



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 01:10 PM GMT

PDB ID : 3D2U
Title : Structure of UL18, a Peptide-Binding Viral MHC Mimic, Bound to a Host Inhibitory Receptor
Authors : Yang, Z.; Bjorkman, P.J.
Deposited on : 2008-05-08
Resolution : 2.21 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

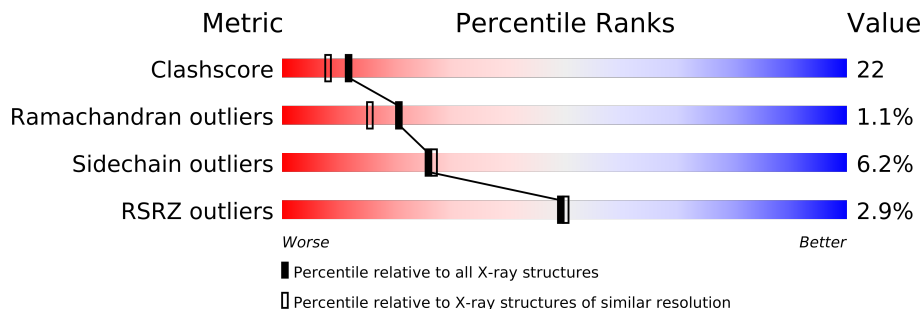
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.21 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))
Clashscore	79885	4208 (2.24-2.20)
Ramachandran outliers	78287	4135 (2.24-2.20)
Sidechain outliers	78261	4136 (2.24-2.20)
RSRZ outliers	66119	3341 (2.24-2.20)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	281	
1	E	281	
2	B	99	
2	F	99	
3	D	198	
3	H	198	
4	C	9	
4	G	9	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	NAG	A	810	-	X
5	NAG	A	831	-	X
5	NAG	A	861	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
5	NAG	E	871	-	X
5	NAG	E	891	-	X
8	FUC	A	814	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 9681 atoms, of which 0 are hydrogen and 0 are deuterium.

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 UL18 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	4	0	0
			2227	1412	372	434	9			
1	E	279	Total	C	N	O	S	8	0	0
			2209	1402	368	430	9			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	36	GLN	ASN	ENGINEERED	UNP Q4A1U8
A	147	GLN	ASN	ENGINEERED	UNP Q4A1U8
A	186	PRO	THR	VARIANT	UNP Q4A1U8
A	220	GLN	ASN	ENGINEERED	UNP Q4A1U8
A	259	SER	CYS	ENGINEERED	UNP Q4A1U8
E	36	GLN	ASN	ENGINEERED	UNP Q4A1U8
E	147	GLN	ASN	ENGINEERED	UNP Q4A1U8
E	186	PRO	THR	VARIANT	UNP Q4A1U8
E	220	GLN	ASN	ENGINEERED	UNP Q4A1U8
E	259	SER	CYS	ENGINEERED	UNP Q4A1U8

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			825	525	139	158	3			
2	F	99	Total	C	N	O	S	0	0	0
			825	525	139	158	3			

- Molecule 3 is a protein called Leukocyte immunoglobulin-like receptor subfamily B member 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	182	Total	C	N	O	S	0	0	0
			1418	904	238	270	6			
3	H	185	Total	C	N	O	S	4	0	0
			1443	920	243	274	6			

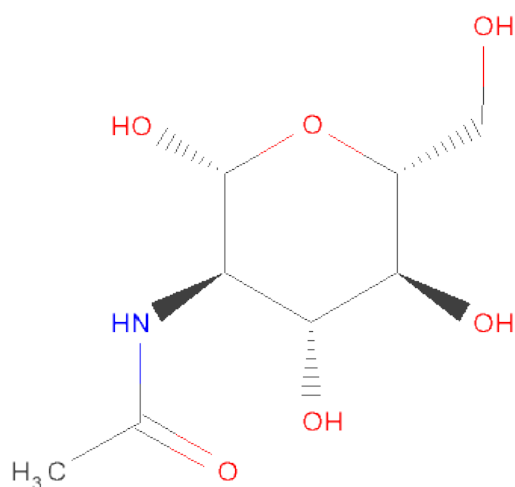
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	45	PRO	LEU	VARIANT	UNP Q8NHL6
D	119	THR	ILE	VARIANT	UNP Q8NHL6
D	132	ILE	SER	VARIANT	UNP Q8NHL6
H	45	PRO	LEU	VARIANT	UNP Q8NHL6
H	119	THR	ILE	VARIANT	UNP Q8NHL6
H	132	ILE	SER	VARIANT	UNP Q8NHL6

