



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:30 PM GMT

PDB ID : 4LN8
Title : The crystal structure of hemagglutinin from a h7n9 influenza virus (a/shanghai/2/2013) in complex with lstb
Authors : Yang, H.; Carney, P.J.; Chang, J.C.; Villanueva, J.M.; Stevens, J.
Deposited on : 2013-07-11
Resolution : 2.50 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

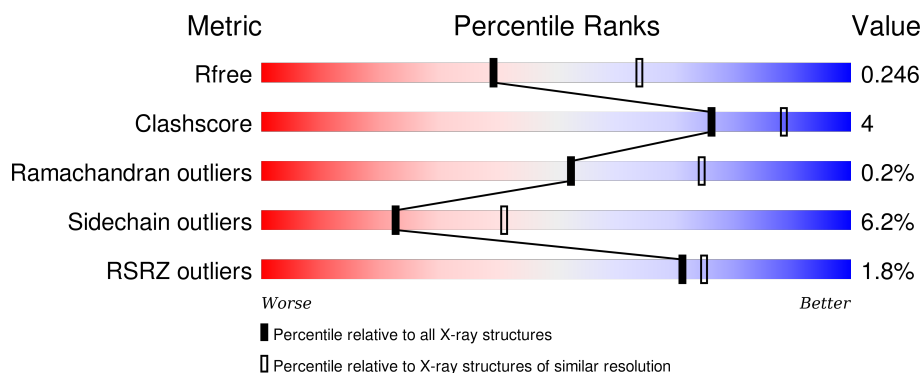
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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. 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	325	<div> <div>2%</div> <div>86%</div> <div>10%</div> <div>••</div> </div>
1	C	325	<div> <div>2%</div> <div>85%</div> <div>12%</div> <div>••</div> </div>
1	E	325	<div> <div>%</div> <div>84%</div> <div>12%</div> <div>••</div> </div>
1	G	325	<div> <div>2%</div> <div>86%</div> <div>10%</div> <div>••</div> </div>
1	I	325	<div> <div>%</div> <div>85%</div> <div>12%</div> <div>••</div> </div>

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Mol	Chain	Length	Quality of chain
1	K	325	
2	B	181	
2	D	181	
2	F	181	
2	H	181	
2	J	181	
2	L	181	

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
3	NAG	A	401	-	-	-	X
3	FUC	A	404	X	-	-	-
3	NAG	E	401	-	-	-	X
3	FUC	E	404	X	-	-	-
7	NAG	B	500	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 23845 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	316	Total	C	N	O	S	1	0	0
			2412	1498	436	463	15			
1	C	316	Total	C	N	O	S	1	0	0
			2412	1498	436	463	15			
1	E	316	Total	C	N	O	S	1	0	0
			2412	1498	436	463	15			
1	G	316	Total	C	N	O	S	1	0	0
			2412	1498	436	463	15			
1	I	316	Total	C	N	O	S	1	0	0
			2412	1498	436	463	15			
1	K	316	Total	C	N	O	S	1	0	0
			2412	1498	436	463	15			

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	167	Total	C	N	O	S	0	0	0
			1360	838	238	277	7			
2	D	167	Total	C	N	O	S	0	0	0
			1360	838	238	277	7			
2	F	167	Total	C	N	O	S	0	0	0
			1360	838	238	277	7			
2	H	167	Total	C	N	O	S	0	0	0
			1360	838	238	277	7			
2	J	167	Total	C	N	O	S	0	0	0
			1360	838	238	277	7			
2	L	167	Total	C	N	O	S	0	0	0
			1360	838	238	277	7			

- Molecule 3 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	4	Total	C	N	O	0	0
			49	28	2	19		
3	C	4	Total	C	N	O	0	0
			49	28	2	19		
3	E	4	Total	C	N	O	0	0
			49	28	2	19		

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	3	Total	C	N	O	0	0
			39	22	2	15		
4	C	3	Total	C	N	O	0	0
			39	22	2	15		
4	E	3	Total	C	N	O	0	0
			39	22	2	15		
4	G	3	Total	C	N	O	0	0
			39	22	2	15		
4	I	3	Total	C	N	O	0	0
			39	22	2	15		
4	K	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	4	Total	C	N	O	0	0
			57	31	2	24		
5	G	4	Total	C	N	O	0	0
			57	31	2	24		
5	K	4	Total	C	N	O	0	0
			57	31	2	24		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	1	Total	Ca	0	0
			1	1		
6	K	1	Total	Ca	0	0
			1	1		
6	E	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	I	1	Total	Ca	0	0
			1	1		
6	C	1	Total	Ca	0	0
			1	1		
6	A	1	Total	Ca	0	0
			1	1		

- Molecule 7 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	D	1	Total	C	N	O	0	0
			14	8	1	5		
7	F	1	Total	C	N	O	0	0
			14	8	1	5		
7	H	1	Total	C	N	O	0	0
			14	8	1	5		
7	J	1	Total	C	N	O	0	0
			14	8	1	5		
7	L	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	3	Total	C	N	O	0	0
			45	25	2	18		
8	I	3	Total	C	N	O	0	0
			45	25	2	18		

- Molecule 9 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	E	2	Total	C	N	O	0	0
			33	19	2	12		

