Full wwPDB X-ray Structure Validation Report ⓘ

Jan 28, 2025 – 04:05 PM EST

PDB ID	:	8V3J
Title	:	Structure-Based Engineering of a Highly Immunogenic, Conformationally Stabilized FimH Antigen for a Urinary Tract Infection Vaccine
Authors	:	Jasti, J.
Deposited on	:	2023-11-28
Resolution	:	1.90 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

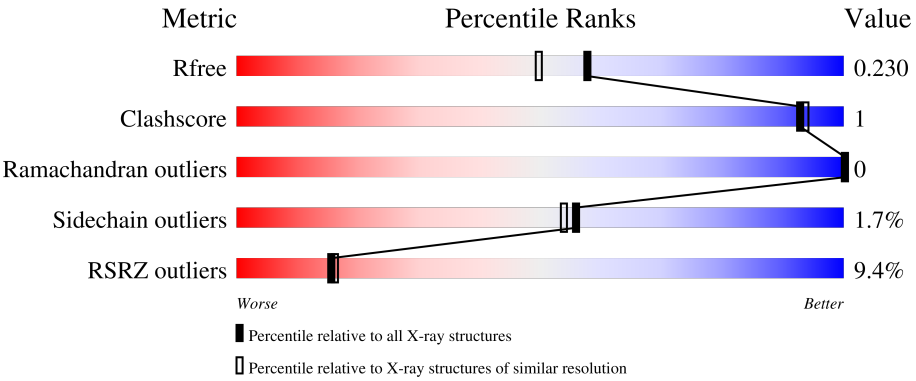
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	164625	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (1.90-1.90)

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 of 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 <=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	310	3% 92% 5% ·
1	B	310	6% 92% 5% ·
1	C	310	7% 93% · ·
1	D	310	16% 64% · 33%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8913 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 Type 1 fimbrin D-mannose specific adhesin,Protein FimG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	300	Total	C	N	O	S	0	1	0
			2185	1379	365	437	4			
1	B	300	Total	C	N	O	S	7	1	0
			2185	1379	365	437	4			
1	C	300	Total	C	N	O	S	7	1	0
			2181	1376	364	437	4			
1	D	208	Total	C	N	O	S	0	1	0
			1449	905	246	296	2			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	SER	ASN	engineered mutation	UNP P08191
A	15	ALA	GLY	engineered mutation	UNP P08191
A	16	ALA	GLY	engineered mutation	UNP P08191
A	27	ALA	VAL	engineered mutation	UNP P08191
A	70	SER	ASN	engineered mutation	UNP P08191
A	228	GLN	ASN	engineered mutation	UNP P08191
A	280	GLY	-	linker	UNP P08191
A	281	GLY	-	linker	UNP P08191
A	282	SER	-	linker	UNP P08191
A	283	SER	-	linker	UNP P08191
A	284	GLY	-	linker	UNP P08191
A	285	GLY	-	linker	UNP P08191
A	286	GLY	-	linker	UNP P08191
A	301	GLY	-	expression tag	UNP P08190
A	302	GLY	-	expression tag	UNP P08190
A	303	HIS	-	expression tag	UNP P08190
A	304	HIS	-	expression tag	UNP P08190
A	305	HIS	-	expression tag	UNP P08190
A	306	HIS	-	expression tag	UNP P08190
A	307	HIS	-	expression tag	UNP P08190
A	308	HIS	-	expression tag	UNP P08190

