



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2017 – 06:02 AM EDT

PDB ID : 5W6R
Title : Crystal structure of the A/Puerto Rico/8/1934 (H1N1) influenza virus hemagglutinin in complex with cyclic peptide CP141099 (P6)
Authors : Wilson, I.A.; Kadam, R.U.
Deposited on : unknown
Resolution : 2.73 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030345

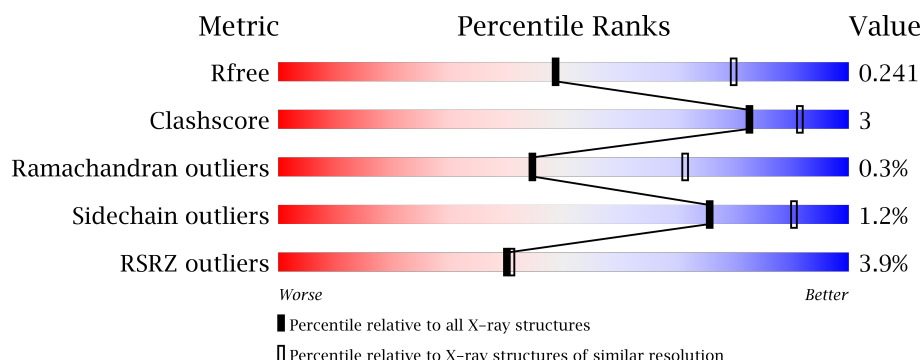
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.73 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}	100719	3342 (2.78-2.70)
Clashscore	112137	3731 (2.78-2.70)
Ramachandran outliers	110173	3670 (2.78-2.70)
Sidechain outliers	110143	3671 (2.78-2.70)
RSRZ outliers	101464	3362 (2.78-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	326	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 91%; height: 10px; background-color: green;"></div> <div style="width: 7%; height: 10px; background-color: yellow;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 0% 91% 7% • </div> </div>
1	C	326	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 88%; height: 10px; background-color: green;"></div> <div style="width: 10%; height: 10px; background-color: yellow;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 0% 88% 10% •• </div> </div>
1	E	326	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 91%; height: 10px; background-color: green;"></div> <div style="width: 7%; height: 10px; background-color: yellow;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 0% 91% 7% •• </div> </div>
1	G	326	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 88%; height: 10px; background-color: green;"></div> <div style="width: 10%; height: 10px; background-color: yellow;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 0% 88% 10% •• </div> </div>
2	B	176	<div> <div style="width: 10%; height: 10px; background-color: red;"></div> <div style="width: 92%; height: 10px; background-color: green;"></div> <div style="width: 5%; height: 10px; background-color: yellow;"></div> <div style="width: 3%; height: 10px; background-color: grey;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 10% 92% 5% • </div> </div>

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Mol	Chain	Length	Quality of chain
2	D	176	
2	F	176	
2	H	176	
3	M	12	
3	N	12	
3	O	12	
3	Q	12	

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
4	NAG	C	405	X	-	-	-
4	NAG	G	405	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16630 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	0	0
			2542	1603	443	483	13			
1	C	322	Total	C	N	O	S	0	0	0
			2542	1603	443	483	13			
1	E	322	Total	C	N	O	S	0	0	0
			2542	1603	443	483	13			
1	G	322	Total	C	N	O	S	0	0	0
			2542	1603	443	483	13			

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	171	Total	C	N	O	S	0	0	0
			1380	866	235	272	7			
2	D	171	Total	C	N	O	S	0	0	0
			1380	866	235	272	7			
2	F	171	Total	C	N	O	S	0	0	0
			1380	866	235	272	7			
2	H	171	Total	C	N	O	S	0	0	0
			1380	866	235	272	7			

- Molecule 3 is a protein called ACE-PH8-ORN-LEU-GLU-TYR-PHE-GLU-TRP-LEU-SER-9WV.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	M	12	Total	C	N	O	0	0	0
			112	78	15	19			
3	O	12	Total	C	N	O	0	0	0
			112	78	15	19			
3	N	12	Total	C	N	O	0	0	0
			112	78	15	19			
3	Q	12	Total	C	N	O	0	0	0
			112	78	15	19			

- Molecule 4 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	H	1	Total	C	N	O	0	0
			14	8	1	5		
4	H	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	21	Total	O	0	0
			21	21		
5	B	2	Total	O	0	0
			2	2		
5	C	21	Total	O	0	0
			21	21		
5	D	7	Total	O	0	0
			7	7		

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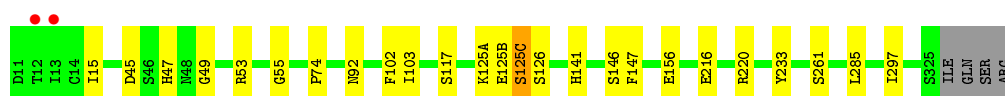
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	20	Total 20	O 20	0	0
5	F	3	Total 3	O 3	0	0
5	G	25	Total 25	O 25	0	0
5	H	3	Total 3	O 3	0	0

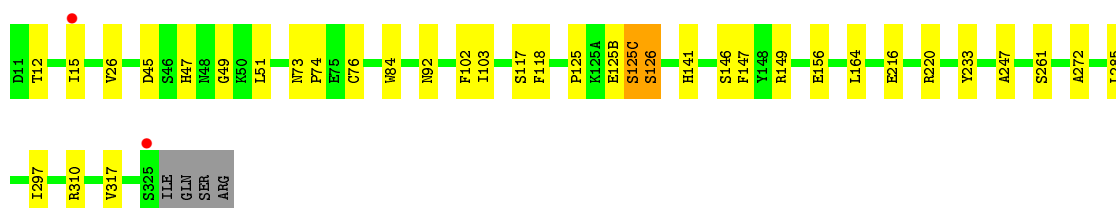
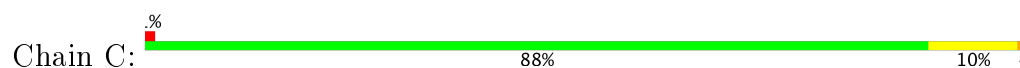
3 Residue-property plots [i](#)

