



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:56 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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

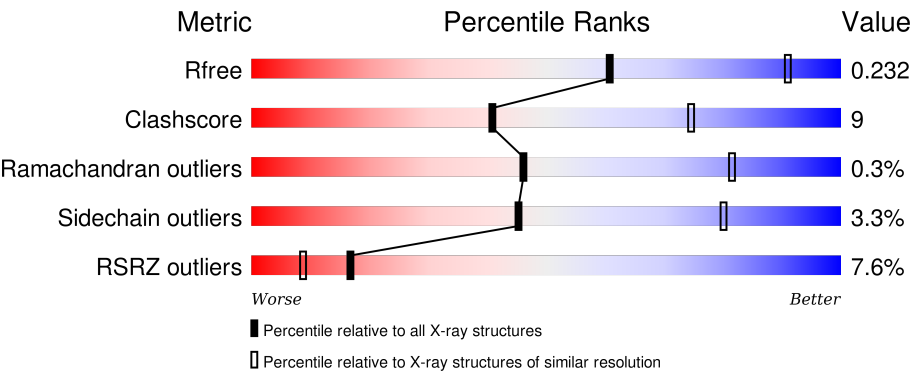
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 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))
R <sub>free</sub>	91344	2184 (3.00-2.92)
Clashscore	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)
RSRZ outliers	91569	2201 (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. 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 <=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	320	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>81%17%..</div></div>
1	C	320	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>78%19%..</div></div>
1	E	320	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>82%16%..</div></div>
2	B	176	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>81%15%..</div></div>
2	D	176	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>77%19%..</div></div>

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Mol	Chain	Length	Quality of chain
2	F	176	
3	L	214	
3	M	214	
3	N	214	
4	H	225	
4	I	225	
4	J	225	

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
12	PG4	E	520	-	-	-	X
5	NAG	B	201	-	-	-	X
8	SO4	B	203	-	-	X	-
8	SO4	C	515	-	-	-	X
9	GOL	B	205	-	-	-	X

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 21460 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	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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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		

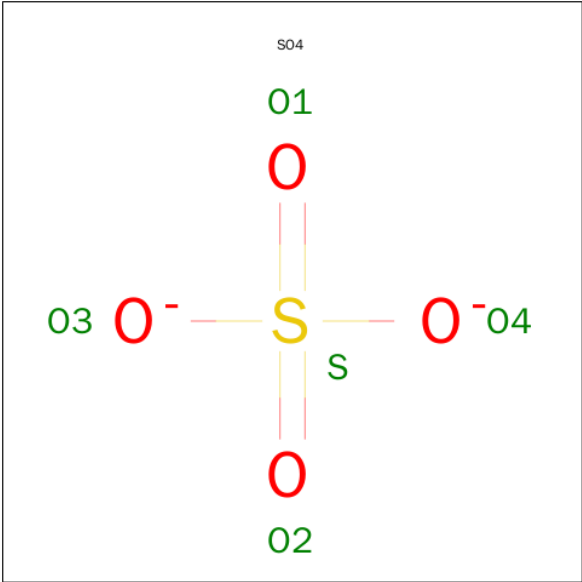
- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

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		

- 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		

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



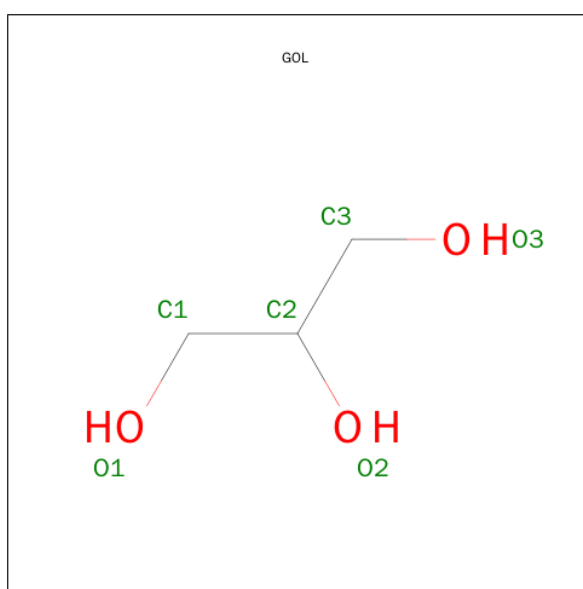
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	B	1	Total	O	S	0	0
			5	4	1		
8	B	1	Total	O	S	0	0
			5	4	1		
8	B	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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).

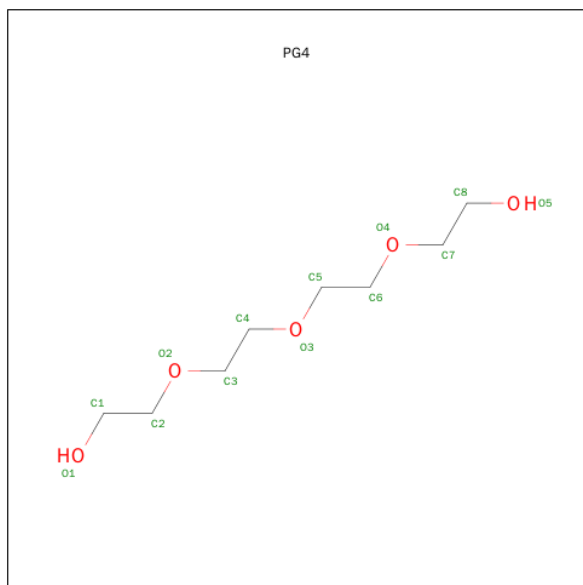
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	C	3	Total	C	N	O	0	0
			39	22	2	15		
10	E	3	Total	C	N	O	0	0
			39	22	2	15		

- 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		

- Molecule 12 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



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		

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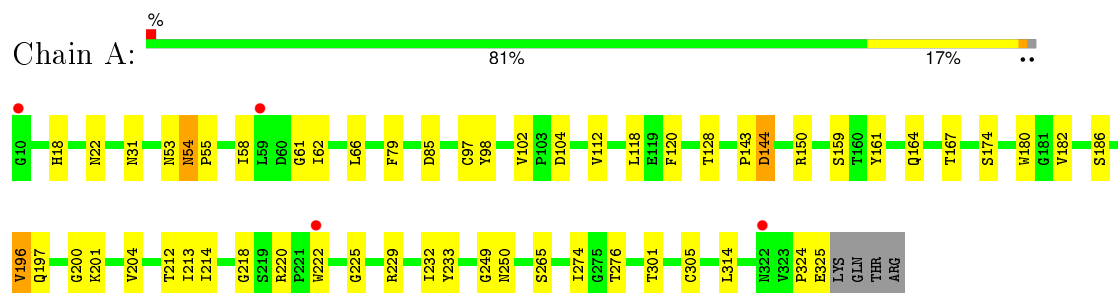
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	N	4	Total	O	0	0
			4	4		
13	J	2	Total	O	0	0
			2	2		

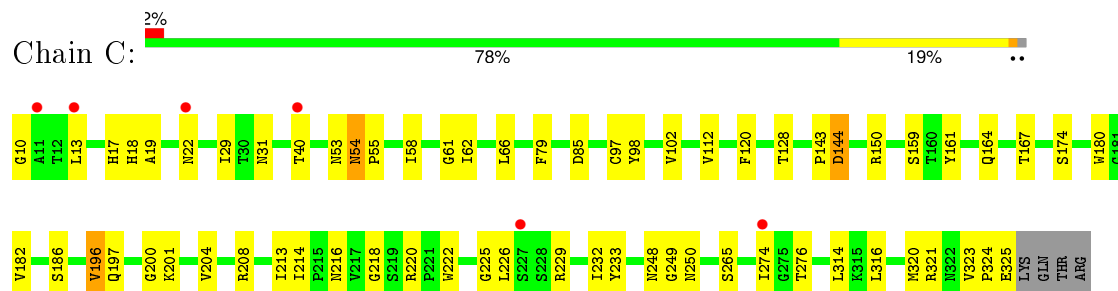
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

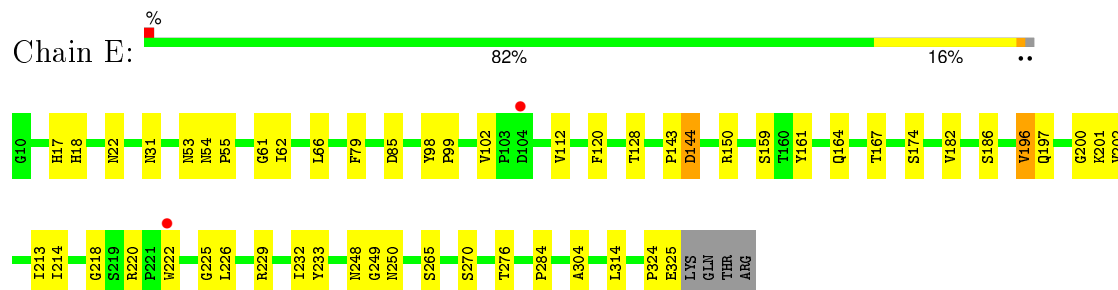
- Molecule 1: Hemagglutinin HA1 chain



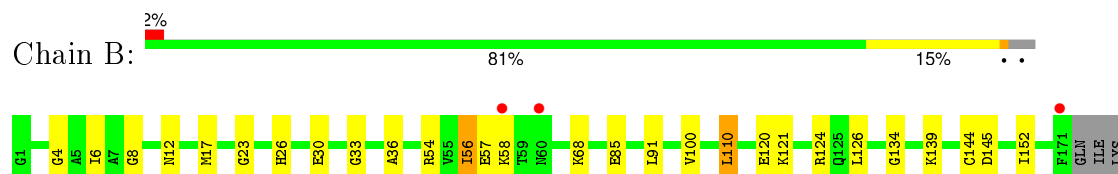
- Molecule 1: Hemagglutinin HA1 chain



- Molecule 1: Hemagglutinin HA1 chain

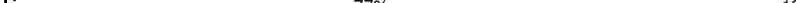


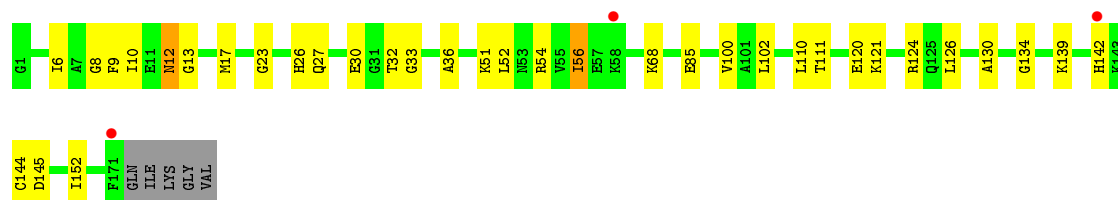
- Molecule 2: Hemagglutinin HA2 chain



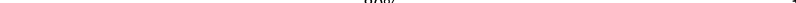
GLY	VAL
1	1
2	2
3	3
4	4
5	5
6	6
7	7
8	8
9	9
10	10
11	11
12	12
13	13
14	14
15	15
16	16
17	17
18	18
19	19
20	20
21	21
22	22
23	23
24	24
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82	82
83	83
84	84
85	85
86	86
87	87
88	88
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94	94
95	95
96	96
97	97
98	98
99	99
100	100

