



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 10:13 PM GMT

PDB ID : 5CEZ
Title : Crystal Structure of the BG505 SOSIP gp140 HIV-1 Env trimer in Complex with an early putative precursor of the PGT121 family at 3.0 Angstrom
Authors : Wilson, I.A.; Garces, F.
Deposited on : 2015-07-08
Resolution : 3.03 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
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) : rb-20026982

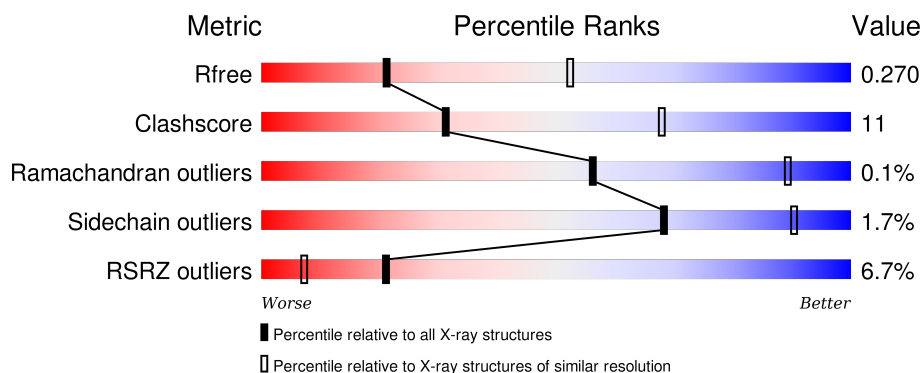
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.03 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	1995 (3.08-3.00)
Clashscore	102246	2351 (3.08-3.00)
Ramachandran outliers	100387	2272 (3.08-3.00)
Sidechain outliers	100360	2275 (3.08-3.00)
RSRZ outliers	91569	2013 (3.08-3.00)

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	G	480	<div> <div>2%</div> <div>73% 21% 6%</div> </div>
2	B	153	<div> <div>3%</div> <div>75% 20% . .</div> </div>
3	L	218	<div> <div>78% 17% . .</div> </div>
4	H	236	<div> <div>2%</div> <div>74% 22% . .</div> </div>
5	D	240	<div> <div>25%</div> <div>86% 14%</div> </div>

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Mol	Chain	Length	Quality of chain
6	E	216	<p>12% 83% 15%</p>

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
9	MAN	L	309	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 12135 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 Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	452	Total	C	N	O	S	0	0	0
			3544	2224	625	668	27			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	137	ALA	ASN	engineered mutation	UNP Q2N0S6
G	332	ASN	THR	engineered mutation	UNP Q2N0S6
G	501	CYS	ALA	engineered mutation	UNP Q2N0S6
G	509	ARG	GLU	insertion	UNP Q2N0S6
G	510	ARG	LYS	insertion	UNP Q2N0S6
G	512	ARG	-	insertion	UNP Q2N0S6
G	513	ARG	-	insertion	UNP Q2N0S6

- Molecule 2 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	147	Total	C	N	O	S	0	0	0
			1171	740	205	220	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	engineered mutation	UNP Q2N0S6
B	605	CYS	THR	engineered mutation	UNP Q2N0S6

- Molecule 3 is a protein called 3H+109L Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	211	Total	C	N	O	S	0	0	0
			1603	1007	276	315	5			

- Molecule 4 is a protein called 3H+109L Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	231	Total	C	N	O	S	0	0	0
			1744	1108	283	347	6			