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



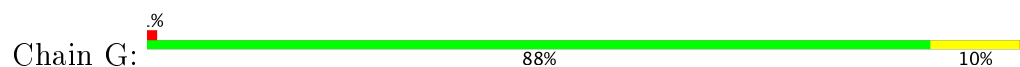
- Molecule 1: Hemagglutinin



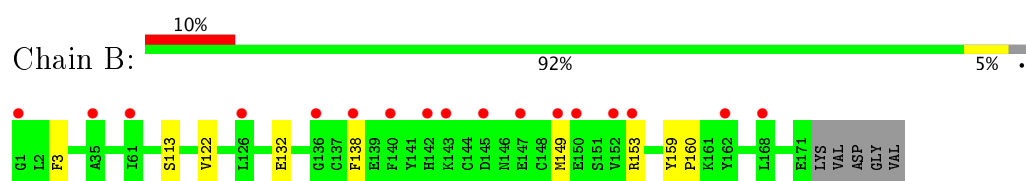
- Molecule 1: Hemagglutinin



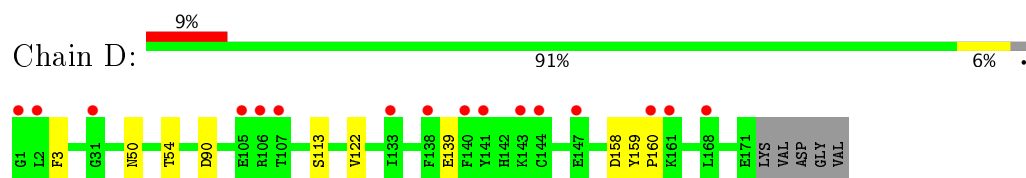
- Molecule 1: Hemagglutinin



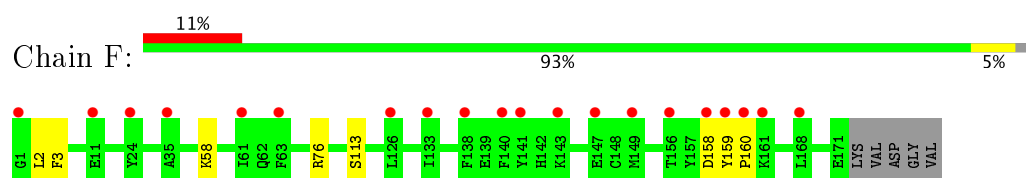
- Molecule 2: Hemagglutinin



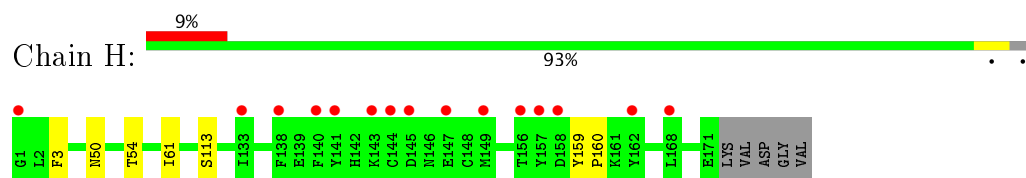
- Molecule 2: Hemagglutinin



- Molecule 2: Hemagglutinin



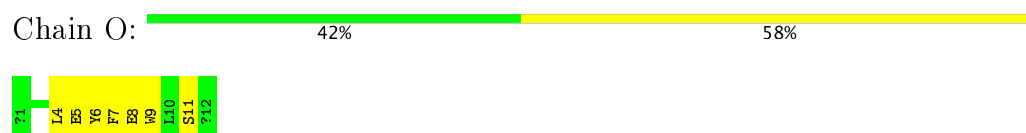
- Molecule 2: Hemagglutinin



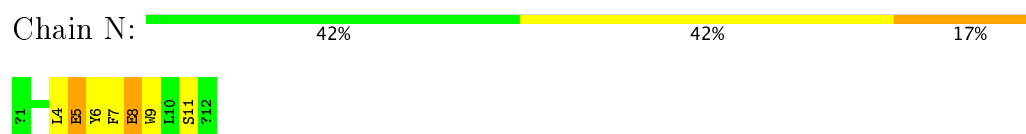
- Molecule 3: ACE-PH8-ORN-LEU-GLU-TYR-PHE-GLU-TRP-LEU-SER-9WV



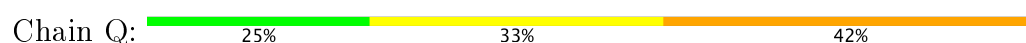
- Molecule 3: ACE-PH8-ORN-LEU-GLU-TYR-PHE-GLU-TRP-LEU-SER-9WV



- Molecule 3: ACE-PH8-ORN-LEU-GLU-TYR-PHE-GLU-TRP-LEU-SER-9WV



- Molecule 3: ACE-PH8-ORN-LEU-GLU-TYR-PHE-GLU-TRP-LEU-SER-9WV





4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	234.46 Å 234.46 Å 144.56 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.34 – 2.73 44.34 – 2.73	Depositor EDS
% Data completeness (in resolution range)	96.8 (44.34-2.73) 96.8 (44.34-2.73)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.73 Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.198 , 0.239 0.204 , 0.241	Depositor DCC
R_{free} test set	3816 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	73.9	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for $-1/3^*h+1/3^*k+4/3^*l, -k, 2/3^*h+1/3^*k+1/3^*l$ 0.024 for $-2/3^*h-1/3^*k-4/3^*l, -1/3^*h-2/3^*k+4/3^*l, -1/3^*h+1/3^*k+1/3^*l$ 0.022 for $-h, 1/3^*h-1/3^*k-4/3^*l, -1/3^*h-2/3^*k+1/3^*l$ 0.398 for $-1/3^*h-2/3^*k+4/3^*l, -2/3^*h-1/3^*k-4/3^*l, 1/3^*h-1/3^*k-1/3^*l$ 0.368 for $-h, 2/3^*h+1/3^*k+4/3^*l, 1/3^*h+2/3^*k-1/3^*l$ 0.379 for $1/3^*h+2/3^*k-4/3^*l, -k, -2/3^*h-1/3^*k-1/3^*l$ 0.026 for $h, -h-k, -l$	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16630	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ORN, 9WV, PH8, NAG, ACE