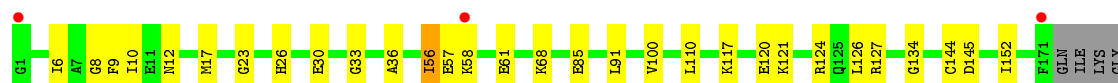
- Molecule 2: Hemagglutinin HA2 chain

Chain D:  2% 77% 19%



- Molecule 2: Hemagglutinin HA2 chain

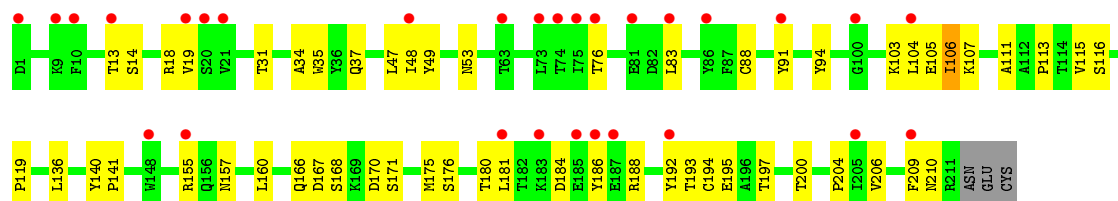
Chain F:  2% 80% 16%



VAL

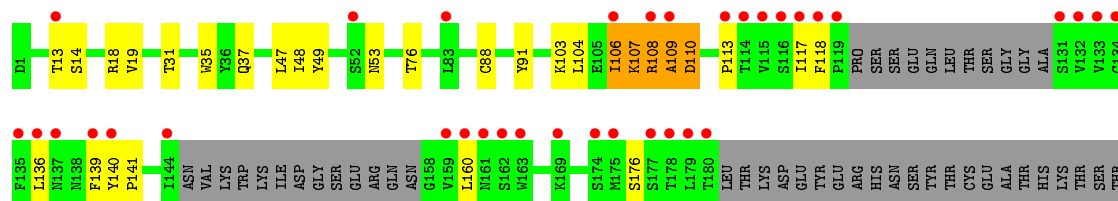
- Molecule 3: Fab S139/1 light chain

Chain L:  14% 73% 25%



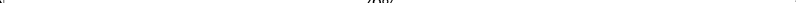
- Molecule 3: Fab S139/1 light chain

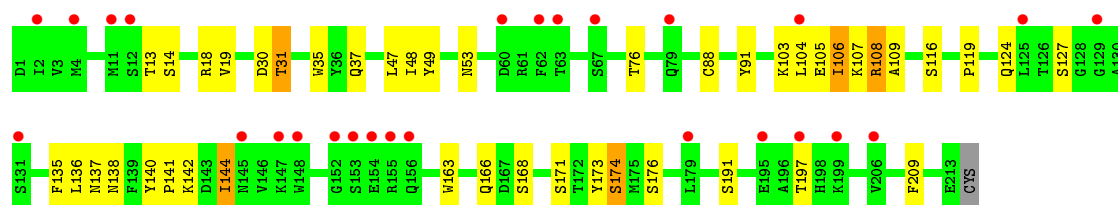
Chain M:  16% 59% 12% 1%



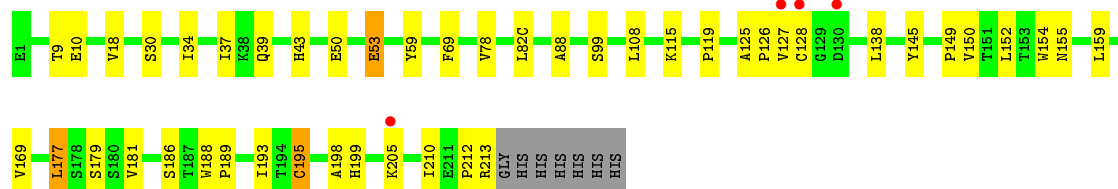
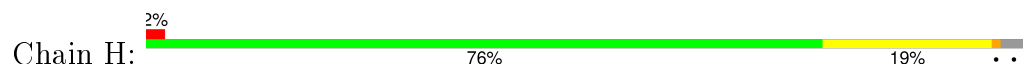
SER  
PRO  
ILE  
VAL  
LYS  
SER  
PHE  
ASN  
ARG  
ASN  
GLU  
CYS

- Molecule 3: Fab S139/1 light chain

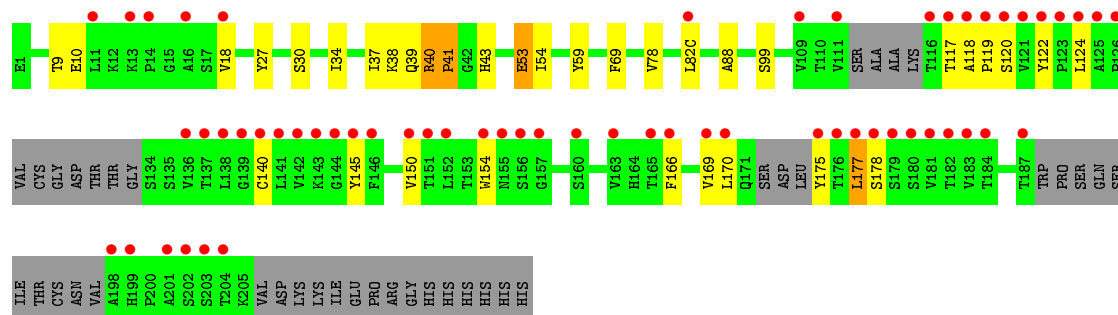
Chain N:  12% 79% 18%



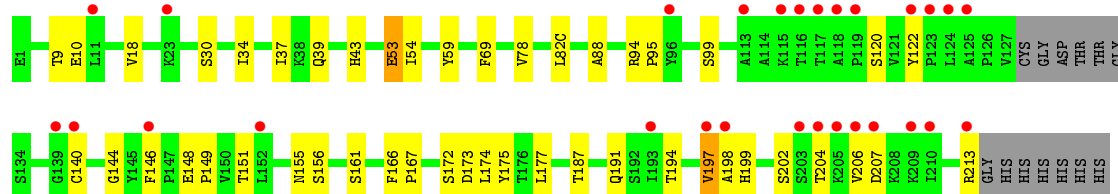
• Molecule 4: Fab S139/1 heavy chain



• Molecule 4: Fab S139/1 heavy chain



• Molecule 4: Fab S139/1 heavy chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	225.51 Å 112.94 Å 196.97 Å 90.00° 118.76° 90.00°	Depositor
Resolution (Å)	48.41 – 2.95 48.41 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.41-2.95) 99.8 (48.41-2.95)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.42 (at 2.96 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, $R_{free}$	0.207 , 0.233 0.208 , 0.232	Depositor DCC
$R_{free}$ test set	4572 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	89.9	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 69.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 91260 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	21460	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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: 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 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	2432	0	2375	35	0
1	C	2432	0	2375	47	0
1	E	2432	0	2375	38	0
2	B	1384	0	1305	21	0
2	D	1384	0	1305	28	0
2	F	1384	0	1305	24	0
3	L	1645	0	1563	41	0
3	M	1209	0	1148	34	0
3	N	1662	0	1575	40	0
4	H	1665	0	1612	38	0
4	I	1429	0	1375	27	0
4	J	1629	0	1582	31	0
5	A	28	0	26	0	0
5	B	14	0	13	0	0
5	C	28	0	26	0	0
5	D	14	0	13	0	0
5	F	14	0	13	0	0
5	I	14	0	13	0	0
5	J	14	0	13	0	0
6	A	56	0	50	0	0
6	C	28	0	25	0	0
6	E	28	0	25	0	0
6	H	28	0	25	0	0
7	A	61	0	52	1	0
7	C	61	0	52	1	0
7	E	61	0	52	1	0
8	A	25	0	0	1	0
8	B	15	0	0	2	0
8	C	15	0	0	0	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	1	0
8	J	5	0	0	0	0
9	B	6	0	8	1	0
9	D	6	0	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	C	39	0	34	0	0
10	E	39	0	34	1	0
11	E	100	0	86	0	0
12	E	13	0	18	1	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	20481	361	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 9.

