



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:12 PM GMT

PDB ID : 4O58
Title : Crystal structure of broadly neutralizing antibody F045-092 in complex with A/Victoria/3/1975 (H3N2) influenza hemagglutinin
Authors : Lee, P.S.; Wilson, I.A.
Deposited on : 2013-12-19
Resolution : 2.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

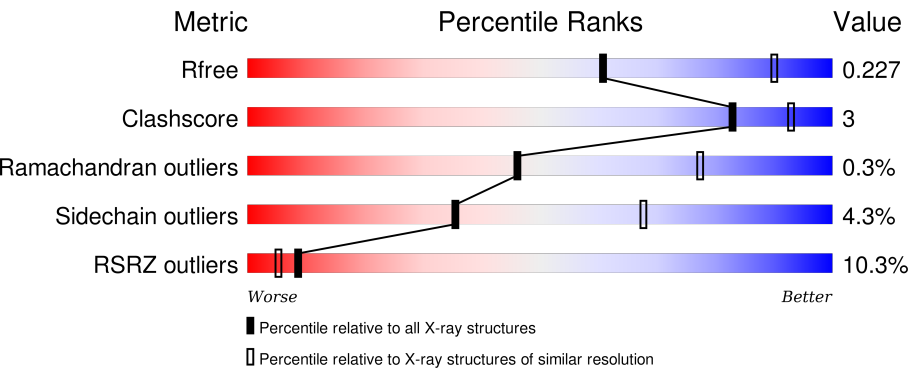
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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	323	<div><div></div><div>89%8%</div><div>..</div></div>
2	B	176	<div><div>%</div><div>90%8%</div><div>.</div></div>
3	L	216	<div><div>32%</div><div>84%13%</div><div>..</div></div>
4	H	240	<div><div>10%</div><div>83%9%7%</div><div>.</div></div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	B	201	-	-	-	X
8	SO4	A	511	-	-	-	X
8	SO4	B	204	-	-	-	X
8	SO4	H	302	-	-	-	X
9	PEG	L	303	-	-	-	X
9	PEG	L	304	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 7390 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 HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total	C	N	O	S	0	0	0
			2439	1526	430	470	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	-	EXPRESSION TAG	UNP P03435
A	8	ASP	-	EXPRESSION TAG	UNP P03435
A	9	PRO	-	EXPRESSION TAG	UNP P03435
A	10	GLY	-	EXPRESSION TAG	UNP P03435

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	0	0
			1393	864	246	277	6			

- Molecule 3 is a protein called Fab F045-092 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	213	Total	C	N	O	S	0	0	0
			1567	973	265	324	5			

- Molecule 4 is a protein called Fab F045-092 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	223	Total	C	N	O	S	0	0	0
			1679	1065	275	331	8			

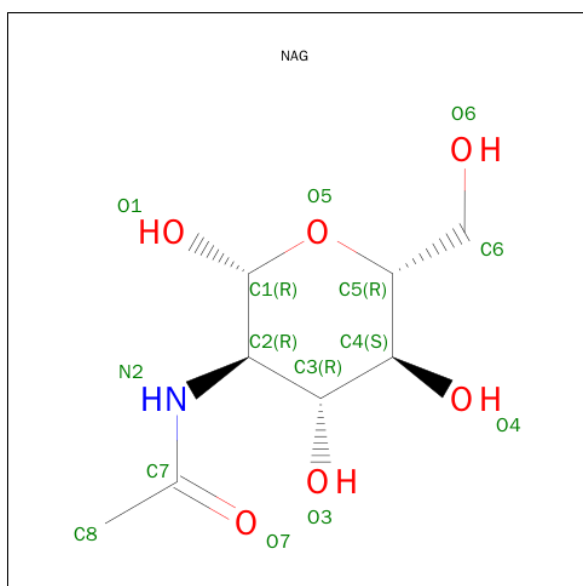
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	217	HIS	-	EXPRESSION TAG	UNP S6C4S0
H	218	HIS	-	EXPRESSION TAG	UNP S6C4S0
H	219	HIS	-	EXPRESSION TAG	UNP S6C4S0
H	220	HIS	-	EXPRESSION TAG	UNP S6C4S0
H	221	HIS	-	EXPRESSION TAG	UNP S6C4S0
H	222	HIS	-	EXPRESSION TAG	UNP S6C4S0

