



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 9, 2020 – 01:42 PM BST

PDB ID : 6D8W
Title : Crystal structure of InvbI.18715.a.KN11: Influenza hemagglutinin from strain A/Jiangsu/ALSI/2011
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2018-04-27
Resolution : 2.35 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

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

with specific help available everywhere you see the ⓘ symbol.

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

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

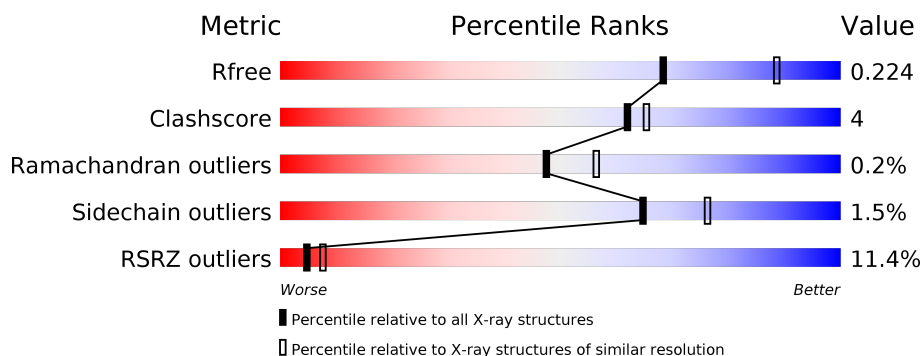
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	499	<div> <div>11%</div> <div> <div></div> <div>81%</div> <div>11%</div> <div>7%</div> </div> </div>
1	B	499	<div> <div>11%</div> <div> <div></div> <div>88%</div> <div>10%</div> <div>•</div> </div> </div>
1	C	499	<div> <div>12%</div> <div> <div></div> <div>86%</div> <div>9%</div> <div>5%</div> </div> </div>
1	D	499	<div> <div>13%</div> <div> <div></div> <div>80%</div> <div>9%</div> <div>11%</div> </div> </div>
1	E	499	<div> <div>8%</div> <div> <div></div> <div>85%</div> <div>10%</div> <div>•</div> </div> </div>
1	F	499	<div> <div>10%</div> <div> <div></div> <div>88%</div> <div>7%</div> <div>5%</div> </div> </div>

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	OXM	F	504	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22584 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	466	Total	C	N	O	S	0	4	0
			3577	2250	625	683	19			
1	B	491	Total	C	N	O	S	0	5	0
			3729	2352	650	708	19			
1	C	476	Total	C	N	O	S	0	7	0
			3630	2292	632	687	19			
1	D	443	Total	C	N	O	S	0	3	0
			3344	2108	582	639	15			
1	E	477	Total	C	N	O	S	0	4	0
			3631	2292	625	695	19			
1	F	476	Total	C	N	O	S	0	3	0
			3636	2286	637	694	19			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP G0Z9B7
A	2	SER	-	expression tag	UNP G0Z9B7
A	493	PHE	-	expression tag	UNP G0Z9B7
A	494	LEU	-	expression tag	UNP G0Z9B7
A	495	VAL	-	expression tag	UNP G0Z9B7
A	496	PRO	-	expression tag	UNP G0Z9B7
A	497	ARG	-	expression tag	UNP G0Z9B7
B	1	GLY	-	expression tag	UNP G0Z9B7
B	2	SER	-	expression tag	UNP G0Z9B7
B	495	PHE	-	expression tag	UNP G0Z9B7
B	496	LEU	-	expression tag	UNP G0Z9B7
B	497	VAL	-	expression tag	UNP G0Z9B7
B	498	PRO	-	expression tag	UNP G0Z9B7
B	499	ARG	-	expression tag	UNP G0Z9B7
C	1	GLY	-	expression tag	UNP G0Z9B7
C	2	SER	-	expression tag	UNP G0Z9B7
C	495	PHE	-	expression tag	UNP G0Z9B7