All (361) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:107:LYS:HB2	3:M:140:TYR:OH	1.72	0.90
2:D:124:ARG:HD3	2:F:134:GLY:HA2	1.64	0.79
3:N:108:ARG:HG2	3:N:108:ARG:HH11	1.48	0.79
3:N:13:THR:O	3:N:106:ILE:HD13	1.87	0.75
3:L:13:THR:O	3:L:106:ILE:HD13	1.88	0.73
2:B:124:ARG:HD3	2:D:134:GLY:HA2	1.72	0.72
3:M:140:TYR:CD1	3:M:141:PRO:HA	2.24	0.72
2:B:17:MET:HE1	2:B:36:ALA:HA	1.70	0.72
2:B:134:GLY:HA2	2:F:124:ARG:HD3	1.70	0.72
2:F:17:MET:HE1	2:F:36:ALA:HA	1.72	0.70
3:M:13:THR:O	3:M:106:ILE:HD13	1.90	0.70
2:D:54:ARG:NH1	9:D:204:GOL:O3	2.27	0.68
2:B:17:MET:HE1	2:B:23:GLY:HA3	1.76	0.68
1:E:222:TRP:CZ2	1:E:225:GLY:HA2	2.28	0.67
4:I:140:CYS:HB2	4:I:154:TRP:CH2	2.30	0.67
1:A:222:TRP:CZ2	1:A:225:GLY:HA2	2.31	0.66
2:D:17:MET:HE1	2:D:23:GLY:HA3	1.77	0.65
1:A:249:GLY:O	1:A:250:ASN:HB2	1.97	0.65
1:C:222:TRP:CZ2	1:C:225:GLY:HA2	2.31	0.65
1:C:226:LEU:HD22	4:I:54:ILE:HG22	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:199:HIS:ND1	4:J:202:SER:HB2	2.11	0.65
3:N:140:TYR:CD1	3:N:141:PRO:HA	2.32	0.65
2:D:17:MET:HE1	2:D:36:ALA:HA	1.77	0.64
2:B:30:GLU:OE2	2:B:145:ASP:HB2	1.98	0.64
1:C:161:TYR:CZ	1:C:249:GLY:HA2	2.32	0.64
1:E:161:TYR:CZ	1:E:249:GLY:HA2	2.33	0.63
1:A:161:TYR:CZ	1:A:249:GLY:HA2	2.32	0.63
3:M:160:LEU:HG	4:I:169:VAL:HG11	1.81	0.63
2:F:17:MET:HE1	2:F:23:GLY:HA3	1.80	0.63
1:C:66:LEU:HD21	1:C:112:VAL:HG12	1.80	0.63
4:H:126:PRO:HD3	4:H:138:LEU:CD2	2.29	0.63
4:H:154:TRP:CZ3	4:H:195:CYS:HB3	2.34	0.63
1:E:53:ASN:HD21	1:E:276:THR:HG22	1.63	0.63
3:M:107:LYS:C	3:M:107:LYS:CD	2.68	0.62
4:J:30:SER:HB2	4:J:53:GLU:HG2	1.80	0.62
1:A:66:LEU:HD21	1:A:112:VAL:HG12	1.81	0.62
1:C:249:GLY:O	1:C:250:ASN:HB2	1.99	0.62
1:A:53:ASN:HD21	1:A:276:THR:HG22	1.66	0.61
4:H:152:LEU:HD21	4:H:179:SER:CB	2.30	0.61
4:H:30:SER:HB2	4:H:53:GLU:HG2	1.81	0.61
2:F:30:GLU:OE2	2:F:145:ASP:HB2	2.01	0.61
2:D:30:GLU:OE2	2:D:145:ASP:HB2	2.01	0.60
4:I:30:SER:HB2	4:I:53:GLU:HG2	1.82	0.60
1:C:182:VAL:HG21	1:C:213:ILE:CG2	2.32	0.60
4:H:177:LEU:HD12	4:H:177:LEU:C	2.22	0.60
1:C:220:ARG:HD3	1:C:229:ARG:CG	2.31	0.60
1:E:66:LEU:HD21	1:E:112:VAL:HG12	1.83	0.60
1:C:53:ASN:HD21	1:C:276:THR:HG22	1.65	0.60
1:E:220:ARG:HD3	1:E:229:ARG:CG	2.32	0.59
4:I:177:LEU:C	4:I:177:LEU:HD12	2.23	0.59
1:C:102:VAL:HG22	1:C:232:ILE:HB	1.85	0.59
1:E:249:GLY:O	1:E:250:ASN:HB2	2.02	0.59
1:C:220:ARG:HD3	1:C:229:ARG:HG3	1.84	0.59
3:N:105:GLU:HG3	3:N:173:TYR:OH	2.02	0.58
3:L:19:VAL:HG21	3:L:104:LEU:HD11	1.85	0.58
3:L:106:ILE:HG22	3:L:166:GLN:HE22	1.68	0.58
4:J:148:GLU:HB3	4:J:149:PRO:HA	1.85	0.58
1:C:314:LEU:HB3	2:D:100:VAL:HG21	1.84	0.58
3:N:142:LYS:HB2	3:N:173:TYR:CE1	2.39	0.57
1:C:143:PRO:HG2	1:C:144:ASP:OD1	2.04	0.57
1:A:220:ARG:HD3	1:A:229:ARG:CG	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:106:ILE:HG22	3:L:166:GLN:NE2	2.19	0.57
3:L:119:PRO:HG2	4:H:213:ARG:CZ	2.35	0.57
3:M:108:ARG:HD3	3:M:109:ALA:HB3	1.87	0.57
3:M:110:ASP:OD1	3:M:110:ASP:N	2.37	0.57
3:N:108:ARG:HG2	3:N:109:ALA:N	2.20	0.56
1:A:182:VAL:HG21	1:A:213:ILE:CG2	2.36	0.56
4:I:27:TYR:HB2	8:I:302:SO4:O1	2.05	0.56
2:B:17:MET:CE	2:B:36:ALA:HA	2.36	0.56
10:E:506:NAG:O3	10:E:507:BMA:O5	2.18	0.56
3:N:19:VAL:HG21	3:N:104:LEU:HD11	1.87	0.56
2:B:68:LYS:HE2	2:B:85:GLU:OE1	2.05	0.56
3:M:19:VAL:HG21	3:M:104:LEU:HD11	1.87	0.56
4:H:152:LEU:CD2	4:H:179:SER:HB2	2.35	0.56
1:E:102:VAL:HG22	1:E:232:ILE:HB	1.86	0.56
1:E:226:LEU:HD22	4:J:54:ILE:HG22	1.88	0.56
1:A:104:ASP:N	8:A:514:SO4:O3	2.37	0.56
1:A:102:VAL:HG22	1:A:232:ILE:HB	1.88	0.56
4:J:177:LEU:HD12	4:J:177:LEU:C	2.26	0.56
2:D:56:ILE:CG2	2:D:56:ILE:O	2.54	0.55
3:M:110:ASP:HA	3:M:140:TYR:HD2	1.72	0.55
3:M:14:SER:HA	3:M:106:ILE:HD12	1.88	0.55
2:B:56:ILE:CG2	2:B:56:ILE:O	2.54	0.55
3:N:108:ARG:CG	3:N:108:ARG:HH11	2.18	0.55
1:E:324:PRO:O	1:E:325:GLU:CB	2.55	0.55
3:N:136:LEU:HD12	3:N:136:LEU:N	2.21	0.55
3:M:108:ARG:HD3	3:M:109:ALA:CB	2.36	0.55
1:A:143:PRO:HG2	1:A:144:ASP:OD1	2.08	0.54
1:C:324:PRO:O	1:C:325:GLU:CB	2.56	0.54
1:C:186:SER:HA	1:C:218:GLY:O	2.08	0.54
3:L:140:TYR:CG	3:L:141:PRO:HA	2.41	0.54
2:D:17:MET:CE	2:D:36:ALA:HA	2.37	0.54
3:N:37:GLN:HB2	3:N:47:LEU:HD11	1.90	0.54
4:I:140:CYS:HB2	4:I:154:TRP:CZ2	2.43	0.54
3:M:35:TRP:CZ3	3:M:88:CYS:HB3	2.43	0.54
4:I:120:SER:HB3	4:I:122:TYR:CZ	2.43	0.54
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.90	0.54
3:N:137:ASN:HA	3:N:174:SER:HB3	1.90	0.54
1:A:212:THR:HG21	1:C:216:ASN:CG	2.28	0.54
1:E:143:PRO:HG2	1:E:144:ASP:OD1	2.06	0.54
1:E:324:PRO:O	1:E:325:GLU:HB2	2.08	0.54
1:A:201:LYS:HG3	1:A:214:ILE:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:209:PHE:HB2	4:H:127:VAL:HG11	1.90	0.53
4:I:38:LYS:HE2	4:I:40:ARG:HD2	1.91	0.53
2:F:17:MET:CE	2:F:36:ALA:HA	2.39	0.53
3:N:35:TRP:CZ3	3:N:88:CYS:HB3	2.44	0.53
1:C:182:VAL:HG21	1:C:213:ILE:HG21	1.91	0.53
1:E:220:ARG:HD3	1:E:229:ARG:HG3	1.89	0.53
2:F:26:HIS:CE1	2:F:33:GLY:HA3	2.43	0.53
3:L:155:ARG:HE	3:L:157:ASN:HB2	1.74	0.52
3:L:106:ILE:HG21	3:L:171:SER:HB3	1.91	0.52
1:C:201:LYS:HG3	1:C:214:ILE:HD13	1.91	0.52
1:C:324:PRO:O	1:C:325:GLU:HB2	2.09	0.52
1:C:200:GLY:HA3	1:C:250:ASN:OD1	2.10	0.52
4:J:37:ILE:HD12	4:J:37:ILE:N	2.24	0.52
1:A:324:PRO:O	1:A:325:GLU:CB	2.58	0.52
4:J:194:THR:HG21	4:J:207:ASP:HB3	1.91	0.52
3:N:138:ASN:H	3:N:174:SER:HB3	1.75	0.52
4:J:187:THR:HG22	4:J:191:GLN:NE2	2.25	0.52
1:E:186:SER:HA	1:E:218:GLY:O	2.10	0.52
3:M:107:LYS:O	3:M:108:ARG:HB2	2.08	0.52
