



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 08:24 PM UTC

PDB ID : 5K9Q / pdb_00005k9q
Title : Crystal structure of multidonor HV1-18-class broadly neutralizing Influenza A antibody 16.a.26 in complex with A/Hong Kong/1-4-MA21-1/1968 (H3N2) Hemagglutinin
Authors : Joyce, M.G.; Thomas, P.V.; Wheatley, A.K.; McDermott, A.B.; Mascola, J.R.; Kwong, P.D.
Deposited on : 2016-06-01
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

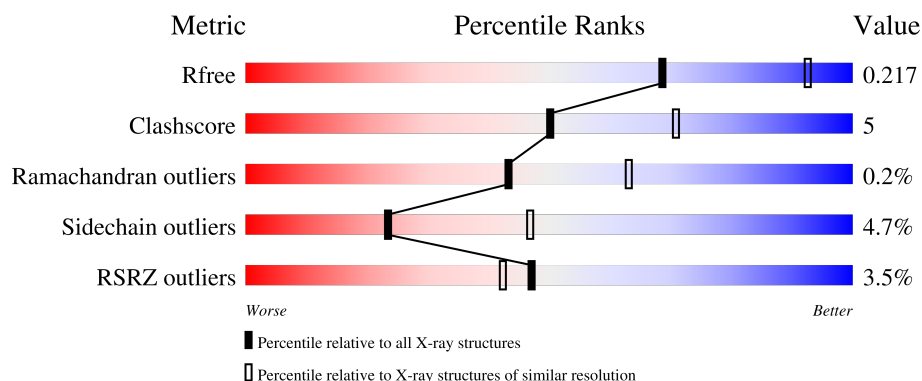
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	320	
1	C	320	
1	E	320	
1	M	320	

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Mol	Chain	Length	Quality of chain
1	O	320	 2% 89% 9% ..
1	Q	320	 % 89% 9% ..
2	B	170	 90% 8% ..
2	D	170	 2% 94% . ..
2	F	170	 % 90% 9% .
2	N	170	 2% 84% 15% ..
2	P	170	 2% 89% 7% .
2	R	170	 3% 89% 9% .
3	G	231	 12% 75% 21% .
3	H	231	 2% 78% 19% ..
3	J	231	 10% 80% 18% .
3	S	231	 8% 80% 17% .
3	U	231	 4% 85% 14% .
3	X	231	 4% 82% 16% .
4	I	214	 6% 85% 15%
4	K	214	 2% 80% 17% .
4	L	214	 2% 77% 20% .
4	T	214	 13% 81% 15% ..
4	V	214	 % 82% 15% .
4	Y	214	 3% 84% 14% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 45420 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	0	0
			2468	1544	433	478	13			
1	C	319	Total	C	N	O	S	0	0	0
			2467	1544	433	477	13			
1	E	318	Total	C	N	O	S	0	0	0
			2458	1538	431	476	13			
1	M	318	Total	C	N	O	S	0	0	0
			2458	1538	431	476	13			
1	O	318	Total	C	N	O	S	0	0	0
			2458	1538	431	476	13			
1	Q	318	Total	C	N	O	S	0	0	0
			2459	1540	431	475	13			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	218	GLU	GLY	conflict	UNP Q91MA7
A	327	ALA	GLN	conflict	UNP Q91MA7
C	218	GLU	GLY	conflict	UNP Q91MA7
C	327	ALA	GLN	conflict	UNP Q91MA7
E	218	GLU	GLY	conflict	UNP Q91MA7
E	327	ALA	GLN	conflict	UNP Q91MA7
M	218	GLU	GLY	conflict	UNP Q91MA7
M	327	ALA	GLN	conflict	UNP Q91MA7
O	218	GLU	GLY	conflict	UNP Q91MA7
O	327	ALA	GLN	conflict	UNP Q91MA7
Q	218	GLU	GLY	conflict	UNP Q91MA7
Q	327	ALA	GLN	conflict	UNP Q91MA7

- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	168	Total	C	N	O	S	0	0	0
			1366	845	241	274	6			
2	D	169	Total	C	N	O	S	0	0	0
			1377	854	242	275	6			
2	F	168	Total	C	N	O	S	0	0	0
			1371	848	242	275	6			
2	N	169	Total	C	N	O	S	0	0	0
			1368	846	240	276	6			
2	P	163	Total	C	N	O	S	0	0	0
			1340	829	236	269	6			
2	R	167	Total	C	N	O	S	0	0	0
			1362	843	240	273	6			

- Molecule 3 is a protein called 16.a.26 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	231	Total	C	N	O	S	0	0	0
			1728	1089	294	338	7			
3	H	228	Total	C	N	O	S	0	0	0
			1707	1077	290	333	7			
3	J	231	Total	C	N	O	S	0	0	0
			1728	1089	294	338	7			
3	S	231	Total	C	N	O	S	0	0	0
			1728	1089	294	338	7			
3	U	231	Total	C	N	O	S	0	0	0
			1728	1089	294	338	7			
3	X	231	Total	C	N	O	S	0	0	0
			1728	1089	294	338	7			

- Molecule 4 is a protein called 16.a.26 Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	214	Total	C	N	O	S	0	0	0
			1658	1034	283	335	6			
4	K	214	Total	C	N	O	S	0	0	0
			1658	1034	283	335	6			
4	L	214	Total	C	N	O	S	0	0	0
			1658	1034	283	335	6			
4	T	214	Total	C	N	O	S	0	0	0
			1658	1034	283	335	6			
4	V	214	Total	C	N	O	S	0	0	0
			1658	1034	283	335	6			
4	Y	214	Total	C	N	O	S	0	0	0
			1658	1034	283	335	6			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: 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	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
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		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	173	Total	O	0	0
			173	173		
6	B	81	Total	O	0	0
			81	81		
6	C	156	Total	O	0	0
			156	156		
6	D	74	Total	O	0	0
			74	74		
6	E	110	Total	O	0	0
			110	110		
6	F	75	Total	O	0	0
			75	75		
6	G	29	Total	O	0	0
			29	29		
6	H	62	Total	O	0	0
			62	62		
6	I	34	Total	O	0	0
			34	34		
6	J	29	Total	O	0	0
			29	29		
6	K	30	Total	O	0	0
			30	30		
6	L	75	Total	O	0	0
			75	75		
6	M	126	Total	O	0	0
			126	126		
6	N	50	Total	O	0	0
			50	50		
6	O	96	Total	O	0	0
			96	96		
6	P	40	Total	O	0	0
			40	40		

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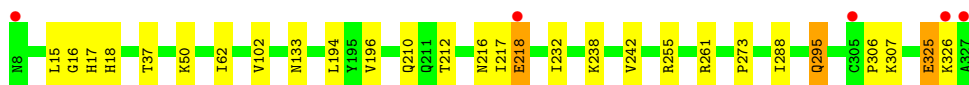
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	Q	128	Total 128	O 128	0	0
6	R	51	Total 51	O 51	0	0
6	S	9	Total 9	O 9	0	0
6	T	19	Total 19	O 19	0	0
6	U	61	Total 61	O 61	0	0
6	V	55	Total 55	O 55	0	0
6	X	55	Total 55	O 55	0	0
6	Y	51	Total 51	O 51	0	0

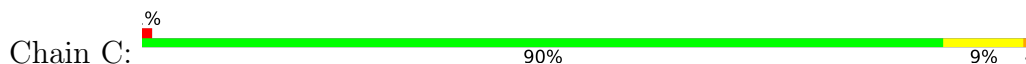
3 Residue-property plots [i](#)

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: Hemagglutinin HA1

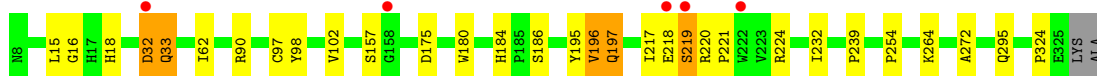


- Molecule 1: Hemagglutinin HA1

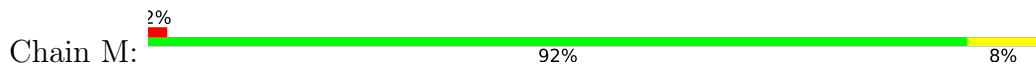


ALA

- Molecule 1: Hemagglutinin HA1



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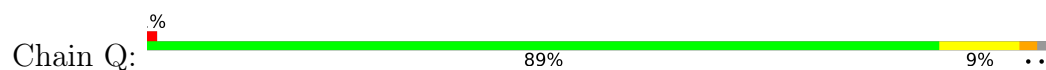


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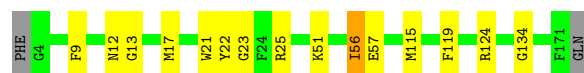
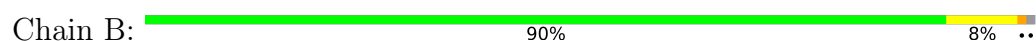




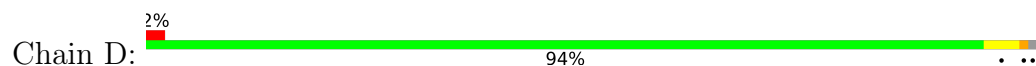
• Molecule 1: Hemagglutinin HA1



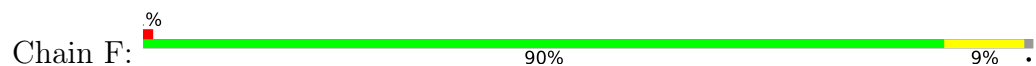
• Molecule 2: Hemagglutinin HA2



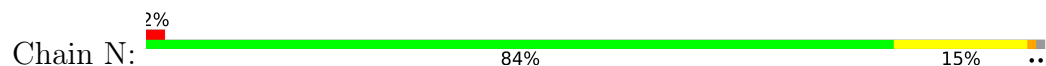
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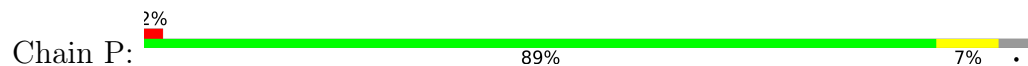
• Molecule 2: Hemagglutinin HA2



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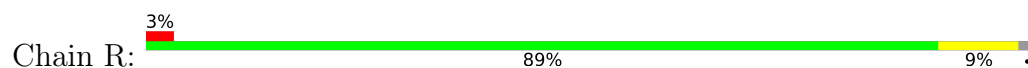


• Molecule 2: Hemagglutinin HA2

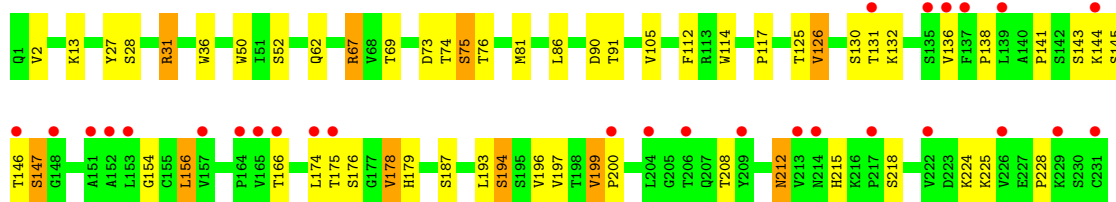
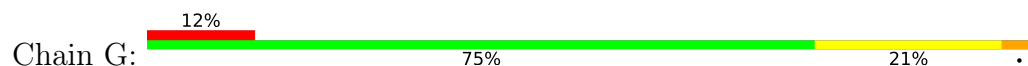




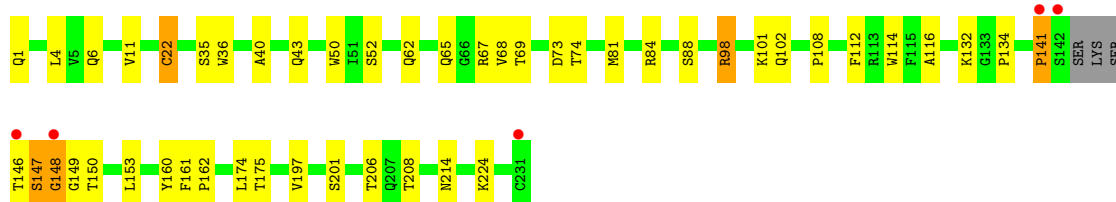
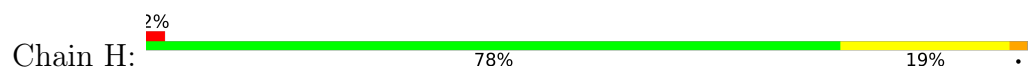
• Molecule 2: Hemagglutinin HA2



