Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2020 – 10:33 AM BST

PDB ID	:	5K9Q
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 following versions of software and data (see references ①) were used in the production of this report:

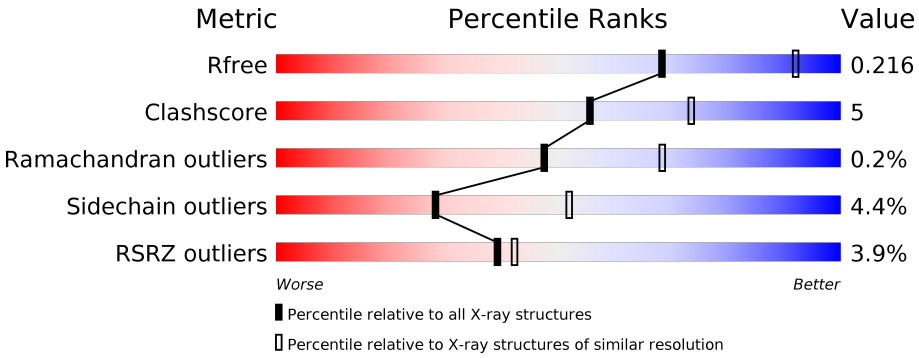
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 on 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 <=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	92% 8%
1	C	320	89% 10%
1	E	320	90% 8%
1	M	320	% 93% 7%
1	O	320	89% 9%
1	Q	320	89% 9%

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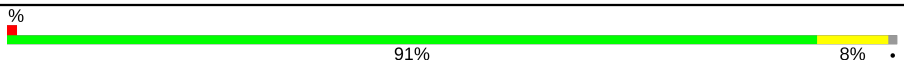
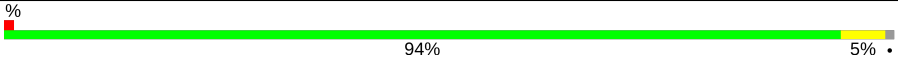
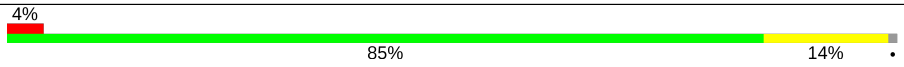
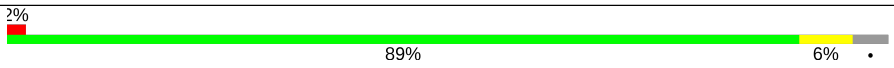
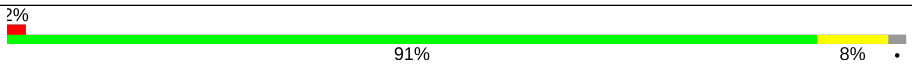
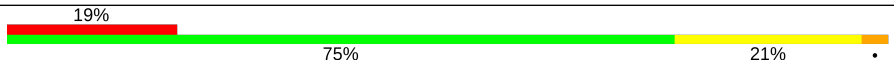
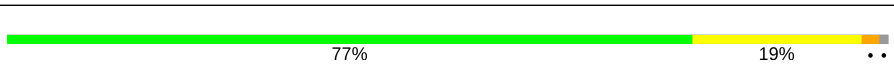
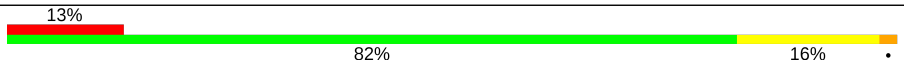
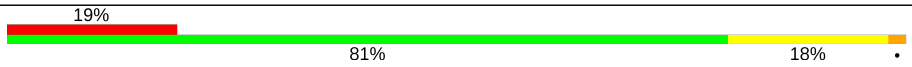
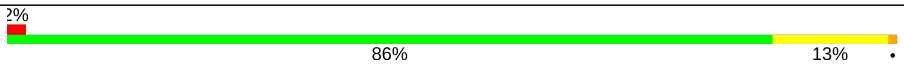
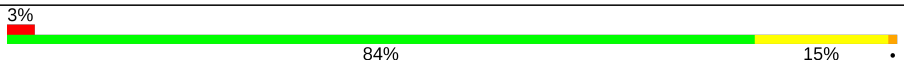
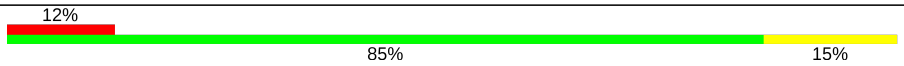
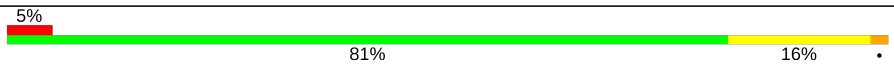
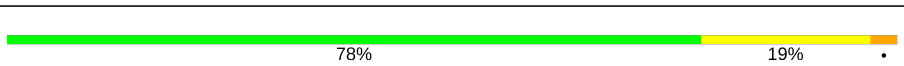
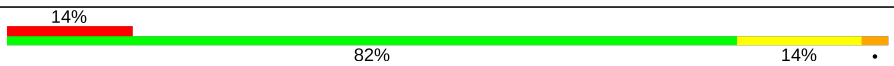
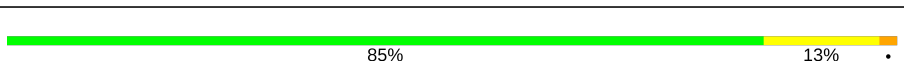
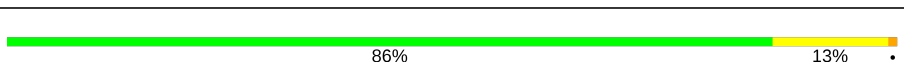
Mol	Chain	Length	Quality of chain
2	B	170	
2	D	170	
2	F	170	
2	N	170	
2	P	170	
2	R	170	
3	G	231	
3	H	231	
3	J	231	
3	S	231	
3	U	231	
3	X	231	
4	I	214	
4	K	214	
4	L	214	
4	T	214	
4	V	214	
4	Y	214	

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	401	-	-	-	X
5	NAG	C	401	-	-	-	X
5	NAG	E	401	-	-	-	X
5	NAG	M	401	-	-	-	X
5	NAG	O	401	-	-	-	X
5	NAG	Q	401	-	-	-	X

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			

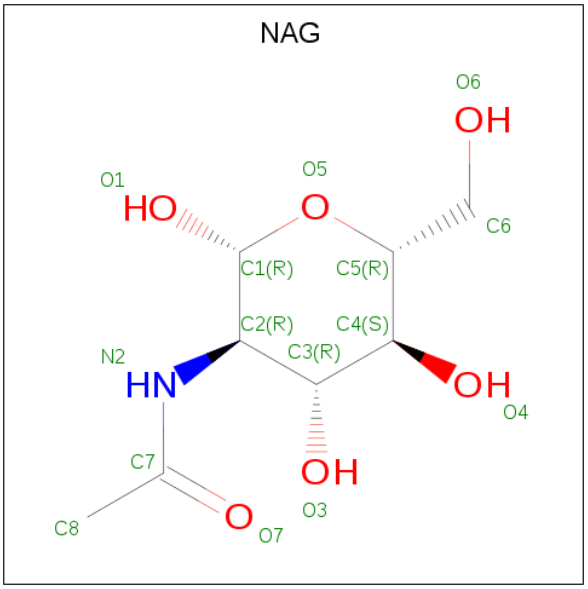
- Molecule 3 is a protein called 16.a.26 Heavy chain.

