



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2017 – 08:44 PM EDT

PDB ID : 5D9Q
Title : Crystal Structure of the BG505 SOSIP gp140 HIV-1 Env trimer in Complex with the Broadly Neutralizing Fab PGT122 and scFv NIH45-46
Authors : Julien, J.-P.; Stanfield, R.L.; Ward, A.B.; Wilson, I.A.
Deposited on : unknown
Resolution : 4.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20029824

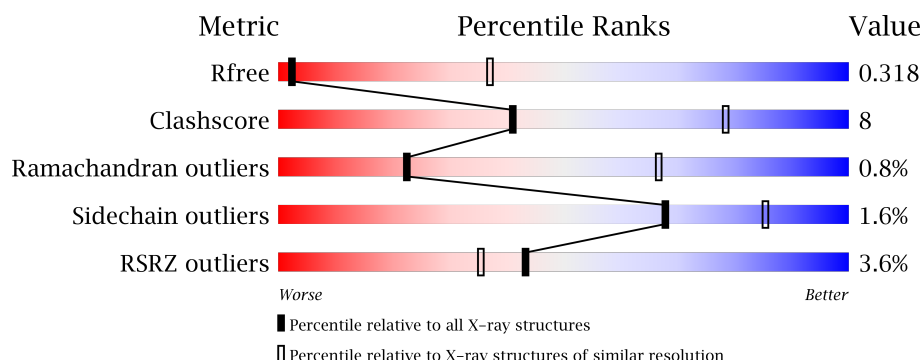
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.40 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}	100719	1024 (5.08-3.62)
Clashscore	112137	1021 (5.08-3.70)
Ramachandran outliers	110173	1018 (5.08-3.66)
Sidechain outliers	110143	1000 (5.08-3.66)
RSRZ outliers	101464	1007 (5.08-3.64)

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

Mol	Chain	Length	Quality of chain
1	A	472	 .% 69% 25% • 5%
1	G	472	 3% 70% 24% • 5%
1	J	472	 2% 67% 27% • 5%
2	B	152	 3% 60% 17% • 20%
2	C	152	 57% 20% • 20%

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Mol	Chain	Length	Quality of chain
2	K	152	
3	E	211	
3	L	211	
3	M	211	
4	F	235	
4	H	235	
4	N	235	
5	D	241	
5	I	241	
5	O	241	

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
6	NAG	A	607	-	-	-	X
6	NAG	A	616	-	-	-	X
6	NAG	A	662	-	-	-	X
6	NAG	G	616	-	-	-	X
6	NAG	G	625	-	-	-	X
6	NAG	G	641	-	-	-	X
6	NAG	G	662	-	-	-	X
6	NAG	J	641	-	-	-	X
6	NAG	J	662	-	-	-	X
6	NAG	J	667	-	-	-	X
6	NAG	J	669	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 31374 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 gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	448	Total	C	N	O	S	0	0	0
			3528	2215	622	663	28			
1	A	448	Total	C	N	O	S	0	0	0
			3528	2215	622	663	28			
1	J	448	Total	C	N	O	S	0	0	0
			3528	2215	622	663	28			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	332	ASN	THR	conflict	UNP Q2N0S6
G	460	ALA	SER	conflict	UNP Q2N0S6
G	461	ASN	THR	conflict	UNP Q2N0S6
G	463	THR	SER	conflict	UNP Q2N0S6
G	464	SER	THR	conflict	UNP Q2N0S6
G	501	CYS	ALA	conflict	UNP Q2N0S6
A	332	ASN	THR	conflict	UNP Q2N0S6
A	460	ALA	SER	conflict	UNP Q2N0S6
A	461	ASN	THR	conflict	UNP Q2N0S6
A	463	THR	SER	conflict	UNP Q2N0S6
A	464	SER	THR	conflict	UNP Q2N0S6
A	501	CYS	ALA	conflict	UNP Q2N0S6
J	332	ASN	THR	conflict	UNP Q2N0S6
J	460	ALA	SER	conflict	UNP Q2N0S6
J	461	ASN	THR	conflict	UNP Q2N0S6
J	463	THR	SER	conflict	UNP Q2N0S6
J	464	SER	THR	conflict	UNP Q2N0S6
J	501	CYS	ALA	conflict	UNP Q2N0S6

- Molecule 2 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	121	Total	C	N	O	S	0	0	0
			968	613	167	182	6			
2	C	121	Total	C	N	O	S	0	0	0
			968	613	167	182	6			
2	K	121	Total	C	N	O	S	0	0	0
			968	613	167	182	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	conflict	UNP Q2N0S9
B	605	CYS	THR	conflict	UNP Q2N0S9
C	559	PRO	ILE	conflict	UNP Q2N0S9
C	605	CYS	THR	conflict	UNP Q2N0S9
K	559	PRO	ILE	conflict	UNP Q2N0S9
K	605	CYS	THR	conflict	UNP Q2N0S9

