



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 12:44 PM GMT

PDB ID : 4GMS
Title : Crystal structure of heterosubtypic Fab S139/1 in complex with influenza A H3 hemagglutinin
Authors : Lee, P.S.; Ekiert, D.C.; Wilson, I.A.
Deposited on : 2012-08-16
Resolution : 2.95 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

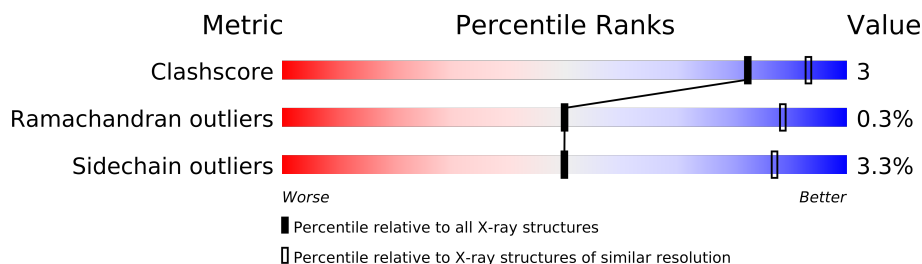
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	FAILED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.95 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))
Clashscore	79885	2029 (3.00-2.92)
Ramachandran outliers	78287	1955 (3.00-2.92)
Sidechain outliers	78261	1958 (3.00-2.92)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	320	
1	C	320	
1	E	320	
2	B	176	
2	D	176	
2	F	176	
3	L	214	
3	M	214	
3	N	214	
4	H	225	
4	I	225	
4	J	225	

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 21460 atoms, of which 0 are hydrogen and 0 are deuterium.

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	316	Total	C	N	O	S	0	0	0
			2432	1521	429	469	13			
1	C	316	Total	C	N	O	S	0	0	0
			2432	1521	429	469	13			
1	E	316	Total	C	N	O	S	0	0	0
			2432	1521	429	469	13			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	GLY	-	EXPRESSION TAG	UNP P03435
C	10	GLY	-	EXPRESSION TAG	UNP P03435
E	10	GLY	-	EXPRESSION TAG	UNP P03435

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	171	Total	C	N	O	S	0	0	0
			1384	859	244	275	6			
2	D	171	Total	C	N	O	S	0	0	0
			1384	859	244	275	6			
2	F	171	Total	C	N	O	S	0	0	0
			1384	859	244	275	6			

- Molecule 3 is a protein called Fab S139/1 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	211	Total	C	N	O	S	0	0	0
			1645	1022	275	341	7			
3	M	156	Total	C	N	O	S	0	0	0
			1209	758	195	250	6			

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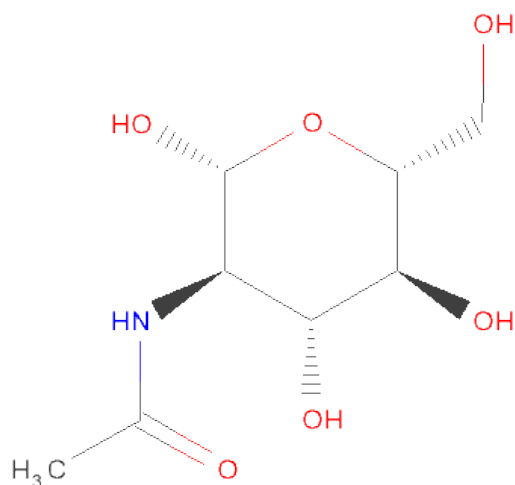
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	213	Total	C	N	O	S	0	0	0
			1662	1031	278	346	7			

- Molecule 4 is a protein called Fab S139/1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	218	Total	C	N	O	S	0	0	0
			1665	1062	267	329	7			
4	I	186	Total	C	N	O	S	0	0	0
			1429	918	226	280	5			
4	J	212	Total	C	N	O	S	0	0	0
			1629	1043	261	319	6			

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



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		
5	I	1	Total	C	N	O	0	0
			14	8	1	5		
5	J	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	GLY	-	EXPRESSION TAG	UNP P03435
A	10	GLY	-	EXPRESSION TAG	UNP P03435
C	10	GLY	-	EXPRESSION TAG	UNP P03435
E	10	GLY	-	EXPRESSION TAG	UNP P03435

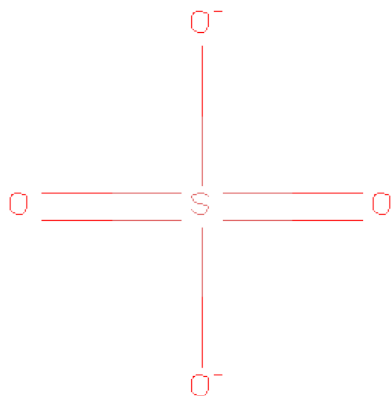
- Molecule 7 is a polymer of unknown type called SUGAR (5-MER).