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

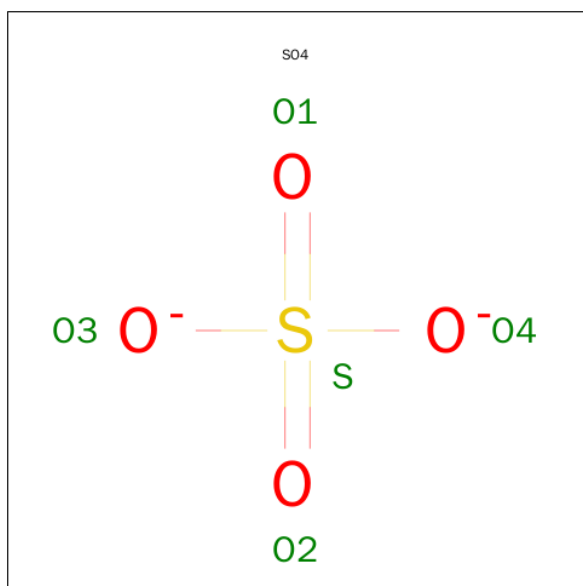


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



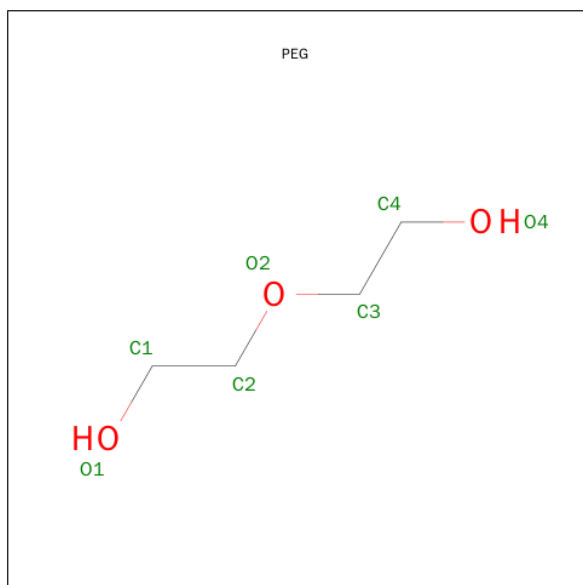
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	B	1	Total	O	S	0	0
			5	4	1		
8	B	1	Total	O	S	0	0
			5	4	1		
8	B	1	Total	O	S	0	0
			5	4	1		
8	L	1	Total	O	S	0	0
			5	4	1		
8	L	1	Total	O	S	0	0
			5	4	1		
8	H	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	H	1	Total	O	S	0	0
			5	4	1		
8	H	1	Total	O	S	0	0
			5	4	1		
8	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			7	4	3		
9	L	1	Total	C	O	0	0
			7	4	3		
9	L	1	Total	C	O	0	0
			7	4	3		

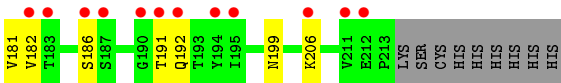
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	42	Total	O	0	0
			42	42		
10	B	16	Total	O	0	0
			16	16		
10	L	4	Total	O	0	0
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	H	14	Total	O	0	0
			14	14		



4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	99.10Å 99.10Å 336.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.02 – 2.75 49.02 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.02-2.75) 99.5 (49.02-2.75)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.177 , 0.224 0.190 , 0.227	Depositor DCC
R_{free} test set	2583 reflections (5.36%)	DCC
Wilson B-factor (Å ²)	58.2	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.1	EDS
Estimated twinning fraction	0.043 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 50815 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7390	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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: PEG, MAN, BMA, NAG, SO4

