



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 04:29 PM GMT

PDB ID : 4F3Z
Title : Crystal structure of a swine H1N2 influenza virus hemagglutinin
Authors : Xu, R.; Wilson, I.A.
Deposited on : 2012-05-09
Resolution : 3.20 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 (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

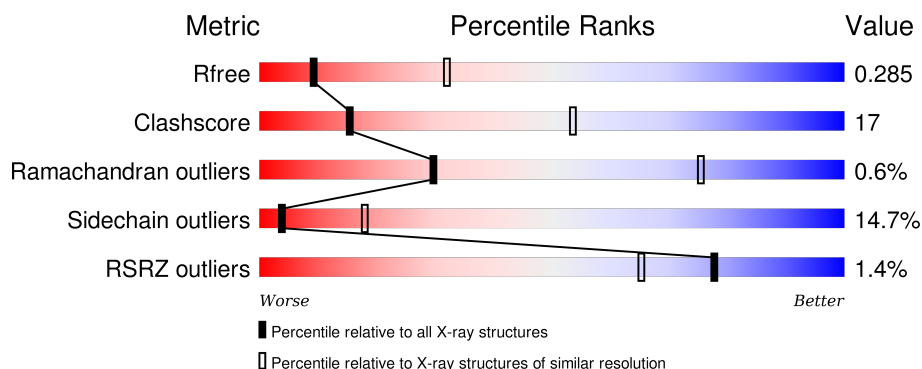
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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.



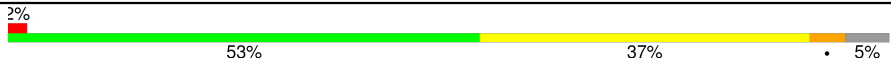
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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>%</div> <div> <div></div> <div>53%</div> <div>36%</div> <div>7%</div> <div>.</div> </div> </div>
1	C	329	<div> <div>53%</div> <div>33%</div> <div>5%</div> <div>9%</div> </div>
1	E	329	<div> <div>3%</div> <div>48%</div> <div>41%</div> <div>9%</div> <div>.</div> </div>
2	B	179	<div> <div>%</div> <div>64%</div> <div>30%</div> <div>.</div> <div>.</div> </div>
2	D	179	<div> <div>2%</div> <div>66%</div> <div>27%</div> <div>.</div> <div>.</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	179	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: a small red segment at the beginning labeled '2%', a large green segment labeled '53%', a large yellow segment labeled '37%', and a small grey segment at the end labeled '5%'.

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11544 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	320	Total	C	N	O	S	0	0	0
			2501	1575	434	479	13			
1	C	301	Total	C	N	O	S	0	0	0
			2364	1492	406	454	12			
1	E	320	Total	C	N	O	S	0	0	0
			2503	1576	434	480	13			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	PRO	-	EXPRESSION TAG	UNP Q8QT89
A	10	GLY	-	EXPRESSION TAG	UNP Q8QT89
A	205	CYS	GLY	ENGINEERED MUTATION	UNP Q8QT89
A	220	CYS	ARG	ENGINEERED MUTATION	UNP Q8QT89
C	9	PRO	-	EXPRESSION TAG	UNP Q8QT89
C	10	GLY	-	EXPRESSION TAG	UNP Q8QT89
C	205	CYS	GLY	ENGINEERED MUTATION	UNP Q8QT89
C	220	CYS	ARG	ENGINEERED MUTATION	UNP Q8QT89
E	9	PRO	-	EXPRESSION TAG	UNP Q8QT89
E	10	GLY	-	EXPRESSION TAG	UNP Q8QT89
E	205	CYS	GLY	ENGINEERED MUTATION	UNP Q8QT89
E	220	CYS	ARG	ENGINEERED MUTATION	UNP Q8QT89