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

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	GLY	-	EXPRESSION TAG	UNP P03435
C	10	GLY	-	EXPRESSION TAG	UNP P03435
E	10	GLY	-	EXPRESSION TAG	UNP P03435

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



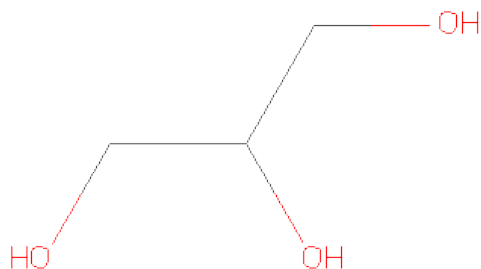
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	B	1	Total	O	S	0	0
			5	4	1		
8	B	1	Total	O	S	0	0
			5	4	1		
8	B	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	O	S	0	0
			5	4	1		
8	D	1	Total	O	S	0	0
			5	4	1		
8	D	1	Total	O	S	0	0
			5	4	1		
8	E	1	Total	O	S	0	0
			5	4	1		
8	F	1	Total	O	S	0	0
			5	4	1		
8	H	1	Total	O	S	0	0
			5	4	1		
8	I	1	Total	O	S	0	0
			5	4	1		
8	J	1	Total	O	S	0	0
			5	4	1		

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



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

- Molecule 10 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	C	3	Total	C	N	O	0	0
			39	22	2	15		
10	E	3	Total	C	N	O	0	0
			39	22	2	15		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	10	GLY	-	EXPRESSION TAG	UNP P03435
E	10	GLY	-	EXPRESSION TAG	UNP P03435

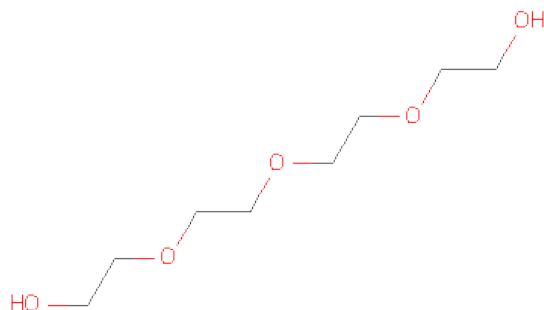
- Molecule 11 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	E	4	Total	C	N	O	0	0
			50	28	2	20		
11	E	4	Total	C	N	O	0	0
			50	28	2	20		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	10	GLY	-	EXPRESSION TAG	UNP P03435
E	10	GLY	-	EXPRESSION TAG	UNP P03435

- Molecule 12 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	E	1	Total	C	O	0	0
			13	8	5		

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	5	Total	O	0	0
			5	5		
13	C	6	Total	O	0	0
			6	6		
13	E	7	Total	O	0	0
			7	7		
13	L	1	Total	O	0	0
			1	1		
13	H	2	Total	O	0	0
			2	2		
13	M	3	Total	O	0	0
			3	3		
13	I	1	Total	O	0	0
			1	1		
13	N	4	Total	O	0	0
			4	4		
13	J	2	Total	O	0	0
			2	2		

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 ($RSRZ > 2$). 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.

Note EDS failed to run properly.

