



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Sep 3, 2017 – 09:27 AM EDT

PDB ID : 5UK1  
EMDB ID: : EMD-8563  
Title : CryoEM structure of an influenza virus receptor-binding site antibody-antigen interface - Class 3  
Authors : Liu, Y.; Pan, J.; Caradonna, T.; Jenni, S.; Raymond, D.D.; Schmidt, A.G.; Harrison, S.C.; Grigorieff, N.  
Deposited on : unknown  
Resolution : 4.80 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

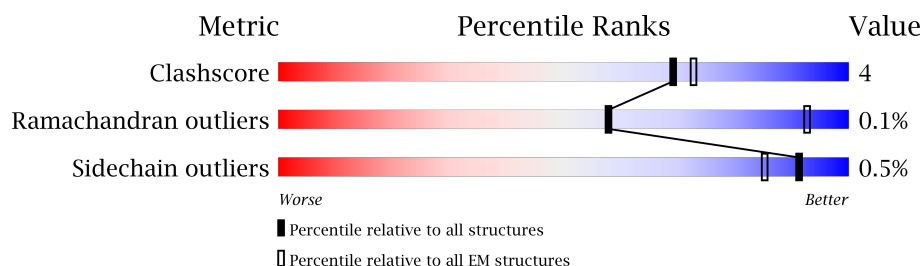
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.80 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)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	323	87% 13%
1	C	323	87% 12% .
1	E	323	88% 11%
2	B	173	85% 15%
2	D	173	84% 16%
2	F	173	86% 14%
3	G	266	77% 10% . 11%
3	H	266	78% 10% 11%
3	I	266	77% 10% . 11%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 34389 atoms, of which 16842 are hydrogens and 0 are deuteriums.

In the tables below, 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 HA1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	323	Total	C	H	N	O	S	0	0
			4973	1597	2438	441	486	11		
1	C	323	Total	C	H	N	O	S	0	0
			4973	1597	2438	441	486	11		
1	E	323	Total	C	H	N	O	S	0	0
			4973	1597	2438	441	486	11		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	GLU	-	expression tag	UNP A7UPX0
C	4	GLU	-	expression tag	UNP A7UPX0
E	4	GLU	-	expression tag	UNP A7UPX0

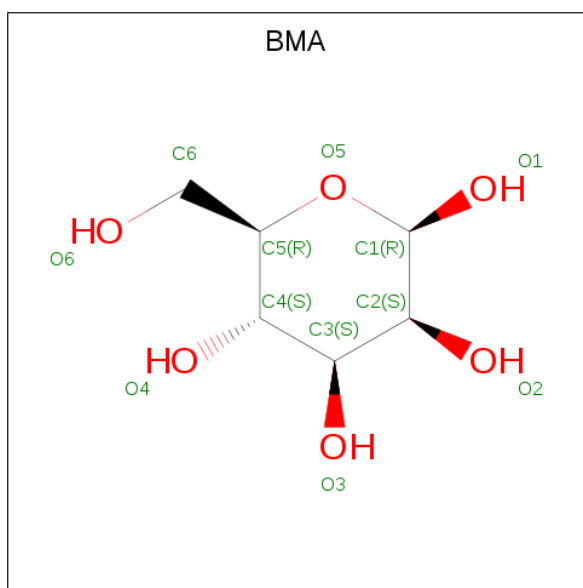
- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	173	Total	C	H	N	O	S	0	0
			2716	874	1322	238	275	7		
2	D	173	Total	C	H	N	O	S	0	0
			2716	874	1322	238	275	7		
2	F	173	Total	C	H	N	O	S	0	0
			2716	874	1322	238	275	7		

- Molecule 3 is a protein called scFv.

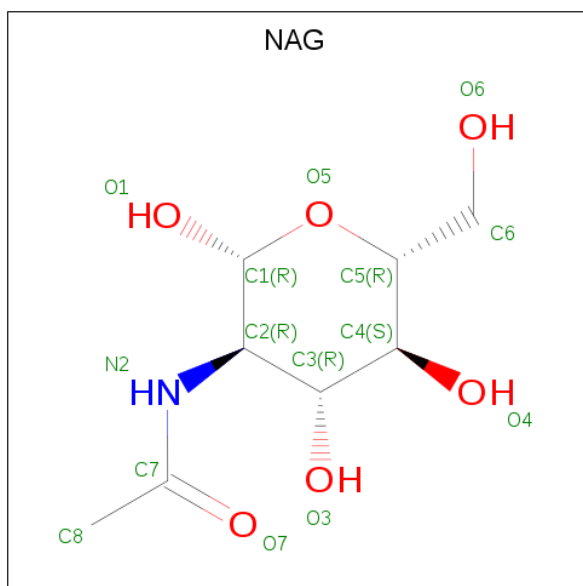
Mol	Chain	Residues	Atoms						AltConf	Trace
3	G	236	Total	C	H	N	O	S	0	0
			3476	1111	1707	306	345	7		
3	H	236	Total	C	H	N	O	S	0	0
			3476	1111	1707	306	345	7		
3	I	236	Total	C	H	N	O	S	0	0
			3476	1111	1707	306	345	7		