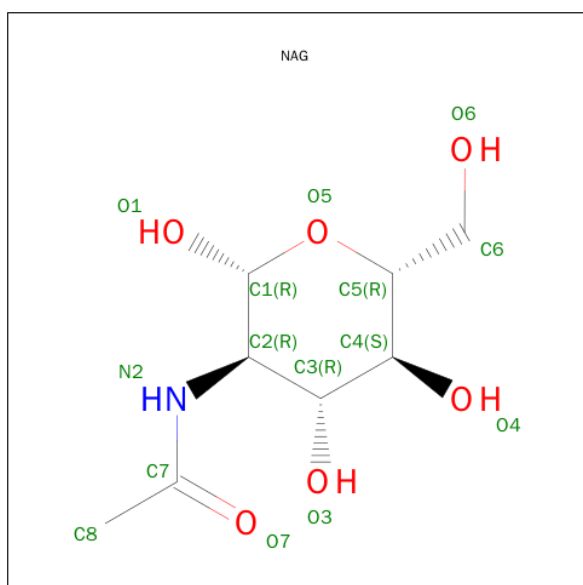
- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	171	Total	C	N	O	S	0	0	0
			1382	869	236	271	6			
2	D	174	Total	C	N	O	S	0	0	0
			1407	884	239	278	6			
2	F	170	Total	C	N	O	S	0	0	0
			1373	864	235	268	6			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	177	SER	-	EXPRESSION TAG	UNP Q8QT89
B	178	GLY	-	EXPRESSION TAG	UNP Q8QT89
B	179	ARG	-	EXPRESSION TAG	UNP Q8QT89
D	177	SER	-	EXPRESSION TAG	UNP Q8QT89
D	178	GLY	-	EXPRESSION TAG	UNP Q8QT89
D	179	ARG	-	EXPRESSION TAG	UNP Q8QT89
F	177	SER	-	EXPRESSION TAG	UNP Q8QT89
F	178	GLY	-	EXPRESSION TAG	UNP Q8QT89
F	179	ARG	-	EXPRESSION TAG	UNP Q8QT89

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

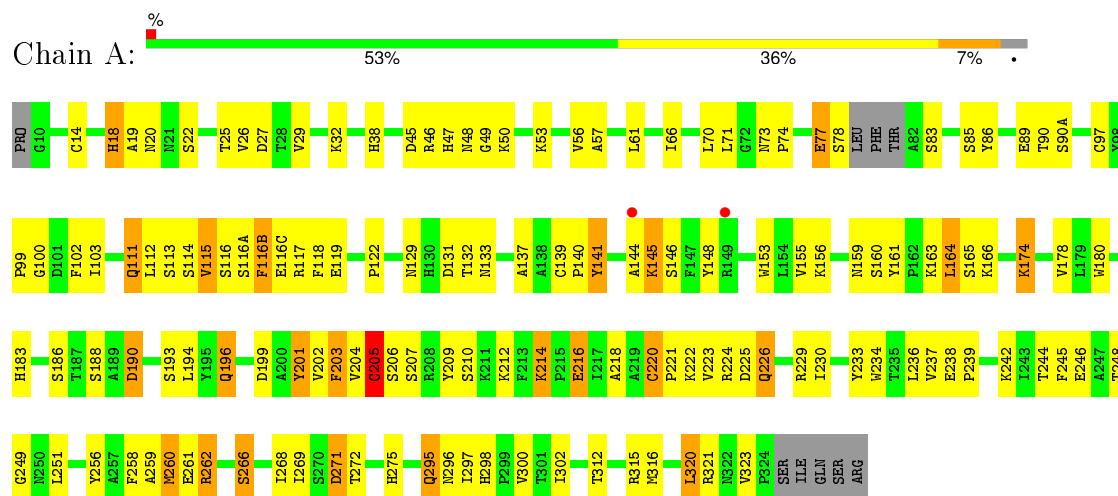


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			14	8	1	5		

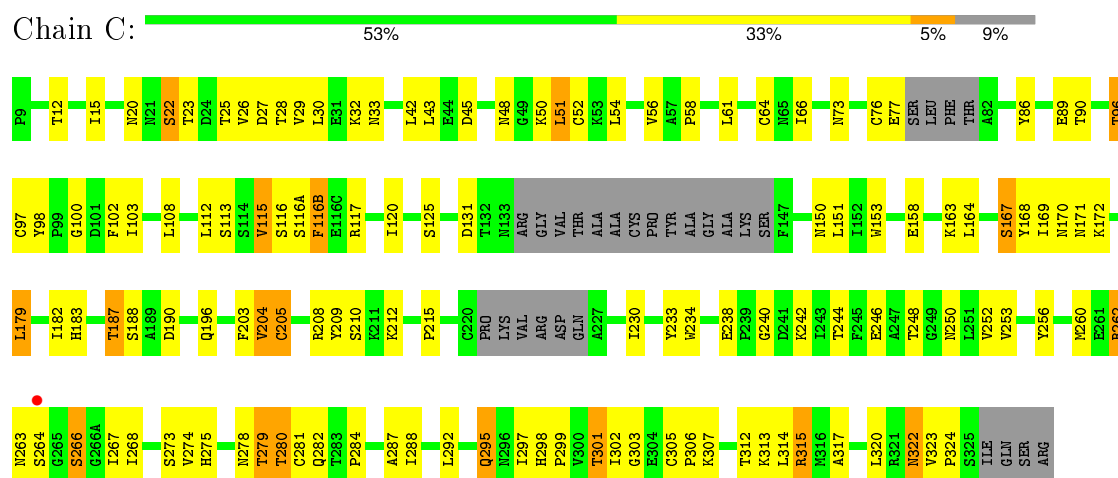
3 Residue-property plots

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.