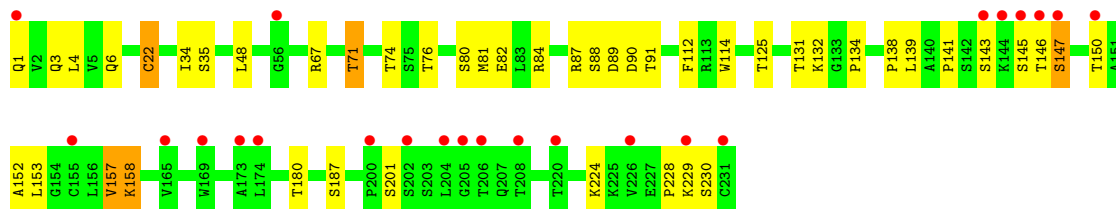
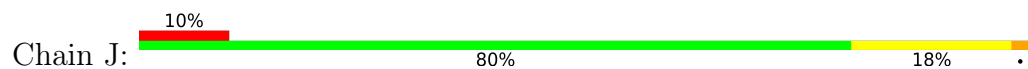
• Molecule 3: 16.a.26 Heavy chain



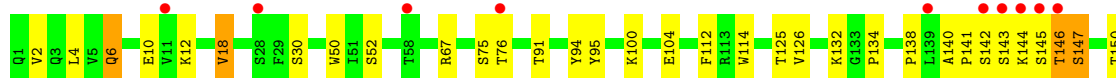
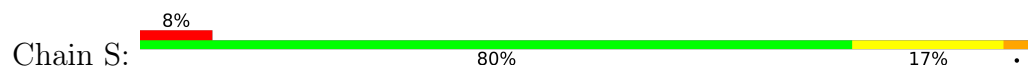
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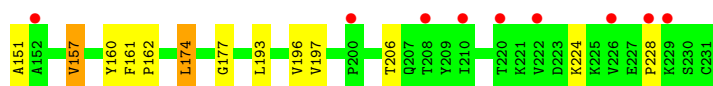


• Molecule 3: 16.a.26 Heavy chain

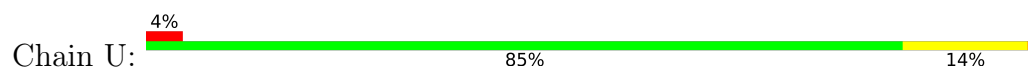


• Molecule 3: 16.a.26 Heavy chain

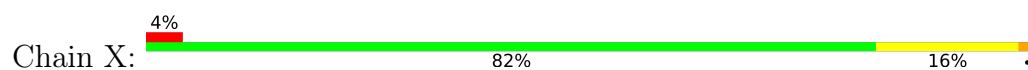




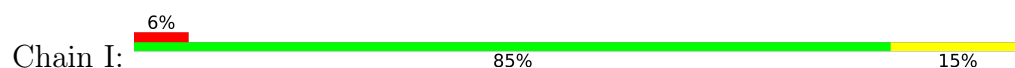
• Molecule 3: 16.a.26 Heavy chain



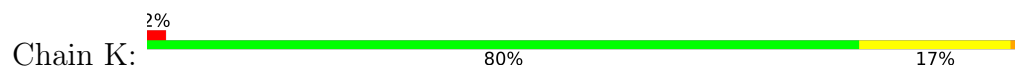
• Molecule 3: 16.a.26 Heavy chain



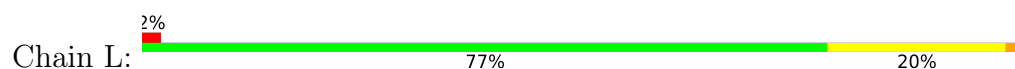
• Molecule 4: 16.a.26 Light chain

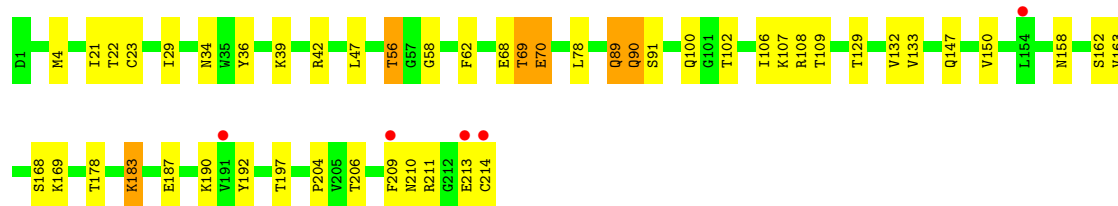


• Molecule 4: 16.a.26 Light chain

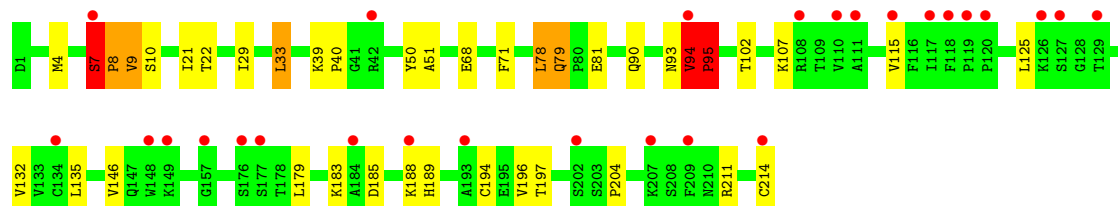
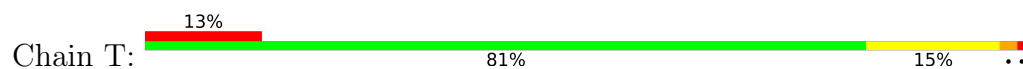


• Molecule 4: 16.a.26 Light chain

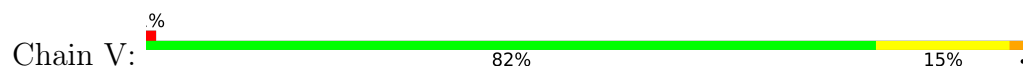




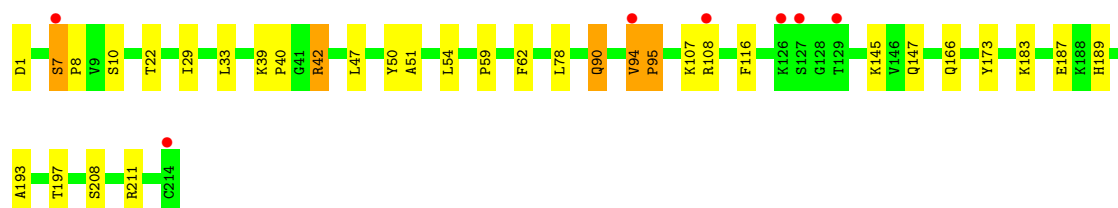
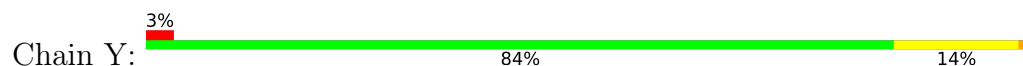
• Molecule 4: 16.a.26 Light chain



• Molecule 4: 16.a.26 Light chain



• Molecule 4: 16.a.26 Light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	121.81Å 233.91Å 302.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.28 – 2.50 49.28 – 2.50	Depositor EDS
% Data completeness (in resolution range)	82.5 (49.28-2.50) 82.5 (49.28-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.182 , 0.218 0.185 , 0.217	Depositor DCC
R_{free} test set	12285 reflections (1.83%)	wwPDB-VP
Wilson B-factor (Å ²)	46.3	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	45420	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.32	0/2524	0.44	2/3441 (0.1%)
1	C	0.35	0/2523	0.39	0/3438
1	E	0.33	0/2514	0.41	1/3427 (0.0%)
1	M	0.30	0/2514	0.42	0/3427
1	O	0.31	0/2514	0.42	1/3427 (0.0%)
1	Q	0.32	0/2515	0.47	3/3427 (0.1%)
2	B	0.21	0/1389	0.35	0/1867
2	D	0.33	0/1401	0.41	1/1883 (0.1%)
2	F	0.38	0/1394	0.45	1/1874 (0.1%)
2	N	0.33	0/1391	0.40	1/1870 (0.1%)
2	P	0.24	0/1363	0.36	0/1832
2	R	0.24	0/1385	0.38	0/1862
3	G	0.27	0/1771	0.43	1/2411 (0.0%)
3	H	0.25	0/1749	0.43	1/2381 (0.0%)
3	J	0.21	0/1771	0.37	0/2411
3	S	0.24	0/1771	0.42	0/2411
3	U	0.26	0/1771	0.42	0/2411
3	X	0.32	0/1771	0.60	4/2411 (0.2%)
4	I	0.30	0/1693	0.42	0/2294
4	K	0.39	2/1693 (0.1%)	0.56	3/2294 (0.1%)
4	L	0.33	1/1693 (0.1%)	0.51	3/2294 (0.1%)
4	T	0.55	4/1693 (0.2%)	0.66	5/2294 (0.2%)
4	V	0.53	3/1693 (0.2%)	0.61	4/2294 (0.2%)
4	Y	0.57	3/1693 (0.2%)	0.63	5/2294 (0.2%)
All	All	0.34	13/44189 (0.0%)	0.46	36/59975 (0.1%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	39	LYS	C-N	5.93	1.40	1.33
4	Y	95	PRO	N-CD	5.64	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	T	95	PRO	N-CD	5.57	1.55	1.47
4	K	8	PRO	N-CD	5.55	1.55	1.47
4	V	39	LYS	C-N	5.55	1.40	1.33
4	Y	8	PRO	N-CD	5.45	1.55	1.47
4	L	58	GLY	C-N	5.40	1.40	1.33
4	T	39	LYS	C-N	5.32	1.40	1.33
4	V	8	PRO	N-CD	5.31	1.55	1.47
4	T	8	PRO	N-CD	5.24	1.55	1.47
4	V	40	PRO	N-CD	5.13	1.54	1.47
4	T	40	PRO	N-CD	5.09	1.54	1.47
4	Y	40	PRO	N-CD	5.01	1.54	1.47

