



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 17, 2020 – 10:09 AM BST

PDB ID : 5K9O
Title : Crystal structure of multidonor HV1-18+HD3-9 class broadly neutralizing Influenza A antibody 31.b.09 in complex with Hemagglutinin H1 A/California/04/2009
Authors : Joyce, M.G.; Thomas, P.V.; Wheatley, A.K.; McDermott, A.B.; Mascola, J.R.; Kwong, P.D.
Deposited on : 2016-06-01
Resolution : 3.39 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

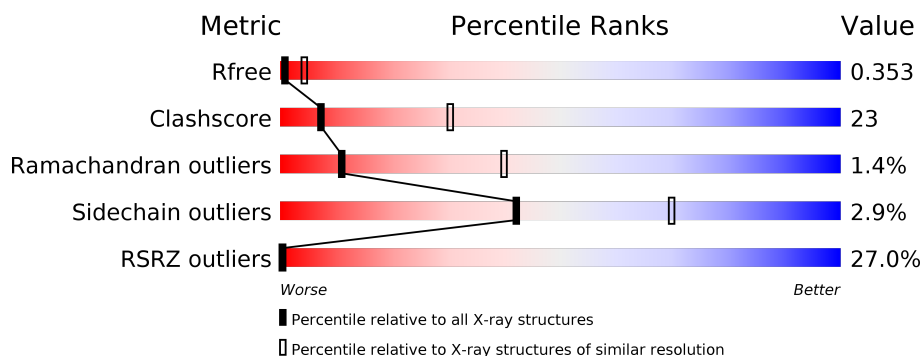
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.39 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	1691 (3.46-3.30)
Clashscore	141614	1762 (3.46-3.30)
Ramachandran outliers	138981	1732 (3.46-3.30)
Sidechain outliers	138945	1731 (3.46-3.30)
RSRZ outliers	127900	1635 (3.46-3.30)

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	227	
1	H	227	
2	B	219	
2	L	219	
3	F	505	
3	I	505	

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Mol	Chain	Length	Quality of chain
4	C	3	<div><div></div><div>33%</div><div>67%</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
4	NAG	C	2	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14056 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 31.b.09 Heavy Fv.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	0
			1655	1043	277	327	8			
1	H	221	Total	C	N	O	S	0	0	0
			1661	1046	280	327	8			

- Molecule 2 is a protein called 31.b.09 Light Fv.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	213	Total	C	N	O	S	0	0	0
			1654	1036	281	331	6			
2	L	217	Total	C	N	O	S	0	0	0
			1684	1055	285	337	7			

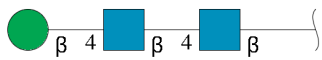
- Molecule 3 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	467	Total	C	N	O	S	0	0	0
			3685	2329	628	711	17			
3	I	466	Total	C	N	O	S	0	0	0
			3678	2317	629	715	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	506	SER	-	expression tag	UNP C3W5S1
F	507	GLY	-	expression tag	UNP C3W5S1
I	506	SER	-	expression tag	UNP C3W5S1
I	507	GLY	-	expression tag	UNP C3W5S1