- Molecule 1: Hemagglutinin HA1 chain

Chain A: 



- Molecule 1: Hemagglutinin HA1 chain

Chain C: 



- Molecule 1: Hemagglutinin HA1 chain

Chain E: 



- Molecule 2: Hemagglutinin HA2 chain

Chain B: 



- Molecule 2: Hemagglutinin HA2 chain

Chain D: 



- Molecule 2: Hemagglutinin HA2 chain

Chain F: 



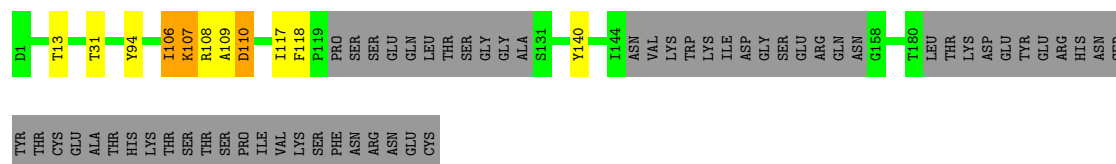
- Molecule 3: Fab S139/1 light chain

Chain L:



- Molecule 3: Fab S139/1 light chain

Chain M:



- Molecule 3: Fab S139/1 light chain

Chain N:



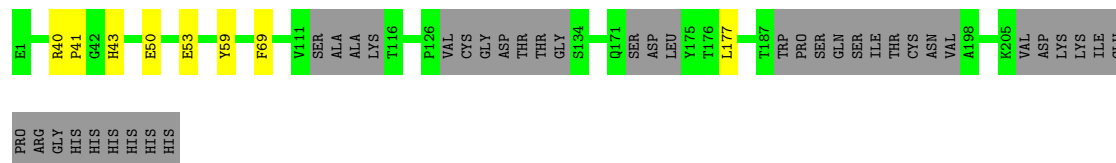
- Molecule 4: Fab S139/1 heavy chain

Chain H:



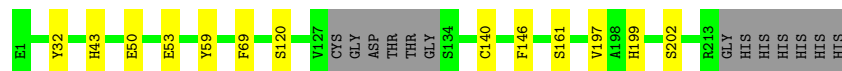
- Molecule 4: Fab S139/1 heavy chain

Chain I:



- Molecule 4: Fab S139/1 heavy chain

Chain J:



4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	225.51Å 112.94Å 196.97Å 90.00° 118.76° 90.00°	Depositor
Resolution (Å)	48.41 – 2.95	Depositor
% Data completeness (in resolution range)	99.8 (48.41-2.95)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.96Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2.869)	Depositor
R, R_{free}	0.207 , 0.233	Depositor
Wilson B-factor (Å ²)	89.9	Xtriage
Anisotropy	0.324	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 91260 reflections	Xtriage
Total number of atoms	21460	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, BMA, NAG, PG4, SO4, PCA, MAN

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	0/2488	0.63	0/3385
1	C	0.50	0/2488	0.61	0/3385
1	E	0.53	0/2488	0.64	0/3385
2	B	0.50	0/1408	0.61	0/1892
2	D	0.50	0/1408	0.59	0/1892
2	F	0.54	0/1408	0.59	0/1892
3	L	0.38	0/1681	0.54	0/2283
3	M	0.38	0/1234	0.53	0/1676
3	N	0.37	0/1698	0.55	0/2306
4	H	0.38	0/1705	0.56	0/2335
4	I	0.33	0/1461	0.53	0/1996
4	J	0.37	0/1668	0.53	0/2283
All	All	0.45	0/21135	0.58	0/28710

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
4	I	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	I	41	PRO	Mainchain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2432	0	0	7	0
1	C	2432	0	0	9	0
1	E	2432	0	0	5	0
2	B	1384	0	0	8	0
2	D	1384	0	0	6	0
2	F	1384	0	0	7	0
3	L	1645	0	0	7	0
3	M	1209	0	0	9	0
3	N	1662	0	0	5	0
4	H	1665	0	0	4	0
4	I	1429	0	0	3	0
4	J	1629	0	0	5	0
5	A	28	0	0	0	0
5	B	14	0	0	0	0
5	C	28	0	0	0	0
5	D	14	0	0	0	0
5	F	14	0	0	0	0
5	I	14	0	0	0	0
5	J	14	0	0	0	0
6	A	56	0	0	0	0
6	C	28	0	0	0	0
6	E	28	0	0	0	0
6	H	28	0	0	0	0
7	A	61	0	0	0	0
7	C	61	0	0	0	0
7	E	61	0	0	0	0
8	A	25	0	0	1	0
8	B	15	0	0	1	0
8	C	15	0	0	2	0
8	D	10	0	0	0	0
8	E	5	0	0	0	0
8	F	5	0	0	0	0
8	H	5	0	0	0	0
8	I	5	0	0	0	0
8	J	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	B	6	0	8	1	0
9	D	6	0	8	1	0
10	C	39	0	0	0	0
10	E	39	0	0	1	0
11	E	100	0	0	1	0
12	E	13	0	18	0	0
13	A	5	0	0	0	0
13	C	6	0	0	0	0
13	E	7	0	0	0	0
13	H	2	0	0	0	0
13	I	1	0	0	0	0
13	J	2	0	0	0	0
13	L	1	0	0	0	0
13	M	3	0	0	0	0
13	N	4	0	0	0	0
All	All	21460	0	34	67	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

