



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 12:54 PM UTC

PDB ID : 6A4K / pdb_00006a4k
Title : Human antibody 32D6 Fab in complex with H1N1 influenza A virus HA1
Authors : Lee, C.C.; Ko, T.P.; Lin, L.L.; Wang, A.H.J.
Deposited on : 2018-06-20
Resolution : 3.15 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 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

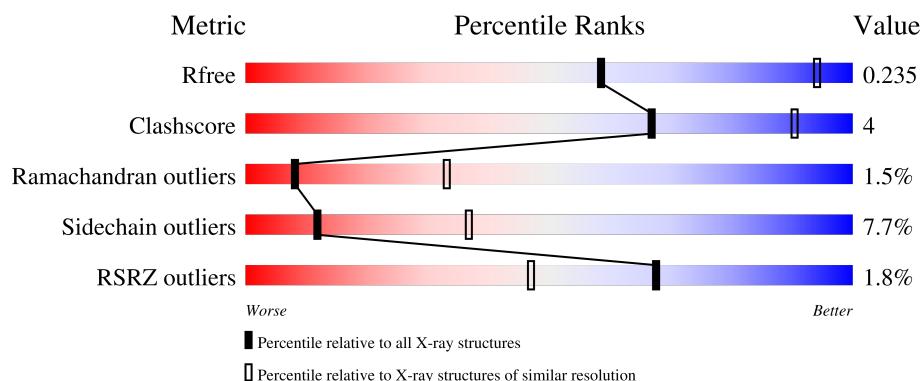
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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}	180053	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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 $\leq 5\%$. 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	235	% 82% 11% • 5%
1	B	235	2% 80% 11% • 6%
1	C	235	% 83% 10% • 5%
1	D	235	% 82% 10% • 6%
2	H	238	% 85% 11% • •

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Mol	Chain	Length	Quality of chain
2	I	238	4% 77% 19% .
2	J	238	2% 81% 13% ..
2	K	238	3% 76% 19% ..
3	L	216	83% 15% .
3	M	216	4% 83% 16% .
3	N	216	% 79% 19% .
3	O	216	% 86% 13% .

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 20618 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	223	Total	C	N	O	S	0	0	0
			1760	1123	296	335	6			
1	B	221	Total	C	N	O	S	0	0	0
			1745	1114	294	331	6			
1	C	223	Total	C	N	O	S	0	0	0
			1760	1123	296	335	6			
1	D	221	Total	C	N	O	S	0	0	0
			1745	1114	294	331	6			

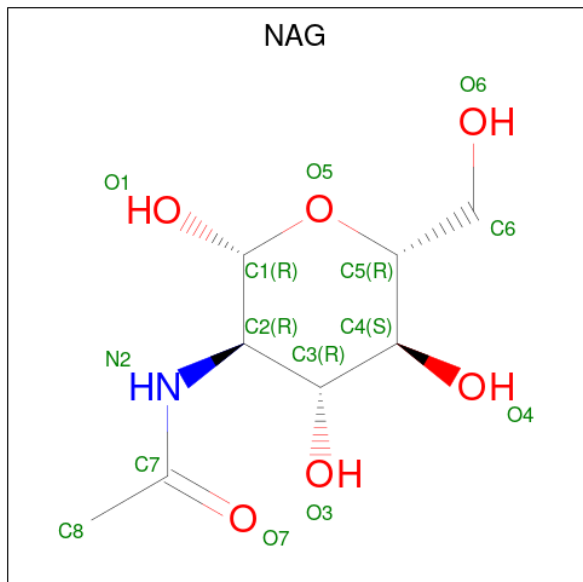
- Molecule 2 is a protein called immunoglobulin Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	230	Total	C	N	O	S	0	0	0
			1722	1091	283	343	5			
2	I	230	Total	C	N	O	S	0	0	0
			1722	1091	283	343	5			
2	J	230	Total	C	N	O	S	0	0	0
			1722	1091	283	343	5			
2	K	230	Total	C	N	O	S	0	0	0
			1722	1091	283	343	5			