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

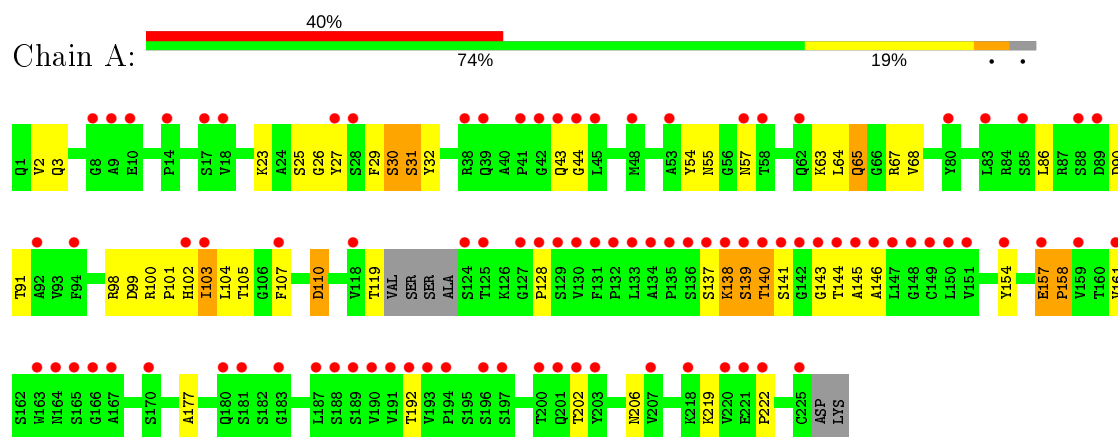


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	C	3	Total	C	N	O	0	0	0
			39	22	2	15			

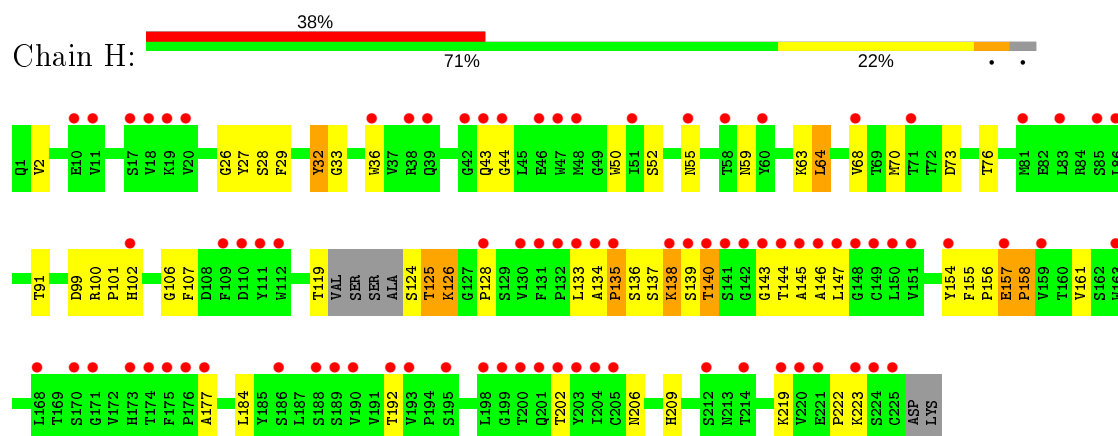
3 Residue-property plots [i](#)

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.