- Molecule 4 is BETA-D-MANNOSE (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	H	O	0
			21	6	10	5	
4	C	1	Total	C	H	O	0
			21	6	10	5	
4	E	1	Total	C	H	O	0
			21	6	10	5	

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



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	H	N	O	0
			249	72	123	9	45	
5	A	1	Total	C	H	N	O	0
			249	72	123	9	45	
5	A	1	Total	C	H	N	O	0
			249	72	123	9	45	
5	A	1	Total	C	H	N	O	0
			249	72	123	9	45	
5	A	1	Total	C	H	N	O	0
			249	72	123	9	45	
5	A	1	Total	C	H	N	O	0
			249	72	123	9	45	
5	A	1	Total	C	H	N	O	0
			249	72	123	9	45	
5	A	1	Total	C	H	N	O	0
			249	72	123	9	45	
5	B	1	Total	C	H	N	O	0
			28	8	14	1	5	
5	C	1	Total	C	H	N	O	0
			249	72	123	9	45	
5	C	1	Total	C	H	N	O	0
			249	72	123	9	45	
5	C	1	Total	C	H	N	O	0
			249	72	123	9	45	
5	C	1	Total	C	H	N	O	0
			249	72	123	9	45	
5	C	1	Total	C	H	N	O	0
			249	72	123	9	45	
5	C	1	Total	C	H	N	O	0
			249	72	123	9	45	
5	C	1	Total	C	H	N	O	0
			249	72	123	9	45	
5	C	1	Total	C	H	N	O	0
			249	72	123	9	45	
5	D	1	Total	C	H	N	O	0
			28	8	14	1	5	
5	E	1	Total	C	H	N	O	0
			249	72	123	9	45	
5	E	1	Total	C	H	N	O	0
			249	72	123	9	45	

Continued on next page...

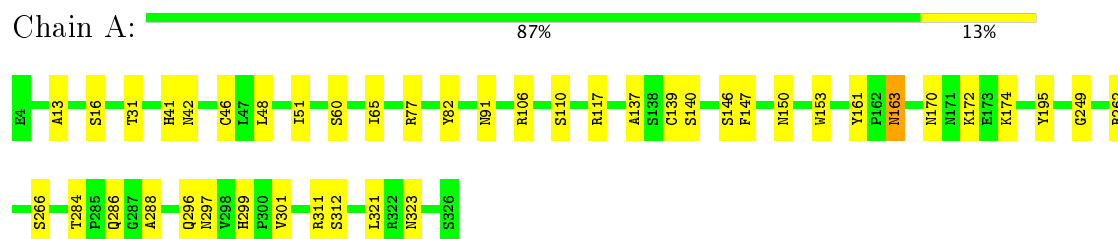
*Continued from previous page...*

Mol	Chain	Residues	Atoms					AltConf
5	E	1	Total	C	H	N	O	0
			249	72	123	9	45	
5	E	1	Total	C	H	N	O	0
			249	72	123	9	45	
5	E	1	Total	C	H	N	O	0
			249	72	123	9	45	
5	E	1	Total	C	H	N	O	0
			249	72	123	9	45	
5	E	1	Total	C	H	N	O	0
			249	72	123	9	45	
5	E	1	Total	C	H	N	O	0
			249	72	123	9	45	
5	F	1	Total	C	H	N	O	0
			28	8	14	1	5	

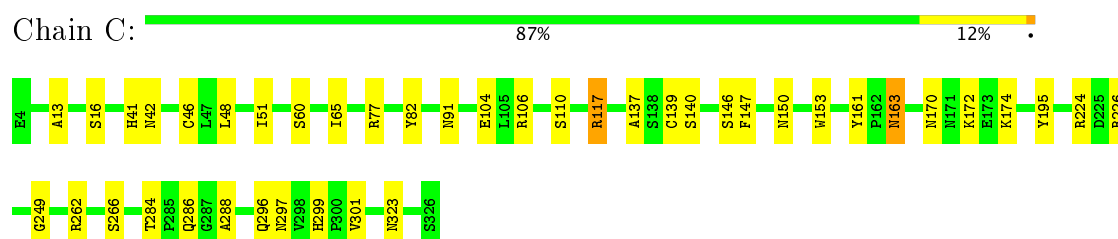
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