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	0.25	0/2606	0.40	0/3544
1	C	0.26	0/2606	0.42	0/3544
1	E	0.26	0/2606	0.41	0/3544
1	G	0.26	0/2606	0.41	0/3544
2	B	0.28	0/1407	0.39	0/1891
2	D	0.28	0/1407	0.40	0/1891
2	F	0.28	0/1407	0.39	0/1891
2	H	0.28	0/1407	0.39	0/1891
3	M	2.57	10/80 (12.5%)	1.39	0/108
3	N	2.59	10/80 (12.5%)	1.37	0/108
3	O	2.58	9/80 (11.2%)	1.35	0/108
3	Q	2.60	12/80 (15.0%)	1.38	0/108
All	All	0.45	41/16372 (0.3%)	0.44	0/22172

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	6	TYR	CB-CG	-7.92	1.39	1.51
3	O	6	TYR	CB-CG	-7.75	1.40	1.51
3	Q	6	TYR	CB-CG	-7.73	1.40	1.51
3	M	6	TYR	CB-CG	-7.67	1.40	1.51
3	Q	7	PHE	CB-CG	-7.03	1.39	1.51
3	O	7	PHE	CB-CG	-6.87	1.39	1.51
3	N	7	PHE	CB-CG	-6.70	1.40	1.51
3	M	7	PHE	CB-CG	-6.67	1.40	1.51
3	N	9	TRP	CG-CD2	-6.34	1.32	1.43
3	O	9	TRP	CG-CD2	-6.25	1.33	1.43
3	M	9	TRP	CG-CD2	-6.25	1.33	1.43
3	M	9	TRP	CD2-CE2	-6.16	1.33	1.41
3	N	9	TRP	CD2-CE2	-6.12	1.34	1.41
3	O	9	TRP	CD2-CE2	-6.10	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Q	9	TRP	CD2-CE2	-6.08	1.34	1.41
3	Q	9	TRP	CG-CD2	-6.08	1.33	1.43
3	Q	10	LEU	CA-C	-5.81	1.37	1.52
3	Q	11	SER	CA-C	-5.46	1.38	1.52
3	N	8	GLU	CA-C	-5.37	1.39	1.52
3	Q	8	GLU	CA-C	-5.37	1.39	1.52
3	Q	9	TRP	CA-C	-5.35	1.39	1.52
3	O	11	SER	CA-C	-5.33	1.39	1.52
3	Q	6	TYR	CA-C	-5.28	1.39	1.52
3	M	11	SER	CA-C	-5.28	1.39	1.52
3	N	11	SER	CA-C	-5.27	1.39	1.52
3	O	6	TYR	CA-C	-5.24	1.39	1.52
3	N	6	TYR	CA-C	-5.24	1.39	1.52
3	M	5	GLU	CA-C	-5.22	1.39	1.52
3	O	8	GLU	CA-C	-5.22	1.39	1.52
3	Q	4	LEU	CA-C	-5.22	1.39	1.52
3	Q	7	PHE	CA-C	-5.21	1.39	1.52
3	N	9	TRP	CA-C	-5.18	1.39	1.52
3	M	4	LEU	CA-C	-5.16	1.39	1.52
3	Q	5	GLU	CA-C	-5.16	1.39	1.52
3	M	6	TYR	CA-C	-5.14	1.39	1.52
3	O	5	GLU	CA-C	-5.11	1.39	1.52
3	O	4	LEU	CA-C	-5.07	1.39	1.52
3	M	8	GLU	CA-C	-5.05	1.39	1.52
3	N	5	GLU	CA-C	-5.02	1.40	1.52
3	N	7	PHE	CA-C	-5.01	1.40	1.52
3	M	10	LEU	CA-C	-5.01	1.40	1.52