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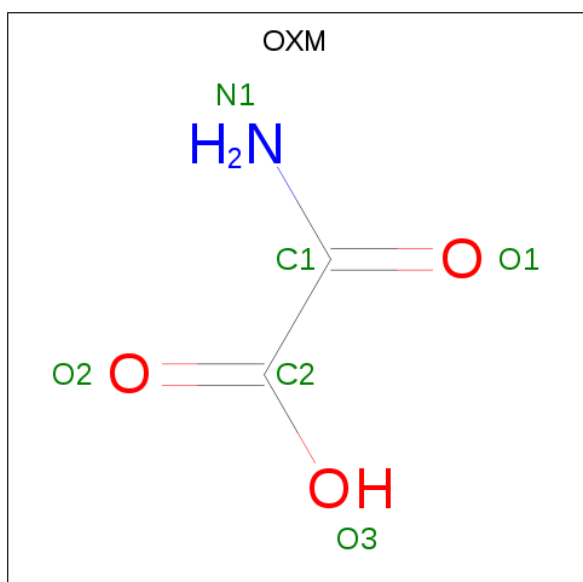
Chain	Residue	Modelled	Actual	Comment	Reference
C	496	LEU	-	expression tag	UNP G0Z9B7
C	497	VAL	-	expression tag	UNP G0Z9B7
C	498	PRO	-	expression tag	UNP G0Z9B7
C	499	ARG	-	expression tag	UNP G0Z9B7
D	1	GLY	-	expression tag	UNP G0Z9B7
D	2	SER	-	expression tag	UNP G0Z9B7
D	495	PHE	-	expression tag	UNP G0Z9B7
D	496	LEU	-	expression tag	UNP G0Z9B7
D	497	VAL	-	expression tag	UNP G0Z9B7
D	498	PRO	-	expression tag	UNP G0Z9B7
D	499	ARG	-	expression tag	UNP G0Z9B7
E	1	GLY	-	expression tag	UNP G0Z9B7
E	2	SER	-	expression tag	UNP G0Z9B7
E	495	PHE	-	expression tag	UNP G0Z9B7
E	496	LEU	-	expression tag	UNP G0Z9B7
E	497	VAL	-	expression tag	UNP G0Z9B7
E	498	PRO	-	expression tag	UNP G0Z9B7
E	499	ARG	-	expression tag	UNP G0Z9B7
F	1	GLY	-	expression tag	UNP G0Z9B7
F	2	SER	-	expression tag	UNP G0Z9B7
F	495	PHE	-	expression tag	UNP G0Z9B7
F	496	LEU	-	expression tag	UNP G0Z9B7
F	497	VAL	-	expression tag	UNP G0Z9B7
F	498	PRO	-	expression tag	UNP G0Z9B7
F	499	ARG	-	expression tag	UNP G0Z9B7

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



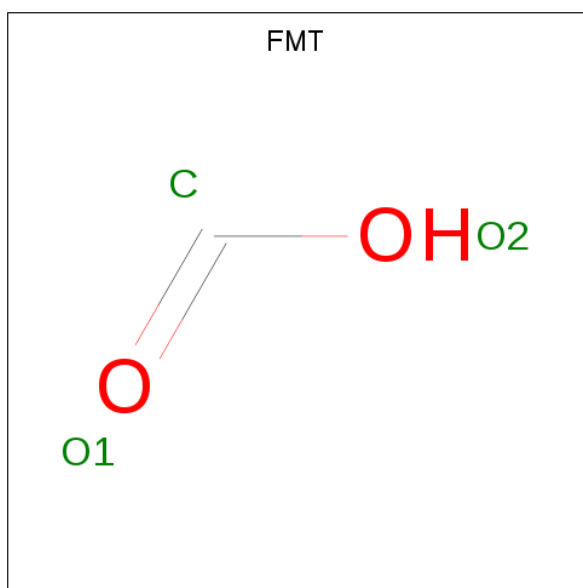
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	E	1	Total	C	N	O	0	0
			14	8	1	5		
2	F	1	Total	C	N	O	0	0
			14	8	1	5		
2	F	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is OXAMIC ACID (three-letter code: OXM) (formula: $C_2H_3NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			6	2	1	3		
3	A	1	Total	C	N	O	0	0
			6	2	1	3		
3	B	1	Total	C	N	O	0	0
			6	2	1	3		
3	C	1	Total	C	N	O	0	0
			6	2	1	3		
3	D	1	Total	C	N	O	0	0
			6	2	1	3		
3	E	1	Total	C	N	O	0	0
			6	2	1	3		
3	F	1	Total	C	N	O	0	0
			6	2	1	3		
3	F	1	Total	C	N	O	0	0
			6	2	1	3		