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 (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	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	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 14 8 1 5	0	0
5	Q	1	Total C N O 14 8 1 5	0	0
5	R	1	Total C N O 14 8 1 5	0	0

- Molecule 6 is water.

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

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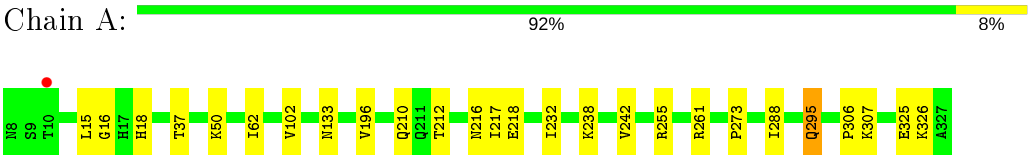
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	Q	128	Total O 128 128	0	0
6	R	51	Total O 51 51	0	0
6	S	9	Total O 9 9	0	0
6	T	19	Total O 19 19	0	0
6	U	61	Total O 61 61	0	0
6	V	55	Total O 55 55	0	0
6	X	55	Total O 55 55	0	0
6	Y	51	Total O 51 51	0	0

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.

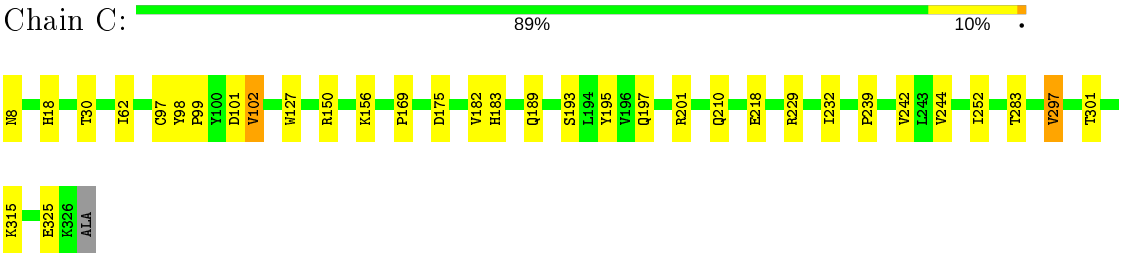
- Molecule 1: Hemagglutinin HA1

Chain A:



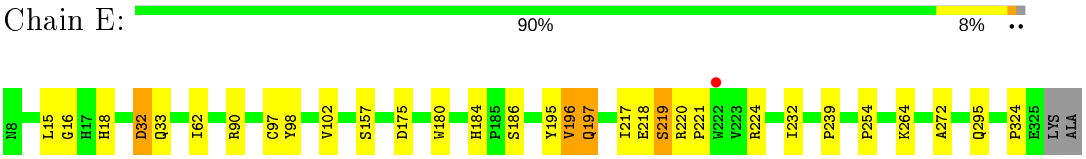
- Molecule 1: Hemagglutinin HA1

Chain C:



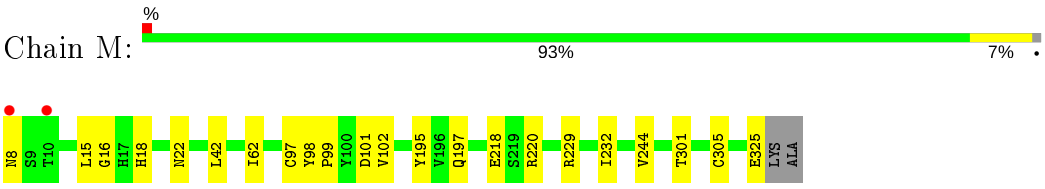
- Molecule 1: Hemagglutinin HA1

Chain E:



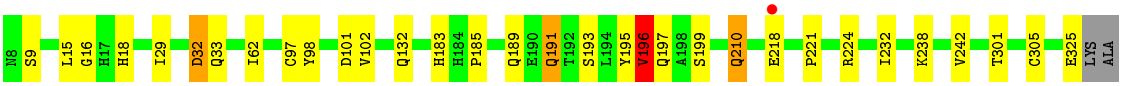
- Molecule 1: Hemagglutinin HA1

Chain M:

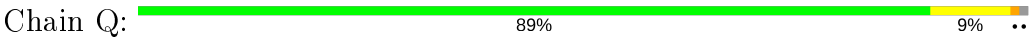


- Molecule 1: Hemagglutinin HA1

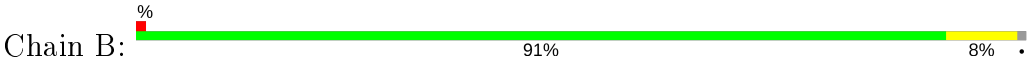
Chain O:

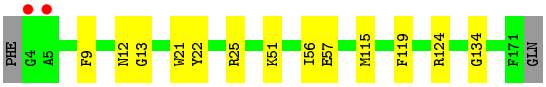


• Molecule 1: Hemagglutinin HA1

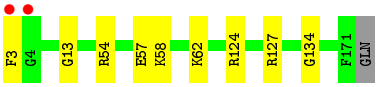


• Molecule 2: Hemagglutinin HA2

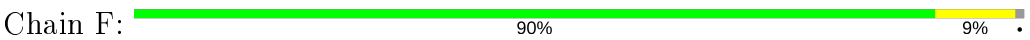


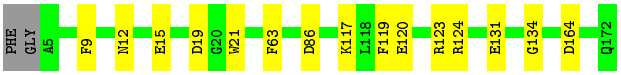


• Molecule 2: Hemagglutinin HA2

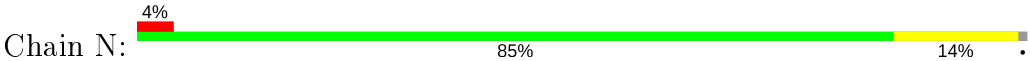


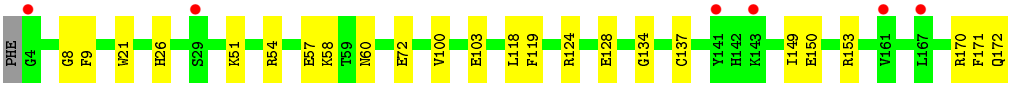
• Molecule 2: Hemagglutinin HA2



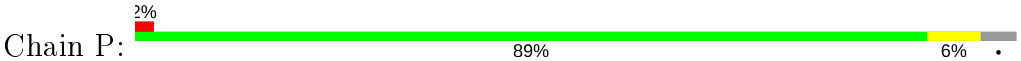


• Molecule 2: Hemagglutinin HA2



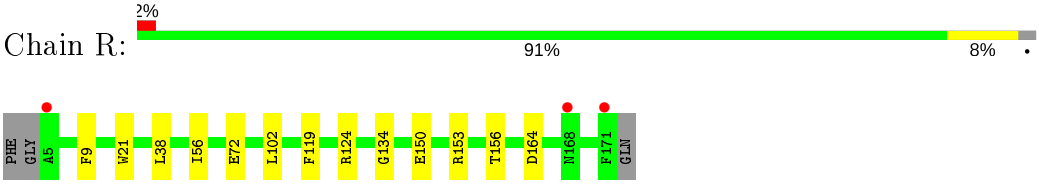


• Molecule 2: Hemagglutinin HA2



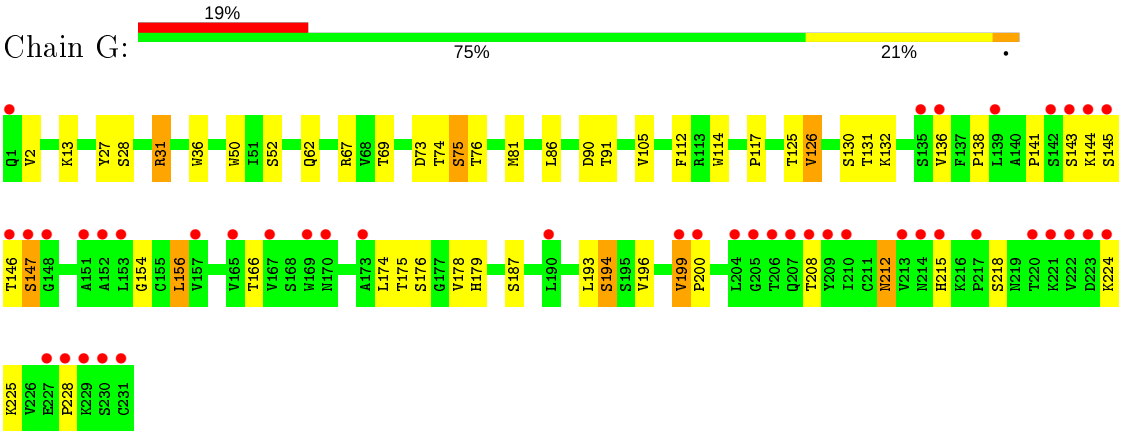
• Molecule 2: Hemagglutinin HA2

Chain R:



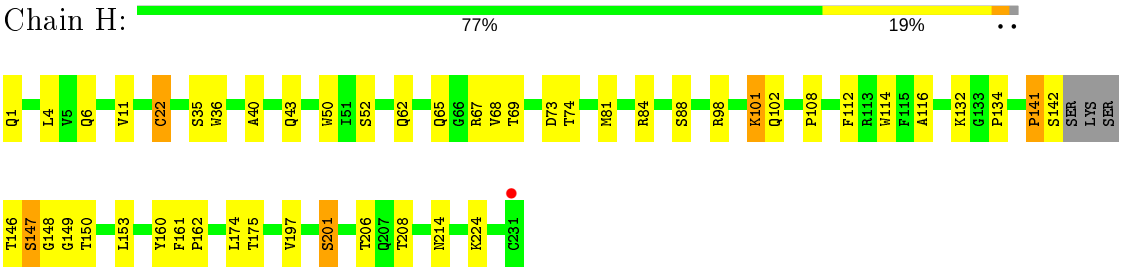
• Molecule 3: 16.a.26 Heavy chain

Chain G:



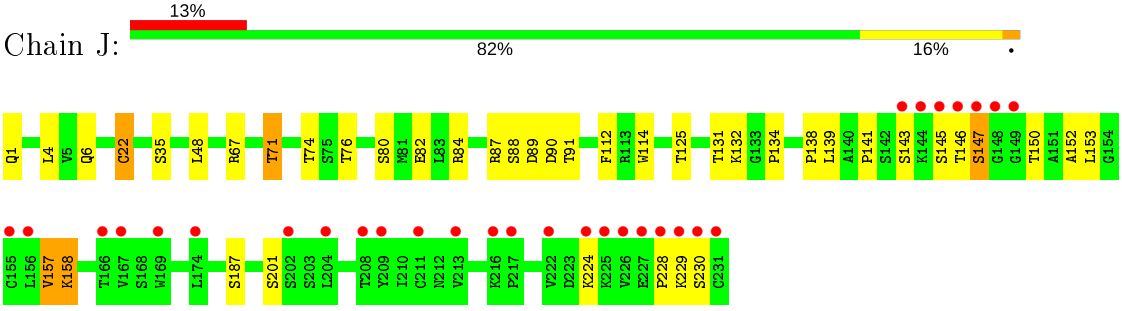
• Molecule 3: 16.a.26 Heavy chain

Chain H:



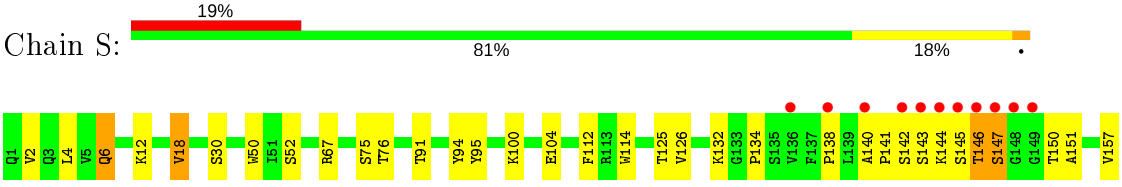
• Molecule 3: 16.a.26 Heavy chain

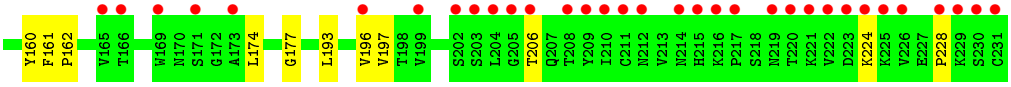
Chain J:



• Molecule 3: 16.a.26 Heavy chain

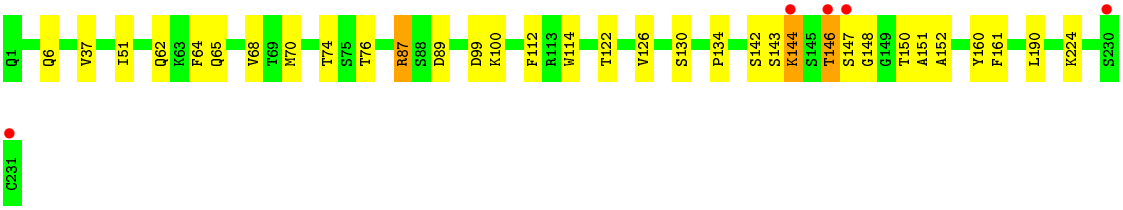
Chain S:





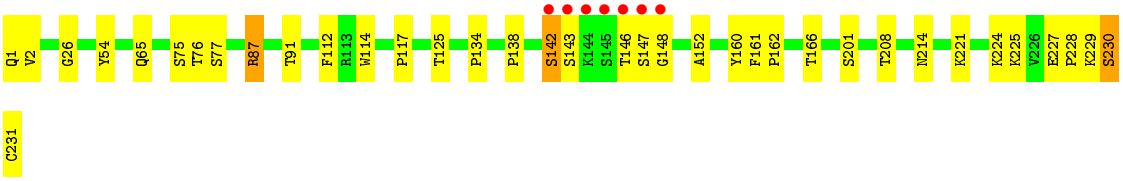
- Molecule 3: 16.a.26 Heavy chain

Chain U:



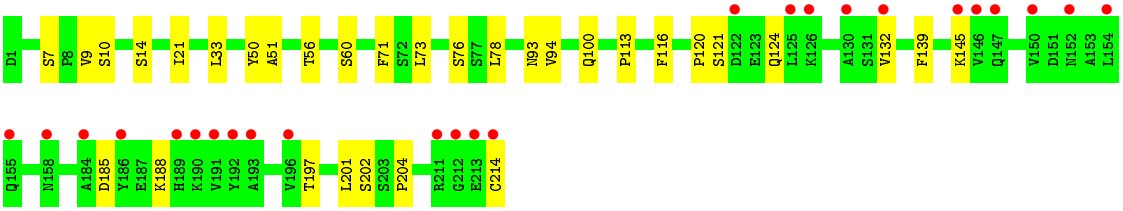
- Molecule 3: 16.a.26 Heavy chain

Chain X:



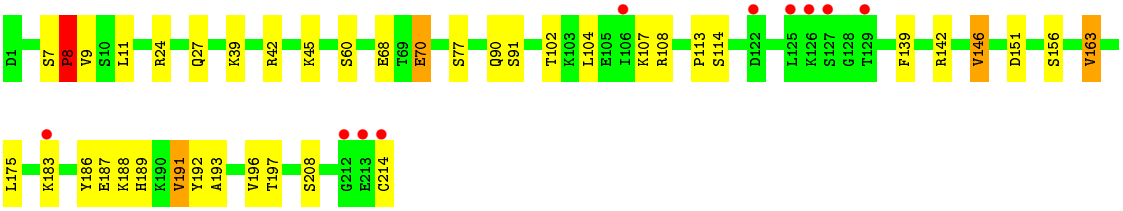
- Molecule 4: 16.a.26 Light chain

Chain I:



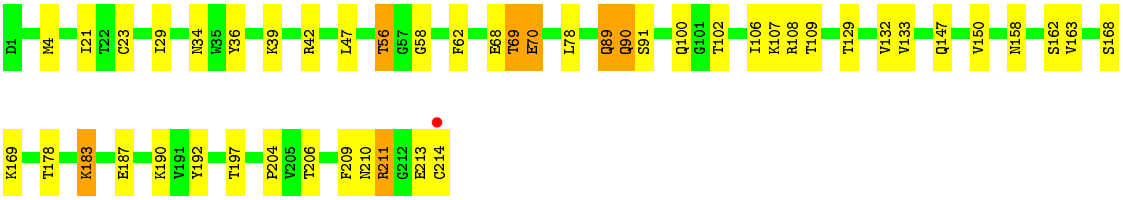
- Molecule 4: 16.a.26 Light chain

Chain K:



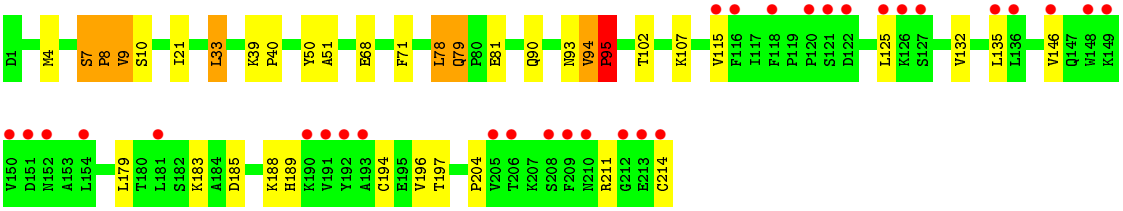
- Molecule 4: 16.a.26 Light chain

Chain L:



• Molecule 4: 16.a.26 Light chain

Chain T:



• Molecule 4: 16.a.26 Light chain

Chain V:

• Molecule 4: 16.a.26 Light chain

Chain Y:

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.02 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.182 , 0.218 0.183 , 0.216	Depositor DCC
R_{free} test set	12282 reflections (5.02%)	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 , 44.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.33	0/2524	0.49	0/3441
1	C	0.35	0/2523	0.47	0/3438
1	E	0.33	0/2514	0.47	0/3427
1	M	0.32	0/2514	0.48	0/3427
1	O	0.32	0/2514	0.47	0/3427
1	Q	0.32	0/2515	0.50	0/3427
2	B	0.28	0/1389	0.42	0/1867
2	D	0.33	0/1401	0.44	0/1883
2	F	0.35	0/1394	0.45	0/1874
2	N	0.33	0/1391	0.42	0/1870
2	P	0.28	0/1363	0.42	0/1832
2	R	0.28	0/1385	0.43	0/1862
3	G	0.33	0/1771	0.50	0/2411
3	H	0.32	0/1749	0.50	0/2381
3	J	0.29	0/1771	0.48	0/2411
3	S	0.30	0/1771	0.48	0/2411
3	U	0.31	0/1771	0.49	0/2411
3	X	0.34	0/1771	0.52	0/2411
4	I	0.34	0/1693	0.49	0/2294
4	K	0.39	1/1693 (0.1%)	0.54	1/2294 (0.0%)
4	L	0.35	0/1693	0.53	1/2294 (0.0%)
4	T	0.48	3/1693 (0.2%)	0.56	1/2294 (0.0%)
4	V	0.47	2/1693 (0.1%)	0.55	1/2294 (0.0%)
4	Y	0.51	2/1693 (0.1%)	0.56	1/2294 (0.0%)
All	All	0.35	8/44189 (0.0%)	0.49	5/59975 (0.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Y	95	PRO	N-CD	5.64	1.55	1.47
4	T	95	PRO	N-CD	5.57	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	8	PRO	N-CD	5.55	1.55	1.47
4	Y	8	PRO	N-CD	5.45	1.55	1.47
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	5.06	1.54	1.47
4	T	40	PRO	N-CD	5.02	1.54	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	K	39	LYS	C-N-CD	5.95	140.89	128.40
4	Y	39	LYS	C-N-CD	5.92	140.82	128.40
4	T	39	LYS	C-N-CD	5.81	140.60	128.40
4	L	58	GLY	C-N-CD	5.67	140.31	128.40
4	V	39	LYS	C-N-CD	5.58	140.13	128.40

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	19	0
1	C	2467	0	2412	21	0
1	E	2458	0	2399	27	0
1	M	2458	0	2399	18	0
1	O	2458	0	2399	29	0
1	Q	2459	0	2406	35	0
2	B	1366	0	1282	15	0
2	D	1377	0	1291	8	0
2	F	1371	0	1287	15	0
2	N	1368	0	1278	17	0
2	P	1340	0	1255	13	0
2	R	1362	0	1279	16	0
3	G	1728	0	1705	36	0
3	H	1707	0	1681	23	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	1728	0	1705	20	0
3	S	1728	0	1705	43	0
3	U	1728	0	1705	24	0
3	X	1728	0	1705	31	2
4	I	1658	0	1609	14	0
4	K	1658	0	1609	12	1
4	L	1658	0	1609	26	0
4	T	1658	0	1611	25	0
4	V	1658	0	1609	19	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	3	0
6	D	74	0	0	0	0
6	E	110	0	0	3	0
6	F	75	0	0	2	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	438	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 (438) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:147:SER:C	3:H:149:GLY:HA2	1.91	0.90
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
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
3:H:148:GLY:N	3:H:149:GLY:HA2	1.94	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:NH1	3:G:31:ARG:HG3	1.95	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
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
4:T:4:MET:HE2	4:T:90:GLN:HG2	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:H:146:THR:N	3:H:201:SER:HG	1.93	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:Q:102:VAL:HG22	1:Q:232:ILE:HB	1.79	0.65
1:O:33:GLN:OE1	4:T:93:ASN:HB3	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:307:LYS:NZ	6:A:508:HOH:O	2.35	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: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:134:PRO:HB3	3:J:157:VAL:HG23	1.85	0.58
3:J:6:GLN:HG2	3:J:22:CYS:SG	2.43	0.58
2:P:124:ARG:HD2	2:R:134:GLY:HA2	1.85	0.58
2:N:134:GLY:HA2	2:R:124:ARG:HD3	1.84	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:O	3:U:144:LYS:HD2	2.04	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:N	3:J:89:ASP:OD1	2.39	0.55
4:L:4:MET:HE2	4:L:23:CYS:SG	2.47	0.55
1:C:102:VAL:HB	1:C:232:ILE:HB	1.88	0.55
2:N:150:GLU:OE1	2:N:153:ARG:NH1	2.40	0.55
3:J:145:SER:HB3	3:J:201:SER:OG	2.08	0.54
1:E:186:SER:HA	1:E:218:GLU:O	2.08	0.54
4:T:4:MET:HE3	4:T:90:GLN:HB3	1.90	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
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:21:ILE:HD12	4:L:102:THR:HG21	1.91	0.53
4:L:4:MET:CE	4:L:23:CYS:SG	2.97	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
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