3:M:106:ILE:O	3:M:106:ILE:HG22	2.10	0.52
2:B:26:HIS:CE1	2:B:33:GLY:HA3	2.45	0.51
4:H:152:LEU:HD21	4:H:179:SER:HB3	1.91	0.51
3:L:35:TRP:CZ3	3:L:88:CYS:HB3	2.45	0.51
2:B:139:LYS:HD2	8:B:203:SO4:O3	2.09	0.51
3:L:167:ASP:OD2	3:L:168:SER:N	2.44	0.51
1:A:220:ARG:HD3	1:A:229:ARG:HG2	1.93	0.51
1:A:186:SER:HA	1:A:218:GLY:O	2.11	0.51
1:E:17:HIS:NE2	2:F:6:ILE:HG23	2.26	0.51
3:M:37:GLN:HB2	3:M:47:LEU:HD11	1.92	0.51
4:H:189:PRO:HB3	4:H:212:PRO:HG3	1.93	0.51
3:M:107:LYS:HB2	3:M:140:TYR:HH	1.75	0.51
1:A:200:GLY:HA3	1:A:250:ASN:OD1	2.11	0.51
1:A:213:ILE:HG12	1:A:233:TYR:CZ	2.45	0.51
1:E:213:ILE:HG12	1:E:233:TYR:CZ	2.46	0.50
3:N:136:LEU:HD23	3:N:144:ILE:HD13	1.94	0.50
2:B:91:LEU:HD13	2:F:91:LEU:HD13	1.92	0.50
4:J:151:THR:OG1	4:J:198:ALA:HB3	2.11	0.50
2:F:56:ILE:CG2	2:F:56:ILE:O	2.59	0.50
4:I:37:ILE:N	4:I:37:ILE:HD12	2.26	0.50
3:N:176:SER:HB2	4:J:166:PHE:CZ	2.47	0.50
4:H:34:ILE:HG13	4:H:78:VAL:HG21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:26:HIS:CE1	2:D:33:GLY:HA3	2.47	0.50
1:A:220:ARG:HD3	1:A:229:ARG:HG3	1.93	0.50
4:H:37:ILE:N	4:H:37:ILE:HD12	2.27	0.50
3:L:18:ARG:HD3	3:L:76:THR:HG22	1.94	0.49
1:E:200:GLY:HA3	1:E:250:ASN:OD1	2.11	0.49
4:J:172:SER:O	4:J:173:ASP:HB2	2.13	0.49
8:B:203:SO4:O4	2:F:127:ARG:NH1	2.41	0.49
3:L:113:PRO:O	3:L:115:VAL:HG23	2.12	0.49
3:N:163:TRP:O	4:J:167:PRO:HD2	2.12	0.49
4:H:108:LEU:HD23	4:H:149:PRO:HD3	1.94	0.49
4:I:170:LEU:HD13	4:I:175:TYR:CD2	2.48	0.49
1:A:324:PRO:O	1:A:325:GLU:HB2	2.11	0.49
1:C:213:ILE:HG12	1:C:233:TYR:CZ	2.47	0.49
1:E:220:ARG:HD3	1:E:229:ARG:HG2	1.94	0.49
1:A:61:GLY:HA2	1:A:79:PHE:CZ	2.48	0.48
4:I:34:ILE:HG13	4:I:78:VAL:HG21	1.95	0.48
1:E:314:LEU:HB3	2:F:100:VAL:HG21	1.96	0.48
2:B:126:LEU:HD21	2:B:152:ILE:HD13	1.95	0.48
1:E:201:LYS:HG3	1:E:214:ILE:HD13	1.94	0.48
4:I:145:TYR:OH	4:I:177:LEU:HD23	2.13	0.48
3:N:107:LYS:HG3	3:N:140:TYR:OH	2.13	0.48
4:I:59:TYR:CE1	4:I:69:PHE:CE2	3.01	0.48
1:C:61:GLY:HA2	1:C:79:PHE:CZ	2.49	0.48
3:M:18:ARG:HD3	3:M:76:THR:HG22	1.96	0.48
3:N:91:TYR:HD1	4:J:99:SER:HB2	1.79	0.48
1:C:196:VAL:HG12	1:C:197:GLN:N	2.28	0.48
4:H:59:TYR:CE1	4:H:69:PHE:CE2	3.01	0.48
1:E:182:VAL:HG21	1:E:213:ILE:CG2	2.43	0.47
1:A:314:LEU:HB3	2:B:100:VAL:HG21	1.96	0.47
4:H:145:TYR:CE2	4:H:150:VAL:HG13	2.49	0.47
4:I:39:GLN:O	4:I:88:ALA:HB1	2.13	0.47
4:H:198:ALA:HB2	4:H:205:LYS:HD2	1.95	0.47
2:B:110:LEU:C	2:B:110:LEU:HD12	2.35	0.47
1:C:40:THR:HG21	2:D:52:LEU:HD11	1.95	0.47
4:H:126:PRO:HD3	4:H:138:LEU:HD22	1.95	0.47
4:H:152:LEU:HD21	4:H:179:SER:HB2	1.96	0.47
3:N:176:SER:HB2	4:J:166:PHE:CE2	2.49	0.47
3:L:184:ASP:O	3:L:188:ARG:HG3	2.15	0.47
4:H:159:LEU:HD23	4:H:181:VAL:HG21	1.95	0.47
3:L:106:ILE:HG21	3:L:171:SER:CB	2.44	0.47
3:L:195:GLU:HG2	3:L:206:VAL:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:61:GLY:HA2	1:E:79:PHE:CZ	2.50	0.47
1:A:128:THR:H	1:A:164:GLN:NE2	2.12	0.47
4:J:197:VAL:O	4:J:197:VAL:HG12	2.15	0.47
3:N:108:ARG:HG2	3:N:109:ALA:H	1.78	0.46
3:N:136:LEU:N	3:N:136:LEU:CD1	2.78	0.46
1:E:167:THR:OG1	7:E:510:NAG:H62	2.15	0.46
4:I:18:VAL:HG12	4:I:82(C):LEU:HD11	1.96	0.46
3:M:107:LYS:HD2	3:M:107:LYS:O	2.15	0.46
3:N:18:ARG:HD3	3:N:76:THR:HG22	1.95	0.46
3:M:107:LYS:CD	3:M:107:LYS:O	2.63	0.46
3:N:106:ILE:HA	3:N:106:ILE:HD13	1.75	0.46
4:J:146:PHE:CD2	4:J:146:PHE:C	2.89	0.46
4:J:34:ILE:HG13	4:J:78:VAL:HG21	1.97	0.46
4:H:138:LEU:HD12	4:H:193:ILE:HG21	1.96	0.46
3:N:135:PHE:HB3	3:N:137:ASN:OD1	2.15	0.46
4:J:146:PHE:CD1	4:J:175:TYR:HE2	2.34	0.46
2:D:126:LEU:HD21	2:D:152:ILE:HD13	1.98	0.46
4:J:199:HIS:ND1	4:J:202:SER:CB	2.77	0.46
1:E:182:VAL:HG22	1:E:202:VAL:HG21	1.97	0.46
2:F:126:LEU:HD21	2:F:152:ILE:HD13	1.98	0.46
4:H:125:ALA:HB2	4:H:210:ILE:HG22	1.97	0.46
3:L:106:ILE:HA	3:L:106:ILE:HD13	1.77	0.46
3:L:14:SER:HA	3:L:106:ILE:HD12	1.98	0.46
1:C:220:ARG:HD3	1:C:229:ARG:HG2	1.98	0.46
2:D:56:ILE:O	2:D:56:ILE:HG22	2.16	0.46
3:N:135:PHE:C	3:N:136:LEU:HD12	2.37	0.46
3:N:14:SER:HA	3:N:106:ILE:HD12	1.97	0.45
4:J:18:VAL:HG12	4:J:82(C):LEU:HD11	1.98	0.45
3:L:197:THR:HG23	3:L:204:PRO:HB3	1.98	0.45
1:A:97:CYS:SG	1:A:98:TYR:N	2.89	0.45
4:I:150:VAL:CG2	4:I:177:LEU:HD21	2.47	0.45
3:N:136:LEU:HD23	3:N:144:ILE:CD1	2.46	0.45
3:M:91:TYR:HD1	4:I:99:SER:HB2	1.81	0.45
4:H:39:GLN:O	4:H:88:ALA:HB1	2.16	0.45
1:E:98:TYR:CZ	1:E:226:LEU:HD13	2.52	0.45
1:A:196:VAL:HG12	1:A:197:GLN:N	2.31	0.45
3:N:103:LYS:HE3	3:N:103:LYS:HB2	1.83	0.45
1:E:200:GLY:O	1:E:201:LYS:HB2	2.17	0.45
3:M:176:SER:HB2	4:I:166:PHE:CE2	2.51	0.45
3:M:103:LYS:HE3	3:M:103:LYS:HB2	1.86	0.45
1:E:248:ASN:C	1:E:248:ASN:OD1	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:196:VAL:HG12	1:E:197:GLN:N	2.31	0.45
3:M:107:LYS:HD2	3:M:107:LYS:C	2.36	0.45
1:C:10:GLY:HA2	2:D:142:HIS:O	2.17	0.45
4:J:59:TYR:CE1	4:J:69:PHE:CE2	3.05	0.45
3:N:166:GLN:HE21	3:N:171:SER:HB3	1.82	0.44
3:L:14:SER:OG	3:L:107:LYS:HG3	2.17	0.44
3:N:140:TYR:CG	3:N:141:PRO:HA	2.52	0.44
1:A:182:VAL:HG21	1:A:213:ILE:HG21	1.98	0.44
2:F:57:GLU:HG2	2:F:58:LYS:N	2.32	0.44
1:A:167:THR:OG1	7:A:505:NAG:H62	2.17	0.44
1:E:128:THR:H	1:E:164:GLN:NE2	2.15	0.44
2:F:110:LEU:C	2:F:110:LEU:HD12	2.38	0.44
4:J:204:THR:CG2	4:J:206:VAL:HG13	2.47	0.44
1:C:323:VAL:O	2:D:12:ASN:HB2	2.18	0.44
1:E:98:TYR:CD1	1:E:99:PRO:HD2	2.53	0.44
1:A:212:THR:HG21	1:C:216:ASN:CB	2.48	0.44
3:M:35:TRP:HB2	3:M:48:ILE:HB	1.99	0.44
3:M:136:LEU:HD12	3:M:136:LEU:N	2.33	0.44
4:H:18:VAL:HG12	4:H:82(C):LEU:HD11	1.99	0.44