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2542	0	2470	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2542	0	2469	22	0
1	E	2542	0	2470	14	0
1	G	2542	0	2469	20	0
2	B	1380	0	1309	6	0
2	D	1380	0	1309	7	0
2	F	1380	0	1309	6	0
2	H	1380	0	1309	5	0
3	M	112	0	89	0	0
3	N	112	0	89	1	0
3	O	112	0	90	0	0
3	Q	112	0	89	1	0
4	A	70	0	64	0	0
4	B	28	0	25	1	0
4	C	70	0	64	0	0
4	D	28	0	25	2	0
4	E	70	0	64	0	0
4	F	28	0	25	1	0
4	G	70	0	64	0	0
4	H	28	0	25	1	0
5	A	21	0	0	0	0
5	B	2	0	0	0	0
5	C	21	0	0	0	0
5	D	7	0	0	0	0
5	E	20	0	0	0	0
5	F	3	0	0	0	0
5	G	25	0	0	1	0
5	H	3	0	0	0	0
All	All	16630	0	15827	95	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (95) 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)
2:D:50:ASN:O	2:D:54:THR:HG23	1.63	0.97
1:A:117:SER:HB3	1:A:261:SER:OG	1.66	0.96
2:H:50:ASN:O	2:H:54:THR:HG23	1.67	0.93
1:C:117:SER:HB3	1:C:261:SER:OG	1.68	0.93
1:G:117:SER:HB3	1:G:261:SER:OG	1.77	0.83
1:E:117:SER:HB3	1:E:261:SER:OG	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:GLU:O	1:A:220:ARG:NH2	2.25	0.70
1:C:125(B):GLU:O	1:C:125(C):SER:HB3	1.91	0.70
1:G:125(B):GLU:O	1:G:125(C):SER:HB3	1.93	0.69
1:C:125:PRO:O	1:C:126:SER:OG	2.11	0.67
1:A:117:SER:CB	1:A:261:SER:OG	2.45	0.63
1:A:117:SER:HB3	1:A:261:SER:HG	1.62	0.63
1:C:216:GLU:O	1:C:220:ARG:NH2	2.33	0.62
4:H:201:NAG:O3	4:H:202:NAG:O5	2.19	0.60
4:F:201:NAG:O3	4:F:202:NAG:O5	2.19	0.59
1:C:117:SER:CB	1:C:261:SER:OG	2.48	0.59
4:B:201:NAG:O3	4:B:202:NAG:O5	2.19	0.57
3:Q:11:SER:O	3:Q:12:9WV:N	2.38	0.57
1:E:125:PRO:O	1:E:126:SER:OG	2.22	0.56
1:E:216:GLU:O	1:E:220:ARG:NH2	2.39	0.55
1:A:47:HIS:HB3	1:A:297:ILE:HD13	1.87	0.55
1:G:117:SER:CB	1:G:261:SER:OG	2.53	0.55
4:D:201:NAG:HO3	4:D:202:NAG:C1	2.21	0.54
1:G:125:PRO:O	1:G:126:SER:OG	2.26	0.54
1:A:53:ARG:NH1	1:A:55:GLY:O	2.42	0.53
1:C:47:HIS:HB3	1:C:297:ILE:HD13	1.90	0.52
1:E:117:SER:HB3	1:E:261:SER:HG	1.72	0.52
1:G:216:GLU:O	1:G:220:ARG:NH2	2.42	0.52
1:E:47:HIS:HB3	1:E:297:ILE:HD13	1.95	0.48
2:F:76:ARG:HB2	5:G:507:HOH:O	2.12	0.48
1:G:47:HIS:HB3	1:G:297:ILE:HD13	1.95	0.48
1:G:51:LEU:HG	1:G:272:ALA:HB3	1.96	0.47
2:B:3:PHE:CE2	2:B:113:SER:HB2	2.49	0.47
1:G:74:PRO:HB2	1:G:141:HIS:HB2	1.95	0.47
1:E:66:ILE:HG12	1:E:89:GLU:OE1	2.15	0.47
2:B:132:GLU:HG2	2:B:138:PHE:CE1	2.50	0.46
1:A:53:ARG:NH2	1:G:119:GLU:OE1	2.39	0.46
4:D:201:NAG:O3	4:D:202:NAG:O5	2.19	0.46
1:C:45:ASP:N	1:C:45:ASP:OD1	2.49	0.46
1:C:125(B):GLU:HA	1:C:125(B):GLU:OE1	2.15	0.46
1:E:76:CYS:O	1:E:149:ARG:NH2	2.38	0.46
1:E:45:ASP:OD1	1:E:45:ASP:N	2.49	0.46
2:F:2:LEU:O	2:H:113:SER:OG	2.28	0.46
1:A:15:ILE:HD11	2:B:122:VAL:HG21	1.98	0.45
1:G:146:SER:OG	1:G:147:PHE:N	2.47	0.45
1:G:103:ILE:HG13	1:G:233:TYR:CE2	2.51	0.45
1:C:103:ILE:HG13	1:C:233:TYR:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:310:ARG:NH1	2:D:90:ASP:OD1	2.38	0.45
1:G:45:ASP:N	1:G:45:ASP:OD1	2.49	0.45
1:G:80:LEU:HB2	1:G:83:ARG:HD3	1.98	0.45
1:C:51:LEU:HG	1:C:272:ALA:HB3	1.98	0.45
1:E:146:SER:OG	1:E:147:PHE:N	2.48	0.45
1:E:73:ASN:HA	1:E:74:PRO:HD3	1.81	0.45
1:A:45:ASP:OD1	1:A:45:ASP:N	2.50	0.45
2:H:159:TYR:HB3	2:H:160:PRO:HD3	1.99	0.45
1:G:92:ASN:N	1:G:92:ASN:OD1	2.49	0.44
2:B:159:TYR:HB3	2:B:160:PRO:HD3	1.99	0.44
2:H:3:PHE:CE2	2:H:113:SER:HB2	2.52	0.44
1:G:73:ASN:HA	1:G:74:PRO:HD3	1.82	0.44
1:C:146:SER:OG	1:C:147:PHE:N	2.47	0.43
1:C:15:ILE:HD11	2:D:122:VAL:HG21	2.00	0.43
2:F:3:PHE:CE2	2:F:113:SER:HB2	2.52	0.43
2:D:159:TYR:HB3	2:D:160:PRO:HD3	1.98	0.43
2:F:159:TYR:HB3	2:F:160:PRO:HD3	2.01	0.43
1:A:49:GLY:HA2	1:A:285:LEU:O	2.19	0.43
1:E:53:ARG:NH1	1:E:55:GLY:O	2.52	0.43
2:D:3:PHE:CE2	2:D:113:SER:HB2	2.53	0.43
1:E:26:VAL:HG21	1:E:317:VAL:HB	2.01	0.43
1:G:53:ARG:NH1	1:G:55:GLY:O	2.52	0.43
2:F:58:LYS:HA	2:F:58:LYS:HD3	1.84	0.43
1:E:74:PRO:HB2	1:E:141:HIS:HB2	2.01	0.43
1:C:74:PRO:HB2	1:C:141:HIS:HB2	2.01	0.42
1:C:12:THR:HG22	2:D:139:GLU:HA	2.01	0.42
2:D:158:ASP:OD1	2:D:160:PRO:HD2	2.18	0.42
1:A:146:SER:OG	1:A:147:PHE:N	2.48	0.42
2:B:132:GLU:HG2	2:B:138:PHE:HE1	1.83	0.42
1:G:304:GLU:HB3	2:H:61:ILE:HG21	2.02	0.42
1:A:74:PRO:HB2	1:A:141:HIS:HB2	2.01	0.42
1:C:26:VAL:HG21	1:C:317:VAL:HB	2.02	0.41
1:A:103:ILE:HG13	1:A:233:TYR:CE2	2.54	0.41
1:C:49:GLY:HA2	1:C:285:LEU:O	2.19	0.41
1:C:76:CYS:O	1:C:149:ARG:NH2	2.40	0.41
1:G:129:ASN:HA	1:G:157:LYS:HD3	2.02	0.41
2:B:149:MET:O	2:B:153:ARG:HG3	2.20	0.41
1:C:84:TRP:CZ3	1:C:118:PHE:HD2	2.39	0.41
1:C:92:ASN:OD1	1:C:92:ASN:N	2.48	0.41
1:G:71:LEU:O	1:G:148:TYR:HB3	2.21	0.41
3:N:4:LEU:HD23	3:N:4:LEU:HA	1.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:158:ASP:OD1	2:F:160:PRO:HD2	2.20	0.40
1:G:66:ILE:HG12	1:G:89:GLU:OE1	2.21	0.40
1:A:92:ASN:OD1	1:A:92:ASN:N	2.48	0.40
1:C:73:ASN:HA	1:C:74:PRO:HD3	1.83	0.40
1:A:125(B):GLU:O	1:A:125(C):SER:CB	2.69	0.40
1:C:164:LEU:HG	1:C:247:ALA:O	2.21	0.40
1:E:125(B):GLU:O	1:E:125(C):SER:CB	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	320/326 (98%)	308 (96%)	10 (3%)	2 (1%)	28	54
1	C	320/326 (98%)	308 (96%)	11 (3%)	1 (0%)	44	71
1	E	320/326 (98%)	307 (96%)	12 (4%)	1 (0%)	44	71
1	G	320/326 (98%)	308 (96%)	10 (3%)	2 (1%)	28	54
2	B	169/176 (96%)	164 (97%)	5 (3%)	0	100	100
2	D	169/176 (96%)	164 (97%)	5 (3%)	0	100	100
2	F	169/176 (96%)	164 (97%)	5 (3%)	0	100	100
2	H	169/176 (96%)	164 (97%)	5 (3%)	0	100	100
3	M	7/12 (58%)	6 (86%)	1 (14%)	0	100	100
3	N	7/12 (58%)	4 (57%)	3 (43%)	0	100	100
3	O	7/12 (58%)	3 (43%)	4 (57%)	0	100	100
3	Q	7/12 (58%)	4 (57%)	3 (43%)	0	100	100
All	All	1984/2056 (96%)	1904 (96%)	74 (4%)	6 (0%)	44	71