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Chain	Residue	Modelled	Actual	Comment	Reference
A	309	HIS	-	expression tag	UNP P08190
A	310	HIS	-	expression tag	UNP P08190
B	7	SER	ASN	engineered mutation	UNP P08191
B	15	ALA	GLY	engineered mutation	UNP P08191
B	16	ALA	GLY	engineered mutation	UNP P08191
B	27	ALA	VAL	engineered mutation	UNP P08191
B	70	SER	ASN	engineered mutation	UNP P08191
B	228	GLN	ASN	engineered mutation	UNP P08191
B	280	GLY	-	linker	UNP P08191
B	281	GLY	-	linker	UNP P08191
B	282	SER	-	linker	UNP P08191
B	283	SER	-	linker	UNP P08191
B	284	GLY	-	linker	UNP P08191
B	285	GLY	-	linker	UNP P08191
B	286	GLY	-	linker	UNP P08191
B	301	GLY	-	expression tag	UNP P08190
B	302	GLY	-	expression tag	UNP P08190
B	303	HIS	-	expression tag	UNP P08190
B	304	HIS	-	expression tag	UNP P08190
B	305	HIS	-	expression tag	UNP P08190
B	306	HIS	-	expression tag	UNP P08190
B	307	HIS	-	expression tag	UNP P08190
B	308	HIS	-	expression tag	UNP P08190
B	309	HIS	-	expression tag	UNP P08190
B	310	HIS	-	expression tag	UNP P08190
C	7	SER	ASN	engineered mutation	UNP P08191
C	15	ALA	GLY	engineered mutation	UNP P08191
C	16	ALA	GLY	engineered mutation	UNP P08191
C	27	ALA	VAL	engineered mutation	UNP P08191
C	70	SER	ASN	engineered mutation	UNP P08191
C	228	GLN	ASN	engineered mutation	UNP P08191
C	280	GLY	-	linker	UNP P08191
C	281	GLY	-	linker	UNP P08191
C	282	SER	-	linker	UNP P08191
C	283	SER	-	linker	UNP P08191
C	284	GLY	-	linker	UNP P08191
C	285	GLY	-	linker	UNP P08191
C	286	GLY	-	linker	UNP P08191
C	301	GLY	-	expression tag	UNP P08190
C	302	GLY	-	expression tag	UNP P08190
C	303	HIS	-	expression tag	UNP P08190
C	304	HIS	-	expression tag	UNP P08190

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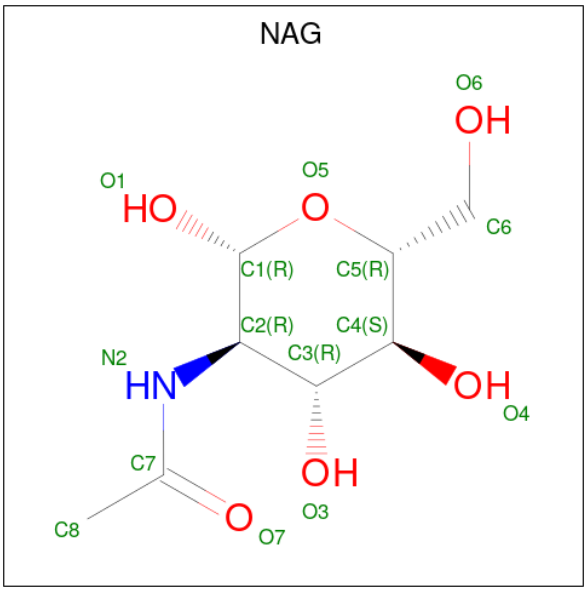
Chain	Residue	Modelled	Actual	Comment	Reference
C	305	HIS	-	expression tag	UNP P08190
C	306	HIS	-	expression tag	UNP P08190
C	307	HIS	-	expression tag	UNP P08190
C	308	HIS	-	expression tag	UNP P08190
C	309	HIS	-	expression tag	UNP P08190
C	310	HIS	-	expression tag	UNP P08190
D	7	SER	ASN	engineered mutation	UNP P08191
D	15	ALA	GLY	engineered mutation	UNP P08191
D	16	ALA	GLY	engineered mutation	UNP P08191
D	27	ALA	VAL	engineered mutation	UNP P08191
D	70	SER	ASN	engineered mutation	UNP P08191
D	228	GLN	ASN	engineered mutation	UNP P08191
D	280	GLY	-	linker	UNP P08191
D	281	GLY	-	linker	UNP P08191
D	282	SER	-	linker	UNP P08191
D	283	SER	-	linker	UNP P08191
D	284	GLY	-	linker	UNP P08191
D	285	GLY	-	linker	UNP P08191
D	286	GLY	-	linker	UNP P08191
D	301	GLY	-	expression tag	UNP P08190
D	302	GLY	-	expression tag	UNP P08190
D	303	HIS	-	expression tag	UNP P08190
D	304	HIS	-	expression tag	UNP P08190
D	305	HIS	-	expression tag	UNP P08190
D	306	HIS	-	expression tag	UNP P08190
D	307	HIS	-	expression tag	UNP P08190
D	308	HIS	-	expression tag	UNP P08190
D	309	HIS	-	expression tag	UNP P08190
D	310	HIS	-	expression tag	UNP P08190