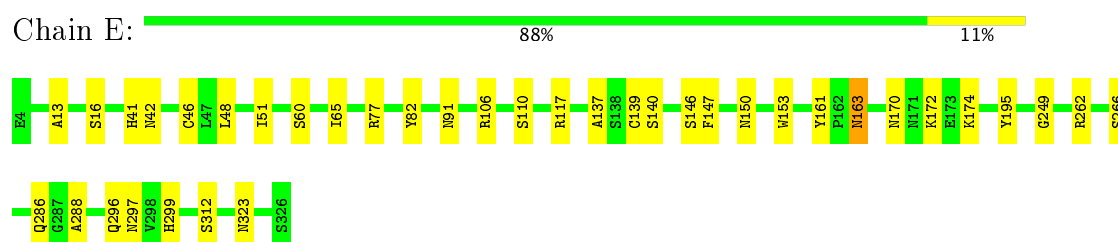
- Molecule 1: Hemagglutinin HA1



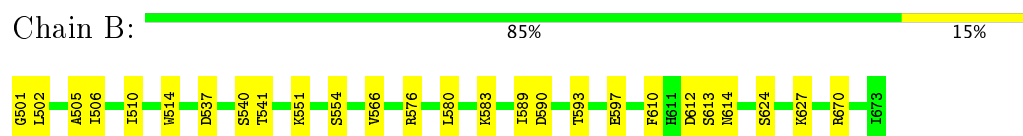
- Molecule 1: Hemagglutinin HA1



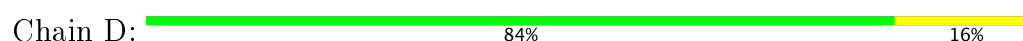
- Molecule 1: Hemagglutinin HA1



- Molecule 2: Hemagglutinin HA2



- Molecule 2: Hemagglutinin HA2





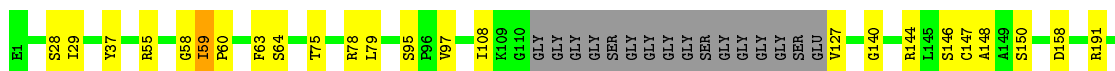
• Molecule 2: Hemagglutinin HA2

Chain F: 86% 14%



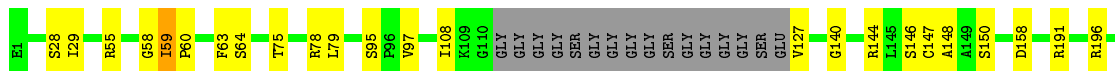
• Molecule 3: scFv

Chain G: 77% 10% 11%



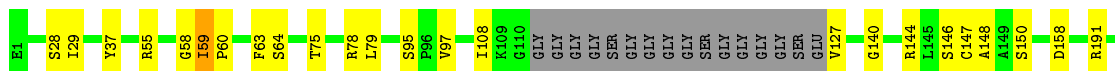
• Molecule 3: scFv

Chain H: 78% 10% 11%



• Molecule 3: scFv

Chain I: 77% 10% 11%





## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	142314	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	9000	Depositor
Magnification	30444	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

## 5 Model quality

### 5.1 Standard geometry

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  >2	RMSZ	# Z  >2
1	A	0.50	0/2601	0.80	3/3540 (0.1%)
1	C	0.50	0/2601	0.80	6/3540 (0.2%)
1	E	0.50	0/2601	0.80	3/3540 (0.1%)
2	B	0.46	0/1421	0.74	1/1909 (0.1%)
2	D	0.46	0/1421	0.74	1/1909 (0.1%)
2	F	0.46	0/1421	0.74	1/1909 (0.1%)
3	G	0.50	0/1808	0.93	6/2452 (0.2%)
3	H	0.50	0/1808	0.93	6/2452 (0.2%)
3	I	0.50	0/1808	0.93	6/2452 (0.2%)
All	All	0.49	0/17490	0.83	33/23703 (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
1	A	0	1
1	C	0	1
1	E	0	1
3	G	0	4
3	H	0	4
3	I	0	4
All	All	0	15