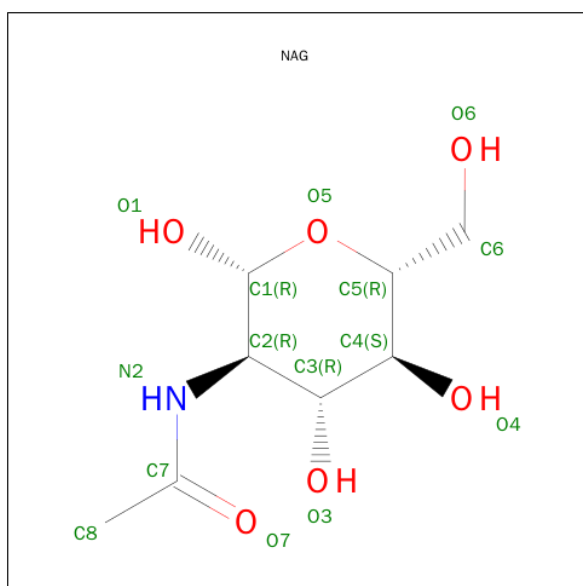
- Molecule 5 is a protein called 35022 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	240	Total	C	N	O	S	0	0	0
			1813	1150	303	352	8			

- Molecule 6 is a protein called 35022 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	213	Total	C	N	O	S	0	0	0
			1615	1012	267	328	8			

- Molecule 7 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

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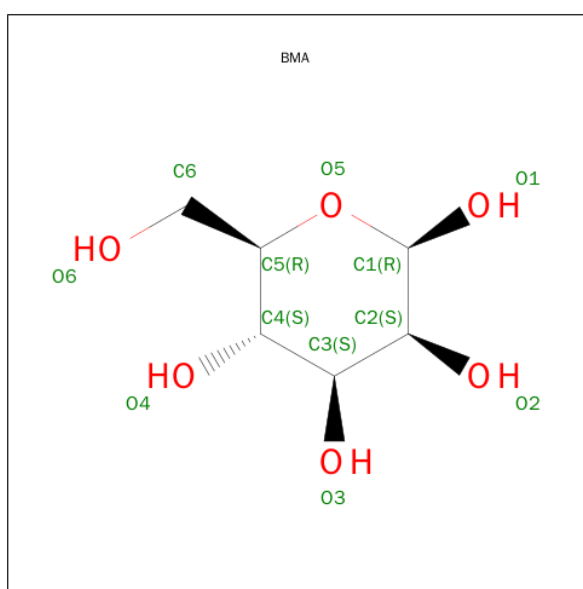
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1	Total	C	N	O	0	0
			14	8	1	5		
7	G	1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

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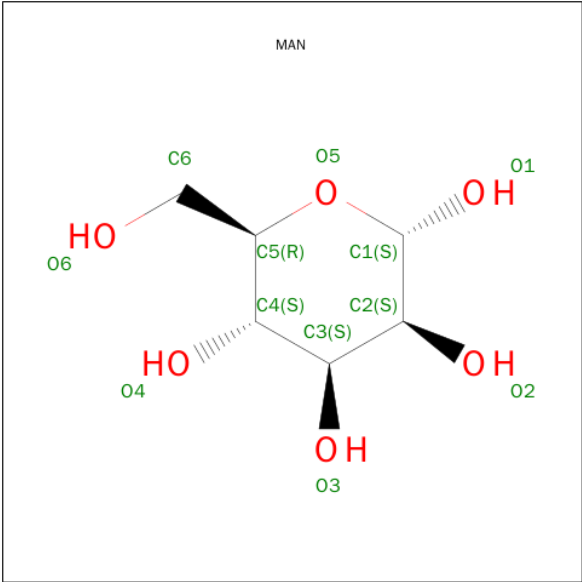
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	L	1	Total	C	N	O	0	0
			14	8	1	5		
7	L	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	G	1	Total	C	O	0	0
			11	6	5		
8	G	1	Total	C	O	0	0
			11	6	5		
8	G	1	Total	C	O	0	0
			11	6	5		
8	G	1	Total	C	O	0	0
			11	6	5		
8	L	1	Total	C	O	0	0
			11	6	5		

- Molecule 9 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).