- Molecule 4 is a protein called Actin.

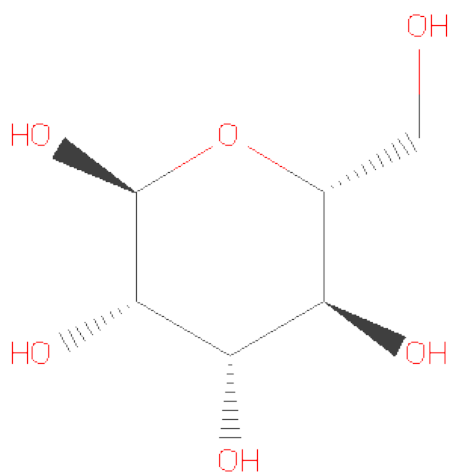
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	9	Total	C	N	O	0	0	0
			71	47	14	10			
4	C	9	Total	C	N	O	0	0	0
			71	47	14	10			

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



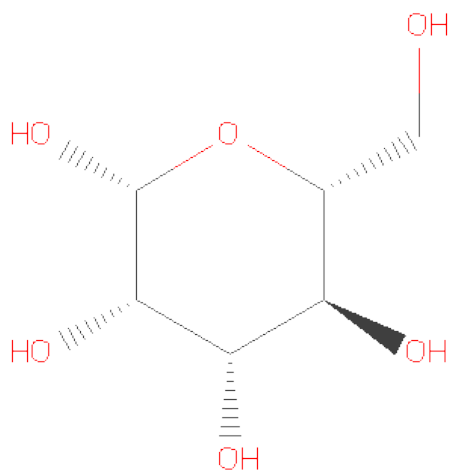
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			15	8	1	6		
5	A	1	Total	C	N	O	0	0
			15	8	1	6		
5	A	1	Total	C	N	O	0	0
			15	8	1	6		
5	A	1	Total	C	N	O	0	0
			15	8	1	6		
5	A	1	Total	C	N	O	0	0
			15	8	1	6		
5	A	1	Total	C	N	O	0	0
			15	8	1	6		
5	E	1	Total	C	N	O	0	0
			15	8	1	6		
5	E	1	Total	C	N	O	0	0
			15	8	1	6		
5	E	1	Total	C	N	O	0	0
			15	8	1	6		
5	E	1	Total	C	N	O	0	0
			15	8	1	6		
5	E	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 6 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (formula: C₆H₁₂O₆).



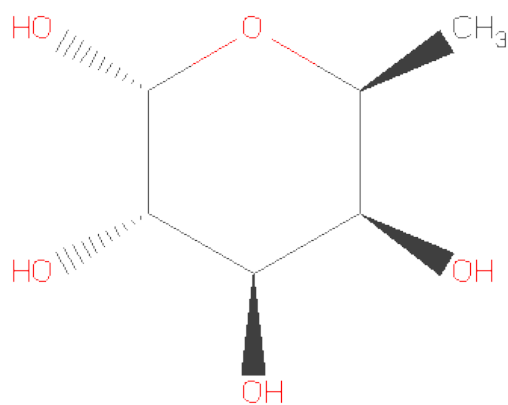
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			12	6	6		

- Molecule 7 is SUGAR (BETA-D-MANNOSE) (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			12	6	6		

- Molecule 8 is SUGAR (ALPHA-L-FUCOSE) (three-letter code: FUC) (formula: $C_6H_{12}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 9 is water.