- 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 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	C	1	Total C N O 14 8 1 5	0	0
2	D	1	Total C N O 14 8 1 5	0	0

- Molecule 3 is water.

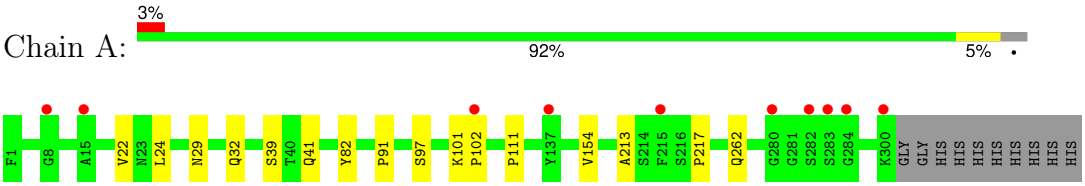
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	280	Total O 280 280	0	0
3	B	222	Total O 222 222	0	0
3	C	228	Total O 228 228	0	0
3	D	127	Total O 127 127	0	0

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.

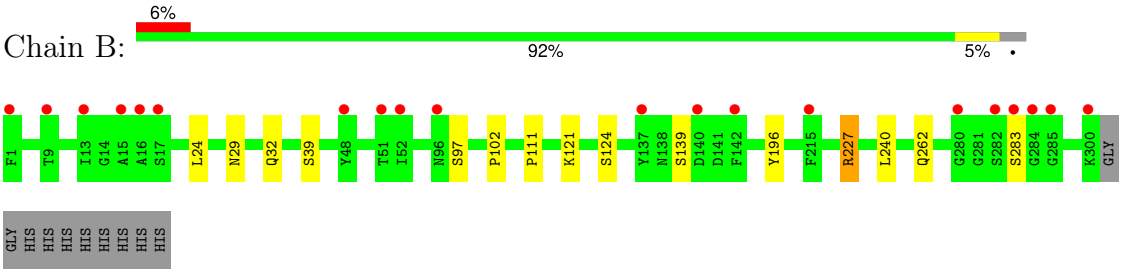
• Molecule 1: Type 1 fimbrin D-mannose specific adhesin,Protein FimG

Chain A:



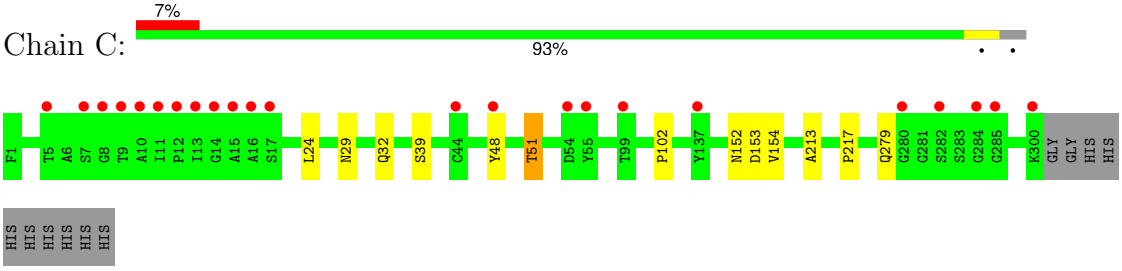
• Molecule 1: Type 1 fimbrin D-mannose specific adhesin,Protein FimG

Chain B:



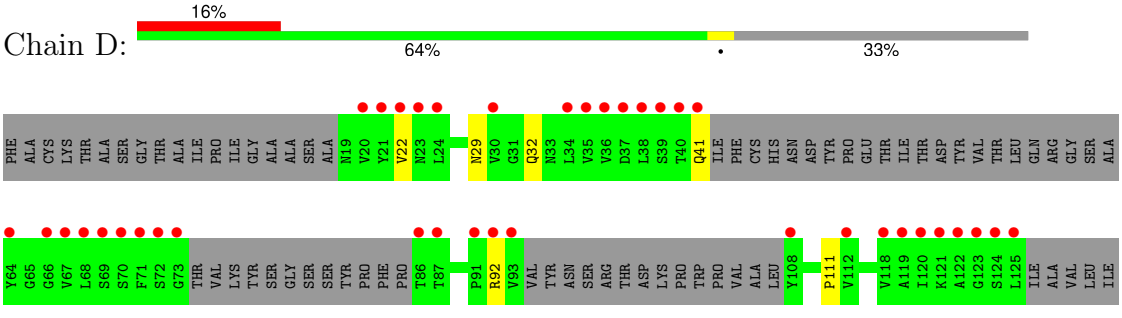
• Molecule 1: Type 1 fimbrin D-mannose specific adhesin,Protein FimG

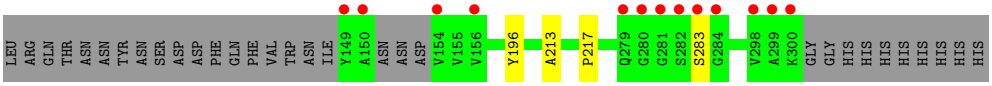
Chain C:



• Molecule 1: Type 1 fimbrin D-mannose specific adhesin,Protein FimG

Chain D:




LEU
ARG
GLN
THR
ASN
ASN
TYR
ASN
SER
ASP
ASP
PHE
GLN
PHE
VAL
TRP
ASN
ILE
Y149
A150
ASN
ASN
ASP
V154
V155
V156
Y196
A213
P217
Q279
G280
G281
S282
S283
G284
V298
A299
K300
GLY
GLY
HIS
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	140.04Å 149.26Å 99.35Å 90.00° 130.03° 90.00°	Depositor
Resolution (Å)	27.50 – 1.90 27.50 – 1.90	Depositor EDS
% Data completeness (in resolution range)	70.4 (27.50-1.90) 70.3 (27.50-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.26 (at 1.89Å)	Xtriage
Refinement program	BUSTER 2.11.8 (22-FEB-2023)	Depositor
R, R_{free}	0.211 , 0.238 0.207 , 0.230	Depositor DCC
R_{free} test set	40901 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å^2)	34.5	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 37.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8913	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 4.15% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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	0.42	0/2230	0.60	0/3062
1	B	0.40	0/2230	0.59	0/3062
1	C	0.42	0/2226	0.59	0/3058
1	D	0.38	0/1465	0.55	0/2003
All	All	0.41	0/8151	0.59	0/11185

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

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	2185	0	2149	7	0
1	B	2185	0	2149	6	0
1	C	2181	0	2138	5	0
1	D	1449	0	1443	5	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
2	C	14	0	13	0	0
2	D	14	0	13	0	0
3	A	280	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	222	0	0	0	0
3	C	228	0	0	0	0
3	D	127	0	0	0	0
All	All	8913	0	7931	22	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 1.