3:L:106:ILE:CG2	3:L:171:SER:HB3	2.48	0.44
3:L:119:PRO:HB3	3:L:209:PHE:CE2	2.52	0.44
2:F:6:ILE:C	2:F:8:GLY:N	2.71	0.44
4:H:155:ASN:HD22	4:H:159:LEU:HD13	1.82	0.44
1:C:58:ILE:HG21	1:C:274:ILE:HD13	1.99	0.44
1:C:180:TRP:CE2	1:C:204:VAL:HG21	2.52	0.44
4:H:126:PRO:HD3	4:H:138:LEU:HD23	1.99	0.44
2:F:57:GLU:CG	2:F:58:LYS:N	2.81	0.44
3:N:13:THR:O	3:N:106:ILE:CD1	2.63	0.43
3:L:209:PHE:CB	4:H:127:VAL:HG11	2.47	0.43
4:I:117:THR:HG22	4:I:118:ALA:N	2.33	0.43
4:I:119:PRO:HB3	4:I:145:TYR:HB3	1.99	0.43
4:J:39:GLN:O	4:J:88:ALA:HB1	2.18	0.43
1:A:120:PHE:CD2	1:A:150:ARG:NH1	2.86	0.43
1:E:304:ALA:HB2	2:F:61:GLU:HG3	1.99	0.43
3:M:106:ILE:HA	3:M:106:ILE:HD13	1.81	0.43
4:H:188:TRP:CG	4:H:189:PRO:HA	2.53	0.43
2:F:57:GLU:CG	2:F:58:LYS:H	2.32	0.43
1:C:19:ALA:HB2	2:D:13:GLY:HA3	2.01	0.43
1:C:17:HIS:NE2	2:D:6:ILE:HG23	2.34	0.43
2:D:27:GLN:HG3	2:D:32:THR:HG22	2.00	0.43
3:N:107:LYS:HA	3:N:140:TYR:OH	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:35:TRP:HB2	3:N:48:ILE:HB	2.01	0.43
4:I:170:LEU:HD13	4:I:175:TYR:CE2	2.53	0.43
1:E:304:ALA:HA	2:F:61:GLU:HA	2.00	0.43
1:C:128:THR:H	1:C:164:GLN:NE2	2.17	0.43
1:A:54:ASN:ND2	1:A:55:PRO:HA	2.33	0.43
2:B:57:GLU:HG2	2:B:58:LYS:N	2.33	0.43
2:B:4:GLY:HA3	2:F:117:LYS:HD3	2.00	0.43
3:N:30:ASP:HB3	3:N:31:THR:H	1.68	0.43
3:L:103:LYS:HE3	3:L:103:LYS:HB2	1.86	0.43
1:E:128:THR:H	1:E:164:GLN:HE22	1.67	0.43
3:L:136:LEU:N	3:L:136:LEU:HD12	2.34	0.43
1:C:54:ASN:ND2	1:C:55:PRO:HA	2.34	0.43
4:I:9:THR:HG22	4:I:10:GLU:N	2.33	0.43
1:A:58:ILE:HG21	1:A:274:ILE:HD13	2.00	0.43
3:M:108:ARG:NE	3:M:109:ALA:HB2	2.34	0.43
4:J:9:THR:HG22	4:J:10:GLU:N	2.34	0.43
4:H:119:PRO:HD3	4:H:199:HIS:ND1	2.33	0.43
1:C:167:THR:OG1	7:C:505:NAG:H62	2.18	0.42
1:C:320:MET:HB3	2:D:111:THR:HB	2.00	0.42
2:D:130:ALA:HA	2:D:139:LYS:O	2.20	0.42
1:C:98:TYR:CZ	1:C:226:LEU:HD13	2.54	0.42
4:I:177:LEU:HD12	4:I:178:SER:N	2.35	0.42
4:J:144:GLY:HA2	4:J:174:LEU:HB3	2.02	0.42
3:N:91:TYR:CD1	4:J:99:SER:HB2	2.55	0.42
1:C:248:ASN:OD1	1:C:248:ASN:C	2.58	0.42
3:M:49:TYR:O	3:M:53:ASN:HB2	2.20	0.42
2:D:9:PHE:CE1	2:D:10:ILE:HG13	2.54	0.42
2:B:6:ILE:C	2:B:8:GLY:N	2.73	0.42
2:B:57:GLU:CG	2:B:58:LYS:N	2.82	0.42
2:B:54:ARG:NH1	9:B:205:GOL:O3	2.52	0.42
3:L:160:LEU:HG	4:H:169:VAL:HG11	2.02	0.42
3:N:49:TYR:O	3:N:53:ASN:HB2	2.20	0.42
3:L:34:ALA:HA	3:L:48:ILE:O	2.20	0.42
1:E:213:ILE:HG12	1:E:233:TYR:CE2	2.54	0.42
4:J:155:ASN:O	4:J:156:SER:HB2	2.20	0.42
2:F:68:LYS:HE2	2:F:85:GLU:OE1	2.19	0.42
2:D:110:LEU:HD12	2:D:110:LEU:C	2.39	0.42
3:L:209:PHE:HB2	4:H:127:VAL:CG1	2.50	0.42
4:J:194:THR:CG2	4:J:207:ASP:HB3	2.50	0.42
2:D:6:ILE:C	2:D:8:GLY:N	2.73	0.42
2:F:9:PHE:CD1	2:F:9:PHE:C	2.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:THR:H	1:A:164:GLN:HE22	1.67	0.41
1:A:180:TRP:CE2	1:A:204:VAL:HG21	2.55	0.41
3:L:94:TYR:OH	4:H:50:GLU:OE2	2.24	0.41
1:A:118:LEU:HA	1:A:118:LEU:HD23	1.91	0.41
1:C:208:ARG:HB3	12:E:520:PG4:H51	2.01	0.41
3:L:111:ALA:C	3:L:200:THR:HG21	2.40	0.41
1:E:85:ASP:O	1:E:265:SER:HA	2.20	0.41
3:N:119:PRO:HB3	3:N:209:PHE:CZ	2.55	0.41
1:C:85:ASP:O	1:C:265:SER:HA	2.20	0.41
1:C:201:LYS:HG3	1:C:214:ILE:CD1	2.50	0.41
4:H:152:LEU:HD23	4:H:179:SER:HB2	2.03	0.41
1:C:13:LEU:CD2	2:D:152:ILE:HG21	2.51	0.41
2:B:57:GLU:CG	2:B:58:LYS:H	2.32	0.41
4:H:9:THR:HG22	4:H:10:GLU:N	2.35	0.41
3:L:91:TYR:HD1	4:H:99:SER:HB2	1.85	0.41
3:L:170:ASP:OD1	3:L:170:ASP:C	2.59	0.41
3:L:180:THR:O	3:L:181:LEU:HG	2.20	0.41
3:M:14:SER:HA	3:M:106:ILE:CD1	2.50	0.41
3:L:35:TRP:HB2	3:L:48:ILE:HB	2.01	0.41
3:M:117:ILE:C	3:M:118:PHE:CD2	2.94	0.41
3:M:113:PRO:HA	3:M:139:PHE:HB3	2.02	0.41
3:N:124:GLN:HB2	4:J:122:TYR:CD1	2.55	0.41
3:M:118:PHE:CD1	4:I:124:LEU:HB3	2.55	0.41
1:C:120:PHE:CD2	1:C:150:ARG:NH1	2.89	0.41
3:N:119:PRO:HG2	4:J:213:ARG:NH2	2.35	0.41
2:D:68:LYS:HE2	2:D:85:GLU:OE1	2.20	0.41
4:H:53:GLU:HA	4:H:53:GLU:OE2	2.20	0.41
4:I:40:ARG:HA	4:I:41:PRO:HD3	1.85	0.41
1:C:316:LEU:HD23	2:D:52:LEU:HD13	2.03	0.41
1:E:120:PHE:CD2	1:E:150:ARG:NH1	2.89	0.41
1:C:29:ILE:HD11	2:D:102:LEU:HD23	2.03	0.41
1:A:85:ASP:O	1:A:265:SER:HA	2.21	0.41
3:N:105:GLU:HG2	3:N:106:ILE:N	2.36	0.41
1:C:200:GLY:O	1:C:201:LYS:HB2	2.21	0.41
1:C:324:PRO:O	1:C:325:GLU:HG3	2.21	0.41
3:L:49:TYR:O	3:L:53:ASN:HB2	2.21	0.41
2:D:9:PHE:CD1	2:D:9:PHE:C	2.95	0.41
3:M:118:PHE:N	3:M:118:PHE:CD2	2.89	0.41
1:E:98:TYR:CE2	1:E:226:LEU:HD13	2.56	0.40
1:A:301:THR:HB	1:A:305:CYS:SG	2.61	0.40
3:L:105:GLU:HG2	3:L:106:ILE:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:270:SER:HB2	1:E:284:PRO:HA	2.02	0.40
3:L:193:THR:HG22	3:L:194:CYS:N	2.36	0.40
4:H:127:VAL:HG12	4:H:128:CYS:N	2.36	0.40
3:L:83:LEU:HD11	3:L:166:GLN:HB3	2.02	0.40
1:C:97:CYS:SG	1:C:98:TYR:N	2.91	0.40
1:E:324:PRO:O	1:E:325:GLU:HG3	2.21	0.40
3:M:91:TYR:CD1	4:I:99:SER:HB2	2.56	0.40
4:H:177:LEU:CD1	4:H:177:LEU:C	2.89	0.40
2:B:56:ILE:HG22	2:B:56:ILE:O	2.20	0.40
2:F:9:PHE:CE1	2:F:10:ILE:HG13	2.57	0.40
3:L:91:TYR:CD1	4:H:99:SER:HB2	2.56	0.40
4:J:94:ARG:HA	4:J:95:PRO:HD3	1.98	0.40
3:L:186:TYR:CE1	3:L:192:TYR:CE2	3.09	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	30	70
1	C	314/320 (98%)	306 (98%)	6 (2%)	2 (1%)	30	70
1	E	314/320 (98%)	306 (98%)	6 (2%)	2 (1%)	30	70
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%)	26	67
3	N	211/214 (99%)	203 (96%)	8 (4%)	0	100	100
4	H	216/225 (96%)	211 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	46	81

