



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 2, 2017 – 07:56 PM EDT

PDB ID : 3UBQ
Title : Influenza hemagglutinin from the 2009 pandemic in complex with ligand 3SLN
Authors : Xu, R.; Wilson, I.A.
Deposited on : unknown
Resolution : 2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

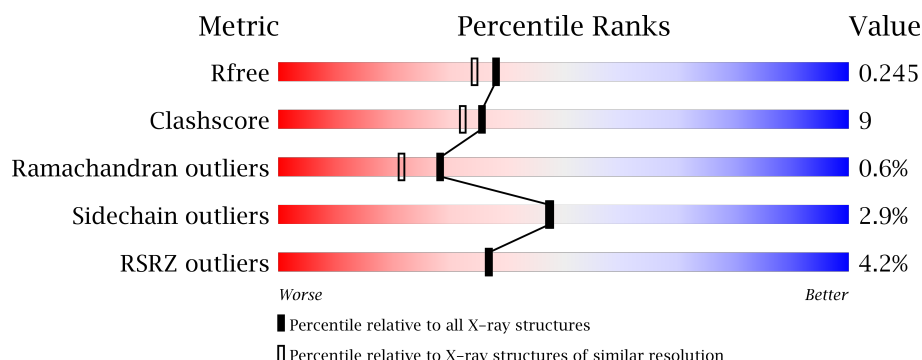
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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	329	<div> <div>2%</div> <div>75%</div> <div>21%</div> <div>..</div> </div>
1	C	329	<div> <div>2%</div> <div>74%</div> <div>22%</div> <div>..</div> </div>
1	E	329	<div> <div>%</div> <div>76%</div> <div>20%</div> <div>..</div> </div>
1	G	329	<div> <div>%</div> <div>78%</div> <div>19%</div> <div>..</div> </div>
1	I	329	<div> <div>%</div> <div>81%</div> <div>15%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	K	329	
2	B	177	
2	D	177	
2	F	177	
2	H	177	
2	J	177	
2	L	177	

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	K	651	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 24675 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called hemagglutinin HA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2522	1595	432	482	13			
1	C	321	Total	C	N	O	S	0	0	0
			2509	1588	430	478	13			
1	E	321	Total	C	N	O	S	0	0	0
			2504	1585	430	476	13			
1	G	323	Total	C	N	O	S	0	0	0
			2522	1595	432	482	13			
1	I	319	Total	C	N	O	S	0	0	0
			2495	1579	428	475	13			
1	K	318	Total	C	N	O	S	0	0	0
			2490	1576	427	474	13			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	PRO	-	EXPRESSION TAG	UNP C3W5S1
A	10	GLY	-	EXPRESSION TAG	UNP C3W5S1
A	205	CYS	GLY	ENGINEERED MUTATION	UNP C3W5S1
A	220	CYS	ARG	ENGINEERED MUTATION	UNP C3W5S1
C	9	PRO	-	EXPRESSION TAG	UNP C3W5S1
C	10	GLY	-	EXPRESSION TAG	UNP C3W5S1
C	205	CYS	GLY	ENGINEERED MUTATION	UNP C3W5S1
C	220	CYS	ARG	ENGINEERED MUTATION	UNP C3W5S1
E	9	PRO	-	EXPRESSION TAG	UNP C3W5S1
E	10	GLY	-	EXPRESSION TAG	UNP C3W5S1
E	205	CYS	GLY	ENGINEERED MUTATION	UNP C3W5S1
E	220	CYS	ARG	ENGINEERED MUTATION	UNP C3W5S1
G	9	PRO	-	EXPRESSION TAG	UNP C3W5S1
G	10	GLY	-	EXPRESSION TAG	UNP C3W5S1
G	205	CYS	GLY	ENGINEERED MUTATION	UNP C3W5S1
G	220	CYS	ARG	ENGINEERED MUTATION	UNP C3W5S1
I	9	PRO	-	EXPRESSION TAG	UNP C3W5S1

