



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 9, 2020 – 05:15 AM BST

PDB ID : 3GBM
Title : Crystal Structure of Fab CR6261 in Complex with a H5N1 influenza virus hemagglutinin.
Authors : Ekiert, D.C.; Elsliger, M.A.; Wilson, I.A.
Deposited on : 2009-02-20
Resolution : 2.70 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

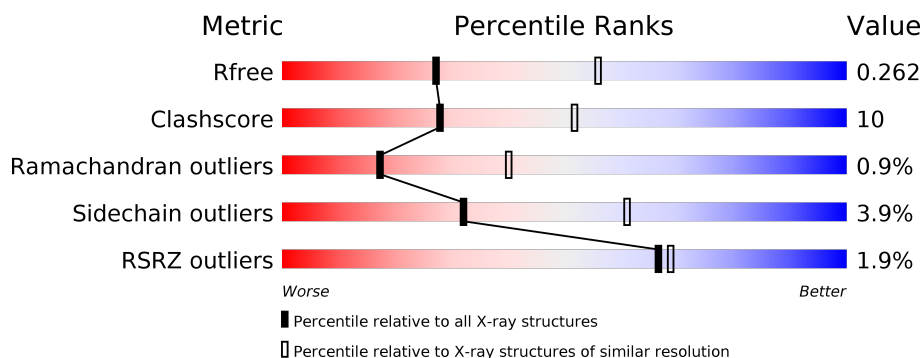
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	334	<div> <div>75%</div> <div>19%</div> <div>• •</div> </div>
1	C	334	<div> <div>73%</div> <div>22%</div> <div>• •</div> </div>
2	B	177	<div> <div>87%</div> <div>12%</div> <div>•</div> </div>
2	D	177	<div> <div>85%</div> <div>12%</div> <div>•</div> </div>
3	H	226	<div> <div>%</div> <div>75%</div> <div>19%</div> <div>• 5%</div> </div>
3	I	226	<div> <div>4%</div> <div>74%</div> <div>18%</div> <div>• 6%</div> </div>

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Mol	Chain	Length	Quality of chain
4	L	221	
4	M	221	
5	E	2	
5	F	2	

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
7	BMA	A	4	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 14189 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	324	Total	C	N	O	S	0	1	0
			2558	1616	438	489	15			
1	C	323	Total	C	N	O	S	0	1	0
			2485	1568	419	483	15			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	-	expression tag	UNP Q6DQ33
A	8	ASP	-	expression tag	UNP Q6DQ33
A	9	PRO	-	expression tag	UNP Q6DQ33
A	10	GLY	-	expression tag	UNP Q6DQ33
C	7	ALA	-	expression tag	UNP Q6DQ33
C	8	ASP	-	expression tag	UNP Q6DQ33
C	9	PRO	-	expression tag	UNP Q6DQ33
C	10	GLY	-	expression tag	UNP Q6DQ33

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	177	Total	C	N	O	S	0	0	0
			1407	874	246	279	8			
2	D	173	Total	C	N	O	S	0	0	0
			1373	852	239	274	8			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	175	SER	-	expression tag	UNP Q6DQ33
B	176	GLY	-	expression tag	UNP Q6DQ33
B	177	ARG	-	expression tag	UNP Q6DQ33
D	175	SER	-	expression tag	UNP Q6DQ33

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Chain	Residue	Modelled	Actual	Comment	Reference
D	176	GLY	-	expression tag	UNP Q6DQ33
D	177	ARG	-	expression tag	UNP Q6DQ33

- Molecule 3 is a protein called antibody (Fab).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	214	Total	C	N	O	S	0	0	0
			1572	1000	257	306	9			
3	I	213	Total	C	N	O	S	0	0	0
			1555	986	255	305	9			

- Molecule 4 is a protein called antibody (Fab).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	208	Total	C	N	O	S	0	0	0
			1498	943	244	307	4			
4	M	197	Total	C	N	O	S	0	0	0
			1415	892	230	289	4			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