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			3	1	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	215	Total	O	0	2
			216	216		

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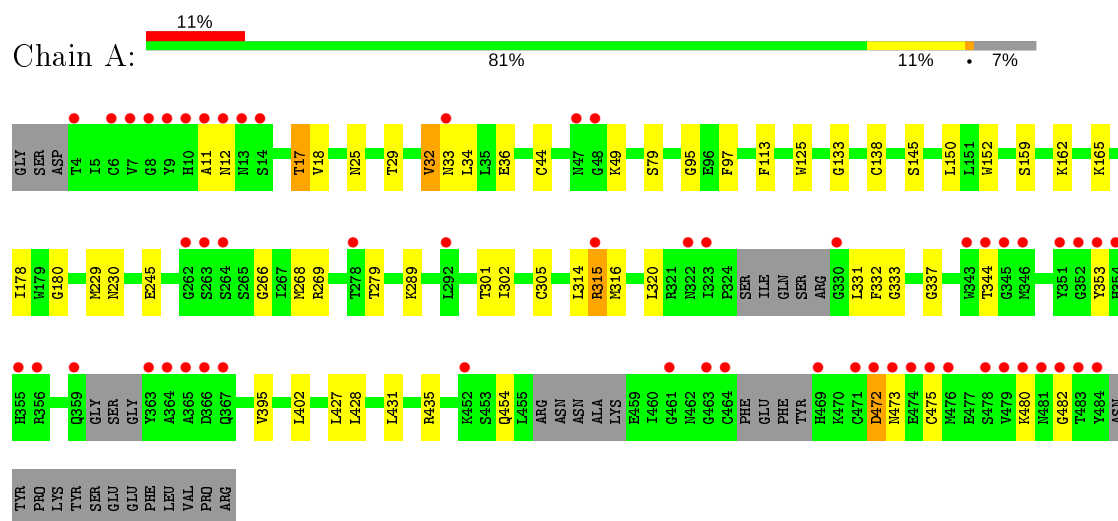
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	96	Total 96	O 96	0	0
5	C	156	Total 156	O 156	0	0
5	D	118	Total 120	O 120	0	2
5	E	152	Total 155	O 155	0	3
5	F	172	Total 173	O 173	0	1

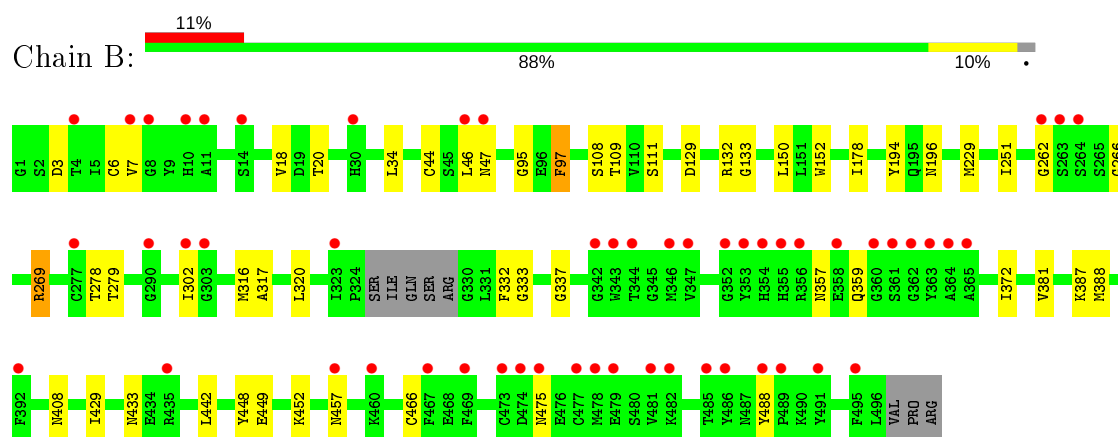
3 Residue-property plots [i](#)