- Molecule 3 is a protein called immunoglobulin Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	216	Total	C	N	O	S	0	0	0
			1614	1000	277	330	7			
3	M	216	Total	C	N	O	S	0	0	0
			1614	1000	277	330	7			
3	N	216	Total	C	N	O	S	0	0	0
			1614	1000	277	330	7			
3	O	216	Total	C	N	O	S	0	0	0
			1614	1000	277	330	7			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

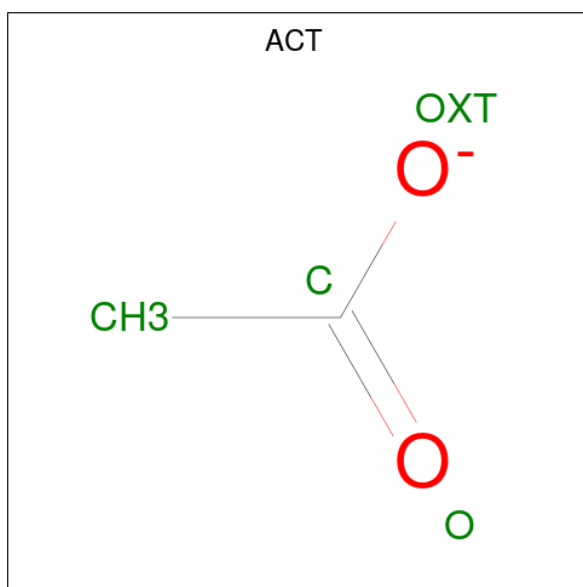


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		
5	B	1	Total	Ca	0	0
			1	1		
5	C	1	Total	Ca	0	0
			1	1		
5	D	1	Total	Ca	0	0
			1	1		
5	O	1	Total	Ca	0	0
			1	1		

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	28	Total	O	0	0
			28	28		
7	H	17	Total	O	0	0
			17	17		
7	L	29	Total	O	0	0
			29	29		
7	B	15	Total	O	0	0
			15	15		
7	I	6	Total	O	0	0
			6	6		
7	M	5	Total	O	0	0
			5	5		
7	C	24	Total	O	0	0
			24	24		
7	N	7	Total	O	0	0
			7	7		
7	D	31	Total	O	0	0
			31	31		
7	K	12	Total	O	0	0
			12	12		

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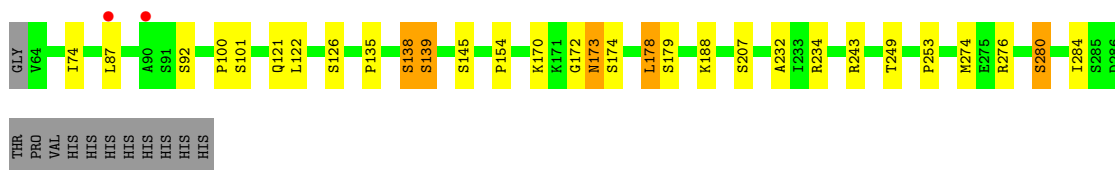
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	O	21	Total	O	0	0
			21	21		

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: Hemagglutinin

Chain A: 



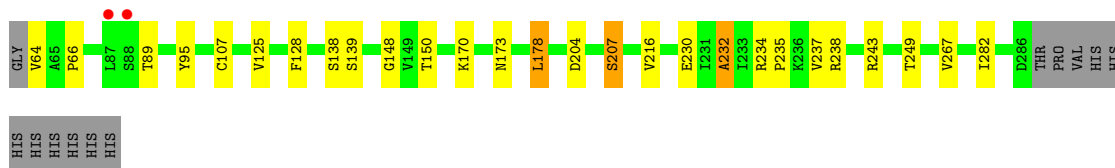
• Molecule 1: Hemagglutinin

Chain B: 



• Molecule 1: Hemagglutinin

Chain C: 



• Molecule 1: Hemagglutinin

Chain D: 



PRO
VAL
HIS
HIS
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HIS

• Molecule 2: immunoglobulin Fab heavy chain

Chain H:  85% 11% . .

