



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:53 PM GMT

PDB ID : 4GEZ
Title : Structure of a neuraminidase-like protein from A/bat/Guatemala/164/2009
Authors : Yang, H.; Carney, P.J.; Donis, R.O.; Stevens, J.
Deposited on : 2012-08-02
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

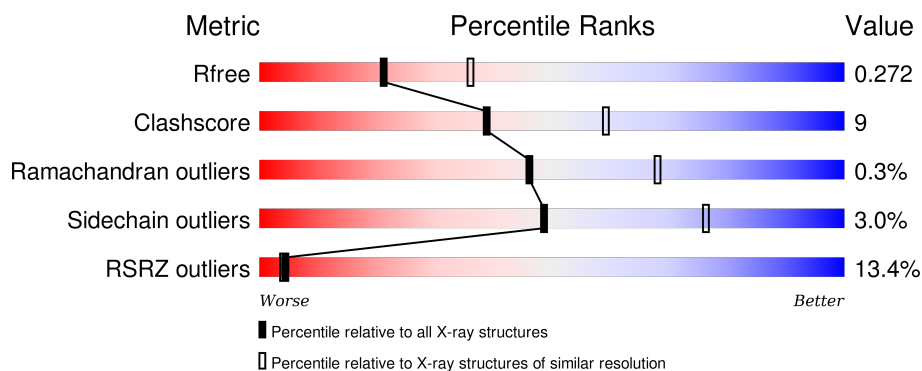
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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. 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	378	<div> <div>7%</div> <div>76%</div> <div>20%</div> <div>..</div> </div>
1	B	378	<div> <div>3%</div> <div>75%</div> <div>20%</div> <div>..</div> </div>
1	C	378	<div> <div>7%</div> <div>79%</div> <div>16%</div> <div>..</div> </div>
1	D	378	<div> <div>10%</div> <div>72%</div> <div>22%</div> <div>..</div> </div>
1	E	378	<div> <div>7%</div> <div>78%</div> <div>17%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	378	
1	G	378	
1	H	378	
1	I	378	
1	J	378	
1	K	378	
1	L	378	

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
3	NAG	A	503	-	-	-	X
4	FUC	I	504	-	-	-	X
6	FUC	D	505	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 35035 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 Neuraminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	365	Total	C	N	O	S	0	0	0
			2858	1804	487	547	20			
1	B	365	Total	C	N	O	S	0	0	0
			2858	1804	487	547	20			
1	C	365	Total	C	N	O	S	0	0	0
			2858	1804	487	547	20			
1	D	365	Total	C	N	O	S	0	0	0
			2858	1804	487	547	20			
1	E	365	Total	C	N	O	S	0	0	0
			2858	1804	487	547	20			
1	F	365	Total	C	N	O	S	0	0	0
			2858	1804	487	547	20			
1	G	365	Total	C	N	O	S	0	0	0
			2858	1804	487	547	20			
1	H	365	Total	C	N	O	S	0	0	0
			2858	1804	487	547	20			
1	I	365	Total	C	N	O	S	0	0	0
			2858	1804	487	547	20			
1	J	363	Total	C	N	O	S	0	0	0
			2832	1784	484	544	20			
1	K	364	Total	C	N	O	S	0	0	0
			2846	1795	486	545	20			
1	L	365	Total	C	N	O	S	0	0	0
			2858	1804	487	547	20			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	65	GLY	-	EXPRESSION TAG	UNP H6QM85
A	66	SER	-	EXPRESSION TAG	UNP H6QM85
A	67	GLY	-	EXPRESSION TAG	UNP H6QM85
A	68	ASP	-	EXPRESSION TAG	UNP H6QM85
A	69	SER	-	EXPRESSION TAG	UNP H6QM85

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Chain	Residue	Modelled	Actual	Comment	Reference
A	70	GLY	-	EXPRESSION TAG	UNP H6QM85
A	71	SER	-	EXPRESSION TAG	UNP H6QM85
A	72	PRO	-	EXPRESSION TAG	UNP H6QM85
A	73	GLY	-	EXPRESSION TAG	UNP H6QM85
B	65	GLY	-	EXPRESSION TAG	UNP H6QM85
B	66	SER	-	EXPRESSION TAG	UNP H6QM85
B	67	GLY	-	EXPRESSION TAG	UNP H6QM85
B	68	ASP	-	EXPRESSION TAG	UNP H6QM85
B	69	SER	-	EXPRESSION TAG	UNP H6QM85
B	70	GLY	-	EXPRESSION TAG	UNP H6QM85
B	71	SER	-	EXPRESSION TAG	UNP H6QM85
B	72	PRO	-	EXPRESSION TAG	UNP H6QM85
B	73	GLY	-	EXPRESSION TAG	UNP H6QM85
C	65	GLY	-	EXPRESSION TAG	UNP H6QM85
C	66	SER	-	EXPRESSION TAG	UNP H6QM85
C	67	GLY	-	EXPRESSION TAG	UNP H6QM85
C	68	ASP	-	EXPRESSION TAG	UNP H6QM85
C	69	SER	-	EXPRESSION TAG	UNP H6QM85
C	70	GLY	-	EXPRESSION TAG	UNP H6QM85
C	71	SER	-	EXPRESSION TAG	UNP H6QM85
C	72	PRO	-	EXPRESSION TAG	UNP H6QM85
C	73	GLY	-	EXPRESSION TAG	UNP H6QM85
D	65	GLY	-	EXPRESSION TAG	UNP H6QM85
D	66	SER	-	EXPRESSION TAG	UNP H6QM85
D	67	GLY	-	EXPRESSION TAG	UNP H6QM85
D	68	ASP	-	EXPRESSION TAG	UNP H6QM85
D	69	SER	-	EXPRESSION TAG	UNP H6QM85
D	70	GLY	-	EXPRESSION TAG	UNP H6QM85
D	71	SER	-	EXPRESSION TAG	UNP H6QM85
D	72	PRO	-	EXPRESSION TAG	UNP H6QM85
D	73	GLY	-	EXPRESSION TAG	UNP H6QM85
E	65	GLY	-	EXPRESSION TAG	UNP H6QM85
E	66	SER	-	EXPRESSION TAG	UNP H6QM85
E	67	GLY	-	EXPRESSION TAG	UNP H6QM85
E	68	ASP	-	EXPRESSION TAG	UNP H6QM85
E	69	SER	-	EXPRESSION TAG	UNP H6QM85
E	70	GLY	-	EXPRESSION TAG	UNP H6QM85
E	71	SER	-	EXPRESSION TAG	UNP H6QM85
E	72	PRO	-	EXPRESSION TAG	UNP H6QM85
E	73	GLY	-	EXPRESSION TAG	UNP H6QM85
F	65	GLY	-	EXPRESSION TAG	UNP H6QM85
F	66	SER	-	EXPRESSION TAG	UNP H6QM85

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Chain	Residue	Modelled	Actual	Comment	Reference
F	67	GLY	-	EXPRESSION TAG	UNP H6QM85
F	68	ASP	-	EXPRESSION TAG	UNP H6QM85
F	69	SER	-	EXPRESSION TAG	UNP H6QM85
F	70	GLY	-	EXPRESSION TAG	UNP H6QM85
F	71	SER	-	EXPRESSION TAG	UNP H6QM85
F	72	PRO	-	EXPRESSION TAG	UNP H6QM85
F	73	GLY	-	EXPRESSION TAG	UNP H6QM85
G	65	GLY	-	EXPRESSION TAG	UNP H6QM85
G	66	SER	-	EXPRESSION TAG	UNP H6QM85
G	67	GLY	-	EXPRESSION TAG	UNP H6QM85
G	68	ASP	-	EXPRESSION TAG	UNP H6QM85
G	69	SER	-	EXPRESSION TAG	UNP H6QM85
G	70	GLY	-	EXPRESSION TAG	UNP H6QM85
G	71	SER	-	EXPRESSION TAG	UNP H6QM85
G	72	PRO	-	EXPRESSION TAG	UNP H6QM85
G	73	GLY	-	EXPRESSION TAG	UNP H6QM85
H	65	GLY	-	EXPRESSION TAG	UNP H6QM85
H	66	SER	-	EXPRESSION TAG	UNP H6QM85
H	67	GLY	-	EXPRESSION TAG	UNP H6QM85
H	68	ASP	-	EXPRESSION TAG	UNP H6QM85
H	69	SER	-	EXPRESSION TAG	UNP H6QM85
H	70	GLY	-	EXPRESSION TAG	UNP H6QM85
H	71	SER	-	EXPRESSION TAG	UNP H6QM85
H	72	PRO	-	EXPRESSION TAG	UNP H6QM85
H	73	GLY	-	EXPRESSION TAG	UNP H6QM85
I	65	GLY	-	EXPRESSION TAG	UNP H6QM85
I	66	SER	-	EXPRESSION TAG	UNP H6QM85
I	67	GLY	-	EXPRESSION TAG	UNP H6QM85
I	68	ASP	-	EXPRESSION TAG	UNP H6QM85
I	69	SER	-	EXPRESSION TAG	UNP H6QM85
I	70	GLY	-	EXPRESSION TAG	UNP H6QM85
I	71	SER	-	EXPRESSION TAG	UNP H6QM85
I	72	PRO	-	EXPRESSION TAG	UNP H6QM85
I	73	GLY	-	EXPRESSION TAG	UNP H6QM85
J	65	GLY	-	EXPRESSION TAG	UNP H6QM85
J	66	SER	-	EXPRESSION TAG	UNP H6QM85
J	67	GLY	-	EXPRESSION TAG	UNP H6QM85
J	68	ASP	-	EXPRESSION TAG	UNP H6QM85
J	69	SER	-	EXPRESSION TAG	UNP H6QM85
J	70	GLY	-	EXPRESSION TAG	UNP H6QM85
J	71	SER	-	EXPRESSION TAG	UNP H6QM85
J	72	PRO	-	EXPRESSION TAG	UNP H6QM85

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Chain	Residue	Modelled	Actual	Comment	Reference
J	73	GLY	-	EXPRESSION TAG	UNP H6QM85
K	65	GLY	-	EXPRESSION TAG	UNP H6QM85
K	66	SER	-	EXPRESSION TAG	UNP H6QM85
K	67	GLY	-	EXPRESSION TAG	UNP H6QM85
K	68	ASP	-	EXPRESSION TAG	UNP H6QM85
K	69	SER	-	EXPRESSION TAG	UNP H6QM85
K	70	GLY	-	EXPRESSION TAG	UNP H6QM85
K	71	SER	-	EXPRESSION TAG	UNP H6QM85
K	72	PRO	-	EXPRESSION TAG	UNP H6QM85
K	73	GLY	-	EXPRESSION TAG	UNP H6QM85
L	65	GLY	-	EXPRESSION TAG	UNP H6QM85
L	66	SER	-	EXPRESSION TAG	UNP H6QM85
L	67	GLY	-	EXPRESSION TAG	UNP H6QM85
L	68	ASP	-	EXPRESSION TAG	UNP H6QM85
L	69	SER	-	EXPRESSION TAG	UNP H6QM85
L	70	GLY	-	EXPRESSION TAG	UNP H6QM85
L	71	SER	-	EXPRESSION TAG	UNP H6QM85
L	72	PRO	-	EXPRESSION TAG	UNP H6QM85
L	73	GLY	-	EXPRESSION TAG	UNP H6QM85

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

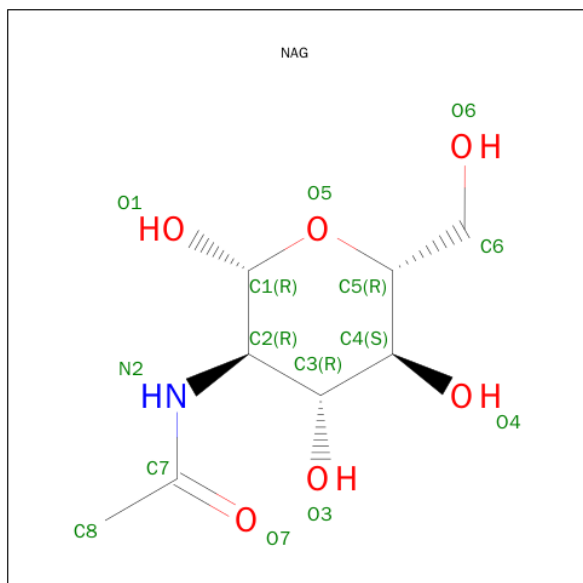
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Ca 1 1	0	0
2	J	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0
2	K	1	Total Ca 1 1	0	0
2	E	1	Total Ca 1 1	0	0
2	H	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0
2	I	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0
2	A	1	Total Ca 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	L	1	Total	Ca	0	0
			1	1		
2	F	1	Total	Ca	0	0
			1	1		

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	G	1	Total	C	N	O	0	0
			14	8	1	5		
3	H	1	Total	C	N	O	0	0
			14	8	1	5		
3	I	1	Total	C	N	O	0	0
			14	8	1	5		
3	K	1	Total	C	N	O	0	0
			14	8	1	5		
3	L	1	Total	C	N	O	0	0
			14	8	1	5		

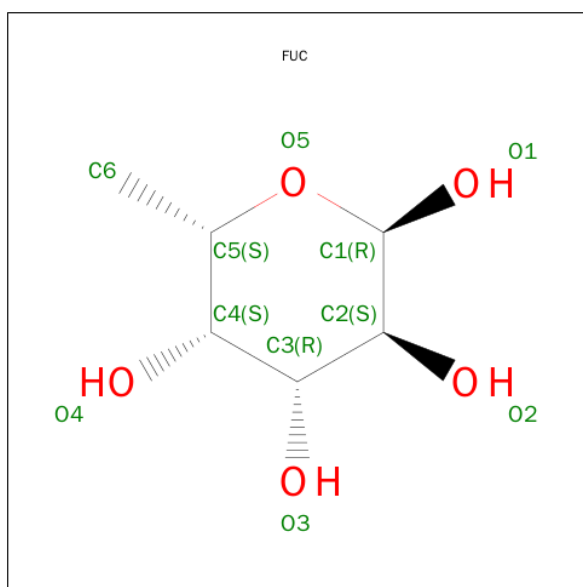
- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			24	14	1	9		
4	E	2	Total	C	N	O	0	0
			24	14	1	9		
4	I	2	Total	C	N	O	0	0
			24	14	1	9		

- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	3	Total	C	N	O	0	0
			38	22	2	14		
5	F	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 6 is SUGAR (ALPHA-L-FUCOSE) (three-letter code: FUC) (formula: C₆H₁₂O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	55	Total	O	0	0
			55	55		
7	B	54	Total	O	0	0
			54	54		
7	C	45	Total	O	0	0
			45	45		
7	D	46	Total	O	0	0
			46	46		
7	E	60	Total	O	0	0
			60	60		
7	F	41	Total	O	0	0
			41	41		
7	G	31	Total	O	0	0
			31	31		
7	H	15	Total	O	0	0
			15	15		
7	I	14	Total	O	0	0
			14	14		
7	J	25	Total	O	0	0
			25	25		
7	K	17	Total	O	0	0
			17	17		