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	0.49	0/2496	0.63	1/3396 (0.0%)
2	B	0.58	0/1417	0.70	1/1904 (0.1%)
3	L	0.36	0/1604	0.54	0/2190
4	H	0.39	0/1721	0.55	1/2349 (0.0%)
All	All	0.46	0/7238	0.60	3/9839 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	LEU	CA-CB-CG	-5.68	102.25	115.30
2	B	170	ARG	NE-CZ-NH1	-5.38	117.61	120.30
4	H	97	ILE	CB-CA-C	-5.06	101.48	111.60

There are no chirality outliers.

There are no planarity outliers.

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	2439	0	2384	13	0
2	B	1393	0	1312	5	0
3	L	1567	0	1515	15	0
4	H	1679	0	1628	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	56	0	50	0	0
6	A	14	0	13	0	0
6	B	14	0	13	0	0
7	A	61	0	52	0	0
8	A	25	0	0	1	0
8	B	15	0	0	0	0
8	H	20	0	0	0	0
8	L	10	0	0	0	0
9	A	7	0	10	0	0
9	L	14	0	20	0	0
10	A	42	0	0	0	0
10	B	16	0	0	0	0
10	H	14	0	0	1	0
10	L	4	0	0	0	0
All	All	7390	0	6997	45	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 3.

All (45) 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)
4:H:70:THR:HG22	4:H:79:TYR:HB2	1.58	0.86
3:L:18:SER:HB3	3:L:76:SER:HA	1.62	0.80
1:A:321:ARG:NH2	8:A:515:SO4:O3	2.20	0.68
2:B:120:GLU:OE1	2:B:123:ARG:NH2	2.20	0.68
1:A:141:ARG:NH1	1:A:147:PHE:O	2.28	0.66
3:L:34:ASN:HD22	3:L:49:TYR:HA	1.63	0.63
1:A:133:ASN:HB3	4:H:100(A):HIS:CD2	2.42	0.55
1:A:66:LEU:HD21	1:A:112:VAL:HG12	1.90	0.53
4:H:163:VAL:HG22	4:H:182:VAL:HG22	1.91	0.53
2:B:54:ARG:NH2	2:B:103:GLU:OE2	2.27	0.52
4:H:36:TRP:CE2	4:H:80:MET:HB2	2.46	0.51
1:A:183:HIS:ND1	1:A:195:TYR:OH	2.39	0.51
3:L:54:ARG:HD3	3:L:60:ASP:HA	1.93	0.51
3:L:149:LYS:HE3	3:L:152:SER:HA	1.95	0.49
3:L:61:ARG:HB2	3:L:76:SER:O	2.13	0.49
4:H:191:THR:OG1	4:H:192:GLN:N	2.44	0.48
1:A:144:ASP:N	1:A:144:ASP:OD1	2.42	0.48
2:B:125:GLN:NE2	2:B:155:GLY:HA2	2.28	0.48
4:H:70:THR:HG21	10:H:401:HOH:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ARG:HH22	1:A:149:SER:HB3	1.77	0.48
3:L:54:ARG:CD	3:L:60:ASP:HA	2.44	0.47
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.97	0.46
3:L:166:LYS:HG3	3:L:172:TYR:CE2	2.51	0.46
2:B:14:TRP:CZ2	2:B:25:ARG:HD2	2.52	0.45
3:L:122:SER:O	3:L:126:GLN:HG3	2.17	0.44
1:A:213:ILE:HG12	1:A:233:TYR:CZ	2.52	0.44
1:A:29:ILE:HA	1:A:29:ILE:HD13	1.83	0.44
4:H:97:ILE:HG13	4:H:97:ILE:H	1.39	0.44
1:A:44:GLN:OE1	1:A:292:LYS:HE2	2.18	0.43
3:L:130:ALA:HB3	3:L:180:LEU:HB2	2.00	0.43
3:L:34:ASN:ND2	3:L:49:TYR:HA	2.33	0.43
1:A:183:HIS:O	1:A:185:PRO:HD3	2.18	0.43
4:H:29:TYR:HD1	4:H:29:TYR:H	1.67	0.43
1:A:175:ASP:OD1	1:A:239:PRO:HD3	2.18	0.43
3:L:95:LEU:HA	3:L:95:LEU:HD23	1.79	0.43
3:L:60:ASP:OD2	3:L:60:ASP:N	2.36	0.42
4:H:7:SER:HB3	4:H:21:SER:OG	2.19	0.42
4:H:199:ASN:OD1	4:H:206:LYS:HG2	2.20	0.42
3:L:108:GLN:HB2	3:L:140:TYR:CE1	2.54	0.42
4:H:145:TYR:OH	4:H:178:LEU:HD23	2.20	0.41
2:B:14:TRP:CE2	2:B:25:ARG:HD2	2.55	0.41
4:H:1:GLU:HG3	4:H:2:VAL:H	1.84	0.41
1:A:22:ASN:N	1:A:22:ASN:OD1	2.53	0.41
3:L:135:LEU:HD13	4:H:181:VAL:HG21	2.03	0.41
4:H:100(F):CYS:HB3	4:H:100(J):ASP:OD2	2.20	0.41