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Chain	Residue	Modelled	Actual	Comment	Reference
I	10	GLY	-	EXPRESSION TAG	UNP C3W5S1
I	205	CYS	GLY	ENGINEERED MUTATION	UNP C3W5S1
I	220	CYS	ARG	ENGINEERED MUTATION	UNP C3W5S1
K	9	PRO	-	EXPRESSION TAG	UNP C3W5S1
K	10	GLY	-	EXPRESSION TAG	UNP C3W5S1
K	205	CYS	GLY	ENGINEERED MUTATION	UNP C3W5S1
K	220	CYS	ARG	ENGINEERED MUTATION	UNP C3W5S1

- Molecule 2 is a protein called hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	169	Total	C	N	O	S	0	0	0
			1360	855	229	270	6			
2	D	170	Total	C	N	O	S	0	0	0
			1371	861	233	271	6			
2	F	170	Total	C	N	O	S	0	0	0
			1371	861	233	271	6			
2	H	172	Total	C	N	O	S	0	0	0
			1389	871	235	277	6			
2	J	170	Total	C	N	O	S	0	0	0
			1371	861	233	271	6			
2	L	169	Total	C	N	O	S	0	0	0
			1360	855	229	270	6			

There are 18 discrepancies between the modelled and reference sequences:

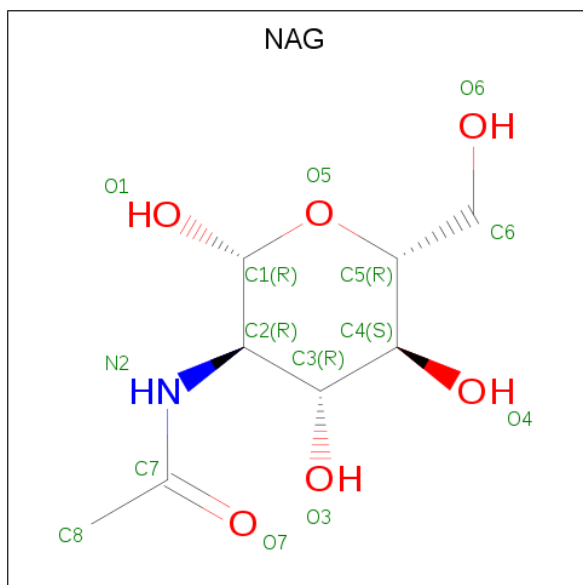
Chain	Residue	Modelled	Actual	Comment	Reference
B	175	SER	-	EXPRESSION TAG	UNP C3W5S1
B	176	GLY	-	EXPRESSION TAG	UNP C3W5S1
B	177	ARG	-	EXPRESSION TAG	UNP C3W5S1
D	175	SER	-	EXPRESSION TAG	UNP C3W5S1
D	176	GLY	-	EXPRESSION TAG	UNP C3W5S1
D	177	ARG	-	EXPRESSION TAG	UNP C3W5S1
F	175	SER	-	EXPRESSION TAG	UNP C3W5S1
F	176	GLY	-	EXPRESSION TAG	UNP C3W5S1
F	177	ARG	-	EXPRESSION TAG	UNP C3W5S1
H	175	SER	-	EXPRESSION TAG	UNP C3W5S1
H	176	GLY	-	EXPRESSION TAG	UNP C3W5S1
H	177	ARG	-	EXPRESSION TAG	UNP C3W5S1
J	175	SER	-	EXPRESSION TAG	UNP C3W5S1
J	176	GLY	-	EXPRESSION TAG	UNP C3W5S1
J	177	ARG	-	EXPRESSION TAG	UNP C3W5S1

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Chain	Residue	Modelled	Actual	Comment	Reference
L	175	SER	-	EXPRESSION TAG	UNP C3W5S1
L	176	GLY	-	EXPRESSION TAG	UNP C3W5S1
L	177	ARG	-	EXPRESSION TAG	UNP C3W5S1