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	191	ARG	NE-CZ-NH1	6.46	123.53	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	191	ARG	NE-CZ-NH1	6.43	123.51	120.30
3	H	191	ARG	NE-CZ-NH1	6.35	123.47	120.30
3	G	158	ASP	CB-CG-OD1	6.23	123.91	118.30
3	I	158	ASP	CB-CG-OD1	6.21	123.89	118.30
3	H	158	ASP	CB-CG-OD1	6.17	123.85	118.30
2	D	670	ARG	NE-CZ-NH1	6.08	123.34	120.30
2	F	670	ARG	NE-CZ-NH1	6.07	123.34	120.30
3	G	196	ARG	NE-CZ-NH1	6.02	123.31	120.30
3	G	78	ARG	NE-CZ-NH1	6.02	123.31	120.30
2	B	670	ARG	NE-CZ-NH1	6.00	123.30	120.30
3	I	196	ARG	NE-CZ-NH1	5.94	123.27	120.30
3	H	225	ARG	NE-CZ-NH1	5.91	123.26	120.30
3	G	225	ARG	NE-CZ-NH1	5.90	123.25	120.30
3	I	78	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	C	106	ARG	NE-CZ-NH1	5.83	123.21	120.30
3	H	78	ARG	NE-CZ-NH1	5.82	123.21	120.30
3	H	196	ARG	NE-CZ-NH1	5.81	123.20	120.30
3	I	225	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	E	106	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	A	106	ARG	NE-CZ-NH1	5.64	123.12	120.30
3	G	196	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	77	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	E	262	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	E	77	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	C	117	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	C	77	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	C	262	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	C	224	ARG	NE-CZ-NH1	5.06	122.83	120.30
3	H	196	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	C	226	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	A	262	ARG	NE-CZ-NH1	5.04	122.82	120.30
3	I	196	ARG	NE-CZ-NH2	-5.03	117.79	120.30

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	297	ASN	Peptide
1	C	297	ASN	Peptide
1	E	297	ASN	Peptide
3	G	28	SER	Peptide
3	G	29	ILE	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
3	G	58	GLY	Peptide
3	G	59	ILE	Peptide
3	H	28	SER	Peptide
3	H	29	ILE	Peptide
3	H	58	GLY	Peptide
3	H	59	ILE	Peptide
3	I	28	SER	Peptide
3	I	29	ILE	Peptide
3	I	58	GLY	Peptide
3	I	59	ILE	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	2535	2438	2438	25	0
1	C	2535	2438	2438	23	0
1	E	2535	2438	2438	22	0
2	B	1394	1322	1322	18	0
2	D	1394	1322	1322	17	0
2	F	1394	1322	1322	16	0
3	G	1769	1707	1711	13	0
3	H	1769	1707	1711	12	0
3	I	1769	1707	1711	13	0
4	A	11	10	10	0	0
4	C	11	10	10	0	0
4	E	11	10	10	0	0
5	A	126	123	114	0	0
5	B	14	14	13	0	0
5	C	126	123	114	0	0
5	D	14	14	13	0	0
5	E	126	123	114	0	0
5	F	14	14	13	0	0
All	All	17547	16842	16824	146	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.