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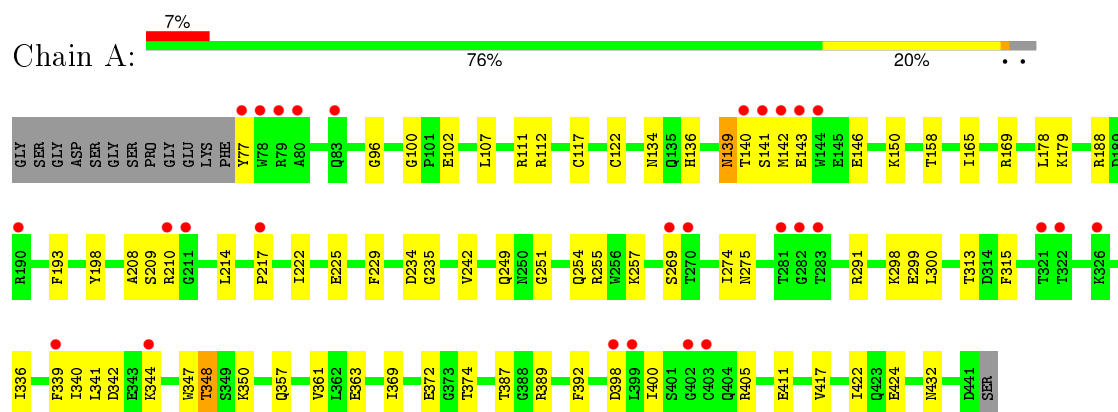
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	L	8	Total	O	0	0
			8	8		

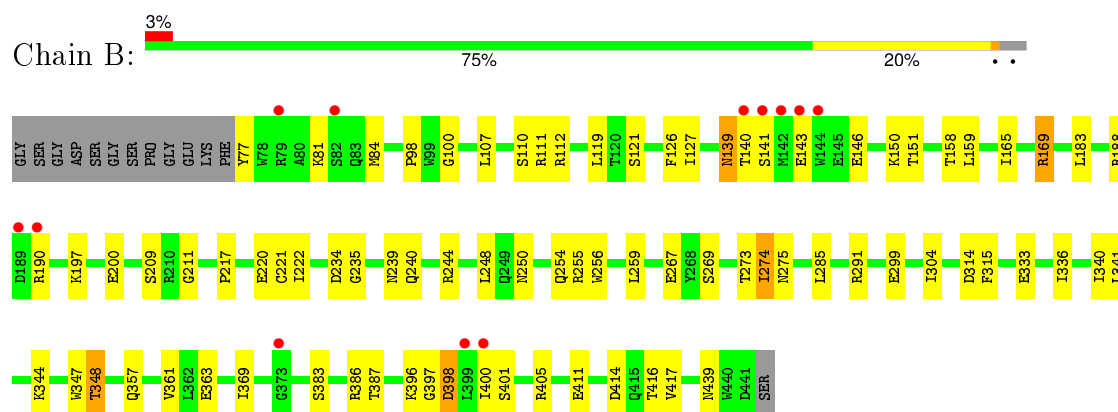
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

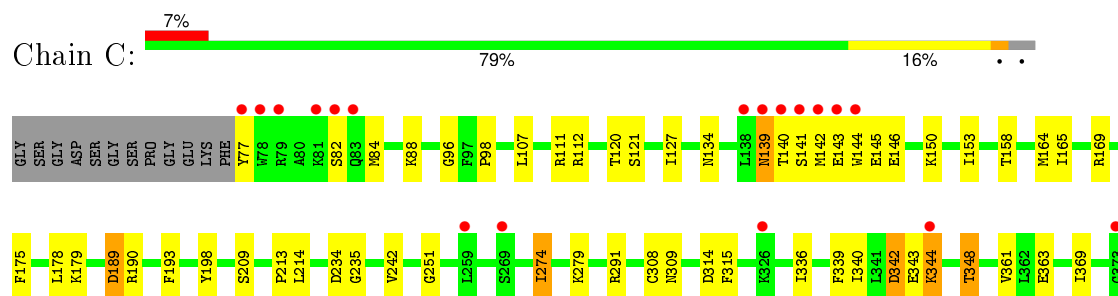
• Molecule 1: Neuraminidase

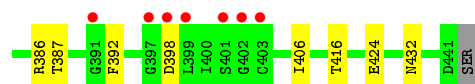


• Molecule 1: Neuraminidase

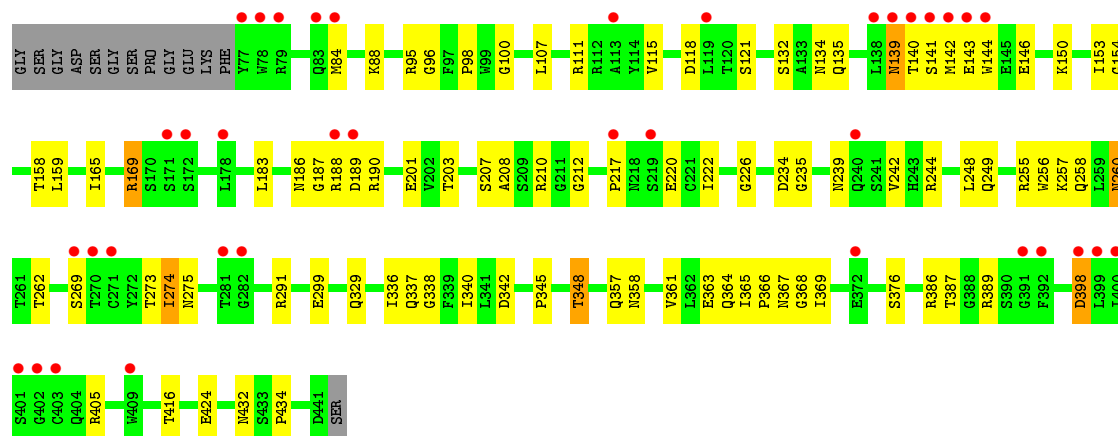


• Molecule 1: Neuraminidase

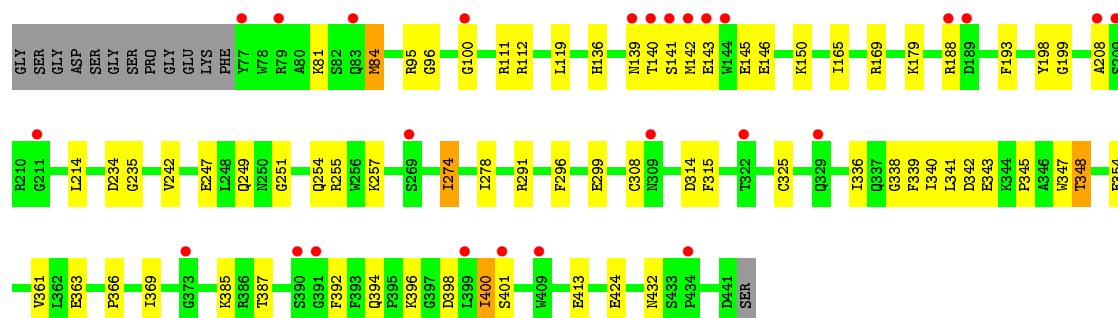
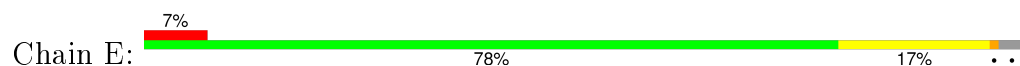




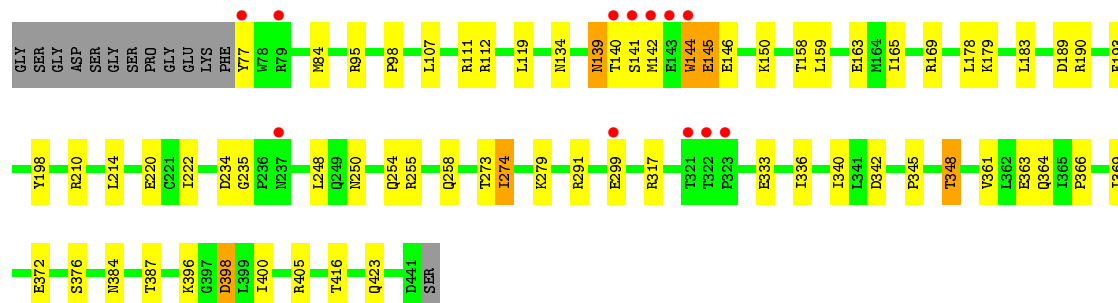
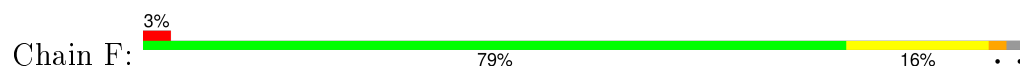
• Molecule 1: Neuraminidase



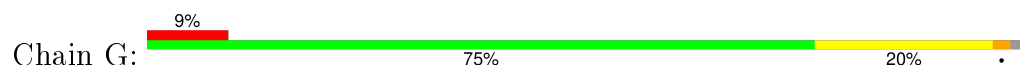
• Molecule 1: Neuraminidase

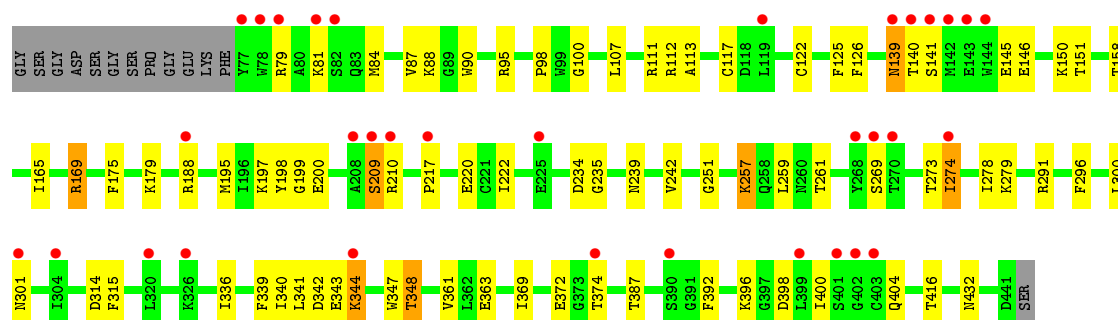


• Molecule 1: Neuraminidase

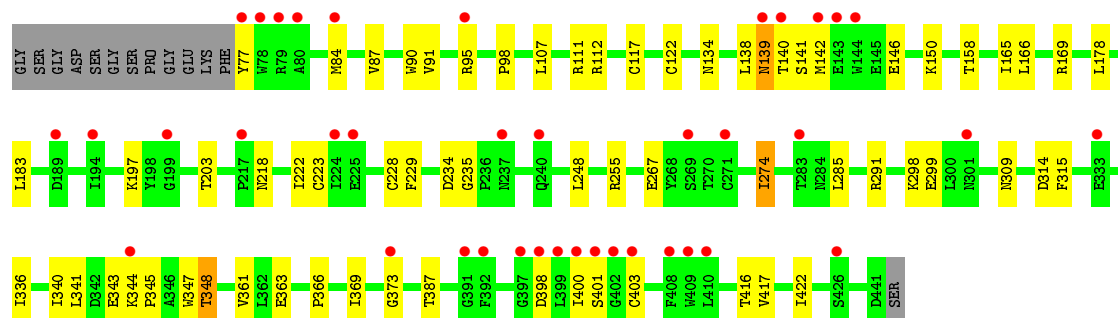
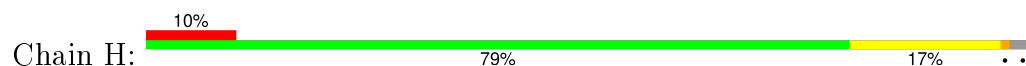


• Molecule 1: Neuraminidase

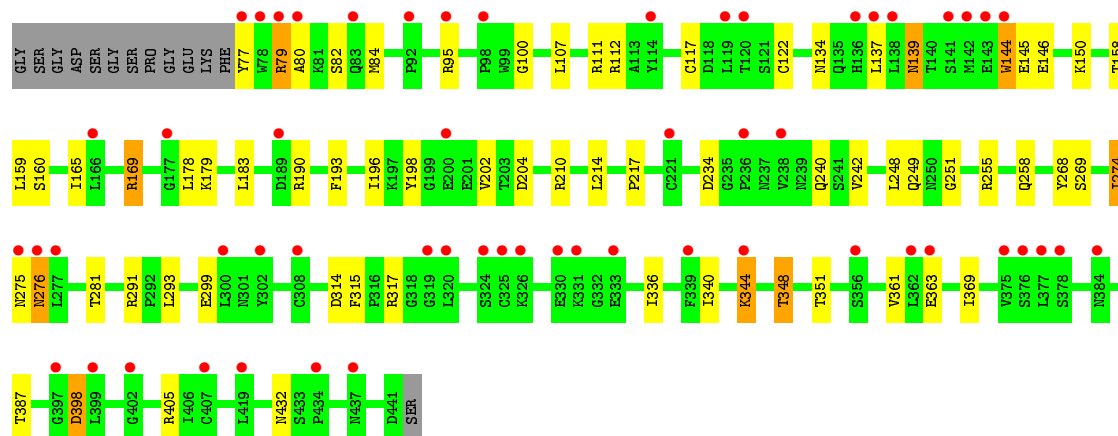
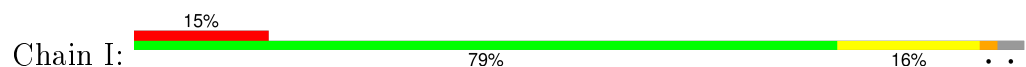




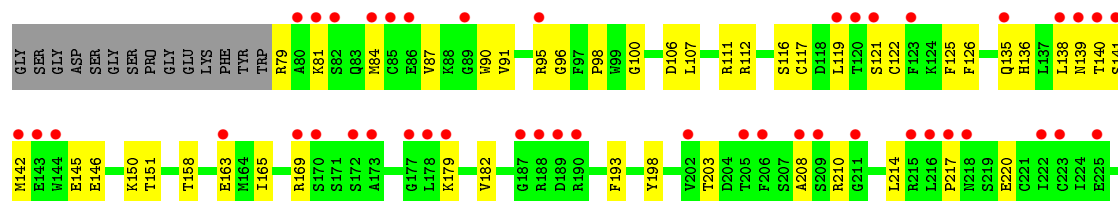
• Molecule 1: Neuraminidase



• Molecule 1: Neuraminidase



• Molecule 1: Neuraminidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	113.33Å 113.33Å 114.31Å 81.47° 81.55° 67.72°	Depositor
Resolution (Å)	29.88 – 2.50 29.88 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.2 (29.88-2.50) 89.1 (29.88-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.94 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.218 , 0.262 0.228 , 0.272	Depositor DCC
R_{free} test set	8775 reflections (5.61%)	DCC
Wilson B-factor (Å ²)	48.6	Xtriage
Anisotropy	0.504	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 54.5	EDS
Estimated twinning fraction	0.370 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 174667 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	35035	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, CA, FUL, 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	0.30	0/2926	0.53	0/3966
1	B	0.29	0/2926	0.51	0/3966
1	C	0.29	0/2926	0.52	0/3966
1	D	0.29	0/2926	0.53	0/3966
1	E	0.29	0/2926	0.52	0/3966
1	F	0.30	0/2926	0.53	0/3966
1	G	0.29	0/2926	0.52	0/3966
1	H	0.28	0/2926	0.54	0/3966
1	I	0.28	0/2926	0.54	0/3966
1	J	0.27	0/2897	0.52	0/3925
1	K	0.27	0/2913	0.53	1/3948 (0.0%)
1	L	0.27	0/2926	0.53	0/3966
All	All	0.29	0/35070	0.53	1/47533 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	G	0	1
1	I	0	1
1	J	0	1
All	All	0	5

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	293	LEU	CA-CB-CG	5.86	128.77	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	344	LYS	Peptide
1	C	344	LYS	Peptide
1	G	344	LYS	Peptide
1	I	344	LYS	Peptide
1	J	344	LYS	Peptide

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	2858	0	2762	49	2
1	B	2858	0	2764	54	2
1	C	2858	0	2764	51	1
1	D	2858	0	2765	67	0
1	E	2858	0	2763	47	2
1	F	2858	0	2764	43	1
1	G	2858	0	2764	51	1
1	H	2858	0	2764	38	0
1	I	2858	0	2763	51	0
1	J	2832	0	2746	64	0
1	K	2846	0	2755	60	0
1	L	2858	0	2763	60	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	A	28	0	26	2	0
3	B	14	0	13	2	0
3	C	14	0	13	1	0
3	D	42	0	39	2	0
3	E	14	0	13	1	0
3	F	14	0	13	1	0
3	G	14	0	13	0	0
3	H	14	0	13	0	0
3	I	14	0	13	2	0
3	K	14	0	13	0	0
3	L	14	0	12	1	0
4	A	24	0	22	0	0
4	E	24	0	22	0	1
4	I	24	0	22	0	0
5	B	38	0	34	2	0
5	F	38	0	34	1	0
6	D	10	0	10	0	0
7	A	55	0	0	9	0
7	B	54	0	0	11	0
7	C	45	0	0	12	0
7	D	46	0	0	16	0
7	E	60	0	0	7	0
7	F	41	0	0	6	0
7	G	31	0	0	7	0
7	H	15	0	0	1	0
7	I	14	0	0	9	0
7	J	25	0	0	14	0
7	K	17	0	0	8	0
7	L	8	0	0	1	0
All	All	35035	0	33462	610	5

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 9.