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



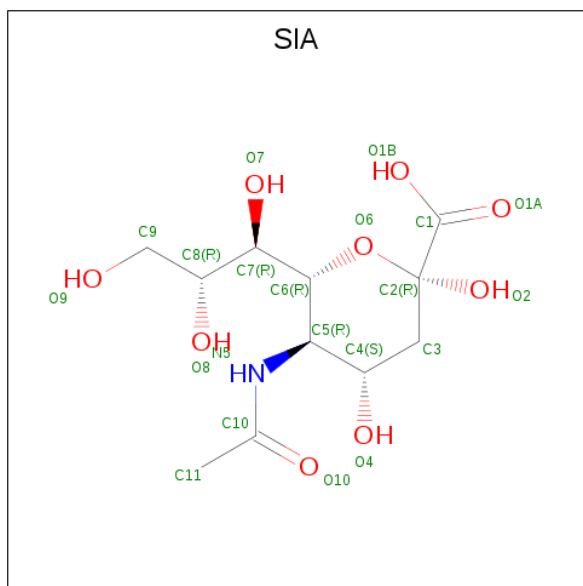
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			15	8	1	6		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	G	1	Total	C	N	O	0	0
			14	8	1	5		
3	G	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	I	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	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	K	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	K	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is O-SIALIC ACID (three-letter code: SIA) (formula: $C_{11}H_{19}NO_9$).



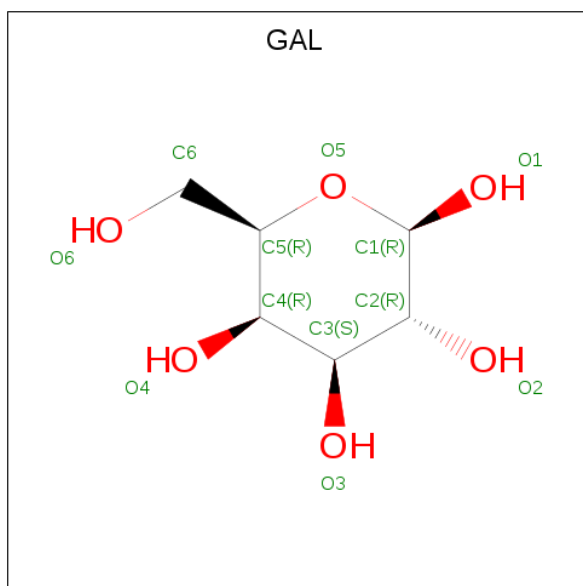
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			20	11	1	8		
4	I	1	Total	C	N	O	0	0
			20	11	1	8		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	K	1	Total	C	N	O	0	0
			20	11	1	8		

- Molecule 5 is BETA-D-GALACTOSE (three-letter code: GAL) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			11	6	5		
5	I	1	Total	C	O	0	0
			11	6	5		
5	K	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	138	Total	O	0	0
			138	138		
6	B	54	Total	O	0	0
			54	54		
6	C	89	Total	O	0	0
			89	89		
6	D	66	Total	O	0	0
			66	66		
6	E	117	Total	O	0	0
			117	117		

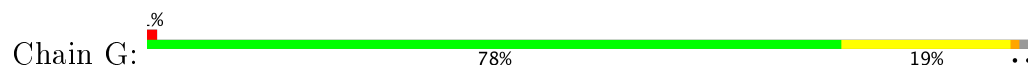
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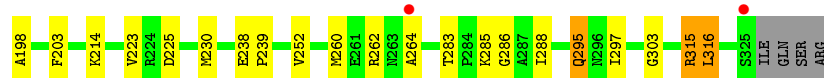
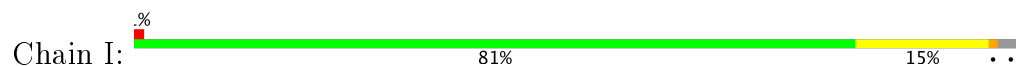
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	62	Total 62	O 62	0	0
6	G	121	Total 121	O 121	0	0
6	H	69	Total 69	O 69	0	0
6	I	127	Total 127	O 127	0	0
6	J	57	Total 57	O 57	0	0
6	K	97	Total 97	O 97	0	0
6	L	54	Total 54	O 54	0	0