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	V	7	SER	C-N-CD	8.21	138.66	120.60
4	T	94	VAL	C-N-CD	8.15	138.53	120.60
4	K	7	SER	C-N-CD	8.11	138.43	120.60
4	T	7	SER	C-N-CD	8.06	138.33	120.60
4	Y	94	VAL	C-N-CD	7.98	138.16	120.60
4	Y	7	SER	C-N-CD	7.98	138.16	120.60
3	X	76	THR	CA-C-N	-7.87	111.18	122.36
3	X	76	THR	C-N-CA	-7.87	111.18	122.36
2	F	57	GLU	N-CA-C	7.21	119.14	111.28
4	V	39	LYS	CA-C-N	-6.77	113.01	119.85
4	V	39	LYS	C-N-CA	-6.77	113.01	119.85
2	D	57	GLU	N-CA-C	6.76	118.65	111.28
4	T	39	LYS	CA-C-N	-6.70	112.86	119.76
4	T	39	LYS	C-N-CA	-6.70	112.86	119.76
4	K	39	LYS	CA-C-N	-6.69	112.61	119.83
4	K	39	LYS	C-N-CA	-6.69	112.61	119.83
4	Y	42	ARG	N-CA-C	6.66	120.24	110.59
2	N	171	PHE	N-CA-C	6.47	118.41	111.36
1	A	325	GLU	N-CA-C	6.46	119.27	110.55
4	L	58	GLY	CA-C-N	-6.01	113.75	119.76
4	L	58	GLY	C-N-CA	-6.01	113.75	119.76
3	G	67	ARG	N-CA-C	5.95	117.85	111.36
1	Q	247	SER	CA-C-N	5.82	132.89	122.06
1	Q	247	SER	C-N-CA	5.82	132.89	122.06
3	X	142	SER	N-CA-C	5.62	118.76	109.94
4	Y	39	LYS	CA-C-N	-5.59	112.85	119.05
4	Y	39	LYS	C-N-CA	-5.59	112.85	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	T	94	VAL	N-CA-C	-5.56	103.85	109.02
1	E	33	GLN	N-CA-C	5.54	117.45	108.26
3	X	143	SER	CB-CA-C	-5.50	110.24	116.63
4	L	58	GLY	N-CA-C	5.48	123.52	112.34
1	A	194	LEU	N-CA-C	5.41	117.25	111.36
4	V	69	THR	N-CA-C	5.35	119.96	113.38
3	H	148	GLY	N-CA-C	5.34	122.46	115.36
1	Q	247	SER	O-C-N	5.05	129.17	123.42
1	O	194	LEU	N-CA-C	5.00	116.55	111.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2468	0	2406	21	0
1	C	2467	0	2412	20	0
1	E	2458	0	2399	27	0
1	M	2458	0	2399	20	0
1	O	2458	0	2399	30	0
1	Q	2459	0	2406	36	0
2	B	1366	0	1282	17	0
2	D	1377	0	1291	8	0
2	F	1371	0	1287	14	0
2	N	1368	0	1278	19	0
2	P	1340	0	1255	14	0
2	R	1362	0	1279	17	0
3	G	1728	0	1705	38	0
3	H	1707	0	1681	22	1
3	J	1728	0	1705	21	0
3	S	1728	0	1705	44	0
3	U	1728	0	1705	27	0
3	X	1728	0	1705	32	2
4	I	1658	0	1609	14	0
4	K	1658	0	1609	13	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	1658	0	1609	27	0
4	T	1658	0	1611	28	0
4	V	1658	0	1609	21	0
4	Y	1658	0	1609	11	0
5	A	70	0	65	0	0
5	B	14	0	13	0	0
5	C	70	0	65	2	0
5	D	14	0	13	0	0
5	E	70	0	65	0	0
5	F	14	0	13	0	0
5	M	70	0	65	1	0
5	N	14	0	13	0	0
5	O	70	0	65	0	0
5	P	14	0	13	0	0
5	Q	70	0	65	0	0
5	R	14	0	13	0	0
6	A	173	0	0	2	0
6	B	81	0	0	1	0
6	C	156	0	0	2	0
6	D	74	0	0	0	0
6	E	110	0	0	3	0
6	F	75	0	0	1	0
6	G	29	0	0	1	0
6	H	62	0	0	2	0
6	I	34	0	0	0	0
6	J	29	0	0	0	0
6	K	30	0	0	1	0
6	L	75	0	0	3	0
6	M	126	0	0	2	0
6	N	50	0	0	1	0
6	O	96	0	0	2	0
6	P	40	0	0	0	0
6	Q	128	0	0	3	0
6	R	51	0	0	2	0
6	S	9	0	0	0	0
6	T	19	0	0	0	0
6	U	61	0	0	2	0
6	V	55	0	0	1	0
6	X	55	0	0	1	0
6	Y	51	0	0	1	0
All	All	45420	0	42423	459	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 5.