All (610) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:187:GLY:O	7:D:612:HOH:O	1.83	0.96
1:C:309:ASN:OD1	7:C:645:HOH:O	1.85	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:226:GLY:O	7:D:626:HOH:O	1.84	0.93
1:B:314:ASP:OD2	7:B:645:HOH:O	1.87	0.93
1:I:291:ARG:NH2	1:I:336:ILE:O	2.02	0.92
1:K:78:TRP:N	7:K:612:HOH:O	2.00	0.92
1:C:82:SER:OG	7:C:616:HOH:O	1.87	0.92
1:D:358:ASN:O	7:D:644:HOH:O	1.88	0.92
1:B:398:ASP:OD2	7:B:617:HOH:O	1.87	0.91
1:I:160:SER:O	7:I:603:HOH:O	1.88	0.91
1:J:220:GLU:OE2	7:J:601:HOH:O	1.89	0.89
1:E:394:GLN:O	7:E:645:HOH:O	1.91	0.88
1:H:291:ARG:NH2	1:H:336:ILE:O	2.07	0.88
1:A:102:GLU:OE2	7:A:612:HOH:O	1.91	0.88
1:G:239:ASN:ND2	7:G:626:HOH:O	1.89	0.87
1:I:340:ILE:HG21	1:I:369:ILE:HD12	1.55	0.87
1:D:345:PRO:HB3	1:D:366:PRO:HA	1.56	0.86
1:I:179:LYS:O	7:I:604:HOH:O	1.91	0.86
1:I:84:MET:HG2	1:I:274:ILE:HG13	1.59	0.85
1:G:291:ARG:NH2	1:G:336:ILE:O	2.09	0.85
1:A:291:ARG:NH2	1:A:336:ILE:O	2.10	0.85
1:J:140:THR:OG1	7:J:622:HOH:O	1.94	0.84
1:B:291:ARG:NH2	1:B:336:ILE:O	2.09	0.84
1:F:291:ARG:NH2	1:F:336:ILE:O	2.11	0.83
1:A:411:GLU:OE2	7:A:646:HOH:O	1.95	0.83
1:D:220:GLU:OE2	7:D:617:HOH:O	1.95	0.83
1:J:106:ASP:OD2	7:J:612:HOH:O	1.95	0.82
1:F:139:ASN:OD1	7:F:625:HOH:O	1.95	0.82
1:E:343:GLU:O	7:E:605:HOH:O	1.97	0.82
1:J:84:MET:HG2	1:J:274:ILE:HG13	1.61	0.82
1:A:340:ILE:HG21	1:A:369:ILE:HD12	1.60	0.82
1:E:340:ILE:HG21	1:E:369:ILE:HD12	1.63	0.81
1:K:220:GLU:OE1	7:K:613:HOH:O	1.97	0.81
1:C:308:CYS:SG	7:C:626:HOH:O	2.38	0.81
1:H:340:ILE:HG21	1:H:369:ILE:HD12	1.62	0.81
1:B:411:GLU:OE2	7:B:608:HOH:O	1.98	0.80
1:F:340:ILE:HG21	1:F:369:ILE:HD12	1.64	0.79
1:H:84:MET:HG2	1:H:274:ILE:HG13	1.64	0.79
1:C:340:ILE:HG21	1:C:369:ILE:HD12	1.61	0.79
1:C:291:ARG:NH2	1:C:336:ILE:O	2.15	0.79
1:E:291:ARG:NH2	1:E:336:ILE:O	2.14	0.78
1:B:259:LEU:O	7:B:640:HOH:O	2.02	0.78
1:D:340:ILE:HG21	1:D:369:ILE:HD12	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:MET:HG2	1:B:274:ILE:HG13	1.65	0.77
1:D:115:VAL:O	7:D:604:HOH:O	2.02	0.77
1:F:255:ARG:NH2	1:F:299:GLU:OE1	2.18	0.77
1:B:414:ASP:OD2	7:B:626:HOH:O	2.03	0.77
1:B:417:VAL:O	7:B:634:HOH:O	2.02	0.77
1:K:399:LEU:O	7:K:617:HOH:O	2.03	0.76
1:C:111:ARG:NH1	1:C:146:GLU:OE1	2.18	0.76
1:G:340:ILE:HG21	1:G:369:ILE:HD12	1.68	0.76
1:F:345:PRO:HB3	1:F:366:PRO:HA	1.68	0.76
1:C:363:GLU:OE1	7:C:628:HOH:O	2.03	0.76
1:J:117:CYS:O	7:J:604:HOH:O	2.04	0.74
1:A:249:GLN:NE2	3:A:503:NAG:O7	2.21	0.73
1:E:249:GLN:NE2	3:E:502:NAG:O7	2.20	0.73
1:B:111:ARG:NH1	1:B:146:GLU:OE1	2.21	0.73
1:K:291:ARG:NH2	1:K:336:ILE:O	2.17	0.73
1:J:121:SER:HB2	7:J:620:HOH:O	1.87	0.72
1:C:121:SER:OG	7:C:640:HOH:O	2.05	0.72
1:J:340:ILE:HG21	1:J:369:ILE:HD12	1.70	0.72
1:G:372:GLU:O	7:G:610:HOH:O	2.08	0.72
1:K:432:ASN:OD1	1:K:432:ASN:N	2.23	0.72
1:E:81:LYS:NZ	1:E:401:SER:O	2.23	0.71
1:C:84:MET:HG2	1:C:274:ILE:HG13	1.72	0.71
1:I:178:LEU:O	7:I:605:HOH:O	2.08	0.70
1:E:255:ARG:HH22	1:E:299:GLU:HA	1.57	0.70
1:C:150:LYS:HB3	1:C:165:ILE:HD11	1.73	0.70
1:G:432:ASN:ND2	7:G:624:HOH:O	1.83	0.69
1:G:150:LYS:HB3	1:G:165:ILE:HD11	1.73	0.69
1:I:77:TYR:OH	7:I:614:HOH:O	2.11	0.69
1:K:150:LYS:HB3	1:K:165:ILE:HD11	1.73	0.69
1:D:255:ARG:HH22	1:D:299:GLU:HA	1.58	0.69
1:K:143:GLU:OE2	1:K:188:ARG:NH1	2.25	0.68
1:D:291:ARG:NH2	1:D:336:ILE:O	2.26	0.68
1:B:340:ILE:HG21	1:B:369:ILE:HD12	1.76	0.68
1:H:111:ARG:HH22	1:H:142:MET:H	1.42	0.68
1:G:112:ARG:O	7:G:602:HOH:O	2.11	0.68
1:D:365:ILE:HG22	7:D:636:HOH:O	1.94	0.67
1:D:153:ILE:O	7:D:622:HOH:O	2.12	0.67
1:E:354:GLU:OE1	7:E:639:HOH:O	2.13	0.67
1:I:111:ARG:NH1	1:I:146:GLU:OE1	2.22	0.67
1:I:281:THR:O	7:I:611:HOH:O	2.12	0.67
1:G:81:LYS:HB2	1:G:404:GLN:HB2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:176:ASP:OD2	1:K:198:TYR:OH	2.07	0.67
1:E:396:LYS:NZ	7:E:651:HOH:O	2.28	0.66
1:C:153:ILE:O	7:C:634:HOH:O	2.13	0.66
3:I:502:NAG:O4	7:I:614:HOH:O	2.12	0.66
1:B:398:ASP:OD1	1:B:405:ARG:NH1	2.29	0.66
1:A:350:LYS:NZ	7:A:629:HOH:O	2.27	0.66
1:L:291:ARG:NH1	7:L:606:HOH:O	2.01	0.66
1:D:368:GLY:N	7:D:636:HOH:O	2.27	0.65
1:F:144:TRP:O	1:F:169:ARG:NH2	2.24	0.65
1:A:400:ILE:HG21	1:D:203:THR:HG22	1.78	0.65
1:J:413:GLU:OE2	7:J:615:HOH:O	2.15	0.65
1:I:107:LEU:HD23	1:I:158:THR:HG22	1.78	0.65
1:G:84:MET:HG2	1:G:274:ILE:HG13	1.78	0.65
1:A:143:GLU:OE2	1:A:188:ARG:NH1	2.28	0.65
1:D:234:ASP:OD1	7:D:646:HOH:O	2.14	0.65
1:I:255:ARG:NH2	1:I:299:GLU:OE1	2.28	0.65
1:E:413:GLU:OE2	7:E:659:HOH:O	2.14	0.65
1:J:283:THR:OG1	7:J:617:HOH:O	2.13	0.65
1:K:340:ILE:HG21	1:K:369:ILE:HD12	1.78	0.64
1:F:220:GLU:OE2	7:F:618:HOH:O	2.14	0.64
1:D:220:GLU:HB2	7:D:604:HOH:O	1.96	0.64
1:D:84:MET:HG2	1:D:274:ILE:HG13	1.79	0.63
1:G:145:GLU:OE2	1:H:95:ARG:NH2	2.26	0.63
1:E:179:LYS:HD3	1:E:199:GLY:HA3	1.79	0.63
1:F:398:ASP:OD2	1:F:405:ARG:NH1	2.29	0.62
1:B:77:TYR:N	7:B:648:HOH:O	2.32	0.62
1:K:346:ALA:HB3	1:K:365:ILE:HB	1.81	0.62
3:A:503:NAG:O4	3:A:503:NAG:N2	2.32	0.62
1:D:398:ASP:OD1	1:D:405:ARG:NH1	2.31	0.62
1:L:405:ARG:NH2	1:L:429:CYS:SG	2.73	0.62
1:H:345:PRO:HB3	1:H:366:PRO:HA	1.81	0.62
1:L:340:ILE:HG21	1:L:369:ILE:HD12	1.81	0.62
1:F:84:MET:HG2	1:F:274:ILE:HG13	1.81	0.61
1:J:341:LEU:HB3	1:J:347:TRP:HB2	1.82	0.61
1:B:143:GLU:OE2	1:B:188:ARG:NH1	2.33	0.61
1:C:279:LYS:HD3	1:C:342:ASP:OD1	2.01	0.61
1:B:112:ARG:NH1	1:B:169:ARG:O	2.34	0.61
1:K:283:THR:OG1	1:K:291:ARG:NH2	2.31	0.61
1:H:150:LYS:NZ	7:H:612:HOH:O	2.07	0.61
1:K:312:PRO:HB2	1:K:317:ARG:HD2	1.83	0.61
1:A:269:SER:OG	7:A:614:HOH:O	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:179:LYS:HD3	1:L:199:GLY:HA3	1.83	0.60
1:I:112:ARG:NH1	1:I:169:ARG:O	2.35	0.60
1:C:84:MET:HE1	1:C:406:ILE:HB	1.83	0.60
1:F:150:LYS:HB3	1:F:165:ILE:HD11	1.84	0.60
1:G:112:ARG:NH1	1:G:169:ARG:O	2.35	0.59
1:G:209:SER:O	1:G:210:ARG:NH1	2.36	0.59
1:B:250:ASN:ND2	3:B:505:NAG:O7	2.36	0.59
1:I:183:LEU:HD21	1:I:248:LEU:HD11	1.84	0.59
1:J:255:ARG:NH2	1:J:299:GLU:OE1	2.33	0.59
1:C:213:PRO:O	7:C:613:HOH:O	2.16	0.59
1:L:106:ASP:N	1:L:106:ASP:OD1	2.36	0.59
1:I:249:GLN:NE2	3:I:502:NAG:O7	2.36	0.59
1:A:405:ARG:NE	7:A:654:HOH:O	2.19	0.59
1:E:143:GLU:OE2	1:E:188:ARG:NH1	2.26	0.58
1:H:223:CYS:HA	1:H:228:CYS:HA	1.85	0.58
1:F:111:ARG:NH1	1:F:142:MET:O	2.37	0.58
1:D:111:ARG:NH1	1:D:146:GLU:OE1	2.37	0.58
1:B:255:ARG:NH2	1:B:299:GLU:OE1	2.36	0.58
1:K:289:ALA:N	1:K:328:ALA:O	2.35	0.58
1:H:348:THR:HG22	1:H:363:GLU:HB2	1.86	0.58
1:G:210:ARG:HG3	1:G:242:VAL:HG21	1.86	0.58
1:D:210:ARG:HG3	1:D:242:VAL:HG21	1.85	0.58
1:G:279:LYS:NZ	1:G:343:GLU:OE2	2.31	0.58
1:E:95:ARG:HH22	1:E:385:LYS:HE3	1.68	0.58
1:D:348:THR:HG22	1:D:363:GLU:HB2	1.86	0.57
1:I:268:TYR:O	7:I:611:HOH:O	2.17	0.57
1:D:139:ASN:HB2	1:D:142:MET:HG3	1.86	0.57
1:C:111:ARG:NH2	1:C:141:SER:HB3	2.20	0.57
1:D:118:ASP:OD2	7:D:629:HOH:O	2.17	0.57
1:I:398:ASP:OD1	1:I:405:ARG:NH1	2.38	0.57
1:K:107:LEU:HD23	1:K:158:THR:HG22	1.85	0.57
1:D:208:ALA:HB1	7:D:646:HOH:O	2.03	0.57
1:H:98:PRO:HB3	1:H:416:THR:HG21	1.86	0.57
1:J:81:LYS:HB2	1:J:404:GLN:HB2	1.87	0.57
1:E:143:GLU:HG2	1:E:188:ARG:HH22	1.70	0.56
1:L:168:GLY:HA2	1:L:186:ASN:ND2	2.20	0.56
1:H:255:ARG:HH22	1:H:299:GLU:HA	1.71	0.56
1:F:250:ASN:ND2	3:F:505:NAG:O5	2.38	0.56
1:D:190:ARG:HH22	1:I:144:TRP:HZ3	1.54	0.56
1:K:348:THR:HG22	1:K:363:GLU:HB2	1.88	0.56
1:A:315:PHE:O	7:A:608:HOH:O	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:179:LYS:HD2	1:J:198:TYR:CE2	2.41	0.56
1:J:258:GLN:NE2	7:J:611:HOH:O	2.38	0.56
1:C:107:LEU:HD23	1:C:158:THR:HG22	1.87	0.56
1:E:150:LYS:HB3	1:E:165:ILE:HD11	1.86	0.56
1:G:107:LEU:HD23	1:G:158:THR:HG22	1.87	0.56
1:A:208:ALA:HB1	7:A:649:HOH:O	2.05	0.55
1:D:150:LYS:HB3	1:D:165:ILE:HD11	1.88	0.55
1:E:111:ARG:NH2	1:E:141:SER:HB3	2.21	0.55
1:B:357:GLN:OE1	1:B:386:ARG:NH2	2.38	0.55
1:A:179:LYS:HD2	1:A:198:TYR:CE2	2.42	0.55
1:B:111:ARG:NH2	1:B:141:SER:HB3	2.21	0.55
1:A:348:THR:HG22	1:A:363:GLU:HB2	1.87	0.55
1:B:126:PHE:HE1	1:B:151:THR:HG1	1.54	0.55
1:J:394:GLN:HG2	7:J:619:HOH:O	2.06	0.55
1:A:255:ARG:HH22	1:A:299:GLU:HA	1.71	0.55
1:L:172:SER:HB2	1:L:217:PRO:HD2	1.88	0.55
1:L:107:LEU:HD23	1:L:158:THR:HG22	1.89	0.55
1:H:84:MET:HG3	1:H:343:GLU:HG3	1.88	0.55
1:J:193:PHE:HA	1:J:214:LEU:HD12	1.88	0.55
1:L:222:ILE:HG21	1:L:273:THR:HB	1.88	0.55
1:L:266:PHE:HE1	1:L:269:SER:HG	1.54	0.54
1:K:193:PHE:HA	1:K:214:LEU:HD12	1.88	0.54
1:D:107:LEU:HD23	1:D:158:THR:HG22	1.89	0.54
1:B:250:ASN:HD21	3:B:505:NAG:C1	2.21	0.54
1:B:81:LYS:NZ	1:B:401:SER:O	2.33	0.54
1:F:210:ARG:HH21	1:F:258:GLN:HE22	1.55	0.54
3:C:502:NAG:O4	7:C:629:HOH:O	2.19	0.54
1:B:348:THR:HG22	1:B:363:GLU:HB2	1.88	0.54
1:J:208:ALA:HB1	7:J:610:HOH:O	2.06	0.54
1:J:150:LYS:HB3	1:J:165:ILE:HD11	1.89	0.54
1:B:220:GLU:OE2	7:B:625:HOH:O	2.17	0.54
1:L:291:ARG:CZ	1:L:338:GLY:HA3	2.38	0.54
1:E:234:ASP:OD1	7:E:631:HOH:O	2.19	0.54
1:A:112:ARG:NH1	1:A:169:ARG:O	2.41	0.54
1:G:279:LYS:HD3	1:G:342:ASP:OD1	2.07	0.53
1:I:95:ARG:NH2	1:L:145:GLU:OE2	2.38	0.53
1:L:255:ARG:NH2	1:L:299:GLU:OE1	2.42	0.53
1:I:234:ASP:HB3	1:I:242:VAL:HG22	1.90	0.53
1:A:357:GLN:HB2	7:A:610:HOH:O	2.07	0.53
1:K:299:GLU:HB2	7:K:614:HOH:O	2.08	0.53
1:I:179:LYS:HD2	1:I:198:TYR:CE2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:196:ILE:HD12	1:I:204:ASP:HB3	1.90	0.53
1:J:138:LEU:O	7:J:622:HOH:O	2.19	0.52
1:J:341:LEU:HD23	1:J:347:TRP:HD1	1.74	0.52
1:I:117:CYS:HA	1:I:122:CYS:HA	1.91	0.52
1:G:175:PHE:N	7:G:615:HOH:O	2.12	0.52
1:G:314:ASP:OD1	1:G:315:PHE:N	2.41	0.52
1:K:196:ILE:HD12	1:K:204:ASP:HB3	1.91	0.52
1:F:189:ASP:OD1	1:F:190:ARG:N	2.42	0.52
1:I:348:THR:HG22	1:I:363:GLU:HB2	1.91	0.52
1:C:348:THR:HG22	1:C:363:GLU:HB2	1.91	0.52
1:H:111:ARG:NH1	1:H:146:GLU:OE1	2.39	0.52
1:D:88:LYS:HD3	1:D:434:PRO:HG3	1.89	0.52
1:L:119:LEU:HA	1:L:396:LYS:O	2.09	0.52
1:J:145:GLU:OE2	1:K:95:ARG:NH2	2.39	0.52
1:F:372:GLU:H	1:F:372:GLU:CD	2.13	0.52
1:C:279:LYS:NZ	1:C:343:GLU:OE2	2.28	0.52
1:H:166:LEU:HD11	1:H:197:LYS:HB2	1.92	0.52
1:F:396:LYS:NZ	7:F:604:HOH:O	2.32	0.52
1:D:226:GLY:O	1:D:249:GLN:HG3	2.09	0.52
1:G:111:ARG:NH2	1:G:141:SER:HB3	2.25	0.52
1:L:168:GLY:HA2	1:L:186:ASN:HD21	1.75	0.52
1:A:225:GLU:OE2	1:A:298:LYS:NZ	2.31	0.52
1:B:183:LEU:HD21	1:B:248:LEU:HD11	1.92	0.52
1:J:112:ARG:NH1	1:J:169:ARG:O	2.43	0.52
1:L:223:CYS:HA	1:L:228:CYS:HA	1.90	0.52
1:G:98:PRO:HB3	1:G:416:THR:HG21	1.92	0.52
1:F:111:ARG:HH22	1:F:142:MET:H	1.58	0.51
1:G:179:LYS:HD2	1:G:198:TYR:CE2	2.45	0.51
1:D:432:ASN:N	1:D:432:ASN:OD1	2.43	0.51
1:H:341:LEU:HB3	1:H:347:TRP:HB2	1.92	0.51
1:J:165:ILE:HG21	1:J:182:VAL:HG11	1.91	0.51
1:C:143:GLU:HG2	1:C:169:ARG:HH11	1.75	0.51
1:G:217:PRO:HB2	1:G:269:SER:O	2.11	0.51
1:J:107:LEU:HD23	1:J:158:THR:HG22	1.91	0.51
1:G:341:LEU:HD23	1:G:347:TRP:HD1	1.74	0.51
1:B:197:LYS:HE2	1:B:200:GLU:HA	1.92	0.51
1:C:198:TYR:HB2	1:C:251:GLY:HA3	1.92	0.51
1:L:183:LEU:HD21	1:L:248:LEU:HD11	1.93	0.51
1:J:135:GLN:HG2	1:J:136:HIS:ND1	2.26	0.51
1:H:77:TYR:CE1	1:H:178:LEU:HD13	2.46	0.51
1:K:98:PRO:HB3	1:K:416:THR:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:292:PRO:HG3	7:J:606:HOH:O	2.11	0.51
1:B:222:ILE:HG21	1:B:273:THR:HB	1.93	0.51
1:E:345:PRO:HB3	1:E:366:PRO:HA	1.92	0.50
1:J:348:THR:HG22	1:J:363:GLU:HB2	1.93	0.50
1:A:139:ASN:N	1:A:139:ASN:OD1	2.44	0.50
1:D:364:GLN:OE1	1:D:376:SER:OG	2.26	0.50
1:K:146:GLU:OE2	1:K:169:ARG:NH1	2.45	0.50
1:F:139:ASN:O	1:F:142:MET:HG3	2.11	0.50
1:C:193:PHE:HA	1:C:214:LEU:HD12	1.94	0.50
1:G:111:ARG:NH1	1:G:146:GLU:OE1	2.44	0.50
1:E:208:ALA:HB1	7:E:631:HOH:O	2.11	0.50
1:K:314:ASP:OD1	1:K:315:PHE:N	2.43	0.50
1:H:255:ARG:NH2	1:H:298:LYS:O	2.44	0.50
1:G:179:LYS:HD3	1:G:199:GLY:HA3	1.94	0.50
1:B:150:LYS:HB3	1:B:165:ILE:HD11	1.93	0.50
1:J:234:ASP:HB3	1:J:242:VAL:HG22	1.94	0.50
1:A:193:PHE:HA	1:A:214:LEU:HD12	1.94	0.50
1:A:107:LEU:HD23	1:A:158:THR:HG22	1.94	0.50
1:L:380:GLU:OE1	1:L:383:SER:OG	2.15	0.50
1:J:234:ASP:OD1	1:J:235:GLY:N	2.42	0.50
1:D:207:SER:O	7:D:632:HOH:O	2.20	0.50
3:L:502:NAG:O4	3:L:502:NAG:O6	2.30	0.50
1:K:217:PRO:HB2	1:K:269:SER:O	2.12	0.50
1:L:234:ASP:OD1	1:L:235:GLY:N	2.43	0.49
1:H:107:LEU:HD23	1:H:158:THR:HG22	1.94	0.49
1:J:373:GLY:N	7:J:625:HOH:O	1.90	0.49
1:E:100:GLY:HA3	1:H:134:ASN:ND2	2.27	0.49
1:D:186:ASN:ND2	7:D:641:HOH:O	2.25	0.49
1:J:291:ARG:NH2	1:J:336:ILE:O	2.45	0.49
1:I:193:PHE:HA	1:I:214:LEU:HD12	1.93	0.49
1:G:257:LYS:HB2	1:G:300:LEU:HD13	1.95	0.49
1:F:364:GLN:OE1	1:F:376:SER:OG	2.27	0.49
3:D:503:NAG:H61	3:D:504:NAG:H82	1.94	0.49
1:J:364:GLN:OE1	1:J:376:SER:OG	2.30	0.49
1:J:87:VAL:HG11	1:J:90:TRP:CZ2	2.48	0.49
1:J:126:PHE:HE1	1:J:151:THR:HG1	1.58	0.49
1:H:134:ASN:O	1:H:138:LEU:HG	2.13	0.49
1:B:98:PRO:HB3	1:B:416:THR:HG21	1.94	0.49
1:D:357:GLN:OE1	1:D:386:ARG:NH2	2.45	0.49
1:B:111:ARG:HH21	1:B:141:SER:HB3	1.77	0.49
1:F:210:ARG:NH2	1:F:258:GLN:HE22	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:276:ASN:OD1	1:I:276:ASN:N	2.46	0.49
1:B:119:LEU:HA	1:B:396:LYS:O	2.12	0.49
1:C:112:ARG:NH1	1:C:169:ARG:O	2.46	0.49
1:L:439:ASN:OD1	1:L:441:ASP:HB2	2.13	0.49
1:J:314:ASP:OD1	1:J:315:PHE:N	2.44	0.49
1:G:396:LYS:NZ	7:G:615:HOH:O	2.45	0.48
1:I:139:ASN:OD1	7:I:609:HOH:O	2.20	0.48
1:K:209:SER:HB3	1:K:210:ARG:NH2	2.28	0.48
1:E:234:ASP:OD1	1:E:235:GLY:N	2.45	0.48
1:J:341:LEU:HD23	1:J:347:TRP:CD1	2.48	0.48
1:L:234:ASP:HB3	1:L:242:VAL:HG22	1.95	0.48
1:A:411:GLU:OE1	7:A:632:HOH:O	2.20	0.48
1:H:111:ARG:NH2	1:H:142:MET:H	2.09	0.48
1:J:140:THR:HA	1:J:141:SER:HA	1.61	0.48
1:C:111:ARG:HH22	1:C:142:MET:H	1.62	0.48