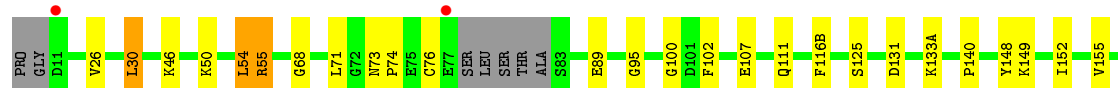
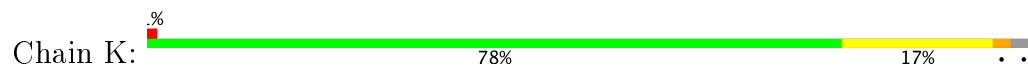
- Molecule 1: hemagglutinin HA1



- Molecule 1: hemagglutinin HA1



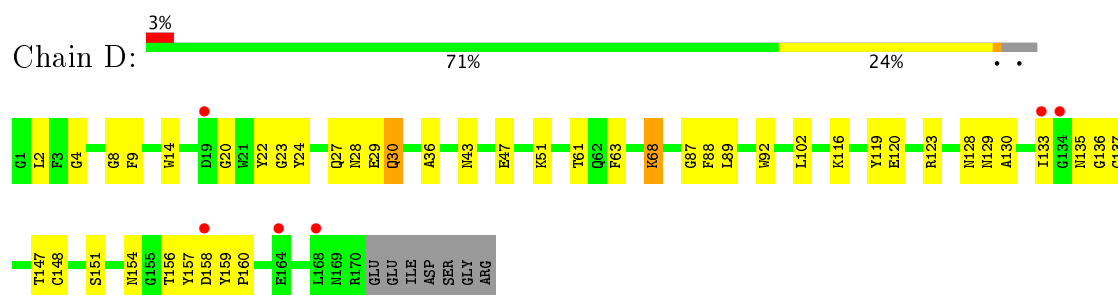
- Molecule 1: hemagglutinin HA1



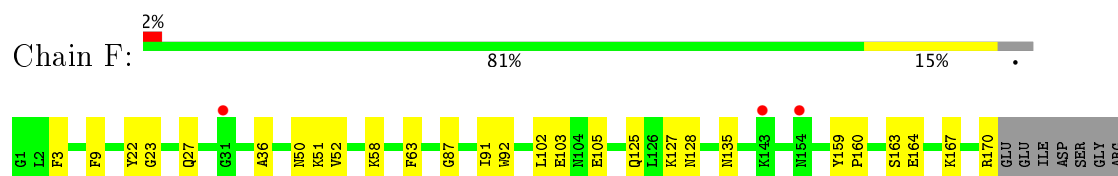
- Molecule 2: hemagglutinin HA2



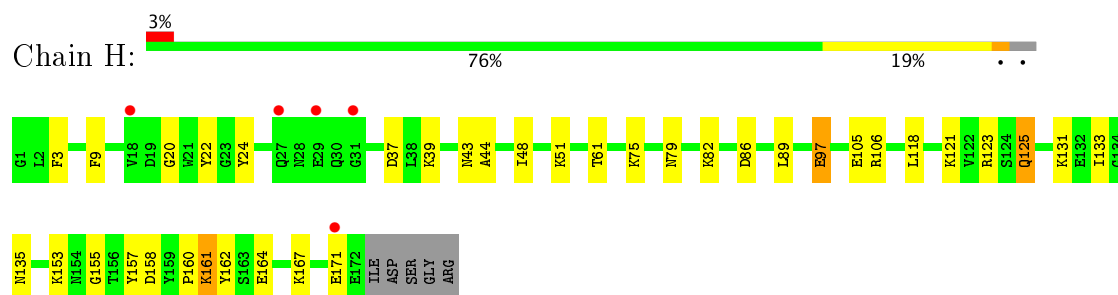
- Molecule 2: hemagglutinin HA2



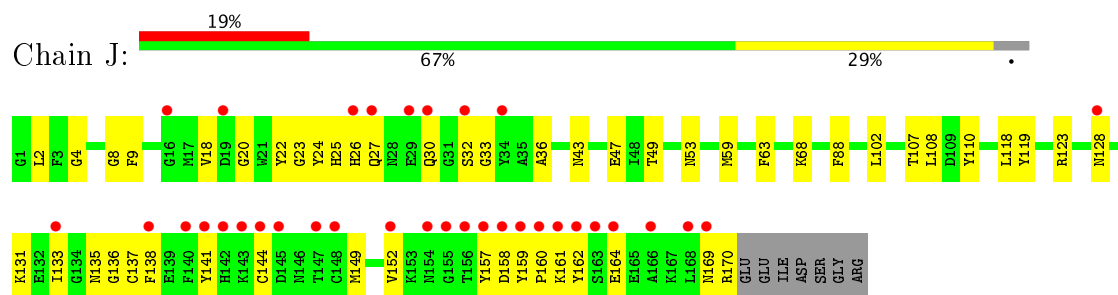
- Molecule 2: hemagglutinin HA2



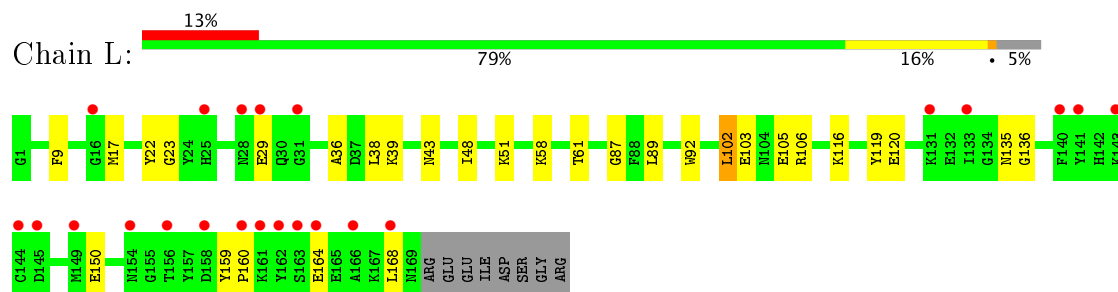
- Molecule 2: hemagglutinin HA2



- Molecule 2: hemagglutinin HA2



- Molecule 2: hemagglutinin HA2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	66.88Å 116.26Å 118.37Å 60.96° 77.13° 80.40°	Depositor
Resolution (Å)	49.24 – 2.00 49.24 – 2.00	Depositor EDS
% Data completeness (in resolution range)	84.2 (49.24-2.00) 77.2 (49.24-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.7 _650	Depositor
R, R_{free}	0.199 , 0.249 0.196 , 0.245	Depositor DCC
R_{free} test set	8641 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	29.5	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	24675	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SIA, GAL, 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	0/2586	0.49	0/3516