All (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
1	E	62	ILE
3	M	109	ALA

### 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%)	55	85
1	C	276/280 (99%)	268 (97%)	8 (3%)	50	82
1	E	276/280 (99%)	268 (97%)	8 (3%)	50	82
2	B	145/149 (97%)	139 (96%)	6 (4%)	37	74
2	D	145/149 (97%)	139 (96%)	6 (4%)	37	74
2	F	145/149 (97%)	140 (97%)	5 (3%)	44	79
3	L	189/192 (98%)	183 (97%)	6 (3%)	46	80
3	M	139/192 (72%)	134 (96%)	5 (4%)	42	78
3	N	191/192 (100%)	181 (95%)	10 (5%)	29	66
4	H	187/193 (97%)	181 (97%)	6 (3%)	46	80
4	I	159/193 (82%)	155 (98%)	4 (2%)	55	85
4	J	183/193 (95%)	177 (97%)	6 (3%)	45	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2311/2442 (95%)	2234 (97%)	77 (3%)	45 80

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	22	ASN
1	A	31	ASN
1	A	54	ASN
1	A	144	ASP
1	A	159	SER
1	A	174	SER
2	B	12	ASN
2	B	56	ILE
2	B	110	LEU
2	B	120	GLU
2	B	121	LYS
2	B	144	CYS
1	C	18	HIS
1	C	22	ASN
1	C	31	ASN
1	C	54	ASN
1	C	144	ASP
1	C	159	SER
1	C	174	SER
1	C	321	ARG
2	D	12	ASN
2	D	51	LYS
2	D	56	ILE
2	D	120	GLU
2	D	121	LYS
2	D	144	CYS
1	E	18	HIS
1	E	22	ASN
1	E	31	ASN
1	E	54	ASN
1	E	55	PRO
1	E	144	ASP
1	E	159	SER
1	E	174	SER
2	F	12	ASN
2	F	56	ILE

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Mol	Chain	Res	Type
2	F	120	GLU
2	F	121	LYS
2	F	144	CYS
3	L	31	THR
3	L	106	ILE
3	L	116	SER
3	L	175	MET
3	L	176	SER
3	L	210	ASN
4	H	43	HIS
4	H	53	GLU
4	H	115	LYS
4	H	177	LEU
4	H	186	SER
4	H	195	CYS
3	M	31	THR
3	M	106	ILE
3	M	107	LYS
3	M	108	ARG
3	M	110	ASP
4	I	40	ARG
4	I	43	HIS
4	I	53	GLU
4	I	177	LEU
3	N	31	THR
3	N	106	ILE
3	N	108	ARG
3	N	116	SER
3	N	127	SER
3	N	144	ILE
3	N	168	SER
3	N	174	SER
3	N	191	SER
3	N	197	THR
4	J	43	HIS
4	J	53	GLU
4	J	120	SER
4	J	140	CYS
4	J	161	SER
4	J	197	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	164	GLN
1	A	246	ASN
2	B	12	ASN
2	B	26	HIS
2	B	27	GLN
2	B	125	GLN
1	C	54	ASN
1	C	122	ASN
1	C	164	GLN
2	D	26	HIS
2	D	27	GLN
2	D	125	GLN
1	E	54	ASN
1	E	164	GLN
2	F	26	HIS
2	F	27	GLN
2	F	125	GLN
3	L	42	GLN
3	L	124	GLN
3	M	42	GLN
3	N	42	GLN
4	J	191	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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	7,8,9	1.92	2 (28%)	9,10,12	2.00	4 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	PCA	I	1	4	7,8,9	1.99	2 (28%)	9,10,12	2.04	5 (55%)
4	PCA	J	1	4	7,8,9	2.07	2 (28%)	9,10,12	1.98	5 (55%)

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1	PCA	CA-N	3.22	1.50	1.46
4	I	1	PCA	CA-N	3.41	1.50	1.46
4	J	1	PCA	CA-N	3.56	1.50	1.46
4	H	1	PCA	CD-N	3.79	1.46	1.33
4	I	1	PCA	CD-N	3.86	1.46	1.33
4	J	1	PCA	CD-N	4.07	1.47	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	1	PCA	CA-N-CD	-3.17	103.17	113.81
4	J	1	PCA	CA-N-CD	-3.13	103.32	113.81
4	H	1	PCA	CA-N-CD	-3.10	103.41	113.81
4	H	1	PCA	CB-CA-C	-2.69	109.09	112.76
4	I	1	PCA	CB-CA-C	-2.53	109.30	112.76
4	I	1	PCA	O-C-CA	-2.36	119.21	125.44
4	J	1	PCA	CB-CA-C	-2.28	109.64	112.76
4	H	1	PCA	O-C-CA	-2.26	119.48	125.44
4	J	1	PCA	O-C-CA	-2.22	119.57	125.44
4	J	1	PCA	OE-CD-CG	-2.19	121.91	126.81
4	I	1	PCA	OE-CD-CG	-2.10	122.11	126.81
4	J	1	PCA	CB-CA-N	2.61	110.83	103.20
4	I	1	PCA	CB-CA-N	2.67	110.98	103.20
4	H	1	PCA	CB-CA-N	2.68	111.03	103.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	14,14,15	0.63	0	15,19,21	0.91	0
6	NAG	A	503	6	14,14,15	0.54	0	15,19,21	0.73	0
7	NAG	A	505	1,7	14,14,15	0.50	0	15,19,21	0.97	1 (6%)
7	NAG	A	506	7	14,14,15	0.59	0	15,19,21	0.95	2 (13%)
7	BMA	A	507	7	11,11,12	0.68	0	14,15,17	0.81	0
7	MAN	A	508	7	11,11,12	0.62	0	14,15,17	0.78	0
7	MAN	A	509	7	11,11,12	0.62	0	14,15,17	1.65	3 (21%)
6	NAG	A	510	1,6	14,14,15	0.49	0	15,19,21	1.49	2 (13%)
6	NAG	A	511	6	14,14,15	0.46	0	15,19,21	0.94	1 (6%)
6	NAG	C	502	1,6	14,14,15	0.58	0	15,19,21	0.86	1 (6%)
6	NAG	C	503	6	14,14,15	0.57	0	15,19,21	0.73	0
7	NAG	C	505	1,7	14,14,15	0.56	0	15,19,21	1.09	1 (6%)
7	NAG	C	506	7	14,14,15	0.59	0	15,19,21	0.98	2 (13%)
7	BMA	C	507	7	11,11,12	0.76	0	14,15,17	1.02	1 (7%)
7	MAN	C	508	7	11,11,12	0.60	0	14,15,17	0.88	0
7	MAN	C	509	7	11,11,12	0.54	0	14,15,17	1.91	4 (28%)
10	NAG	C	510	1,10	14,14,15	0.52	0	15,19,21	1.68	2 (13%)
10	NAG	C	511	10	14,14,15	0.46	0	15,19,21	1.20	1 (6%)
10	BMA	C	512	10	11,11,12	0.61	0	14,15,17	1.19	2 (14%)
11	NAG	E	501	11,1	14,14,15	0.50	0	15,19,21	1.25	2 (13%)
11	NAG	E	502	11	14,14,15	0.54	0	15,19,21	0.84	1 (6%)
11	BMA	E	503	11	11,11,12	0.64	0	14,15,17	0.85	0
11	MAN	E	504	11	11,11,12	0.62	0	14,15,17	0.84	1 (7%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	NAG	E	505	1,10	14,14,15	0.68	0	15,19,21	0.90	1 (6%)
10	NAG	E	506	10	14,14,15	0.52	0	15,19,21	0.79	0
10	BMA	E	507	10	11,11,12	0.49	0	14,15,17	0.98	1 (7%)
6	NAG	E	508	1,6	14,14,15	0.51	0	15,19,21	1.01	2 (13%)
6	NAG	E	509	6	14,14,15	0.71	1 (7%)	15,19,21	0.99	0
7	NAG	E	510	1,7	14,14,15	0.61	0	15,19,21	1.10	1 (6%)
7	NAG	E	511	7	14,14,15	0.60	0	15,19,21	0.95	1 (6%)
7	BMA	E	512	7	11,11,12	0.85	1 (9%)	14,15,17	1.02	0
7	MAN	E	513	7	11,11,12	0.62	0	14,15,17	0.73	0
7	MAN	E	514	7	11,11,12	0.59	0	14,15,17	1.76	3 (21%)
11	NAG	E	515	11,1	14,14,15	0.43	0	15,19,21	1.66	2 (13%)
11	NAG	E	516	11	14,14,15	0.46	0	15,19,21	1.23	2 (13%)
11	BMA	E	517	11	11,11,12	0.53	0	14,15,17	1.02	2 (14%)
11	MAN	E	518	11	11,11,12	0.59	0	14,15,17	0.76	0
6	NAG	H	301	4,6	14,14,15	0.63	0	15,19,21	0.83	0
6	NAG	H	302	6	14,14,15	0.51	0	15,19,21	1.14	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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	512	BMA	O5-C1	-2.03	1.40	1.43
6	E	509	NAG	C1-C2	2.25	1.55	1.52