1:B:140:THR:HA	1:B:141:SER:HA	1.58	0.48
1:F:112:ARG:NH1	1:F:169:ARG:O	2.47	0.48
1:L:222:ILE:O	1:L:229:PHE:N	2.42	0.48
1:L:210:ARG:HG3	1:L:242:VAL:HG21	1.95	0.48
1:H:234:ASP:OD1	1:H:235:GLY:N	2.45	0.48
1:J:98:PRO:HB3	1:J:416:THR:HG21	1.96	0.48
1:D:258:GLN:H	1:I:240:GLN:NE2	2.12	0.48
1:H:140:THR:HA	1:H:141:SER:HA	1.60	0.48
1:B:190:ARG:HG3	1:B:211:GLY:HA2	1.95	0.48
1:K:144:TRP:O	1:K:169:ARG:NH2	2.42	0.48
1:F:183:LEU:HD21	1:F:248:LEU:HD11	1.96	0.48
1:K:122:CYS:HB2	1:K:153:ILE:HG21	1.96	0.48
1:L:118:ASP:OD1	1:L:121:SER:N	2.28	0.48
1:E:119:LEU:HA	1:E:396:LYS:O	2.14	0.47
1:L:243:HIS:CD2	1:L:261:THR:HG21	2.49	0.47
1:J:116:SER:HB3	1:J:125:PHE:CE1	2.49	0.47
1:H:150:LYS:HB3	1:H:165:ILE:HD11	1.96	0.47
1:K:279:LYS:HD3	1:K:342:ASP:OD1	2.14	0.47
1:F:107:LEU:HD23	1:F:158:THR:HG22	1.94	0.47
1:E:341:LEU:HB3	1:E:347:TRP:HB2	1.96	0.47
1:F:348:THR:HG22	1:F:363:GLU:HB2	1.95	0.47
1:I:202:VAL:HG11	1:J:91:VAL:HG21	1.95	0.47
1:C:98:PRO:HB3	1:C:416:THR:HG21	1.95	0.47
1:F:384:ASN:ND2	7:F:615:HOH:O	2.47	0.47
1:B:217:PRO:HB2	1:B:269:SER:O	2.14	0.47
1:D:234:ASP:OD1	1:D:235:GLY:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:95:ARG:NH2	1:E:385:LYS:HE3	2.29	0.47
1:F:145:GLU:OE2	1:G:95:ARG:NH2	2.38	0.47
1:J:79:ARG:N	7:J:618:HOH:O	2.47	0.47
1:J:290:LYS:NZ	1:J:324:SER:O	2.48	0.47
1:K:369:ILE:HG22	7:K:611:HOH:O	2.13	0.47
1:E:193:PHE:HA	1:E:214:LEU:HD12	1.96	0.47
5:B:503:NAG:N2	7:B:637:HOH:O	2.35	0.47
1:K:257:LYS:HZ1	1:K:302:TYR:HE1	1.63	0.47
1:D:96:GLY:N	1:D:424:GLU:OE2	2.34	0.47
1:C:144:TRP:O	1:C:169:ARG:NH2	2.33	0.47
1:C:164:MET:HB3	1:D:154:GLY:HA2	1.96	0.47
1:C:140:THR:HA	1:C:141:SER:HA	1.52	0.47
1:C:146:GLU:OE2	1:C:169:ARG:HG3	2.15	0.47
1:D:244:ARG:HD3	1:D:256:TRP:CE3	2.49	0.47
5:F:502:NAG:H61	5:F:504:FUL:O2	2.15	0.47
1:D:260:ASN:ND2	1:D:262:THR:OG1	2.44	0.47
1:A:417:VAL:HG11	1:A:422:ILE:HG12	1.96	0.47
1:E:348:THR:HG22	1:E:363:GLU:HB2	1.95	0.47
1:A:111:ARG:HH22	1:A:142:MET:H	1.62	0.47
1:K:364:GLN:OE1	1:K:376:SER:OG	2.32	0.47
1:B:234:ASP:OD1	1:B:235:GLY:N	2.44	0.47
1:K:341:LEU:HD23	1:K:347:TRP:CD1	2.50	0.47
1:K:140:THR:HA	1:K:141:SER:HA	1.55	0.47
1:K:111:ARG:NH1	1:K:142:MET:O	2.44	0.47
1:F:317:ARG:NH1	7:F:606:HOH:O	2.44	0.47
1:K:293:LEU:HD21	1:K:369:ILE:HG21	1.97	0.47
1:D:118:ASP:OD1	1:D:121:SER:N	2.34	0.47
1:H:417:VAL:HG11	1:H:422:ILE:HG12	1.97	0.47
1:K:288:ASP:OD1	1:K:328:ALA:N	2.47	0.47
1:I:82:SER:O	1:I:275:ASN:HB2	2.15	0.47
1:L:314:ASP:OD1	1:L:315:PHE:N	2.48	0.47
1:H:139:ASN:OD1	1:H:139:ASN:N	2.48	0.47
1:E:234:ASP:HB3	1:E:242:VAL:HG22	1.96	0.46
1:I:145:GLU:OE2	1:J:95:ARG:NH2	2.32	0.46
1:E:145:GLU:OE2	1:F:95:ARG:NH2	2.26	0.46
1:L:143:GLU:HG2	1:L:169:ARG:NH1	2.30	0.46
1:L:210:ARG:CZ	1:L:244:ARG:HH21	2.27	0.46
1:I:150:LYS:HB3	1:I:165:ILE:HD11	1.97	0.46
1:J:117:CYS:HA	1:J:122:CYS:HA	1.97	0.46
1:L:117:CYS:HA	1:L:122:CYS:HA	1.97	0.46
1:K:341:LEU:HD23	1:K:347:TRP:HD1	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:398:ASP:OD2	1:K:405:ARG:NH1	2.48	0.46
1:B:81:LYS:NZ	1:B:398:ASP:O	2.47	0.46
1:G:341:LEU:HB3	1:G:347:TRP:HB2	1.97	0.46
1:L:142:MET:HB3	1:L:144:TRP:CD1	2.51	0.46
1:J:398:ASP:OD2	1:J:405:ARG:HD3	2.16	0.46
1:D:239:ASN:HD21	3:D:502:NAG:C1	2.29	0.46
1:H:183:LEU:HD21	1:H:248:LEU:HD11	1.96	0.46
1:E:339:PHE:HB2	1:E:392:PHE:CE2	2.50	0.46
1:E:432:ASN:N	1:E:432:ASN:OD1	2.49	0.46
1:K:438:ILE:HD13	1:K:440:TRP:CZ2	2.51	0.46
1:K:309:ASN:OD1	1:K:373:GLY:HA3	2.15	0.46
1:D:275:ASN:O	1:D:275:ASN:ND2	2.49	0.46
1:L:308:CYS:HB2	1:L:371:SER:O	2.16	0.46
1:A:210:ARG:HG3	1:A:242:VAL:HG21	1.98	0.46
1:E:84:MET:HG2	1:E:274:ILE:HG13	1.97	0.46
1:K:317:ARG:O	1:K:331:LYS:HD2	2.16	0.46
1:K:405:ARG:HH21	1:K:429:CYS:HB3	1.81	0.46
1:D:132:SER:O	1:D:135:GLN:HB2	2.16	0.46
1:F:222:ILE:HG21	1:F:273:THR:HB	1.97	0.46
1:I:134:ASN:HA	1:I:137:LEU:HD12	1.97	0.46
1:D:217:PRO:HB2	1:D:269:SER:O	2.15	0.46
1:B:110:SER:HB2	1:B:126:PHE:HB2	1.97	0.45
1:J:119:LEU:HA	1:J:396:LYS:O	2.16	0.45
1:L:190:ARG:HG3	1:L:211:GLY:O	2.16	0.45
1:C:139:ASN:O	1:C:142:MET:HG3	2.15	0.45
1:D:139:ASN:OD1	1:D:139:ASN:N	2.49	0.45
1:G:234:ASP:OD1	1:G:235:GLY:N	2.48	0.45
1:D:210:ARG:NH2	1:D:258:GLN:HE22	2.15	0.45
1:B:244:ARG:HD3	1:B:256:TRP:CD1	2.51	0.45
1:A:400:ILE:HG22	1:D:201:GLU:OE1	2.16	0.45
1:C:175:PHE:N	7:C:601:HOH:O	2.36	0.45
1:A:432:ASN:N	1:A:432:ASN:OD1	2.47	0.45
1:D:367:ASN:N	7:D:636:HOH:O	2.50	0.45
1:J:145:GLU:OE1	1:K:98:PRO:HG3	2.17	0.45
1:F:119:LEU:HA	1:F:396:LYS:O	2.17	0.45
1:G:126:PHE:HE1	1:G:151:THR:HG1	1.63	0.45
1:C:189:ASP:OD1	1:C:190:ARG:N	2.50	0.45
1:D:98:PRO:HB3	1:D:416:THR:HG21	1.99	0.45
1:L:111:ARG:NH2	1:L:141:SER:OG	2.49	0.45
1:A:136:HIS:CD2	1:E:136:HIS:CD2	3.05	0.45
1:A:234:ASP:OD1	1:A:235:GLY:N	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:98:PRO:HB3	1:F:416:THR:HG21	1.97	0.45
1:D:222:ILE:HG21	1:D:273:THR:HB	1.98	0.45
1:J:138:LEU:HD13	1:J:142:MET:SD	2.57	0.45
1:G:146:GLU:OE2	1:G:169:ARG:HG3	2.17	0.45
1:D:212:GLY:O	7:D:646:HOH:O	2.21	0.45
1:J:146:GLU:OE2	1:J:169:ARG:HG3	2.16	0.45
1:J:234:ASP:HB3	1:J:242:VAL:CG2	2.47	0.45
1:C:314:ASP:OD1	1:C:315:PHE:N	2.49	0.45
1:J:96:GLY:N	1:J:424:GLU:OE2	2.39	0.45
1:F:134:ASN:ND2	1:G:100:GLY:HA3	2.32	0.45
1:I:100:GLY:HA3	1:L:134:ASN:ND2	2.32	0.45
1:J:111:ARG:NH1	1:J:142:MET:O	2.44	0.45
1:I:314:ASP:OD1	1:I:315:PHE:N	2.50	0.45
1:L:290:LYS:HE3	1:L:328:ALA:HB2	1.97	0.45
1:A:100:GLY:HA3	1:D:134:ASN:ND2	2.32	0.45
1:L:150:LYS:HB3	1:L:165:ILE:HD11	1.99	0.45
1:I:198:TYR:HB2	1:I:251:GLY:HA3	1.98	0.45
1:A:389:ARG:NH1	1:A:411:GLU:OE1	2.44	0.45
1:G:432:ASN:N	1:G:432:ASN:OD1	2.46	0.45
1:K:279:LYS:NZ	1:K:342:ASP:O	2.44	0.45
1:L:122:CYS:HB2	1:L:153:ILE:HG21	1.98	0.45
1:I:317:ARG:NH2	1:I:351:THR:OG1	2.47	0.45
1:I:432:ASN:N	1:I:432:ASN:OD1	2.48	0.45
1:L:346:ALA:HB3	1:L:365:ILE:HB	1.99	0.44
1:K:252:THR:OG1	7:K:604:HOH:O	2.21	0.44
1:A:198:TYR:HB2	1:A:251:GLY:HA3	1.98	0.44
1:G:341:LEU:HD23	1:G:347:TRP:CD1	2.52	0.44
1:F:234:ASP:OD1	1:F:235:GLY:N	2.44	0.44
1:C:386:ARG:NH1	7:C:638:HOH:O	2.51	0.44
1:C:234:ASP:OD1	1:C:235:GLY:N	2.45	0.44
1:G:117:CYS:HA	1:G:122:CYS:HA	1.99	0.44
1:G:222:ILE:HG21	1:G:273:THR:HB	2.00	0.44
1:J:313:THR:HG22	1:J:350:LYS:HD3	2.00	0.44
1:C:432:ASN:OD1	1:C:432:ASN:N	2.46	0.44
1:E:278:ILE:HD13	1:E:296:PHE:CE2	2.53	0.44
1:J:217:PRO:HB2	1:J:269:SER:O	2.17	0.44
1:A:111:ARG:NH1	1:A:146:GLU:OE1	2.46	0.44
1:K:341:LEU:HB3	1:K:347:TRP:HB2	2.00	0.44
1:J:198:TYR:HB3	1:J:203:THR:HG21	2.00	0.44
1:D:143:GLU:O	1:D:188:ARG:NH2	2.51	0.44
1:L:197:LYS:HE2	1:L:200:GLU:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:ILE:O	5:B:504:FUL:H62	2.18	0.44
1:D:144:TRP:O	1:D:169:ARG:NH2	2.44	0.43
1:L:212:GLY:HA3	1:L:235:GLY:C	2.38	0.43
1:C:190:ARG:H	1:C:190:ARG:HG3	1.33	0.43
1:L:140:THR:HA	1:L:141:SER:HA	1.40	0.43
1:J:229:PHE:CE2	1:J:300:LEU:HD21	2.53	0.43
1:A:96:GLY:N	1:A:424:GLU:OE2	2.43	0.43
1:A:150:LYS:HB3	1:A:165:ILE:HD11	2.00	0.43
1:D:183:LEU:HD21	1:D:248:LEU:HD11	2.00	0.43
1:I:144:TRP:HA	1:I:144:TRP:CE3	2.52	0.43
1:B:220:GLU:HG2	1:B:221:CYS:O	2.18	0.43
1:E:140:THR:HA	1:E:141:SER:HA	1.46	0.43
1:A:140:THR:HA	1:A:141:SER:HA	1.54	0.43
1:K:291:ARG:HA	1:K:292:PRO:HD2	1.88	0.43
1:B:159:LEU:HD13	1:C:107:LEU:HD21	2.00	0.43
1:K:146:GLU:OE2	1:K:169:ARG:HG3	2.18	0.43
1:L:265:ASN:HB3	1:L:284:ASN:OD1	2.19	0.43
1:G:197:LYS:HE2	1:G:200:GLU:HA	2.00	0.43
1:H:117:CYS:HA	1:H:122:CYS:HA	2.01	0.43
1:L:243:HIS:HD2	1:L:261:THR:HG21	1.82	0.43
1:E:84:MET:HB3	1:E:84:MET:HE3	1.93	0.43
1:K:278:ILE:HD13	1:K:296:PHE:CE2	2.54	0.43
1:K:116:SER:OG	1:K:220:GLU:HG3	2.18	0.43
1:C:145:GLU:OE2	1:D:95:ARG:NH2	2.32	0.43
1:L:432:ASN:N	1:L:432:ASN:OD1	2.46	0.43
1:C:143:GLU:HG2	1:C:169:ARG:NH1	2.34	0.43
1:A:117:CYS:HA	1:A:122:CYS:HA	2.00	0.43
1:H:112:ARG:HD3	1:H:218:ASN:ND2	2.34	0.43
1:F:146:GLU:OE2	1:F:169:ARG:HG3	2.19	0.43
1:L:186:ASN:O	1:L:192:SER:HA	2.18	0.43
1:G:198:TYR:HB2	1:G:251:GLY:HA3	2.01	0.43
1:F:423:GLN:OE1	7:F:621:HOH:O	2.21	0.43
1:J:274:ILE:HA	1:J:274:ILE:HD13	1.92	0.43
1:E:111:ARG:HH22	1:E:142:MET:H	1.67	0.43
1:L:244:ARG:HD3	1:L:256:TRP:CE3	2.53	0.43
1:K:134:ASN:HA	1:K:137:LEU:HD12	2.00	0.43
1:D:291:ARG:CZ	1:D:338:GLY:HA3	2.48	0.42
1:L:119:LEU:HD23	1:L:396:LYS:O	2.19	0.42
1:A:134:ASN:ND2	1:B:100:GLY:HA3	2.34	0.42
1:I:274:ILE:HD13	1:I:274:ILE:HA	1.93	0.42
1:C:120:THR:OG1	7:C:640:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:348:THR:HG22	1:G:363:GLU:HB2	2.00	0.42
1:A:107:LEU:HD21	1:D:159:LEU:HD13	2.02	0.42
1:A:257:LYS:HB2	1:A:300:LEU:HD13	2.00	0.42
1:E:314:ASP:OD1	1:E:315:PHE:N	2.52	0.42
1:C:77:TYR:CE1	1:C:178:LEU:HD13	2.54	0.42
1:G:139:ASN:OD1	1:G:139:ASN:N	2.51	0.42
1:G:220:GLU:O	7:G:623:HOH:O	2.22	0.42
1:D:146:GLU:OE2	1:D:169:ARG:HG3	2.20	0.42
1:L:143:GLU:HG2	1:L:169:ARG:HH12	1.84	0.42
1:I:144:TRP:HE3	1:I:144:TRP:HA	1.84	0.42
1:I:193:PHE:HE1	1:J:438:ILE:HG21	1.85	0.42
1:C:339:PHE:HB2	1:C:392:PHE:CE2	2.55	0.42
1:I:255:ARG:HH22	1:I:299:GLU:HA	1.84	0.42
1:K:107:LEU:HB2	1:K:132:SER:HB3	2.02	0.42
1:D:190:ARG:HG3	1:D:190:ARG:H	1.57	0.42
1:L:309:ASN:OD1	1:L:310:GLY:N	2.49	0.42
1:C:179:LYS:HD2	1:C:198:TYR:CE2	2.55	0.42
1:E:341:LEU:HD23	1:E:347:TRP:CD1	2.54	0.42
1:C:77:TYR:CD1	1:C:178:LEU:HD13	2.55	0.42
1:H:314:ASP:OD1	1:H:315:PHE:N	2.53	0.42
1:G:259:LEU:HB2	1:G:261:THR:HG23	2.01	0.42
1:B:107:LEU:HD23	1:B:158:THR:HG22	2.02	0.42
1:K:81:LYS:HD2	1:K:402:GLY:O	2.19	0.42
1:F:77:TYR:CE1	1:F:178:LEU:HD13	2.55	0.42
1:E:96:GLY:N	1:E:424:GLU:OE2	2.49	0.42
1:G:278:ILE:HD13	1:G:296:PHE:CE2	2.55	0.42
1:L:308:CYS:HA	1:L:325:CYS:HA	2.01	0.42
1:F:193:PHE:HA	1:F:214:LEU:HD12	2.01	0.42
1:K:200:GLU:N	7:K:602:HOH:O	2.37	0.42
1:D:337:GLN:OE1	1:D:389:ARG:NH2	2.53	0.42
1:L:225:GLU:OE2	1:L:298:LYS:NZ	2.32	0.42
1:G:87:VAL:HG11	1:G:90:TRP:CZ2	2.55	0.42
1:L:139:ASN:OD1	1:L:139:ASN:N	2.52	0.42
1:B:127:ILE:CG2	1:B:146:GLU:HB3	2.50	0.41
1:I:210:ARG:HG3	1:I:242:VAL:HG21	2.02	0.41
1:I:134:ASN:ND2	1:J:100:GLY:HA3	2.34	0.41
1:F:179:LYS:HD2	1:F:198:TYR:CE2	2.55	0.41
1:B:239:ASN:OD1	1:B:240:GLN:HG2	2.20	0.41
1:B:383:SER:OG	1:B:439:ASN:ND2	2.53	0.41
1:L:313:THR:HB	1:L:349:SER:O	2.20	0.41
1:I:293:LEU:HD21	1:I:369:ILE:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:301:ASN:ND2	7:K:614:HOH:O	2.49	0.41
1:E:247:GLU:OE1	1:E:255:ARG:NE	2.45	0.41
1:D:84:MET:CG	1:D:274:ILE:HG13	2.49	0.41
1:F:145:GLU:HG2	1:G:98:PRO:HD3	2.02	0.41
1:E:341:LEU:HD23	1:E:347:TRP:HD1	1.85	0.41
1:H:417:VAL:HG21	1:H:422:ILE:HG13	2.01	0.41
1:I:79:ARG:HG3	1:I:80:ALA:O	2.20	0.41
1:C:96:GLY:N	1:C:424:GLU:OE2	2.52	0.41
1:E:400:ILE:HG21	1:H:203:THR:HG22	2.02	0.41
1:E:291:ARG:CZ	1:E:338:GLY:HA3	2.50	0.41
1:C:111:ARG:HH21	1:C:141:SER:HB3	1.86	0.41
1:I:159:LEU:HD13	1:J:107:LEU:HD21	2.02	0.41
1:E:198:TYR:HB2	1:E:251:GLY:HA3	2.00	0.41
1:K:201:GLU:OE2	1:L:400:ILE:HG22	2.20	0.41
1:L:386:ARG:HD3	1:L:413:GLU:OE1	2.20	0.41
1:I:217:PRO:HB2	1:I:269:SER:O	2.21	0.41
1:G:113:ALA:HA	1:G:125:PHE:O	2.20	0.41
1:A:222:ILE:O	1:A:229:PHE:N	2.47	0.41
1:C:291:ARG:N	7:C:602:HOH:O	2.34	0.41
1:B:274:ILE:HD13	1:B:274:ILE:HA	1.91	0.41
1:D:398:ASP:CG	1:D:405:ARG:HH11	2.23	0.41
1:A:217:PRO:HB2	1:A:269:SER:O	2.21	0.41
1:F:140:THR:HA	1:F:141:SER:HA	1.43	0.41
1:B:291:ARG:NH1	7:B:636:HOH:O	2.54	0.41
1:I:240:GLN:OE1	7:I:607:HOH:O	2.22	0.41
1:L:104:PRO:HG2	1:L:107:LEU:HG	2.03	0.41
1:A:339:PHE:HB2	1:A:392:PHE:CE2	2.56	0.41
1:K:264:ILE:HG22	1:K:327:MET:SD	2.61	0.41
1:C:139:ASN:OD1	1:C:139:ASN:N	2.53	0.41
1:G:140:THR:HA	1:G:141:SER:HA	1.42	0.41
1:B:77:TYR:HA	1:B:77:TYR:HD1	1.72	0.41
1:I:210:ARG:NH2	1:I:258:GLN:HE22	2.19	0.41
1:G:339:PHE:HB2	1:G:392:PHE:CE2	2.56	0.41
1:E:112:ARG:NH1	1:E:169:ARG:O	2.54	0.41
1:H:267:GLU:HG3	1:H:285:LEU:HD12	2.03	0.41
1:H:309:ASN:OD1	1:H:373:GLY:HA3	2.19	0.41
1:C:127:ILE:CG2	1:C:146:GLU:HB3	2.51	0.41
1:H:401:SER:HB2	1:H:403:CYS:SG	2.61	0.41
1:H:222:ILE:O	1:H:229:PHE:N	2.43	0.41
1:G:195:MET:SD	1:H:91:VAL:HB	2.60	0.41
1:D:140:THR:HA	1:D:141:SER:HA	1.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:116:SER:HB3	1:L:125:PHE:CE1	2.56	0.41
1:J:210:ARG:HE	1:J:244:ARG:NH2	2.19	0.41
1:E:146:GLU:OE2	1:E:169:ARG:HG3	2.21	0.41
1:K:339:PHE:HB2	1:K:392:PHE:CE2	2.56	0.41
1:L:291:ARG:NH2	1:L:338:GLY:HA3	2.35	0.41
1:F:84:MET:CG	1:F:274:ILE:HG13	2.49	0.41
1:D:244:ARG:HG2	1:D:258:GLN:HA	2.03	0.41
1:K:245:ILE:HB	1:K:257:LYS:HB3	2.02	0.41
1:B:139:ASN:N	1:B:139:ASN:OD1	2.53	0.41
1:B:121:SER:HB2	7:B:650:HOH:O	2.20	0.41
1:J:198:TYR:CZ	1:J:250:ASN:HA	2.55	0.40
1:E:308:CYS:HA	1:E:325:CYS:HA	2.03	0.40
1:A:372:GLU:HG2	1:A:374:THR:HG23	2.03	0.40
1:A:77:TYR:CE1	1:A:178:LEU:HD13	2.55	0.40
1:L:291:ARG:HA	1:L:292:PRO:HD2	1.87	0.40
1:F:159:LEU:HD13	1:G:107:LEU:HD21	2.03	0.40
1:A:111:ARG:NH1	1:A:142:MET:O	2.48	0.40
1:A:234:ASP:HB3	1:A:242:VAL:HG22	2.02	0.40
1:F:279:LYS:HD3	1:F:342:ASP:OD1	2.21	0.40
1:B:314:ASP:OD1	1:B:315:PHE:N	2.55	0.40
1:L:395:PRO:HG2	1:L:405:ARG:NH1	2.37	0.40
1:J:210:ARG:HG3	1:J:242:VAL:HG21	2.03	0.40
1:C:134:ASN:ND2	1:D:100:GLY:HA3	2.36	0.40
1:K:308:CYS:HA	1:K:324:SER:O	2.21	0.40
1:J:389:ARG:HD3	1:J:411:GLU:OE1	2.20	0.40
1:B:267:GLU:HG3	1:B:285:LEU:HD12	2.03	0.40
1:D:190:ARG:NH2	1:I:144:TRP:HZ3	2.17	0.40
1:A:313:THR:HG21	1:A:348:THR:OG1	2.21	0.40
1:A:341:LEU:HD23	1:A:347:TRP:HD1	1.86	0.40
1:B:341:LEU:HB3	1:B:347:TRP:HB2	2.04	0.40
1:K:223:CYS:HA	1:K:227:SER:O	2.22	0.40
1:C:234:ASP:HB3	1:C:242:VAL:HG22	2.03	0.40
1:H:87:VAL:HG11	1:H:90:TRP:CZ2	2.56	0.40
1:B:344:LYS:HB3	1:B:344:LYS:HE3	1.88	0.40