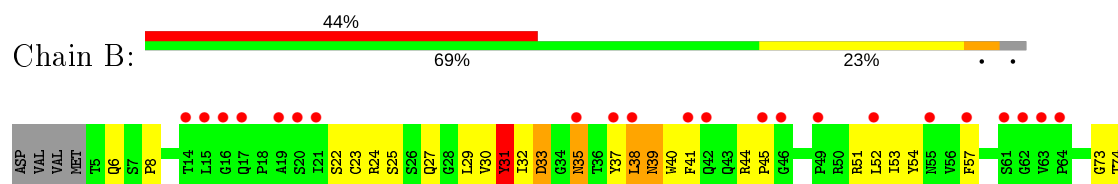
• Molecule 1: 31.b.09 Heavy Fv

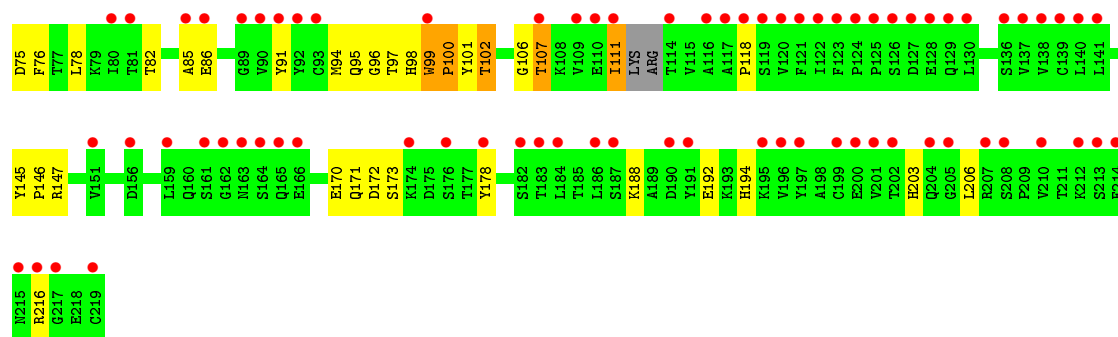


• Molecule 1: 31.b.09 Heavy Fv

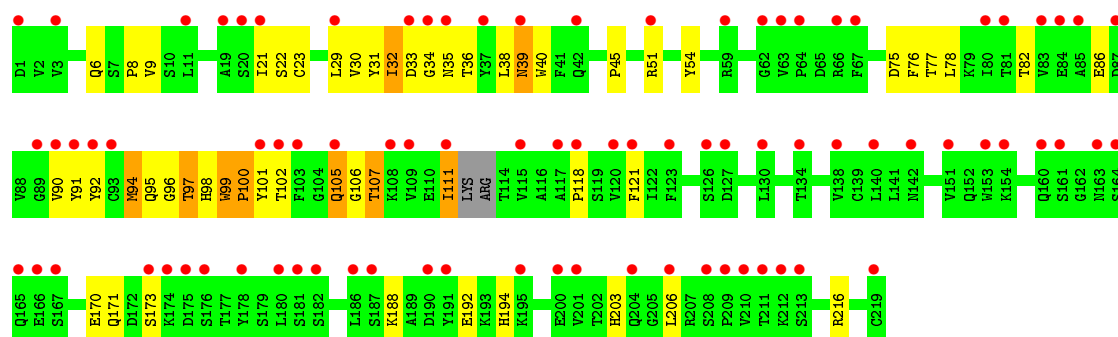
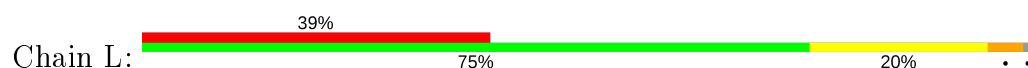


• Molecule 2: 31.b.09 Light Fv

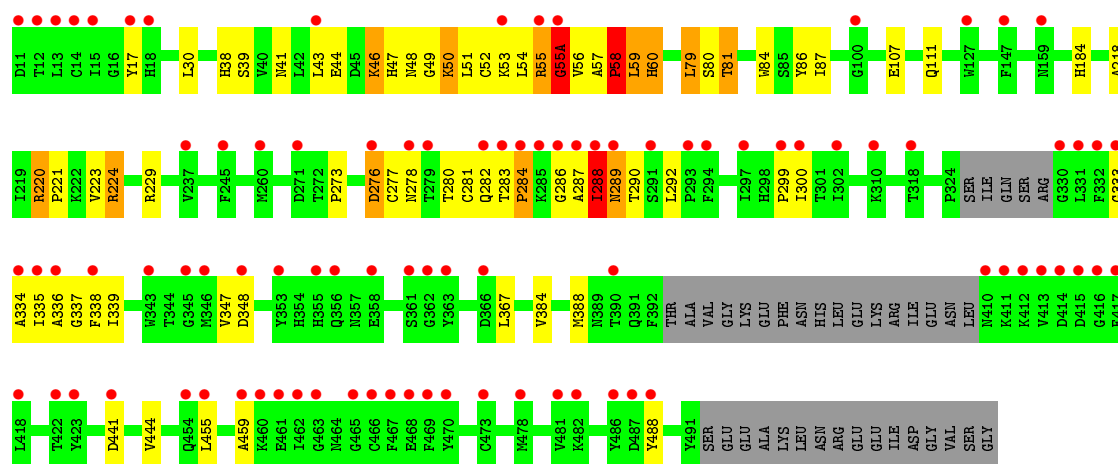
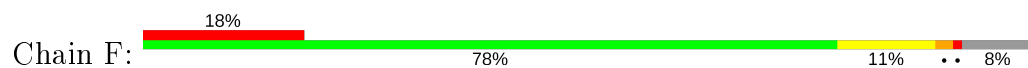