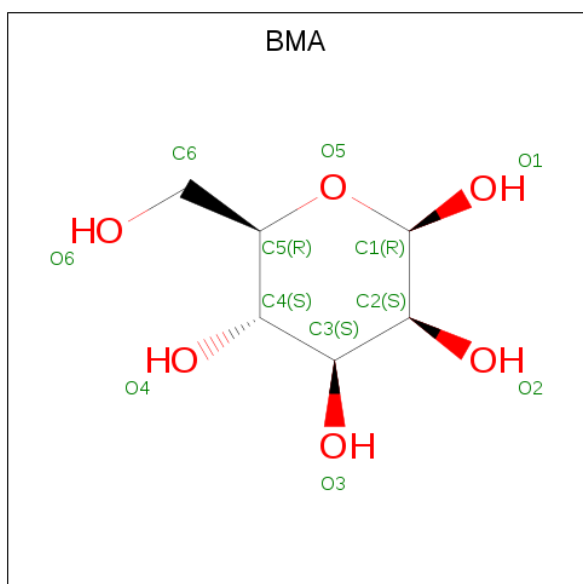
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
5	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		

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



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

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			4	2	2		
8	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			6	3	3		

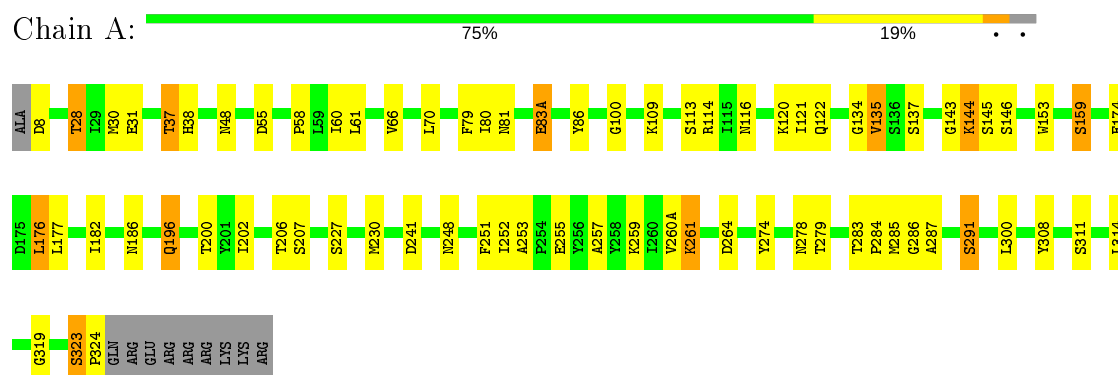
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	52	Total	O	0	0
			52	52		
10	B	38	Total	O	0	0
			38	38		
10	C	5	Total	O	0	0
			5	5		
10	D	24	Total	O	0	0
			24	24		
10	H	17	Total	O	0	0
			17	17		
10	L	6	Total	O	0	0
			6	6		
10	I	13	Total	O	0	0
			13	13		
10	M	9	Total	O	0	0
			9	9		

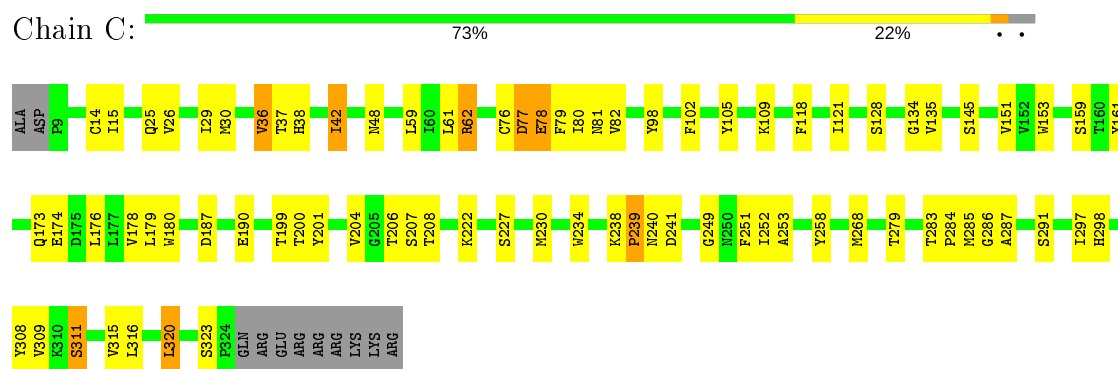
3 Residue-property plots

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.