All (5) 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)
1:A:254:GLN:OE1	1:G:88:LYS:NZ[1_455]	2.12	0.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:LYS:NZ	1:F:254:GLN:O[1_455]	2.15	0.05
1:B:299:GLU:OE2	4:E:504:FUC:O3[1_545]	2.15	0.05
1:C:88:LYS:NZ	1:E:254:GLN:OE1[1_545]	2.17	0.03
1:B:254:GLN:O	1:E:257:LYS:NZ[1_545]	2.19	0.01

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	363/378 (96%)	340 (94%)	22 (6%)	1 (0%)	46	68
1	B	363/378 (96%)	339 (93%)	22 (6%)	2 (1%)	30	50
1	C	363/378 (96%)	342 (94%)	20 (6%)	1 (0%)	46	68
1	D	363/378 (96%)	344 (95%)	18 (5%)	1 (0%)	46	68
1	E	363/378 (96%)	343 (94%)	19 (5%)	1 (0%)	46	68
1	F	363/378 (96%)	342 (94%)	20 (6%)	1 (0%)	46	68
1	G	363/378 (96%)	340 (94%)	22 (6%)	1 (0%)	46	68
1	H	363/378 (96%)	341 (94%)	21 (6%)	1 (0%)	46	68
1	I	363/378 (96%)	338 (93%)	24 (7%)	1 (0%)	46	68
1	J	361/378 (96%)	338 (94%)	21 (6%)	2 (1%)	30	50
1	K	362/378 (96%)	339 (94%)	22 (6%)	1 (0%)	46	68
1	L	363/378 (96%)	344 (95%)	18 (5%)	1 (0%)	46	68
All	All	4353/4536 (96%)	4090 (94%)	249 (6%)	14 (0%)	46	68

