



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:34 PM GMT

PDB ID : 4P9H
Title : Crystal structure of 8ANC195 Fab in complex with gp120 of 93TH057 HIV-1 and soluble CD4 D1D2
Authors : Scharf, L.; Bjorkman, P.J.
Deposited on : 2014-04-04
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

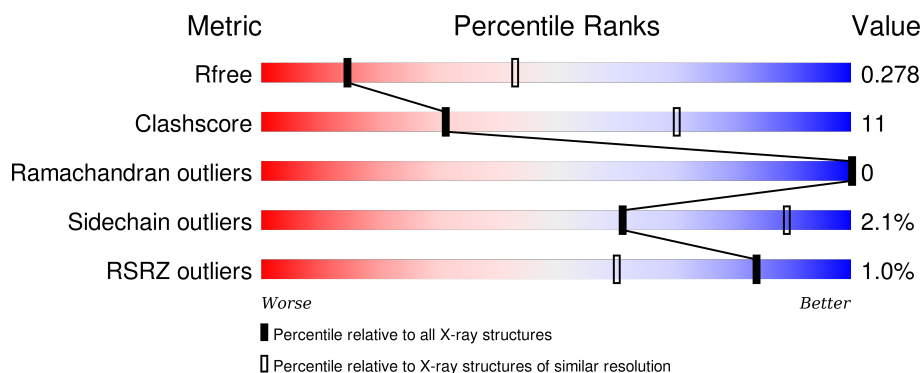
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	192	<div> <div>2%</div> <div>68%</div> <div>18%</div> <div>13%</div> </div>
2	G	361	<div> <div>80%</div> <div>13%</div> <div>6%</div> </div>
3	H	244	<div> <div>66%</div> <div>23%</div> <div>12%</div> </div>
4	L	215	<div> <div>2%</div> <div>80%</div> <div>19%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	BAM	G	602	-	-	-	X
7	BAM	G	603	-	-	-	X

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 7371 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 T-cell surface glycoprotein CD4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	167	Total	C	N	O	S	0	0	0
			1225	763	207	251	4			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	75	THR	LYS	engineered mutation	UNP P01730
C	183	ILE	-	expression tag	UNP P01730
C	184	ASP	-	expression tag	UNP P01730
C	185	GLY	-	expression tag	UNP P01730
C	186	ARG	-	expression tag	UNP P01730
C	187	HIS	-	expression tag	UNP P01730
C	188	HIS	-	expression tag	UNP P01730
C	189	HIS	-	expression tag	UNP P01730
C	190	HIS	-	expression tag	UNP P01730
C	191	HIS	-	expression tag	UNP P01730
C	192	HIS	-	expression tag	UNP P01730

- Molecule 2 is a protein called Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	338	Total	C	N	O	S	0	0	0
			2616	1639	453	500	24			

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	65	CYS	VAL	engineered mutation	UNP Q0ED31
G	88	GLN	ASN	engineered mutation	UNP Q0ED31
G	115	CYS	SER	engineered mutation	UNP Q0ED31
G	124	GLY	-	linker	UNP Q0ED31
G	198	GLY	-	linker	UNP Q0ED31

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Chain	Residue	Modelled	Actual	Comment	Reference
G	289	GLN	ASN	engineered mutation	UNP Q0ED31
G	318	GLY	-	linker	UNP Q0ED31
G	319	GLY	-	linker	UNP Q0ED31
G	320	SER	-	linker	UNP Q0ED31
G	321	GLY	-	linker	UNP Q0ED31
G	322	SER	-	linker	UNP Q0ED31
G	323	GLY	-	linker	UNP Q0ED31
G	334	GLN	ASN	engineered mutation	UNP Q0ED31
G	392	GLN	ASN	engineered mutation	UNP Q0ED31
G	448	GLN	ASN	engineered mutation	UNP Q0ED31
G	493	GLY	-	expression tag	UNP Q0ED31
G	494	SER	-	expression tag	UNP Q0ED31
G	495	HIS	-	expression tag	UNP Q0ED31
G	496	HIS	-	expression tag	UNP Q0ED31
G	497	HIS	-	expression tag	UNP Q0ED31
G	498	HIS	-	expression tag	UNP Q0ED31
G	499	HIS	-	expression tag	UNP Q0ED31
G	500	HIS	-	expression tag	UNP Q0ED31

- Molecule 3 is a protein called Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	215	Total	C	N	O	S	0	0	0
			1573	1000	262	306	5			