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	E	501	NAG	C2-N2-C7	-3.76	118.20	123.04
7	C	509	MAN	O2-C2-C3	-2.98	104.13	110.12
6	H	302	NAG	C4-C3-C2	-2.62	107.15	111.23
6	A	510	NAG	C2-N2-C7	-2.55	119.76	123.04
7	C	506	NAG	C2-N2-C7	-2.50	119.83	123.04
7	A	509	MAN	O5-C5-C6	-2.48	101.97	107.35
10	E	505	NAG	C2-N2-C7	-2.40	119.96	123.04
7	A	506	NAG	C2-N2-C7	-2.32	120.06	123.04
7	E	511	NAG	C2-N2-C7	-2.29	120.10	123.04
10	C	510	NAG	C2-N2-C7	-2.28	120.11	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	E	516	NAG	C2-N2-C7	-2.28	120.11	123.04
6	C	502	NAG	C2-N2-C7	-2.25	120.14	123.04
11	E	515	NAG	C2-N2-C7	-2.15	120.28	123.04
7	E	514	MAN	O5-C5-C6	-2.13	102.74	107.35
7	C	509	MAN	C2-C3-C4	-2.09	107.49	111.04
7	A	509	MAN	C2-C3-C4	-2.09	107.50	111.04
11	E	502	NAG	C2-N2-C7	-2.01	120.45	123.04
7	C	507	BMA	O5-C5-C6	2.01	111.69	107.35
7	C	506	NAG	O5-C5-C6	2.01	111.70	107.35
7	A	506	NAG	O5-C5-C6	2.02	111.73	107.35
6	E	508	NAG	C1-O5-C5	2.09	114.90	112.25
11	E	517	BMA	O5-C5-C6	2.19	112.09	107.35
11	E	501	NAG	C1-O5-C5	2.20	115.05	112.25
11	E	504	MAN	C1-C2-C3	2.32	112.28	109.54
7	C	509	MAN	C1-C2-C3	2.39	112.36	109.54
10	C	512	BMA	O5-C5-C6	2.41	112.56	107.35
6	E	508	NAG	C4-C3-C2	2.51	115.13	111.23
10	E	507	BMA	O5-C5-C6	2.55	112.86	107.35
11	E	517	BMA	C1-C2-C3	2.72	112.75	109.54
7	E	514	MAN	C1-C2-C3	2.74	112.79	109.54
6	A	511	NAG	C1-O5-C5	2.82	115.83	112.25
7	A	505	NAG	C1-O5-C5	3.14	116.23	112.25
10	C	512	BMA	C1-C2-C3	3.46	113.63	109.54
7	C	505	NAG	C1-O5-C5	3.50	116.68	112.25
7	E	510	NAG	C1-O5-C5	3.59	116.80	112.25
7	A	509	MAN	C1-O5-C5	3.80	117.06	112.25
11	E	516	NAG	C1-O5-C5	3.94	117.25	112.25
10	C	511	NAG	C1-O5-C5	3.96	117.27	112.25
6	A	510	NAG	C1-O5-C5	4.39	117.82	112.25
7	E	514	MAN	C1-O5-C5	4.54	118.01	112.25
7	C	509	MAN	C1-O5-C5	4.61	118.10	112.25
11	E	515	NAG	C1-O5-C5	5.52	119.25	112.25
10	C	510	NAG	C1-O5-C5	5.78	119.59	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	505	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	505	NAG	1	0
10	E	506	NAG	1	0
10	E	507	BMA	1	0
7	E	510	NAG	1	0

## 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	14,14,15	0.50	0	15,19,21	0.88	1 (6%)
5	NAG	A	504	1	14,14,15	0.51	0	15,19,21	0.90	0
8	SO4	A	512	-	4,4,4	0.19	0	6,6,6	0.08	0
8	SO4	A	513	-	4,4,4	0.16	0	6,6,6	0.47	0
8	SO4	A	514	-	4,4,4	0.09	0	6,6,6	0.15	0
8	SO4	A	515	-	4,4,4	0.12	0	6,6,6	0.35	0
8	SO4	A	516	-	4,4,4	0.11	0	6,6,6	0.40	0
5	NAG	B	201	2	14,14,15	0.54	0	15,19,21	0.98	1 (6%)
8	SO4	B	202	-	4,4,4	0.24	0	6,6,6	0.21	0
8	SO4	B	203	-	4,4,4	0.24	0	6,6,6	0.08	0
8	SO4	B	204	-	4,4,4	0.19	0	6,6,6	0.22	0
9	GOL	B	205	-	5,5,5	0.48	0	5,5,5	0.70	0
5	NAG	C	501	1	14,14,15	0.51	0	15,19,21	0.87	0
5	NAG	C	504	1	14,14,15	0.52	0	15,19,21	0.90	1 (6%)
8	SO4	C	513	-	4,4,4	0.22	0	6,6,6	0.16	0
8	SO4	C	514	-	4,4,4	0.20	0	6,6,6	0.22	0
8	SO4	C	515	-	4,4,4	0.06	0	6,6,6	0.51	0
5	NAG	D	201	2	14,14,15	0.52	0	15,19,21	1.00	1 (6%)
8	SO4	D	202	-	4,4,4	0.22	0	6,6,6	0.21	0
8	SO4	D	203	-	4,4,4	0.19	0	6,6,6	0.34	0
9	GOL	D	204	-	5,5,5	0.51	0	5,5,5	0.72	0
8	SO4	E	519	-	4,4,4	0.29	0	6,6,6	0.55	0
12	PG4	E	520	-	12,12,12	0.54	0	11,11,11	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	F	201	2	14,14,15	0.53	0	15,19,21	0.95	1 (6%)
8	SO4	F	202	-	4,4,4	0.13	0	6,6,6	0.29	0
8	SO4	H	303	-	4,4,4	0.20	0	6,6,6	0.19	0
5	NAG	I	301	4	14,14,15	0.48	0	15,19,21	0.89	0
8	SO4	I	302	-	4,4,4	0.19	0	6,6,6	0.19	0
5	NAG	J	301	4	14,14,15	0.55	0	15,19,21	1.17	1 (6%)
8	SO4	J	302	-	4,4,4	0.20	0	6,6,6	0.15	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	NAG	C2-N2-C7	-2.56	119.75	123.04
5	J	301	NAG	C2-N2-C7	-2.31	120.07	123.04
5	C	504	NAG	C1-O5-C5	2.13	114.96	112.25
5	F	201	NAG	C1-O5-C5	3.13	116.22	112.25
5	B	201	NAG	C1-O5-C5	3.15	116.25	112.25
5	D	201	NAG	C1-O5-C5	3.20	116.31	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	514	SO4	1	0
8	B	203	SO4	2	0
9	B	205	GOL	1	0
9	D	204	GOL	1	0
12	E	520	PG4	1	0
8	I	302	SO4	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	316/320 (98%)	0.25	4 (1%) 79 61	62, 83, 113, 146	0
1	C	316/320 (98%)	0.28	6 (1%) 70 50	60, 83, 120, 188	0
1	E	316/320 (98%)	0.17	2 (0%) 90 78	49, 74, 105, 166	0
2	B	171/176 (97%)	0.15	3 (1%) 71 51	52, 86, 118, 189	0
2	D	171/176 (97%)	0.22	3 (1%) 71 51	56, 92, 128, 160	0
2	F	171/176 (97%)	0.20	3 (1%) 71 51	53, 82, 116, 166	0
3	L	211/214 (98%)	0.83	29 (13%) 4 2	84, 122, 154, 196	0
3	M	156/214 (72%)	1.31	35 (22%) 1 1	66, 132, 197, 239	0
3	N	213/214 (99%)	0.81	26 (12%) 5 3	85, 131, 174, 199	0
4	H	217/225 (96%)	0.20	4 (1%) 71 51	78, 101, 135, 200	0
4	I	185/225 (82%)	1.72	60 (32%) 1 0	85, 141, 218, 287	0
4	J	211/225 (93%)	0.73	28 (13%) 4 2	74, 129, 188, 226	0
All	All	2654/2805 (94%)	0.52	203 (7%) 17 9	49, 97, 174, 287	0

All (203) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	I	152	LEU	9.2
4	I	141	LEU	8.9
3	M	136	LEU	8.4
4	I	183	VAL	8.3
4	I	144	GLY	8.2
4	I	151	THR	7.3
3	M	135	PHE	7.0
4	I	121	VAL	6.9
4	I	202	SER	6.9
4	I	123	PRO	6.8
4	I	126	PRO	6.8

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Mol	Chain	Res	Type	RSRZ
3	M	132	VAL	6.8
3	M	159	VAL	6.6
4	I	118	ALA	6.4
3	M	114	THR	6.4
3	M	134	CYS	6.4
4	I	124	LEU	6.3
3	M	160	LEU	6.0
4	I	119	PRO	5.7
4	I	203	SER	5.7
4	I	140	CYS	5.6
4	I	150	VAL	5.6
4	I	179	SER	5.5
2	B	58	LYS	5.4
3	M	180	THR	5.3
4	I	136	VAL	5.3
3	M	118	PHE	5.2
3	M	161	ASN	5.2
3	M	133	VAL	5.1
4	J	213	ARG	5.1
3	M	113	PRO	5.0
4	I	111	VAL	4.9
4	I	175	TYR	4.8
3	M	116	SER	4.7
4	J	197	VAL	4.6
4	I	122	TYR	4.6
4	I	125	ALA	4.5
3	N	104	LEU	4.5
3	L	186	TYR	4.5
3	L	155	ARG	4.4
4	I	165	THR	4.4
3	L	19	VAL	4.4
4	J	203	SER	4.4
4	I	145	TYR	4.3
4	J	152	LEU	4.3
3	M	144	ILE	4.3
4	I	82(C)	LEU	4.3
4	J	205	LYS	4.2
4	I	170	LEU	4.2
4	I	137	THR	4.1
4	I	138	LEU	4.0
3	M	119	PRO	4.0
4	I	142	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
4	I	156	SER	3.9
4	J	123	PRO	3.9
3	M	179	LEU	3.9
4	H	205	LYS	3.8
4	I	166	PHE	3.8
4	J	117	THR	3.8
4	I	181	VAL	3.7
3	M	178	THR	3.7
4	I	184	THR	3.6
3	M	109	ALA	3.6
4	I	169	VAL	3.6
2	D	171	PHE	3.6
4	I	155	ASN	3.5
3	N	179	LEU	3.5
3	M	131	SER	3.5
4	I	176	THR	3.5
3	N	147	LYS	3.4
4	J	118	ALA	3.4
4	I	198	ALA	3.4
3	L	76	THR	3.4
3	L	148	TRP	3.4
3	N	11	MET	3.4
3	N	12	SER	3.4
3	M	115	VAL	3.4
4	J	206	VAL	3.3
4	J	210	ILE	3.3
4	J	124	LEU	3.3
3	L	13	THR	3.3
3	M	117	ILE	3.3
4	I	117	THR	3.2
4	J	207	ASP	3.2
4	I	16	ALA	3.2
4	J	139	GLY	3.2
3	N	153	SER	3.2
3	L	73	LEU	3.1
4	I	139	GLY	3.1
4	I	180	SER	3.1
1	E	222	TRP	3.1
4	I	154	TRP	3.1
4	J	193	ILE	3.1
4	I	11	LEU	3.1
4	J	140	CYS	3.0