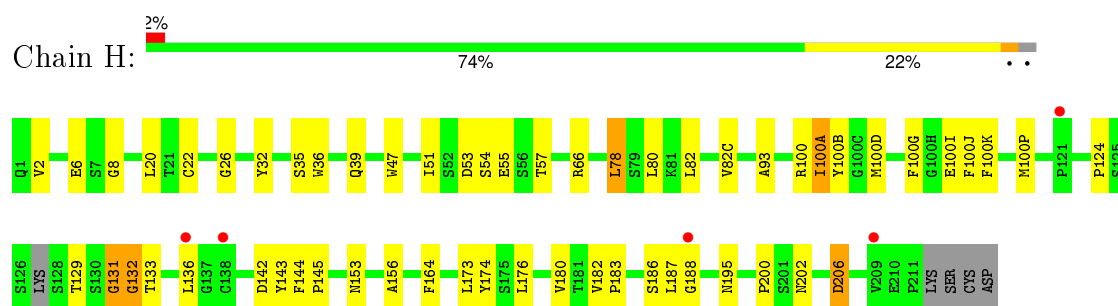


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	G	1	Total	C	O	0	0
			11	6	5		
9	G	1	Total	C	O	0	0
			11	6	5		
9	G	1	Total	C	O	0	0
			11	6	5		
9	G	1	Total	C	O	0	0
			11	6	5		
9	G	1	Total	C	O	0	0
			11	6	5		
9	G	1	Total	C	O	0	0
			11	6	5		
9	G	1	Total	C	O	0	0
			11	6	5		
9	L	1	Total	C	O	0	0
			11	6	5		
9	L	1	Total	C	O	0	0
			11	6	5		
9	L	1	Total	C	O	0	0
			11	6	5		
9	L	1	Total	C	O	0	0
			11	6	5		

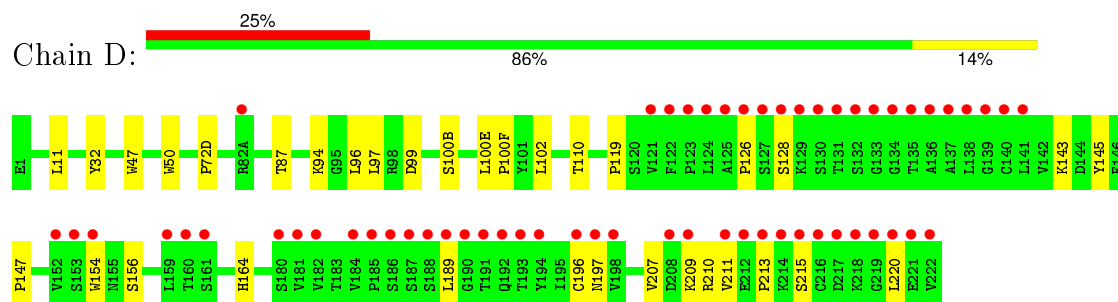
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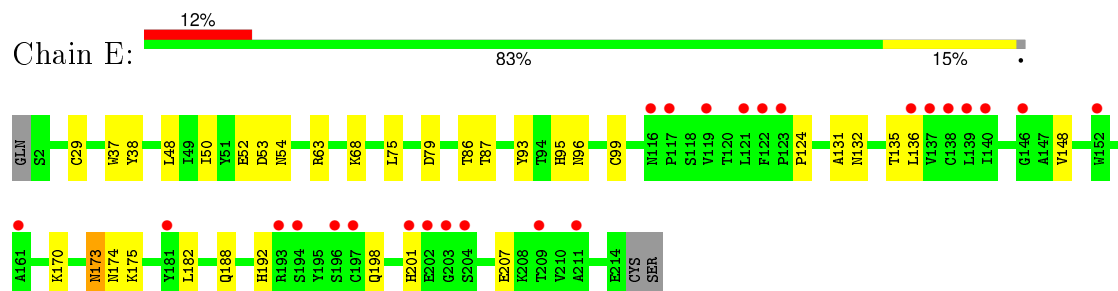
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	L	1	Total	C	O	0	0
			11	6	5		
9	L	1	Total	C	O	0	0
			11	6	5		
9	H	1	Total	C	O	0	0
			11	6	5		
9	D	1	Total	C	O	0	0
			11	6	5		