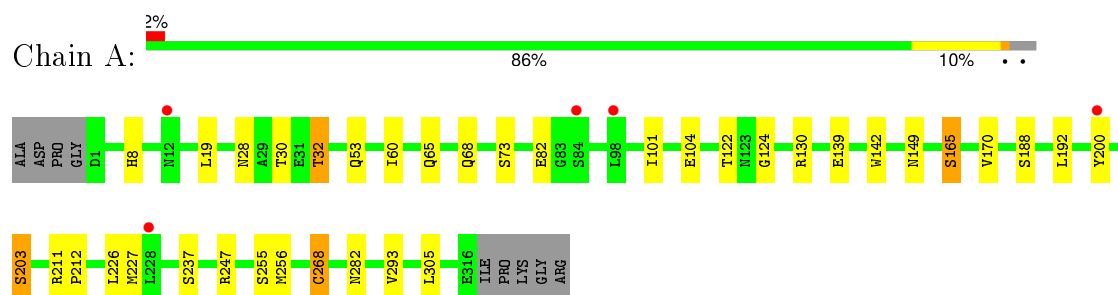
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	48	Total	O	0	0
			48	48		
10	B	28	Total	O	0	0
			28	28		
10	C	39	Total	O	0	0
			39	39		
10	D	25	Total	O	0	0
			25	25		
10	E	52	Total	O	0	0
			52	52		
10	F	28	Total	O	0	0
			28	28		
10	G	48	Total	O	0	0
			48	48		
10	H	25	Total	O	0	0
			25	25		
10	I	51	Total	O	0	0
			51	51		
10	J	27	Total	O	0	0
			27	27		
10	K	53	Total	O	0	0
			53	53		
10	L	24	Total	O	0	0
			24	24		

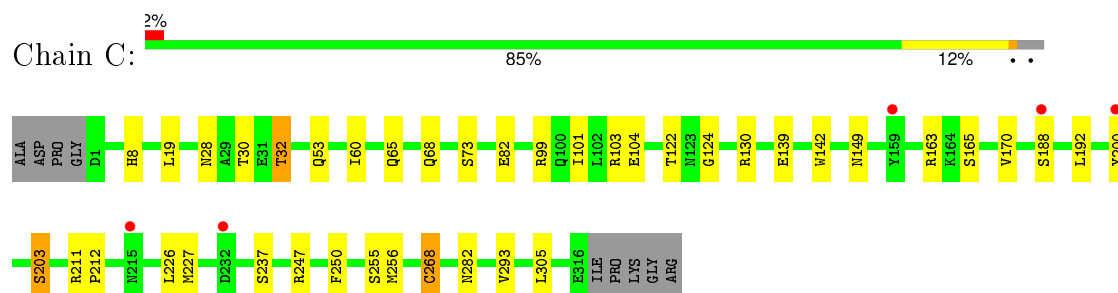
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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.

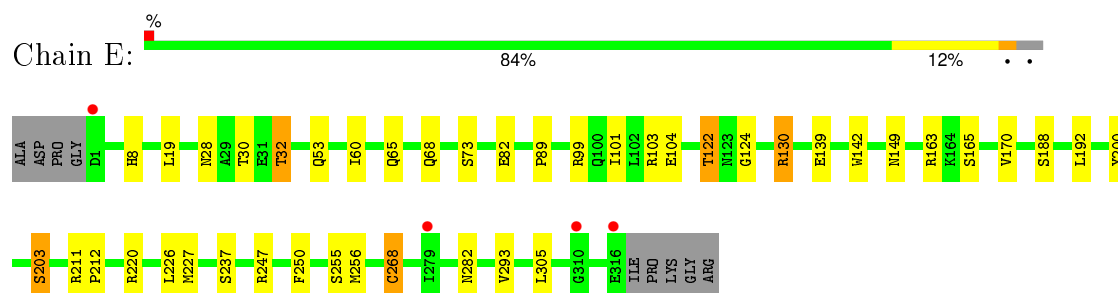
• Molecule 1: Hemagglutinin



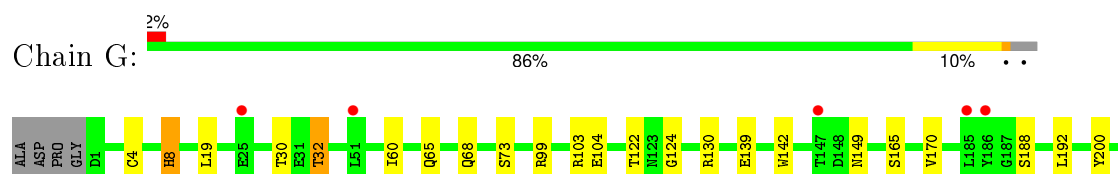
• Molecule 1: Hemagglutinin



• Molecule 1: Hemagglutinin

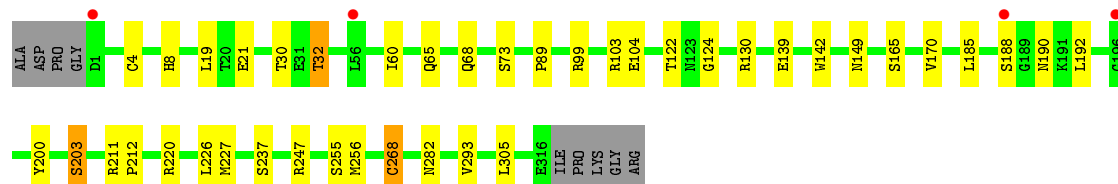
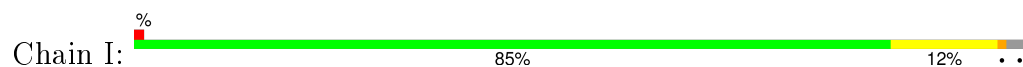