Q1 S15 L18 T23 N30 T31 T58 S67 T75 F110 V120 L135 L141 A142 A147 L152 V153 L170 L189 L195 P196 S197 S198 S199 N208 K212 K217 K220 K225 S226 C227 T230 HIS HIS HIS HIS HIS

HIS
HIS

• Molecule 2: immunoglobulin Fab heavy chain

Chain I:  77% 19% .

Q1 Q5 V12 T17 L18 T23 N30 W33 A51 S56 G57 S67 L71 S83 S86 V87 T88 T92 L100 D103 T106 F110 Q116 V120 I121 S126 P130 S131 V132 L135 P137 S141 A142 S143 G144 T146 A147 L148 L149 L152 V153 K154 S167 V180 L181 Q182 L186 Y187 S188 V195 P196 S199 T204 Y205 I206 V209 V218 V219 K220 R221 V222 T230 HIS HIS HIS HIS HIS HIS HIS

• Molecule 2: immunoglobulin Fab heavy chain

Chain J:  81% 13% . .

Q1 V2 Q3 L4 Q5 T17 L18 S19 L20 T23 V24 T31 A51 Y52 S59 N60 L65 T70 N78 T88 V94 I104 Q116 V120 T127 P134 L135 A136 P137 A142 L152 D155 V163 T171 Q182 L186 L189 P196 S199 V209 K217 R221 P224 C227 T230 HIS HIS HIS HIS HIS HIS HIS

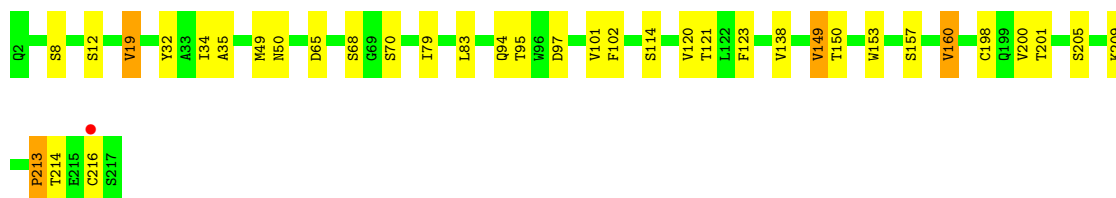
• Molecule 2: immunoglobulin Fab heavy chain

Chain K:  76% 19% . .

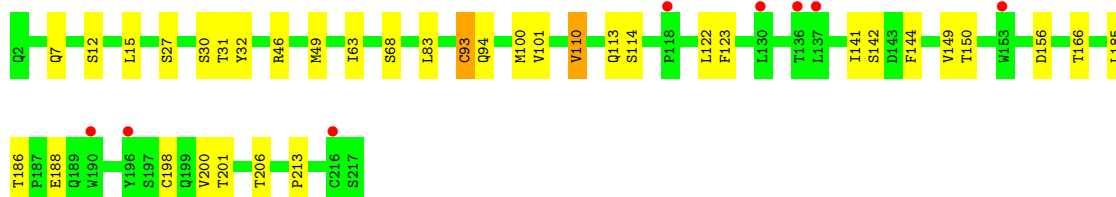
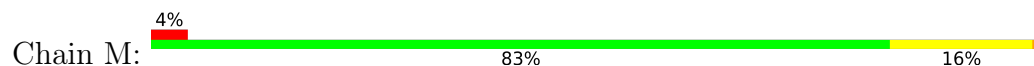
Q1 V2 Q3 L4 S15 L18 S19 S25 V29 G32 S33 Y34 A51 S64 L65 L71 L72 V73 D74 T75 R85 T88 T92 L105 I121 V122 A125 S126 T127 K128 G129 P130 V132 P137 K140 S141 A142 G145 A148 L149 G150 C151 Y156 V161 S164 S172 V180 L181 Y187 S188 L189 T194 V195 Y205 I206 C207 N208 V209 P213 S214 V218 P224 C227 D228 K229 T230 HIS HIS HIS HIS HIS HIS HIS