• Molecule 2: 31.b.09 Light Fv

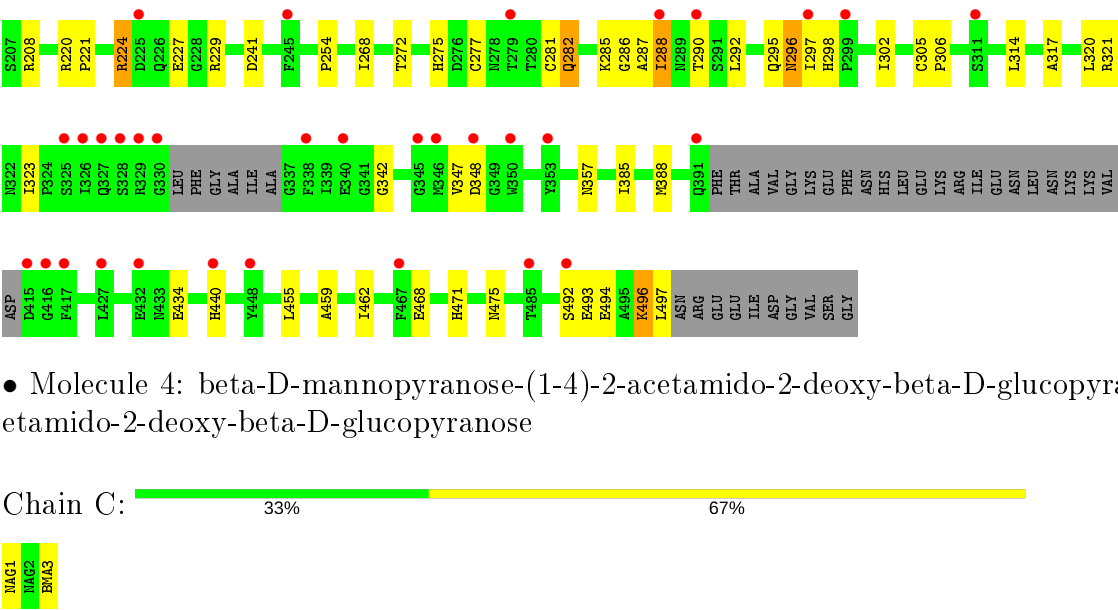


• Molecule 3: Hemagglutinin



• Molecule 3: Hemagglutinin





● Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

4 Data and refinement statistics

Property	Value	Source
Space group	P 6 2 2	Depositor
Cell constants a, b, c, α , β , γ	208.65Å 208.65Å 252.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.97 – 3.39 46.57 – 3.39	Depositor EDS
% Data completeness (in resolution range)	63.8 (38.97-3.39) 63.8 (46.57-3.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 3.40Å)	Xtriage
Refinement program	PHENIX (1.10 _2155: ???)	Depositor
R, R_{free}	0.291 , 0.346 0.304 , 0.353	Depositor DCC
R_{free} test set	1432 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	102.9	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 160.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	14056	wwPDB-VP
Average B, all atoms (Å ²)	207.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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: BMA, 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	0.31	0/1695	0.55	3/2308 (0.1%)
1	H	0.32	0/1701	0.59	3/2315 (0.1%)
2	B	0.33	1/1692 (0.1%)	0.58	2/2299 (0.1%)
2	L	0.28	0/1722	0.54	0/2340
3	F	0.32	0/3774	0.69	5/5117 (0.1%)
3	I	0.28	0/3765	0.49	0/5104
All	All	0.30	1/14349 (0.0%)	0.59	13/19483 (0.1%)

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
3	F	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	100	PRO	N-CD	5.08	1.54	1.47

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	55(A)	GLY	C-N-CA	-25.34	58.34	121.70
3	F	55(A)	GLY	CA-C-N	-19.58	74.12	117.20
1	H	134	ALA	C-N-CD	-11.96	94.30	120.60
3	F	55(A)	GLY	O-C-N	6.33	132.83	122.70
3	F	57	ALA	C-N-CD	6.33	141.69	128.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	F	55(A)	GLY	Mainchain

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	1655	0	1611	76	0
1	H	1661	0	1621	119	0
2	B	1654	0	1584	120	0
2	L	1684	0	1621	111	0
3	F	3685	0	3557	139	0
3	I	3678	0	3546	104	0
4	C	39	0	34	0	0
All	All	14056	0	13574	622	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 23.