The worst 5 of 67 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:54:ARG:NH1	9:D:204:GOL:O3	2.27	0.68
8:C:514:SO4:O3	4:I:59:TYR:OH	2.15	0.64
3:M:107:LYS:C	3:M:107:LYS:CD	2.68	0.62
10:E:506:NAG:O3	10:E:507:BMA:O5	2.18	0.62
1:A:104:ASP:N	8:A:514:SO4:O3	2.37	0.58

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	314/320 (98%)	305 (97%)	7 (2%)	2 (1%)	33 79

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	314/320 (98%)	306 (98%)	6 (2%)	2 (1%)	33	79
1	E	314/320 (98%)	306 (98%)	6 (2%)	2 (1%)	33	79
2	B	169/176 (96%)	164 (97%)	5 (3%)	0	100	100
2	D	169/176 (96%)	165 (98%)	4 (2%)	0	100	100
2	F	169/176 (96%)	165 (98%)	4 (2%)	0	100	100
3	L	209/214 (98%)	200 (96%)	9 (4%)	0	100	100
3	M	150/214 (70%)	140 (93%)	9 (6%)	1 (1%)	30	76
3	N	211/214 (99%)	203 (96%)	8 (4%)	0	100	100
4	H	216/225 (96%)	211 (98%)	5 (2%)	0	100	100
4	I	176/225 (78%)	170 (97%)	6 (3%)	0	100	100
4	J	208/225 (92%)	197 (95%)	11 (5%)	0	100	100
All	All	2619/2805 (93%)	2532 (97%)	80 (3%)	7 (0%)	50	88

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	VAL
1	C	196	VAL
1	E	196	VAL
1	A	62	ILE
1	C	62	ILE

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	276/280 (99%)	269 (98%)	7 (2%)	60	91
1	C	276/280 (99%)	268 (97%)	8 (3%)	55	89
1	E	276/280 (99%)	268 (97%)	8 (3%)	55	89
2	B	145/149 (97%)	139 (96%)	6 (4%)	41	82
2	D	145/149 (97%)	139 (96%)	6 (4%)	41	82
2	F	145/149 (97%)	140 (97%)	5 (3%)	49	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	L	189/192 (98%)	183 (97%)	6 (3%)	51	87
3	M	139/192 (72%)	134 (96%)	5 (4%)	47	85
3	N	191/192 (100%)	181 (95%)	10 (5%)	32	74
4	H	187/193 (97%)	181 (97%)	6 (3%)	51	87
4	I	159/193 (82%)	155 (98%)	4 (2%)	60	91
4	J	183/193 (95%)	177 (97%)	6 (3%)	50	87
All	All	2311/2442 (95%)	2234 (97%)	77 (3%)	50	87

5 of 77 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	174	SER
3	L	175	MET
4	J	43	HIS
2	F	12	ASN
2	F	144	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

3 non-standard protein/DNA/RNA residues 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	PCA	H	1	4	8,8,9	6.81	3 (37%)	8,10,12	8.03	4 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PCA	I	1	4	8,8,9	6.76	3 (37%)	8,10,12	7.22	4 (50%)
4	PCA	J	1	4	8,8,9	6.73	4 (50%)	8,10,12	7.32	4 (50%)

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	PCA	H	1	4	-	0/0/11/13	0/1/1/1
4	PCA	I	1	4	-	0/0/11/13	0/1/1/1
4	PCA	J	1	4	-	0/0/11/13	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1	PCA	O-C	18.18	1.23	1.11
4	I	1	PCA	O-C	18.01	1.23	1.11
4	J	1	PCA	O-C	17.83	1.23	1.11
4	J	1	PCA	CD-N	6.03	1.47	1.34
4	I	1	PCA	CD-N	5.73	1.46	1.34