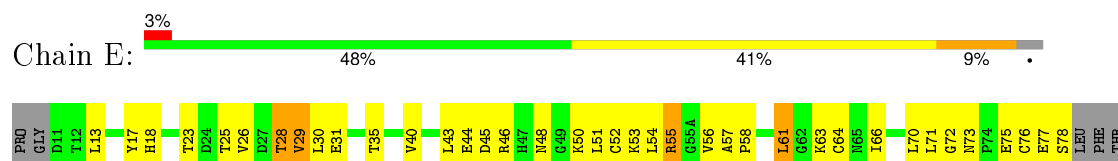
• Molecule 1: Hemagglutinin

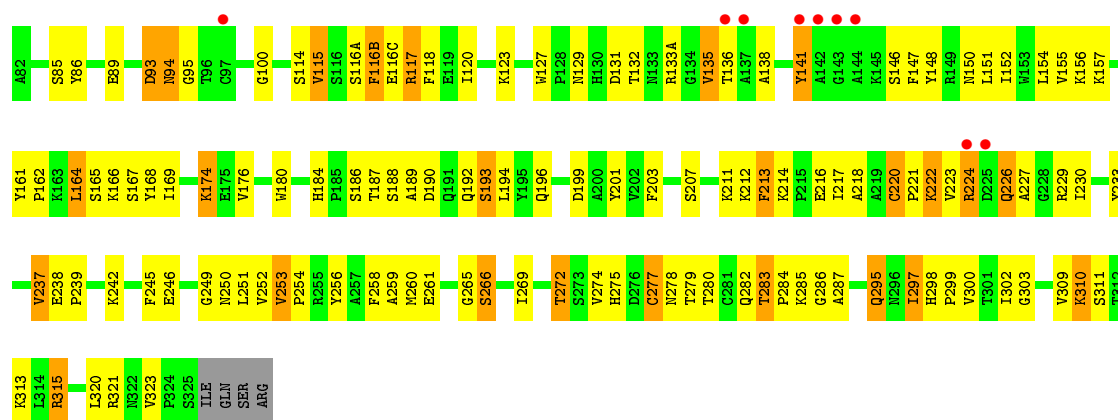


• Molecule 1: Hemagglutinin

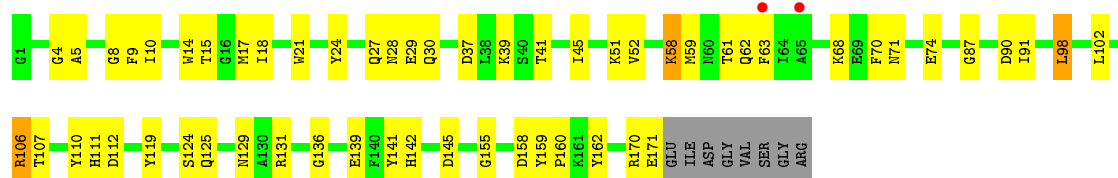


• Molecule 1: Hemagglutinin

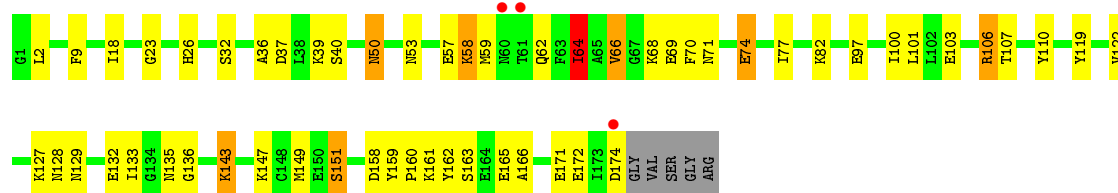




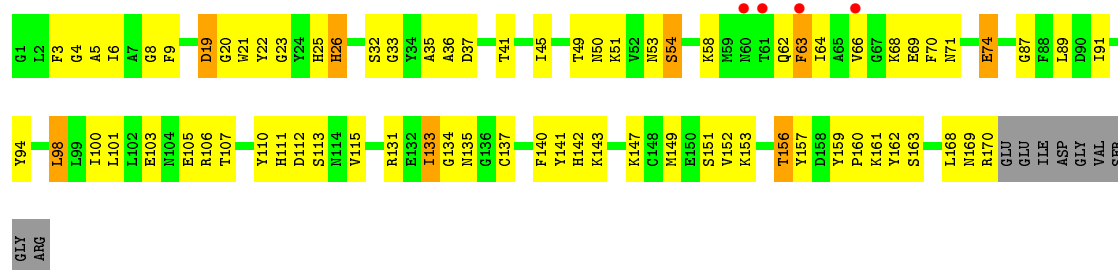
• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	93.44Å 94.92Å 220.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.27 – 3.20 34.28 – 3.19	Depositor EDS
% Data completeness (in resolution range)	93.2 (34.27-3.20) 91.6 (34.28-3.19)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.73 (at 3.18Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.234 , 0.293 0.227 , 0.285	Depositor DCC
R_{free} test set	1566 reflections (5.08%)	DCC
Wilson B-factor (Å ²)	43.9	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 22.6	EDS
Estimated twinning fraction	0.013 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 30965 reflections (0.006%)	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	11544	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% 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: 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	0.26	0/2562	0.45	0/3482
1	C	0.25	0/2421	0.46	0/3288
1	E	0.26	0/2564	0.44	0/3485
2	B	0.25	0/1410	0.40	0/1897
2	D	0.26	0/1435	0.40	0/1931
2	F	0.27	0/1401	0.41	0/1885
All	All	0.26	0/11793	0.44	0/15968