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	315/323 (98%)	303 (96%)	10 (3%)	2 (1%)	30	62
2	B	170/176 (97%)	161 (95%)	9 (5%)	0	100	100
3	L	211/216 (98%)	202 (96%)	8 (4%)	1 (0%)	34	67
4	H	219/240 (91%)	213 (97%)	6 (3%)	0	100	100
All	All	915/955 (96%)	879 (96%)	33 (4%)	3 (0%)	46	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	ILE
1	A	143	PRO
3	L	151	ASP

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	277/282 (98%)	266 (96%)	11 (4%)	38	71
2	B	146/149 (98%)	141 (97%)	5 (3%)	44	76
3	L	178/181 (98%)	166 (93%)	12 (7%)	20	46
4	H	186/201 (92%)	180 (97%)	6 (3%)	46	78
All	All	787/813 (97%)	753 (96%)	34 (4%)	35	68

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	18	HIS
1	A	24	THR
1	A	27	LYS
1	A	31	ASN
1	A	141	ARG
1	A	144	ASP
1	A	160	THR

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Mol	Chain	Res	Type
1	A	174	SER
1	A	222	TRP
1	A	259	LYS
2	B	2	ILE
2	B	12	ASN
2	B	17	MET
2	B	160	ASP
2	B	172	GLN
3	L	2	SER
3	L	18	SER
3	L	39	LEU
3	L	60	ASP
3	L	72	SER
3	L	76	SER
3	L	78	LEU
3	L	90	SER
3	L	95(A)	ASN
3	L	162	THR
3	L	189	ARG
3	L	209	THR
4	H	3	GLN
4	H	27	THR
4	H	29	TYR
4	H	70	THR
4	H	97	ILE
4	H	186	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	193	ASN
2	B	53	ASN
4	H	100(A)	HIS