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	PCA	C-CA-N	-17.31	106.80	110.71
4	J	1	PCA	C-CA-N	-14.40	107.46	110.71
4	I	1	PCA	CA-N-CD	-14.33	103.17	114.37
4	J	1	PCA	CA-N-CD	-14.14	103.32	114.37
4	H	1	PCA	CA-N-CD	-14.02	103.41	114.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

39 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
6	NAG	A	502	1,6	12,14,15	0.76	1 (8%)	15,19,21	0.92	0
6	NAG	A	503	6	12,14,15	0.71	1 (8%)	15,19,21	0.89	1 (6%)
7	NAG	A	505	1,7	12,14,15	0.70	1 (8%)	15,19,21	0.80	1 (6%)
7	NAG	A	506	7	12,14,15	0.73	1 (8%)	15,19,21	1.33	1 (6%)
7	BMA	A	507	7	10,11,12	0.82	1 (10%)	11,15,17	1.34	1 (9%)
7	MAN	A	508	7	10,11,12	0.84	1 (10%)	11,15,17	1.09	1 (9%)
7	MAN	A	509	7	10,11,12	0.86	1 (10%)	11,15,17	1.88	3 (27%)
6	NAG	A	510	1,6	12,14,15	0.61	0	15,19,21	1.00	0
6	NAG	A	511	6	12,14,15	0.62	0	15,19,21	0.78	0
6	NAG	C	502	1,6	12,14,15	0.79	1 (8%)	15,19,21	1.00	0
6	NAG	C	503	6	12,14,15	0.69	1 (8%)	15,19,21	0.85	1 (6%)
7	NAG	C	505	1,7	12,14,15	0.71	1 (8%)	15,19,21	0.84	1 (6%)
7	NAG	C	506	7	12,14,15	0.67	0	15,19,21	1.38	1 (6%)
7	BMA	C	507	7	10,11,12	0.90	0	11,15,17	1.63	1 (9%)
7	MAN	C	508	7	10,11,12	0.80	1 (10%)	11,15,17	1.15	1 (9%)
7	MAN	C	509	7	10,11,12	0.83	0	11,15,17	1.54	3 (27%)
10	NAG	C	510	1,10	12,14,15	0.66	0	15,19,21	0.80	0
10	NAG	C	511	10	12,14,15	0.55	0	15,19,21	0.87	1 (6%)
10	BMA	C	512	10	10,11,12	0.79	0	11,15,17	1.76	1 (9%)
11	NAG	E	501	11,1	12,14,15	0.70	0	15,19,21	1.02	1 (6%)
11	NAG	E	502	11	12,14,15	0.73	0	15,19,21	1.25	1 (6%)
11	BMA	E	503	11	10,11,12	0.81	1 (10%)	11,15,17	1.24	1 (9%)
11	MAN	E	504	11	10,11,12	0.83	1 (10%)	11,15,17	0.70	0
10	NAG	E	505	1,10	12,14,15	0.93	1 (8%)	15,19,21	0.99	0
10	NAG	E	506	10	12,14,15	0.68	1 (8%)	15,19,21	0.89	1 (6%)
10	BMA	E	507	10	10,11,12	0.70	0	11,15,17	1.76	1 (9%)
6	NAG	E	508	1,6	12,14,15	0.65	0	15,19,21	1.05	2 (13%)
6	NAG	E	509	6	12,14,15	0.58	0	15,19,21	1.41	2 (13%)
7	NAG	E	510	1,7	12,14,15	0.74	0	15,19,21	0.84	0
7	NAG	E	511	7	12,14,15	0.79	1 (8%)	15,19,21	1.24	1 (6%)