All (459) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:146:THR:HG21	3:S:151:ALA:CA	1.48	1.43
3:S:146:THR:CG2	3:S:151:ALA:HA	1.52	1.38
3:S:146:THR:HG21	3:S:151:ALA:CB	1.54	1.36
3:J:147:SER:CB	3:J:150:THR:O	1.77	1.32
3:J:147:SER:HB2	3:J:150:THR:O	1.27	1.28
1:E:219:SER:OG	6:E:501:HOH:O	1.63	1.15
3:S:147:SER:HB2	3:S:150:THR:O	1.46	1.14
1:Q:15:LEU:HD12	2:R:119:PHE:CD1	1.83	1.11
1:O:325:GLU:HA	2:P:12:ASN:HD21	1.08	1.10
2:F:120:GLU:OE2	2:F:123:ARG:NH2	1.86	1.09
1:Q:15:LEU:HD12	2:R:119:PHE:HD1	1.07	1.08
3:J:147:SER:HB3	3:J:150:THR:O	1.59	1.03
1:M:218:GLU:OE1	1:Q:201:ARG:NH1	1.91	1.02
1:E:32:ASP:OD2	6:E:502:HOH:O	1.76	1.01
2:D:62:LYS:NZ	2:F:86:ASP:OD2	1.94	0.99
1:A:216:ASN:OD1	1:A:218:GLU:HG3	1.64	0.97
1:O:210:GLN:HE22	1:Q:220:ARG:HE	1.09	0.97
3:S:142:SER:O	3:S:146:THR:HA	1.63	0.97
3:S:146:THR:HG23	3:S:151:ALA:HA	1.44	0.97
3:X:146:THR:HG22	3:X:147:SER:H	1.27	0.97
1:O:210:GLN:NE2	1:Q:220:ARG:HE	1.60	0.96
3:X:142:SER:O	3:X:146:THR:HA	1.66	0.96
1:O:325:GLU:HA	2:P:12:ASN:ND2	1.81	0.95
3:H:147:SER:C	3:H:149:GLY:HA2	1.91	0.95
3:G:31:ARG:HG3	3:G:31:ARG:HH11	1.28	0.94
3:S:146:THR:CG2	3:S:151:ALA:CB	2.43	0.94
3:X:142:SER:O	3:X:146:THR:CA	2.16	0.93
3:S:146:THR:CG2	3:S:151:ALA:CA	2.25	0.93
1:C:201:ARG:NH1	1:E:218:GLU:OE2	2.03	0.91
2:N:51:LYS:HD3	2:N:103:GLU:OE1	1.71	0.91
3:S:146:THR:HG21	3:S:151:ALA:HA	1.08	0.89
3:U:147:SER:HB3	3:U:150:THR:O	1.75	0.86
1:Q:15:LEU:CD1	2:R:119:PHE:HA	2.07	0.85
3:G:146:THR:HG22	3:G:147:SER:OG	1.75	0.85
1:O:18:HIS:HD2	2:P:21:TRP:HA	1.41	0.85
3:U:146:THR:HG21	3:U:152:ALA:H	1.42	0.85
1:O:185:PRO:HG2	1:O:191:GLN:HG2	1.59	0.85
4:T:79:GLN:HB3	4:T:81:GLU:OE1	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:142:SER:O	3:X:146:THR:N	2.10	0.85
1:Q:18:HIS:HD2	2:R:21:TRP:HA	1.42	0.84
3:X:148:GLY:O	3:X:201:SER:HB3	1.79	0.83
1:M:18:HIS:HD2	2:N:21:TRP:HA	1.42	0.83
2:D:127:ARG:NH2	2:F:131:GLU:OE2	2.11	0.83
4:T:21:ILE:HD12	4:T:102:THR:HG21	1.60	0.82
1:A:18:HIS:HD2	2:B:21:TRP:HA	1.46	0.81
3:G:31:ARG:HG3	3:G:31:ARG:NH1	1.95	0.80
3:H:148:GLY:N	3:H:149:GLY:HA2	1.94	0.80
1:A:325:GLU:HB3	2:B:13:GLY:O	1.82	0.80
2:N:128:GLU:O	2:N:170:ARG:NH1	2.15	0.79
4:T:4:MET:HE3	4:T:90:GLN:HG2	1.63	0.79
1:A:326:LYS:H	2:B:12:ASN:HD22	1.29	0.79
1:O:210:GLN:NE2	1:Q:220:ARG:NE	2.31	0.78
3:S:141:PRO:HD2	3:S:228:PRO:HA	1.64	0.78
3:X:148:GLY:O	3:X:201:SER:CB	2.32	0.78
3:U:146:THR:HB	3:U:151:ALA:HA	1.65	0.78
4:L:197:THR:HG22	4:L:204:PRO:HB3	1.67	0.77
3:U:148:GLY:O	6:U:301:HOH:O	2.02	0.77
3:H:141:PRO:HB3	3:H:153:LEU:HB3	1.67	0.77
3:S:141:PRO:HG2	3:S:228:PRO:HB3	1.64	0.77
3:S:140:ALA:HB1	3:S:141:PRO:HD2	1.67	0.76
2:B:124:ARG:HD2	2:D:134:GLY:HA2	1.67	0.76
3:S:6:GLN:NE2	3:S:94:TYR:O	2.18	0.76
1:O:16:GLY:HA2	2:P:9:PHE:HB3	1.65	0.76
1:M:301:THR:OG1	1:M:305:CYS:SG	2.44	0.75
3:X:146:THR:HG22	3:X:147:SER:N	2.00	0.75
3:S:146:THR:HG21	3:S:151:ALA:HB1	1.64	0.75
3:S:147:SER:CB	3:S:150:THR:O	2.33	0.75
1:M:16:GLY:HA2	2:N:9:PHE:HB3	1.69	0.75
3:G:146:THR:HG21	4:I:116:PHE:HE2	1.50	0.74
1:O:325:GLU:OE2	2:P:13:GLY:O	2.05	0.74
3:S:146:THR:HG21	3:S:151:ALA:HB2	1.63	0.73
3:S:174:LEU:HD11	3:S:197:VAL:HG21	1.71	0.72
1:E:18:HIS:HD2	2:F:21:TRP:HA	1.55	0.72
3:S:145:SER:HB3	3:S:147:SER:O	1.92	0.70
4:T:185:ASP:HA	4:T:188:LYS:HE2	1.74	0.70
2:D:54:ARG:HA	2:D:57:GLU:HG2	1.72	0.69
3:S:141:PRO:CG	3:S:228:PRO:HB3	2.22	0.69
1:M:99:PRO:HB2	1:M:229:ARG:HD3	1.72	0.69
2:B:134:GLY:HA2	2:F:124:ARG:HD2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:4:MET:HE3	4:T:90:GLN:CG	2.23	0.69
3:S:145:SER:O	3:S:146:THR:HG22	1.92	0.68
1:C:8:ASN:N	6:C:505:HOH:O	2.27	0.67
3:S:144:LYS:O	3:S:145:SER:HB2	1.93	0.67
3:H:69:THR:OG1	3:H:84:ARG:NH2	2.28	0.67
3:X:1:GLN:N	6:X:302:HOH:O	2.27	0.67
3:H:65:GLN:OE1	6:H:301:HOH:O	2.14	0.66
4:T:4:MET:CE	4:T:90:GLN:HG2	2.26	0.66
4:L:187:GLU:O	4:L:211:ARG:NH2	2.26	0.66
4:Y:29:ILE:HG21	4:Y:90:GLN:HG3	1.76	0.66
4:Y:189:HIS:O	4:Y:211:ARG:NH1	2.29	0.66
1:E:157:SER:O	6:E:503:HOH:O	2.14	0.66
1:C:150:ARG:HH12	5:C:403:NAG:H81	1.61	0.65
1:Q:15:LEU:HD13	2:R:119:PHE:HA	1.77	0.65
1:A:133:ASN:OD1	1:A:255:ARG:NH2	2.24	0.65
1:O:33:GLN:OE1	4:T:93:ASN:HB3	1.96	0.65
1:Q:102:VAL:HG22	1:Q:232:ILE:HB	1.79	0.65
2:D:124:ARG:HD2	2:F:134:GLY:HA2	1.79	0.65
1:Q:133:ASN:OD1	1:Q:255:ARG:NH2	2.27	0.64
1:Q:83:THR:HG22	1:Q:117:THR:HG22	1.77	0.64
3:S:146:THR:CG2	3:S:151:ALA:HB2	2.21	0.64
1:E:195:TYR:O	1:E:196:VAL:HG13	1.98	0.64
4:L:56:THR:O	6:L:301:HOH:O	2.15	0.64
3:G:144:LYS:NZ	6:G:302:HOH:O	2.29	0.63
4:I:185:ASP:HA	4:I:188:LYS:HE2	1.79	0.63
1:M:8:ASN:N	6:M:503:HOH:O	2.31	0.63
1:O:325:GLU:HA	1:O:325:GLU:OE2	1.99	0.63
4:V:147:GLN:OE1	4:V:154:LEU:HD11	1.98	0.63
4:V:108:ARG:HD2	4:V:170:ASP:O	1.99	0.63
1:E:32:ASP:HB3	4:I:93:ASN:HD21	1.64	0.63
4:L:183:LYS:O	4:L:187:GLU:HG2	1.98	0.63
3:S:134:PRO:HB3	3:S:160:TYR:HB3	1.80	0.63
3:J:146:THR:HG21	3:J:152:ALA:H	1.64	0.62
3:X:148:GLY:O	3:X:201:SER:OG	2.17	0.61
1:E:16:GLY:HA2	2:F:9:PHE:HB3	1.82	0.61
4:I:120:PRO:HD3	4:I:132:VAL:HG22	1.81	0.61
4:K:8:PRO:O	4:K:102:THR:HG23	2.00	0.61
4:L:34:ASN:HD22	4:L:89:GLN:HE22	1.48	0.61
2:N:171:PHE:O	2:N:172:GLN:HB2	1.99	0.61
3:X:147:SER:HB3	4:Y:116:PHE:HE1	1.66	0.60
4:K:186:TYR:O	4:K:192:TYR:OH	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:192:TYR:HB2	4:L:209:PHE:CE1	2.36	0.60
4:L:100:GLN:NE2	6:L:303:HOH:O	2.31	0.60
3:J:82:GLU:OE1	3:J:84:ARG:NH1	2.33	0.59
4:L:36:TYR:HE2	4:L:89:GLN:HE21	1.49	0.59
3:X:142:SER:N	3:X:146:THR:OG1	2.36	0.59
3:G:91:THR:HG23	3:G:125:THR:HA	1.85	0.59
3:U:99:ASP:O	3:U:100:LYS:HB2	2.03	0.59
1:A:216:ASN:OD1	1:A:218:GLU:CG	2.46	0.59
3:H:146:THR:N	3:H:201:SER:HG	2.00	0.59
4:T:4:MET:HE1	4:T:29:ILE:HD13	1.85	0.59
3:X:76:THR:O	3:X:76:THR:HG22	2.02	0.59
3:G:215:HIS:CD2	3:G:218:SER:H	2.20	0.58
3:J:6:GLN:HG2	3:J:22:CYS:SG	2.43	0.58
3:J:134:PRO:HB3	3:J:157:VAL:HG23	1.85	0.58
2:N:134:GLY:HA2	2:R:124:ARG:HD3	1.84	0.58
2:P:124:ARG:HD2	2:R:134:GLY:HA2	1.85	0.58
1:Q:97:CYS:O	1:Q:224:ARG:NH1	2.37	0.58
1:C:210:GLN:HE22	1:E:220:ARG:HE	1.52	0.58
1:Q:224:ARG:NH2	6:Q:504:HOH:O	2.35	0.58
3:S:196:VAL:HG21	4:T:135:LEU:HD22	1.85	0.58
3:U:144:LYS:HD2	3:U:144:LYS:O	2.04	0.58
3:G:146:THR:HG22	3:G:147:SER:HG	1.69	0.58
4:V:164:THR:HG22	4:V:174:SER:H	1.69	0.58
4:L:39:LYS:NZ	6:L:305:HOH:O	2.35	0.57
1:A:325:GLU:HA	2:B:12:ASN:HB2	1.86	0.57
1:Q:62:ILE:HG22	1:Q:63:ASP:N	2.19	0.57
4:T:8:PRO:O	4:T:9:VAL:HG23	2.05	0.57
3:G:154:GLY:HA3	3:G:196:VAL:HG12	1.85	0.57
4:L:69:THR:HG22	4:L:70:GLU:OE1	2.04	0.57
3:J:71:THR:HG23	3:J:80:SER:HB2	1.85	0.57
3:H:6:GLN:HG2	3:H:22:CYS:SG	2.45	0.57
3:H:40:ALA:HB3	3:H:43:GLN:HG3	1.86	0.57
1:C:325:GLU:HB3	2:D:13:GLY:O	2.05	0.56
1:Q:15:LEU:HD11	2:R:119:PHE:HA	1.87	0.56
3:G:143:SER:HB2	3:G:146:THR:HA	1.86	0.56
1:O:325:GLU:OE2	2:P:12:ASN:ND2	2.37	0.56
1:E:102:VAL:HG22	1:E:232:ILE:HB	1.88	0.56
1:A:307:LYS:NZ	6:A:508:HOH:O	2.35	0.56
1:Q:210:GLN:HG3	6:Q:523:HOH:O	2.05	0.56
3:G:199:VAL:HG22	3:G:200:PRO:HD2	1.87	0.56
3:J:89:ASP:OD1	3:J:89:ASP:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:VAL:HB	1:C:232:ILE:HB	1.88	0.55
2:F:120:GLU:CD	2:F:123:ARG:HH21	2.14	0.55
2:N:150:GLU:OE1	2:N:153:ARG:NH1	2.40	0.55
4:T:7:SER:HA	4:T:8:PRO:C	2.32	0.54
1:A:217:ILE:C	1:A:218:GLU:HG2	2.32	0.54
3:J:145:SER:HB3	3:J:201:SER:OG	2.08	0.54
2:P:9:PHE:C	2:P:9:PHE:CD2	2.85	0.54
1:E:186:SER:HA	1:E:218:GLU:O	2.08	0.54
3:H:134:PRO:HB3	3:H:160:TYR:HB3	1.89	0.54
1:Q:16:GLY:HA2	2:R:9:PHE:HB3	1.88	0.54
4:V:108:ARG:HG3	4:V:171:SER:HB2	1.88	0.54
1:A:238:LYS:NZ	6:A:511:HOH:O	2.41	0.53
4:T:189:HIS:O	4:T:211:ARG:NH1	2.41	0.53
1:Q:168:MET:HE2	1:Q:168:MET:HA	1.90	0.53
3:S:12:LYS:HG3	3:S:18:VAL:HG13	1.90	0.53
3:U:6:GLN:NE2	3:U:122:THR:HG23	2.24	0.53
4:L:4:MET:CE	4:L:23:CYS:SG	2.97	0.53
4:L:21:ILE:HD12	4:L:102:THR:HG21	1.91	0.53
3:S:141:PRO:CD	3:S:228:PRO:HA	2.36	0.53
1:C:283:THR:HG22	1:C:301:THR:HG22	1.91	0.53
1:Q:9:SER:N	6:Q:505:HOH:O	2.42	0.53
1:A:326:LYS:H	2:B:12:ASN:ND2	2.01	0.52
1:C:169:PRO:HB3	1:C:242:VAL:HG22	1.91	0.52
1:E:18:HIS:CD2	2:F:21:TRP:HA	2.39	0.52
2:F:15:GLU:OE2	6:F:301:HOH:O	2.19	0.52
3:J:67:ARG:NH1	3:J:90:ASP:OD2	2.42	0.52
1:M:12:THR:HG23	2:N:133:MET:HE1	1.90	0.52
3:U:36:TRP:CD1	3:U:70:MET:HE3	2.43	0.52
4:V:90:GLN:NE2	4:V:97:THR:OG1	2.43	0.52
1:E:15:LEU:HD22	2:F:119:PHE:HA	1.92	0.52
1:O:210:GLN:HE21	1:Q:220:ARG:HD3	1.73	0.52
4:K:163:VAL:HG23	4:K:175:LEU:HD12	1.91	0.52
3:J:143:SER:HB2	3:J:146:THR:HA	1.91	0.52
1:M:195:TYR:O	1:M:197:GLN:N	2.39	0.52
2:N:51:LYS:CD	2:N:103:GLU:OE1	2.51	0.52
4:V:29:ILE:HG21	4:V:90:GLN:HG3	1.92	0.52
1:C:127:TRP:O	6:C:501:HOH:O	2.19	0.52
1:Q:15:LEU:CD1	2:R:119:PHE:CD1	2.75	0.52
4:K:188:LYS:HB2	4:K:189:HIS:CE1	2.45	0.51
1:O:210:GLN:HE22	1:Q:220:ARG:NE	1.90	0.51
3:G:2:VAL:HG13	3:G:27:TYR:HD1	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:141:PRO:HG2	3:G:228:PRO:HB3	1.92	0.51
1:O:132:GLN:NE2	6:O:504:HOH:O	2.40	0.51
4:T:197:THR:HG22	4:T:204:PRO:HG3	1.93	0.51
3:U:87:ARG:HD2	3:U:89:ASP:OD1	2.10	0.51
4:T:94:VAL:HG23	4:T:95:PRO:HA	1.93	0.51
3:X:76:THR:O	3:X:77:SER:C	2.48	0.51
1:E:196:VAL:HG22	1:E:197:GLN:OE1	2.11	0.51
3:G:145:SER:O	3:G:146:THR:HB	2.10	0.51
3:U:146:THR:CB	3:U:151:ALA:HA	2.36	0.51
3:G:138:PRO:HD3	3:G:224:LYS:NZ	2.25	0.51
3:U:146:THR:HG22	4:V:116:PHE:CD1	2.45	0.51
3:U:134:PRO:HB3	3:U:160:TYR:HB3	1.93	0.51
1:E:90:ARG:NH1	1:E:272:ALA:O	2.42	0.51
1:O:210:GLN:HE21	1:Q:220:ARG:CD	2.23	0.50
4:K:24:ARG:HG3	4:K:70:GLU:OE2	2.10	0.50
4:T:4:MET:HE3	4:T:90:GLN:HB3	1.93	0.50
3:X:148:GLY:C	3:X:201:SER:HG	2.19	0.50
4:L:34:ASN:HD22	4:L:89:GLN:NE2	2.09	0.50
3:X:2:VAL:HG12	3:X:117:PRO:HG3	1.93	0.50
3:X:230:SER:O	3:X:231:CYS:SG	2.69	0.50
3:J:141:PRO:HG2	3:J:228:PRO:HB3	1.94	0.50
4:K:183:LYS:NZ	4:K:187:GLU:OE2	2.28	0.50
3:S:146:THR:CG2	3:S:147:SER:N	2.74	0.50
3:J:91:THR:HG23	3:J:125:THR:HA	1.92	0.50
1:A:102:VAL:HG22	1:A:232:ILE:HB	1.93	0.50
2:B:22:TYR:HD1	2:B:115:MET:HE2	1.76	0.50
3:U:148:GLY:HA2	6:U:317:HOH:O	2.12	0.50