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	125(A)	LYS
1	A	125(C)	SER
1	C	125(C)	SER
1	E	125(C)	SER
1	G	125(C)	SER
1	G	125(A)	LYS

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	285/289 (99%)	282 (99%)	3 (1%)	78	91
1	C	285/289 (99%)	282 (99%)	3 (1%)	78	91
1	E	285/289 (99%)	282 (99%)	3 (1%)	78	91
1	G	285/289 (99%)	280 (98%)	5 (2%)	64	86
2	B	147/151 (97%)	147 (100%)	0	100	100
2	D	147/151 (97%)	147 (100%)	0	100	100
2	F	147/151 (97%)	147 (100%)	0	100	100
2	H	147/151 (97%)	147 (100%)	0	100	100
3	M	8/8 (100%)	7 (88%)	1 (12%)	5	11
3	N	8/8 (100%)	6 (75%)	2 (25%)	1	1
3	O	8/8 (100%)	8 (100%)	0	100	100
3	Q	8/8 (100%)	4 (50%)	4 (50%)	0	0
All	All	1760/1792 (98%)	1739 (99%)	21 (1%)	75	90

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	PHE
1	A	126	SER
1	A	156	GLU
1	C	102	PHE
1	C	126	SER

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Mol	Chain	Res	Type
1	C	156	GLU
1	E	102	PHE
1	E	126	SER
1	E	156	GLU
1	G	102	PHE
1	G	125(C)	SER
1	G	126	SER
1	G	156	GLU
1	G	261	SER
3	M	5	GLU
3	N	5	GLU
3	N	8	GLU
3	Q	4	LEU
3	Q	5	GLU
3	Q	8	GLU
3	Q	10	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	9WV	M	12	3	9,10,11	2.80	1 (11%)	6,11,13	1.14	0
3	PH8	M	2	3	13,13,14	1.40	2 (15%)	12,15,17	0.78	0
3	ORN	M	3	3	7,7,8	3.16	1 (14%)	4,7,9	1.38	1 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	9WV	N	12	3	9,10,11	3.06	1 (11%)	6,11,13	0.91	0
3	PH8	N	2	3	13,13,14	1.42	2 (15%)	12,15,17	0.86	0
3	ORN	N	3	3	7,7,8	2.87	1 (14%)	4,7,9	1.00	0
3	9WV	O	12	3	9,10,11	2.92	1 (11%)	6,11,13	0.92	0
3	PH8	O	2	3	13,13,14	1.42	2 (15%)	12,15,17	0.79	0
3	ORN	O	3	3	7,7,8	3.10	1 (14%)	4,7,9	1.44	1 (25%)
3	9WV	Q	12	3	9,10,11	2.71	1 (11%)	6,11,13	1.21	1 (16%)
3	PH8	Q	2	3	13,13,14	1.40	2 (15%)	12,15,17	0.81	0
3	ORN	Q	3	3	7,7,8	3.24	1 (14%)	4,7,9	1.12	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
3	9WV	M	12	3	-	0/9/11/13	0/0/0/0
3	PH8	M	2	3	-	0/6/8/10	0/1/1/1
3	ORN	M	3	3	-	0/4/6/8	0/0/0/0
3	9WV	N	12	3	-	0/9/11/13	0/0/0/0
3	PH8	N	2	3	-	0/6/8/10	0/1/1/1
3	ORN	N	3	3	-	0/4/6/8	0/0/0/0
3	9WV	O	12	3	-	0/9/11/13	0/0/0/0
3	PH8	O	2	3	-	0/6/8/10	0/1/1/1
3	ORN	O	3	3	-	0/4/6/8	0/0/0/0
3	9WV	Q	12	3	-	0/9/11/13	0/0/0/0
3	PH8	Q	2	3	-	0/6/8/10	0/1/1/1
3	ORN	Q	3	3	-	0/4/6/8	0/0/0/0

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	12	9WV	CA-C	-8.93	1.38	1.50
3	O	12	9WV	CA-C	-8.54	1.39	1.50
3	Q	3	ORN	CA-C	-8.49	1.39	1.50
3	M	3	ORN	CA-C	-8.30	1.39	1.50
3	M	12	9WV	CA-C	-8.17	1.39	1.50
3	O	3	ORN	CA-C	-8.08	1.39	1.50
3	Q	12	9WV	CA-C	-7.92	1.39	1.50
3	N	3	ORN	CA-C	-7.43	1.40	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	2	PH8	CJ-CG	-4.25	1.39	1.51
3	Q	2	PH8	CJ-CG	-4.15	1.39	1.51
3	O	2	PH8	CJ-CG	-4.13	1.39	1.51
3	M	2	PH8	CJ-CG	-4.08	1.39	1.51
3	N	2	PH8	CA-C	2.53	1.53	1.50
3	Q	2	PH8	CA-C	2.55	1.53	1.50
3	M	2	PH8	CA-C	2.60	1.53	1.50
3	O	2	PH8	CA-C	2.67	1.53	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	12	9WV	O-C-CA	-2.29	119.81	125.15
3	O	3	ORN	CB-CA-C	-2.27	107.91	111.65
3	M	3	ORN	CB-CA-C	-2.25	107.94	111.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Q	12	9WV	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