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	398	ASP
1	E	398	ASP
1	F	398	ASP

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Mol	Chain	Res	Type
1	B	398	ASP
1	C	398	ASP
1	G	398	ASP
1	H	398	ASP
1	J	398	ASP
1	K	398	ASP
1	D	398	ASP
1	I	398	ASP
1	L	398	ASP
1	J	345	PRO
1	B	397	GLY

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	318/327 (97%)	310 (98%)	8 (2%)	55	82
1	B	318/327 (97%)	308 (97%)	10 (3%)	47	75
1	C	318/327 (97%)	309 (97%)	9 (3%)	51	78
1	D	318/327 (97%)	307 (96%)	11 (4%)	43	70
1	E	318/327 (97%)	310 (98%)	8 (2%)	55	82
1	F	318/327 (97%)	308 (97%)	10 (3%)	47	75
1	G	318/327 (97%)	304 (96%)	14 (4%)	35	60
1	H	318/327 (97%)	310 (98%)	8 (2%)	55	82
1	I	318/327 (97%)	307 (96%)	11 (4%)	43	70
1	J	316/327 (97%)	308 (98%)	8 (2%)	55	82
1	K	317/327 (97%)	306 (96%)	11 (4%)	43	70
1	L	318/327 (97%)	311 (98%)	7 (2%)	60	84
All	All	3813/3924 (97%)	3698 (97%)	115 (3%)	48	76

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	139	ASN
1	A	209	SER
1	A	274	ILE
1	A	275	ASN
1	A	342	ASP
1	A	348	THR
1	A	361	VAL
1	A	387	THR
1	B	139	ASN
1	B	169	ARG
1	B	209	SER
1	B	274	ILE
1	B	275	ASN
1	B	333	GLU
1	B	348	THR
1	B	361	VAL
1	B	387	THR
1	B	400	ILE
1	C	139	ASN
1	C	189	ASP
1	C	209	SER
1	C	274	ILE
1	C	342	ASP
1	C	344	LYS
1	C	348	THR
1	C	361	VAL
1	C	387	THR
1	D	139	ASN
1	D	169	ARG
1	D	189	ASP
1	D	257	LYS
1	D	260	ASN
1	D	274	ILE
1	D	329	GLN
1	D	342	ASP
1	D	348	THR
1	D	361	VAL
1	D	387	THR
1	E	84	MET
1	E	139	ASN
1	E	274	ILE
1	E	342	ASP
1	E	348	THR

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Mol	Chain	Res	Type
1	E	361	VAL
1	E	387	THR
1	E	400	ILE
1	F	139	ASN
1	F	144	TRP
1	F	145	GLU
1	F	163	GLU
1	F	274	ILE
1	F	333	GLU
1	F	348	THR
1	F	361	VAL
1	F	387	THR
1	F	400	ILE
1	G	79	ARG
1	G	139	ASN
1	G	169	ARG
1	G	188	ARG
1	G	209	SER
1	G	257	LYS
1	G	274	ILE
1	G	301	ASN
1	G	344	LYS
1	G	348	THR
1	G	361	VAL
1	G	374	THR
1	G	387	THR
1	G	400	ILE
1	H	139	ASN
1	H	169	ARG
1	H	274	ILE
1	H	344	LYS
1	H	348	THR
1	H	361	VAL
1	H	387	THR
1	H	400	ILE
1	I	79	ARG
1	I	139	ASN
1	I	144	TRP
1	I	169	ARG
1	I	190	ARG
1	I	274	ILE
1	I	276	ASN

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Mol	Chain	Res	Type
1	I	344	LYS
1	I	348	THR
1	I	361	VAL
1	I	387	THR
1	J	139	ASN
1	J	163	GLU
1	J	274	ILE
1	J	344	LYS
1	J	348	THR
1	J	361	VAL
1	J	387	THR
1	J	400	ILE
1	K	84	MET
1	K	139	ASN
1	K	169	ARG
1	K	274	ILE
1	K	293	LEU
1	K	344	LYS
1	K	348	THR
1	K	361	VAL
1	K	387	THR
1	K	400	ILE
1	K	432	ASN
1	L	106	ASP
1	L	139	ASN
1	L	274	ILE
1	L	342	ASP
1	L	348	THR
1	L	361	VAL
1	L	387	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	HIS
1	A	258	GLN
1	B	250	ASN
1	C	136	HIS
1	D	260	ASN
1	D	275	ASN
1	E	136	HIS
1	F	250	ASN

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Mol	Chain	Res	Type
1	G	136	HIS
1	I	240	GLN

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 ⓘ

12 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	A	504	1,4	14,14,15	0.48	0	15,19,21	1.10	1 (6%)
4	FUC	A	505	4	10,10,11	0.66	0	14,14,16	1.04	1 (7%)
5	NAG	B	502	1,5	14,14,15	0.49	0	15,19,21	1.25	2 (13%)
5	NAG	B	503	5	14,14,15	0.43	0	15,19,21	1.73	3 (20%)
5	FUL	B	504	5	10,10,11	1.43	2 (20%)	14,14,16	1.75	4 (28%)
4	NAG	E	503	1,4	14,14,15	0.67	0	15,19,21	1.55	3 (20%)
4	FUC	E	504	4	10,10,11	0.91	0	14,14,16	0.96	0
5	NAG	F	502	1,5	14,14,15	0.46	0	15,19,21	1.35	2 (13%)
5	NAG	F	503	5	14,14,15	0.50	0	15,19,21	1.49	3 (20%)
5	FUL	F	504	5	10,10,11	1.40	1 (10%)	14,14,16	2.01	4 (28%)
4	NAG	I	503	1,4	14,14,15	0.50	0	15,19,21	1.93	2 (13%)
4	FUC	I	504	4	10,10,11	1.10	1 (10%)	14,14,16	0.72	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	504	1,4	-	0/6/23/26	0/1/1/1
4	FUC	A	505	4	-	0/0/17/20	0/1/1/1
5	NAG	B	502	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	503	5	-	0/6/23/26	0/1/1/1
5	FUL	B	504	5	-	0/0/17/20	0/1/1/1
4	NAG	E	503	1,4	-	0/6/23/26	0/1/1/1
4	FUC	E	504	4	-	0/0/17/20	0/1/1/1
5	NAG	F	502	1,5	-	0/6/23/26	0/1/1/1
5	NAG	F	503	5	-	0/6/23/26	0/1/1/1
5	FUL	F	504	5	-	0/0/17/20	0/1/1/1
4	NAG	I	503	1,4	-	0/6/23/26	0/1/1/1
4	FUC	I	504	4	-	0/0/17/20	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	504	FUC	O5-C1	-2.46	1.39	1.43
5	B	504	FUL	C4-C3	2.08	1.57	1.52
5	F	504	FUL	C4-C5	2.56	1.58	1.52
5	B	504	FUL	C4-C5	2.87	1.58	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	503	NAG	C6-C5-C4	-2.28	107.39	113.02
4	E	503	NAG	O6-C6-C5	-2.03	104.64	111.33
5	B	504	FUL	C3-C4-C5	2.44	113.83	109.72
5	B	503	NAG	C2-N2-C7	2.48	126.23	123.04
4	E	503	NAG	C3-C4-C5	2.58	114.70	110.20
4	A	505	FUC	C1-O5-C5	2.62	116.42	112.38
5	F	503	NAG	C4-C3-C2	2.65	115.34	111.23
5	B	503	NAG	C3-C4-C5	2.65	114.81	110.20
5	B	502	NAG	C1-O5-C5	2.68	115.65	112.25
5	F	502	NAG	C1-O5-C5	2.75	115.73	112.25
5	B	502	NAG	O5-C5-C6	2.87	113.57	107.35
5	F	503	NAG	C1-O5-C5	2.94	115.97	112.25
5	B	504	FUL	C1-O5-C5	3.02	117.04	112.38
5	B	504	FUL	O2-C2-C1	3.09	115.39	109.21
5	F	504	FUL	C3-C4-C5	3.19	115.10	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	503	NAG	C4-C3-C2	3.23	116.25	111.23
5	F	502	NAG	O5-C5-C6	3.29	114.48	107.35
5	F	504	FUL	O2-C2-C1	3.40	116.02	109.21
5	B	504	FUL	O5-C5-C4	3.46	115.53	109.53
4	A	504	NAG	C1-O5-C5	3.47	116.65	112.25
5	F	503	NAG	C3-C4-C5	3.48	116.26	110.20
5	F	504	FUL	C1-O5-C5	3.70	118.10	112.38
5	F	504	FUL	O5-C5-C4	4.06	116.56	109.53
5	B	503	NAG	C1-O5-C5	4.40	117.83	112.25
4	I	503	NAG	C1-O5-C5	6.29	120.23	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	503	NAG	1	0
5	B	504	FUL	1	0
4	E	504	FUC	0	1
5	F	502	NAG	1	0
5	F	504	FUL	1	0