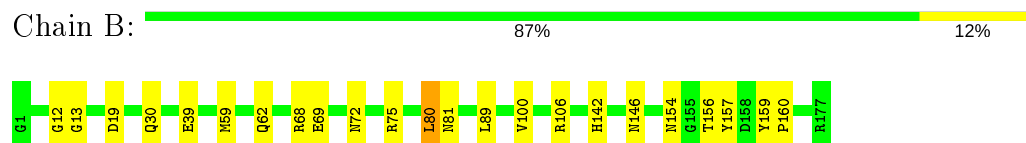
• Molecule 1: Hemagglutinin



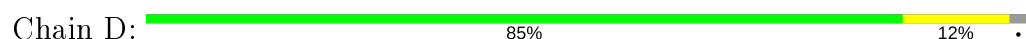
• Molecule 1: Hemagglutinin



• Molecule 2: Hemagglutinin

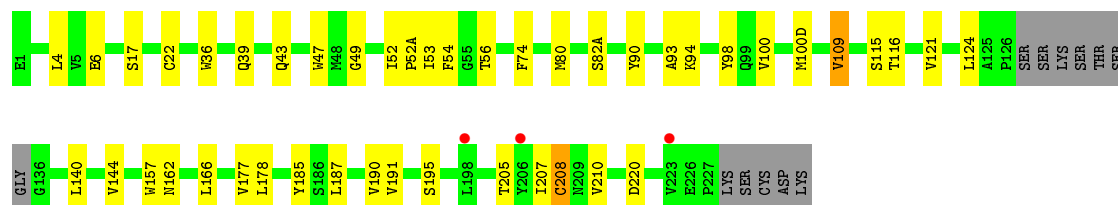
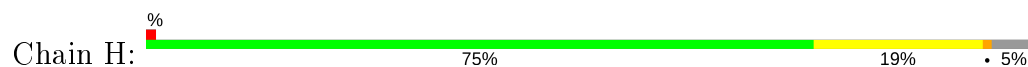


• Molecule 2: Hemagglutinin

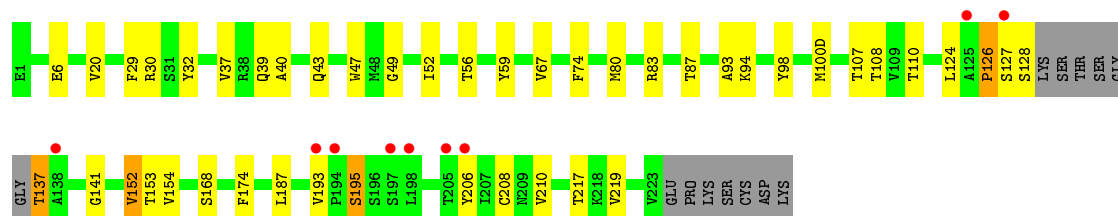
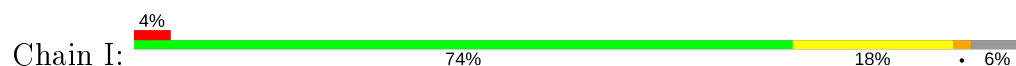




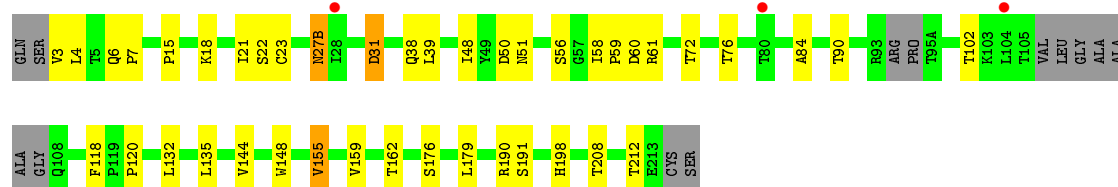
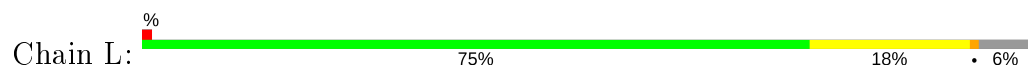
- Molecule 3: antibody (Fab)