7	BMA	E	512	7	10,11,12	0.86	0	11,15,17	1.52	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MAN	E	513	7	10,11,12	0.87	1 (10%)	11,15,17	0.99	0
7	MAN	E	514	7	10,11,12	0.78	0	11,15,17	1.65	2 (18%)
11	NAG	E	515	11,1	12,14,15	0.63	0	15,19,21	0.92	0
11	NAG	E	516	11	12,14,15	0.66	0	15,19,21	0.90	1 (6%)
11	BMA	E	517	11	10,11,12	0.73	0	11,15,17	1.58	1 (9%)
11	MAN	E	518	11	10,11,12	0.78	0	11,15,17	0.78	0
6	NAG	H	301	4,6	12,14,15	0.77	1 (8%)	15,19,21	0.84	0
6	NAG	H	302	6	12,14,15	0.62	0	15,19,21	0.98	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	502	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	503	6	-	0/6/23/26	0/1/1/1
7	NAG	A	505	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	506	7	-	0/6/23/26	0/1/1/1
7	BMA	A	507	7	-	0/2/19/22	0/1/1/1
7	MAN	A	508	7	-	0/2/19/22	0/1/1/1
7	MAN	A	509	7	-	0/2/19/22	0/1/1/1
6	NAG	A	510	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	511	6	-	0/6/23/26	0/1/1/1
6	NAG	C	502	1,6	-	0/6/23/26	0/1/1/1
6	NAG	C	503	6	-	0/6/23/26	0/1/1/1
7	NAG	C	505	1,7	-	0/6/23/26	0/1/1/1
7	NAG	C	506	7	-	0/6/23/26	0/1/1/1
7	BMA	C	507	7	-	0/2/19/22	0/1/1/1
7	MAN	C	508	7	-	0/2/19/22	0/1/1/1
7	MAN	C	509	7	-	0/2/19/22	0/1/1/1
10	NAG	C	510	1,10	-	0/6/23/26	0/1/1/1
10	NAG	C	511	10	-	0/6/23/26	0/1/1/1
10	BMA	C	512	10	-	0/2/19/22	0/1/1/1
11	NAG	E	501	11,1	-	0/6/23/26	0/1/1/1
11	NAG	E	502	11	-	0/6/23/26	0/1/1/1
11	BMA	E	503	11	-	0/2/19/22	0/1/1/1
11	MAN	E	504	11	-	0/2/19/22	0/1/1/1
10	NAG	E	505	1,10	-	0/6/23/26	0/1/1/1
10	NAG	E	506	10	-	0/6/23/26	0/1/1/1
10	BMA	E	507	10	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	E	508	1,6	-	0/6/23/26	0/1/1/1
6	NAG	E	509	6	-	0/6/23/26	0/1/1/1
7	NAG	E	510	1,7	-	0/6/23/26	0/1/1/1
7	NAG	E	511	7	-	0/6/23/26	0/1/1/1
7	BMA	E	512	7	-	0/2/19/22	0/1/1/1
7	MAN	E	513	7	-	0/2/19/22	0/1/1/1
7	MAN	E	514	7	-	0/2/19/22	0/1/1/1
11	NAG	E	515	11,1	-	0/6/23/26	0/1/1/1
11	NAG	E	516	11	-	0/6/23/26	0/1/1/1
11	BMA	E	517	11	-	0/2/19/22	0/1/1/1
11	MAN	E	518	11	-	0/2/19/22	0/1/1/1
6	NAG	H	301	4,6	-	0/6/23/26	0/1/1/1
6	NAG	H	302	6	-	0/6/23/26	0/1/1/1