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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
3:G:2:VAL:HG13	3:G:27:TYR:HD1	1.75	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
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: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
2:F:120:GLU:CD	2:F:123:ARG:HH21	2.14	0.50
1:A:102:VAL:HG22	1:A:232:ILE:HB	1.93	0.50
4:T:7:SER:HA	4:T:8:PRO:C	2.32	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
1:A:217:ILE:C	1:A:218:GLU:HG2	2.32	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
2:P:9:PHE:CD2	2:P:9:PHE:C	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: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
1:C:315:LYS:NZ	6:C:508:HOH:O	2.41	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
3:X:76:THR:O	3:X:77:SER:C	2.48	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: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:193:ALA:HB2	4:K:208:SER:HB3	1.96	0.47
4:K:77:SER:OG	6:K:301:HOH:O	2.21	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:X:142:SER:N	3:X:146:THR:HG1	2.14	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:N	3:G:212:ASN:OD1	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
4:T:33:LEU:HD22	4:T:71:PHE:CG	2.52	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
2:F:117:LYS:NZ	6:F:302:HOH:O	2.50	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:C:175:ASP:OD1	1:C:239:PRO:HD3	2.17	0.44
1:E:195:TYR:C	1:E:196:VAL:CG1	2.85	0.44
4:I:50:TYR:O	4:I:51:ALA:HB3	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:HA	4:L:78:LEU:HD12	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
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:HA	2:D:58:LYS:HD2	1.66	0.43
4:Y:183:LYS:HE2	4:Y:187:GLU:OE2	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:M:220:ARG:HD2	1:Q:210:GLN:OE1	2.18	0.43
1:A:288:ILE:CD1	1:A:295:GLN:HG3	2.48	0.43
3:G:2:VAL:HG12	3:G:117:PRO:HG3	2.01	0.43
3:H:50:TRP:CH2	3:H:52:SER:HB2	2.53	0.43
3:S:112:PHE:HA	3:S:114:TRP:CE2	2.53	0.43
3:S:12:LYS:O	3:S:126:VAL:HA	2.18	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:O:29:ILE:HD11	2:P:102:LEU:HD23	2.01	0.43
3:S:146:THR:HG22	3:S:147:SER:H	1.83	0.43
3:S:50:TRP:CH2	3:S:52:SER:HB2	2.54	0.43
4:V:147:GLN:OE1	4:V:154:LEU:CD1	2.65	0.43
3:X:87:ARG:HB2	3:X:87:ARG:HE	1.67	0.43
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
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:HA	3:U:224:LYS:HD2	1.83	0.43
2:N:8:GLY:N	2:N:137:CYS:SG	2.92	0.43
2:B:115:MET:HB2	2:B:115:MET:HE2	1.90	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:36:TYR:OH	4:L:89:GLN:NE2	2.52	0.42
1:A:295:GLN:HB2	1:A:306:PRO:HB2	2.01	0.42
1:A:18:HIS:CE1	1:A:37:THR:HG21	2.55	0.42
3:U:64:PHE:HB3	3:U:68:VAL:HG23	2.02	0.42
3:X:148:GLY:C	3:X:201:SER:HG	2.19	0.42
3:X:230:SER:O	3:X:231:CYS:CB	2.67	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:R:150:GLU:OE1	6:R:301:HOH:O	2.21	0.42
3:S:145:SER:C	3:S:147:SER:N	2.73	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:HD3	3:J:229:LYS:HA	1.60	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
2:R:38:LEU:HD22	3:X:54:TYR:CZ	2.55	0.42
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
3:U:51:ILE:HB	3:U:70:MET:HE2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HB3	4:L:90:GLN:HE21	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
2:B:22:TYR:HD1	2:B:115:MET:HE1	1.85	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: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
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:G:146:THR:HG22	3:G:147:SER:HG	1.81	0.41
3:H:101:LYS:HG3	3:H:102:GLN:N	2.35	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
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
2:R:56:ILE:HA	2:R:56:ILE:HD12	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
3:H:141:PRO:O	3:H:142:SER:CB	2.70	0.40
1:Q:192:THR:O	1:Q:195:TYR:O	2.39	0.40
3:S:145:SER:C	3:S:147:SER:H	2.24	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 sym-

metry 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 (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	318/320 (99%)	306 (96%)	11 (4%)	1 (0%)	41	61
1	C	317/320 (99%)	308 (97%)	8 (2%)	1 (0%)	41	61
1	E	316/320 (99%)	306 (97%)	9 (3%)	1 (0%)	41	61
1	M	316/320 (99%)	306 (97%)	9 (3%)	1 (0%)	41	61
1	O	316/320 (99%)	308 (98%)	6 (2%)	2 (1%)	25	43
1	Q	316/320 (99%)	307 (97%)	8 (2%)	1 (0%)	41	61
2	B	166/170 (98%)	160 (96%)	6 (4%)	0	100	100
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%)	34	54
3	J	229/231 (99%)	222 (97%)	7 (3%)	0	100	100
3	S	229/231 (99%)	218 (95%)	10 (4%)	1 (0%)	34	54
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	K	212/214 (99%)	207 (98%)	5 (2%)	0	100 100
4	L	212/214 (99%)	208 (98%)	3 (1%)	1 (0%)	29 48
4	T	212/214 (99%)	204 (96%)	7 (3%)	1 (0%)	29 48
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%)	47 68

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	281/282 (100%)	275 (98%)	6 (2%)	53 78
1	C	282/282 (100%)	275 (98%)	7 (2%)	47 73
1	E	281/282 (100%)	275 (98%)	6 (2%)	53 78
1	M	281/282 (100%)	280 (100%)	1 (0%)	91 97
1	O	281/282 (100%)	269 (96%)	12 (4%)	29 53
1	Q	281/282 (100%)	273 (97%)	8 (3%)	43 70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	144/146 (99%)	143 (99%)	1 (1%)	84 94
2	D	145/146 (99%)	145 (100%)	0	100 100
2	F	145/146 (99%)	144 (99%)	1 (1%)	84 94
2	N	144/146 (99%)	142 (99%)	2 (1%)	67 86
2	P	143/146 (98%)	141 (99%)	2 (1%)	67 86
2	R	144/146 (99%)	141 (98%)	3 (2%)	53 78
3	G	194/194 (100%)	172 (89%)	22 (11%)	6 11
3	H	191/194 (98%)	175 (92%)	16 (8%)	11 21
3	J	194/194 (100%)	175 (90%)	19 (10%)	8 15
3	S	194/194 (100%)	183 (94%)	11 (6%)	20 39
3	U	194/194 (100%)	188 (97%)	6 (3%)	40 67
3	X	194/194 (100%)	187 (96%)	7 (4%)	35 61
4	I	189/189 (100%)	174 (92%)	15 (8%)	12 24
4	K	189/189 (100%)	169 (89%)	20 (11%)	6 13
4	L	189/189 (100%)	169 (89%)	20 (11%)	6 13
4	T	189/189 (100%)	179 (95%)	10 (5%)	22 43
4	V	189/189 (100%)	181 (96%)	8 (4%)	30 54
4	Y	189/189 (100%)	180 (95%)	9 (5%)	25 48
All	All	4847/4866 (100%)	4635 (96%)	212 (4%)	28 52