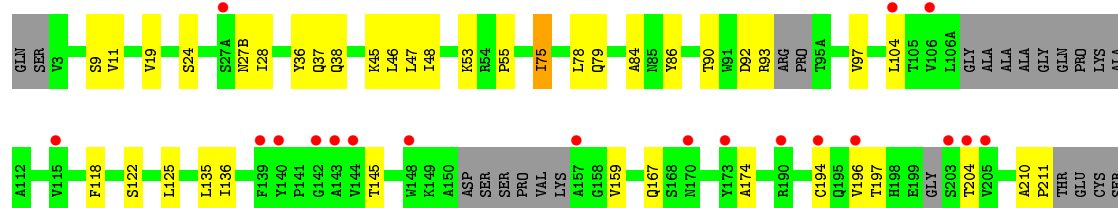
- Molecule 3: antibody (Fab)



- Molecule 4: antibody (Fab)



- Molecule 4: antibody (Fab)



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  100%

HA01
HA02

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  100%

HA01
HA02

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	202.76 Å 202.76 Å 202.76 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.00 – 2.70 49.18 – 2.70	Depositor EDS
% Data completeness (in resolution range)	94.0 (49.00-2.70) 94.1 (49.18-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.69 Å)	Xtriage
Refinement program	REFMAC 5.5.0044	Depositor
R, R_{free}	0.203 , 0.261 0.205 , 0.262	Depositor DCC
R_{free} test set	3645 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	65.7	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 57.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.021 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14189	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.20% 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

5.1 Standard geometry

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

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	0.64	0/2624	0.75	0/3569
1	C	0.53	0/2551	0.63	0/3481
2	B	0.74	0/1434	0.82	2/1930 (0.1%)
2	D	0.61	0/1400	0.66	0/1888
3	H	0.65	0/1612	0.67	0/2201
3	I	0.57	0/1594	0.65	0/2177
4	L	0.64	1/1535 (0.1%)	0.68	1/2109 (0.0%)
4	M	0.51	0/1447	0.60	0/1984
All	All	0.61	1/14197 (0.0%)	0.69	3/19339 (0.0%)

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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	190	ARG	NE-CZ	13.00	1.50	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	190	ARG	CD-NE-CZ	-8.54	111.65	123.60
2	B	106	ARG	NE-CZ-NH2	-6.75	116.93	120.30
2	B	106	ARG	NE-CZ-NH1	5.66	123.13	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	323	SER	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	2558	0	2468	63	0
1	C	2485	0	2322	75	0
2	B	1407	0	1295	17	0
2	D	1373	0	1233	18	0
3	H	1572	0	1520	38	0
3	I	1555	0	1490	31	0
4	L	1498	0	1376	30	0
4	M	1415	0	1298	23	0
5	E	28	0	25	0	0
5	F	28	0	25	0	0
6	A	28	0	26	0	0
6	B	14	0	13	0	0
6	C	14	0	13	1	0
6	D	14	0	13	0	0
7	A	11	0	10	0	0
7	C	11	0	10	0	0
8	A	4	0	6	0	0
8	C	4	0	6	0	0
9	B	6	0	8	1	0
10	A	52	0	0	3	0
10	B	38	0	0	0	0
10	C	5	0	0	0	0
10	D	24	0	0	0	0
10	H	17	0	0	0	0
10	I	13	0	0	0	0
10	L	6	0	0	0	0
10	M	9	0	0	1	0
All	All	14189	0	13157	268	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 10.