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

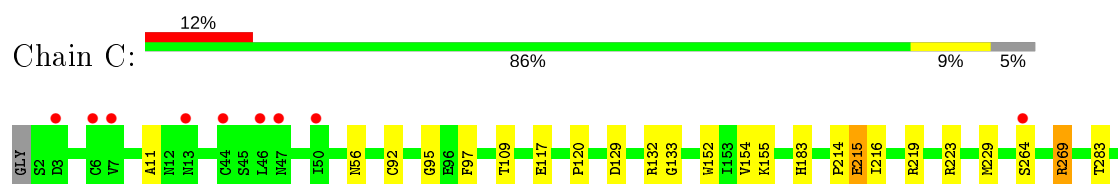
• Molecule 1: Hemagglutinin

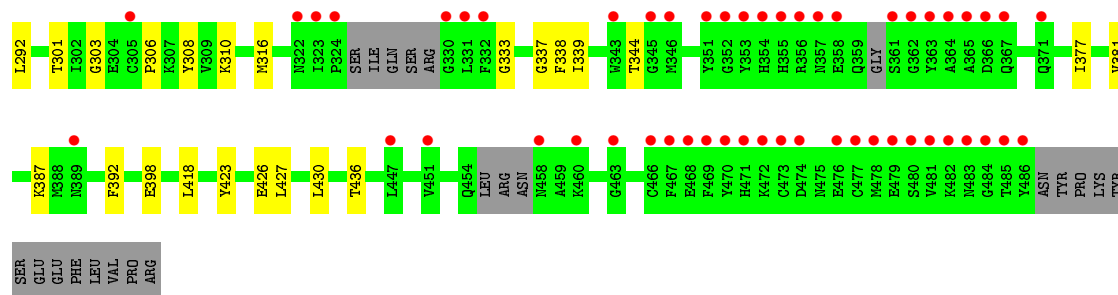


• Molecule 1: Hemagglutinin

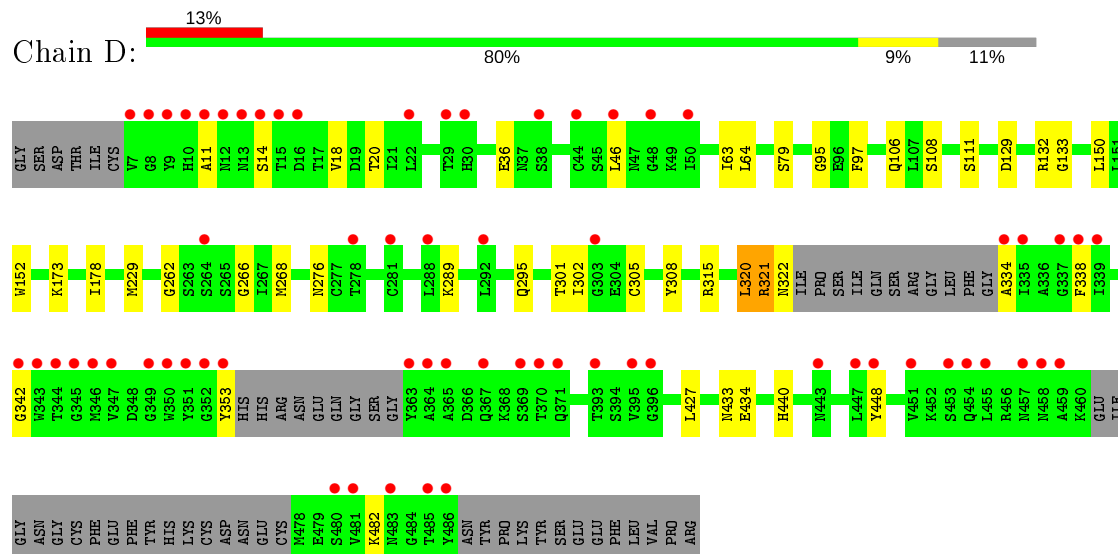


• Molecule 1: Hemagglutinin

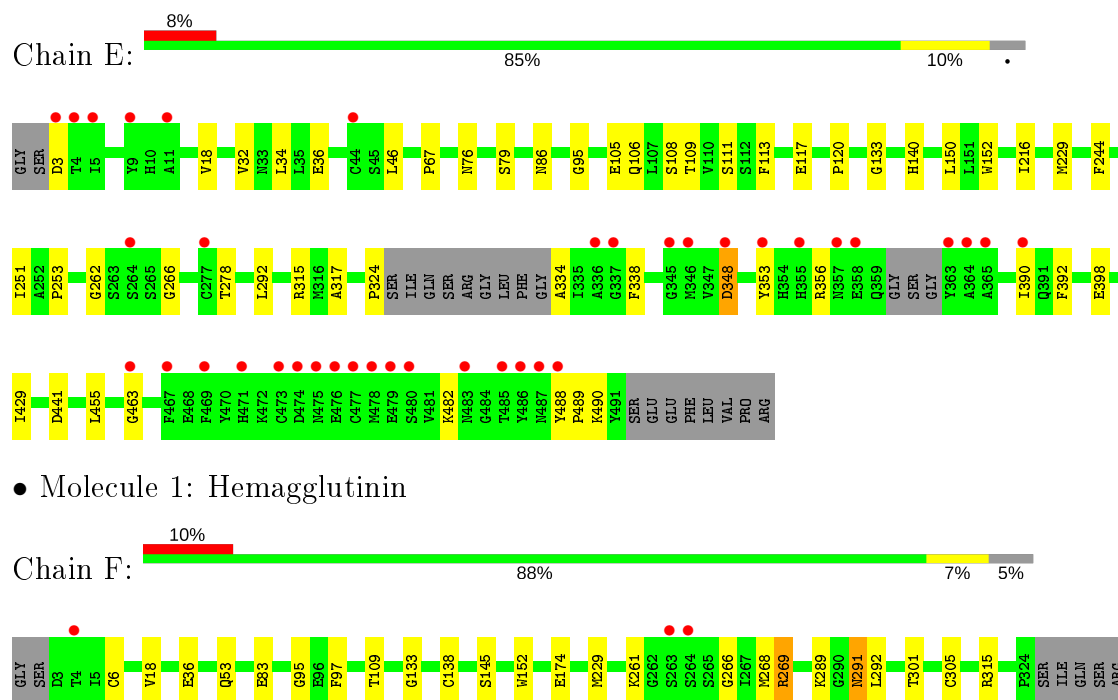


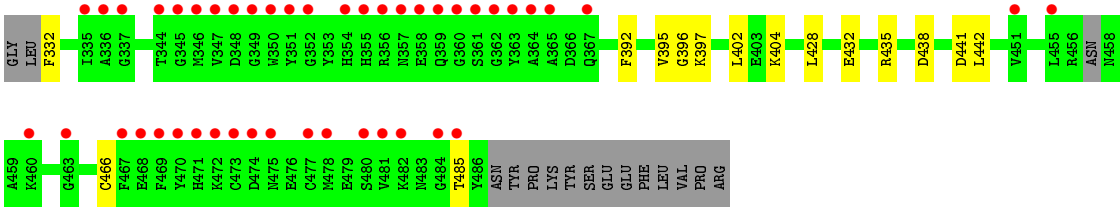


- Molecule 1: Hemagglutinin



- Molecule 1: Hemagglutinin





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	67.30Å 113.33Å 130.12Å 110.16° 90.85° 90.28°	Depositor
Resolution (Å)	43.29 – 2.35 46.34 – 2.35	Depositor EDS
% Data completeness (in resolution range)	97.5 (43.29-2.35) 97.5 (46.34-2.35)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.179 , 0.225 0.180 , 0.224	Depositor DCC
R_{free} test set	2044 reflections (1.39%)	wwPDB-VP
Wilson B-factor (Å ²)	40.1	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 54.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	22584	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.75 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.3547e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: OXM, FMT, 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	0.43	0/3668	0.61	0/4985
1	B	0.39	0/3830	0.56	0/5216
1	C	0.41	0/3736	0.59	0/5086
1	D	0.40	0/3429	0.58	0/4672
1	E	0.41	0/3730	0.58	0/5086
1	F	0.43	0/3725	0.60	0/5066
All	All	0.41	0/22118	0.59	0/30111