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Mol	Chain	Res	Type	RSRZ
4	I	163	VAL	3.0
3	L	81	GLU	3.0
4	I	13	LYS	3.0
3	N	152	GLY	2.9
3	M	137	ASN	2.9
4	J	122	TYR	2.9
3	L	1	ASP	2.9
3	N	62	PHE	2.9
4	I	201	ALA	2.9
3	M	139	PHE	2.9
3	N	145	ASN	2.9
4	H	128	CYS	2.9
4	J	146	PHE	2.9
2	F	58	LYS	2.8
4	J	116	THR	2.8
4	J	204	THR	2.8
2	B	171	PHE	2.8
3	L	20	SER	2.7
4	J	96	TYR	2.7
3	L	9	LYS	2.7
3	L	104	LEU	2.7
1	A	322	ASN	2.7
3	M	175	MET	2.7
1	C	40	THR	2.7
1	C	227	SER	2.7
4	I	182	THR	2.6
1	A	10	GLY	2.6
3	L	21	VAL	2.6
4	J	125	ALA	2.6
4	I	160	SER	2.6
1	A	222	TRP	2.6
3	L	91	TYR	2.6
4	I	204	THR	2.5
4	J	113	ALA	2.5
3	N	155	ARG	2.5
4	J	11	LEU	2.5
3	M	177	SER	2.5
4	I	120	SER	2.5
4	H	130	ASP	2.5
4	I	146	PHE	2.5
3	L	86	TYR	2.5
3	N	4	MET	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	58	LYS	2.5
2	F	171	PHE	2.4
1	C	22	ASN	2.4
4	J	209	LYS	2.4
3	L	74	THR	2.4
3	M	13	THR	2.4
4	I	187	THR	2.4
3	L	63	THR	2.4
3	L	185	GLU	2.4
4	I	116	THR	2.4
3	N	79	GLN	2.4
3	M	163	TRP	2.4
4	I	14	PRO	2.4
3	M	169	LYS	2.4
4	J	115	LYS	2.4
4	J	119	PRO	2.4
3	N	67	SER	2.4
4	I	18	VAL	2.4
3	M	83	LEU	2.3
4	I	143	LYS	2.3
1	E	104	ASP	2.3
3	N	129	GLY	2.3
3	N	131	SER	2.3
1	C	11	ALA	2.3
4	J	198	ALA	2.3
3	L	10	PHE	2.3
3	N	63	THR	2.3
3	N	148	TRP	2.3
3	L	183	LYS	2.3
3	M	162	SER	2.2
3	M	140	TYR	2.2
4	I	177	LEU	2.2
4	J	23	LYS	2.2
4	I	199	HIS	2.2
3	N	199	LYS	2.2
2	F	1	GLY	2.2
3	L	187	GLU	2.2
3	N	156	GLN	2.2
3	N	206	VAL	2.2
3	N	60	ASP	2.2
3	N	154	GLU	2.2
3	L	205	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	60	ASN	2.1
4	I	178	SER	2.1
3	N	195	GLU	2.1
1	C	274	ILE	2.1
3	L	75	ILE	2.1
1	A	59	LEU	2.1
3	L	83	LEU	2.1
3	L	100	GLY	2.1
4	H	127	VAL	2.1
4	I	109	VAL	2.1
3	L	181	LEU	2.1
3	L	192	TYR	2.1
1	C	13	LEU	2.1
2	D	142	HIS	2.0
3	L	48	ILE	2.0
3	M	174	SER	2.0
3	L	209	PHE	2.0
4	I	157	GLY	2.0
3	M	106	ILE	2.0
3	N	2	ILE	2.0
3	N	197	THR	2.0
3	M	52	SER	2.0
3	M	108	ARG	2.0
3	N	125	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	PCA	H	1	8/9	0.95	0.16	-	123,125,127,127	0
4	PCA	I	1	8/9	0.92	0.18	-	152,156,161,164	0
4	PCA	J	1	8/9	0.91	0.30	-	160,164,167,168	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
11	NAG	E	515	14/15	0.96	0.20	0.81	72,87,94,96	0
7	NAG	C	506	14/15	0.94	0.22	-0.22	102,128,147,149	0
6	NAG	A	510	14/15	0.98	0.19	-0.25	81,98,105,105	0
10	NAG	C	510	14/15	0.94	0.18	-0.51	88,109,112,114	0
7	NAG	A	506	14/15	0.92	0.23	-0.58	103,137,158,163	0
7	NAG	E	511	14/15	0.95	0.20	-0.80	92,122,139,145	0
7	NAG	A	505	14/15	0.95	0.21	-	94,113,128,129	0
7	MAN	C	509	11/12	0.68	0.40	-	209,225,234,235	0
7	MAN	A	509	11/12	0.71	0.36	-	182,197,207,208	0
7	MAN	E	513	11/12	0.75	0.29	-	132,157,187,187	0
10	NAG	C	511	14/15	0.88	0.21	-	128,155,169,173	0
6	NAG	A	511	14/15	0.87	0.19	-	125,148,161,162	0
11	BMA	E	503	11/12	0.72	0.36	-	179,190,194,196	0
10	NAG	E	506	14/15	0.79	0.34	-	158,178,183,190	0
11	MAN	E	518	11/12	0.59	0.52	-	214,234,255,259	0
7	BMA	E	512	11/12	0.91	0.16	-	97,110,121,128	0
10	BMA	C	512	11/12	0.71	0.41	-	209,215,227,230	0
6	NAG	E	509	14/15	0.75	0.30	-	154,181,201,201	0
6	NAG	E	508	14/15	0.89	0.40	-	153,173,185,186	0
11	NAG	E	501	14/15	0.90	0.21	-	102,124,133,136	0
7	BMA	C	507	11/12	0.90	0.20	-	116,126,136,143	0
10	NAG	E	505	14/15	0.93	0.18	-	76,97,110,115	0
6	NAG	C	502	14/15	0.91	0.19	-	91,113,128,134	0
7	BMA	A	507	11/12	0.89	0.22	-	123,134,148,158	0
11	BMA	E	517	11/12	0.87	0.38	-	186,193,200,204	0
6	NAG	A	502	14/15	0.84	0.28	-	99,117,131,137	0
6	NAG	C	503	14/15	0.81	0.22	-	150,173,177,185	0
6	NAG	H	301	14/15	0.92	0.12	-	131,141,153,160	0
11	MAN	E	504	11/12	0.73	0.30	-	142,168,179,197	0
10	BMA	E	507	11/12	0.66	0.29	-	195,200,206,208	0
6	NAG	A	503	14/15	0.75	0.38	-	164,187,198,205	0
11	NAG	E	502	14/15	0.88	0.20	-	111,132,137,138	0
7	NAG	C	505	14/15	0.95	0.19	-	88,106,117,118	0
7	MAN	A	508	11/12	0.73	0.35	-	134,157,185,188	0
7	NAG	E	510	14/15	0.96	0.18	-	80,98,111,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	NAG	H	302	14/15	0.88	0.22	-	165,171,175,177	0
7	MAN	E	514	11/12	0.87	0.23	-	155,166,182,191	0
7	MAN	C	508	11/12	0.80	0.33	-	125,145,170,174	0
11	NAG	E	516	14/15	0.75	0.27	-	121,142,150,156	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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
8	SO4	C	515	5/5	0.76	0.35	4.18	181,181,181,181	0
5	NAG	B	201	14/15	0.67	0.29	2.55	152,166,178,185	0
9	GOL	B	205	6/6	0.64	0.34	2.45	100,100,100,100	0
12	PG4	E	520	13/13	0.82	0.31	2.32	110,110,110,110	0
9	GOL	D	204	6/6	0.68	0.32	1.94	103,103,103,103	0
5	NAG	F	201	14/15	0.89	0.27	1.90	125,136,146,152	0
8	SO4	C	514	5/5	0.93	0.20	-0.24	133,133,133,133	0
8	SO4	D	202	5/5	0.87	0.17	-0.67	159,159,159,159	0
8	SO4	J	302	5/5	0.86	0.19	-0.76	168,168,168,168	0
8	SO4	D	203	5/5	0.92	0.14	-0.82	109,109,109,109	0
8	SO4	F	202	5/5	0.95	0.16	-1.08	106,106,106,106	0
8	SO4	E	519	5/5	0.94	0.17	-1.16	101,101,101,101	0
8	SO4	B	204	5/5	0.97	0.15	-1.16	104,104,104,104	0
8	SO4	A	513	5/5	0.96	0.14	-1.26	98,98,98,98	0
8	SO4	H	303	5/5	0.93	0.10	-1.39	155,155,155,155	0
8	SO4	B	202	5/5	0.93	0.12	-1.59	149,149,149,149	0
8	SO4	B	203	5/5	0.98	0.09	-2.20	115,115,115,115	0
5	NAG	I	301	14/15	0.82	0.17	-	166,184,208,216	0
5	NAG	J	301	14/15	0.92	0.19	-	126,139,155,161	0
8	SO4	A	514	5/5	0.78	0.76	-	181,181,181,181	0
8	SO4	A	516	5/5	0.88	0.20	-	166,166,166,166	0
8	SO4	C	513	5/5	0.81	0.21	-	183,183,183,183	0
8	SO4	I	302	5/5	0.76	0.19	-	161,161,161,161	0
8	SO4	A	512	5/5	0.94	0.15	-	178,178,178,178	0
5	NAG	C	504	14/15	0.83	0.39	-	145,168,179,183	0
8	SO4	A	515	5/5	0.58	0.48	-	197,197,197,197	0
5	NAG	C	501	14/15	0.75	0.30	-	145,168,180,184	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	D	201	14/15	0.84	0.30	-	146,155,171,178	0
5	NAG	A	504	14/15	0.82	0.48	-	160,181,195,195	0
5	NAG	A	501	14/15	0.82	0.28	-	132,153,159,160	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.