• Molecule 3: immunoglobulin Fab light chain

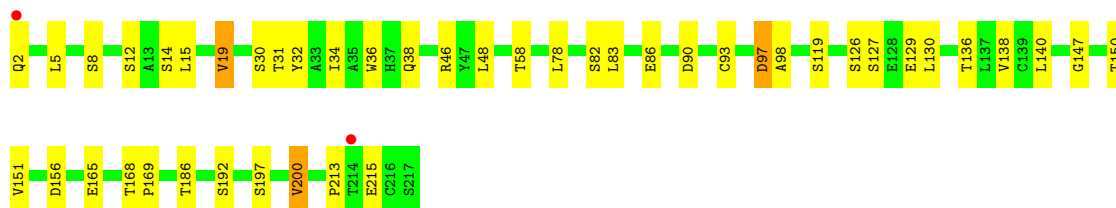
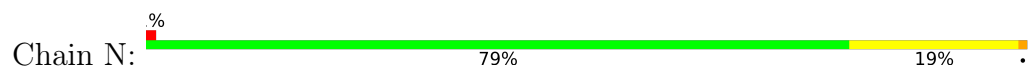
Chain L:  83% 15% .



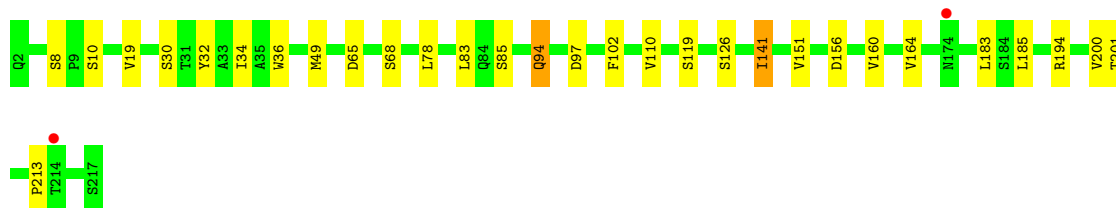
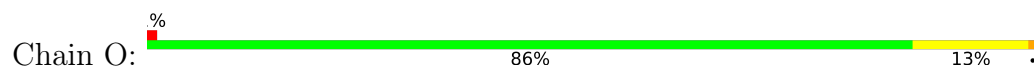
- Molecule 3: immunoglobulin Fab light chain



- Molecule 3: immunoglobulin Fab light chain



- Molecule 3: immunoglobulin Fab light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, α , β , γ	181.74Å 181.74Å 248.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.15 20.00 – 3.15	Depositor EDS
% Data completeness (in resolution range)	94.5 (20.00-3.15) 94.5 (20.00-3.15)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 3.15Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.175 , 0.233 0.178 , 0.235	Depositor DCC
R_{free} test set	3830 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å ²)	65.1	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 58.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	20618	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.87% 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: CA, ACT, 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	0.70	0/1810	0.89	2/2457 (0.1%)
1	B	0.70	0/1795	0.90	1/2436 (0.0%)
1	C	0.69	0/1810	0.91	2/2457 (0.1%)
1	D	0.72	0/1795	0.92	1/2436 (0.0%)
2	H	0.72	0/1766	0.96	0/2414
2	I	0.80	0/1766	0.92	0/2414
2	J	0.71	0/1766	0.90	0/2414
2	K	0.78	0/1766	0.94	2/2414 (0.1%)
3	L	0.75	0/1651	0.97	0/2246
3	M	0.80	0/1651	0.95	1/2246 (0.0%)
3	N	0.73	0/1651	0.90	0/2246
3	O	0.79	0/1651	0.95	0/2246
All	All	0.74	0/20878	0.93	9/28426 (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
1	C	0	1
1	D	0	1
2	H	0	1
3	L	0	1
3	N	0	1
All	All	0	6

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	173	ASN	N-CA-CB	-7.55	101.01	110.98
2	K	150	GLY	N-CA-C	6.90	121.20	111.19
1	A	173	ASN	N-CA-CB	-6.75	102.03	111.00
1	C	232	ALA	N-CA-C	6.75	118.65	108.46
2	K	105	LEU	N-CA-C	6.34	117.86	111.07