- Molecule 3 is a protein called PGT122 light chain,Ig lambda-3 chain C regions.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	208	Total	C	N	O	S	0	0	0
			1577	990	265	318	4			
3	E	208	Total	C	N	O	S	0	0	0
			1577	990	265	318	4			
3	M	208	Total	C	N	O	S	0	0	0
			1577	990	265	318	4			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	156	VAL	ALA	conflict	UNP P0CG06
E	156	VAL	ALA	conflict	UNP P0CG06
M	156	VAL	ALA	conflict	UNP P0CG06

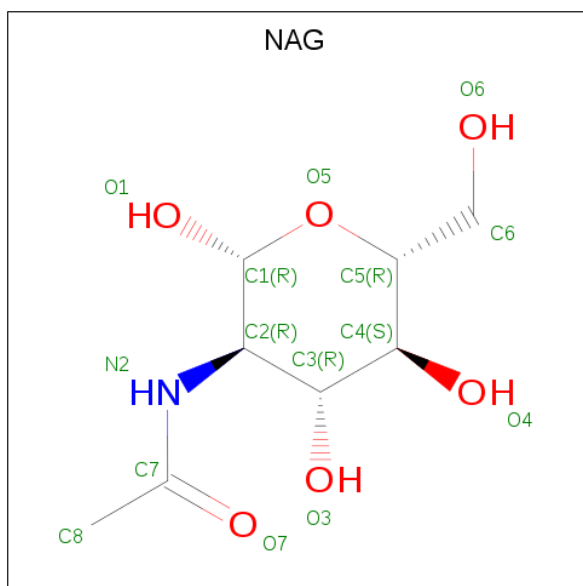
- Molecule 4 is a protein called PGT122 heavy chain,IgG H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	227	Total	C	N	O	S	0	0	0
			1738	1108	293	332	5			
4	F	227	Total	C	N	O	S	0	0	0
			1738	1108	293	332	5			
4	N	227	Total	C	N	O	S	0	0	0
			1738	1108	293	332	5			

- Molecule 5 is a protein called NIH45-46 single chain Fv.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	222	Total	C	N	O	S	0	0	0
			1753	1103	315	325	10			
5	I	222	Total	C	N	O	S	0	0	0
			1753	1103	315	325	10			
5	O	222	Total	C	N	O	S	0	0	0
			1753	1103	315	325	10			

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



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

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

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

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

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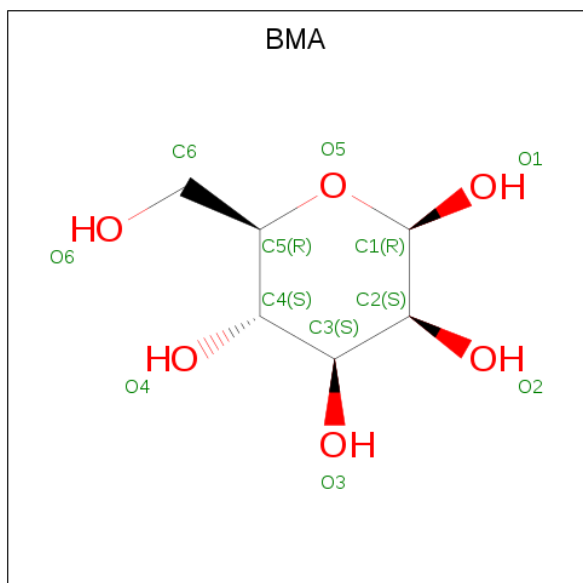
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	J	1	Total	C	N	O	0	0
			14	8	1	5		
6	J	1	Total	C	N	O	0	0
			14	8	1	5		
6	J	1	Total	C	N	O	0	0
			14	8	1	5		
6	J	1	Total	C	N	O	0	0
			14	8	1	5		
6	J	1	Total	C	N	O	0	0
			14	8	1	5		
6	J	1	Total	C	N	O	0	0
			14	8	1	5		
6	J	1	Total	C	N	O	0	0
			14	8	1	5		
6	J	1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