The worst 5 of 622 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)
3:F:59:LEU:CD2	3:F:81:THR:HA	1.24	1.65
1:A:107:PHE:CZ	2:B:99:TRP:CH2	1.76	1.64
1:H:124:SER:CA	1:H:155:PHE:HE1	1.05	1.59
1:A:107:PHE:CE2	2:B:99:TRP:CZ3	1.90	1.57
1:H:124:SER:HA	1:H:155:PHE:CE1	0.98	1.51

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	217/227 (96%)	196 (90%)	18 (8%)	3 (1%)	11	40
1	H	217/227 (96%)	193 (89%)	21 (10%)	3 (1%)	11	40
2	B	209/219 (95%)	187 (90%)	19 (9%)	3 (1%)	11	40
2	L	213/219 (97%)	186 (87%)	20 (9%)	7 (3%)	4	24
3	F	461/505 (91%)	422 (92%)	33 (7%)	6 (1%)	12	42
3	I	460/505 (91%)	426 (93%)	32 (7%)	2 (0%)	34	68
All	All	1777/1902 (93%)	1610 (91%)	143 (8%)	24 (1%)	11	40

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	140	THR
2	B	82	THR
3	F	60	HIS
3	F	288	ILE
2	L	34	GLY

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	186/192 (97%)	180 (97%)	6 (3%)	39	68
1	H	187/192 (97%)	181 (97%)	6 (3%)	39	68
2	B	188/194 (97%)	181 (96%)	7 (4%)	34	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	192/194 (99%)	187 (97%)	5 (3%)	46	72
3	F	407/440 (92%)	395 (97%)	12 (3%)	42	70
3	I	408/440 (93%)	398 (98%)	10 (2%)	47	73
All	All	1568/1652 (95%)	1522 (97%)	46 (3%)	42	70

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	276	ASP
1	H	32	TYR
2	L	99	TRP
3	F	288	ILE
3	F	348	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
3	I	275	HIS
3	I	296	ASN
2	L	39	ASN
3	I	41	ASN
2	L	35	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 ⓘ

3 monosaccharides 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	NAG	C	1	3,4	14,14,15	0.94	1 (7%)	17,19,21	1.18	1 (5%)
4	NAG	C	2	4	14,14,15	0.26	0	17,19,21	0.69	0
4	BMA	C	3	4	11,11,12	0.68	0	15,15,17	0.96	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
4	NAG	C	1	3,4	-	1/6/23/26	0/1/1/1
4	NAG	C	2	4	-	1/6/23/26	0/1/1/1
4	BMA	C	3	4	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1	NAG	O5-C1	3.26	1.48	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1	NAG	C1-O5-C5	4.63	118.47	112.19
4	C	3	BMA	C1-O5-C5	2.16	115.12	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1	NAG	O5-C5-C6-O6
4	C	2	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	221/227 (97%)	2.24	91 (41%) 0 0	110, 280, 411, 476	0
1	H	221/227 (97%)	1.77	86 (38%) 0 0	146, 249, 355, 409	3 (1%)
2	B	213/219 (97%)	2.55	96 (45%) 0 0	164, 287, 364, 434	2 (0%)
2	L	217/219 (99%)	1.89	85 (39%) 0 0	143, 256, 349, 411	3 (1%)
3	F	467/505 (92%)	1.13	92 (19%) 1 1	54, 156, 288, 362	9 (1%)
3	I	466/505 (92%)	0.66	38 (8%) 11 14	47, 123, 238, 322	10 (2%)
All	All	1805/1902 (94%)	1.48	488 (27%) 0 0	47, 210, 352, 476	27 (1%)

The worst 5 of 488 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	334	ALA	15.9
1	A	130	VAL	14.2
1	A	134	ALA	13.4
2	B	138	VAL	12.9
1	A	147	LEU	12.8

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](#)

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(\AA^2)	Q<0.9
4	BMA	C	3	11/12	0.47	0.39	247,256,270,274	0
4	NAG	C	2	14/15	0.49	0.62	250,259,274,277	0
4	NAG	C	1	14/15	0.59	0.30	212,224,243,250	0

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.