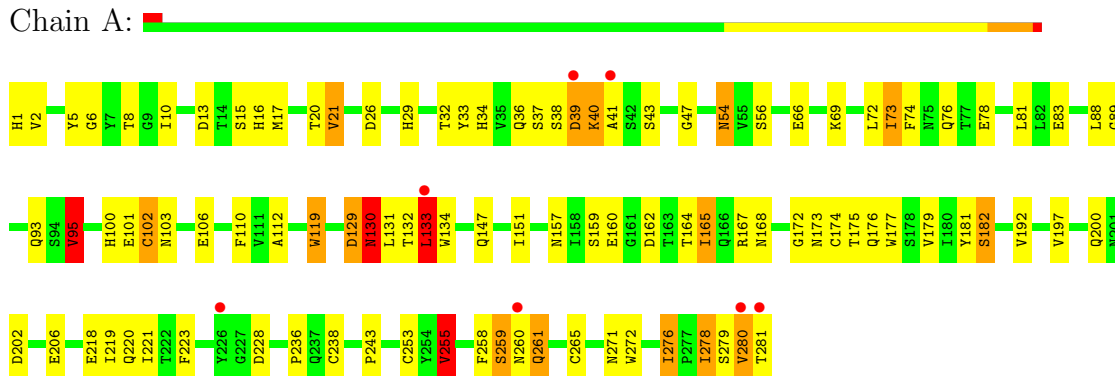
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	90	Total	O	0	0
			90	90		
9	B	48	Total	O	0	0
			48	48		
9	D	46	Total	O	0	0
			46	46		
9	E	62	Total	O	0	0
			62	62		
9	F	58	Total	O	0	0
			58	58		
9	H	58	Total	O	0	0
			58	58		

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.

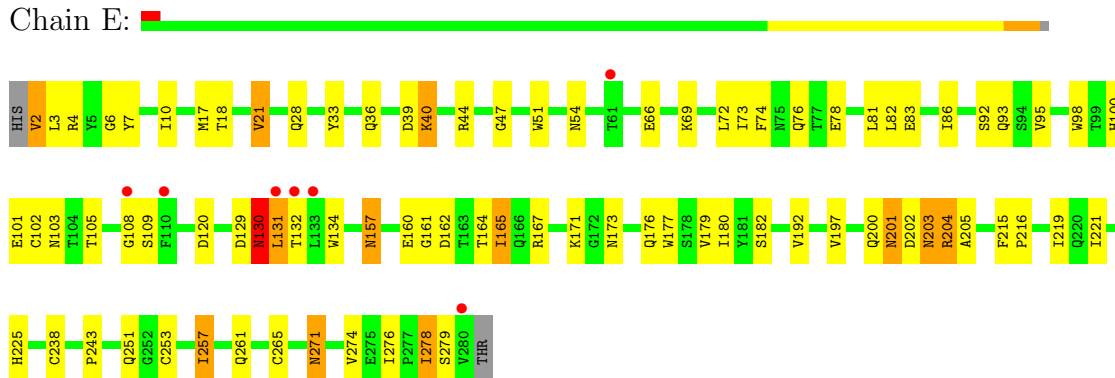
• Molecule 1: UL18 protein

Chain A:



• Molecule 1: UL18 protein

Chain E:



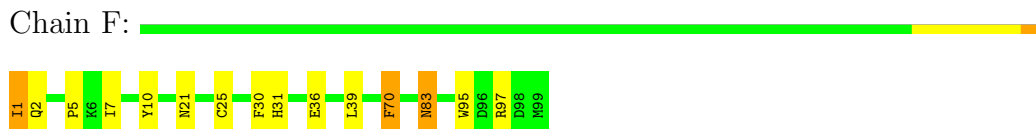
• Molecule 2: Beta-2-microglobulin

Chain B:



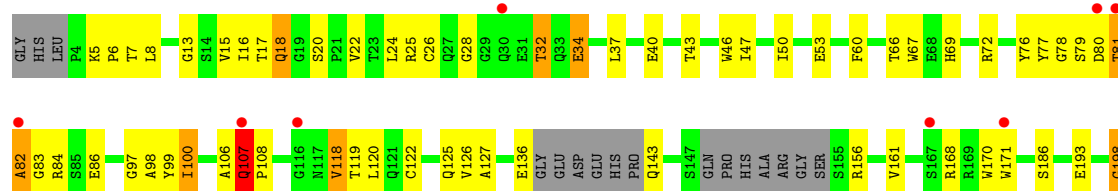
• Molecule 2: Beta-2-microglobulin

Chain F:



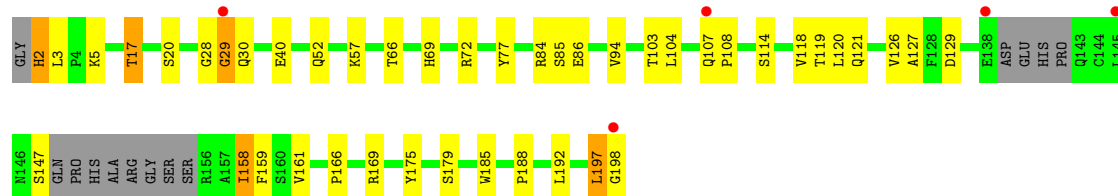
- Molecule 3: Leukocyte immunoglobulin-like receptor subfamily B member 1

Chain D:



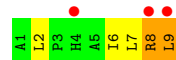
- Molecule 3: Leukocyte immunoglobulin-like receptor subfamily B member 1

Chain H:



- Molecule 4: Actin

Chain G:



- Molecule 4: Actin

Chain C:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.37Å 98.11Å 172.15Å 90.00° 98.46° 90.00°	Depositor
Resolution (Å)	47.46 – 2.21 47.46 – 2.21	Depositor EDS
% Data completeness (in resolution range)	97.0 (47.46-2.21) 94.2 (47.46-2.21)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.66 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.241 , 0.259 0.237 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	35.3	Xtriage
Anisotropy	0.734	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 46.9	EDS
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	3 of 84329 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9681	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, BMA, NAG, MAN

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	0.48	0/2289	0.83	8/3120 (0.3%)
1	E	0.45	0/2270	0.76	3/3095 (0.1%)
2	B	0.43	0/848	0.74	0/1148
2	F	0.49	0/848	0.74	0/1148
3	D	0.45	0/1458	0.83	1/1988 (0.1%)
3	H	0.42	0/1484	0.80	1/2024 (0.0%)
4	C	0.49	0/72	1.01	0/96
4	G	0.46	0/72	0.88	0/96
All	All	0.46	0/9341	0.80	13/12715 (0.1%)

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	30	GLN	N-CA-C	-10.30	83.19	111.00
3	D	198	GLY	N-CA-C	-6.80	96.09	113.10
1	A	174	CYS	CA-CB-SG	-6.66	102.02	114.00
1	A	255	VAL	CB-CA-C	-6.46	99.12	111.40
1	A	102	CYS	CA-CB-SG	6.35	125.43	114.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2227	0	2080	131	0
1	E	2209	0	2063	106	0
2	B	825	0	783	17	0
2	F	825	0	783	19	0
3	D	1418	0	1365	56	0
3	H	1443	0	1386	42	0
4	C	71	0	83	6	0
4	G	71	0	83	9	0
5	A	105	0	105	53	0
5	E	90	0	90	24	0
6	A	12	0	12	13	0
7	A	12	0	12	8	0
8	A	11	0	12	6	0
9	A	90	0	0	1	0
9	B	48	0	0	3	0
9	D	46	0	0	2	0
9	E	62	0	0	3	0
9	F	58	0	0	0	0
9	H	58	0	0	3	0
All	All	9681	0	8857	396	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 22.