5.6 Ligand geometry ⓘ

Of 27 ligands modelled in this entry, 12 are monoatomic - leaving 15 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	NAG	A	502	1	14,14,15	0.45	0	15,19,21	0.96	1 (6%)
3	NAG	A	503	1	14,14,15	0.42	0	15,19,21	1.78	3 (20%)
3	NAG	B	505	-	14,14,15	0.54	0	15,19,21	1.02	0
3	NAG	C	502	1	14,14,15	0.57	0	15,19,21	1.00	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	D	502	-	14,14,15	0.49	0	15,19,21	1.30	2 (13%)
3	NAG	D	503	-	14,14,15	0.61	0	15,19,21	1.24	1 (6%)
3	NAG	D	504	-	14,14,15	0.44	0	15,19,21	3.74	4 (26%)
6	FUC	D	505	-	10,10,11	2.05	2 (20%)	14,14,16	4.62	3 (21%)
3	NAG	E	502	1	14,14,15	0.43	0	15,19,21	0.72	0
3	NAG	F	505	-	14,14,15	0.49	0	15,19,21	0.70	0
3	NAG	G	502	1	14,14,15	0.49	0	15,19,21	1.00	1 (6%)
3	NAG	H	502	1	14,14,15	0.50	0	15,19,21	1.04	1 (6%)
3	NAG	I	502	1	14,14,15	0.51	0	15,19,21	1.44	1 (6%)
3	NAG	K	502	1	14,14,15	0.53	0	15,19,21	1.13	2 (13%)
3	NAG	L	502	1	14,14,15	0.51	0	15,19,21	1.18	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	502	1	-	0/6/23/26	0/1/1/1
3	NAG	A	503	1	-	0/6/23/26	0/1/1/1
3	NAG	B	505	-	-	0/6/23/26	0/1/1/1
3	NAG	C	502	1	-	0/6/23/26	0/1/1/1
3	NAG	D	502	-	-	0/6/23/26	0/1/1/1
3	NAG	D	503	-	-	0/6/23/26	0/1/1/1
3	NAG	D	504	-	-	0/6/23/26	0/1/1/1
6	FUC	D	505	-	-	0/0/17/20	0/1/1/1
3	NAG	E	502	1	-	0/6/23/26	0/1/1/1
3	NAG	F	505	-	-	0/6/23/26	0/1/1/1
3	NAG	G	502	1	-	0/6/23/26	0/1/1/1
3	NAG	H	502	1	-	0/6/23/26	0/1/1/1
3	NAG	I	502	1	-	0/6/23/26	0/1/1/1
3	NAG	K	502	1	-	0/6/23/26	0/1/1/1
3	NAG	L	502	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)
6	D	505	FUC	C1-C2	3.91	1.61	1.52
6	D	505	FUC	C2-C3	4.84	1.59	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	505	FUC	O5-C1-C2	-15.99	84.91	110.86
3	A	503	NAG	C4-C3-C2	-2.58	107.22	111.23
3	D	504	NAG	C3-C4-C5	-2.35	106.10	110.20
3	D	504	NAG	C4-C3-C2	-2.16	107.87	111.23
3	D	502	NAG	C2-N2-C7	-2.07	120.38	123.04
3	K	502	NAG	C2-N2-C7	2.09	125.73	123.04
6	D	505	FUC	C1-O5-C5	2.21	115.79	112.38
3	C	502	NAG	C1-O5-C5	2.52	115.45	112.25
3	G	502	NAG	C1-O5-C5	2.93	115.96	112.25
3	A	502	NAG	C1-O5-C5	2.99	116.04	112.25
3	K	502	NAG	C1-O5-C5	3.22	116.34	112.25
3	H	502	NAG	C1-O5-C5	3.28	116.42	112.25
3	D	503	NAG	C1-O5-C5	3.33	116.47	112.25
3	D	502	NAG	C1-O5-C5	3.39	116.55	112.25
3	D	504	NAG	O5-C5-C6	3.55	115.04	107.35
3	L	502	NAG	C1-O5-C5	3.85	117.13	112.25
3	A	503	NAG	C2-N2-C7	3.95	128.12	123.04
3	A	503	NAG	C1-O5-C5	4.09	117.44	112.25
3	I	502	NAG	C1-O5-C5	4.46	117.90	112.25
6	D	505	FUC	C1-C2-C3	5.11	115.59	109.54
3	D	504	NAG	C1-O5-C5	13.45	129.32	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	NAG	2	0
3	B	505	NAG	2	0
3	C	502	NAG	1	0
3	D	502	NAG	1	0
3	D	503	NAG	1	0
3	D	504	NAG	1	0
3	E	502	NAG	1	0
3	F	505	NAG	1	0
3	I	502	NAG	2	0
3	L	502	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	365/378 (96%)	0.31	28 (7%) 16 18	10, 33, 79, 133	0
1	B	365/378 (96%)	0.18	12 (3%) 50 55	11, 34, 71, 137	0
1	C	365/378 (96%)	0.28	25 (6%) 20 23	12, 39, 81, 141	0
1	D	365/378 (96%)	0.42	37 (10%) 9 9	11, 38, 88, 148	0
1	E	365/378 (96%)	0.26	26 (7%) 19 21	11, 34, 82, 133	0
1	F	365/378 (96%)	0.18	12 (3%) 50 55	12, 34, 69, 140	0
1	G	365/378 (96%)	0.51	33 (9%) 12 12	14, 46, 93, 135	0
1	H	365/378 (96%)	0.57	39 (10%) 8 8	13, 45, 96, 139	0
1	I	365/378 (96%)	0.94	56 (15%) 3 3	39, 65, 106, 137	0
1	J	363/378 (96%)	1.51	107 (29%) 1 0	47, 75, 104, 146	0
1	K	364/378 (96%)	1.64	115 (31%) 1 0	45, 87, 112, 149	0
1	L	365/378 (96%)	1.46	98 (26%) 1 1	45, 84, 116, 145	0
All	All	4377/4536 (96%)	0.69	588 (13%) 4 4	10, 51, 104, 149	0

All (588) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	399	LEU	13.8
1	A	140	THR	12.7
1	C	140	THR	10.9
1	L	400	ILE	10.8
1	G	142	MET	10.7
1	K	142	MET	10.5
1	D	401	SER	10.1
1	J	399	LEU	9.9
1	L	320	LEU	9.8
1	K	141	SER	9.6
1	G	140	THR	9.6

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Mol	Chain	Res	Type	RSRZ
1	H	399	LEU	9.2
1	D	142	MET	9.1
1	E	140	THR	9.0
1	K	140	THR	9.0
1	D	400	ILE	8.9
1	I	119	LEU	8.8
1	J	144	TRP	8.8
1	C	399	LEU	8.7
1	K	305	VAL	8.6
1	L	143	GLU	8.5
1	J	178	LEU	8.5
1	K	430	GLY	8.4
1	I	419	LEU	8.1
1	J	188	ARG	8.0
1	K	375	VAL	7.9
1	C	141	SER	7.7
1	I	143	GLU	7.5
1	K	377	LEU	7.5
1	H	77	TYR	7.5
1	L	142	MET	7.4
1	L	327	MET	7.4
1	L	83	GLN	7.3
1	B	142	MET	7.3
1	G	141	SER	7.1
1	H	142	MET	7.0
1	K	78	TRP	7.0
1	H	140	THR	6.9
1	C	402	GLY	6.8
1	L	119	LEU	6.8
1	L	80	ALA	6.7
1	K	401	SER	6.7
1	J	325	CYS	6.7
1	K	376	SER	6.7
1	I	137	LEU	6.6
1	J	208	ALA	6.6
1	H	403	CYS	6.4
1	B	140	THR	6.4
1	D	144	TRP	6.3
1	I	144	TRP	6.3
1	D	399	LEU	6.3
1	E	79	ARG	6.3
1	J	82	SER	6.2

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Mol	Chain	Res	Type	RSRZ
1	L	178	LEU	6.2
1	J	143	GLU	6.2
1	E	144	TRP	6.2
1	L	81	LYS	6.1
1	J	344	LYS	6.1
1	C	77	TYR	6.1
1	J	140	THR	5.9
1	D	402	GLY	5.9
1	J	119	LEU	5.9
1	K	144	TRP	5.9
1	B	189	ASP	5.8
1	J	339	PHE	5.8
1	G	399	LEU	5.7
1	K	326	LYS	5.7
1	L	398	ASP	5.7
1	L	321	THR	5.6
1	L	82	SER	5.6
1	I	397	GLY	5.6
1	G	78	TRP	5.5
1	F	142	MET	5.5
1	J	398	ASP	5.5
1	A	141	SER	5.4
1	L	319	GLY	5.4
1	C	139	ASN	5.4
1	H	78	TRP	5.3
1	K	339	PHE	5.3
1	L	144	TRP	5.3
1	B	144	TRP	5.2
1	L	271	CYS	5.1
1	L	308	CYS	5.1
1	K	271	CYS	5.1
1	F	143	GLU	5.1
1	K	379	TYR	5.1
1	A	144	TRP	5.1
1	D	77	TYR	5.1
1	A	402	GLY	5.1
1	F	140	THR	5.0
1	G	139	ASN	5.0
1	K	341	LEU	5.0
1	D	78	TRP	5.0
1	L	286	TRP	5.0
1	H	397	GLY	4.9