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

- Molecule 7 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



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

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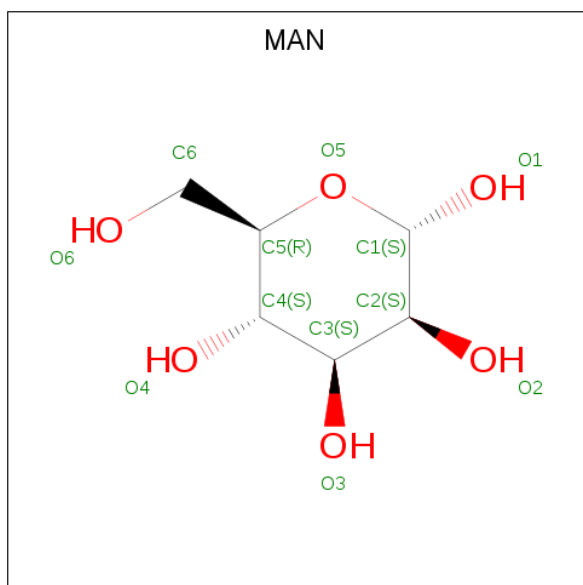
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	G	1	Total	C	O	0	0
			11	6	5		
7	G	1	Total	C	O	0	0
			11	6	5		
7	G	1	Total	C	O	0	0
			11	6	5		
7	G	1	Total	C	O	0	0
			11	6	5		
7	G	1	Total	C	O	0	0
			11	6	5		
7	G	1	Total	C	O	0	0
			11	6	5		
7	A	1	Total	C	O	0	0
			11	6	5		
7	A	1	Total	C	O	0	0
			11	6	5		
7	A	1	Total	C	O	0	0
			11	6	5		
7	A	1	Total	C	O	0	0
			11	6	5		
7	A	1	Total	C	O	0	0
			11	6	5		
7	A	1	Total	C	O	0	0
			11	6	5		
7	A	1	Total	C	O	0	0
			11	6	5		
7	J	1	Total	C	O	0	0
			11	6	5		
7	J	1	Total	C	O	0	0
			11	6	5		
7	J	1	Total	C	O	0	0
			11	6	5		
7	J	1	Total	C	O	0	0
			11	6	5		
7	J	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	J	1	Total	C	O	0	0
			11	6	5		
7	J	1	Total	C	O	0	0
			11	6	5		

- Molecule 8 is ALPHA-D-MANNOSE (three-letter code: MAN) (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	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		

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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	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	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	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	G	1	Total	C	O	0	0
			11	6	5		

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			11	6	5		
8	A	1	Total	C	O	0	0
			11	6	5		
8	A	1	Total	C	O	0	0
			11	6	5		
8	A	1	Total	C	O	0	0
			11	6	5		
8	A	1	Total	C	O	0	0
			11	6	5		
8	A	1	Total	C	O	0	0
			11	6	5		
8	A	1	Total	C	O	0	0
			11	6	5		
8	J	1	Total	C	O	0	0
			11	6	5		
8	J	1	Total	C	O	0	0
			11	6	5		
8	J	1	Total	C	O	0	0
			11	6	5		
8	J	1	Total	C	O	0	0
			11	6	5		
8	J	1	Total	C	O	0	0
			11	6	5		
8	J	1	Total	C	O	0	0
			11	6	5		
8	J	1	Total	C	O	0	0
			11	6	5		
8	J	1	Total	C	O	0	0
			11	6	5		
8	J	1	Total	C	O	0	0
			11	6	5		
8	J	1	Total	C	O	0	0
			11	6	5		

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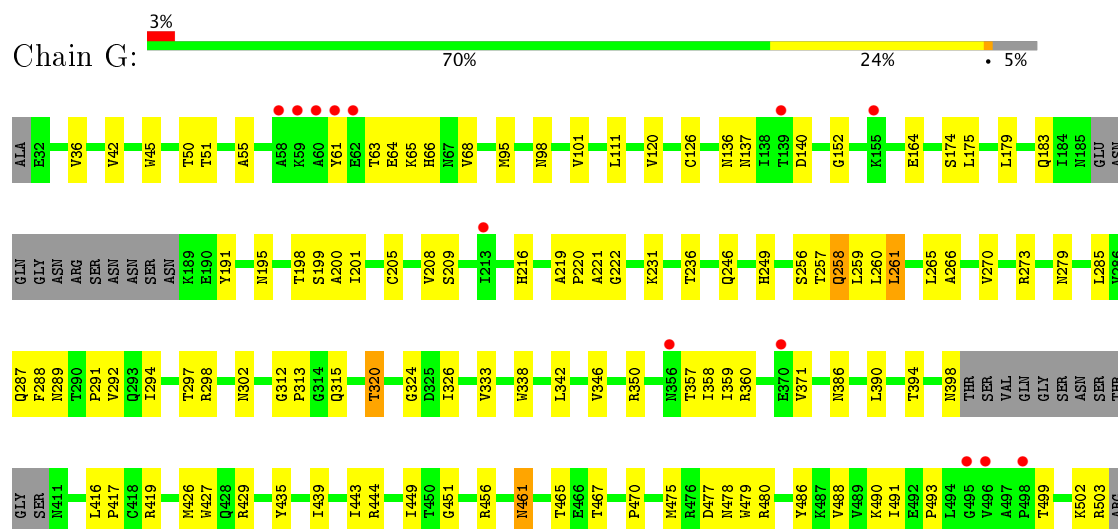
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	J	1	Total	C	O	0	0
			11	6	5		
8	J	1	Total	C	O	0	0
			11	6	5		
8	J	1	Total	C	O	0	0
			11	6	5		
8	J	1	Total	C	O	0	0
			11	6	5		
8	J	1	Total	C	O	0	0
			11	6	5		
8	J	1	Total	C	O	0	0
			11	6	5		
8	J	1	Total	C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