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	E	505	NAG	O5-C5	-2.81	1.40	1.45
6	H	301	NAG	O5-C5	-2.43	1.40	1.45
6	C	502	NAG	O5-C5	-2.34	1.41	1.45
7	E	513	MAN	O5-C5	-2.26	1.41	1.45
6	A	502	NAG	O5-C5	-2.24	1.41	1.45

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	E	507	BMA	O5-C5-C6	5.60	112.86	106.98
10	C	512	BMA	O5-C5-C6	5.32	112.56	106.98
11	E	517	BMA	O5-C5-C6	4.87	112.09	106.98
7	A	509	MAN	O5-C5-C6	-4.78	101.97	106.98
7	A	506	NAG	O5-C5-C6	4.52	111.73	106.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry

30 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$
5	NAG	A	501	1	12,14,15	0.66	0	15,19,21	0.75	0
5	NAG	A	504	1	12,14,15	0.66	1 (8%)	15,19,21	1.10	2 (13%)
8	SO4	A	512	-	4,4,4	0.17	0	6,6,6	0.07	0
8	SO4	A	513	-	4,4,4	0.14	0	6,6,6	0.45	0
8	SO4	A	514	-	4,4,4	0.09	0	6,6,6	0.15	0
8	SO4	A	515	-	4,4,4	0.10	0	6,6,6	0.33	0
8	SO4	A	516	-	4,4,4	0.08	0	6,6,6	0.39	0
5	NAG	B	201	2	12,14,15	0.61	0	15,19,21	1.00	2 (13%)
8	SO4	B	202	-	4,4,4	0.22	0	6,6,6	0.19	0
8	SO4	B	203	-	4,4,4	0.23	0	6,6,6	0.07	0
8	SO4	B	204	-	4,4,4	0.18	0	6,6,6	0.22	0
9	GOL	B	205	-	5,5,5	0.44	0	5,5,5	0.77	0
5	NAG	C	501	1	12,14,15	0.63	0	15,19,21	0.80	0
5	NAG	C	504	1	12,14,15	0.63	0	15,19,21	1.11	2 (13%)
8	SO4	C	513	-	4,4,4	0.20	0	6,6,6	0.15	0
8	SO4	C	514	-	4,4,4	0.18	0	6,6,6	0.22	0
8	SO4	C	515	-	4,4,4	0.07	0	6,6,6	0.50	0
5	NAG	D	201	2	12,14,15	0.65	0	15,19,21	1.00	2 (13%)
8	SO4	D	202	-	4,4,4	0.20	0	6,6,6	0.19	0
8	SO4	D	203	-	4,4,4	0.17	0	6,6,6	0.35	0
9	GOL	D	204	-	5,5,5	0.46	0	5,5,5	0.80	0
8	SO4	E	519	-	4,4,4	0.29	0	6,6,6	0.53	0
12	PG4	E	520	-	12,12,12	0.54	0	11,11,11	0.29	0
5	NAG	F	201	2	12,14,15	0.58	0	15,19,21	0.83	1 (6%)
8	SO4	F	202	-	4,4,4	0.11	0	6,6,6	0.28	0
8	SO4	H	303	-	4,4,4	0.18	0	6,6,6	0.19	0
5	NAG	I	301	4	12,14,15	0.57	0	15,19,21	1.08	1 (6%)
8	SO4	I	302	-	4,4,4	0.17	0	6,6,6	0.18	0
5	NAG	J	301	4	12,14,15	0.56	0	15,19,21	1.22	1 (6%)
8	SO4	J	302	-	4,4,4	0.18	0	6,6,6	0.14	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
5	NAG	A	501	1	-	0/6/23/26	0/1/1/1
5	NAG	A	504	1	-	0/6/23/26	0/1/1/1
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
8	SO4	A	516	-	-	0/0/0/0	0/0/0/0
5	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
9	GOL	B	205	-	-	0/4/4/4	0/0/0/0
5	NAG	C	501	1	-	0/6/23/26	0/1/1/1
5	NAG	C	504	1	-	0/6/23/26	0/1/1/1
8	SO4	C	513	-	-	0/0/0/0	0/0/0/0
8	SO4	C	514	-	-	0/0/0/0	0/0/0/0
8	SO4	C	515	-	-	0/0/0/0	0/0/0/0
5	NAG	D	201	2	-	0/6/23/26	0/1/1/1
8	SO4	D	202	-	-	0/0/0/0	0/0/0/0
8	SO4	D	203	-	-	0/0/0/0	0/0/0/0
9	GOL	D	204	-	-	0/4/4/4	0/0/0/0
8	SO4	E	519	-	-	0/0/0/0	0/0/0/0
12	PG4	E	520	-	-	0/10/10/10	0/0/0/0
5	NAG	F	201	2	-	0/6/23/26	0/1/1/1
8	SO4	F	202	-	-	0/0/0/0	0/0/0/0
8	SO4	H	303	-	-	0/0/0/0	0/0/0/0
5	NAG	I	301	4	-	0/6/23/26	0/1/1/1
8	SO4	I	302	-	-	0/0/0/0	0/0/0/0
5	NAG	J	301	4	-	0/6/23/26	0/1/1/1
8	SO4	J	302	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	504	NAG	O5-C5	-2.01	1.41	1.45

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	301	NAG	O5-C5-C6	3.64	110.80	106.98
5	J	301	NAG	O5-C5-C6	3.30	110.44	106.98
5	C	504	NAG	O5-C5-C6	3.21	110.35	106.98
5	A	504	NAG	O5-C5-C6	2.97	110.09	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	201	NAG	O5-C5-C6	2.66	109.77	106.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

EDS failed to run properly - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS failed to run properly - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.