• Molecule 5: 35022 Fab Heavy Chain



• Molecule 6: 35022 Fab Light Chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	127.98Å 127.98Å 316.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.49 – 3.03 44.97 – 3.03	Depositor EDS
% Data completeness (in resolution range)	99.5 (40.49-3.03) 99.7 (44.97-3.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.233 , 0.266 0.245 , 0.270	Depositor DCC
R_{free} test set	2813 reflections (5.24%)	DCC
Wilson B-factor (Å ²)	92.6	Xtriage
Anisotropy	0.668	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 66.6	EDS
Estimated twinning fraction	0.046 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 56481 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12135	wwPDB-VP
Average B, all atoms (Å ²)	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, 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	G	0.26	0/3617	0.46	0/4911
2	B	0.24	0/1192	0.42	0/1618
3	L	0.25	0/1646	0.45	1/2247 (0.0%)
4	H	0.25	0/1787	0.45	0/2436
5	D	0.25	0/1860	0.45	0/2533
6	E	0.25	0/1659	0.47	0/2269
All	All	0.25	0/11761	0.45	1/16014 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	L	0	3
4	H	0	2
6	E	0	1
All	All	0	6

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	46	LEU	CA-CB-CG	5.67	128.33	115.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	H	131	GLY	Peptide
4	H	132	GLY	Peptide
3	L	150	LYS	Peptide
3	L	50	ASN	Peptide
3	L	52	GLN	Peptide

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	G	3544	0	3474	106	0
2	B	1171	0	1158	48	0
3	L	1603	0	1545	39	0
4	H	1744	0	1710	39	0
5	D	1813	0	1784	21	0
6	E	1615	0	1544	24	0
7	B	42	0	38	1	0
7	G	322	0	285	3	0
7	L	28	0	24	5	0
8	G	44	0	33	1	0
8	L	11	0	7	0	0
9	D	11	0	10	0	0
9	G	110	0	95	7	0
9	H	11	0	10	4	0
9	L	66	0	54	12	0
All	All	12135	0	11771	257	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 257 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)
1:G:259:LEU:HD13	1:G:449:ILE:CD1	1.74	1.16
1:G:259:LEU:CD1	1:G:449:ILE:HD12	1.75	1.14
1:G:65:LYS:HD2	2:B:563:GLN:NE2	1.65	1.11
1:G:259:LEU:HD13	1:G:449:ILE:HD12	1.31	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:71:THR:HG22	1:G:72:HIS:H	1.21	1.03

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	G	444/480 (92%)	423 (95%)	21 (5%)	0	100	100
2	B	145/153 (95%)	136 (94%)	9 (6%)	0	100	100
3	L	209/218 (96%)	201 (96%)	7 (3%)	1 (0%)	34	74
4	H	227/236 (96%)	222 (98%)	5 (2%)	0	100	100
5	D	238/240 (99%)	236 (99%)	2 (1%)	0	100	100
6	E	211/216 (98%)	206 (98%)	5 (2%)	0	100	100
All	All	1474/1543 (96%)	1424 (97%)	49 (3%)	1 (0%)	56	89

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	84	ALA

5.3.2 Protein sidechains [i](#)

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	G	401/427 (94%)	394 (98%)	7 (2%)	68	90
2	B	127/129 (98%)	125 (98%)	2 (2%)	70	91
3	L	175/181 (97%)	171 (98%)	4 (2%)	58	86
4	H	200/205 (98%)	194 (97%)	6 (3%)	48	82
5	D	203/203 (100%)	202 (100%)	1 (0%)	92	97
6	E	186/189 (98%)	184 (99%)	2 (1%)	80	94
All	All	1292/1334 (97%)	1270 (98%)	22 (2%)	68	90