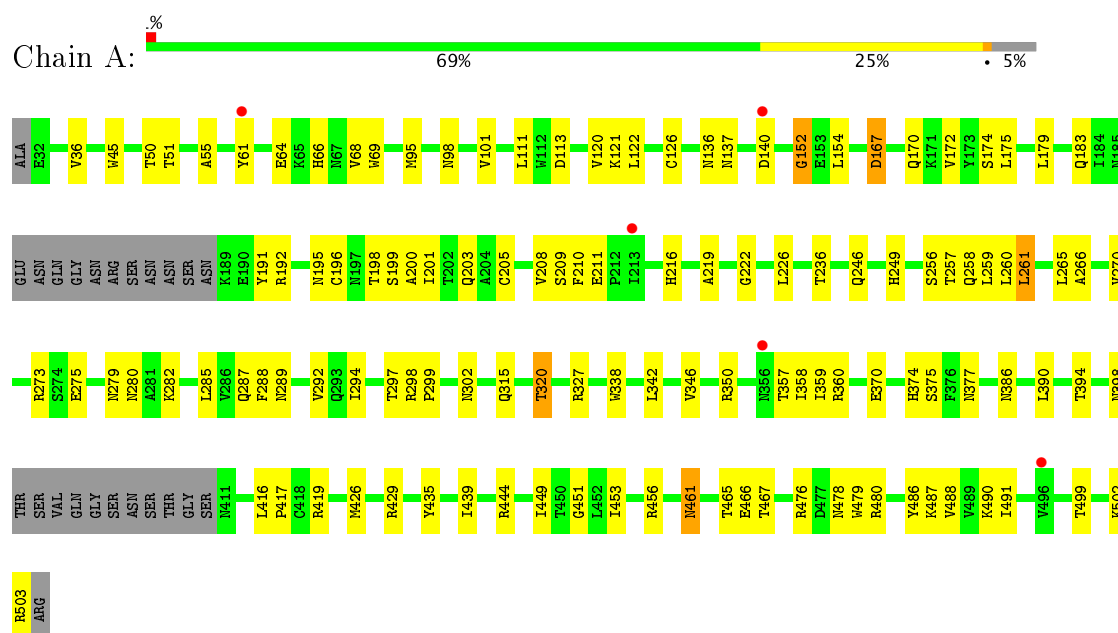
3 Residue-property plots

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

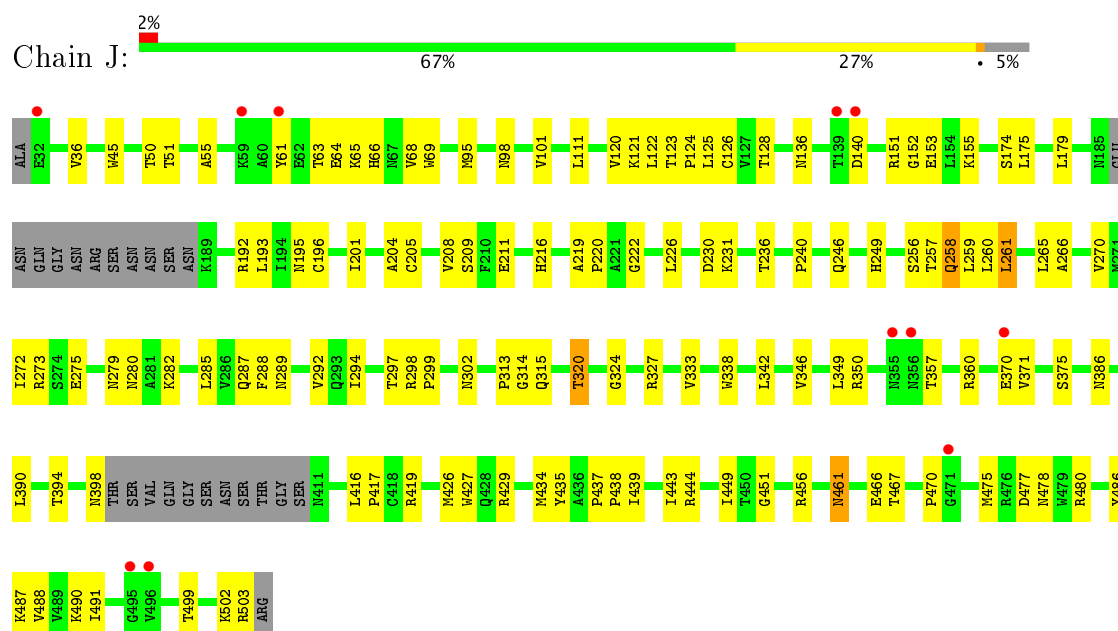
- Molecule 1: Envelope glycoprotein gp120