The worst 5 of 396 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:A:831:NAG:O4	5:A:832:NAG:H1	1.33	1.26
5:A:811:NAG:O4	6:A:812:MAN:H1	1.14	1.25
1:A:271:ASN:HD21	5:A:891:NAG:C1	1.51	1.21
1:E:164:THR:HG22	1:E:167:ARG:NH2	1.63	1.14
5:A:831:NAG:O4	5:A:832:NAG:C1	1.95	1.14

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	279/281 (99%)	263 (94%)	13 (5%)	3 (1%)	21	15
1	E	277/281 (99%)	253 (91%)	20 (7%)	4 (1%)	16	11
2	B	97/99 (98%)	95 (98%)	2 (2%)	0	100	100
2	F	97/99 (98%)	96 (99%)	1 (1%)	0	100	100
3	D	176/198 (89%)	166 (94%)	7 (4%)	3 (2%)	14	8
3	H	179/198 (90%)	174 (97%)	3 (2%)	2 (1%)	21	15
4	C	7/9 (78%)	7 (100%)	0	0	100	100
4	G	7/9 (78%)	7 (100%)	0	0	100	100
All	All	1119/1174 (95%)	1061 (95%)	46 (4%)	12 (1%)	21	15

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	LYS
3	D	82	ALA
1	E	130	ASN
3	D	81	THR
1	E	40	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	242/244 (99%)	219 (90%)	23 (10%)	12	10
1	E	240/244 (98%)	226 (94%)	14 (6%)	28	30
2	B	93/94 (99%)	90 (97%)	3 (3%)	51	62
2	F	93/94 (99%)	90 (97%)	3 (3%)	51	62
3	D	156/171 (91%)	147 (94%)	9 (6%)	28	30
3	H	158/171 (92%)	151 (96%)	7 (4%)	39	45
4	C	7/7 (100%)	6 (86%)	1 (14%)	5	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	G	7/7 (100%)	5 (71%)	2 (29%)	0	0
All	All	996/1032 (96%)	934 (94%)	62 (6%)	26	27

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	34	GLU
3	D	143	GLN
3	H	169	ARG
3	D	107	GLN
1	E	3	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	146	ASN
1	E	76	GLN
3	H	69	HIS
3	D	180	ASN
1	E	28	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

16 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
5	NAG	A	810	-	15,15,15	0.65	0	21,21,21	1.12	2 (9%)
5	NAG	A	811	-	15,15,15	0.63	0	21,21,21	1.35	2 (9%)
6	MAN	A	812	-	12,12,12	0.35	0	17,17,17	1.00	1 (5%)
7	BMA	A	813	-	12,12,12	0.43	0	17,17,17	0.58	0
8	FUC	A	814	-	11,11,11	0.56	0	16,16,16	1.26	2 (12%)
5	NAG	A	831	-	15,15,15	0.82	0	21,21,21	1.55	2 (9%)
5	NAG	A	832	-	15,15,15	0.69	0	21,21,21	1.94	3 (14%)
5	NAG	A	861	-	15,15,15	0.83	1 (6%)	21,21,21	1.94	3 (14%)
5	NAG	A	871	-	15,15,15	0.35	0	21,21,21	1.22	4 (19%)
5	NAG	A	891	-	15,15,15	0.66	0	21,21,21	1.53	3 (14%)
5	NAG	E	810	-	15,15,15	0.45	0	21,21,21	0.68	0
5	NAG	E	831	-	15,15,15	0.89	1 (6%)	21,21,21	1.43	2 (9%)
5	NAG	E	832	-	15,15,15	0.78	1 (6%)	21,21,21	0.86	1 (4%)
5	NAG	E	861	-	15,15,15	0.71	1 (6%)	21,21,21	0.86	1 (4%)
5	NAG	E	871	-	15,15,15	0.46	0	21,21,21	1.04	2 (9%)
5	NAG	E	891	-	15,15,15	0.51	0	21,21,21	0.89	1 (4%)