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	L	31	ARG
3	L	152	ASP
6	E	99	CYS
3	L	51	ASN
3	L	95(B)	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
3	L	127	GLN
3	L	170	ASN
6	E	95	HIS
2	B	607	ASN
5	D	197	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

51 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$
7	NAG	B	701	2	14,14,15	2.64	3 (21%)	15,19,21	0.55	0
7	NAG	B	702	2	14,14,15	2.05	2 (14%)	15,19,21	1.33	1 (6%)
7	NAG	B	703	2	14,14,15	0.18	0	15,19,21	0.31	0
9	MAN	D	301	-	11,11,12	0.63	0	15,15,17	1.08	2 (13%)
7	NAG	G	601	1,7	14,14,15	0.25	0	15,19,21	0.41	0
7	NAG	G	602	8,7	14,14,15	0.32	0	15,19,21	0.31	0
8	BMA	G	603	9,7	11,11,12	0.65	0	15,15,17	0.69	0
9	MAN	G	604	8	11,11,12	0.65	0	15,15,17	1.09	2 (13%)
9	MAN	G	605	9,8	11,11,12	0.67	0	15,15,17	1.02	2 (13%)
9	MAN	G	606	9	11,11,12	0.52	0	15,15,17	0.68	0
9	MAN	G	607	9	11,11,12	0.62	0	15,15,17	0.60	0
7	NAG	G	608	1,7	14,14,15	0.18	0	15,19,21	0.42	0
7	NAG	G	609	7	14,14,15	0.26	0	15,19,21	0.25	0
7	NAG	G	610	1	14,14,15	0.16	0	15,19,21	0.32	0
7	NAG	G	611	1	14,14,15	0.16	0	15,19,21	0.33	0
7	NAG	G	612	1,7	14,14,15	0.26	0	15,19,21	0.40	0
7	NAG	G	613	7	14,14,15	0.17	0	15,19,21	0.30	0
7	NAG	G	614	1,7	14,14,15	0.24	0	15,19,21	0.55	0
7	NAG	G	615	7	14,14,15	1.37	1 (7%)	15,19,21	0.31	0
7	NAG	G	616	1	14,14,15	0.20	0	15,19,21	0.23	0
7	NAG	G	617	1,7	14,14,15	0.16	0	15,19,21	0.34	0
7	NAG	G	618	7	14,14,15	2.66	3 (21%)	15,19,21	0.81	1 (6%)
7	NAG	G	619	1,7	14,14,15	0.22	0	15,19,21	0.26	0
7	NAG	G	620	7	14,14,15	0.18	0	15,19,21	0.34	0
7	NAG	G	621	1,7	14,14,15	0.21	0	15,19,21	0.26	0
7	NAG	G	622	7	14,14,15	0.22	0	15,19,21	0.35	0
7	NAG	G	623	1,7	14,14,15	0.25	0	15,19,21	0.26	0
7	NAG	G	624	8,7	14,14,15	0.20	0	15,19,21	0.26	0
8	BMA	G	625	9,7	11,11,12	0.59	0	15,15,17	0.78	0
9	MAN	G	626	8	11,11,12	0.68	0	15,15,17	1.09	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	MAN	G	627	8	11,11,12	0.68	0	15,15,17	1.04	2 (13%)
7	NAG	G	628	1,7	14,14,15	0.26	0	15,19,21	0.26	0
7	NAG	G	629	8,7	14,14,15	0.23	0	15,19,21	0.26	0
8	BMA	G	630	9,7	11,11,12	0.61	0	15,15,17	0.78	0
9	MAN	G	631	8	11,11,12	0.67	0	15,15,17	1.04	2 (13%)
7	NAG	G	632	1,7	14,14,15	0.30	0	15,19,21	0.31	0
7	NAG	G	633	8,7	14,14,15	0.90	1 (7%)	15,19,21	1.29	1 (6%)
8	BMA	G	634	9,7	11,11,12	0.67	0	15,15,17	0.75	0
9	MAN	G	635	8	11,11,12	0.62	0	15,15,17	1.17	2 (13%)
9	MAN	G	636	9,8	11,11,12	0.81	1 (9%)	15,15,17	1.29	3 (20%)
9	MAN	G	637	9	11,11,12	0.69	0	15,15,17	1.01	1 (6%)
9	MAN	H	301	-	11,11,12	0.25	0	15,15,17	0.64	0
7	NAG	L	301	1,7	14,14,15	0.34	0	15,19,21	0.80	0