- Molecule 4 is a protein called Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	212	Total	C	N	O	S	0	0	0
			1549	969	263	312	5			

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

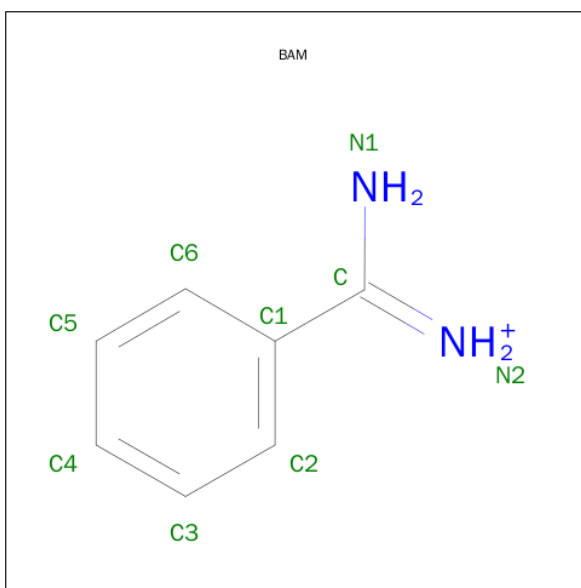
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	2	Total	C	N	O	0	0
			28	16	2	10		
5	G	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	G	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 7 is BENZAMIDINE (three-letter code: BAM) (formula: $C_7H_9N_2$).

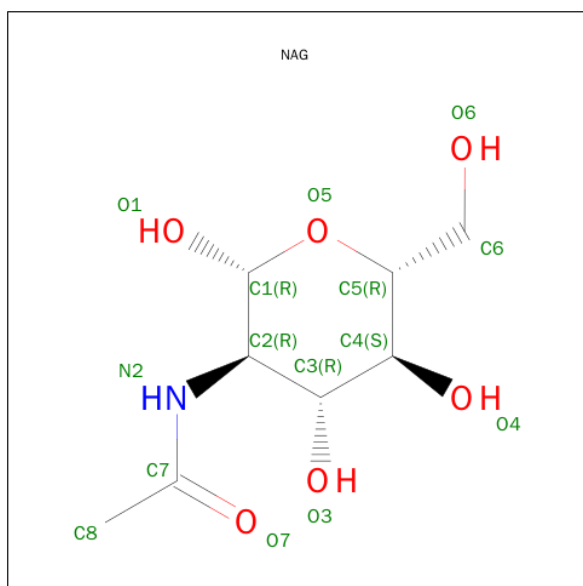


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	G	1	Total	C	N	0	0
			9	7	2		
7	G	1	Total	C	N	0	0
			9	7	2		

- Molecule 8 is a polymer of unknown type called SUGAR (10-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	G	10	Total	C	N	O	0	0
			116	64	2	50		

- Molecule 9 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	G	1	Total	C	N	O	0	0
			14	8	1	5		
9	G	1	Total	C	N	O	0	0
			14	8	1	5		
9	H	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 10 is a polymer of unknown type called SUGAR (4-MER).

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

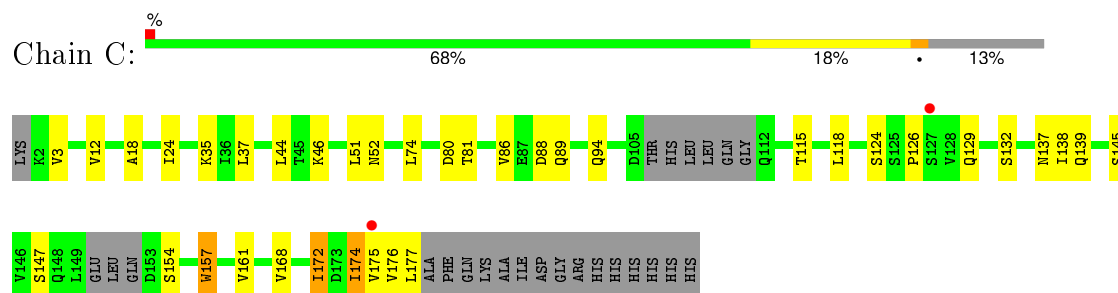
- Molecule 11 is a polymer of unknown type called SUGAR (5-MER).