3:J:138:PRO:HD3	3:J:224:LYS:NZ	2.27	0.49
4:T:125:LEU:O	4:T:183:LYS:HD2	2.12	0.49
4:Y:50:TYR:O	4:Y:51:ALA:HB3	2.12	0.49
3:G:67:ARG:NH1	3:G:90:ASP:OD2	2.45	0.49
1:O:238:LYS:NZ	6:O:506:HOH:O	2.44	0.49
1:C:297:VAL:HB	5:C:405:NAG:H82	1.94	0.49
4:V:166:GLN:HG3	4:V:173:TYR:CZ	2.47	0.49
3:J:145:SER:O	3:J:147:SER:N	2.41	0.49
1:Q:29:ILE:HD11	2:R:102:LEU:HD23	1.93	0.49
3:G:2:VAL:HG13	3:G:27:TYR:CD1	2.48	0.49
1:E:195:TYR:C	1:E:196:VAL:CG1	2.85	0.49
3:S:140:ALA:HB1	3:S:141:PRO:CD	2.42	0.49
3:G:146:THR:CG2	4:I:116:PHE:HE2	2.22	0.49
4:I:197:THR:HG22	4:I:204:PRO:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:60:ASN:ND2	6:N:302:HOH:O	2.44	0.49
4:T:21:ILE:CD1	4:T:102:THR:HG21	2.37	0.49
4:T:146:VAL:HG22	4:T:196:VAL:HG12	1.93	0.49
1:A:16:GLY:C	2:B:115:MET:HE1	2.38	0.48
1:C:99:PRO:HB2	1:C:229:ARG:HD3	1.95	0.48
3:U:6:GLN:HE21	3:U:122:THR:HG23	1.78	0.48
3:G:146:THR:HG21	4:I:116:PHE:CE2	2.40	0.48
3:S:157:VAL:HG13	3:S:193:LEU:HB3	1.95	0.48
4:T:50:TYR:O	4:T:51:ALA:HB3	2.13	0.48
3:S:142:SER:O	3:S:143:SER:HB2	2.12	0.48
4:V:33:LEU:HD22	4:V:71:PHE:CG	2.49	0.48
3:X:91:THR:HG23	3:X:125:THR:HA	1.94	0.48
3:J:81:MET:HE3	3:J:81:MET:HB3	1.82	0.48
3:S:138:PRO:HD3	3:S:224:LYS:NZ	2.28	0.48
3:S:6:GLN:HE22	3:S:95:TYR:HA	1.79	0.48
4:V:105:GLU:OE1	4:V:173:TYR:OH	2.28	0.48
4:T:115:VAL:HG21	4:T:196:VAL:HG21	1.95	0.48
4:L:108:ARG:NH2	4:L:109:THR:O	2.46	0.47
1:M:244:VAL:HG21	1:O:221:PRO:HD3	1.96	0.47
1:O:210:GLN:NE2	1:Q:220:ARG:CD	2.77	0.47
1:E:97:CYS:O	1:E:224:ARG:NH1	2.48	0.47
1:C:210:GLN:HE22	1:E:220:ARG:NE	2.10	0.47
1:Q:28:THR:HG22	1:Q:31:ASP:H	1.79	0.47
3:S:145:SER:C	3:S:147:SER:N	2.73	0.47
3:G:50:TRP:CH2	3:G:52:SER:HB2	2.50	0.47
3:J:112:PHE:HA	3:J:114:TRP:CE2	2.49	0.47
3:X:166:THR:OG1	3:X:214:ASN:HB2	2.15	0.47
4:K:77:SER:OG	6:K:301:HOH:O	2.21	0.47
4:K:193:ALA:HB2	4:K:208:SER:HB3	1.96	0.47
1:O:183:HIS:ND1	1:O:195:TYR:OH	2.43	0.47
4:Y:166:GLN:HG3	4:Y:173:TYR:CZ	2.50	0.47
4:L:133:VAL:HG22	4:L:178:THR:HG22	1.97	0.46
4:V:113:PRO:HB3	4:V:139:PHE:HB3	1.97	0.46
3:X:134:PRO:HB3	3:X:160:TYR:HB3	1.96	0.46
4:Y:145:LYS:HB3	4:Y:197:THR:OG1	2.15	0.46
4:L:190:LYS:HA	4:L:211:ARG:HG2	1.98	0.46
4:L:4:MET:HE3	4:L:23:CYS:SG	2.55	0.46
3:X:146:THR:CG2	3:X:147:SER:N	2.73	0.46
1:C:183:HIS:HB2	1:C:252:ILE:HD11	1.98	0.46
4:Y:1:ASP:OD2	6:Y:301:HOH:O	2.21	0.46
3:G:73:ASP:OD1	3:G:75:SER:OG	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:97:CYS:O	1:O:224:ARG:NH1	2.48	0.46
1:Q:15:LEU:HD13	2:R:119:PHE:CA	2.46	0.46
3:U:51:ILE:HB	3:U:70:MET:HE2	1.97	0.46
4:K:11:LEU:HB3	4:K:104:LEU:HD12	1.98	0.46
4:K:113:PRO:HB3	4:K:139:PHE:HB3	1.97	0.46
3:G:178:VAL:O	3:G:179:HIS:ND1	2.49	0.45
3:G:193:LEU:HD23	3:G:194:SER:N	2.32	0.45
4:L:29:ILE:HG21	4:L:90:GLN:HG3	1.98	0.45
1:M:325:GLU:O	6:M:501:HOH:O	2.21	0.45
3:U:74:THR:O	3:U:76:THR:HA	2.17	0.45
4:Y:193:ALA:HB2	4:Y:208:SER:HB3	1.97	0.45
1:A:50:LYS:HG2	1:A:273:PRO:HG2	1.98	0.45
3:G:36:TRP:CE2	3:G:81:MET:HB2	2.51	0.45
3:H:224:LYS:HD2	3:H:224:LYS:HA	1.70	0.45
4:T:146:VAL:HG13	4:T:194:CYS:SG	2.57	0.45
1:A:16:GLY:HA2	2:B:9:PHE:HB3	1.99	0.45
4:V:193:ALA:HB2	4:V:208:SER:HB3	1.97	0.45
1:C:156:LYS:HE3	1:C:193:SER:O	2.17	0.45
1:M:15:LEU:HD22	2:N:119:PHE:HA	1.99	0.45
4:V:12:SER:HA	4:V:105:GLU:O	2.17	0.45
1:A:15:LEU:HD22	2:B:119:PHE:HA	1.98	0.45
3:G:212:ASN:OD1	3:G:212:ASN:N	2.49	0.45
4:L:158:ASN:OD1	4:L:158:ASN:N	2.46	0.45
1:O:97:CYS:SG	1:O:98:TYR:N	2.87	0.45
1:O:102:VAL:HG22	1:O:232:ILE:HB	1.99	0.45
1:Q:62:ILE:HG22	1:Q:63:ASP:H	1.81	0.45
3:U:161:PHE:HB2	3:U:190:LEU:HD23	1.98	0.45
3:X:112:PHE:HA	3:X:114:TRP:CE2	2.51	0.45
3:G:208:THR:HG23	3:G:225:LYS:HE3	1.98	0.45
1:M:218:GLU:OE1	1:Q:201:ARG:CZ	2.61	0.45
3:S:145:SER:C	3:S:147:SER:H	2.24	0.45
4:T:33:LEU:HD22	4:T:71:PHE:CG	2.52	0.45
2:P:17:MET:HE1	2:P:23:GLY:HA3	1.99	0.45
3:H:98:ARG:HD2	3:H:116:ALA:O	2.17	0.45
3:J:158:LYS:HE2	3:J:158:LYS:HB2	1.78	0.45
3:H:112:PHE:HA	3:H:114:TRP:CE2	2.52	0.44
4:V:36:TYR:HE2	4:V:89:GLN:HB3	1.83	0.44
3:H:148:GLY:N	3:H:149:GLY:CA	2.72	0.44
4:Y:47:LEU:HD21	4:Y:62:PHE:CD2	2.52	0.44
1:A:17:HIS:HD2	2:B:115:MET:HE3	1.83	0.44
1:C:175:ASP:OD1	1:C:239:PRO:HD3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:50:TYR:O	4:I:51:ALA:HB3	2.16	0.44
1:O:195:TYR:C	1:O:196:VAL:HG13	2.42	0.44
2:B:56:ILE:HD11	3:H:108:PRO:HG2	1.99	0.44
1:E:33:GLN:HG2	4:I:93:ASN:ND2	2.33	0.44
2:R:133:MET:HE3	2:R:137:CYS:HB2	1.98	0.44
3:U:112:PHE:HA	3:U:114:TRP:CE2	2.53	0.44
2:D:3:PHE:CD2	2:D:3:PHE:O	2.70	0.44
1:E:97:CYS:SG	1:E:98:TYR:N	2.88	0.44
1:O:32:ASP:HB3	4:T:93:ASN:HD21	1.83	0.44
4:V:4:MET:HE1	4:V:25:ALA:HB2	1.99	0.44
1:A:18:HIS:CD2	2:B:21:TRP:HA	2.38	0.44
3:G:215:HIS:HD2	3:G:218:SER:H	1.66	0.44
4:L:78:LEU:HD12	4:L:78:LEU:HA	1.87	0.44
2:N:124:ARG:HD2	2:P:134:GLY:HA2	2.00	0.44
2:B:51:LYS:HG3	1:C:30:THR:HG22	1.99	0.44
4:T:4:MET:HE3	4:T:90:GLN:CB	2.48	0.44
1:C:210:GLN:NE2	1:E:220:ARG:HE	2.16	0.44
4:I:33:LEU:HD22	4:I:71:PHE:CG	2.53	0.44
1:M:18:HIS:CD2	2:N:21:TRP:HA	2.34	0.44
3:S:75:SER:HA	3:S:76:THR:HA	1.68	0.44
2:D:58:LYS:HD2	2:D:58:LYS:HA	1.66	0.43
4:Y:183:LYS:HE2	4:Y:187:GLU:OE2	2.18	0.43
4:K:4:MET:HE1	4:K:25:ALA:HB2	2.00	0.43
1:M:220:ARG:HD2	1:Q:210:GLN:OE1	2.18	0.43
1:O:15:LEU:HD22	2:P:119:PHE:HA	1.98	0.43
1:O:18:HIS:CD2	2:P:21:TRP:HA	2.34	0.43
1:A:288:ILE:CD1	1:A:295:GLN:HG3	2.48	0.43
2:B:17:MET:HE1	2:B:23:GLY:HA3	1.99	0.43
3:G:2:VAL:HG12	3:G:117:PRO:HG3	2.01	0.43
3:G:81:MET:HE3	3:G:81:MET:HB3	1.93	0.43
3:H:50:TRP:CH2	3:H:52:SER:HB2	2.53	0.43
3:S:12:LYS:O	3:S:126:VAL:HA	2.18	0.43
3:S:112:PHE:HA	3:S:114:TRP:CE2	2.53	0.43
4:T:125:LEU:HD22	4:T:183:LYS:HG3	2.00	0.43
4:K:151:ASP:OD1	4:K:191:VAL:HG13	2.19	0.43
1:M:260:MET:HE2	1:M:260:MET:HB3	1.93	0.43
1:O:29:ILE:HD11	2:P:102:LEU:HD23	2.01	0.43
3:S:50:TRP:CH2	3:S:52:SER:HB2	2.54	0.43
3:S:146:THR:HG22	3:S:147:SER:H	1.83	0.43
4:V:147:GLN:OE1	4:V:154:LEU:CD1	2.65	0.43
3:X:87:ARG:HE	3:X:87:ARG:HB2	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:138:PRO:HD3	3:J:224:LYS:HZ1	1.84	0.43
4:V:50:TYR:O	4:V:51:ALA:HB3	2.19	0.43
4:V:124:GLN:O	4:V:127:SER:OG	2.32	0.43
1:E:175:ASP:OD1	1:E:239:PRO:HD3	2.19	0.43
1:Q:27:LYS:HG3	1:Q:32:ASP:O	2.18	0.43
3:U:146:THR:HG22	4:V:116:PHE:HD1	1.84	0.43
3:U:224:LYS:HD2	3:U:224:LYS:HA	1.83	0.43
2:N:8:GLY:N	2:N:137:CYS:SG	2.92	0.43
1:C:244:VAL:HG21	1:E:221:PRO:HD3	2.01	0.42
4:I:21:ILE:HD11	4:I:73:LEU:HD23	2.00	0.42
1:Q:175:ASP:OD1	1:Q:239:PRO:HD3	2.19	0.42
3:U:36:TRP:HD1	3:U:70:MET:HE3	1.83	0.42
4:L:36:TYR:OH	4:L:89:GLN:NE2	2.52	0.42
1:A:18:HIS:CE1	1:A:37:THR:HG21	2.55	0.42
1:A:295:GLN:HB2	1:A:306:PRO:HB2	2.01	0.42
3:U:64:PHE:HB3	3:U:68:VAL:HG23	2.02	0.42
3:X:230:SER:O	3:X:231:CYS:CB	2.67	0.42
3:G:145:SER:C	3:G:147:SER:H	2.26	0.42
4:L:150:VAL:HG12	4:L:192:TYR:CD2	2.54	0.42
3:H:67:ARG:HD2	3:H:84:ARG:O	2.19	0.42
3:U:146:THR:HG21	3:U:152:ALA:N	2.22	0.42
1:C:195:TYR:O	1:C:197:GLN:N	2.47	0.42
1:E:180:TRP:HB3	1:E:254:PRO:HD3	2.01	0.42
4:L:210:ASN:HB3	4:L:213:GLU:HB3	2.01	0.42
1:O:301:THR:HB	1:O:305:CYS:SG	2.60	0.42
4:I:113:PRO:HB3	4:I:139:PHE:HB3	2.01	0.42
4:L:47:LEU:HD21	4:L:62:PHE:CD1	2.55	0.42
2:N:26:HIS:CG	2:N:149:ILE:HD13	2.55	0.42
2:N:133:MET:HE3	2:N:137:CYS:HB2	2.02	0.42
2:R:150:GLU:OE1	6:R:301:HOH:O	2.21	0.42
3:X:81:MET:HE3	3:X:81:MET:HB3	1.78	0.42
3:X:146:THR:HG21	3:X:152:ALA:H	1.84	0.42
1:E:264:LYS:HB3	2:F:63:PHE:CD1	2.55	0.42
1:M:15:LEU:HD23	2:N:118:LEU:HG	2.01	0.42
3:U:62:GLN:HA	3:U:65:GLN:HG2	2.01	0.42
3:G:112:PHE:HA	3:G:114:TRP:CE2	2.55	0.42
3:G:145:SER:O	3:G:147:SER:N	2.43	0.42
3:J:229:LYS:HA	3:J:229:LYS:HD3	1.60	0.42
2:R:38:LEU:HD22	3:X:54:TYR:CZ	2.55	0.42
3:S:91:THR:HG23	3:S:125:THR:HA	2.02	0.42
4:T:78:LEU:HD12	4:T:78:LEU:HA	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:CYS:SG	1:C:98:TYR:N	2.89	0.41
4:L:150:VAL:O	4:L:150:VAL:HG23	2.20	0.41
3:X:227:GLU:HA	3:X:228:PRO:HD3	1.90	0.41
2:F:19:ASP:OD1	2:F:19:ASP:N	2.48	0.41
3:H:36:TRP:CE2	3:H:81:MET:HB2	2.55	0.41
4:K:146:VAL:HG13	4:K:196:VAL:HG22	2.02	0.41
3:U:142:SER:OG	3:U:143:SER:O	2.36	0.41
3:G:86:LEU:HB3	3:G:126:VAL:HG11	2.01	0.41
2:N:54:ARG:O	2:N:57:GLU:HG2	2.21	0.41
3:G:138:PRO:HD3	3:G:224:LYS:HZ3	1.84	0.41
3:H:62:GLN:HA	3:H:65:GLN:HG3	2.03	0.41
4:I:145:LYS:HB3	4:I:197:THR:OG1	2.21	0.41
4:V:10:SER:O	6:V:301:HOH:O	2.22	0.41
3:X:208:THR:HG23	3:X:225:LYS:HE3	2.02	0.41
1:Q:28:THR:HG23	1:Q:29:ILE:N	2.36	0.41
1:E:324:PRO:O	2:F:12:ASN:HB2	2.21	0.41
3:H:73:ASP:OD1	6:H:302:HOH:O	2.22	0.41
4:L:90:GLN:HE21	4:L:90:GLN:HB3	1.76	0.41
1:M:97:CYS:SG	1:M:98:TYR:N	2.92	0.41
3:X:214:ASN:OD1	3:X:221:LYS:HE3	2.21	0.41
4:Y:54:LEU:HD21	4:Y:59:PRO:O	2.21	0.41
1:M:102:VAL:HG22	1:M:232:ILE:HB	2.01	0.41
4:V:90:GLN:HE21	4:V:90:GLN:HB3	1.67	0.41
3:X:138:PRO:HD3	3:X:224:LYS:HE2	2.03	0.41
3:X:141:PRO:C	3:X:146:THR:OG1	2.64	0.41
3:G:31:ARG:HA	3:G:31:ARG:HD2	1.70	0.41
3:S:161:PHE:HA	3:S:162:PRO:HA	1.80	0.41
3:U:142:SER:HB3	3:U:146:THR:HA	2.03	0.41
3:G:174:LEU:HD12	3:G:174:LEU:HA	1.86	0.41
3:H:161:PHE:HA	3:H:162:PRO:HA	1.82	0.41
4:L:187:GLU:C	4:L:211:ARG:HH21	2.25	0.41
1:M:42:LEU:HD12	2:N:100:VAL:HG12	2.03	0.41
2:P:51:LYS:HB3	2:P:51:LYS:HE2	1.87	0.41
4:T:132:VAL:HG13	4:T:179:LEU:HB3	2.02	0.41
1:E:184:HIS:HB3	1:E:220:ARG:NH1	2.35	0.41
3:G:136:VAL:HA	3:G:156:LEU:O	2.21	0.41
3:G:146:THR:CG2	4:I:116:PHE:CE2	3.00	0.41
3:H:101:LYS:HG3	3:H:102:GLN:N	2.35	0.41
3:U:81:MET:HE3	3:U:81:MET:HB3	1.89	0.41
2:B:25:ARG:NH1	6:B:306:HOH:O	2.44	0.40
1:O:196:VAL:O	1:O:196:VAL:HG23	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:221:PRO:O	1:Q:229:ARG:NH2	2.48	0.40
2:R:153:ARG:NE	6:R:301:HOH:O	2.39	0.40
3:S:138:PRO:HD3	3:S:224:LYS:HZ3	1.85	0.40
2:R:56:ILE:HD12	2:R:56:ILE:HA	1.98	0.40
3:H:174:LEU:HD21	3:H:197:VAL:HG21	2.03	0.40
1:M:22:ASN:OD1	5:M:401:NAG:N2	2.55	0.40
3:S:134:PRO:HB2	3:S:157:VAL:HG23	2.04	0.40
3:S:177:GLY:O	3:S:197:VAL:HA	2.21	0.40
3:X:161:PHE:HA	3:X:162:PRO:HA	1.84	0.40
1:Q:192:THR:O	1:Q:195:TYR:O	2.39	0.40
4:T:8:PRO:O	4:T:9:VAL:CB	2.69	0.40