7	NAG	L	302	8,7	14,14,15	0.37	0	15,19,21	0.88	0
8	BMA	L	303	9,7	11,11,12	1.44	2 (18%)	15,15,17	4.41	4 (26%)
9	MAN	L	304	9,8	11,11,12	0.23	0	15,15,17	0.77	0
9	MAN	L	305	9	11,11,12	0.27	0	15,15,17	0.76	0
9	MAN	L	306	9	11,11,12	0.23	0	15,15,17	0.64	0
9	MAN	L	307	9,8	11,11,12	0.22	0	15,15,17	0.69	0
9	MAN	L	308	9,3	11,11,12	0.29	0	15,15,17	0.70	0
9	MAN	L	309	9	11,11,12	0.35	0	15,15,17	0.68	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
7	NAG	B	701	2	-	0/6/23/26	0/1/1/1
7	NAG	B	702	2	-	0/6/23/26	0/1/1/1
7	NAG	B	703	2	-	0/6/23/26	0/1/1/1
9	MAN	D	301	-	-	0/2/19/22	0/1/1/1
7	NAG	G	601	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	602	8,7	-	0/6/23/26	0/1/1/1
8	BMA	G	603	9,7	-	0/2/19/22	0/1/1/1
9	MAN	G	604	8	-	0/2/19/22	0/1/1/1
9	MAN	G	605	9,8	-	0/2/19/22	0/1/1/1
9	MAN	G	606	9	-	0/2/19/22	0/1/1/1
9	MAN	G	607	9	-	0/2/19/22	0/1/1/1
7	NAG	G	608	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	609	7	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	G	610	1	-	0/6/23/26	0/1/1/1
7	NAG	G	611	1	-	0/6/23/26	0/1/1/1
7	NAG	G	612	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	613	7	-	0/6/23/26	0/1/1/1
7	NAG	G	614	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	615	7	-	0/6/23/26	0/1/1/1
7	NAG	G	616	1	-	0/6/23/26	0/1/1/1
7	NAG	G	617	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	618	7	-	0/6/23/26	0/1/1/1
7	NAG	G	619	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	620	7	-	0/6/23/26	0/1/1/1
7	NAG	G	621	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	622	7	-	0/6/23/26	0/1/1/1
7	NAG	G	623	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	624	8,7	-	0/6/23/26	0/1/1/1
8	BMA	G	625	9,7	-	0/2/19/22	0/1/1/1
9	MAN	G	626	8	-	0/2/19/22	0/1/1/1
9	MAN	G	627	8	-	0/2/19/22	0/1/1/1
7	NAG	G	628	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	629	8,7	-	0/6/23/26	0/1/1/1
8	BMA	G	630	9,7	-	0/2/19/22	0/1/1/1
9	MAN	G	631	8	-	0/2/19/22	0/1/1/1
7	NAG	G	632	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	633	8,7	-	0/6/23/26	0/1/1/1
8	BMA	G	634	9,7	-	0/2/19/22	0/1/1/1
9	MAN	G	635	8	-	0/2/19/22	0/1/1/1
9	MAN	G	636	9,8	-	0/2/19/22	0/1/1/1
9	MAN	G	637	9	-	0/2/19/22	0/1/1/1
9	MAN	H	301	-	-	0/2/19/22	0/1/1/1
7	NAG	L	301	1,7	-	1/6/23/26	0/1/1/1
7	NAG	L	302	8,7	-	0/6/23/26	0/1/1/1
8	BMA	L	303	9,7	-	0/2/19/22	0/1/1/1
9	MAN	L	304	9,8	-	0/2/19/22	0/1/1/1
9	MAN	L	305	9	-	0/2/19/22	0/1/1/1
9	MAN	L	306	9	-	0/2/19/22	0/1/1/1
9	MAN	L	307	9,8	-	0/2/19/22	0/1/1/1
9	MAN	L	308	9,3	-	0/2/19/22	0/1/1/1
9	MAN	L	309	9	-	0/2/19/22	0/1/1/1