28 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
4	NAG	A	401	1	14,14,15	1.04	0	15,19,21	1.38	2 (13%)
4	NAG	A	402	1,4	14,14,15	0.57	0	15,19,21	1.20	2 (13%)
4	NAG	A	403	4	14,14,15	1.18	2 (14%)	15,19,21	1.61	2 (13%)
4	NAG	A	404	1	14,14,15	0.26	0	15,19,21	0.60	0
4	NAG	A	405	1	14,14,15	1.06	1 (7%)	15,19,21	1.66	3 (20%)
4	NAG	B	201	2,4	14,14,15	0.63	0	15,19,21	1.54	2 (13%)
4	NAG	B	202	4	14,14,15	0.56	0	15,19,21	1.71	3 (20%)
4	NAG	C	401	1	14,14,15	1.04	1 (7%)	15,19,21	1.39	2 (13%)
4	NAG	C	402	1,4	14,14,15	0.55	0	15,19,21	1.21	2 (13%)
4	NAG	C	403	4	14,14,15	1.17	2 (14%)	15,19,21	1.61	2 (13%)
4	NAG	C	404	1	14,14,15	0.27	0	15,19,21	0.60	0
4	NAG	C	405	1	14,14,15	1.04	1 (7%)	15,19,21	1.66	3 (20%)
4	NAG	D	201	2,4	14,14,15	0.63	0	15,19,21	1.55	2 (13%)
4	NAG	D	202	4	14,14,15	0.56	0	15,19,21	1.71	3 (20%)
4	NAG	E	401	1	14,14,15	1.04	1 (7%)	15,19,21	1.38	2 (13%)
4	NAG	E	402	1,4	14,14,15	0.57	0	15,19,21	1.20	2 (13%)
4	NAG	E	403	4	14,14,15	1.17	2 (14%)	15,19,21	1.60	2 (13%)
4	NAG	E	404	1	14,14,15	0.25	0	15,19,21	0.60	0
4	NAG	E	405	1	14,14,15	1.05	1 (7%)	15,19,21	1.66	3 (20%)
4	NAG	F	201	2,4	14,14,15	0.63	0	15,19,21	1.53	2 (13%)
4	NAG	F	202	4	14,14,15	0.55	0	15,19,21	1.71	3 (20%)
4	NAG	G	401	1	14,14,15	1.04	1 (7%)	15,19,21	1.38	2 (13%)
4	NAG	G	402	1,4	14,14,15	0.56	0	15,19,21	1.22	3 (20%)
4	NAG	G	403	4	14,14,15	1.17	2 (14%)	15,19,21	1.60	2 (13%)
4	NAG	G	404	1	14,14,15	0.26	0	15,19,21	0.60	0
4	NAG	G	405	1	14,14,15	1.06	1 (7%)	15,19,21	1.65	3 (20%)
4	NAG	H	201	2,4	14,14,15	0.64	0	15,19,21	1.54	2 (13%)
4	NAG	H	202	4	14,14,15	0.57	0	15,19,21	1.70	3 (20%)

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	401	1	-	0/6/23/26	0/1/1/1
4	NAG	A	402	1,4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	403	4	-	0/6/23/26	0/1/1/1
4	NAG	A	404	1	-	0/6/23/26	0/1/1/1
4	NAG	A	405	1	-	0/6/23/26	0/1/1/1
4	NAG	B	201	2,4	-	0/6/23/26	0/1/1/1
4	NAG	B	202	4	-	0/6/23/26	0/1/1/1
4	NAG	C	401	1	-	0/6/23/26	0/1/1/1
4	NAG	C	402	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	403	4	-	0/6/23/26	0/1/1/1
4	NAG	C	404	1	-	0/6/23/26	0/1/1/1
4	NAG	C	405	1	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	D	201	2,4	-	0/6/23/26	0/1/1/1
4	NAG	D	202	4	-	0/6/23/26	0/1/1/1
4	NAG	E	401	1	-	0/6/23/26	0/1/1/1
4	NAG	E	402	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	403	4	-	0/6/23/26	0/1/1/1
4	NAG	E	404	1	-	0/6/23/26	0/1/1/1
4	NAG	E	405	1	-	0/6/23/26	0/1/1/1
4	NAG	F	201	2,4	-	0/6/23/26	0/1/1/1
4	NAG	F	202	4	-	0/6/23/26	0/1/1/1
4	NAG	G	401	1	-	0/6/23/26	0/1/1/1
4	NAG	G	402	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	403	4	-	0/6/23/26	0/1/1/1
4	NAG	G	404	1	-	0/6/23/26	0/1/1/1
4	NAG	G	405	1	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	H	201	2,4	-	0/6/23/26	0/1/1/1
4	NAG	H	202	4	-	0/6/23/26	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	403	NAG	O5-C1	-2.28	1.40	1.43
4	A	403	NAG	O5-C1	-2.27	1.40	1.43
4	E	403	NAG	O5-C1	-2.24	1.40	1.43
4	C	403	NAG	O5-C1	-2.22	1.40	1.43
4	G	405	NAG	C2-N2	-2.20	1.42	1.46
4	A	405	NAG	C2-N2	-2.17	1.42	1.46
4	C	405	NAG	C2-N2	-2.14	1.42	1.46
4	G	403	NAG	C2-N2	-2.14	1.42	1.46
4	E	405	NAG	C2-N2	-2.14	1.42	1.46
4	E	403	NAG	C2-N2	-2.13	1.42	1.46
4	C	403	NAG	C2-N2	-2.11	1.42	1.46
4	A	403	NAG	C2-N2	-2.10	1.42	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	401	NAG	C2-N2	-2.02	1.42	1.46
4	G	401	NAG	C2-N2	-2.01	1.42	1.46
4	E	401	NAG	C2-N2	-2.00	1.42	1.46