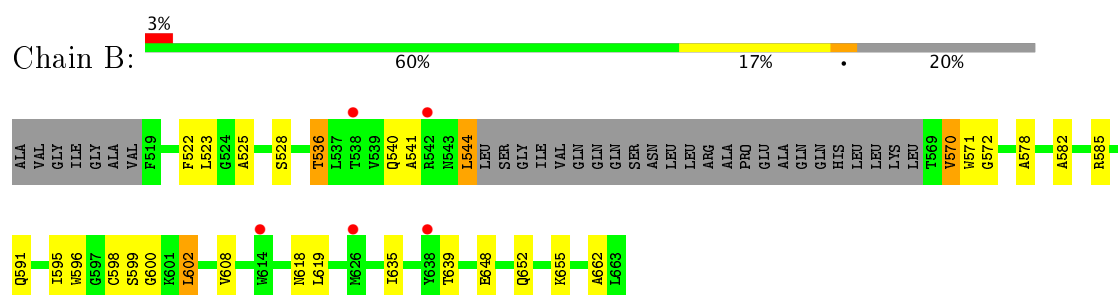
- Molecule 1: Envelope glycoprotein gp120



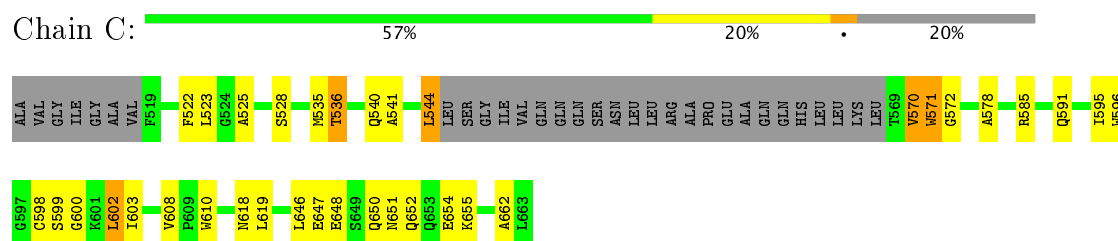
- Molecule 1: Envelope glycoprotein gp120



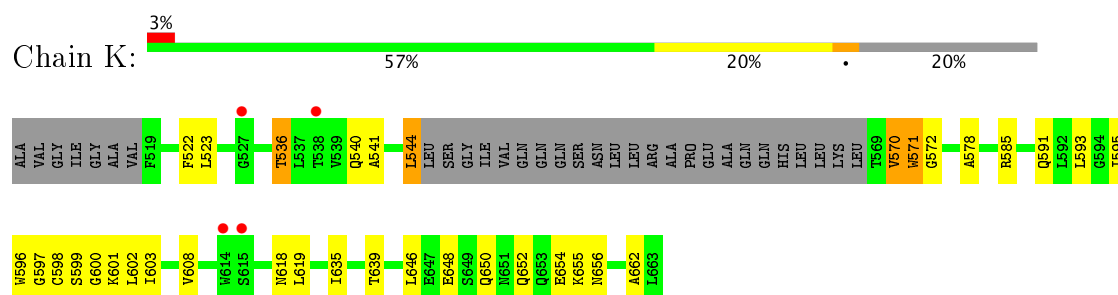
- Molecule 2: Envelope glycoprotein gp41