• Molecule 1: Hemagglutinin

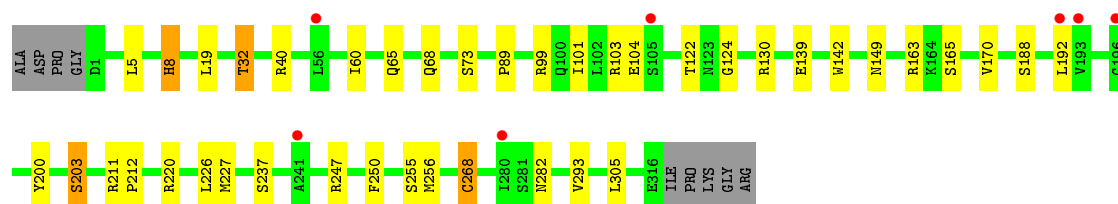
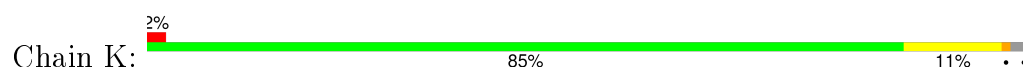




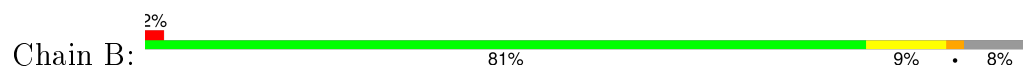
- Molecule 1: Hemagglutinin



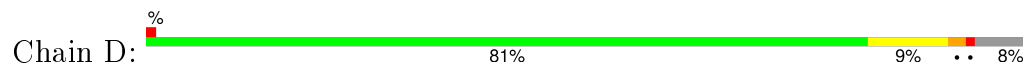
- Molecule 1: Hemagglutinin



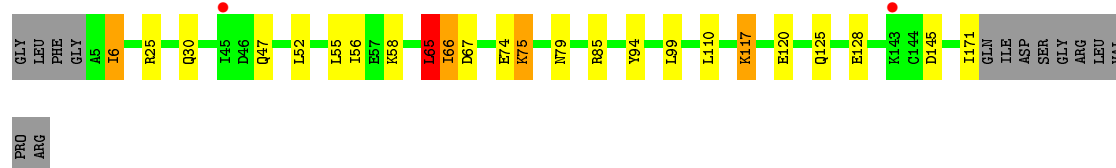
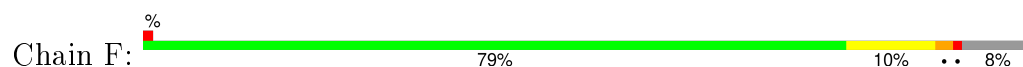
- Molecule 2: Hemagglutinin