1	C	0.27	0/2572	0.47	0/3495
1	E	0.30	0/2568	0.51	0/3490
1	G	0.31	0/2586	0.49	0/3516
1	I	0.30	0/2558	0.49	0/3476
1	K	0.28	0/2553	0.48	0/3469
2	B	0.27	0/1388	0.42	0/1871
2	D	0.28	0/1399	0.43	0/1885
2	F	0.29	0/1399	0.43	0/1885
2	H	0.29	0/1417	0.43	0/1909
2	J	0.27	0/1399	0.42	0/1885
2	L	0.27	0/1388	0.41	0/1871
All	All	0.29	0/23813	0.47	0/32268

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2522	0	2466	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2509	0	2455	56	0
1	E	2504	0	2449	54	0
1	G	2522	0	2465	52	0
1	I	2495	0	2436	39	0
1	K	2490	0	2430	49	0
2	B	1360	0	1284	31	0
2	D	1371	0	1296	36	0
2	F	1371	0	1297	21	0
2	H	1389	0	1309	33	0
2	J	1371	0	1297	35	0
2	L	1360	0	1284	20	0
3	A	42	0	38	1	0
3	C	15	0	14	0	0
3	D	14	0	13	0	0
3	E	42	0	38	0	0
3	G	42	0	39	3	0
3	I	42	0	39	0	0
3	K	70	0	64	2	0
4	C	20	0	17	1	0
4	I	20	0	17	2	0
4	K	20	0	17	1	0
5	C	11	0	9	0	0
5	I	11	0	9	0	0
5	K	11	0	9	0	0
6	A	138	0	0	5	0
6	B	54	0	0	1	0
6	C	89	0	0	2	0
6	D	66	0	0	1	0
6	E	117	0	0	3	0
6	F	62	0	0	0	0
6	G	121	0	0	2	0
6	H	69	0	0	2	0
6	I	127	0	0	1	0
6	J	57	0	0	0	0
6	K	97	0	0	1	0
6	L	54	0	0	2	0
All	All	24675	0	22791	426	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 9.