All (2) 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:K:156:SER:OG	3:X:231:CYS:SG[1_455]	1.94	0.26
3:H:1:GLN:N	3:X:26:GLY:O[1_455]	2.15	0.05

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	318/320 (99%)	306 (96%)	11 (4%)	1 (0%)	36	55
1	C	317/320 (99%)	308 (97%)	8 (2%)	1 (0%)	36	55
1	E	316/320 (99%)	306 (97%)	9 (3%)	1 (0%)	36	55
1	M	316/320 (99%)	306 (97%)	9 (3%)	1 (0%)	36	55
1	O	316/320 (99%)	308 (98%)	6 (2%)	2 (1%)	21	38
1	Q	316/320 (99%)	307 (97%)	8 (2%)	1 (0%)	36	55
2	B	166/170 (98%)	160 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	167/170 (98%)	159 (95%)	8 (5%)	0	100	100
2	F	166/170 (98%)	160 (96%)	6 (4%)	0	100	100
2	N	167/170 (98%)	160 (96%)	7 (4%)	0	100	100
2	P	161/170 (95%)	155 (96%)	6 (4%)	0	100	100
2	R	165/170 (97%)	158 (96%)	7 (4%)	0	100	100
3	G	229/231 (99%)	218 (95%)	11 (5%)	0	100	100
3	H	224/231 (97%)	217 (97%)	6 (3%)	1 (0%)	30	49
3	J	229/231 (99%)	222 (97%)	7 (3%)	0	100	100
3	S	229/231 (99%)	218 (95%)	10 (4%)	1 (0%)	30	49
3	U	229/231 (99%)	219 (96%)	10 (4%)	0	100	100
3	X	229/231 (99%)	219 (96%)	10 (4%)	0	100	100
4	I	212/214 (99%)	206 (97%)	6 (3%)	0	100	100
4	K	212/214 (99%)	207 (98%)	5 (2%)	0	100	100
4	L	212/214 (99%)	208 (98%)	3 (1%)	1 (0%)	24	43
4	T	212/214 (99%)	204 (96%)	7 (3%)	1 (0%)	24	43
4	V	212/214 (99%)	207 (98%)	5 (2%)	0	100	100
4	Y	212/214 (99%)	208 (98%)	4 (2%)	0	100	100
All	All	5532/5610 (99%)	5346 (97%)	175 (3%)	11 (0%)	43	63

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	T	9	VAL
1	O	196	VAL
1	A	62	ILE
1	C	62	ILE
1	E	62	ILE
4	L	68	GLU
1	M	62	ILE
1	O	62	ILE
1	Q	62	ILE
3	S	100	LYS
3	H	141	PRO

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	281/282 (100%)	274 (98%)	7 (2%)	42	69
1	C	282/282 (100%)	277 (98%)	5 (2%)	51	77
1	E	281/282 (100%)	275 (98%)	6 (2%)	47	74
1	M	281/282 (100%)	280 (100%)	1 (0%)	84	93
1	O	281/282 (100%)	269 (96%)	12 (4%)	26	51
1	Q	281/282 (100%)	273 (97%)	8 (3%)	38	66
2	B	144/146 (99%)	142 (99%)	2 (1%)	59	81
2	D	145/146 (99%)	144 (99%)	1 (1%)	76	89
2	F	145/146 (99%)	144 (99%)	1 (1%)	76	89
2	N	144/146 (99%)	141 (98%)	3 (2%)	47	74
2	P	143/146 (98%)	142 (99%)	1 (1%)	76	89
2	R	144/146 (99%)	141 (98%)	3 (2%)	47	74
3	G	194/194 (100%)	170 (88%)	24 (12%)	4	9
3	H	191/194 (98%)	176 (92%)	15 (8%)	11	24
3	J	194/194 (100%)	172 (89%)	22 (11%)	5	12
3	S	194/194 (100%)	180 (93%)	14 (7%)	13	28
3	U	194/194 (100%)	189 (97%)	5 (3%)	40	68
3	X	194/194 (100%)	185 (95%)	9 (5%)	24	48
4	I	189/189 (100%)	174 (92%)	15 (8%)	11	24
4	K	189/189 (100%)	169 (89%)	20 (11%)	6	14
4	L	189/189 (100%)	169 (89%)	20 (11%)	6	14
4	T	189/189 (100%)	178 (94%)	11 (6%)	18	38
4	V	189/189 (100%)	179 (95%)	10 (5%)	20	42
4	Y	189/189 (100%)	177 (94%)	12 (6%)	16	34
All	All	4847/4866 (100%)	4620 (95%)	227 (5%)	23	47

All (227) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	196	VAL
1	A	210	GLN
1	A	212	THR
1	A	218	GLU
1	A	242	VAL
1	A	261	ARG
1	A	295	GLN
2	B	56	ILE
2	B	57	GLU
1	C	102	VAL
1	C	182	VAL
1	C	189	GLN
1	C	218	GLU
1	C	297	VAL
2	D	58	LYS
1	E	32	ASP
1	E	196	VAL
1	E	197	GLN
1	E	217	ILE
1	E	219	SER
1	E	295	GLN
2	F	150	GLU
3	G	13	LYS
3	G	28	SER
3	G	31	ARG
3	G	62	GLN
3	G	69	THR
3	G	74	THR
3	G	75	SER
3	G	76	THR
3	G	105	VAL
3	G	126	VAL
3	G	130	SER
3	G	131	THR
3	G	132	LYS
3	G	147	SER
3	G	156	LEU
3	G	166	THR
3	G	175	THR
3	G	176	SER
3	G	178	VAL
3	G	187	SER
3	G	194	SER

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Mol	Chain	Res	Type
3	G	197	VAL
3	G	199	VAL
3	G	212	ASN
3	H	4	LEU
3	H	11	VAL
3	H	22	CYS
3	H	35	SER
3	H	68	VAL
3	H	74	THR
3	H	88	SER
3	H	98	ARG
3	H	132	LYS
3	H	147	SER
3	H	150	THR
3	H	175	THR
3	H	206	THR
3	H	208	THR
3	H	214	ASN
4	I	7	SER
4	I	9	VAL
4	I	14	SER
4	I	42	ARG
4	I	56	THR
4	I	60	SER
4	I	76	SER
4	I	78	LEU
4	I	94	VAL
4	I	100	GLN
4	I	121	SER
4	I	124	GLN
4	I	201	LEU
4	I	202	SER
4	I	214	CYS
3	J	1	GLN
3	J	3	GLN
3	J	4	LEU
3	J	22	CYS
3	J	34	ILE
3	J	35	SER
3	J	48	LEU
3	J	71	THR
3	J	74	THR

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Mol	Chain	Res	Type
3	J	76	THR
3	J	87	ARG
3	J	88	SER
3	J	131	THR
3	J	132	LYS
3	J	139	LEU
3	J	147	SER
3	J	153	LEU
3	J	157	VAL
3	J	158	LYS
3	J	180	THR
3	J	187	SER
3	J	230	SER
4	K	7	SER
4	K	8	PRO
4	K	9	VAL
4	K	27	GLN
4	K	42	ARG
4	K	48	ILE
4	K	60	SER
4	K	68	GLU
4	K	70	GLU
4	K	90	GLN
4	K	91	SER
4	K	107	LYS
4	K	108	ARG
4	K	109	THR
4	K	114	SER
4	K	142	ARG
4	K	146	VAL
4	K	163	VAL
4	K	191	VAL
4	K	197	THR
4	L	22	THR
4	L	42	ARG
4	L	56	THR
4	L	69	THR
4	L	70	GLU
4	L	89	GLN
4	L	90	GLN
4	L	91	SER
4	L	106	ILE