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 ⓘ

9 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$
5	NAG	A	501	1,5	14,14,15	0.62	0	15,19,21	2.16	4 (26%)
5	NAG	A	502	5	14,14,15	0.50	0	15,19,21	1.29	2 (13%)
7	NAG	A	504	1,7	14,14,15	0.70	0	15,19,21	1.19	1 (6%)
7	NAG	A	505	7	14,14,15	0.59	0	15,19,21	1.06	2 (13%)
7	BMA	A	506	7	11,11,12	0.80	0	14,15,17	1.35	1 (7%)
7	MAN	A	507	7	11,11,12	0.59	0	14,15,17	0.99	1 (7%)
7	MAN	A	508	7	11,11,12	0.59	0	14,15,17	0.99	1 (7%)
5	NAG	A	509	1,5	14,14,15	0.45	0	15,19,21	1.04	1 (6%)
5	NAG	A	510	5	14,14,15	0.44	0	15,19,21	0.97	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	501	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	502	5	-	0/6/23/26	0/1/1/1
7	NAG	A	504	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	505	7	-	0/6/23/26	0/1/1/1
7	BMA	A	506	7	-	0/2/19/22	0/1/1/1
7	MAN	A	507	7	-	0/2/19/22	0/1/1/1
7	MAN	A	508	7	-	0/2/19/22	0/1/1/1
5	NAG	A	509	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	510	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	NAG	C2-N2-C7	-2.94	119.27	123.04
7	A	505	NAG	O7-C7-C8	-2.28	117.88	122.06
7	A	504	NAG	C6-C5-C4	-2.21	107.57	113.02
5	A	510	NAG	O5-C5-C6	2.31	112.35	107.35
7	A	505	NAG	C1-O5-C5	2.33	115.20	112.25
7	A	507	MAN	C1-C2-C3	2.42	112.41	109.54
7	A	508	MAN	O5-C5-C6	2.52	112.80	107.35
5	A	509	NAG	C1-O5-C5	2.58	115.53	112.25
5	A	502	NAG	O5-C5-C6	2.72	113.24	107.35
5	A	502	NAG	C1-O5-C5	3.25	116.37	112.25
7	A	506	BMA	C1-C2-C3	3.44	113.61	109.54
5	A	501	NAG	C3-C4-C5	3.98	117.13	110.20
5	A	501	NAG	C4-C3-C2	4.20	117.76	111.23
5	A	501	NAG	C1-O5-C5	4.67	118.17	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry [i](#)

19 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	A	503	1	14,14,15	0.55	0	15,19,21	2.16	2 (13%)
8	SO4	A	511	-	4,4,4	0.16	0	6,6,6	0.29	0
8	SO4	A	512	-	4,4,4	0.13	0	6,6,6	0.18	0
8	SO4	A	513	-	4,4,4	0.17	0	6,6,6	0.09	0
8	SO4	A	514	-	4,4,4	0.20	0	6,6,6	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	SO4	A	515	-	4,4,4	0.06	0	6,6,6	0.16	0
9	PEG	A	516	-	6,6,6	0.78	0	5,5,5	0.48	0
6	NAG	B	201	2	14,14,15	0.50	0	15,19,21	0.79	0
8	SO4	B	202	-	4,4,4	0.29	0	6,6,6	0.23	0
8	SO4	B	203	-	4,4,4	0.41	0	6,6,6	0.30	0
8	SO4	B	204	-	4,4,4	0.26	0	6,6,6	0.35	0
8	SO4	H	301	-	4,4,4	0.13	0	6,6,6	0.34	0
8	SO4	H	302	-	4,4,4	0.23	0	6,6,6	0.41	0
8	SO4	H	303	-	4,4,4	0.14	0	6,6,6	0.23	0
8	SO4	H	304	-	4,4,4	0.15	0	6,6,6	0.19	0
8	SO4	L	301	-	4,4,4	0.22	0	6,6,6	0.25	0
8	SO4	L	302	-	4,4,4	0.13	0	6,6,6	0.15	0
9	PEG	L	303	-	6,6,6	0.43	0	5,5,5	0.36	0
9	PEG	L	304	-	6,6,6	0.67	0	5,5,5	0.39	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
6	NAG	A	503	1	-	0/6/23/26	0/1/1/1
8	SO4	A	511	-	-	0/0/0/0	0/0/0/0
8	SO4	A	512	-	-	0/0/0/0	0/0/0/0
8	SO4	A	513	-	-	0/0/0/0	0/0/0/0
8	SO4	A	514	-	-	0/0/0/0	0/0/0/0
8	SO4	A	515	-	-	0/0/0/0	0/0/0/0
9	PEG	A	516	-	-	0/4/4/4	0/0/0/0
6	NAG	B	201	2	-	0/6/23/26	0/1/1/1
8	SO4	B	202	-	-	0/0/0/0	0/0/0/0
8	SO4	B	203	-	-	0/0/0/0	0/0/0/0
8	SO4	B	204	-	-	0/0/0/0	0/0/0/0
8	SO4	H	301	-	-	0/0/0/0	0/0/0/0
8	SO4	H	302	-	-	0/0/0/0	0/0/0/0
8	SO4	H	303	-	-	0/0/0/0	0/0/0/0
8	SO4	H	304	-	-	0/0/0/0	0/0/0/0
8	SO4	L	301	-	-	0/0/0/0	0/0/0/0
8	SO4	L	302	-	-	0/0/0/0	0/0/0/0
9	PEG	L	303	-	-	0/4/4/4	0/0/0/0
9	PEG	L	304	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	503	NAG	O5-C5-C6	-2.16	102.67	107.35
6	A	503	NAG	C1-O5-C5	7.19	121.37	112.25