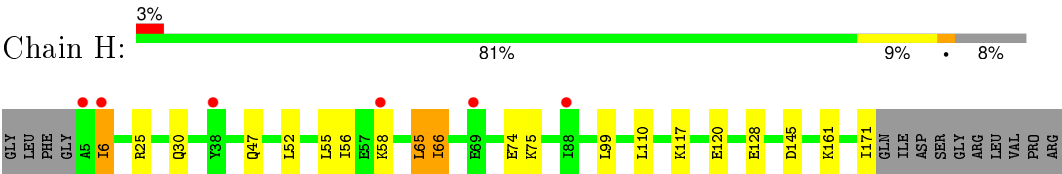
- Molecule 2: Hemagglutinin



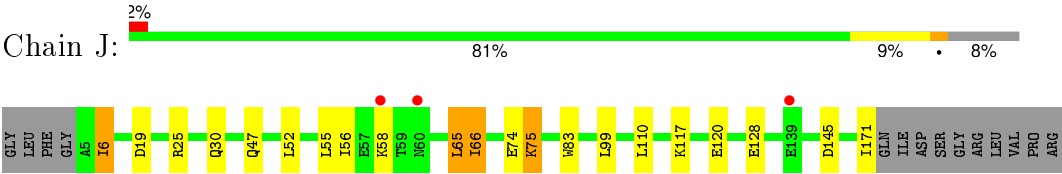
- Molecule 2: Hemagglutinin



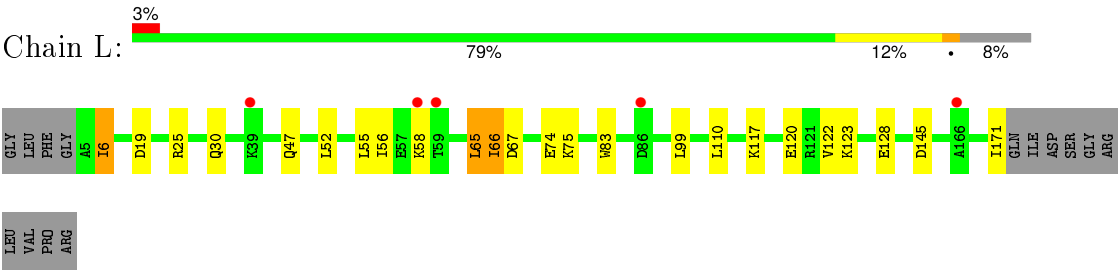
- Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	154.36Å 154.44Å 154.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.62 – 2.50 38.59 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.2 (38.62-2.50) 97.6 (38.59-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.217 , 0.246 0.217 , 0.246	Depositor DCC
R_{free} test set	6406 reflections (5.39%)	DCC
Wilson B-factor (Å ²)	57.1	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 20.3	EDS
Estimated twinning fraction	0.024 for k,h,-l 0.021 for -h,-l,-k 0.023 for l,-k,h 0.447 for k,l,h 0.447 for l,h,k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 125218 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	23845	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.94% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: BMA, NAG, CA, SIA, GAL, FUC

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	0.79	1/2458 (0.0%)	0.79	1/3322 (0.0%)
1	C	0.78	1/2458 (0.0%)	0.79	0/3322
1	E	0.78	1/2458 (0.0%)	0.79	1/3322 (0.0%)
1	G	0.86	1/2458 (0.0%)	0.80	1/3322 (0.0%)
1	I	0.82	1/2458 (0.0%)	0.80	1/3322 (0.0%)
1	K	0.83	1/2458 (0.0%)	0.80	1/3322 (0.0%)
2	B	0.73	1/1383 (0.1%)	0.77	1/1864 (0.1%)
2	D	0.74	1/1383 (0.1%)	0.77	2/1864 (0.1%)
2	F	0.75	1/1383 (0.1%)	0.78	2/1864 (0.1%)
2	H	0.75	1/1383 (0.1%)	0.78	0/1864
2	J	0.77	3/1383 (0.2%)	0.78	0/1864
2	L	0.78	3/1383 (0.2%)	0.78	0/1864
All	All	0.79	16/23046 (0.1%)	0.79	10/31116 (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
3	A	1	0
3	E	1	0
All	All	2	0

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	268	CYS	CB-SG	-25.39	1.39	1.82
1	K	268	CYS	CB-SG	-24.16	1.41	1.82
1	I	268	CYS	CB-SG	-22.43	1.44	1.82
1	A	268	CYS	CB-SG	-19.58	1.49	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	268	CYS	CB-SG	-18.99	1.50	1.82

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	268	CYS	CA-CB-SG	7.30	127.14	114.00
1	K	268	CYS	CA-CB-SG	7.26	127.06	114.00
1	I	268	CYS	CA-CB-SG	7.12	126.81	114.00
2	D	85	ARG	NE-CZ-NH2	-5.51	117.55	120.30
2	B	85	ARG	NE-CZ-NH2	-5.47	117.56	120.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	404	FUC	C1
3	E	404	FUC	C1

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2412	0	2374	15	1
1	C	2412	0	2374	17	1
1	E	2412	0	2374	20	1
1	G	2412	0	2375	15	1
1	I	2412	0	2375	17	1
1	K	2412	0	2375	18	1
2	B	1360	0	1262	13	0
2	D	1360	0	1262	18	0
2	F	1360	0	1262	18	0
2	H	1360	0	1262	14	0
2	J	1360	0	1262	13	0
2	L	1360	0	1262	14	0
3	A	49	0	43	1	0
3	C	49	0	43	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	49	0	43	1	0
4	A	39	0	34	0	0
4	C	39	0	34	0	0
4	E	39	0	34	0	0
4	G	39	0	34	0	0
4	I	39	0	34	0	0
4	K	39	0	34	0	0
5	A	57	0	49	0	0
5	G	57	0	49	0	0
5	K	57	0	49	0	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
6	E	1	0	0	0	0
6	G	1	0	0	0	0
6	I	1	0	0	0	0
6	K	1	0	0	0	0
7	B	14	0	13	0	0
7	D	14	0	13	0	0
7	F	14	0	13	1	0
7	H	14	0	13	0	0
7	J	14	0	13	0	0
7	L	14	0	13	0	0
8	C	45	0	38	0	0
8	I	45	0	38	2	0
9	E	33	0	27	0	0
10	A	48	0	0	2	0
10	B	28	0	0	0	0
10	C	39	0	0	0	0
10	D	25	0	0	3	0
10	E	52	0	0	2	0
10	F	28	0	0	3	0
10	G	48	0	0	0	0
10	H	25	0	0	2	0
10	I	51	0	0	2	0
10	J	27	0	0	0	0
10	K	53	0	0	1	0
10	L	24	0	0	2	0
All	All	23845	0	22480	172	3

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 172 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)
2:D:58:LYS:HA	10:D:612:HOH:O	1.80	0.80
1:I:139:GLU:OE1	1:I:247:ARG:HD3	1.82	0.79
1:G:139:GLU:OE1	1:G:247:ARG:HD3	1.83	0.78
1:K:139:GLU:OE1	1:K:247:ARG:HD3	1.83	0.77
1:C:139:GLU:OE1	1:C:247:ARG:HD3	1.84	0.77