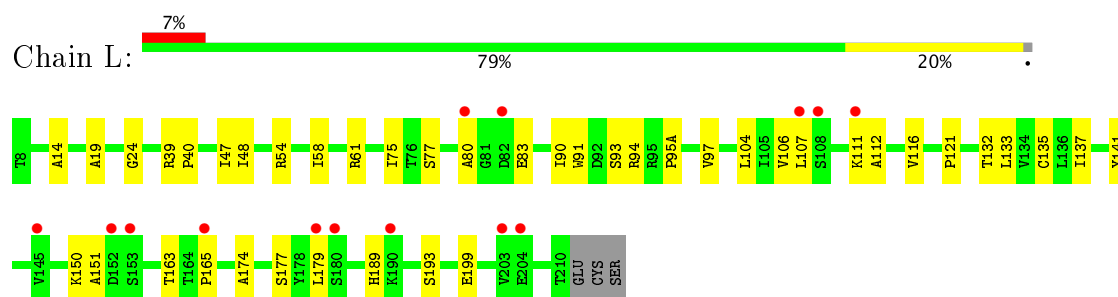
- Molecule 2: Envelope glycoprotein gp41



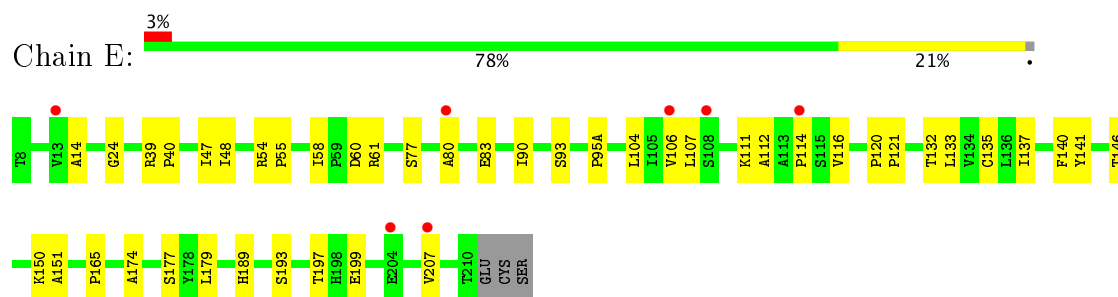
- Molecule 2: Envelope glycoprotein gp41



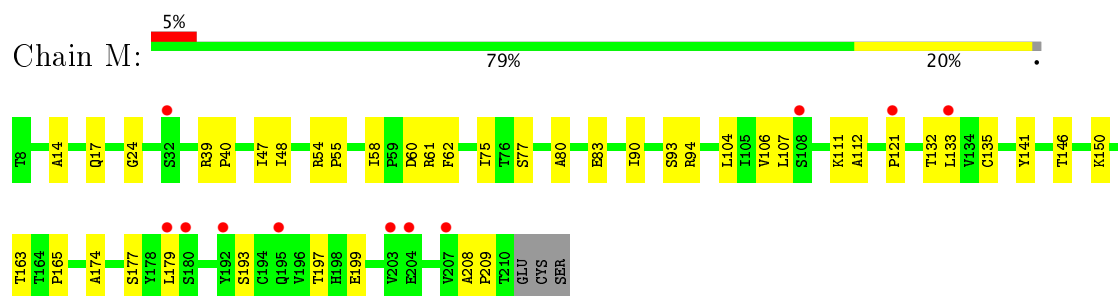
- Molecule 3: PGT122 light chain,Ig lambda-3 chain C regions



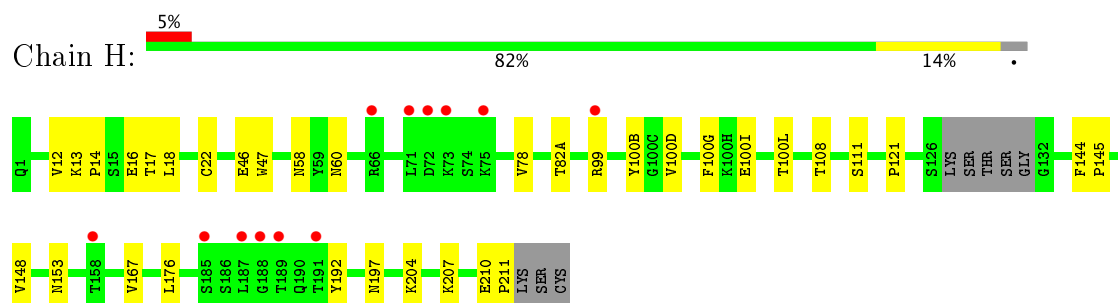
- Molecule 3: PGT122 light chain,Ig lambda-3 chain C regions