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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	701	NAG	O6-C6	-7.90	1.08	1.42
7	G	615	NAG	C8-C7	-5.04	1.40	1.50
7	G	618	NAG	C2-N2	-4.84	1.37	1.46
7	B	702	NAG	C1-C2	-4.83	1.45	1.52
7	G	618	NAG	C3-C2	-2.09	1.47	1.52

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	303	BMA	O3-C3-C2	-13.11	85.99	110.01
9	G	605	MAN	O2-C2-C3	-2.72	104.71	110.19
8	L	303	BMA	O2-C2-C3	-2.71	104.73	110.19
9	D	301	MAN	O2-C2-C3	-2.33	105.50	110.19
9	G	635	MAN	O2-C2-C3	-2.31	105.53	110.19

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	L	301	NAG	O7-C7-N2-C2

There are no ring outliers.

16 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	702	NAG	1	0
7	G	601	NAG	1	0
7	G	602	NAG	1	0
9	G	605	MAN	1	0
9	G	607	MAN	4	0
7	G	623	NAG	1	0
7	G	633	NAG	1	0
8	G	634	BMA	1	0
9	G	635	MAN	1	0
9	G	636	MAN	1	0
9	H	301	MAN	4	0
7	L	301	NAG	4	0
7	L	302	NAG	2	0
9	L	304	MAN	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	L	308	MAN	2	0
9	L	309	MAN	6	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	G	452/480 (94%)	0.01	7 (1%) 76 49	58, 95, 164, 244	0
2	B	147/153 (96%)	0.09	4 (2%) 58 28	61, 95, 200, 230	0
3	L	211/218 (96%)	-0.26	0 100 100	77, 113, 140, 169	0
4	H	231/236 (97%)	-0.06	5 (2%) 65 35	81, 118, 171, 189	0
5	D	240/240 (100%)	1.12	59 (24%) 1 0	71, 143, 294, 323	0
6	E	213/216 (98%)	0.55	25 (11%) 6 2	74, 145, 223, 240	0
All	All	1494/1543 (96%)	0.22	100 (6%) 21 7	58, 111, 217, 323	0

The worst 5 of 100 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	D	213	PRO	12.5
5	D	214	LYS	11.0
5	D	132	SER	10.5
5	D	215	SER	9.8
5	D	212	GLU	9.7

