,32,41,42	0
7	NAG	M	508	14/15	0.82	0.42	-	70,79,89,89	0
6	MAN	Q	506	11/12	0.69	0.36	-	92,96,98,98	0
6	NAG	W	603	14/15	0.79	0.28	-	43,52,61,63	0
7	NAG	C	507	14/15	0.81	0.30	-	45,52,59,60	0
6	BMA	I	504	11/12	0.75	0.23	-	65,69,73,73	0
7	NAG	Q	508	14/15	0.79	0.41	-	59,67,73,73	0
6	MAN	A	605	11/12	0.69	0.51	-	78,80,84,84	0
7	NAG	G	508	14/15	0.62	0.58	-	49,58,66,66	0
7	NAG	K	607	14/15	0.61	0.46	-	54,62,69,69	0
6	BMA	U	505	11/12	0.62	0.30	-	62,67,72,72	0
6	NAG	E	603	14/15	0.92	0.29	-	46,50,58,60	0
6	BMA	A	604	11/12	0.63	0.26	-	70,74,78,78	0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
5	NAG	G	502	14/15	0.34	0.83	4.31	42,47,49,51	0
5	NAG	D	201	14/15	0.74	0.49	3.67	73,75,77,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	NAG	T	201	14/15	0.53	0.52	3.04	93,100,105,107	0
5	NAG	N	201	14/15	0.48	0.38	2.94	109,114,121,122	0
5	NAG	O	501	14/15	0.61	0.63	2.86	90,98,105,108	0
5	NAG	S	501	14/15	0.65	0.49	1.86	71,78,84,87	0
5	NAG	U	501	14/15	0.78	0.33	1.59	66,70,75,78	0
5	NAG	C	501	14/15	0.70	0.52	1.49	66,69,74,76	0
5	NAG	L	201	14/15	0.66	0.51	1.39	81,89,95,96	0
5	NAG	P	201	14/15	0.62	0.38	1.15	96,101,106,107	0
5	NAG	J	201	14/15	0.73	0.34	0.82	73,75,79,80	0
5	NAG	X	201	14/15	0.66	0.36	0.67	119,129,138,140	0
5	NAG	A	601	14/15	0.49	0.56	0.53	38,44,45,46	0
5	NAG	I	501	14/15	0.61	0.42	0.01	66,74,81,84	0
5	NAG	B	201	14/15	0.78	0.24	-0.06	80,89,94,96	0
5	NAG	Q	501	14/15	0.84	0.23	-0.56	66,74,80,83	0
5	NAG	G	501	14/15	0.84	0.25	-0.73	68,75,84,87	0
5	NAG	M	501	14/15	0.74	0.35	-1.16	89,92,96,98	0
5	NAG	R	201	14/15	0.43	0.63	-	100,111,117,117	0
5	NAG	V	201	14/15	0.63	0.53	-	83,85,91,93	0
5	NAG	E	601	14/15	0.51	0.46	-	59,64,66,67	0
5	NAG	H	201	14/15	0.73	0.25	-	115,125,133,134	0
5	NAG	O	502	14/15	0.56	0.50	-	74,78,81,83	0
5	NAG	U	502	14/15	0.43	0.58	-	46,48,50,51	0
5	NAG	S	502	14/15	0.52	0.48	-	65,69,74,75	0
5	NAG	W	601	14/15	0.55	0.36	-	45,51,52,54	0
5	NAG	K	601	14/15	0.66	0.42	-	58,64,66,68	0
5	NAG	M	502	14/15	0.35	0.50	-	75,76,77,78	0
5	NAG	Q	502	14/15	0.42	0.69	-	61,67,70,71	0
5	NAG	F	201	14/15	0.65	0.62	-	88,93,99,100	0

6.5 Other polymers ⓘ

There are no such residues in this entry.