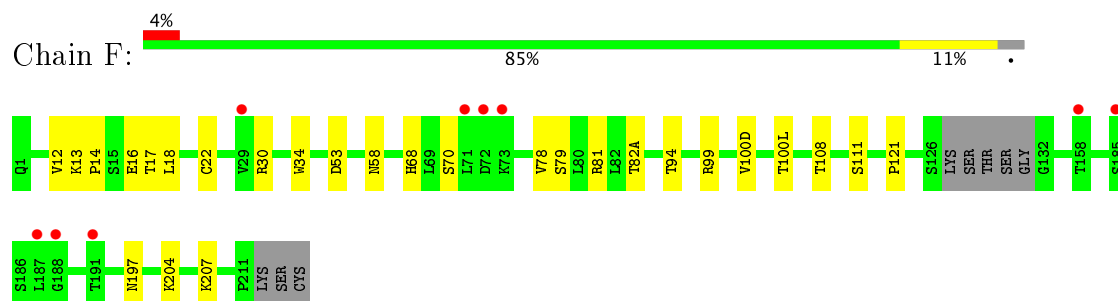
- Molecule 3: PGT122 light chain,Ig lambda-3 chain C regions



- Molecule 4: PGT122 heavy chain,IgG H chain



- Molecule 4: PGT122 heavy chain,IgG H chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	153.76Å 254.35Å 283.55Å 90.00° 100.96° 90.00°	Depositor
Resolution (Å)	39.89 – 4.40 39.89 – 4.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.89-4.40) 100.0 (39.89-4.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 4.44Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.290 , 0.320 0.294 , 0.318	Depositor DCC
R_{free} test set	1008 reflections (1.49%)	DCC
Wilson B-factor (Å ²)	144.8	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 99.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.29$, $\langle L^2 \rangle = 0.13$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	31374	wwPDB-VP
Average B, all atoms (Å ²)	217.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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, 0.333 respectively for untwinned datasets, and 0.375, 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, PCA, 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	A	0.28	0/3602	0.48	0/4891
1	G	0.27	0/3602	0.47	0/4891
1	J	0.27	0/3602	0.48	0/4891
2	B	0.26	0/986	0.44	0/1337
2	C	0.26	0/986	0.45	0/1337
2	K	0.27	0/986	0.44	0/1337
3	E	0.24	0/1619	0.42	0/2217
3	L	0.24	0/1619	0.41	0/2217
3	M	0.25	0/1619	0.42	0/2217
4	F	0.26	0/1785	0.45	0/2437
4	H	0.26	0/1785	0.44	0/2437
4	N	0.25	0/1785	0.44	0/2437
5	D	0.24	0/1792	0.41	0/2428
5	I	0.25	0/1792	0.41	0/2428
5	O	0.24	0/1792	0.41	0/2428
All	All	0.26	0/29352	0.45	0/39930

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3528	0	3456	84	0
1	G	3528	0	3456	79	0
1	J	3528	0	3456	89	0
2	B	968	0	944	23	0
2	C	968	0	944	30	0
2	K	968	0	944	29	0
3	E	1577	0	1518	24	0
3	L	1577	0	1518	25	0
3	M	1577	0	1518	25	0
4	F	1738	0	1711	16	0
4	H	1738	0	1711	21	0
4	N	1738	0	1711	21	0
5	D	1753	0	1678	28	0
5	I	1753	0	1678	30	0
5	O	1753	0	1678	27	0
6	A	448	0	394	7	0
6	B	28	0	26	0	0
6	C	28	0	26	0	0
6	G	448	0	394	8	0
6	J	448	0	394	6	0
6	K	28	0	26	0	0
7	A	88	0	65	0	0
7	G	88	0	65	0	0
7	J	88	0	65	0	0
8	A	330	0	285	0	0
8	G	330	0	285	3	0
8	J	330	0	285	2	0
All	All	31374	0	30231	496	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 8.