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:ASN:OD1	1:I:149:ASN:OD1[4_445]	2.00	0.20
1:E:149:ASN:OD1	1:G:149:ASN:OD1[2_444]	2.03	0.17
1:A:149:ASN:OD1	1:K:149:ASN:OD1[4_445]	2.03	0.17

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	314/325 (97%)	305 (97%)	8 (2%)	1 (0%)	46	68
1	C	314/325 (97%)	306 (98%)	7 (2%)	1 (0%)	46	68
1	E	314/325 (97%)	304 (97%)	9 (3%)	1 (0%)	46	68
1	G	314/325 (97%)	306 (98%)	7 (2%)	1 (0%)	46	68
1	I	314/325 (97%)	304 (97%)	9 (3%)	1 (0%)	46	68
1	K	314/325 (97%)	304 (97%)	9 (3%)	1 (0%)	46	68
2	B	165/181 (91%)	158 (96%)	7 (4%)	0	100	100
2	D	165/181 (91%)	158 (96%)	7 (4%)	0	100	100
2	F	165/181 (91%)	158 (96%)	7 (4%)	0	100	100
2	H	165/181 (91%)	157 (95%)	8 (5%)	0	100	100
2	J	165/181 (91%)	157 (95%)	8 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	165/181 (91%)	158 (96%)	7 (4%)	0	100	100
All	All	2874/3036 (95%)	2775 (97%)	93 (3%)	6 (0%)	52	75

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	200	TYR
1	A	200	TYR
1	C	200	TYR
1	E	200	TYR
1	G	200	TYR

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	265/271 (98%)	249 (94%)	16 (6%)	24	43
1	C	265/271 (98%)	249 (94%)	16 (6%)	24	43
1	E	265/271 (98%)	249 (94%)	16 (6%)	24	43
1	G	265/271 (98%)	249 (94%)	16 (6%)	24	43
1	I	265/271 (98%)	249 (94%)	16 (6%)	24	43
1	K	265/271 (98%)	250 (94%)	15 (6%)	25	46
2	B	144/155 (93%)	135 (94%)	9 (6%)	22	40
2	D	144/155 (93%)	135 (94%)	9 (6%)	22	40
2	F	144/155 (93%)	135 (94%)	9 (6%)	22	40
2	H	144/155 (93%)	135 (94%)	9 (6%)	22	40
2	J	144/155 (93%)	134 (93%)	10 (7%)	19	35
2	L	144/155 (93%)	134 (93%)	10 (7%)	19	35
All	All	2454/2556 (96%)	2303 (94%)	151 (6%)	23	41

5 of 151 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	65	LEU
1	G	165	SER
1	K	256	MET
2	F	75	LYS
1	G	19	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	J	76	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 ⓘ