The worst 5 of 426 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:H:97:GLU:HG2	2:L:58:LYS:HD2	1.37	1.06
1:C:283:THR:HG22	1:C:285:LYS:H	1.20	1.03
1:I:283:THR:HG22	1:I:285:LYS:H	1.20	1.02
1:A:283:THR:HG22	1:A:285:LYS:H	1.28	0.97
1:A:79:LEU:HD12	1:A:81:THR:HB	1.49	0.92

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	321/329 (98%)	303 (94%)	13 (4%)	5 (2%)	11	5
1	C	317/329 (96%)	301 (95%)	15 (5%)	1 (0%)	44	40
1	E	317/329 (96%)	306 (96%)	10 (3%)	1 (0%)	44	40
1	G	321/329 (98%)	305 (95%)	16 (5%)	0	100	100
1	I	315/329 (96%)	300 (95%)	12 (4%)	3 (1%)	18	10
1	K	314/329 (95%)	295 (94%)	17 (5%)	2 (1%)	28	21
2	B	167/177 (94%)	161 (96%)	5 (3%)	1 (1%)	28	21
2	D	168/177 (95%)	160 (95%)	6 (4%)	2 (1%)	15	8
2	F	168/177 (95%)	159 (95%)	9 (5%)	0	100	100
2	H	170/177 (96%)	164 (96%)	6 (4%)	0	100	100
2	J	168/177 (95%)	157 (94%)	9 (5%)	2 (1%)	15	8
2	L	167/177 (94%)	157 (94%)	10 (6%)	0	100	100
All	All	2913/3036 (96%)	2768 (95%)	128 (4%)	17 (1%)	28	21

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	81	THR

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Mol	Chain	Res	Type
1	A	265	GLY
2	B	127	LYS
1	C	94	ASN
1	E	116(A)	SER

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	285/290 (98%)	280 (98%)	5 (2%)	64	68
1	C	283/290 (98%)	272 (96%)	11 (4%)	37	34
1	E	282/290 (97%)	273 (97%)	9 (3%)	44	42
1	G	285/290 (98%)	277 (97%)	8 (3%)	49	49
1	I	281/290 (97%)	274 (98%)	7 (2%)	53	54
1	K	281/290 (97%)	274 (98%)	7 (2%)	53	54
2	B	145/152 (95%)	139 (96%)	6 (4%)	35	31
2	D	146/152 (96%)	141 (97%)	5 (3%)	42	40
2	F	146/152 (96%)	144 (99%)	2 (1%)	71	76
2	H	148/152 (97%)	143 (97%)	5 (3%)	42	40
2	J	146/152 (96%)	140 (96%)	6 (4%)	35	31
2	L	145/152 (95%)	141 (97%)	4 (3%)	49	49
All	All	2573/2652 (97%)	2498 (97%)	75 (3%)	48	47

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	283	THR
1	G	115	VAL
1	K	283	THR
1	E	295	GLN
1	G	11	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	196	GLN
2	H	27	GLN
2	J	53	ASN
2	D	117	ASN
2	F	95	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