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

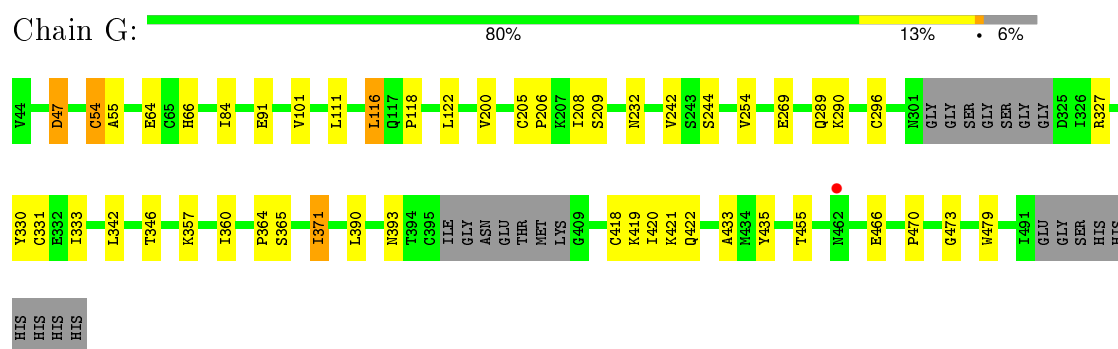
3 Residue-property plots [i](#)

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 ($RSRZ > 2$). 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.

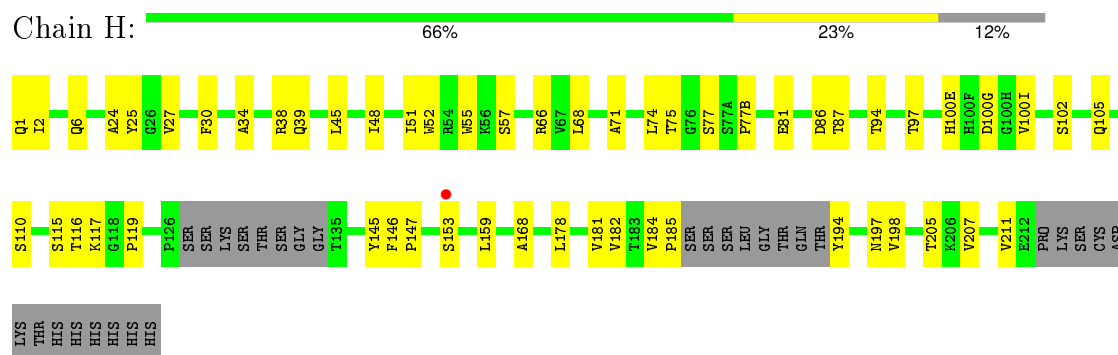
- Molecule 1: T-cell surface glycoprotein CD4



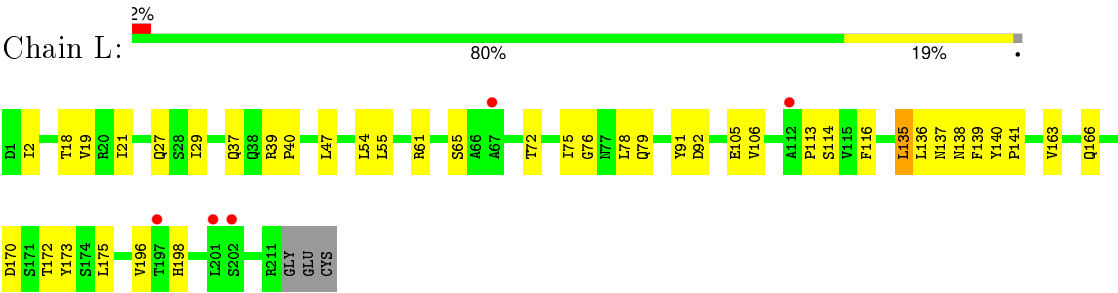
- Molecule 2: Envelope glycoprotein gp120



- Molecule 3: Fab heavy chain



- Molecule 4: Fab light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.53Å 132.49Å 142.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.22 – 3.00 39.22 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.22-3.00) 97.6 (39.22-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 2.65Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.235 , 0.272 0.245 , 0.278	Depositor DCC
R_{free} test set	1414 reflections (5.76%)	DCC
Wilson B-factor (Å ²)	61.6	Xtriage
Anisotropy	0.642	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 36730 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7371	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EPE, BAM, NAG, BMA, 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	C	0.37	0/1241	0.57	1/1686 (0.1%)
2	G	0.43	0/2672	0.54	0/3637
3	H	0.39	0/1615	0.49	0/2214
4	L	0.34	0/1583	0.50	0/2165
All	All	0.39	0/7111	0.52	1/9702 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	88	ASP	CB-CG-OD2	5.14	122.92	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1225	0	1162	36	0
2	G	2616	0	2495	38	0
3	H	1573	0	1491	37	0
4	L	1549	0	1434	47	0
5	C	28	0	25	2	0
5	G	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	G	15	0	18	1	0
7	G	18	0	18	0	0
8	G	116	0	97	3	0
9	G	28	0	26	0	0
9	H	14	0	13	0	0
10	G	100	0	86	1	0
11	G	61	0	52	0	0
All	All	7371	0	6942	155	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 11.