50 carbohydrates 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	$\# Z > 2$
3	NAG	A	401	1,3	14,14,15	0.99	1 (7%)	15,19,21	2.86	1 (6%)
3	NAG	A	402	3	14,14,15	0.83	1 (7%)	15,19,21	1.24	3 (20%)
3	BMA	A	403	3	11,11,12	0.88	0	14,15,17	2.67	4 (28%)
3	FUC	A	404	3	10,10,11	1.01	0	14,14,16	1.92	4 (28%)
4	NAG	A	405	1,4	14,14,15	0.86	0	15,19,21	1.02	2 (13%)
4	NAG	A	406	4	14,14,15	0.47	0	15,19,21	1.19	0
4	BMA	A	407	4	11,11,12	0.81	0	14,15,17	1.81	6 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SIA	A	408	5	16,20,21	0.50	0	18,28,31	1.36	3 (16%)
5	NAG	A	409	5	13,13,15	0.66	0	15,17,21	1.09	1 (6%)
5	GAL	A	410	5	12,12,12	0.59	0	17,17,17	0.86	0
5	GAL	A	411	5	12,12,12	0.89	1 (8%)	17,17,17	1.92	5 (29%)
3	NAG	C	401	1,3	14,14,15	0.94	1 (7%)	15,19,21	2.69	3 (20%)
3	NAG	C	402	3	14,14,15	0.88	1 (7%)	15,19,21	1.39	1 (6%)
3	BMA	C	403	3	11,11,12	0.58	0	14,15,17	1.95	2 (14%)
3	FUC	C	404	3	10,10,11	0.68	0	14,14,16	2.19	4 (28%)
4	NAG	C	405	1,4	14,14,15	0.72	0	15,19,21	1.73	3 (20%)
4	NAG	C	406	4	14,14,15	0.46	0	15,19,21	1.09	2 (13%)
4	BMA	C	407	4	11,11,12	0.65	0	14,15,17	1.13	0
8	SIA	C	408	8	16,20,21	0.67	0	18,28,31	1.49	3 (16%)
8	NAG	C	409	8	13,13,15	0.63	0	15,17,21	1.78	3 (20%)
8	GAL	C	410	8	12,12,12	0.57	0	17,17,17	1.09	1 (5%)
3	NAG	E	401	1,3	14,14,15	0.92	1 (7%)	15,19,21	2.68	3 (20%)
3	NAG	E	402	3	14,14,15	0.77	0	15,19,21	1.13	1 (6%)
3	BMA	E	403	3	11,11,12	0.49	0	14,15,17	2.46	1 (7%)
3	FUC	E	404	3	10,10,11	0.92	0	14,14,16	2.14	6 (42%)
4	NAG	E	405	1,4	14,14,15	0.78	0	15,19,21	1.02	1 (6%)
4	NAG	E	406	4	14,14,15	0.56	0	15,19,21	1.40	2 (13%)
4	BMA	E	407	4	11,11,12	0.67	0	14,15,17	2.42	4 (28%)
9	SIA	E	408	9	16,20,21	0.61	0	18,28,31	1.40	3 (16%)
9	NAG	E	409	9	13,13,15	0.89	1 (7%)	15,17,21	2.00	3 (20%)
4	NAG	G	401	1,4	14,14,15	0.57	0	15,19,21	1.25	1 (6%)
4	NAG	G	402	4	14,14,15	0.61	0	15,19,21	0.89	0
4	BMA	G	403	4	11,11,12	0.72	0	14,15,17	1.44	3 (21%)
5	SIA	G	404	5	16,20,21	0.56	0	18,28,31	1.06	1 (5%)
5	NAG	G	405	5	13,13,15	0.66	0	15,17,21	2.20	5 (33%)
5	GAL	G	406	5	12,12,12	0.52	0	17,17,17	1.24	1 (5%)
5	GAL	G	407	5	12,12,12	0.57	0	17,17,17	1.28	2 (11%)
4	NAG	I	401	1,4	14,14,15	0.63	0	15,19,21	0.91	0
4	NAG	I	402	4	14,14,15	0.68	0	15,19,21	1.06	1 (6%)
4	BMA	I	403	4	11,11,12	0.61	0	14,15,17	1.57	2 (14%)
8	SIA	I	404	8	16,20,21	0.53	0	18,28,31	1.35	3 (16%)
8	NAG	I	405	8	13,13,15	0.72	0	15,17,21	2.92	6 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	GAL	I	406	8	12,12,12	0.58	0	17,17,17	1.13	1 (5%)
4	NAG	K	401	1,4	14,14,15	0.59	0	15,19,21	1.09	1 (6%)
4	NAG	K	402	4	14,14,15	0.69	0	15,19,21	1.37	3 (20%)
4	BMA	K	403	4	11,11,12	0.71	0	14,15,17	1.52	3 (21%)
5	SIA	K	404	5	16,20,21	0.42	0	18,28,31	1.17	2 (11%)
5	NAG	K	405	5	13,13,15	0.74	0	15,17,21	1.58	2 (13%)
5	GAL	K	406	5	12,12,12	0.62	0	17,17,17	1.45	3 (17%)
5	GAL	K	407	5	12,12,12	0.79	0	17,17,17	1.71	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
3	NAG	A	401	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	402	3	-	0/6/23/26	0/1/1/1
3	BMA	A	403	3	-	0/2/19/22	0/1/1/1
3	FUC	A	404	3	1/1/4/5	0/0/17/20	0/1/1/1
4	NAG	A	405	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	406	4	-	0/6/23/26	0/1/1/1
4	BMA	A	407	4	-	0/2/19/22	0/1/1/1
5	SIA	A	408	5	-	0/14/34/38	0/1/1/1
5	NAG	A	409	5	-	0/6/19/26	0/1/1/1
5	GAL	A	410	5	-	0/2/22/22	0/1/1/1
5	GAL	A	411	5	-	0/2/22/22	0/1/1/1
3	NAG	C	401	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	402	3	-	0/6/23/26	0/1/1/1
3	BMA	C	403	3	-	0/2/19/22	0/1/1/1
3	FUC	C	404	3	-	0/0/17/20	0/1/1/1
4	NAG	C	405	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	406	4	-	0/6/23/26	0/1/1/1
4	BMA	C	407	4	-	0/2/19/22	0/1/1/1
8	SIA	C	408	8	-	0/14/34/38	0/1/1/1
8	NAG	C	409	8	-	0/6/19/26	0/1/1/1
8	GAL	C	410	8	-	0/2/22/22	0/1/1/1
3	NAG	E	401	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	402	3	-	0/6/23/26	0/1/1/1
3	BMA	E	403	3	-	0/2/19/22	0/1/1/1
3	FUC	E	404	3	1/1/4/5	0/0/17/20	0/1/1/1
4	NAG	E	405	1,4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	E	406	4	-	0/6/23/26	0/1/1/1
4	BMA	E	407	4	-	0/2/19/22	0/1/1/1
9	SIA	E	408	9	-	0/14/34/38	0/1/1/1
9	NAG	E	409	9	-	0/6/19/26	0/1/1/1
4	NAG	G	401	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	402	4	-	0/6/23/26	0/1/1/1
4	BMA	G	403	4	-	0/2/19/22	0/1/1/1
5	SIA	G	404	5	-	0/14/34/38	0/1/1/1
5	NAG	G	405	5	-	0/6/19/26	0/1/1/1
5	GAL	G	406	5	-	0/2/22/22	0/1/1/1
5	GAL	G	407	5	-	0/2/22/22	0/1/1/1
4	NAG	I	401	1,4	-	0/6/23/26	0/1/1/1
4	NAG	I	402	4	-	0/6/23/26	0/1/1/1
4	BMA	I	403	4	-	0/2/19/22	0/1/1/1
8	SIA	I	404	8	-	0/14/34/38	0/1/1/1
8	NAG	I	405	8	-	0/6/19/26	0/1/1/1
8	GAL	I	406	8	-	0/2/22/22	0/1/1/1
4	NAG	K	401	1,4	-	0/6/23/26	0/1/1/1
4	NAG	K	402	4	-	0/6/23/26	0/1/1/1
4	BMA	K	403	4	-	0/2/19/22	0/1/1/1
5	SIA	K	404	5	-	0/14/34/38	0/1/1/1
5	NAG	K	405	5	-	0/6/19/26	0/1/1/1
5	GAL	K	406	5	-	0/2/22/22	0/1/1/1
5	GAL	K	407	5	-	0/2/22/22	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	411	GAL	C4-C5	2.05	1.57	1.53
3	A	402	NAG	C1-C2	2.09	1.55	1.52
3	C	402	NAG	C1-C2	2.21	1.55	1.52
9	E	409	NAG	C1-C2	2.26	1.55	1.52
3	C	401	NAG	C1-C2	2.40	1.55	1.52