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
7	NAG	G	617	14/15	0.88	0.25	0.43	132,143,176,177	0
7	NAG	G	621	14/15	0.88	0.29	0.34	136,156,163,166	0
7	NAG	G	619	14/15	0.90	0.20	0.26	120,145,166,169	0
7	NAG	G	610	14/15	0.86	0.23	0.23	104,132,154,161	0
7	NAG	L	301	14/15	0.92	0.22	0.23	92,106,116,116	0
9	MAN	D	301	11/12	0.88	0.20	0.12	118,135,149,151	0
7	NAG	G	632	14/15	0.96	0.21	-0.05	65,79,91,93	0
7	NAG	G	633	14/15	0.96	0.22	-0.24	60,84,92,97	0
7	NAG	G	612	14/15	0.97	0.19	-0.49	83,104,137,143	0
7	NAG	G	601	14/15	0.96	0.23	-0.61	77,92,110,113	0
7	NAG	G	623	14/15	0.94	0.18	-0.65	108,145,179,182	0
9	MAN	L	308	11/12	0.95	0.16	-0.70	88,98,116,118	0
9	MAN	L	307	11/12	0.96	0.14	-1.30	73,78,107,108	0
7	NAG	L	302	14/15	0.94	0.15	-1.58	79,100,119,122	0
9	MAN	G	635	11/12	0.94	0.18	-	74,92,101,105	0
7	NAG	G	609	14/15	0.87	0.23	-	163,176,183,206	0
7	NAG	G	611	14/15	0.93	0.27	-	128,151,164,173	0
7	NAG	G	608	14/15	0.85	0.23	-	118,152,170,174	0
7	NAG	G	614	14/15	0.90	0.17	-	92,142,163,169	0
7	NAG	G	613	14/15	0.91	0.16	-	137,156,165,178	0
8	BMA	G	603	11/12	0.83	0.14	-	176,187,196,202	0
7	NAG	G	628	14/15	0.96	0.19	-	86,118,135,138	0
9	MAN	G	637	11/12	0.94	0.23	-	125,148,163,164	0
9	MAN	G	605	11/12	0.90	0.16	-	173,199,206,215	0
7	NAG	B	701	14/15	0.89	0.12	-	129,150,172,172	0
9	MAN	L	306	11/12	0.90	0.30	-	136,147,157,161	0
7	NAG	G	616	14/15	0.92	0.19	-	101,141,154,157	0
7	NAG	G	618	14/15	0.81	0.27	-	143,184,189,202	0
8	BMA	G	630	11/12	0.75	0.28	-	188,209,222,228	0
7	NAG	G	622	14/15	0.82	0.39	-	157,175,191,195	0
9	MAN	L	305	11/12	0.96	0.11	-	108,123,130,135	0
8	BMA	G	625	11/12	0.61	0.24	-	229,237,248,259	0
9	MAN	G	627	11/12	0.73	0.23	-	195,215,230,234	0
9	MAN	L	304	11/12	0.90	0.12	-	119,124,135,140	0
9	MAN	G	607	11/12	0.68	0.48	-	223,233,240,249	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	NAG	G	615	14/15	0.82	0.26	-	129,176,187,190	0
9	MAN	G	636	11/12	0.81	0.17	-	119,129,145,159	0
8	BMA	L	303	11/12	0.94	0.17	-	93,96,121,125	0
7	NAG	B	702	14/15	0.90	0.13	-	116,143,159,164	0
9	MAN	G	631	11/12	0.73	0.38	-	191,222,229,231	0
9	MAN	G	604	11/12	0.69	0.32	-	173,200,215,218	0
8	BMA	G	634	11/12	0.91	0.23	-	78,87,127,130	0
7	NAG	G	624	14/15	0.90	0.25	-	154,200,221,233	0
9	MAN	G	626	11/12	0.74	0.61	-	251,264,271,276	0
9	MAN	H	301	11/12	0.92	0.14	-	134,138,155,160	0
7	NAG	G	629	14/15	0.91	0.14	-	135,146,175,197	0
9	MAN	L	309	11/12	0.96	0.12	-	89,107,112,113	0
7	NAG	G	620	14/15	0.91	0.17	-	134,170,177,179	0
7	NAG	G	602	14/15	0.94	0.16	-	108,133,150,163	0
7	NAG	B	703	14/15	0.85	0.27	-	150,170,188,199	0
9	MAN	G	606	11/12	0.78	0.21	-	171,199,222,235	0

6.5 Other polymers

There are no such residues in this entry.