The worst 5 of 155 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:419:LYS:HE3	2:G:421:LYS:HD2	1.36	1.07
1:C:175:VAL:HG12	1:C:176:VAL:H	1.17	1.05
1:C:175:VAL:HG12	1:C:176:VAL:N	1.73	0.95
2:G:419:LYS:CE	2:G:421:LYS:HD3	1.98	0.94
2:G:419:LYS:HE3	2:G:421:LYS:CD	1.97	0.94

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	C	161/192 (84%)	153 (95%)	8 (5%)	0	100	100
2	G	332/361 (92%)	315 (95%)	17 (5%)	0	100	100
3	H	209/244 (86%)	207 (99%)	2 (1%)	0	100	100
4	L	210/215 (98%)	207 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	912/1012 (90%)	882 (97%)	30 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	C	136/173 (79%)	127 (93%)	9 (7%)	21	57
2	G	293/318 (92%)	289 (99%)	4 (1%)	74	93
3	H	173/210 (82%)	171 (99%)	2 (1%)	78	94
4	L	162/182 (89%)	161 (99%)	1 (1%)	90	97
All	All	764/883 (86%)	748 (98%)	16 (2%)	61	89

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	172	ILE
1	C	174	ILE
2	G	371	ILE
1	C	157	TRP
3	H	100(G)	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	89	GLN
2	G	229	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

27 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	NAG	C	1001	1,5	14,14,15	1.23	3 (21%)	15,19,21	1.81	4 (26%)
5	NAG	C	1002	5	14,14,15	1.30	2 (14%)	15,19,21	1.74	2 (13%)
8	NAG	G	604	8,2	14,14,15	1.39	3 (21%)	15,19,21	0.87	1 (6%)
8	NAG	G	605	8	14,14,15	1.29	2 (14%)	15,19,21	0.97	1 (6%)
8	BMA	G	606	8	11,11,12	1.46	2 (18%)	14,15,17	1.33	1 (7%)
8	MAN	G	607	8	11,11,12	1.55	2 (18%)	14,15,17	1.08	1 (7%)
8	MAN	G	608	8	11,11,12	1.34	2 (18%)	14,15,17	1.62	1 (7%)
8	MAN	G	609	8	11,11,12	1.43	2 (18%)	14,15,17	0.67	0
8	MAN	G	610	8	11,11,12	1.46	2 (18%)	14,15,17	1.07	2 (14%)
8	MAN	G	611	8	11,11,12	1.69	2 (18%)	14,15,17	1.52	3 (21%)
8	MAN	G	612	8	11,11,12	1.33	2 (18%)	14,15,17	0.67	0
8	MAN	G	613	8	11,11,12	1.21	2 (18%)	14,15,17	1.03	2 (14%)
10	NAG	G	615	10,2	14,14,15	1.37	2 (14%)	15,19,21	1.10	1 (6%)
10	NAG	G	616	10	14,14,15	1.33	3 (21%)	15,19,21	1.22	1 (6%)
10	BMA	G	617	10	11,11,12	1.28	2 (18%)	14,15,17	1.88	1 (7%)
10	MAN	G	618	10	11,11,12	1.37	2 (18%)	14,15,17	1.01	1 (7%)
11	NAG	G	619	11,2	14,14,15	1.46	3 (21%)	15,19,21	1.57	4 (26%)
11	NAG	G	620	11	14,14,15	1.39	1 (7%)	15,19,21	3.45	6 (40%)
11	BMA	G	621	11	11,11,12	1.44	2 (18%)	14,15,17	1.17	2 (14%)
11	MAN	G	622	11	11,11,12	1.84	2 (18%)	14,15,17	2.75	3 (21%)
11	MAN	G	623	11	11,11,12	1.85	2 (18%)	14,15,17	2.27	2 (14%)
5	NAG	G	624	2,5	14,14,15	1.20	3 (21%)	15,19,21	1.29	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	G	625	5	14,14,15	1.43	3 (21%)	15,19,21	0.87	0
10	NAG	G	627	10,2	14,14,15	1.36	2 (14%)	15,19,21	1.32	2 (13%)
10	NAG	G	628	10	14,14,15	1.36	3 (21%)	15,19,21	0.99	1 (6%)
10	BMA	G	629	10	11,11,12	1.35	2 (18%)	14,15,17	0.89	0
10	MAN	G	630	10	11,11,12	1.40	2 (18%)	14,15,17	1.01	1 (7%)