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Mol	Chain	Res	Type
4	L	107	LYS
4	L	129	THR
4	L	132	VAL
4	L	147	GLN
4	L	162	SER
4	L	163	VAL
4	L	168	SER
4	L	169	LYS
4	L	183	LYS
4	L	206	THR
4	L	214	CYS
1	M	101	ASP
2	N	55	VAL
2	N	58	LYS
2	N	72	GLU
1	O	9	SER
1	O	32	ASP
1	O	101	ASP
1	O	189	GLN
1	O	191	GLN
1	O	193	SER
1	O	196	VAL
1	O	197	GLN
1	O	199	SER
1	O	210	GLN
1	O	218	GLU
1	O	242	VAL
2	P	123	ARG
1	Q	27	LYS
1	Q	28	THR
1	Q	168	MET
1	Q	195	TYR
1	Q	196	VAL
1	Q	248	ASN
1	Q	295	GLN
1	Q	326	LYS
2	R	72	GLU
2	R	156	THR
2	R	164	ASP
3	S	2	VAL
3	S	4	LEU
3	S	6	GLN

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Mol	Chain	Res	Type
3	S	10	GLU
3	S	18	VAL
3	S	30	SER
3	S	67	ARG
3	S	104	GLU
3	S	132	LYS
3	S	146	THR
3	S	147	SER
3	S	157	VAL
3	S	174	LEU
3	S	206	THR
4	T	7	SER
4	T	10	SER
4	T	22	THR
4	T	33	LEU
4	T	68	GLU
4	T	78	LEU
4	T	79	GLN
4	T	94	VAL
4	T	95	PRO
4	T	107	LYS
4	T	214	CYS
3	U	37	VAL
3	U	126	VAL
3	U	130	SER
3	U	144	LYS
3	U	146	THR
4	V	7	SER
4	V	8	PRO
4	V	22	THR
4	V	33	LEU
4	V	75	ILE
4	V	90	GLN
4	V	105	GLU
4	V	108	ARG
4	V	142	ARG
4	V	214	CYS
3	X	13	LYS
3	X	65	GLN
3	X	75	SER
3	X	87	ARG
3	X	105	VAL

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Mol	Chain	Res	Type
3	X	142	SER
3	X	143	SER
3	X	229	LYS
3	X	230	SER
4	Y	7	SER
4	Y	10	SER
4	Y	22	THR
4	Y	33	LEU
4	Y	42	ARG
4	Y	78	LEU
4	Y	90	GLN
4	Y	94	VAL
4	Y	95	PRO
4	Y	107	LYS
4	Y	108	ARG
4	Y	147	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	75	HIS
1	A	210	GLN
2	B	12	ASN
2	B	60	ASN
2	B	116	ASN
1	C	189	GLN
1	C	210	GLN
2	D	47	GLN
2	D	105	GLN
2	D	159	HIS
1	E	18	HIS
1	E	33	GLN
1	E	216	ASN
2	F	105	GLN
3	G	43	GLN
3	G	219	ASN
3	H	214	ASN
4	I	37	GLN
4	I	53	ASN
4	I	92	ASN
4	I	93	ASN

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Mol	Chain	Res	Type
3	J	39	GLN
4	K	34	ASN
4	K	38	GLN
4	K	53	ASN
4	K	92	ASN
4	L	37	GLN
4	L	89	GLN
1	M	18	HIS
1	M	75	HIS
1	M	210	GLN
1	M	296	ASN
2	N	105	GLN
1	O	18	HIS
1	O	75	HIS
1	O	80	GLN
1	O	210	GLN
1	O	296	ASN
2	P	12	ASN
2	P	65	GLN
2	P	78	GLN
1	Q	18	HIS
1	Q	75	HIS
1	Q	211	GLN
1	Q	248	ASN
1	Q	296	ASN
4	T	79	GLN
3	U	102	GLN
3	U	186	GLN
4	V	53	ASN
4	V	79	GLN
4	V	90	GLN
4	V	92	ASN
4	V	189	HIS
3	X	65	GLN
3	X	179	HIS
4	Y	53	ASN
4	Y	137	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

36 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	E	405	1	14,14,15	0.24	0	17,19,21	0.47	0
5	NAG	F	201	2	14,14,15	0.20	0	17,19,21	0.49	0
5	NAG	O	405	1	14,14,15	0.29	0	17,19,21	0.39	0
5	NAG	O	402	1	14,14,15	0.41	0	17,19,21	0.46	0
5	NAG	E	403	1	14,14,15	0.18	0	17,19,21	0.43	0
5	NAG	C	404	1	14,14,15	0.27	0	17,19,21	0.39	0
5	NAG	M	403	1	14,14,15	0.95	1 (7%)	17,19,21	1.26	1 (5%)
5	NAG	E	402	1	14,14,15	0.32	0	17,19,21	0.37	0
5	NAG	A	402	1	14,14,15	0.35	0	17,19,21	0.41	0
5	NAG	E	401	1	14,14,15	0.40	0	17,19,21	0.60	1 (5%)
5	NAG	A	405	1	14,14,15	0.23	0	17,19,21	0.35	0
5	NAG	P	201	2	14,14,15	0.24	0	17,19,21	0.47	0
5	NAG	C	402	1	14,14,15	0.43	0	17,19,21	0.51	0
5	NAG	C	405	1	14,14,15	0.22	0	17,19,21	0.37	0
5	NAG	M	401	1	14,14,15	0.51	0	17,19,21	0.53	0
5	NAG	Q	403	1	14,14,15	0.17	0	17,19,21	0.42	0
5	NAG	Q	401	1	14,14,15	0.34	0	17,19,21	0.36	0
5	NAG	D	201	2	14,14,15	0.19	0	17,19,21	0.41	0
5	NAG	C	403	1	14,14,15	1.28	1 (7%)	17,19,21	1.16	3 (17%)
5	NAG	Q	402	1	14,14,15	0.36	0	17,19,21	0.49	0
5	NAG	N	201	2	14,14,15	0.20	0	17,19,21	0.43	0
5	NAG	O	403	1	14,14,15	0.21	0	17,19,21	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	C	401	1	14,14,15	0.43	0	17,19,21	0.52	0
5	NAG	A	403	1	14,14,15	0.24	0	17,19,21	0.46	0
5	NAG	O	401	1	14,14,15	0.27	0	17,19,21	0.44	0
5	NAG	M	404	1	14,14,15	0.29	0	17,19,21	0.37	0
5	NAG	Q	404	1	14,14,15	0.30	0	17,19,21	0.41	0
5	NAG	A	401	1	14,14,15	0.19	0	17,19,21	0.71	1 (5%)
5	NAG	M	402	1	14,14,15	0.45	0	17,19,21	0.52	0
5	NAG	M	405	1	14,14,15	0.24	0	17,19,21	0.45	0
5	NAG	Q	405	1	14,14,15	0.21	0	17,19,21	0.41	0
5	NAG	E	404	1	14,14,15	0.35	0	17,19,21	0.37	0
5	NAG	B	201	2	14,14,15	0.28	0	17,19,21	0.38	0
5	NAG	O	404	1	14,14,15	0.27	0	17,19,21	0.36	0
5	NAG	R	201	2	14,14,15	0.17	0	17,19,21	0.53	0
5	NAG	A	404	1	14,14,15	0.49	0	17,19,21	0.69	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	E	405	1	-	0/6/23/26	0/1/1/1
5	NAG	F	201	2	-	0/6/23/26	0/1/1/1
5	NAG	O	405	1	-	0/6/23/26	0/1/1/1
5	NAG	O	402	1	-	2/6/23/26	0/1/1/1
5	NAG	E	403	1	-	2/6/23/26	0/1/1/1
5	NAG	C	404	1	-	1/6/23/26	0/1/1/1
5	NAG	M	403	1	-	1/6/23/26	0/1/1/1
5	NAG	E	402	1	-	2/6/23/26	0/1/1/1
5	NAG	A	402	1	-	2/6/23/26	0/1/1/1
5	NAG	E	401	1	-	1/6/23/26	0/1/1/1
5	NAG	A	405	1	-	0/6/23/26	0/1/1/1
5	NAG	P	201	2	-	0/6/23/26	0/1/1/1
5	NAG	C	402	1	-	2/6/23/26	0/1/1/1
5	NAG	C	405	1	-	0/6/23/26	0/1/1/1
5	NAG	M	401	1	-	0/6/23/26	0/1/1/1
5	NAG	Q	403	1	-	0/6/23/26	0/1/1/1
5	NAG	Q	401	1	-	2/6/23/26	0/1/1/1
5	NAG	D	201	2	-	0/6/23/26	0/1/1/1
5	NAG	C	403	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	Q	402	1	-	2/6/23/26	0/1/1/1
5	NAG	N	201	2	-	0/6/23/26	0/1/1/1
5	NAG	O	403	1	-	0/6/23/26	0/1/1/1
5	NAG	C	401	1	-	2/6/23/26	0/1/1/1
5	NAG	A	403	1	-	1/6/23/26	0/1/1/1
5	NAG	O	401	1	-	2/6/23/26	0/1/1/1
5	NAG	M	404	1	-	2/6/23/26	0/1/1/1
5	NAG	Q	404	1	-	0/6/23/26	0/1/1/1
5	NAG	A	401	1	-	0/6/23/26	0/1/1/1
5	NAG	M	402	1	-	2/6/23/26	0/1/1/1
5	NAG	M	405	1	-	0/6/23/26	0/1/1/1
5	NAG	Q	405	1	-	0/6/23/26	0/1/1/1
5	NAG	E	404	1	-	0/6/23/26	0/1/1/1
5	NAG	B	201	2	-	0/6/23/26	0/1/1/1
5	NAG	O	404	1	-	0/6/23/26	0/1/1/1
5	NAG	R	201	2	-	0/6/23/26	0/1/1/1
5	NAG	A	404	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	403	NAG	C1-C2	4.30	1.58	1.52
5	M	403	NAG	O5-C1	3.28	1.49	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	403	NAG	C1-O5-C5	4.91	118.77	112.19
5	C	403	NAG	C1-O5-C5	2.87	116.03	112.19
5	A	404	NAG	C1-O5-C5	2.25	115.20	112.19
5	C	403	NAG	O5-C5-C4	-2.22	105.44	110.83
5	A	401	NAG	C1-O5-C5	2.19	115.12	112.19
5	C	403	NAG	C4-C3-C2	2.17	114.20	111.02
5	E	401	NAG	C1-O5-C5	2.01	114.88	112.19