The worst 5 of 119 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	405	NAG	C4-C3-C2	-7.04	105.58	112.53
9	E	409	NAG	C4-C3-C2	-5.90	106.70	112.53
5	K	405	NAG	C4-C3-C2	-5.20	107.40	112.53
5	G	405	NAG	C4-C3-C2	-4.67	107.92	112.53
8	I	405	NAG	C6-C5-C4	-4.54	107.50	113.29

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	E	404	FUC	C1
3	A	404	FUC	C1

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	NAG	1	0
3	C	401	NAG	1	0
3	E	401	NAG	1	0
8	I	404	SIA	2	0

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 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
7	NAG	B	500	2	14,14,15	0.95	1 (7%)	15,19,21	1.71	4 (26%)
7	NAG	D	500	2	14,14,15	0.85	1 (7%)	15,19,21	1.83	3 (20%)
7	NAG	F	500	2	14,14,15	0.95	1 (7%)	15,19,21	2.01	4 (26%)
7	NAG	H	500	2	14,14,15	1.09	2 (14%)	15,19,21	2.53	7 (46%)
7	NAG	J	500	2	14,14,15	1.21	2 (14%)	15,19,21	2.59	7 (46%)
7	NAG	L	500	2	14,14,15	1.18	2 (14%)	15,19,21	3.02	4 (26%)

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
7	NAG	B	500	2	-	0/6/23/26	0/1/1/1
7	NAG	D	500	2	-	0/6/23/26	0/1/1/1
7	NAG	F	500	2	-	0/6/23/26	0/1/1/1
7	NAG	H	500	2	-	0/6/23/26	0/1/1/1
7	NAG	J	500	2	-	0/6/23/26	0/1/1/1
7	NAG	L	500	2	-	0/6/23/26	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	H	500	NAG	C1-C2	2.10	1.55	1.52
7	J	500	NAG	O7-C7	2.14	1.28	1.23
7	L	500	NAG	C1-C2	2.38	1.55	1.52
7	D	500	NAG	C1-C2	2.44	1.55	1.52
7	L	500	NAG	O7-C7	2.47	1.28	1.23

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	500	NAG	C8-C7-N2	-4.00	108.46	116.11
7	J	500	NAG	C8-C7-N2	-3.44	109.52	116.11
7	H	500	NAG	C8-C7-N2	-3.43	109.54	116.11
7	F	500	NAG	O7-C7-C8	-3.05	116.46	122.06
7	H	500	NAG	C4-C3-C2	-2.79	106.90	111.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	500	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	316/325 (97%)	0.20	5 (1%) 74 78	39, 59, 82, 97	1 (0%)
1	C	316/325 (97%)	0.21	5 (1%) 74 78	38, 58, 83, 97	1 (0%)
1	E	316/325 (97%)	0.16	4 (1%) 79 82	39, 58, 81, 98	1 (0%)
1	G	316/325 (97%)	0.25	7 (2%) 65 69	42, 60, 83, 104	1 (0%)
1	I	316/325 (97%)	0.23	4 (1%) 79 82	43, 60, 85, 101	1 (0%)
1	K	316/325 (97%)	0.27	7 (2%) 65 69	41, 60, 83, 105	1 (0%)
2	B	167/181 (92%)	0.33	3 (1%) 71 75	35, 60, 89, 129	0
2	D	167/181 (92%)	0.30	1 (0%) 90 91	34, 59, 87, 124	0
2	F	167/181 (92%)	0.29	2 (1%) 81 83	34, 60, 88, 120	0
2	H	167/181 (92%)	0.30	6 (3%) 46 51	37, 58, 80, 135	0
2	J	167/181 (92%)	0.23	3 (1%) 71 75	35, 58, 84, 138	0
2	L	167/181 (92%)	0.31	5 (2%) 54 59	36, 59, 81, 133	0
All	All	2898/3036 (95%)	0.24	52 (1%) 71 75	34, 59, 85, 138	6 (0%)