All (146) 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:A:42:ASN:HD21	1:A:288:ALA:HB3	1.54	0.73
1:E:42:ASN:HD21	1:E:288:ALA:HB3	1.54	0.72
1:C:42:ASN:HD21	1:C:288:ALA:HB3	1.54	0.72
1:E:296:GLN:NE2	1:E:299:HIS:O	2.25	0.70
1:A:296:GLN:NE2	1:A:299:HIS:O	2.25	0.70
1:C:296:GLN:NE2	1:C:299:HIS:O	2.25	0.69
1:A:137:ALA:O	1:A:140:SER:OG	2.12	0.68
1:C:137:ALA:O	1:C:140:SER:OG	2.12	0.68
3:I:127:VAL:N	3:I:150:SER:O	2.28	0.67
2:F:624:SER:O	2:F:627:LYS:NZ	2.25	0.67
3:H:127:VAL:N	3:H:150:SER:O	2.28	0.67
3:G:127:VAL:N	3:G:150:SER:O	2.28	0.66
1:E:137:ALA:O	1:E:140:SER:OG	2.12	0.66
1:E:170:ASN:ND2	1:E:174:LYS:O	2.29	0.66
2:B:624:SER:O	2:B:627:LYS:NZ	2.25	0.66
1:C:170:ASN:ND2	1:C:174:LYS:O	2.29	0.65
1:A:170:ASN:ND2	1:A:174:LYS:O	2.29	0.65
2:D:502:LEU:O	2:F:613:SER:OG	2.14	0.65
2:F:537:ASP:O	2:F:541:THR:OG1	2.13	0.65
2:B:502:LEU:O	2:D:613:SER:OG	2.15	0.64
2:D:589:ILE:O	2:D:593:THR:OG1	2.11	0.64
3:G:64:SER:O	3:G:75:THR:OG1	2.11	0.63
2:B:537:ASP:OD2	2:B:540:SER:OG	2.15	0.62
2:B:576:ARG:NE	1:C:104:GLU:OE2	2.32	0.62
2:D:624:SER:O	2:D:627:LYS:NZ	2.25	0.62
1:A:312:SER:OG	2:B:597:GLU:OE2	2.11	0.61
1:E:65:ILE:O	1:E:150:ASN:ND2	2.34	0.61
1:C:65:ILE:O	1:C:150:ASN:ND2	2.34	0.60
1:A:65:ILE:O	1:A:150:ASN:ND2	2.34	0.60
2:B:589:ILE:O	2:B:593:THR:OG1	2.11	0.60
3:I:64:SER:O	3:I:75:THR:OG1	2.11	0.59
2:B:610:PHE:O	2:B:614:ASN:ND2	2.36	0.59
2:B:613:SER:OG	2:F:502:LEU:O	2.21	0.59
2:D:610:PHE:O	2:D:614:ASN:ND2	2.36	0.59
3:H:225:ARG:NE	3:H:227:VAL:O	2.36	0.58
3:H:64:SER:O	3:H:75:THR:OG1	2.11	0.58
2:F:610:PHE:O	2:F:614:ASN:ND2	2.36	0.58
3:G:225:ARG:NE	3:G:227:VAL:O	2.36	0.58
3:I:225:ARG:NE	3:I:227:VAL:O	2.36	0.58
2:B:580:LEU:O	2:B:583:LYS:N	2.37	0.58
2:D:580:LEU:O	2:D:583:LYS:N	2.37	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:501:GLY:N	2:B:506:ILE:O	2.37	0.57
1:C:46:CYS:O	1:C:82:TYR:OH	2.22	0.57
1:A:46:CYS:O	1:A:82:TYR:OH	2.22	0.57
1:E:46:CYS:O	1:E:82:TYR:OH	2.22	0.57
2:F:501:GLY:N	2:F:506:ILE:O	2.37	0.57
2:D:501:GLY:N	2:D:506:ILE:O	2.37	0.57
2:F:580:LEU:O	2:F:583:LYS:N	2.37	0.57
1:E:110:SER:OG	1:E:266:SER:O	2.22	0.57
2:F:537:ASP:OD2	2:F:540:SER:OG	2.14	0.57
1:C:284:THR:OG1	1:C:301:VAL:O	2.14	0.56
2:F:589:ILE:O	2:F:593:THR:OG1	2.11	0.56
1:E:139:CYS:O	1:E:146:SER:N	2.40	0.55
1:A:139:CYS:O	1:A:146:SER:N	2.39	0.55
1:E:42:ASN:ND2	1:E:288:ALA:HB3	2.21	0.54
3:I:37:TYR:OH	3:I:239:MET:SD	2.59	0.54
1:C:60:SER:OG	1:C:91:ASN:O	2.17	0.54
1:E:170:ASN:OD1	1:E:172:LYS:N	2.41	0.54
1:C:139:CYS:O	1:C:146:SER:N	2.39	0.54
1:C:42:ASN:ND2	1:C:288:ALA:HB3	2.21	0.54
1:C:110:SER:OG	1:C:266:SER:O	2.22	0.53
1:C:42:ASN:OD1	1:C:288:ALA:N	2.41	0.53
3:I:144:ARG:NH1	3:I:146:SER:OG	2.42	0.53
1:E:42:ASN:OD1	1:E:288:ALA:N	2.41	0.53
1:E:60:SER:OG	1:E:91:ASN:O	2.17	0.53
3:G:144:ARG:NH1	3:G:146:SER:OG	2.42	0.53
1:A:42:ASN:ND2	1:A:288:ALA:HB3	2.21	0.53
2:B:583:LYS:NZ	2:D:566:VAL:O	2.41	0.53
2:D:583:LYS:NZ	2:F:566:VAL:O	2.42	0.53
1:E:48:LEU:O	1:E:51:ILE:N	2.41	0.53
1:A:110:SER:OG	1:A:266:SER:O	2.22	0.53
1:C:170:ASN:OD1	1:C:172:LYS:N	2.41	0.52
3:H:144:ARG:NH1	3:H:146:SER:OG	2.42	0.52