25 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	$\# Z > 2$
3	NAG	A	330	1,3	14,14,15	0.59	0	15,19,21	1.05	1 (6%)
3	NAG	A	331	3	14,14,15	0.53	0	15,19,21	0.76	1 (6%)
3	NAG	A	332	1	14,14,15	0.54	0	15,19,21	0.76	0
4	SIA	C	330	5	17,20,21	0.24	0	19,28,31	0.78	0
5	GAL	C	331	3,4	11,11,12	0.67	0	13,15,17	1.28	2 (15%)
3	NAG	C	332	5	15,15,15	0.51	0	21,21,21	0.79	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	D	261	2	14,14,15	0.46	0	15,19,21	0.89	1 (6%)
3	NAG	E	331	1,3	14,14,15	0.50	0	15,19,21	0.84	1 (6%)
3	NAG	E	332	3	14,14,15	0.53	0	15,19,21	1.09	1 (6%)
3	NAG	E	341	1	14,14,15	0.50	0	15,19,21	1.09	1 (6%)
3	NAG	G	411	1	14,14,15	0.48	0	15,19,21	0.87	1 (6%)
3	NAG	G	431	1	14,14,15	0.52	0	15,19,21	1.00	2 (13%)
3	NAG	G	451	1	14,14,15	0.49	0	15,19,21	0.77	1 (6%)
4	SIA	I	501	5	17,20,21	0.30	0	19,28,31	0.79	1 (5%)
5	GAL	I	502	4	11,11,12	0.66	0	13,15,17	1.00	0
3	NAG	I	521	1	14,14,15	0.46	0	15,19,21	0.60	0
3	NAG	I	531	1	14,14,15	0.48	0	15,19,21	1.08	1 (6%)
3	NAG	I	541	1	14,14,15	0.46	0	15,19,21	0.91	0
4	SIA	K	601	5	17,20,21	0.25	0	19,28,31	0.79	1 (5%)
5	GAL	K	602	4	11,11,12	0.59	0	13,15,17	0.63	0
3	NAG	K	621	1	14,14,15	0.43	0	15,19,21	0.83	1 (6%)
3	NAG	K	631	1,3	14,14,15	0.50	0	15,19,21	0.91	0
3	NAG	K	632	3	14,14,15	0.53	0	15,19,21	0.71	0
3	NAG	K	641	1	14,14,15	0.50	0	15,19,21	0.72	0
3	NAG	K	651	1	14,14,15	0.45	0	15,19,21	0.79	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	NAG	A	330	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	331	3	-	0/6/23/26	0/1/1/1
3	NAG	A	332	1	-	0/6/23/26	0/1/1/1
4	SIA	C	330	5	-	0/14/34/38	0/1/1/1
5	GAL	C	331	3,4	-	0/2/19/22	0/1/1/1
3	NAG	C	332	5	-	0/6/26/26	0/1/1/1
3	NAG	D	261	2	-	0/6/23/26	0/1/1/1
3	NAG	E	331	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	332	3	-	0/6/23/26	0/1/1/1
3	NAG	E	341	1	-	0/6/23/26	0/1/1/1
3	NAG	G	411	1	-	0/6/23/26	0/1/1/1
3	NAG	G	431	1	-	0/6/23/26	0/1/1/1
3	NAG	G	451	1	-	0/6/23/26	0/1/1/1
4	SIA	I	501	5	-	0/14/34/38	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GAL	I	502	4	-	0/2/19/22	0/1/1/1
3	NAG	I	521	1	-	0/6/23/26	0/1/1/1
3	NAG	I	531	1	-	0/6/23/26	0/1/1/1
3	NAG	I	541	1	-	0/6/23/26	0/1/1/1
4	SIA	K	601	5	-	0/14/34/38	0/1/1/1
5	GAL	K	602	4	-	0/2/19/22	0/1/1/1
3	NAG	K	621	1	-	0/6/23/26	0/1/1/1
3	NAG	K	631	1,3	-	0/6/23/26	0/1/1/1
3	NAG	K	632	3	-	0/6/23/26	0/1/1/1
3	NAG	K	641	1	-	0/6/23/26	0/1/1/1
3	NAG	K	651	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	331	GAL	O3-C3-C2	-3.60	103.47	110.02
3	A	330	NAG	O5-C1-C2	-2.78	107.60	111.47
3	E	332	NAG	O5-C1-C2	-2.71	107.70	111.47
3	E	341	NAG	O5-C1-C2	-2.42	108.11	111.47
4	I	501	SIA	C8-C7-C6	-2.31	108.55	113.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	332	NAG	1	0
4	C	330	SIA	1	0
3	G	431	NAG	1	0
3	G	451	NAG	2	0
4	I	501	SIA	2	0
4	K	601	SIA	1	0
3	K	631	NAG	1	0
3	K	632	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	323/329 (98%)	-0.06	8 (2%) 58 57	22, 35, 56, 75	0
1	C	321/329 (97%)	-0.13	5 (1%) 72 71	27, 42, 58, 76	0
1	E	321/329 (97%)	-0.13	4 (1%) 79 78	24, 35, 51, 69	0
1	G	323/329 (98%)	-0.13	2 (0%) 89 88	24, 36, 50, 70	0
1	I	319/329 (96%)	-0.25	4 (1%) 77 77	24, 36, 54, 76	0
1	K	318/329 (96%)	-0.08	2 (0%) 89 88	27, 40, 58, 74	0
2	B	169/177 (95%)	0.92	28 (16%) 2 2	23, 45, 90, 106	0
2	D	170/177 (96%)	0.18	6 (3%) 44 45	25, 46, 63, 75	0
2	F	170/177 (96%)	0.06	3 (1%) 69 68	24, 40, 60, 67	0
2	H	172/177 (97%)	-0.02	5 (2%) 52 52	24, 43, 58, 68	0
2	J	170/177 (96%)	0.73	34 (20%) 1 1	24, 46, 78, 83	0
2	L	169/177 (95%)	0.49	23 (13%) 3 3	26, 45, 81, 94	0
All	All	2945/3036 (97%)	0.05	124 (4%) 37 37	22, 39, 68, 106	0