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	3577	0	3354	44	0
1	B	3729	0	3430	30	0
1	C	3630	0	3349	31	0
1	D	3344	0	3075	29	0
1	E	3631	0	3340	26	0
1	F	3636	0	3383	26	0
2	A	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	14	0	13	0	0
2	E	14	0	13	0	0
2	F	28	0	26	1	0
3	A	12	0	4	2	0
3	B	6	0	2	0	0
3	C	6	0	2	1	0
3	D	6	0	2	1	0
3	E	6	0	2	0	0
3	F	12	0	4	2	0
4	B	3	0	1	0	0
5	A	216	0	0	2	0
5	B	96	0	0	0	0
5	C	156	0	0	6	0
5	D	120	0	0	5	0
5	E	155	0	0	3	0
5	F	173	0	0	5	0
All	All	22584	0	20013	183	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 4.

The worst 5 of 183 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:A:315:ARG:CZ	1:A:315:ARG:HA	1.90	1.00
1:A:33:ASN:HA	1:A:315:ARG:NH2	1.82	0.94
1:D:64:LEU:HD23	1:D:178[B]:ILE:HD11	1.51	0.91
1:A:32:VAL:O	1:A:315:ARG:NH1	2.12	0.82
1:F:266:GLY:HA3	1:F:395:VAL:HG11	1.61	0.79

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	460/499 (92%)	443 (96%)	16 (4%)	1 (0%)	47	56
1	B	492/499 (99%)	474 (96%)	17 (4%)	1 (0%)	47	56
1	C	475/499 (95%)	463 (98%)	12 (2%)	0	100	100
1	D	438/499 (88%)	425 (97%)	13 (3%)	0	100	100
1	E	475/499 (95%)	457 (96%)	16 (3%)	2 (0%)	34	38
1	F	473/499 (95%)	458 (97%)	14 (3%)	1 (0%)	47	56
All	All	2813/2994 (94%)	2720 (97%)	88 (3%)	5 (0%)	47	56

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	392	PHE
1	B	47	ASN
1	A	472	ASP
1	E	489	PRO
1	E	392	PHE

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	376/435 (86%)	368 (98%)	8 (2%)	53	65
1	B	378/435 (87%)	373 (99%)	5 (1%)	69	80
1	C	370/435 (85%)	364 (98%)	6 (2%)	62	75
1	D	337/435 (78%)	333 (99%)	4 (1%)	71	82
1	E	375/435 (86%)	369 (98%)	6 (2%)	62	75
1	F	377/435 (87%)	373 (99%)	4 (1%)	73	84
All	All	2213/2610 (85%)	2180 (98%)	33 (2%)	65	76

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	215[A]	GLU
1	C	430	LEU
1	F	268	MET
1	C	215[B]	GLU
1	C	216	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	487	ASN
1	F	291	ASN
1	E	471	HIS
1	A	454	GLN
1	E	483	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

14 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	FMT	B	503	-	0,2,2	0.00	-	0,1,1	0.00	-
3	OXM	E	502	-	2,5,5	0.40	0	2,6,6	1.71	1 (50%)
2	NAG	F	502	1	14,14,15	0.53	0	17,19,21	1.49	2 (11%)
3	OXM	D	700	-	2,5,5	0.31	0	2,6,6	1.76	1 (50%)
3	OXM	A	502	-	2,5,5	0.34	0	2,6,6	2.02	1 (50%)
3	OXM	F	504	-	2,5,5	0.58	0	2,6,6	1.00	0
2	NAG	B	501	1	14,14,15	0.68	1 (7%)	17,19,21	0.44	0
2	NAG	E	501	1	14,14,15	0.33	0	17,19,21	0.36	0
3	OXM	F	503	-	2,5,5	0.70	0	2,6,6	1.04	0
2	NAG	F	501	1	14,14,15	0.59	0	17,19,21	0.68	1 (5%)
3	OXM	A	503	-	2,5,5	0.70	0	2,6,6	1.74	1 (50%)
2	NAG	A	501	1	14,14,15	0.24	0	17,19,21	0.38	0
3	OXM	C	700	-	2,5,5	0.19	0	2,6,6	2.45	1 (50%)
3	OXM	B	502	-	2,5,5	0.21	0	2,6,6	2.28	1 (50%)