All (212) 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	242	VAL
1	A	261	ARG
1	A	295	GLN
2	B	57	GLU
1	C	18	HIS
1	C	101	ASP
1	C	102	VAL
1	C	182	VAL
1	C	189	GLN
1	C	218	GLU

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Mol	Chain	Res	Type
1	C	297	VAL
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	164	ASP
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	187	SER
3	G	194	SER
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	101	LYS
3	H	132	LYS
3	H	147	SER
3	H	150	THR
3	H	175	THR

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Mol	Chain	Res	Type
3	H	201	SER
3	H	206	THR
3	H	208	THR
3	H	214	ASN
4	I	7	SER
4	I	9	VAL
4	I	10	SER
4	I	14	SER
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	4	LEU
3	J	22	CYS
3	J	35	SER
3	J	48	LEU
3	J	71	THR
3	J	74	THR
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	187	SER
3	J	230	SER
4	K	7	SER
4	K	8	PRO
4	K	9	VAL
4	K	27	GLN

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Mol	Chain	Res	Type
4	K	42	ARG
4	K	45	LYS
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	114	SER
4	K	142	ARG
4	K	146	VAL
4	K	163	VAL
4	K	191	VAL
4	K	197	THR
4	K	214	CYS
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
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	211	ARG
4	L	214	CYS
1	M	101	ASP
2	N	58	LYS
2	N	72	GLU
1	O	9	SER
1	O	32	ASP
1	O	101	ASP

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Mol	Chain	Res	Type
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
2	P	164	ASP
1	Q	27	LYS
1	Q	28	THR
1	Q	195	TYR
1	Q	196	VAL
1	Q	248	ASN
1	Q	295	GLN
1	Q	321	ARG
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
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	206	THR
4	T	7	SER
4	T	10	SER
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

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Mol	Chain	Res	Type
4	T	214	CYS
3	U	37	VAL
3	U	87	ARG
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	33	LEU
4	V	90	GLN
4	V	105	GLU
4	V	108	ARG
4	V	142	ARG
4	V	214	CYS
3	X	65	GLN
3	X	75	SER
3	X	87	ARG
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	33	LEU
4	Y	42	ARG
4	Y	90	GLN
4	Y	95	PRO
4	Y	107	LYS
4	Y	108	ARG
4	Y	147	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	210	GLN
2	B	12	ASN
1	C	189	GLN
1	C	210	GLN
1	E	18	HIS
1	E	33	GLN

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Mol	Chain	Res	Type
1	E	216	ASN
3	G	215	HIS
4	I	92	ASN
4	I	93	ASN
4	L	89	GLN
1	M	18	HIS
1	M	197	GLN
1	O	18	HIS
1	O	210	GLN
2	P	12	ASN
2	P	65	GLN
1	Q	18	HIS
4	T	79	GLN
4	V	90	GLN
3	X	65	GLN
4	Y	53	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	P	201	2	14,14,15	0.23	0	17,19,21	0.45	0
5	NAG	E	404	1	14,14,15	0.33	0	17,19,21	0.36	0
5	NAG	M	401	1	14,14,15	0.48	0	17,19,21	0.52	0
5	NAG	D	201	2	14,14,15	0.19	0	17,19,21	0.39	0
5	NAG	A	405	1	14,14,15	0.23	0	17,19,21	0.33	0
5	NAG	M	404	1	14,14,15	0.27	0	17,19,21	0.35	0
5	NAG	O	404	1	14,14,15	0.26	0	17,19,21	0.35	0
5	NAG	C	403	1	14,14,15	1.19	1 (7%)	17,19,21	1.15	3 (17%)
5	NAG	Q	403	1	14,14,15	0.17	0	17,19,21	0.40	0
5	NAG	O	402	1	14,14,15	0.38	0	17,19,21	0.45	0
5	NAG	M	402	1	14,14,15	0.42	0	17,19,21	0.51	0
5	NAG	M	403	1	14,14,15	0.98	1 (7%)	17,19,21	1.24	1 (5%)
5	NAG	A	402	1	14,14,15	0.33	0	17,19,21	0.39	0
5	NAG	Q	405	1	14,14,15	0.20	0	17,19,21	0.39	0
5	NAG	N	201	2	14,14,15	0.20	0	17,19,21	0.41	0
5	NAG	Q	401	1	14,14,15	0.32	0	17,19,21	0.34	0
5	NAG	M	405	1	14,14,15	0.23	0	17,19,21	0.43	0
5	NAG	F	201	2	14,14,15	0.20	0	17,19,21	0.47	0
5	NAG	E	405	1	14,14,15	0.23	0	17,19,21	0.45	0
5	NAG	B	201	2	14,14,15	0.27	0	17,19,21	0.36	0
5	NAG	O	405	1	14,14,15	0.28	0	17,19,21	0.37	0
5	NAG	C	402	1	14,14,15	0.40	0	17,19,21	0.49	0
5	NAG	Q	404	1	14,14,15	0.29	0	17,19,21	0.40	0
5	NAG	C	401	1	14,14,15	0.41	0	17,19,21	0.51	0
5	NAG	E	402	1	14,14,15	0.30	0	17,19,21	0.36	0
5	NAG	E	403	1	14,14,15	0.18	0	17,19,21	0.41	0
5	NAG	R	201	2	14,14,15	0.17	0	17,19,21	0.51	0
5	NAG	O	401	1	14,14,15	0.26	0	17,19,21	0.42	0
5	NAG	Q	402	1	14,14,15	0.34	0	17,19,21	0.48	0
5	NAG	A	404	1	14,14,15	0.45	0	17,19,21	0.68	1 (5%)
5	NAG	A	403	1	14,14,15	0.23	0	17,19,21	0.45	0
5	NAG	C	404	1	14,14,15	0.25	0	17,19,21	0.37	0
5	NAG	C	405	1	14,14,15	0.21	0	17,19,21	0.35	0
5	NAG	A	401	1	14,14,15	0.19	0	17,19,21	0.69	1 (5%)
5	NAG	E	401	1	14,14,15	0.38	0	17,19,21	0.59	0
5	NAG	O	403	1	14,14,15	0.20	0	17,19,21	0.52	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	P	201	2	-	0/6/23/26	0/1/1/1
5	NAG	E	404	1	-	0/6/23/26	0/1/1/1
5	NAG	M	401	1	-	0/6/23/26	0/1/1/1
5	NAG	D	201	2	-	0/6/23/26	0/1/1/1
5	NAG	A	405	1	-	0/6/23/26	0/1/1/1
5	NAG	M	404	1	-	2/6/23/26	0/1/1/1
5	NAG	O	404	1	-	0/6/23/26	0/1/1/1
5	NAG	C	403	1	-	2/6/23/26	0/1/1/1
5	NAG	Q	403	1	-	0/6/23/26	0/1/1/1
5	NAG	O	402	1	-	2/6/23/26	0/1/1/1
5	NAG	M	402	1	-	2/6/23/26	0/1/1/1
5	NAG	M	403	1	-	1/6/23/26	0/1/1/1
5	NAG	A	402	1	-	2/6/23/26	0/1/1/1
5	NAG	Q	405	1	-	0/6/23/26	0/1/1/1
5	NAG	N	201	2	-	0/6/23/26	0/1/1/1
5	NAG	Q	401	1	-	2/6/23/26	0/1/1/1
5	NAG	M	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	E	405	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	405	1	-	0/6/23/26	0/1/1/1
5	NAG	C	402	1	-	2/6/23/26	0/1/1/1
5	NAG	Q	404	1	-	0/6/23/26	0/1/1/1
5	NAG	C	401	1	-	2/6/23/26	0/1/1/1
5	NAG	E	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	R	201	2	-	0/6/23/26	0/1/1/1
5	NAG	O	401	1	-	2/6/23/26	0/1/1/1
5	NAG	Q	402	1	-	2/6/23/26	0/1/1/1
5	NAG	A	404	1	-	2/6/23/26	0/1/1/1
5	NAG	A	403	1	-	1/6/23/26	0/1/1/1
5	NAG	C	404	1	-	1/6/23/26	0/1/1/1
5	NAG	C	405	1	-	0/6/23/26	0/1/1/1
5	NAG	A	401	1	-	0/6/23/26	0/1/1/1
5	NAG	E	401	1	-	1/6/23/26	0/1/1/1
5	NAG	O	403	1	-	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	C	403	NAG	C1-C2	3.93	1.58	1.52
5	M	403	NAG	O5-C1	3.44	1.49	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	403	NAG	C1-O5-C5	4.85	118.77	112.19
5	C	403	NAG	C1-O5-C5	2.83	116.03	112.19
5	A	404	NAG	C1-O5-C5	2.22	115.20	112.19
5	C	403	NAG	O5-C5-C4	-2.22	105.44	110.83
5	C	403	NAG	C4-C3-C2	2.17	114.20	111.02
5	A	401	NAG	C1-O5-C5	2.16	115.12	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
5	O	402	NAG	O5-C5-C6-O6
5	M	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	C	403	NAG	O5-C5-C6-O6
5	Q	402	NAG	C4-C5-C6-O6
5	C	402	NAG	O5-C5-C6-O6
5	O	402	NAG	C4-C5-C6-O6
5	C	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	A	404	NAG	O5-C5-C6-O6
5	E	402	NAG	C4-C5-C6-O6
5	C	403	NAG	C4-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