All (22) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:VAL:HG13	1:D:41:GLN:HG3	1.75	0.68
1:A:82:TYR:OH	1:A:91:PRO:HD3	1.95	0.65
1:A:22:VAL:HG22	1:A:41:GLN:HB3	1.82	0.60
1:D:32:GLN:HA	1:D:111:PRO:HD3	1.87	0.56
1:A:32:GLN:HA	1:A:111:PRO:HD3	1.87	0.56
1:B:32:GLN:HA	1:B:111:PRO:HD3	1.88	0.53
1:B:121:LYS:O	1:B:124:SER:OG	2.27	0.51
1:C:48:TYR:HB3	1:C:51:THR:HG23	1.93	0.50
1:C:29:ASN:HB2	1:C:32:GLN:O	2.11	0.50
1:A:39:SER:O	1:A:102:PRO:HB3	2.14	0.48
1:B:39:SER:O	1:B:102:PRO:HB3	2.14	0.47
1:C:39:SER:O	1:C:102:PRO:HB3	2.15	0.47
1:B:29:ASN:HB2	1:B:32:GLN:O	2.14	0.47
1:A:101:LYS:HD2	1:C:152:ASN:HB3	1.95	0.46
1:C:213:ALA:HB3	1:C:217:PRO:HB3	1.98	0.46
1:D:213:ALA:HB3	1:D:217:PRO:HB3	1.98	0.45
1:A:29:ASN:HB2	1:A:32:GLN:O	2.17	0.45
1:B:227:ARG:HH12	1:B:240:LEU:CD2	2.30	0.45
1:B:196:TYR:OH	1:B:283:SER:HB3	2.18	0.43
1:D:29:ASN:HB2	1:D:32:GLN:O	2.20	0.42
1:D:196:TYR:OH	1:D:283:SER:HB3	2.20	0.41
1:A:213:ALA:HB3	1:A:217:PRO:HB3	2.03	0.41

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	299/310 (96%)	297 (99%)	2 (1%)	0	100	100
1	B	299/310 (96%)	299 (100%)	0	0	100	100
1	C	299/310 (96%)	296 (99%)	3 (1%)	0	100	100
1	D	197/310 (64%)	194 (98%)	3 (2%)	0	100	100
All	All	1094/1240 (88%)	1086 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	239/246 (97%)	235 (98%)	4 (2%)	56	54
1	B	239/246 (97%)	234 (98%)	5 (2%)	48	45
1	C	238/246 (97%)	233 (98%)	5 (2%)	48	45
1	D	158/246 (64%)	157 (99%)	1 (1%)	84	86
All	All	874/984 (89%)	859 (98%)	15 (2%)	56	54

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	97	SER

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Mol	Chain	Res	Type
1	A	154	VAL
1	A	262	GLN
1	B	24	LEU
1	B	97	SER
1	B	139	SER
1	B	227	ARG
1	B	262	GLN
1	C	24	LEU
1	C	51	THR
1	C	153	ASP
1	C	154	VAL
1	C	279	GLN
1	D	92	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	32	GLN
1	C	96	ASN
1	D	32	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

4 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	$\#\|Z\| > 2$
2	NAG	C	401	1	14,14,15	0.33	0	17,19,21	1.05	1 (5%)
2	NAG	D	401	1	14,14,15	0.34	0	17,19,21	1.06	1 (5%)
2	NAG	B	401	1	14,14,15	0.31	0	17,19,21	0.57	0
2	NAG	A	401	1	14,14,15	0.28	0	17,19,21	0.58	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
2	NAG	C	401	1	-	1/6/23/26	0/1/1/1
2	NAG	D	401	1	-	2/6/23/26	0/1/1/1
2	NAG	B	401	1	-	0/6/23/26	0/1/1/1
2	NAG	A	401	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	401	NAG	C2-N2-C7	2.94	126.84	122.90
2	D	401	NAG	C2-N2-C7	2.71	126.53	122.90

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	401	NAG	C1-C2-N2-C7
2	D	401	NAG	C1-C2-N2-C7
2	D	401	NAG	O5-C5-C6-O6

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, 95^{th} 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	300/310 (96%)	0.17	10 (3%) 49 51	18, 35, 50, 71	1 (0%)
1	B	300/310 (96%)	0.29	20 (6%) 25 26	18, 36, 67, 79	1 (0%)
1	C	299/310 (96%)	0.31	23 (7%) 21 22	25, 34, 64, 72	0
1	D	208/310 (67%)	1.01	51 (24%) 2 2	21, 39, 100, 115	1 (0%)
All	All	1107/1240 (89%)	0.40	104 (9%) 15 16	18, 35, 70, 115	3 (0%)