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	201	NAG	C6-C5-C4	-4.80	101.78	113.00
4	B	201	NAG	C6-C5-C4	-4.77	101.83	113.00
4	H	201	NAG	C6-C5-C4	-4.77	101.84	113.00
4	F	201	NAG	C6-C5-C4	-4.76	101.86	113.00
4	D	202	NAG	C2-N2-C7	-4.66	116.14	122.94
4	F	202	NAG	C2-N2-C7	-4.65	116.17	122.94
4	B	202	NAG	C2-N2-C7	-4.64	116.18	122.94
4	A	403	NAG	O5-C1-C2	-4.63	105.04	111.47
4	C	403	NAG	O5-C1-C2	-4.62	105.04	111.47
4	H	202	NAG	C2-N2-C7	-4.62	116.21	122.94
4	G	403	NAG	O5-C1-C2	-4.61	105.06	111.47
4	E	403	NAG	O5-C1-C2	-4.60	105.07	111.47
4	H	202	NAG	C4-C3-C2	-3.09	106.49	111.02
4	B	202	NAG	C4-C3-C2	-3.08	106.50	111.02
4	F	202	NAG	C4-C3-C2	-3.06	106.53	111.02
4	D	202	NAG	C4-C3-C2	-3.05	106.54	111.02
4	A	405	NAG	C6-C5-C4	-2.88	106.26	113.00
4	E	405	NAG	C6-C5-C4	-2.87	106.28	113.00
4	C	405	NAG	C6-C5-C4	-2.87	106.28	113.00
4	G	405	NAG	C6-C5-C4	-2.86	106.31	113.00
4	C	405	NAG	O5-C1-C2	-2.73	107.67	111.47
4	E	405	NAG	O5-C1-C2	-2.68	107.74	111.47
4	A	405	NAG	O5-C1-C2	-2.66	107.77	111.47
4	G	405	NAG	O5-C1-C2	-2.64	107.80	111.47
4	C	401	NAG	O5-C1-C2	-2.59	107.87	111.47
4	G	401	NAG	O5-C1-C2	-2.58	107.88	111.47
4	A	401	NAG	O5-C1-C2	-2.57	107.89	111.47
4	E	401	NAG	O5-C1-C2	-2.57	107.89	111.47
4	D	202	NAG	C3-C4-C5	-2.56	105.70	110.22
4	F	202	NAG	C3-C4-C5	-2.55	105.72	110.22
4	B	202	NAG	C3-C4-C5	-2.55	105.73	110.22
4	H	202	NAG	C3-C4-C5	-2.53	105.76	110.22
4	B	201	NAG	O5-C1-C2	-2.39	108.14	111.47
4	D	201	NAG	O5-C1-C2	-2.39	108.15	111.47
4	H	201	NAG	O5-C1-C2	-2.38	108.17	111.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	201	NAG	O5-C1-C2	-2.36	108.19	111.47
4	C	402	NAG	O5-C1-C2	-2.30	108.28	111.47
4	G	402	NAG	O5-C1-C2	-2.29	108.28	111.47
4	A	402	NAG	O5-C1-C2	-2.28	108.30	111.47
4	E	402	NAG	O5-C1-C2	-2.28	108.30	111.47
4	G	402	NAG	O4-C4-C3	-2.08	105.83	110.36
4	A	402	NAG	O4-C4-C3	-2.05	105.89	110.36
4	E	402	NAG	O4-C4-C3	-2.05	105.89	110.36
4	C	402	NAG	O4-C4-C3	-2.05	105.90	110.36
4	G	402	NAG	C2-N2-C7	-2.03	119.98	122.94
4	G	403	NAG	C1-O5-C5	2.06	115.00	112.17
4	E	403	NAG	C1-O5-C5	2.09	115.05	112.17
4	C	403	NAG	C1-O5-C5	2.11	115.07	112.17
4	A	403	NAG	C1-O5-C5	2.12	115.08	112.17
4	E	401	NAG	C1-O5-C5	2.91	116.17	112.17
4	A	401	NAG	C1-O5-C5	2.94	116.22	112.17
4	G	401	NAG	C1-O5-C5	2.95	116.24	112.17
4	C	401	NAG	C1-O5-C5	2.96	116.25	112.17
4	G	405	NAG	C1-O5-C5	3.24	116.63	112.17
4	A	405	NAG	C1-O5-C5	3.24	116.64	112.17
4	E	405	NAG	C1-O5-C5	3.25	116.65	112.17
4	C	405	NAG	C1-O5-C5	3.26	116.66	112.17

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	C	405	NAG	C1
4	G	405	NAG	C1