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
8	A	515	SO4	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	317/323 (98%)	-0.07	0 100 100	20, 38, 59, 85	0
2	B	172/176 (97%)	0.03	1 (0%) 90 88	16, 27, 53, 95	0
3	L	213/216 (98%)	1.36	69 (32%) 1 0	36, 85, 151, 170	0
4	H	223/240 (92%)	0.59	25 (11%) 7 4	31, 63, 135, 169	0
All	All	925/955 (96%)	0.44	95 (10%) 9 5	16, 43, 130, 170	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	193	CYS	7.3
3	L	132	LEU	6.1
3	L	146	VAL	5.9
3	L	117	LEU	5.4
3	L	157	ALA	5.4
3	L	155	VAL	5.3
3	L	203	GLU	5.1
3	L	202	VAL	5.0
3	L	180	LEU	4.7
3	L	148	TRP	4.6
4	H	211	VAL	4.6
3	L	178	LEU	4.6
3	L	190	SER	4.6
3	L	206	VAL	4.5
3	L	182	PRO	4.5
3	L	189	ARG	4.4
4	H	159	LEU	4.3
4	H	206	LYS	4.3
3	L	129	LYS	4.3
3	L	185	TRP	4.3
3	L	156	LYS	4.3

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Mol	Chain	Res	Type	RSRZ
3	L	125	LEU	4.2
3	L	147	ALA	4.2
4	H	183	THR	4.2
4	H	124	LEU	4.2
4	H	137	ALA	4.1
3	L	158	GLY	4.1
3	L	201	THR	4.1
4	H	135	THR	4.1
3	L	149	LYS	4.0
4	H	194	TYR	4.0
3	L	133	VAL	4.0
3	L	200	SER	4.0
3	L	153	SER	3.9
3	L	181	THR	3.8
3	L	118	PHE	3.8
3	L	130	ALA	3.8
3	L	139	PHE	3.8
3	L	154	PRO	3.7
3	L	191	TYR	3.7
3	L	199	GLY	3.7
3	L	209	THR	3.7
3	L	207	ALA	3.7
4	H	195	ILE	3.6
3	L	186	LYS	3.6
3	L	177	TYR	3.6
3	L	143	ALA	3.6
3	L	195	VAL	3.5
3	L	159	VAL	3.5
4	H	192	GLN	3.5
3	L	150	ALA	3.4
3	L	194	GLN	3.4
3	L	204	LYS	3.4
4	H	138	LEU	3.3
3	L	135	LEU	3.3
3	L	116	THR	3.3
4	H	160	THR	3.3
3	L	187	SER	3.3
3	L	205	THR	3.2
3	L	192	SER	3.1
4	H	187	SER	3.0
3	L	152	SER	3.0
4	H	154	TRP	2.9