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Mol	Chain	Res	Type	Atoms
5	E	403	NAG	C4-C5-C6-O6
5	A	403	NAG	O5-C5-C6-O6
5	M	404	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	M	401	NAG	1	0
5	C	403	NAG	1	0
5	C	405	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	-0.42	1 (0%) 94 94	27, 38, 64, 120	0
1	C	319/320 (99%)	-0.42	0 100 100	27, 43, 68, 109	1 (0%)
1	E	318/320 (99%)	-0.35	1 (0%) 94 94	33, 50, 79, 106	0
1	M	318/320 (99%)	-0.38	2 (0%) 89 90	30, 43, 72, 124	2 (0%)
1	O	318/320 (99%)	-0.26	1 (0%) 94 94	36, 53, 87, 134	1 (0%)
1	Q	318/320 (99%)	-0.39	0 100 100	31, 44, 66, 102	2 (0%)
2	B	168/170 (98%)	-0.11	2 (1%) 79 80	28, 45, 70, 161	2 (1%)
2	D	169/170 (99%)	-0.13	2 (1%) 79 80	28, 47, 72, 167	0
2	F	168/170 (98%)	-0.22	0 100 100	31, 46, 65, 131	2 (1%)
2	N	169/170 (99%)	0.04	6 (3%) 42 46	32, 69, 105, 139	2 (1%)
2	P	163/170 (95%)	-0.01	3 (1%) 68 71	31, 64, 101, 148	2 (1%)
2	R	167/170 (98%)	-0.16	3 (1%) 68 71	30, 55, 98, 122	0
3	G	231/231 (100%)	0.57	44 (19%) 1 1	35, 78, 164, 266	0
3	H	228/231 (98%)	-0.35	1 (0%) 92 93	28, 52, 86, 142	0
3	J	231/231 (100%)	0.43	30 (12%) 3 3	35, 77, 166, 268	1 (0%)
3	S	231/231 (100%)	0.87	44 (19%) 1 1	51, 94, 161, 280	0
3	U	231/231 (100%)	-0.20	5 (2%) 62 65	33, 54, 88, 174	0
3	X	231/231 (100%)	-0.22	7 (3%) 50 53	35, 57, 100, 201	0
4	I	214/214 (100%)	0.26	25 (11%) 4 4	34, 74, 161, 221	1 (0%)
4	K	214/214 (100%)	0.07	10 (4%) 31 33	33, 79, 114, 187	0
4	L	214/214 (100%)	-0.24	1 (0%) 91 91	25, 52, 105, 163	0
4	T	214/214 (100%)	0.50	31 (14%) 2 2	24, 83, 169, 223	2 (0%)
4	V	214/214 (100%)	-0.24	1 (0%) 91 91	24, 51, 79, 153	0
4	Y	214/214 (100%)	-0.27	0 100 100	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%)	-0.10	220 (3%) 39 42	24, 53, 125, 280	19 (0%)

All (220) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	T	214	CYS	11.1
3	J	148	GLY	10.9
3	G	204	LEU	10.7
3	S	146	THR	9.5
3	J	231	CYS	8.8
3	S	222	VAL	8.1
3	J	144	LYS	7.7
3	S	231	CYS	7.2
3	S	230	SER	7.1
4	L	214	CYS	7.1
3	J	147	SER	7.1
4	I	214	CYS	6.9
3	G	146	THR	6.8
3	U	147	SER	6.5
3	G	206	THR	6.3
3	J	146	THR	6.1
3	J	145	SER	6.1
3	X	148	GLY	6.0
3	U	146	THR	6.0
3	G	205	GLY	6.0
3	G	135	SER	5.6
4	K	214	CYS	5.6
3	S	145	SER	5.6
2	D	3	PHE	5.3
3	U	231	CYS	5.3
3	J	229	LYS	5.2
4	K	126	LYS	5.2
4	T	193	ALA	5.0
3	G	209	TYR	4.8
2	R	171	PHE	4.8
3	S	223	ASP	4.7
3	G	144	LYS	4.7
4	T	192	TYR	4.6
2	R	5	ALA	4.6
3	H	231	CYS	4.6
3	X	146	THR	4.5
3	X	147	SER	4.5