The worst 5 of 268 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:C:37:THR:HG22	1:C:38:HIS:CD2	1.70	1.24
1:C:42:ILE:CD1	1:C:316:LEU:HD12	1.82	1.09
1:A:37:THR:CG2	1:A:38:HIS:CD2	2.37	1.07
1:A:279:THR:HG21	1:A:287:ALA:HB1	1.36	1.05
1:C:37:THR:CG2	1:C:38:HIS:CD2	2.45	0.99

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	323/334 (97%)	306 (95%)	15 (5%)	2 (1%)	25	50
1	C	322/334 (96%)	293 (91%)	22 (7%)	7 (2%)	6	17
2	B	175/177 (99%)	170 (97%)	4 (2%)	1 (1%)	25	50
2	D	171/177 (97%)	167 (98%)	3 (2%)	1 (1%)	25	50
3	H	210/226 (93%)	201 (96%)	8 (4%)	1 (0%)	29	54
3	I	209/226 (92%)	195 (93%)	12 (6%)	2 (1%)	15	37
4	L	202/221 (91%)	187 (93%)	13 (6%)	2 (1%)	15	37
4	M	187/221 (85%)	165 (88%)	21 (11%)	1 (0%)	29	54
All	All	1799/1916 (94%)	1684 (94%)	98 (5%)	17 (1%)	17	40

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	80	ILE
3	I	127	SER

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Mol	Chain	Res	Type
1	C	62	ARG
1	C	77	ASP
1	C	78	GLU

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	286/300 (95%)	274 (96%)	12 (4%)	30	58
1	C	271/300 (90%)	260 (96%)	11 (4%)	30	59
2	B	145/151 (96%)	144 (99%)	1 (1%)	84	94
2	D	138/151 (91%)	136 (99%)	2 (1%)	67	86
3	H	170/189 (90%)	160 (94%)	10 (6%)	19	43
3	I	168/189 (89%)	158 (94%)	10 (6%)	19	42
4	L	156/182 (86%)	149 (96%)	7 (4%)	27	55
4	M	146/182 (80%)	142 (97%)	4 (3%)	44	74
All	All	1480/1644 (90%)	1423 (96%)	57 (4%)	32	61

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	27	SER
3	H	115	SER
3	I	208	CYS
3	H	6	GLU
3	H	56	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	150	ASN
2	D	50	ASN

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Mol	Chain	Res	Type
4	M	38	GLN
1	C	278	ASN
2	D	72	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 ⓘ

4 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
5	NAG	E	1	1,5	14,14,15	0.49	0	17,19,21	1.78	2 (11%)
5	NAG	E	2	5	14,14,15	0.74	0	17,19,21	1.47	4 (23%)
5	NAG	F	1	1,5	14,14,15	0.44	0	17,19,21	1.43	3 (17%)
5	NAG	F	2	5	14,14,15	0.58	0	17,19,21	2.59	4 (23%)

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	E	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	2	5	-	1/6/23/26	0/1/1/1
5	NAG	F	1	1,5	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	F	2	5	-	1/6/23/26	0/1/1/1

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(°)
5	F	2	NAG	C1-O5-C5	7.73	122.67	112.19
5	E	1	NAG	C1-O5-C5	5.20	119.24	112.19
5	F	2	NAG	C4-C3-C2	-5.11	103.52	111.02
5	E	2	NAG	O5-C1-C2	3.33	116.54	111.29
5	F	1	NAG	C3-C4-C5	-2.97	104.93	110.24

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	1	NAG	O5-C5-C6-O6
5	F	2	NAG	O5-C5-C6-O6
5	F	1	NAG	C4-C5-C6-O6
5	E	2	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry [i](#)

10 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
6	NAG	C	334	1	14,14,15	0.93	1 (7%)	17,19,21	1.68	4 (23%)
6	NAG	D	182	2	14,14,15	1.19	1 (7%)	17,19,21	1.85	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	B	182	2	14,14,15	0.58	0	17,19,21	2.26	2 (11%)
8	EDO	C	335	-	3,3,3	0.43	0	2,2,2	0.33	0
8	EDO	A	336	-	3,3,3	0.42	0	2,2,2	0.72	0
6	NAG	A	335	1	14,14,15	0.55	0	17,19,21	2.32	2 (11%)
7	BMA	A	4	-	11,11,12	0.40	0	15,15,17	0.98	0
9	GOL	B	183	-	5,5,5	0.36	0	5,5,5	0.47	0
7	BMA	C	4	-	11,11,12	0.42	0	15,15,17	1.45	4 (26%)
6	NAG	A	1	1	14,14,15	0.69	0	17,19,21	1.31	1 (5%)