1:E:13:ALA:N	2:F:514:TRP:O	2.40	0.52
1:A:170:ASN:OD1	1:A:172:LYS:N	2.41	0.52
3:G:95:SER:O	3:G:97:VAL:N	2.43	0.52
1:A:42:ASN:OD1	1:A:288:ALA:N	2.41	0.52
3:I:95:SER:O	3:I:97:VAL:N	2.43	0.52
2:D:537:ASP:OD2	2:D:540:SER:OG	2.15	0.51
3:H:95:SER:O	3:H:97:VAL:N	2.43	0.51
1:A:163:ASN:OD1	1:A:163:ASN:N	2.44	0.51
1:C:48:LEU:O	1:C:51:ILE:N	2.41	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:LEU:O	1:A:51:ILE:N	2.41	0.50
1:A:60:SER:OG	1:A:91:ASN:O	2.17	0.50
1:E:163:ASN:OD1	1:E:163:ASN:N	2.44	0.50
1:E:153:TRP:CZ2	1:E:195:TYR:OH	2.65	0.50
1:A:153:TRP:CZ2	1:A:195:TYR:OH	2.65	0.50
1:C:163:ASN:OD1	1:C:163:ASN:N	2.44	0.50
2:B:537:ASP:O	2:B:541:THR:OG1	2.13	0.49
1:C:153:TRP:CZ2	1:C:195:TYR:OH	2.65	0.49
1:E:117:ARG:NE	1:E:150:ASN:OD1	2.43	0.49
1:E:312:SER:OG	2:F:597:GLU:OE2	2.26	0.49
1:E:146:SER:OG	1:E:147:PHE:N	2.46	0.49
1:A:146:SER:OG	1:A:147:PHE:N	2.46	0.48
1:C:146:SER:OG	1:C:147:PHE:N	2.46	0.48
2:D:502:LEU:N	2:D:612:ASP:OD2	2.47	0.48
2:D:603:GLU:O	2:D:607:THR:OG1	2.24	0.48
2:F:502:LEU:N	2:F:612:ASP:OD2	2.47	0.47
2:D:537:ASP:O	2:D:541:THR:OG1	2.13	0.47
1:A:117:ARG:NE	1:A:150:ASN:OD1	2.43	0.47
2:B:502:LEU:N	2:B:612:ASP:OD2	2.47	0.47
3:G:140:GLY:N	3:G:210:LEU:O	2.44	0.47
1:C:117:ARG:NE	1:C:150:ASN:OD1	2.43	0.46
3:G:37:TYR:OH	3:G:239:MET:SD	2.59	0.46
1:A:161:TYR:OH	1:A:249:GLY:N	2.49	0.46
3:I:140:GLY:N	3:I:210:LEU:O	2.44	0.45
1:A:284:THR:OG1	1:A:301:VAL:O	2.14	0.45
1:E:16:SER:O	1:E:323:ASN:ND2	2.48	0.45
1:A:16:SER:O	1:A:323:ASN:ND2	2.48	0.45
3:G:147:CYS:SG	3:G:148:ALA:N	2.90	0.45
2:D:551:LYS:O	2:D:554:SER:N	2.50	0.45
3:G:225:ARG:HB3	3:G:235:PHE:HB3	1.99	0.45
3:H:147:CYS:SG	3:H:148:ALA:N	2.90	0.45
3:H:225:ARG:HB3	3:H:235:PHE:HB3	1.99	0.45
1:C:161:TYR:OH	1:C:249:GLY:N	2.49	0.44
2:F:551:LYS:O	2:F:554:SER:N	2.50	0.44
3:I:225:ARG:HB3	3:I:235:PHE:HB3	2.00	0.44
3:I:147:CYS:SG	3:I:148:ALA:N	2.90	0.44
2:B:505:ALA:O	2:B:510:ILE:N	2.48	0.44
2:B:551:LYS:O	2:B:554:SER:N	2.50	0.44
1:E:161:TYR:OH	1:E:249:GLY:N	2.49	0.44
2:B:566:VAL:O	2:F:583:LYS:NZ	2.51	0.44
2:F:505:ALA:O	2:F:510:ILE:N	2.48	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:55:ARG:NH1	3:H:63:PHE:O	2.51	0.44
1:C:16:SER:O	1:C:323:ASN:ND2	2.49	0.43
3:I:55:ARG:NH1	3:I:63:PHE:O	2.51	0.43
3:G:55:ARG:NH1	3:G:63:PHE:O	2.51	0.42
3:H:79:LEU:HD21	3:H:108:ILE:HG13	2.02	0.42
2:D:629:ASN:O	2:D:666:SER:OG	2.34	0.42
3:H:140:GLY:N	3:H:210:LEU:O	2.44	0.42
1:C:13:ALA:N	2:D:514:TRP:O	2.51	0.41
1:E:41:HIS:ND1	1:E:286:GLN:O	2.53	0.41
3:I:79:LEU:HD21	3:I:108:ILE:HG13	2.02	0.41
3:H:79:LEU:HD21	3:H:108:ILE:CG1	2.51	0.41
1:A:13:ALA:N	2:B:514:TRP:O	2.53	0.41
3:G:79:LEU:HD21	3:G:108:ILE:CG1	2.51	0.41
1:A:31:THR:N	1:A:321:LEU:O	2.48	0.41
1:C:41:HIS:ND1	1:C:286:GLN:O	2.53	0.41
3:G:79:LEU:HD21	3:G:108:ILE:HG13	2.02	0.41
3:I:55:ARG:HE	3:I:59:ILE:HB	1.86	0.40
3:I:79:LEU:HD21	3:I:108:ILE:CG1	2.51	0.40
2:D:505:ALA:O	2:D:510:ILE:N	2.48	0.40
1:A:41:HIS:ND1	1:A:286:GLN:O	2.53	0.40
3:H:55:ARG:HE	3:H:59:ILE:HB	1.86	0.40
1:A:311:ARG:NH1	2:B:590:ASP:OD1	2.55	0.40
3:G:55:ARG:HE	3:G:59:ILE:HB	1.86	0.40