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Mol	Chain	Res	Type	RSRZ
1	D	79	ARG	4.9
1	H	80	ALA	4.9
1	I	434	PRO	4.9
1	C	144	TRP	4.9
1	D	403	CYS	4.9
1	C	398	ASP	4.9
1	J	286	TRP	4.9
1	E	143	GLU	4.8
1	K	391	GLY	4.8
1	K	403	CYS	4.8
1	H	398	ASP	4.8
1	J	310	GLY	4.8
1	J	390	SER	4.8
1	K	139	ASN	4.7
1	G	77	TYR	4.7
1	C	78	TRP	4.7
1	L	401	SER	4.7
1	D	140	THR	4.7
1	K	392	PHE	4.6
1	L	79	ARG	4.6
1	K	383	SER	4.6
1	I	141	SER	4.6
1	J	408	PHE	4.5
1	L	190	ARG	4.5
1	C	401	SER	4.5
1	G	269	SER	4.5
1	H	269	SER	4.4
1	J	142	MET	4.4
1	I	399	LEU	4.4
1	K	86	GLU	4.4
1	B	373	GLY	4.4
1	E	139	ASN	4.4
1	K	262	THR	4.4
1	D	398	ASP	4.4
1	K	286	TRP	4.4
1	K	255	ARG	4.3
1	K	264	ILE	4.3
1	K	434	PRO	4.3
1	D	141	SER	4.3
1	H	400	ILE	4.3
1	K	355	SER	4.3
1	J	263	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
1	J	407	CYS	4.2
1	J	120	THR	4.2
1	L	274	ILE	4.2
1	L	251	GLY	4.2
1	A	77	TYR	4.2
1	J	392	PHE	4.2
1	I	120	THR	4.2
1	G	143	GLU	4.2
1	H	84	MET	4.2
1	G	79	ARG	4.1
1	L	396	LYS	4.1
1	L	297	THR	4.1
1	J	209	SER	4.1
1	K	178	LEU	4.1
1	D	143	GLU	4.1
1	L	392	PHE	4.1
1	K	407	CYS	4.0
1	F	79	ARG	4.0
1	D	84	MET	4.0
1	K	80	ALA	4.0
1	L	261	THR	4.0
1	C	373	GLY	4.0
1	K	269	SER	4.0
1	K	279	LYS	4.0
1	J	187	GLY	4.0
1	K	328	ALA	3.9
1	L	223	CYS	3.9
1	K	400	ILE	3.9
1	I	326	LYS	3.9
1	I	324	SER	3.9
1	L	84	MET	3.9
1	H	79	ARG	3.9
1	K	222	ILE	3.9
1	L	432	ASN	3.8
1	H	144	TRP	3.8
1	E	211	GLY	3.8
1	J	338	GLY	3.8
1	K	304	ILE	3.7
1	K	143	GLU	3.7
1	L	333	GLU	3.7
1	J	373	GLY	3.7
1	L	329	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
1	K	327	MET	3.7
1	K	404	GLN	3.7
1	L	408	PHE	3.7
1	L	231	ILE	3.7
1	I	136	HIS	3.7
1	J	355	SER	3.7
1	K	390	SER	3.7
1	L	139	ASN	3.7
1	K	254	GLN	3.6
1	D	391	GLY	3.6
1	L	89	GLY	3.6
1	J	429	CYS	3.6
1	J	216	LEU	3.6
1	J	205	THR	3.6
1	A	344	LYS	3.6
1	J	333	GLU	3.6
1	K	318	GLY	3.6
1	E	399	LEU	3.6
1	L	270	THR	3.5
1	D	219	SER	3.5
1	K	408	PHE	3.5
1	L	326	LYS	3.5
1	I	277	LEU	3.5
1	L	78	TRP	3.5
1	J	395	PRO	3.5
1	A	322	THR	3.5
1	E	141	SER	3.5
1	J	218	ASN	3.5
1	I	302	TYR	3.5
1	J	354	GLU	3.5
1	K	431	ILE	3.5
1	K	176	ASP	3.5
1	K	270	THR	3.5
1	J	391	GLY	3.4
1	K	315	PHE	3.4
1	G	144	TRP	3.4
1	H	344	LYS	3.4
1	G	81	LYS	3.4
1	K	239	ASN	3.4
1	L	344	LYS	3.4
1	L	363	GLU	3.4
1	J	189	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	188	ARG	3.4
1	A	142	MET	3.4
1	K	154	GLY	3.4
1	J	256	TRP	3.3
1	L	120	THR	3.3
1	K	365	ILE	3.3
1	K	276	ASN	3.3
1	E	434	PRO	3.3
1	K	384	ASN	3.3
1	K	198	TYR	3.3
1	L	301	ASN	3.3
1	A	80	ALA	3.3
1	I	331	LYS	3.3
1	J	84	MET	3.3
1	J	276	ASN	3.3
1	H	401	SER	3.2
1	G	374	THR	3.2
1	J	215	ARG	3.2
1	K	251	GLY	3.2
1	C	79	ARG	3.2
1	L	93	THR	3.2
1	K	329	GLN	3.2
1	L	272	TYR	3.2
1	L	309	ASN	3.2
1	J	85	CYS	3.2
1	J	306	GLU	3.2
1	E	142	MET	3.2
1	A	143	GLU	3.2
1	J	190	ARG	3.2
1	L	199	GLY	3.2
1	L	373	GLY	3.2
1	J	340	ILE	3.2
1	K	330	GLU	3.2
1	H	189	ASP	3.1
1	L	310	GLY	3.1
1	L	238	VAL	3.1
1	A	321	THR	3.1
1	I	221	CYS	3.1
1	F	77	TYR	3.1
1	H	402	GLY	3.1
1	B	82	SER	3.1
1	G	403	CYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	400	ILE	3.1
1	L	239	ASN	3.1
1	F	321	THR	3.1
1	L	264	ILE	3.1
1	D	281	THR	3.0
1	D	269	SER	3.0
1	J	123	PHE	3.0
1	K	405	ARG	3.0
1	K	344	LYS	3.0
1	I	142	MET	3.0
1	K	120	THR	3.0
1	L	334	GLY	3.0
1	K	421	MET	3.0
1	K	121	SER	3.0
1	I	78	TRP	3.0
1	K	277	LEU	3.0
1	I	95	ARG	3.0
1	K	321	THR	3.0
1	L	123	PHE	2.9
1	J	177	GLY	2.9
1	L	386	ARG	2.9
1	H	143	GLU	2.9
1	J	80	ALA	2.9
1	K	340	ILE	2.9
1	D	139	ASN	2.9
1	C	344	LYS	2.9
1	L	262	THR	2.9
1	J	403	CYS	2.9
1	K	272	TYR	2.9
1	L	86	GLU	2.9
1	I	437	ASN	2.9
1	K	280	CYS	2.9
1	K	338	GLY	2.9
1	I	320	LEU	2.9
1	J	86	GLU	2.9
1	C	81	LYS	2.9
1	I	319	GLY	2.9
1	J	121	SER	2.8
1	L	298	LYS	2.8
1	J	217	PRO	2.8
1	L	307	PRO	2.8
1	G	274	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	K	238	VAL	2.8
1	K	281	THR	2.8
1	K	368	GLY	2.8
1	I	330	GLU	2.8
1	K	409	TRP	2.8
1	J	139	ASN	2.8
1	L	77	TYR	2.8
1	I	375	VAL	2.8
1	K	283	THR	2.8
1	L	240	GLN	2.8
1	I	77	TYR	2.8
1	H	408	PHE	2.8
1	J	328	ALA	2.8
1	I	378	SER	2.8
1	J	343	GLU	2.8
1	L	225	GLU	2.8
1	A	281	THR	2.7
1	L	208	ALA	2.7
1	B	399	LEU	2.7
1	B	141	SER	2.7
1	A	403	CYS	2.7
1	G	402	GLY	2.7
1	J	264	ILE	2.7
1	E	409	TRP	2.7
1	K	362	LEU	2.7
1	B	143	GLU	2.7
1	L	176	ASP	2.7
1	C	138	LEU	2.7
1	I	377	LEU	2.7
1	G	209	SER	2.7
1	I	402	GLY	2.7
1	I	344	LYS	2.7
1	G	210	ARG	2.7
1	H	409	TRP	2.7
1	L	409	TRP	2.7
1	E	77	TYR	2.7
1	J	300	LEU	2.7
1	J	141	SER	2.7
1	K	366	PRO	2.7
1	D	409	TRP	2.7
1	H	391	GLY	2.7
1	D	189	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	I	384	ASN	2.7
1	J	301	ASN	2.7
1	K	136	HIS	2.6
1	J	401	SER	2.6
1	C	143	GLU	2.6
1	K	268	TYR	2.6
1	D	188	ARG	2.6
1	J	393	PHE	2.6
1	K	220	GLU	2.6
1	L	339	PHE	2.6
1	I	308	CYS	2.6
1	L	280	CYS	2.6
1	A	190	ARG	2.6
1	J	242	VAL	2.6
1	E	390	SER	2.6
1	J	170	SER	2.6
1	J	172	SER	2.6
1	J	337	GLN	2.6
1	K	200	GLU	2.6
1	D	271	CYS	2.6
1	E	100	GLY	2.6
1	I	407	CYS	2.6
1	E	209	SER	2.6
1	F	141	SER	2.6
1	K	189	ASP	2.6
1	G	326	LYS	2.6
1	K	119	LEU	2.6
1	A	78	TRP	2.6
1	G	268	TYR	2.5
1	H	373	GLY	2.5
1	H	426	SER	2.5
1	K	219	SER	2.5
1	L	259	LEU	2.5
1	D	113	ALA	2.5
1	J	428	PHE	2.5
1	L	402	GLY	2.5
1	F	323	PRO	2.5
1	I	114	TYR	2.5
1	C	142	MET	2.5
1	K	282	GLY	2.5
1	C	83	GLN	2.5
1	G	188	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	J	345	PRO	2.5
1	J	138	LEU	2.5
1	J	259	LEU	2.5
1	L	145	GLU	2.5
1	H	224	ILE	2.5
1	K	117	CYS	2.5
1	H	139	ASN	2.5
1	L	433	SER	2.5
1	D	178	LEU	2.5
1	K	216	LEU	2.5
1	J	270	THR	2.5
1	E	391	GLY	2.5
1	K	221	CYS	2.5
1	C	82	SER	2.5
1	G	401	SER	2.5
1	K	410	LEU	2.5
1	G	270	THR	2.5
1	L	252	THR	2.5
1	I	79	ARG	2.5
1	C	403	CYS	2.4
1	K	201	GLU	2.4
1	F	322	THR	2.4
1	J	241	SER	2.4
1	J	371	SER	2.4
1	L	404	GLN	2.4
1	K	180	TRP	2.4
1	K	274	ILE	2.4
1	I	80	ALA	2.4
1	J	341	LEU	2.4
1	K	214	LEU	2.4
1	J	225	GLU	2.4
1	L	140	THR	2.4
1	A	79	ARG	2.4
1	I	376	SER	2.4
1	H	283	THR	2.4
1	J	389	ARG	2.4
1	E	329	GLN	2.4
1	L	390	SER	2.4
1	K	406	ILE	2.4
1	L	222	ILE	2.4
1	L	256	TRP	2.4
1	D	217	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	217	PRO	2.4
1	G	301	ASN	2.4
1	A	282	GLY	2.4
1	D	270	THR	2.4
1	K	278	ILE	2.4
1	J	409	TRP	2.3
1	A	339	PHE	2.3
1	D	138	LEU	2.3
1	J	299	GLU	2.3
1	K	356	SER	2.3
1	J	358	ASN	2.3
1	K	237	ASN	2.3
1	L	173	ALA	2.3
1	E	83	GLN	2.3
1	I	325	CYS	2.3
1	I	333	GLU	2.3
1	J	372	GLU	2.3
1	H	410	LEU	2.3
1	G	390	SER	2.3
1	F	237	ASN	2.3
1	L	260	ASN	2.3
1	K	346	ALA	2.3
1	I	83	GLN	2.3
1	F	144	TRP	2.3
1	E	322	THR	2.3
1	G	217	PRO	2.3
1	I	92	PRO	2.3
1	D	392	PHE	2.3
1	J	202	VAL	2.3
1	F	299	GLU	2.3
1	A	211	GLY	2.3
1	C	391	GLY	2.3
1	L	257	LYS	2.3
1	H	95	ARG	2.3
1	E	401	SER	2.3
1	I	138	LEU	2.3
1	A	398	ASP	2.3
1	G	344	LYS	2.3
1	E	208	ALA	2.3
1	J	231	ILE	2.3
1	H	240	GLN	2.3
1	I	300	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	J	179	LYS	2.3
1	J	260	ASN	2.3
1	J	298	LYS	2.3
1	K	137	LEU	2.3
1	K	101	PRO	2.3
1	L	210	ARG	2.3
1	J	222	ILE	2.2
1	A	326	LYS	2.2
1	J	135	GLN	2.2
1	D	171	SER	2.2
1	I	339	PHE	2.2
1	J	206	PHE	2.2
1	K	175	PHE	2.2
1	C	259	LEU	2.2
1	A	210	ARG	2.2
1	J	173	ALA	2.2
1	H	237	ASN	2.2
1	A	217	PRO	2.2
1	K	353	ALA	2.2
1	C	269	SER	2.2
1	G	82	SER	2.2
1	J	163	GLU	2.2
1	J	169	ARG	2.2
1	I	166	LEU	2.2
1	J	410	LEU	2.2
1	L	203	THR	2.2
1	L	220	GLU	2.2
1	I	356	SER	2.2
1	J	95	ARG	2.2
1	L	340	ILE	2.2
1	K	399	LEU	2.2
1	I	238	VAL	2.2
1	A	83	GLN	2.2
1	H	392	PHE	2.2
1	K	229	PHE	2.2
1	L	273	THR	2.2
1	L	405	ARG	2.2
1	L	96	GLY	2.2
1	D	240	GLN	2.2
1	E	189	ASP	2.2
1	I	189	ASP	2.2
1	K	213	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	K	432	ASN	2.2
1	K	82	SER	2.1
1	L	141	SER	2.1
1	G	304	ILE	2.1
1	J	400	ILE	2.1
1	C	326	LYS	2.1
1	K	428	PHE	2.1
1	I	98	PRO	2.1
1	K	236	PRO	2.1
1	L	250	ASN	2.1
1	J	375	VAL	2.1
1	K	115	VAL	2.1
1	J	81	LYS	2.1
1	B	190	ARG	2.1
1	A	399	LEU	2.1
1	K	217	PRO	2.1
1	C	397	GLY	2.1
1	J	211	GLY	2.1
1	A	269	SER	2.1
1	H	225	GLU	2.1
1	J	237	ASN	2.1
1	G	320	LEU	2.1
1	I	362	LEU	2.1
1	A	270	THR	2.1
1	A	283	THR	2.1
1	K	316	PRO	2.1
1	H	199	GLY	2.1
1	J	223	CYS	2.1
1	K	295	ARG	2.1
1	J	247	GLU	2.1
1	D	119	LEU	2.1
1	J	350	LYS	2.1
1	J	250	ASN	2.1
1	L	367	ASN	2.1
1	G	119	LEU	2.1
1	J	89	GLY	2.1
1	I	200	GLU	2.1
1	D	172	SER	2.1
1	G	208	ALA	2.1
1	D	83	GLN	2.1
1	L	275	ASN	2.1
1	B	79	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	255	ARG	2.1
1	K	79	ARG	2.1
1	L	325	CYS	2.1
1	H	333	GLU	2.1
1	I	236	PRO	2.1
1	L	378	SER	2.1
1	K	83	GLN	2.0
1	I	276	ASN	2.0
1	G	225	GLU	2.0
1	E	373	GLY	2.0
1	I	177	GLY	2.0
1	H	271	CYS	2.0
1	J	249	GLN	2.0
1	D	372	GLU	2.0
1	E	309	ASN	2.0
1	I	363	GLU	2.0
1	K	331	LYS	2.0
1	L	87	VAL	2.0
1	D	282	GLY	2.0
1	E	269	SER	2.0
1	J	329	GLN	2.0
1	L	296	PHE	2.0
1	L	188	ARG	2.0
1	H	301	ASN	2.0
1	I	275	ASN	2.0
1	J	282	GLY	2.0
1	L	397	GLY	2.0
1	H	194	ILE	2.0
1	J	396	LYS	2.0
1	K	172	SER	2.0
1	J	284	ASN	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	FUC	I	504	10/11	0.86	0.27	2.32	74,79,86,87	0
4	NAG	I	503	14/15	0.86	0.22	1.06	35,55,67,68	0
4	FUC	E	504	10/11	0.88	0.16	0.67	54,57,61,63	0
4	FUC	A	505	10/11	0.91	0.17	-0.09	26,46,53,63	0
4	NAG	A	504	14/15	0.91	0.15	-0.14	38,48,52,52	0
4	NAG	E	503	14/15	0.91	0.15	-0.16	45,48,54,55	0
5	NAG	F	503	14/15	0.65	0.37	-	89,95,101,102	0
5	FUL	B	504	10/11	0.90	0.18	-	68,80,83,84	0
5	NAG	B	503	14/15	0.89	0.24	-	86,92,96,96	0
5	NAG	B	502	14/15	0.94	0.16	-	60,69,80,83	0
5	NAG	F	502	14/15	0.89	0.21	-	55,67,75,82	0
5	FUL	F	504	10/11	0.87	0.13	-	54,61,69,70	0

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	FUC	D	505	10/11	0.89	0.24	5.49	46,59,84,86	0
3	NAG	A	503	14/15	0.76	0.43	2.19	83,99,103,104	0
3	NAG	E	502	14/15	0.80	0.31	1.50	83,97,100,101	0
2	CA	C	501	1/1	0.99	0.17	0.40	37,37,37,37	0
2	CA	A	501	1/1	0.98	0.17	0.16	34,34,34,34	0
2	CA	H	501	1/1	0.98	0.13	-0.25	37,37,37,37	0
2	CA	B	501	1/1	0.97	0.12	-0.38	42,42,42,42	0
2	CA	D	501	1/1	0.99	0.11	-0.55	33,33,33,33	0
2	CA	F	501	1/1	0.97	0.12	-0.71	45,45,45,45	0
2	CA	E	501	1/1	0.96	0.11	-0.72	41,41,41,41	0
2	CA	I	501	1/1	0.97	0.08	-1.23	51,51,51,51	0
2	CA	L	501	1/1	0.75	0.08	-1.38	84,84,84,84	0
2	CA	G	501	1/1	0.98	0.03	-2.00	28,28,28,28	0
2	CA	J	501	1/1	0.94	0.05	-2.17	65,65,65,65	0
2	CA	K	501	1/1	0.98	0.03	-3.05	51,51,51,51	0
3	NAG	L	502	14/15	0.61	0.31	-	75,86,94,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	B	505	14/15	0.78	0.20	-	64,76,81,83	0
3	NAG	D	502	14/15	0.71	0.21	-	75,87,90,91	0
3	NAG	C	502	14/15	0.84	0.22	-	44,53,61,64	0
3	NAG	D	503	14/15	0.79	0.22	-	49,73,79,83	0
3	NAG	G	502	14/15	0.80	0.18	-	64,72,75,75	0
3	NAG	D	504	14/15	0.82	0.17	-	30,81,85,85	0
3	NAG	I	502	14/15	0.68	0.37	-	79,85,89,91	0
3	NAG	H	502	14/15	0.83	0.21	-	54,67,82,84	0
3	NAG	F	505	14/15	0.82	0.23	-	63,81,85,86	0
3	NAG	A	502	14/15	0.56	0.37	-	82,102,105,105	0
3	NAG	K	502	14/15	0.69	0.51	-	73,86,92,93	0

6.5 Other polymers [i](#)

There are no such residues in this entry.