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	C	1001	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	1002	5	-	0/6/23/26	0/1/1/1
8	NAG	G	604	8,2	-	0/6/23/26	0/1/1/1
8	NAG	G	605	8	-	0/6/23/26	0/1/1/1
8	BMA	G	606	8	-	0/2/19/22	0/1/1/1
8	MAN	G	607	8	-	0/2/19/22	0/1/1/1
8	MAN	G	608	8	-	0/2/19/22	0/1/1/1
8	MAN	G	609	8	-	0/2/19/22	0/1/1/1
8	MAN	G	610	8	-	0/2/19/22	0/1/1/1
8	MAN	G	611	8	-	0/2/19/22	0/1/1/1
8	MAN	G	612	8	-	0/2/19/22	0/1/1/1
8	MAN	G	613	8	-	0/2/19/22	0/1/1/1
10	NAG	G	615	10,2	-	0/6/23/26	0/1/1/1
10	NAG	G	616	10	-	0/6/23/26	0/1/1/1
10	BMA	G	617	10	-	0/2/19/22	0/1/1/1
10	MAN	G	618	10	-	0/2/19/22	0/1/1/1
11	NAG	G	619	11,2	-	0/6/23/26	0/1/1/1
11	NAG	G	620	11	-	0/6/23/26	0/1/1/1
11	BMA	G	621	11	-	0/2/19/22	0/1/1/1
11	MAN	G	622	11	-	0/2/19/22	0/1/1/1
11	MAN	G	623	11	-	0/2/19/22	0/1/1/1
5	NAG	G	624	2,5	-	0/6/23/26	0/1/1/1
5	NAG	G	625	5	-	0/6/23/26	0/1/1/1
10	NAG	G	627	10,2	-	0/6/23/26	0/1/1/1
10	NAG	G	628	10	-	0/6/23/26	0/1/1/1
10	BMA	G	629	10	-	0/2/19/22	0/1/1/1
10	MAN	G	630	10	-	0/2/19/22	0/1/1/1

The worst 5 of 60 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	G	610	MAN	C2-C3	-3.43	1.47	1.52
11	G	622	MAN	C2-C3	-3.28	1.48	1.52
8	G	606	BMA	C2-C3	-3.16	1.48	1.52
8	G	611	MAN	C2-C3	-3.15	1.48	1.52
8	G	609	MAN	C2-C3	-3.08	1.48	1.52

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	G	617	BMA	C1-O5-C5	-6.39	104.14	112.25
5	C	1001	NAG	C1-O5-C5	-5.01	105.89	112.25
11	G	620	NAG	O7-C7-N2	-4.04	113.64	121.86
10	G	627	NAG	C1-O5-C5	-3.81	107.41	112.25
8	G	606	BMA	C1-O5-C5	-3.32	108.03	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
5	C	1001	NAG	2	0
5	C	1002	NAG	2	0
8	G	611	MAN	1	0
8	G	613	MAN	2	0
10	G	615	NAG	1	0
5	G	625	NAG	1	0

5.6 Ligand geometry

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	EPE	G	601	-	14,15,15	1.30	1 (7%)	18,20,20	1.51	3 (16%)
7	BAM	G	602	-	9,9,9	1.44	2 (22%)	9,11,11	0.93	0
7	BAM	G	603	-	9,9,9	1.50	2 (22%)	9,11,11	0.64	0
9	NAG	G	614	2	14,14,15	1.38	3 (21%)	15,19,21	0.79	0
9	NAG	G	626	2	14,14,15	1.35	2 (14%)	15,19,21	1.73	1 (6%)
9	NAG	H	1001	3	14,14,15	1.40	3 (21%)	15,19,21	0.97	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	EPE	G	601	-	-	0/9/19/19	0/1/1/1
7	BAM	G	602	-	-	0/4/4/4	0/1/1/1
7	BAM	G	603	-	-	0/4/4/4	0/1/1/1
9	NAG	G	614	2	-	0/6/23/26	0/1/1/1
9	NAG	G	626	2	-	0/6/23/26	0/1/1/1
9	NAG	H	1001	3	-	0/6/23/26	0/1/1/1