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 PDB entries followed by that with respect to all EM entries.

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	321/323 (99%)	302 (94%)	19 (6%)	0	100	100
1	C	321/323 (99%)	303 (94%)	18 (6%)	0	100	100

*Continued on next page...*



Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	321/323 (99%)	302 (94%)	19 (6%)	0	100	100
2	B	171/173 (99%)	157 (92%)	14 (8%)	0	100	100
2	D	171/173 (99%)	157 (92%)	14 (8%)	0	100	100
2	F	171/173 (99%)	158 (92%)	13 (8%)	0	100	100
3	G	232/266 (87%)	205 (88%)	26 (11%)	1 (0%)	38	77
3	H	232/266 (87%)	205 (88%)	26 (11%)	1 (0%)	38	77
3	I	232/266 (87%)	205 (88%)	26 (11%)	1 (0%)	38	77
All	All	2172/2286 (95%)	1994 (92%)	175 (8%)	3 (0%)	58	88

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	60	PRO
3	H	60	PRO
3	I	60	PRO

### 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 PDB entries followed by that with respect to all EM entries.

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	283/283 (100%)	282 (100%)	1 (0%)	93	95
1	C	283/283 (100%)	282 (100%)	1 (0%)	93	95
1	E	283/283 (100%)	282 (100%)	1 (0%)	93	95
2	B	149/149 (100%)	149 (100%)	0	100	100
2	D	149/149 (100%)	149 (100%)	0	100	100
2	F	149/149 (100%)	149 (100%)	0	100	100
3	G	186/200 (93%)	184 (99%)	2 (1%)	78	89
3	H	186/200 (93%)	184 (99%)	2 (1%)	78	89
3	I	186/200 (93%)	184 (99%)	2 (1%)	78	89
All	All	1854/1896 (98%)	1845 (100%)	9 (0%)	91	95

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	163	ASN
1	C	163	ASN
1	E	163	ASN
3	G	225	ARG
3	G	239	MET
3	H	225	ARG
3	H	239	MET
3	I	225	ARG
3	I	239	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	542	GLN
2	B	546	ASN
2	B	595	ASN
2	B	614	ASN
2	D	542	GLN
2	D	546	ASN
2	D	595	ASN
2	D	614	ASN
2	F	542	GLN
2	F	546	ASN
2	F	595	ASN
2	F	614	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