The worst 5 of 52 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	228	LEU	4.9
2	L	59	THR	4.3
2	L	58	LYS	4.3
2	D	171	ILE	3.6
1	C	215	ASN	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 ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	NAG	A	401	14/15	0.69	0.44	3.56	86,96,104,105	0
3	NAG	E	401	14/15	0.73	0.23	2.02	96,103,107,109	0
3	NAG	C	401	14/15	0.74	0.22	1.11	96,102,108,110	0
5	SIA	A	408	20/21	0.89	0.21	0.73	62,78,93,98	0
5	SIA	G	404	20/21	0.89	0.18	0.13	64,70,83,88	0
5	SIA	K	404	20/21	0.92	0.15	-0.19	66,72,78,78	0
8	SIA	C	408	20/21	0.93	0.15	-0.26	67,82,97,99	0
8	SIA	I	404	20/21	0.93	0.15	-0.61	64,73,81,82	0
9	SIA	E	408	20/21	0.92	0.13	-0.72	60,76,87,89	0
3	BMA	A	403	11/12	0.72	0.37	-	117,135,146,147	0
5	GAL	A	411	12/12	0.63	0.21	-	105,137,151,153	0
3	FUC	E	404	10/11	0.76	0.30	-	103,109,115,119	0
3	FUC	C	404	10/11	0.86	0.21	-	109,116,118,118	0
4	NAG	I	401	14/15	0.90	0.12	-	79,89,94,101	0
4	NAG	A	406	14/15	0.92	0.15	-	94,99,109,114	0
5	GAL	G	406	12/12	0.73	0.25	-	114,128,131,132	0
4	NAG	E	405	14/15	0.89	0.13	-	72,79,90,91	0
3	BMA	C	403	11/12	0.72	0.38	-	122,135,143,145	0
4	BMA	G	403	11/12	0.75	0.54	-	132,146,150,150	0
4	NAG	C	406	14/15	0.92	0.21	-	86,94,102,103	0
8	NAG	C	409	13/15	0.80	0.16	-	106,125,142,143	0
3	NAG	E	402	14/15	0.78	0.17	-	86,118,126,139	0
3	BMA	E	403	11/12	0.68	0.37	-	124,147,153,156	0
4	NAG	C	405	14/15	0.92	0.16	-	77,93,99,99	0
4	BMA	I	403	11/12	0.82	0.24	-	113,131,137,139	0
5	GAL	G	407	12/12	0.68	0.27	-	113,134,148,152	0
4	NAG	I	402	14/15	0.90	0.22	-	82,107,120,130	0
8	GAL	C	410	12/12	0.79	0.33	-	116,136,144,147	0
8	GAL	I	406	12/12	0.80	0.15	-	97,120,125,130	0
4	NAG	E	406	14/15	0.90	0.19	-	88,95,106,110	0
5	GAL	K	407	12/12	0.65	0.23	-	105,126,136,138	0
4	BMA	C	407	11/12	0.79	0.17	-	92,110,114,116	0
4	NAG	G	402	14/15	0.84	0.29	-	86,109,124,138	0
4	BMA	K	403	11/12	0.69	0.35	-	112,134,138,140	0
4	BMA	A	407	11/12	0.71	0.19	-	102,115,119,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	C	402	14/15	0.89	0.15	-	102,122,127,131	0
4	NAG	G	401	14/15	0.95	0.21	-	83,90,97,102	0
3	NAG	A	402	14/15	0.78	0.29	-	91,117,125,131	0
5	NAG	A	409	13/15	0.88	0.14	-	104,122,136,136	0
4	NAG	K	402	14/15	0.86	0.34	-	94,112,129,129	0
5	NAG	K	405	13/15	0.88	0.14	-	85,109,133,133	0
5	GAL	K	406	12/12	0.88	0.11	-	112,123,125,126	0
5	GAL	A	410	12/12	0.73	0.33	-	109,131,133,134	0
8	NAG	I	405	13/15	0.86	0.20	-	97,111,148,155	0
3	FUC	A	404	10/11	0.84	0.29	-	102,110,116,116	0
5	NAG	G	405	13/15	0.88	0.15	-	99,111,128,128	0
4	NAG	A	405	14/15	0.86	0.24	-	78,91,97,100	0
9	NAG	E	409	13/15	0.79	0.25	-	90,109,134,138	0
4	BMA	E	407	11/12	0.72	0.18	-	96,111,117,118	0
4	NAG	K	401	14/15	0.88	0.18	-	76,87,98,106	0

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	NAG	B	500	14/15	0.69	0.26	2.02	70,81,92,94	0
7	NAG	F	500	14/15	0.72	0.23	1.89	78,87,98,100	0
7	NAG	D	500	14/15	0.81	0.23	1.13	65,86,97,105	0
7	NAG	J	500	14/15	0.72	0.21	0.85	76,87,94,99	0
7	NAG	L	500	14/15	0.70	0.18	0.30	72,78,82,82	0
7	NAG	H	500	14/15	0.79	0.17	-0.36	65,73,76,76	0
6	CA	A	412	1/1	0.95	0.17	-	75,75,75,75	0
6	CA	I	407	1/1	0.93	0.17	-	77,77,77,77	0
6	CA	K	408	1/1	0.93	0.18	-	77,77,77,77	0
6	CA	E	410	1/1	0.94	0.25	-	75,75,75,75	0
6	CA	C	411	1/1	0.96	0.20	-	76,76,76,76	0
6	CA	G	408	1/1	0.89	0.16	-	77,77,77,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.