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
6	NAG	C	334	1	-	0/6/23/26	0/1/1/1
6	NAG	D	182	2	-	2/6/23/26	0/1/1/1
6	NAG	B	182	2	-	2/6/23/26	0/1/1/1
8	EDO	C	335	-	-	0/1/1/1	-
8	EDO	A	336	-	-	1/1/1/1	-
6	NAG	A	335	1	-	1/6/23/26	0/1/1/1
7	BMA	A	4	-	-	2/2/19/22	0/1/1/1
9	GOL	B	183	-	-	4/4/4/4	-
7	BMA	C	4	-	-	0/2/19/22	0/1/1/1
6	NAG	A	1	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	182	NAG	C1-C2	3.54	1.57	1.52
6	C	334	NAG	O5-C1	-2.14	1.40	1.43

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	335	NAG	C1-O5-C5	7.83	122.80	112.19
6	B	182	NAG	C1-O5-C5	7.78	122.74	112.19
6	D	182	NAG	C1-O5-C5	4.16	117.83	112.19
6	A	335	NAG	C4-C3-C2	-3.65	105.67	111.02
6	C	334	NAG	C4-C3-C2	3.42	116.04	111.02

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	183	GOL	C1-C2-C3-O3
6	B	182	NAG	C4-C5-C6-O6
6	D	182	NAG	O5-C5-C6-O6
6	D	182	NAG	C4-C5-C6-O6
6	B	182	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	334	NAG	1	0
9	B	183	GOL	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 ⓘ

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	324/334 (97%)	-0.18	0 100 100	22, 45, 53, 60	0
1	C	323/334 (96%)	-0.06	0 100 100	31, 57, 66, 70	0
2	B	177/177 (100%)	0.11	0 100 100	18, 34, 46, 53	0
2	D	173/177 (97%)	0.09	0 100 100	30, 45, 56, 62	0
3	H	214/226 (94%)	-0.13	3 (1%) 75 77	28, 44, 65, 67	0
3	I	213/226 (94%)	0.01	9 (4%) 36 35	37, 49, 72, 74	0
4	L	208/221 (94%)	0.11	3 (1%) 75 77	47, 59, 78, 87	0
4	M	197/221 (89%)	0.44	19 (9%) 8 6	49, 61, 75, 79	0
All	All	1829/1916 (95%)	0.02	34 (1%) 66 69	18, 50, 70, 87	0

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	M	27(A)	SER	5.1
3	I	198	LEU	5.0
4	M	104	LEU	4.6
4	M	144	VAL	4.5
4	M	142	GLY	4.4

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 ⓘ

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
5	NAG	E	2	14/15	0.84	0.27	92,96,97,98	0
5	NAG	F	2	14/15	0.85	0.26	100,102,103,103	0
5	NAG	E	1	14/15	0.94	0.14	69,74,79,85	0
5	NAG	F	1	14/15	0.95	0.15	85,88,92,96	0

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
7	BMA	A	4	11/12	0.73	0.42	42,47,48,48	11
6	NAG	D	182	14/15	0.78	0.23	71,74,80,81	0
6	NAG	C	334	14/15	0.89	0.26	74,80,83,84	0
7	BMA	C	4	11/12	0.90	0.32	30,32,33,33	11
6	NAG	B	182	14/15	0.91	0.20	62,68,71,72	0
6	NAG	A	335	14/15	0.91	0.11	69,73,74,74	0
6	NAG	A	1	14/15	0.92	0.13	60,68,70,71	0
9	GOL	B	183	6/6	0.94	0.14	63,65,65,66	0
8	EDO	C	335	4/4	0.96	0.21	56,58,59,60	0
8	EDO	A	336	4/4	0.98	0.21	41,43,43,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.