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	2
1	C	0	2
1	E	0	2
2	D	0	1
All	All	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	205	CYS	Peptide
1	A	262	ARG	Peptide
1	C	262	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	C	96	THR	Peptide
2	D	64	ILE	Peptide

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	2501	0	2429	103	0
1	C	2364	0	2288	81	0
1	E	2503	0	2431	121	0
2	B	1382	0	1312	40	0
2	D	1407	0	1333	33	0
2	F	1373	0	1306	47	0
3	C	14	0	13	0	0
All	All	11544	0	11112	391	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 17.

The worst 5 of 391 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:E:189:ALA:O	1:E:193:SER:HB3	1.50	1.11
1:C:96:THR:HA	1:C:97:CYS:HB2	1.37	1.01
1:E:116(A):SER:HB3	1:E:261:GLU:HB3	1.39	1.00
1:E:141:TYR:HB2	1:E:146:SER:HB2	1.46	0.97
1:A:70:LEU:HD11	1:A:112:LEU:HD11	1.53	0.91

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	316/329 (96%)	293 (93%)	20 (6%)	3 (1%)	21	67
1	C	293/329 (89%)	273 (93%)	18 (6%)	2 (1%)	26	72
1	E	316/329 (96%)	283 (90%)	29 (9%)	4 (1%)	15	59
2	B	169/179 (94%)	164 (97%)	5 (3%)	0	100	100
2	D	172/179 (96%)	156 (91%)	16 (9%)	0	100	100
2	F	168/179 (94%)	156 (93%)	12 (7%)	0	100	100
All	All	1434/1524 (94%)	1325 (92%)	100 (7%)	9 (1%)	30	75

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	116(B)	PHE
1	A	266	SER
1	E	116(B)	PHE
1	E	266	SER
1	A	115	VAL

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	280/289 (97%)	235 (84%)	45 (16%)	3	14
1	C	267/289 (92%)	223 (84%)	44 (16%)	3	13
1	E	281/289 (97%)	236 (84%)	45 (16%)	3	14
2	B	146/152 (96%)	132 (90%)	14 (10%)	10	39
2	D	149/152 (98%)	130 (87%)	19 (13%)	5	25
2	F	145/152 (95%)	126 (87%)	19 (13%)	5	24
All	All	1268/1323 (96%)	1082 (85%)	186 (15%)	4	18

5 of 186 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	204	VAL
2	D	50	ASN
2	F	58	LYS
1	C	210	SER
1	C	288	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	169	ASN
1	C	150	ASN
1	E	192	GLN
2	B	30	GLN
1	E	94	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

1 ligand is 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	C	401	1	14,14,15	0.51	0	15,19,21	0.86	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	C	401	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	401	NAG	C2-N2-C7	-2.12	120.32	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	320/329 (97%)	-0.15	2 (0%) 90 84	23, 48, 89, 124	0
1	C	301/329 (91%)	-0.37	1 (0%) 94 93	21, 34, 70, 109	0
1	E	320/329 (97%)	0.05	9 (2%) 56 42	31, 66, 111, 156	0
2	B	171/179 (95%)	-0.31	2 (1%) 81 69	22, 41, 79, 145	0
2	D	174/179 (97%)	-0.24	3 (1%) 73 60	16, 38, 90, 153	0
2	F	170/179 (94%)	-0.16	4 (2%) 62 47	19, 51, 109, 157	0
All	All	1456/1524 (95%)	-0.18	21 (1%) 78 65	16, 46, 96, 157	0

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	142	ALA	3.6
1	A	144	ALA	3.4
2	F	63	PHE	3.3
1	E	143	GLY	3.2
2	D	174	ASP	3.1

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 ⓘ

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
3	NAG	C	401	14/15	0.94	0.16	-0.93	23,37,41,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.