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	280	SER	Peptide
1	C	89	THR	Peptide
2	H	198	SER	Peptide
3	L	213	PRO	Peptide
3	N	215	GLU	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	1760	0	1696	11	0
1	B	1745	0	1683	13	0
1	C	1760	0	1696	9	0
1	D	1745	0	1683	14	0
2	H	1722	0	1687	8	0
2	I	1722	0	1687	19	0
2	J	1722	0	1687	13	0
2	K	1722	0	1687	18	0
3	L	1614	0	1553	14	0
3	M	1614	0	1553	16	0
3	N	1614	0	1553	15	0
3	O	1614	0	1553	10	0
4	A	14	0	13	1	0
4	B	14	0	13	0	0
4	C	14	0	13	0	0
4	D	14	0	13	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	O	1	0	0	0	0
6	B	4	0	3	0	0
6	D	4	0	3	0	0
7	A	28	0	0	0	0
7	B	15	0	0	1	0
7	C	24	0	0	0	0
7	D	31	0	0	0	0
7	H	17	0	0	1	0
7	I	6	0	0	0	0
7	K	12	0	0	0	0
7	L	29	0	0	1	0
7	M	5	0	0	0	0
7	N	7	0	0	1	0
7	O	21	0	0	0	0
All	All	20618	0	19776	150	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 4.

The worst 5 of 150 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:M:7:GLN:NE2	3:M:93:CYS:SG	2.48	0.87
3:M:7:GLN:HE22	3:M:93:CYS:H	1.31	0.78
2:I:218:VAL:HG12	2:I:220:LYS:HG2	1.73	0.71
3:O:151:VAL:HG12	3:O:200:VAL:HG12	1.72	0.70
2:H:110:PHE:HA	3:L:94:GLN:HE22	1.59	0.67

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	221/235 (94%)	202 (91%)	16 (7%)	3 (1%)	9	34
1	B	219/235 (93%)	197 (90%)	19 (9%)	3 (1%)	9	34
1	C	221/235 (94%)	203 (92%)	17 (8%)	1 (0%)	24	55
1	D	219/235 (93%)	201 (92%)	15 (7%)	3 (1%)	9	34
2	H	228/238 (96%)	200 (88%)	23 (10%)	5 (2%)	5	25
2	I	228/238 (96%)	198 (87%)	26 (11%)	4 (2%)	6	29
2	J	228/238 (96%)	203 (89%)	20 (9%)	5 (2%)	5	25
2	K	228/238 (96%)	197 (86%)	25 (11%)	6 (3%)	4	21
3	L	214/216 (99%)	200 (94%)	12 (6%)	2 (1%)	14	43
3	M	214/216 (99%)	193 (90%)	19 (9%)	2 (1%)	14	43
3	N	214/216 (99%)	201 (94%)	10 (5%)	3 (1%)	9	34
3	O	214/216 (99%)	204 (95%)	7 (3%)	3 (1%)	9	34
All	All	2648/2756 (96%)	2399 (91%)	209 (8%)	40 (2%)	8	33

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	15	SER
2	H	225	LYS
2	H	227	CYS
3	L	213	PRO
1	B	86	SER

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	192/203 (95%)	179 (93%)	13 (7%)	14	41
1	B	190/203 (94%)	177 (93%)	13 (7%)	14	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	192/203 (95%)	181 (94%)	11 (6%)	18	47
1	D	190/203 (94%)	181 (95%)	9 (5%)	23	52
2	H	199/207 (96%)	184 (92%)	15 (8%)	12	38
2	I	199/207 (96%)	183 (92%)	16 (8%)	11	35
2	J	199/207 (96%)	182 (92%)	17 (8%)	10	33
2	K	199/207 (96%)	184 (92%)	15 (8%)	12	38
3	L	180/180 (100%)	163 (91%)	17 (9%)	8	29
3	M	180/180 (100%)	165 (92%)	15 (8%)	10	34
3	N	180/180 (100%)	158 (88%)	22 (12%)	5	19
3	O	180/180 (100%)	167 (93%)	13 (7%)	13	39
All	All	2280/2360 (97%)	2104 (92%)	176 (8%)	12	37

5 of 176 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	J	217	LYS
1	D	179	SER
3	N	15	LEU
3	N	127	SER
2	K	75	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	173	ASN
1	D	206	GLN
2	K	166	ASN
2	I	208	ASN
2	I	182	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 for Mogul analysis.