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	601	EPE	C2-N1	-2.20	1.40	1.46
9	G	626	NAG	C7-N2	2.11	1.42	1.34
7	G	602	BAM	C1-C	2.11	1.51	1.47
9	H	1001	NAG	C7-N2	2.15	1.42	1.34
9	H	1001	NAG	O7-C7	2.18	1.28	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	G	626	NAG	C1-O5-C5	-5.80	104.89	112.25
6	G	601	EPE	O3S-S-O2S	-2.29	106.27	111.61
6	G	601	EPE	O2S-S-C10	3.02	109.49	106.91
6	G	601	EPE	O1S-S-C10	4.03	110.34	106.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	601	EPE	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	C	167/192 (86%)	-0.11	2 (1%) 81 55	42, 74, 105, 120	0
2	G	338/361 (93%)	-0.33	1 (0%) 94 84	28, 47, 75, 136	0
3	H	215/244 (88%)	-0.28	1 (0%) 91 76	41, 60, 108, 113	0
4	L	212/215 (98%)	-0.18	5 (2%) 62 32	50, 77, 110, 155	0
All	All	932/1012 (92%)	-0.24	9 (0%) 84 60	28, 61, 106, 155	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	462	ASN	3.3
1	C	127	SER	3.0
4	L	202	SER	2.8
4	L	112	ALA	2.7
1	C	175	VAL	2.5

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

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

6.3 Carbohydrates ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
10	NAG	G	615	14/15	0.94	0.25	1.72	56,72,105,131	0
8	MAN	G	613	11/12	0.89	0.22	1.37	53,63,65,68	11
5	NAG	G	624	14/15	0.89	0.20	1.18	83,94,106,117	0
11	NAG	G	619	14/15	0.91	0.19	0.23	46,57,77,98	0
8	NAG	G	604	14/15	0.94	0.23	0.11	46,50,59,67	0
8	MAN	G	608	11/12	0.93	0.21	-0.14	65,69,79,81	0
8	MAN	G	609	11/12	0.91	0.19	-0.52	65,69,74,74	0
11	NAG	G	620	14/15	0.94	0.18	-0.66	58,66,76,78	0
5	NAG	C	1002	14/15	0.71	0.31	-	118,129,132,133	0
10	NAG	G	616	14/15	0.92	0.19	-	66,82,92,98	0
8	MAN	G	612	11/12	0.85	0.35	-	88,97,104,105	0
10	MAN	G	630	11/12	0.73	0.32	-	118,125,131,131	0
8	BMA	G	606	11/12	0.89	0.17	-	63,66,72,76	0
10	NAG	G	627	14/15	0.91	0.19	-	58,68,78,93	0
10	NAG	G	628	14/15	0.90	0.24	-	103,117,127,129	0
11	MAN	G	622	11/12	0.86	0.24	-	81,88,98,101	11
5	NAG	C	1001	14/15	0.72	0.20	-	106,114,125,127	0
5	NAG	G	625	14/15	0.65	0.33	-	122,136,140,141	0
8	MAN	G	610	11/12	0.90	0.14	-	60,72,78,81	0
10	BMA	G	629	11/12	0.78	0.24	-	127,131,133,138	0
8	MAN	G	607	11/12	0.90	0.20	-	71,78,87,100	0
11	BMA	G	621	11/12	0.87	0.14	-	83,92,105,106	0
8	NAG	G	605	14/15	0.93	0.20	-	51,56,65,82	0
10	BMA	G	617	11/12	0.80	0.25	-	100,115,120,123	0
10	MAN	G	618	11/12	0.82	0.28	-	86,119,124,129	0
11	MAN	G	623	11/12	0.55	0.30	-	98,115,126,129	0
8	MAN	G	611	11/12	0.82	0.20	-	66,80,86,94	11

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	BAM	G	602	9/9	0.91	0.33	4.01	33,38,43,45	9
7	BAM	G	603	9/9	0.89	0.28	3.76	40,43,52,55	9
9	NAG	G	614	14/15	0.78	0.30	1.37	100,105,116,120	0
6	EPE	G	601	15/15	0.94	0.23	0.28	37,45,63,73	0
9	NAG	G	626	14/15	0.76	0.30	0.21	110,120,134,145	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
9	NAG	H	1001	14/15	0.76	0.27	-	90,108,112,113	0

6.5 Other polymers [i](#)

There are no such residues in this entry.