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
5	NAG	A	810	-	-	0/6/26/26	0/1/1/1
5	NAG	A	811	-	-	0/6/26/26	0/1/1/1
6	MAN	A	812	-	-	0/2/22/22	0/1/1/1
7	BMA	A	813	-	-	0/2/22/22	0/1/1/1
8	FUC	A	814	-	-	0/0/20/20	0/1/1/1
5	NAG	A	831	-	-	0/6/26/26	0/1/1/1
5	NAG	A	832	-	-	0/6/26/26	0/1/1/1
5	NAG	A	861	-	-	0/6/26/26	0/1/1/1
5	NAG	A	871	-	-	0/6/26/26	0/1/1/1
5	NAG	A	891	-	-	0/6/26/26	0/1/1/1
5	NAG	E	810	-	-	0/6/26/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	E	831	-	-	0/6/26/26	0/1/1/1
5	NAG	E	832	-	-	0/6/26/26	0/1/1/1
5	NAG	E	861	-	-	0/6/26/26	0/1/1/1
5	NAG	E	871	-	-	0/6/26/26	0/1/1/1
5	NAG	E	891	-	-	2/6/26/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	861	NAG	C1-C2	2.70	1.56	1.53
5	E	832	NAG	C1-C2	-2.31	1.50	1.53
5	E	861	NAG	C1-C2	2.13	1.55	1.53
5	E	831	NAG	O4-C4	-2.10	1.37	1.43

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	832	NAG	O5-C1-C2	6.93	116.63	109.61
5	A	831	NAG	C1-C2-C3	-5.70	102.43	110.59
5	A	861	NAG	O5-C1-C2	5.37	115.06	109.61
5	A	861	NAG	C1-C2-C3	5.29	118.17	110.59
5	E	831	NAG	O5-C1-C2	4.11	113.78	109.61

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	891	NAG	C1-C2-N2-C7
5	E	891	NAG	O7-C7-N2-C2

There are no ring outliers.

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	281/281 (100%)	0.26	7 (2%) 54 55	29, 42, 55, 61	1 (0%)
1	E	279/281 (99%)	0.32	7 (2%) 54 55	26, 42, 57, 63	2 (0%)
2	B	99/99 (100%)	0.31	0 100 100	28, 38, 51, 56	0
2	F	99/99 (100%)	0.51	0 100 100	22, 36, 49, 55	0
3	D	182/198 (91%)	0.31	8 (4%) 33 33	32, 45, 57, 65	0
3	H	185/198 (93%)	0.21	5 (2%) 52 53	23, 37, 52, 62	1 (0%)
4	C	9/9 (100%)	1.19	4 (44%) 1 0	45, 52, 58, 61	0
4	G	9/9 (100%)	1.51	3 (33%) 1 1	48, 54, 60, 63	0
All	All	1143/1174 (97%)	0.32	34 (2%) 49 49	22, 41, 56, 65	4 (0%)

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	280	VAL	4.8
3	H	29	GLY	4.8
1	E	133	LEU	4.1
1	A	281	THR	4.0
4	G	4	HIS	3.8

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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	NAG	E	891	15/15	0.35	411.00	52,59,69,71	0
5	NAG	E	871	15/15	0.36	11.84	55,62,78,78	0
5	NAG	A	831	15/15	0.21	4.29	41,51,71,76	0
5	NAG	A	861	15/15	0.28	3.08	52,61,73,73	0
5	NAG	A	810	15/15	0.18	2.94	37,50,69,70	0
8	FUC	A	814	11/11	0.20	2.05	51,55,72,74	0
5	NAG	A	891	15/15	0.30	1.86	46,60,71,74	0
5	NAG	A	871	15/15	0.26	1.50	50,61,74,81	0
5	NAG	E	861	15/15	0.30	1.47	46,63,72,74	0
6	MAN	A	812	12/12	0.17	0.77	39,49,72,73	0
7	BMA	A	813	12/12	0.16	0.60	34,47,56,67	0
5	NAG	E	831	15/15	0.19	0.44	43,55,62,71	0
5	NAG	A	811	15/15	0.16	-	39,50,59,59	0
5	NAG	A	832	15/15	0.18	-	44,54,66,75	0
5	NAG	E	810	15/15	0.14	-	46,57,64,64	0
5	NAG	E	832	15/15	0.20	-	44,55,69,69	0

6.5 Other polymers ⓘ

There are no such residues in this entry.