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	201	NAG	1	0
4	B	202	NAG	1	0
4	D	201	NAG	2	0
4	D	202	NAG	2	0
4	F	201	NAG	1	0
4	F	202	NAG	1	0
4	H	201	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	202	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, 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	322/326 (98%)	0.10	2 (0%) 89 91	51, 71, 104, 145	0
1	C	322/326 (98%)	0.01	2 (0%) 89 91	49, 71, 102, 141	0
1	E	322/326 (98%)	0.08	4 (1%) 79 81	51, 71, 105, 144	0
1	G	322/326 (98%)	-0.02	3 (0%) 84 86	51, 70, 101, 133	0
2	B	171/176 (97%)	0.65	17 (9%) 8 7	46, 100, 141, 153	0
2	D	171/176 (97%)	0.78	16 (9%) 9 8	44, 100, 143, 158	0
2	F	171/176 (97%)	0.69	20 (11%) 5 4	44, 98, 137, 153	0
2	H	171/176 (97%)	0.63	15 (8%) 11 9	44, 97, 140, 156	0
3	M	8/12 (66%)	0.65	0 100 100	85, 100, 109, 126	0
3	N	8/12 (66%)	0.20	0 100 100	93, 101, 109, 118	0
3	O	8/12 (66%)	0.07	0 100 100	88, 97, 106, 117	0
3	Q	8/12 (66%)	-0.16	0 100 100	86, 99, 105, 111	0
All	All	2004/2056 (97%)	0.27	79 (3%) 40 41	44, 78, 133, 158	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	138	PHE	6.1
2	F	138	PHE	5.8
2	D	143	LYS	5.1
2	B	143	LYS	5.0
2	B	138	PHE	4.8
2	D	147	GLU	4.4
2	H	138	PHE	4.3
2	D	1	GLY	4.3
2	F	147	GLU	4.2
2	B	147	GLU	4.1
2	H	168	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
2	D	141	TYR	3.9
2	D	140	PHE	3.8
2	H	147	GLU	3.7
2	B	35	ALA	3.3
2	D	160	PRO	3.3
2	H	143	LYS	3.1
2	D	144	CYS	3.0
2	H	133	ILE	2.9
2	B	136	GLY	2.9
2	F	143	LYS	2.9
2	B	140	PHE	2.9
1	C	325	SER	2.8
2	B	126	LEU	2.8
2	B	149	MET	2.8
2	F	63	PHE	2.7
2	F	158	ASP	2.7
2	D	168	LEU	2.7
2	F	61	ILE	2.7
2	F	149	MET	2.7
1	G	325	SER	2.7
1	A	12	THR	2.7
2	B	162	TYR	2.7
1	E	12	THR	2.6
2	F	1	GLY	2.6
2	H	157	TYR	2.5
2	H	158	ASP	2.5
1	E	325	SER	2.5
2	F	140	PHE	2.5
2	F	126	LEU	2.5
2	D	31	GLY	2.5
2	D	133	ILE	2.5
2	F	168	LEU	2.4
1	E	15	ILE	2.4
2	H	156	THR	2.4
2	B	61	ILE	2.4
1	G	12	THR	2.4
2	F	133	ILE	2.4
2	H	162	TYR	2.4
2	D	2	LEU	2.4
2	H	140	PHE	2.3
2	F	159	TYR	2.3
1	C	15	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	142	HIS	2.3
2	F	156	THR	2.3
2	F	161	LYS	2.3
1	G	142	GLU	2.3
2	H	145	ASP	2.3
2	D	161	LYS	2.2
2	B	168	LEU	2.2
2	B	152	VAL	2.2
2	F	35	ALA	2.2
2	F	24	TYR	2.2
2	F	141	TYR	2.2
2	B	1	GLY	2.2
2	D	106	ARG	2.2
2	B	153	ARG	2.2
2	D	107	THR	2.2
2	H	144	CYS	2.1
2	D	105	GLU	2.1
2	H	1	GLY	2.1
2	F	160	PRO	2.1
2	B	150	GLU	2.1
1	A	13	ILE	2.1
2	F	11	GLU	2.1
2	H	141	TYR	2.1
1	E	142	GLU	2.1
2	B	145	ASP	2.0
2	H	149	MET	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
3	PH8	Q	2	13/14	0.91	0.26	-	83,97,104,105	0
3	PH8	M	2	13/14	0.95	0.33	-	81,95,102,105	0
3	9WV	O	12	11/12	0.92	0.16	-	96,107,110,113	0
3	PH8	N	2	13/14	0.89	0.28	-	81,92,107,108	0
3	ORN	O	3	8/9	0.90	0.14	-	86,88,99,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	ORN	M	3	8/9	0.91	0.19	-	91,97,115,119	0
3	9WV	M	12	11/12	0.89	0.17	-	101,111,117,122	0
3	9WV	Q	12	11/12	0.90	0.12	-	98,105,112,115	0
3	ORN	Q	3	8/9	0.94	0.19	-	86,91,101,107	0
3	ORN	N	3	8/9	0.90	0.17	-	93,97,110,118	0
3	PH8	O	2	13/14	0.96	0.21	-	80,91,104,104	0
3	9WV	N	12	11/12	0.85	0.14	-	87,104,116,118	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	G	402	14/15	0.86	0.29	-	134,144,162,163	0
4	NAG	A	405	14/15	0.73	0.34	-	126,142,155,158	0
4	NAG	D	202	14/15	0.76	0.42	-	150,181,194,197	0
4	NAG	A	404	14/15	0.70	0.33	-	126,142,155,157	0
4	NAG	G	404	14/15	0.79	0.28	-	134,141,149,150	0
4	NAG	A	401	14/15	0.86	0.37	-	115,154,165,165	0
4	NAG	B	201	14/15	0.83	0.34	-	153,164,180,182	0
4	NAG	E	402	14/15	0.78	0.27	-	132,143,159,167	0
4	NAG	A	402	14/15	0.87	0.18	-	125,145,165,170	0
4	NAG	E	401	14/15	0.86	0.50	-	124,160,175,181	0
4	NAG	C	402	14/15	0.81	0.19	-	127,142,162,164	0
4	NAG	C	403	14/15	0.76	0.47	-	126,169,190,199	0
4	NAG	G	403	14/15	0.75	0.44	-	129,165,193,201	0
4	NAG	E	404	14/15	0.77	0.25	-	132,145,151,155	0
4	NAG	H	201	14/15	0.82	0.36	-	140,169,177,180	0
4	NAG	E	405	14/15	0.80	0.26	-	122,138,145,146	0
4	NAG	C	405	14/15	0.66	0.37	-	109,132,142,146	0
4	NAG	F	201	14/15	0.83	0.34	-	161,171,176,177	0
4	NAG	C	401	14/15	0.85	0.32	-	150,167,175,179	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	E	403	14/15	0.62	0.42	-	126,165,187,194	0
4	NAG	C	404	14/15	0.80	0.34	-	135,147,153,154	0
4	NAG	B	202	14/15	0.76	0.36	-	136,170,177,179	0
4	NAG	H	202	14/15	0.64	0.44	-	148,169,185,185	0
4	NAG	F	202	14/15	0.59	0.48	-	150,176,191,192	0
4	NAG	G	401	14/15	0.82	0.37	-	125,154,164,166	0
4	NAG	G	405	14/15	0.71	0.36	-	120,137,147,149	0
4	NAG	A	403	14/15	0.81	0.39	-	154,170,195,205	0
4	NAG	D	201	14/15	0.83	0.35	-	159,173,183,183	0

6.5 Other polymers [i](#)

There are no such residues in this entry.