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	OXM	E	502	-	-	0/0/4/4	-
2	NAG	F	502	1	-	5/6/23/26	0/1/1/1
3	OXM	D	700	-	-	0/0/4/4	-
3	OXM	A	502	-	-	0/0/4/4	-
3	OXM	F	504	-	-	0/0/4/4	-
2	NAG	B	501	1	-	2/6/23/26	0/1/1/1
2	NAG	E	501	1	-	2/6/23/26	0/1/1/1
3	OXM	F	503	-	-	0/0/4/4	-
2	NAG	F	501	1	-	2/6/23/26	0/1/1/1
3	OXM	A	503	-	-	0/0/4/4	-
2	NAG	A	501	1	-	2/6/23/26	0/1/1/1
3	OXM	C	700	-	-	0/0/4/4	-
3	OXM	B	502	-	-	0/0/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NAG	O5-C1	-2.29	1.40	1.43

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	F	502	NAG	C2-N2-C7	4.43	129.21	122.90
3	C	700	OXM	O1-C1-N1	3.20	127.12	122.58
2	F	502	NAG	C1-C2-N2	2.90	115.45	110.49
3	B	502	OXM	C2-C1-N1	2.84	120.58	115.85
3	A	502	OXM	O1-C1-N1	2.80	126.56	122.58

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	501	NAG	C4-C5-C6-O6
2	F	502	NAG	O5-C5-C6-O6
2	E	501	NAG	O5-C5-C6-O6
2	F	502	NAG	C4-C5-C6-O6
2	F	502	NAG	C8-C7-N2-C2

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	502	NAG	1	0
3	D	700	OXM	1	0
3	A	502	OXM	1	0
3	F	504	OXM	2	0
3	A	503	OXM	1	0
3	C	700	OXM	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	466/499 (93%)	0.67	56 (12%) 4 7	21, 50, 123, 145	0
1	B	491/499 (98%)	0.53	54 (10%) 5 8	28, 65, 108, 125	0
1	C	476/499 (95%)	0.60	61 (12%) 3 6	22, 58, 116, 150	0
1	D	443/499 (88%)	0.67	65 (14%) 2 3	26, 61, 129, 151	0
1	E	477/499 (95%)	0.38	38 (7%) 12 18	25, 55, 104, 132	0
1	F	476/499 (95%)	0.45	48 (10%) 7 11	23, 51, 108, 133	0
All	All	2829/2994 (94%)	0.55	322 (11%) 5 7	21, 57, 115, 151	0

The worst 5 of 322 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	484	TYR	10.9
1	D	345	GLY	9.5
1	A	352	GLY	9.0
1	C	467	PHE	7.6
1	D	8	GLY	7.4

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	F	502	14/15	0.72	0.27	92,104,110,113	0
2	NAG	E	501	14/15	0.75	0.34	78,102,109,111	0
2	NAG	F	501	14/15	0.76	0.35	85,102,110,113	0
4	FMT	B	503	3/3	0.79	0.12	91,91,92,93	0
3	OXM	A	503	6/6	0.85	0.40	90,90,93,96	0
3	OXM	F	504	6/6	0.86	0.24	75,81,82,87	0
2	NAG	B	501	14/15	0.87	0.23	73,94,110,113	0
2	NAG	A	501	14/15	0.89	0.18	75,85,89,91	0
3	OXM	D	700	6/6	0.92	0.29	61,65,83,93	0
3	OXM	F	503	6/6	0.93	0.28	56,61,76,80	0
3	OXM	C	700	6/6	0.93	0.29	50,65,83,84	0
3	OXM	B	502	6/6	0.94	0.26	47,55,61,74	0
3	OXM	A	502	6/6	0.95	0.25	44,55,60,64	0
3	OXM	E	502	6/6	0.96	0.17	45,56,63,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.