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	Q	402	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	M	402	NAG	O5-C5-C6-O6
5	O	402	NAG	O5-C5-C6-O6
5	A	402	NAG	O5-C5-C6-O6
5	Q	401	NAG	O5-C5-C6-O6
5	E	402	NAG	O5-C5-C6-O6
5	Q	402	NAG	C4-C5-C6-O6
5	C	403	NAG	O5-C5-C6-O6
5	C	402	NAG	O5-C5-C6-O6
5	O	402	NAG	C4-C5-C6-O6
5	M	402	NAG	C4-C5-C6-O6
5	A	402	NAG	C4-C5-C6-O6
5	Q	401	NAG	C4-C5-C6-O6
5	C	402	NAG	C4-C5-C6-O6
5	E	402	NAG	C4-C5-C6-O6
5	C	403	NAG	C4-C5-C6-O6
5	A	404	NAG	O5-C5-C6-O6
5	A	404	NAG	C4-C5-C6-O6
5	E	403	NAG	O5-C5-C6-O6
5	O	401	NAG	C4-C5-C6-O6
5	O	401	NAG	O5-C5-C6-O6
5	C	401	NAG	O5-C5-C6-O6
5	C	401	NAG	C4-C5-C6-O6
5	M	404	NAG	C4-C5-C6-O6
5	C	404	NAG	C4-C5-C6-O6
5	E	403	NAG	C4-C5-C6-O6
5	M	404	NAG	O5-C5-C6-O6
5	A	403	NAG	O5-C5-C6-O6
5	M	403	NAG	O5-C5-C6-O6
5	E	401	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	405	NAG	1	0
5	M	401	NAG	1	0
5	C	403	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	320/320 (100%)	-0.35	5 (1%) 70 67	27, 38, 64, 116	0
1	C	319/320 (99%)	-0.26	4 (1%) 75 71	27, 43, 67, 109	1 (0%)
1	E	318/320 (99%)	-0.09	5 (1%) 70 67	33, 50, 79, 106	0
1	M	318/320 (99%)	-0.25	5 (1%) 70 67	30, 42, 72, 124	2 (0%)
1	O	318/320 (99%)	-0.02	7 (2%) 62 58	36, 53, 87, 134	1 (0%)
1	Q	318/320 (99%)	-0.25	2 (0%) 85 83	31, 44, 66, 102	2 (0%)
2	B	168/170 (98%)	-0.25	0 100 100	28, 45, 66, 161	2 (1%)
2	D	169/170 (99%)	-0.19	3 (1%) 67 64	28, 46, 71, 167	0
2	F	168/170 (98%)	-0.21	1 (0%) 85 83	31, 46, 65, 131	2 (1%)
2	N	169/170 (99%)	0.17	4 (2%) 59 55	32, 68, 105, 139	2 (1%)
2	P	163/170 (95%)	0.11	4 (2%) 58 54	31, 64, 101, 144	2 (1%)
2	R	167/170 (98%)	0.04	5 (2%) 52 48	30, 55, 98, 114	0
3	G	231/231 (100%)	0.63	28 (12%) 8 7	34, 78, 164, 266	0
3	H	228/231 (98%)	-0.05	5 (2%) 62 58	28, 52, 86, 142	0
3	J	231/231 (100%)	0.53	23 (9%) 12 10	35, 77, 164, 268	1 (0%)
3	S	231/231 (100%)	0.87	19 (8%) 17 15	51, 94, 161, 280	0
3	U	231/231 (100%)	0.16	9 (3%) 43 38	32, 54, 88, 174	0
3	X	231/231 (100%)	0.02	9 (3%) 43 38	35, 57, 98, 201	0
4	I	214/214 (100%)	0.53	12 (5%) 30 26	34, 74, 161, 216	1 (0%)
4	K	214/214 (100%)	0.38	4 (1%) 66 62	33, 79, 114, 174	0
4	L	214/214 (100%)	0.10	5 (2%) 61 57	25, 51, 105, 158	0
4	T	214/214 (100%)	0.85	27 (12%) 8 6	24, 83, 169, 219	2 (0%)
4	V	214/214 (100%)	0.02	3 (1%) 73 70	24, 50, 79, 152	0
4	Y	214/214 (100%)	0.11	7 (3%) 49 45	24, 56, 91, 118	1 (0%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
All	All	5582/5610 (99%)	0.09	196 (3%)	47	42	24, 52, 125, 280	19 (0%)

All (196) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	U	146	THR	6.2
2	R	5	ALA	6.1
3	X	146	THR	5.4
3	H	146	THR	5.3
1	O	218	GLU	5.3
4	L	214	CYS	5.2
4	K	214	CYS	5.0
3	J	146	THR	4.9
3	U	147	SER	4.7
1	C	218	GLU	4.6
1	E	218	GLU	4.5
1	Q	218	GLU	4.5
3	H	142	SER	4.2
2	P	171	PHE	4.2
3	U	143	SER	4.1
1	A	305	CYS	4.1
3	X	148	GLY	4.0
3	S	229	LYS	4.0
3	G	166	THR	3.8
1	C	326	LYS	3.8
3	H	231	CYS	3.8
3	G	135	SER	3.7
4	V	214	CYS	3.7
3	X	143	SER	3.7
4	I	193	ALA	3.6
1	M	218	GLU	3.6
4	T	184	ALA	3.6
1	A	327	ALA	3.5
1	O	32	ASP	3.5
4	Y	126	LYS	3.5
3	J	231	CYS	3.5
4	T	108	ARG	3.5
2	D	3	PHE	3.4
1	A	8	ASN	3.3
1	E	219	SER	3.3
3	X	144	LYS	3.3
3	U	229	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
3	X	231	CYS	3.2
3	S	146	THR	3.2
4	Y	127	SER	3.2
3	S	226	VAL	3.2
4	T	94	VAL	3.2
3	X	142	SER	3.2
2	P	123	ARG	3.1
3	S	76	THR	3.1
3	X	145	SER	3.1
3	G	148	GLY	3.1
4	T	202	SER	3.1
4	Y	7	SER	3.1
3	J	145	SER	3.1
3	S	142	SER	3.1
3	H	148	GLY	3.1
3	S	222	VAL	3.1
4	I	149	LYS	3.0
3	G	200	PRO	3.0
3	J	205	GLY	3.0
3	X	147	SER	3.0
2	R	6	ILE	2.9
3	G	222	VAL	2.9
4	Y	94	VAL	2.9
2	R	171	PHE	2.9
1	C	9	SER	2.9
4	T	120	PRO	2.9
3	G	214	ASN	2.8
3	G	165	VAL	2.8
4	I	197	THR	2.8
2	P	11	GLU	2.8
3	U	148	GLY	2.8
3	J	208	THR	2.8
4	L	154	LEU	2.8
2	N	172	GLN	2.8
1	C	8	ASN	2.7
3	J	202	SER	2.7
3	S	143	SER	2.7
4	T	110	VAL	2.7
3	G	151	ALA	2.7
3	J	229	LYS	2.7
4	Y	214	CYS	2.7
2	F	10	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
3	S	228	PRO	2.7
2	N	29	SER	2.7
3	G	226	VAL	2.7
4	T	7	SER	2.7
3	G	146	THR	2.7
4	T	207	LYS	2.6
2	R	123	ARG	2.6
3	J	1	GLN	2.6
4	T	119	PRO	2.6
2	N	144	CYS	2.6
4	I	132	VAL	2.6
1	O	219	SER	2.6
3	J	173	ALA	2.6
1	A	218	GLU	2.6
3	J	165	VAL	2.6
1	O	325	GLU	2.6
1	O	277	CYS	2.6
3	J	143	SER	2.6
3	S	139	LEU	2.5
4	V	154	LEU	2.5
4	V	3	GLN	2.5
3	G	136	VAL	2.5
4	T	193	ALA	2.5
3	S	210	ILE	2.5
4	T	117	ILE	2.5
3	G	157	VAL	2.5
4	T	42	ARG	2.5
3	U	128	SER	2.5
3	G	204	LEU	2.5
4	T	149	LYS	2.5
4	T	148	TRP	2.5
3	S	200	PRO	2.4
4	I	154	LEU	2.4
4	L	191	VAL	2.4
3	X	230	SER	2.4
4	T	127	SER	2.4
2	P	144	CYS	2.4
3	G	137	PHE	2.4
3	G	213	VAL	2.4
4	K	126	LYS	2.4
2	R	7	ALA	2.4
3	J	147	SER	2.4

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Mol	Chain	Res	Type	RSRZ
3	G	144	LYS	2.4
3	U	145	SER	2.3
4	I	212	GLY	2.3
4	L	209	PHE	2.3
4	I	205	VAL	2.3
3	J	200	PRO	2.3
3	J	56	GLY	2.3
3	G	139	LEU	2.3
3	G	153	LEU	2.3
4	I	207	LYS	2.3
4	T	134	CYS	2.3
3	G	209	TYR	2.3
4	T	115	VAL	2.3
3	J	150	THR	2.3
3	J	226	VAL	2.3
1	M	8	ASN	2.3
3	G	152	ALA	2.3
3	G	217	PRO	2.3
3	G	206	THR	2.3
1	E	222	TRP	2.3
3	U	231	CYS	2.3
3	S	58	THR	2.2
3	G	174	LEU	2.2
3	J	204	LEU	2.2
1	M	321	ARG	2.2
3	J	169	TRP	2.2
3	S	144	LYS	2.2
4	T	126	LYS	2.2
3	G	131	THR	2.2
1	O	9	SER	2.2
4	T	118	PHE	2.2
3	S	152	ALA	2.2
3	S	208	THR	2.2
1	Q	305	CYS	2.2
3	J	174	LEU	2.2
4	K	7	SER	2.2
4	I	122	ASP	2.2
2	D	171	PHE	2.2
3	G	229	LYS	2.2
3	U	144	LYS	2.2
4	T	209	PHE	2.2
4	T	111	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	158	GLY	2.1
3	J	206	THR	2.1
4	Y	129	THR	2.1
4	T	214	CYS	2.1
3	J	220	THR	2.1
3	S	220	THR	2.1
4	I	129	THR	2.1
3	J	155	CYS	2.1
1	E	32	ASP	2.1
3	G	164	PRO	2.1
3	H	141	PRO	2.1
3	G	175	THR	2.1
4	T	129	THR	2.1
1	M	220	ARG	2.1
3	J	144	LYS	2.1
4	T	188	LYS	2.1
3	G	231	CYS	2.1
4	T	177	SER	2.1
3	S	11	VAL	2.1
2	N	5	ALA	2.1
4	L	213	GLU	2.1
3	S	28	SER	2.1
4	Y	108	ARG	2.0
1	M	22	ASN	2.0
4	I	181	LEU	2.0
1	O	222	TRP	2.0
2	D	4	GLY	2.0
4	T	157	GLY	2.0
4	I	125	LEU	2.0
1	A	326	LYS	2.0
4	K	129	THR	2.0
3	S	145	SER	2.0
4	T	176	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	M	401	14/15	0.27	0.21	142,162,166,166	0
5	NAG	E	401	14/15	0.35	0.18	144,157,161,163	0
5	NAG	A	401	14/15	0.36	0.22	143,153,161,163	0
5	NAG	O	401	14/15	0.39	0.16	149,162,172,172	0
5	NAG	C	401	14/15	0.48	0.20	144,160,163,163	0
5	NAG	Q	401	14/15	0.57	0.20	138,157,160,161	0
5	NAG	O	404	14/15	0.69	0.18	93,109,116,121	0
5	NAG	M	403	14/15	0.72	0.18	95,104,111,111	0
5	NAG	Q	404	14/15	0.72	0.19	102,123,131,135	0
5	NAG	C	403	14/15	0.74	0.20	105,118,126,127	0
5	NAG	A	404	14/15	0.75	0.21	93,112,127,130	0
5	NAG	R	201	14/15	0.75	0.15	87,101,112,118	0
5	NAG	M	404	14/15	0.78	0.17	93,104,108,110	0
5	NAG	E	404	14/15	0.78	0.14	89,105,123,129	0
5	NAG	M	402	14/15	0.79	0.16	77,88,91,92	0
5	NAG	O	402	14/15	0.80	0.18	80,99,106,109	0
5	NAG	P	201	14/15	0.81	0.14	79,93,96,100	0
5	NAG	C	404	14/15	0.81	0.17	104,126,132,137	0
5	NAG	E	402	14/15	0.82	0.17	72,82,91,92	0
5	NAG	Q	402	14/15	0.82	0.18	81,93,105,110	0
5	NAG	Q	405	14/15	0.83	0.12	62,76,87,97	0
5	NAG	Q	403	14/15	0.83	0.17	86,95,107,113	0
5	NAG	A	402	14/15	0.84	0.16	76,87,92,97	0
5	NAG	N	201	14/15	0.84	0.12	83,94,99,105	0
5	NAG	A	403	14/15	0.84	0.15	78,94,104,106	0
5	NAG	C	402	14/15	0.85	0.14	65,77,83,93	0
5	NAG	A	405	14/15	0.86	0.11	56,67,76,83	0
5	NAG	B	201	14/15	0.87	0.12	52,62,73,85	0
5	NAG	M	405	14/15	0.88	0.11	59,72,86,86	0
5	NAG	C	405	14/15	0.88	0.12	64,69,85,86	0
5	NAG	D	201	14/15	0.89	0.10	52,67,75,78	0
5	NAG	E	405	14/15	0.90	0.10	49,62,70,76	0
5	NAG	O	405	14/15	0.92	0.10	59,75,87,88	0
5	NAG	F	201	14/15	0.92	0.08	48,66,72,75	0
5	NAG	O	403	14/15	0.92	0.09	53,62,70,72	0
5	NAG	E	403	14/15	0.92	0.10	57,72,79,82	0

6.5 Other polymers [i](#)

There are no such residues in this entry.