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	A	501	1	14,14,15	0.58	0	17,19,21	1.99	2 (11%)
6	ACT	B	503	-	3,3,3	0.83	0	3,3,3	0.88	0
4	NAG	B	501	1	14,14,15	0.94	0	17,19,21	1.74	3 (17%)
4	NAG	C	501	1	14,14,15	0.58	0	17,19,21	1.06	1 (5%)
4	NAG	D	501	1	14,14,15	0.61	0	17,19,21	1.26	1 (5%)
6	ACT	D	503	-	3,3,3	0.80	0	3,3,3	0.79	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
4	NAG	C	501	1	-	2/6/23/26	0/1/1/1
4	NAG	D	501	1	-	0/6/23/26	0/1/1/1
4	NAG	B	501	1	-	2/6/23/26	0/1/1/1
4	NAG	A	501	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	A	501	NAG	C1-O5-C5	7.30	121.97	112.19
4	B	501	NAG	C2-N2-C7	3.77	127.96	122.90
4	C	501	NAG	C1-O5-C5	2.86	116.02	112.19
4	B	501	NAG	C1-O5-C5	2.71	115.82	112.19
4	B	501	NAG	C1-C2-N2	2.65	114.61	110.43

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	501	NAG	C4-C5-C6-O6
4	B	501	NAG	O5-C5-C6-O6
4	A	501	NAG	O5-C5-C6-O6
4	C	501	NAG	O5-C5-C6-O6
4	A	501	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	NAG	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	223/235 (94%)	-0.59	2 (0%) 81 64	34, 55, 110, 171	0
1	B	221/235 (94%)	-0.32	5 (2%) 61 40	42, 72, 155, 183	0
1	C	223/235 (94%)	-0.49	2 (0%) 81 64	40, 62, 112, 169	0
1	D	221/235 (94%)	-0.57	3 (1%) 73 53	33, 60, 136, 196	0
2	H	230/238 (96%)	-0.46	2 (0%) 81 64	33, 67, 150, 226	0
2	I	230/238 (96%)	0.04	10 (4%) 40 23	43, 76, 223, 261	0
2	J	230/238 (96%)	-0.07	4 (1%) 69 48	46, 95, 186, 200	0
2	K	230/238 (96%)	-0.03	7 (3%) 52 32	33, 86, 182, 212	0
3	L	216/216 (100%)	-0.69	1 (0%) 87 75	32, 56, 88, 202	0
3	M	216/216 (100%)	0.04	8 (3%) 45 26	43, 81, 219, 268	0
3	N	216/216 (100%)	-0.19	2 (0%) 81 64	43, 95, 145, 197	0
3	O	216/216 (100%)	-0.32	2 (0%) 81 64	30, 65, 155, 191	0
All	All	2672/2756 (96%)	-0.30	48 (1%) 67 47	30, 69, 183, 268	0

The worst 5 of 48 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	227	CYS	4.7
2	I	218	VAL	4.1
2	J	142	ALA	4.1
1	D	282	ILE	3.7
1	C	87	LEU	3.6

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 [i](#)

There are no oligosaccharides 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, 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
4	NAG	A	501	14/15	0.85	0.12	80,103,112,117	0
4	NAG	B	501	14/15	0.85	0.13	97,120,125,127	0
4	NAG	D	501	14/15	0.87	0.13	116,127,130,132	0
5	CA	O	301	1/1	0.89	0.36	122,122,122,122	1
4	NAG	C	501	14/15	0.90	0.12	111,122,127,129	0
6	ACT	B	503	4/4	0.93	0.15	58,60,63,66	0
5	CA	C	502	1/1	0.95	0.05	71,71,71,71	0
5	CA	B	502	1/1	0.97	0.06	72,72,72,72	0
6	ACT	D	503	4/4	0.97	0.08	51,51,57,58	0
5	CA	D	502	1/1	0.98	0.04	71,71,71,71	0
5	CA	A	502	1/1	0.99	0.08	69,69,69,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.