The worst 5 of 124 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	168	LEU	8.7
2	B	166	ALA	7.4
2	B	160	PRO	7.3
2	B	168	LEU	7.2
2	J	147	THR	6.8

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

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

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(Å ²)	Q<0.9
3	NAG	K	651	14/15	0.72	0.23	5.59	53,74,82,85	0
3	NAG	I	531	14/15	0.84	0.15	1.57	41,53,63,64	0
3	NAG	E	331	14/15	0.79	0.25	1.47	55,63,71,71	0
3	NAG	I	541	14/15	0.86	0.15	1.04	57,67,75,80	0
4	SIA	K	601	20/21	0.88	0.13	0.37	42,51,57,57	0
4	SIA	I	501	20/21	0.91	0.11	0.32	36,45,49,51	0
3	NAG	K	631	14/15	0.92	0.12	-0.15	51,58,66,69	0
3	NAG	G	431	14/15	0.92	0.10	-0.38	40,52,62,64	0
4	SIA	C	330	20/21	0.94	0.10	-0.76	33,43,47,50	0
3	NAG	A	330	14/15	0.96	0.08	-1.60	32,39,46,48	0
3	NAG	I	521	14/15	0.71	0.19	-	73,83,88,92	0
3	NAG	A	332	14/15	0.76	0.38	-	51,62,69,70	0
3	NAG	K	621	14/15	0.79	0.18	-	53,67,77,83	0
3	NAG	G	451	14/15	0.69	0.38	-	65,84,90,94	0
5	GAL	K	602	11/12	0.85	0.20	-	59,70,77,77	0
5	GAL	I	502	11/12	0.85	0.13	-	55,60,68,69	0
3	NAG	E	341	14/15	0.76	0.32	-	76,79,87,89	0
3	NAG	A	331	14/15	0.89	0.14	-	44,53,62,67	0
3	NAG	K	641	14/15	0.82	0.20	-	57,63,74,78	0
3	NAG	C	332	15/15	0.83	0.26	-	74,83,91,94	0
3	NAG	G	411	14/15	0.85	0.31	-	70,75,82,84	0
5	GAL	C	331	11/12	0.82	0.13	-	53,65,70,76	0
3	NAG	D	261	14/15	0.86	0.14	-	65,68,72,76	0
3	NAG	K	632	14/15	0.81	0.18	-	67,75,84,85	0
3	NAG	E	332	14/15	0.77	0.36	-	62,77,84,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.