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Mol	Chain	Res	Type	RSRZ
3	G	231	CYS	4.4
3	S	143	SER	4.4
4	T	212	GLY	4.4
3	X	143	SER	4.4
4	T	116	PHE	4.3
2	P	171	PHE	4.3
3	X	142	SER	4.3
3	J	169	TRP	4.2
3	S	211	CYS	4.2
3	S	220	THR	4.1
4	I	132	VAL	4.0
2	N	29	SER	4.0
3	G	153	LEU	4.0
4	I	192	TYR	4.0
3	S	144	LYS	3.9
3	J	222	VAL	3.9
3	G	208	THR	3.9
4	T	213	GLU	3.9
3	S	221	LYS	3.9
3	S	225	LYS	3.9
3	S	142	SER	3.9
3	U	230	SER	3.9
3	S	169	TRP	3.9
3	S	209	TYR	3.9
4	T	209	PHE	3.9
3	S	228	PRO	3.9
3	S	210	ILE	3.9
3	G	151	ALA	3.8
3	G	210	ILE	3.8
3	S	205	GLY	3.8
3	J	226	VAL	3.8
4	T	127	SER	3.8
3	J	174	LEU	3.7
3	G	145	SER	3.7
4	V	214	CYS	3.7
4	T	151	ASP	3.7
3	X	144	LYS	3.6
2	B	4	GLY	3.6
3	S	204	LEU	3.6
4	I	130	ALA	3.6
4	I	184	ALA	3.6
4	T	150	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
4	I	122	ASP	3.5
4	T	154	LEU	3.5
3	S	226	VAL	3.5
3	G	147	SER	3.5
3	J	216	LYS	3.5
3	G	217	PRO	3.5
3	G	214	ASN	3.5
4	T	191	VAL	3.4
3	S	138	PRO	3.4
4	I	213	GLU	3.4
3	J	149	GLY	3.3
4	T	125	LEU	3.3
4	I	154	LEU	3.3
3	J	211	CYS	3.2
4	T	210	ASN	3.2
3	S	173	ALA	3.2
3	G	227	GLU	3.2
3	S	224	LYS	3.2
3	S	199	VAL	3.2
3	G	230	SER	3.2
4	T	115	VAL	3.2
3	S	148	GLY	3.2
3	S	214	ASN	3.2
3	G	207	GLN	3.1
1	M	10	THR	3.1
3	S	208	THR	3.1
4	T	146	VAL	3.1
2	P	141	TYR	3.1
4	T	190	LYS	3.1
3	G	213	VAL	3.1
4	K	212	GLY	3.1
3	S	229	LYS	3.1
4	I	190	LYS	3.1
3	G	229	LYS	3.1
3	J	224	LYS	3.1
3	J	225	LYS	3.1
3	S	149	GLY	3.1
3	J	208	THR	3.1
3	G	165	VAL	3.0
3	G	223	ASP	3.0
4	I	152	ASN	3.0
3	G	221	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
4	I	193	ALA	3.0
3	G	200	PRO	3.0
3	J	204	LEU	3.0
4	I	191	VAL	3.0
3	G	148	GLY	3.0
4	I	150	VAL	2.9
4	K	213	GLU	2.9
4	I	126	LYS	2.9
4	T	148	TRP	2.9
2	R	168	ASN	2.9
3	G	215	HIS	2.8
3	S	206	THR	2.8
4	I	211	ARG	2.8
3	G	157	VAL	2.8
4	I	145	LYS	2.7
3	S	203	SER	2.7
3	J	209	TYR	2.7
4	K	127	SER	2.7
2	P	140	ILE	2.7
3	J	202	SER	2.7
4	I	186	TYR	2.7
3	X	145	SER	2.7
3	J	217	PRO	2.7
3	G	152	ALA	2.6
3	J	143	SER	2.6
3	S	212	ASN	2.6
4	T	118	PHE	2.6
4	T	121	SER	2.6
3	S	219	ASN	2.6
2	N	143	LYS	2.6
4	T	208	SER	2.6
4	I	125	LEU	2.6
4	I	155	GLN	2.6
4	T	126	LYS	2.6
2	N	4	GLY	2.5
3	S	147	SER	2.5
3	G	169	TRP	2.5
4	T	120	PRO	2.5
2	N	161	VAL	2.5
3	J	155	CYS	2.5
4	T	206	THR	2.5
3	G	190	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
3	G	199	VAL	2.5
3	S	136	VAL	2.5
4	T	135	LEU	2.4
4	T	122	ASP	2.4
4	I	147	GLN	2.4
3	G	167	VAL	2.4
2	N	141	TYR	2.4
1	M	8	ASN	2.4
2	D	4	GLY	2.4
2	B	5	ALA	2.4
1	E	222	TRP	2.4
3	J	227	GLU	2.4
3	J	167	VAL	2.4
4	T	149	LYS	2.4
4	I	212	GLY	2.4
3	G	220	THR	2.4
3	G	142	SER	2.4
3	G	170	ASN	2.3
3	S	140	ALA	2.3
4	K	183	LYS	2.3
4	T	152	ASN	2.3
4	I	146	VAL	2.3
3	S	217	PRO	2.3
4	T	181	LEU	2.3
3	J	166	THR	2.2
3	S	215	HIS	2.2
3	G	228	PRO	2.2
4	T	205	VAL	2.2
3	G	136	VAL	2.2
3	S	202	SER	2.2
3	G	139	LEU	2.2
4	K	125	LEU	2.2
3	J	156	LEU	2.2
4	I	158	ASN	2.2
4	K	106	ILE	2.2
4	T	136	LEU	2.2
3	G	143	SER	2.2
3	J	230	SER	2.2
4	I	189	HIS	2.1
3	J	228	PRO	2.1
1	A	10	THR	2.1
3	G	173	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
3	S	196	VAL	2.1
4	I	196	VAL	2.1
3	U	144	LYS	2.1
4	K	122	ASP	2.1
3	G	1	GLN	2.1
3	G	222	VAL	2.1
3	G	224	LYS	2.1
2	N	167	LEU	2.1
3	S	166	THR	2.1
3	S	171	SER	2.1
3	S	216	LYS	2.0
3	S	165	VAL	2.0
4	K	129	THR	2.0
3	J	213	VAL	2.0
1	O	218	GLU	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	C	401	14/15	0.43	0.72	144,160,163,163	0
5	NAG	E	401	14/15	0.53	0.45	144,157,161,163	0
5	NAG	O	401	14/15	0.59	0.65	149,162,172,172	0
5	NAG	A	401	14/15	0.61	0.61	143,153,161,163	0
5	NAG	C	403	14/15	0.73	0.27	105,118,126,127	0
5	NAG	Q	401	14/15	0.74	0.59	138,157,160,161	0
5	NAG	A	404	14/15	0.74	0.24	93,112,127,130	0
5	NAG	M	401	14/15	0.75	0.57	142,162,166,166	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	M	404	14/15	0.82	0.21	93,104,108,110	0
5	NAG	M	403	14/15	0.83	0.23	95,104,111,111	0
5	NAG	Q	404	14/15	0.84	0.24	102,123,131,135	0
5	NAG	O	404	14/15	0.84	0.18	93,109,116,121	0
5	NAG	O	402	14/15	0.86	0.17	80,99,106,109	0
5	NAG	A	403	14/15	0.86	0.28	78,94,104,106	0
5	NAG	Q	403	14/15	0.87	0.26	86,95,107,113	0
5	NAG	Q	402	14/15	0.87	0.18	81,93,105,110	0
5	NAG	P	201	14/15	0.87	0.23	79,93,96,100	0
5	NAG	C	404	14/15	0.88	0.34	104,126,132,137	0
5	NAG	A	402	14/15	0.89	0.23	76,87,92,97	0
5	NAG	E	404	14/15	0.90	0.17	89,105,123,129	0
5	NAG	R	201	14/15	0.91	0.18	87,101,112,118	0
5	NAG	N	201	14/15	0.92	0.17	83,94,99,105	0
5	NAG	E	402	14/15	0.92	0.18	72,82,91,92	0
5	NAG	A	405	14/15	0.92	0.13	56,67,76,83	0
5	NAG	C	402	14/15	0.92	0.17	65,77,83,93	0
5	NAG	M	402	14/15	0.92	0.12	77,88,91,92	0
5	NAG	M	405	14/15	0.93	0.18	59,72,86,86	0
5	NAG	C	405	14/15	0.93	0.17	64,69,85,86	0
5	NAG	D	201	14/15	0.94	0.15	52,67,75,78	0
5	NAG	B	201	14/15	0.94	0.12	52,62,73,85	0
5	NAG	O	405	14/15	0.94	0.13	59,75,87,88	0
5	NAG	Q	405	14/15	0.94	0.19	62,76,87,97	0
5	NAG	E	403	14/15	0.95	0.18	57,72,79,82	0
5	NAG	E	405	14/15	0.95	0.10	49,62,70,76	0
5	NAG	O	403	14/15	0.96	0.17	53,62,70,72	0
5	NAG	F	201	14/15	0.97	0.08	48,66,72,75	0

6.5 Other polymers (i)

There are no such residues in this entry.