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Mol	Chain	Res	Type	RSRZ
3	L	188	HIS	2.9
3	L	183	GLU	2.8
4	H	182	VAL	2.8
3	L	108	GLN	2.8
4	H	161	SER	2.8
3	L	112	ALA	2.8
3	L	179	SER	2.6
3	L	115	VAL	2.6
4	H	191	THR	2.6
3	L	151	ASP	2.6
2	B	58	LYS	2.6
3	L	136	ILE	2.5
3	L	141	PRO	2.5
4	H	125	ALA	2.5
4	H	126	PRO	2.5
3	L	144	VAL	2.4
4	H	190	GLY	2.4
4	H	212	GLU	2.4
3	L	138	ASP	2.4
3	L	131	THR	2.4
4	H	186	SER	2.3
3	L	111	ALA	2.3
3	L	196	THR	2.2
3	L	145	THR	2.2
3	L	134	CYS	2.1
3	L	171	LYS	2.1
3	L	197	HIS	2.1
3	L	140	TYR	2.1
4	H	121	VAL	2.0
4	H	119	PRO	2.0
4	H	155	ASN	2.0
3	L	56	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
5	NAG	A	509	14/15	0.95	0.14	-0.28	42,52,67,72	0
7	NAG	A	504	14/15	0.97	0.16	-0.60	41,51,63,64	0
7	NAG	A	505	14/15	0.96	0.15	-1.06	49,55,67,70	0
5	NAG	A	502	14/15	0.70	0.34	-	98,112,120,124	0
7	MAN	A	508	11/12	0.87	0.23	-	106,116,121,124	0
5	NAG	A	501	14/15	0.81	0.20	-	71,80,91,96	0
7	MAN	A	507	11/12	0.79	0.25	-	111,117,122,126	0
5	NAG	A	510	14/15	0.89	0.17	-	66,95,99,101	0
7	BMA	A	506	11/12	0.87	0.13	-	82,95,104,111	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(Å ²)	Q<0.9
6	NAG	B	201	14/15	0.85	0.31	7.86	81,97,111,112	0
8	SO4	A	511	5/5	0.92	0.33	5.17	104,107,110,111	0
8	SO4	B	204	5/5	0.88	0.27	3.69	83,93,98,99	0
8	SO4	H	302	5/5	0.93	0.24	3.67	83,87,89,92	0
9	PEG	L	303	7/7	0.94	0.21	2.88	59,60,71,73	0
9	PEG	L	304	7/7	0.87	0.23	2.56	56,68,73,74	0
8	SO4	H	301	5/5	0.90	0.18	0.23	97,97,103,106	0
9	PEG	A	516	7/7	0.90	0.18	0.07	30,45,50,53	0
8	SO4	L	301	5/5	0.97	0.13	-1.86	80,81,83,83	0
8	SO4	B	202	5/5	0.98	0.14	-2.12	56,61,64,64	0
8	SO4	B	203	5/5	0.98	0.13	-2.38	30,36,45,56	0
8	SO4	A	515	5/5	0.94	0.12	-	76,78,82,83	0
8	SO4	H	304	5/5	0.81	0.26	-	117,119,122,122	0
6	NAG	A	503	14/15	0.96	0.15	-	45,51,60,60	0
8	SO4	L	302	5/5	0.87	0.20	-	119,122,123,125	0
8	SO4	H	303	5/5	0.92	0.17	-	103,103,105,109	0
8	SO4	A	512	5/5	0.86	0.22	-	108,109,110,111	0
8	SO4	A	514	5/5	0.92	0.36	-	141,142,142,143	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
8	SO4	A	513	5/5	0.91	0.23	-	122,122,125,126	0

6.5 Other polymers [i](#)

There are no such residues in this entry.