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	21	TYR	7.0
1	D	73	GLY	6.6
1	C	137	TYR	6.3
1	D	93	VAL	6.0
1	D	122	ALA	5.7
1	D	91	PRO	5.4
1	B	137	TYR	5.1
1	C	13	ILE	5.1
1	D	150	ALA	5.0
1	D	123	GLY	5.0
1	B	51	THR	4.9
1	D	108	TYR	4.9
1	D	20	VAL	4.9
1	D	149	TYR	4.9
1	D	125	LEU	4.8
1	A	280	GLY	4.8
1	A	283	SER	4.7
1	D	22	VAL	4.5
1	D	23	ASN	4.4
1	D	24	LEU	4.3
1	D	40	THR	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	68	LEU	4.2
1	D	35	VAL	4.2
1	C	14	GLY	4.1
1	B	284	GLY	4.0
1	D	280	GLY	3.8
1	C	280	GLY	3.8
1	D	64	TYR	3.7
1	B	215	PHE	3.6
1	D	92	ARG	3.6
1	B	285	GLY	3.6
1	D	71	PHE	3.6
1	B	283	SER	3.6
1	D	38	LEU	3.5
1	C	10	ALA	3.5
1	C	8	GLY	3.5
1	D	41	GLN	3.4
1	B	48	TYR	3.4
1	B	280	GLY	3.4
1	D	300	LYS	3.4
1	D	299	ALA	3.4
1	D	284	GLY	3.3
1	A	137	TYR	3.3
1	C	16	ALA	3.2
1	D	86	THR	3.2
1	B	52	ILE	3.2
1	D	87	THR	3.1
1	C	300	LYS	3.1
1	D	72	SER	3.1
1	D	283	SER	3.0
1	B	282	SER	2.9
1	D	154	VAL	2.9
1	B	300	LYS	2.9
1	C	9	THR	2.8
1	B	142	PHE	2.8
1	D	121	LYS	2.8
1	D	36	VAL	2.8
1	C	285	GLY	2.8
1	D	124	SER	2.8
1	B	140	ASP	2.7
1	A	215	PHE	2.7
1	D	70	SER	2.7
1	D	282	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	11	ILE	2.6
1	A	284	GLY	2.6
1	D	67	VAL	2.6
1	D	112	VAL	2.6
1	C	282	SER	2.6
1	D	69	SER	2.6
1	B	9	THR	2.5
1	C	284	GLY	2.5
1	C	55	TYR	2.5
1	C	15	ALA	2.5
1	B	1	PHE	2.5
1	A	8	GLY	2.5
1	B	15	ALA	2.5
1	D	39	SER	2.4
1	C	5	THR	2.4
1	B	16	ALA	2.4
1	C	7	SER	2.4
1	D	156	VAL	2.3
1	D	66	GLY	2.3
1	D	30	VAL	2.3
1	B	96	ASN	2.2
1	D	279	GLN	2.2
1	C	54	ASP	2.2
1	C	44	CYS	2.2
1	A	300	LYS	2.2
1	C	48	TYR	2.2
1	C	99	THR	2.1
1	A	282	SER	2.1
1	D	281	GLY	2.1
1	A	15	ALA	2.1
1	B	17	SER	2.1
1	D	34	LEU	2.1
1	B	13	ILE	2.1
1	C	17	SER	2.1
1	D	37	ASP	2.0
1	D	118	VAL	2.0
1	C	12	PRO	2.0
1	D	120	ILE	2.0
1	A	102	PRO	2.0
1	D	119	ALA	2.0
1	D	298	VAL	2.0

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

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

6.3 Carbohydrates (i)

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, 95^{th} 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	B	401	14/15	0.29	0.20	70,73,73,74	0
2	NAG	A	401	14/15	0.52	0.16	66,68,70,70	0
2	NAG	D	401	14/15	0.73	0.13	48,52,55,57	0
2	NAG	C	401	14/15	0.78	0.12	51,53,54,55	0

6.5 Other polymers (i)

There are no such residues in this entry.