33 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$
4	BMA	A	401	5	11,11,12	0.95	1 (9%)	13,15,17	0.91	0
5	NAG	A	402	5,4	14,14,15	0.36	0	15,19,21	0.46	0
5	NAG	A	403	1,5	14,14,15	0.50	0	15,19,21	0.63	0
5	NAG	A	404	5	14,14,15	0.18	0	15,19,21	0.60	0
5	NAG	A	405	1,5	14,14,15	0.35	0	15,19,21	0.69	0
5	NAG	A	406	1	14,14,15	0.30	0	15,19,21	0.65	0
5	NAG	A	407	1	14,14,15	0.19	0	15,19,21	0.55	0
5	NAG	A	408	1	14,14,15	0.38	0	15,19,21	0.53	0
5	NAG	A	409	1	14,14,15	0.60	0	15,19,21	0.73	0
5	NAG	A	410	1	14,14,15	0.39	0	15,19,21	0.65	0
5	NAG	B	701	2	14,14,15	0.14	0	15,19,21	0.54	0
4	BMA	C	401	5	11,11,12	0.97	1 (9%)	13,15,17	0.92	0
5	NAG	C	402	5,4	14,14,15	0.39	0	15,19,21	0.48	0
5	NAG	C	403	1,5	14,14,15	0.48	0	15,19,21	0.65	0
5	NAG	C	404	5	14,14,15	0.19	0	15,19,21	0.59	0
5	NAG	C	405	1,5	14,14,15	0.39	0	15,19,21	0.69	0
5	NAG	C	406	1	14,14,15	0.33	0	15,19,21	0.70	0
5	NAG	C	407	1	14,14,15	0.16	0	15,19,21	0.58	0
5	NAG	C	408	1	14,14,15	0.38	0	15,19,21	0.52	0
5	NAG	C	409	1	14,14,15	0.63	1 (7%)	15,19,21	0.70	0
5	NAG	C	410	1	14,14,15	0.40	0	15,19,21	0.64	0
5	NAG	D	701	2	14,14,15	0.17	0	15,19,21	0.51	0
4	BMA	E	401	5	11,11,12	0.98	1 (9%)	13,15,17	0.92	0
5	NAG	E	402	5,4	14,14,15	0.34	0	15,19,21	0.47	0
5	NAG	E	403	1,5	14,14,15	0.54	0	15,19,21	0.63	0
5	NAG	E	404	5	14,14,15	0.18	0	15,19,21	0.61	0
5	NAG	E	405	1,5	14,14,15	0.32	0	15,19,21	0.69	0
5	NAG	E	406	1	14,14,15	0.31	0	15,19,21	0.68	0
5	NAG	E	407	1	14,14,15	0.18	0	15,19,21	0.56	0
5	NAG	E	408	1	14,14,15	0.36	0	15,19,21	0.51	0
5	NAG	E	409	1	14,14,15	0.58	0	15,19,21	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	E	410	1	14,14,15	0.41	0	15,19,21	0.65	0
5	NAG	F	701	2	14,14,15	0.15	0	15,19,21	0.51	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	BMA	A	401	5	-	0/2/19/22	0/1/1/1
5	NAG	A	402	5,4	-	0/6/23/26	0/1/1/1
5	NAG	A	403	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	404	5	-	0/6/23/26	0/1/1/1
5	NAG	A	405	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	406	1	-	0/6/23/26	0/1/1/1
5	NAG	A	407	1	-	0/6/23/26	0/1/1/1
5	NAG	A	408	1	-	0/6/23/26	0/1/1/1
5	NAG	A	409	1	-	0/6/23/26	0/1/1/1
5	NAG	A	410	1	-	0/6/23/26	0/1/1/1
5	NAG	B	701	2	-	0/6/23/26	0/1/1/1
4	BMA	C	401	5	-	0/2/19/22	0/1/1/1
5	NAG	C	402	5,4	-	0/6/23/26	0/1/1/1
5	NAG	C	403	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	404	5	-	0/6/23/26	0/1/1/1
5	NAG	C	405	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	406	1	-	0/6/23/26	0/1/1/1
5	NAG	C	407	1	-	0/6/23/26	0/1/1/1
5	NAG	C	408	1	-	0/6/23/26	0/1/1/1
5	NAG	C	409	1	-	0/6/23/26	0/1/1/1
5	NAG	C	410	1	-	0/6/23/26	0/1/1/1
5	NAG	D	701	2	-	0/6/23/26	0/1/1/1
4	BMA	E	401	5	-	0/2/19/22	0/1/1/1
5	NAG	E	402	5,4	-	0/6/23/26	0/1/1/1
5	NAG	E	403	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	404	5	-	0/6/23/26	0/1/1/1
5	NAG	E	405	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	406	1	-	0/6/23/26	0/1/1/1
5	NAG	E	407	1	-	0/6/23/26	0/1/1/1
5	NAG	E	408	1	-	0/6/23/26	0/1/1/1
5	NAG	E	409	1	-	0/6/23/26	0/1/1/1
5	NAG	E	410	1	-	0/6/23/26	0/1/1/1
5	NAG	F	701	2	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	401	BMA	O5-C1	-2.67	1.39	1.43
4	C	401	BMA	O5-C1	-2.61	1.39	1.43
4	A	401	BMA	O5-C1	-2.59	1.39	1.43
5	C	409	NAG	O5-C1	-2.05	1.40	1.43

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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.