All (496) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:197:ASN:HD22	4:N:204:LYS:HG2	1.48	0.78
4:H:14:PRO:HG3	4:H:111:SER:HB3	1.67	0.77
1:J:68:VAL:HG22	1:J:209:SER:HB3	1.67	0.76
3:E:39:ARG:HD3	3:E:40:PRO:HD2	1.68	0.76
1:J:279:ASN:OD1	5:O:102:TRP:NE1	2.15	0.76
3:L:39:ARG:HD3	3:L:40:PRO:HD2	1.68	0.76
1:A:222:GLY:HA2	2:C:544:LEU:HD12	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:ASN:OD1	5:I:102:TRP:NE1	2.18	0.74
3:L:150:LYS:HB2	3:L:193:SER:HB2	1.70	0.74
1:A:261:LEU:HD21	1:A:294:ILE:HD11	1.69	0.74
1:G:222:GLY:HA2	2:B:544:LEU:HD12	1.69	0.73
1:G:55:ALA:HB3	1:G:216:HIS:HB2	1.69	0.73
1:J:55:ALA:HB3	1:J:216:HIS:HB2	1.70	0.73
4:F:14:PRO:HG3	4:F:111:SER:HB3	1.69	0.72
3:M:150:LYS:HB2	3:M:193:SER:HB2	1.70	0.72
4:F:197:ASN:HD22	4:F:204:LYS:HG2	1.55	0.72
1:J:456:ARG:O	5:O:58:ASN:ND2	2.23	0.72
1:A:256:SER:O	1:A:478:ASN:ND2	2.20	0.72
5:D:236:GLN:HB3	5:D:283:VAL:HG13	1.71	0.71
1:A:456:ARG:O	5:I:58:ASN:ND2	2.21	0.70
3:E:150:LYS:HB2	3:E:193:SER:HB2	1.74	0.70
4:N:99:ARG:HG2	4:N:100(L):THR:HG22	1.73	0.70
1:G:279:ASN:OD1	5:D:102:TRP:NE1	2.19	0.70
1:J:222:GLY:HA2	2:K:544:LEU:HD12	1.73	0.70
1:A:175:LEU:HB3	1:A:320:THR:HB	1.72	0.69
1:G:360:ARG:HG2	1:G:394:THR:HG23	1.73	0.69
1:J:261:LEU:HD21	1:J:294:ILE:HD11	1.73	0.69
1:G:256:SER:O	1:G:478:ASN:ND2	2.23	0.69
1:A:55:ALA:HB3	1:A:216:HIS:HB2	1.75	0.69
1:G:261:LEU:HD21	1:G:294:ILE:HD11	1.74	0.69
5:I:236:GLN:HB3	5:I:283:VAL:HG13	1.75	0.68
3:E:47:ILE:HG22	3:E:48:ILE:HG13	1.75	0.68
3:M:39:ARG:HD3	3:M:40:PRO:HD2	1.75	0.68
3:E:24:GLY:HA3	3:E:90:ILE:HD11	1.76	0.68
2:C:541:ALA:O	2:K:591:GLN:NE2	2.26	0.68
1:G:456:ARG:O	5:D:58:ASN:ND2	2.25	0.68
3:L:133:LEU:HD12	3:L:179:LEU:HD23	1.76	0.68
1:J:360:ARG:HG2	1:J:394:THR:HG23	1.76	0.67
1:A:360:ARG:HG2	1:A:394:THR:HG23	1.76	0.67
1:G:68:VAL:HG22	1:G:209:SER:HB3	1.75	0.67
3:L:47:ILE:HG22	3:L:48:ILE:HG13	1.77	0.67
2:C:523:LEU:H	2:C:540:GLN:HG3	1.58	0.67
5:D:96:LYS:HE2	5:D:247:TYR:CZ	2.30	0.66
1:G:249:HIS:ND1	1:G:486:TYR:OH	2.27	0.66
1:G:175:LEU:HB3	1:G:320:THR:HB	1.77	0.66
1:G:499:THR:OG1	2:C:662:ALA:O	2.13	0.66
1:J:360:ARG:HB2	1:J:467:THR:HG22	1.77	0.66
1:J:201:ILE:HD11	1:J:435:TYR:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:VAL:HG22	1:A:209:SER:HB3	1.78	0.65
2:K:536:THR:O	2:K:540:GLN:NE2	2.25	0.65
1:A:360:ARG:HB2	1:A:467:THR:HG22	1.79	0.65
4:H:197:ASN:HD22	4:H:204:LYS:HG2	1.62	0.65
5:D:245:VAL:HG12	5:D:246:ILE:HG13	1.78	0.65
1:J:175:LEU:HB3	1:J:320:THR:HB	1.79	0.64
3:M:24:GLY:HA3	3:M:90:ILE:HD11	1.79	0.64
5:O:236:GLN:HB3	5:O:283:VAL:HG13	1.78	0.64
2:K:523:LEU:H	2:K:540:GLN:HG3	1.62	0.64
1:G:297:THR:HG22	1:G:444:ARG:HG2	1.78	0.64
1:G:260:LEU:HD12	1:G:451:GLY:HA3	1.79	0.64
2:K:523:LEU:HD23	2:K:540:GLN:HG2	1.79	0.64
3:M:80:ALA:HA	3:M:106:VAL:HG21	1.79	0.63
1:A:64:GLU:O	1:A:66:HIS:N	2.31	0.63
3:M:47:ILE:HG22	3:M:48:ILE:HG13	1.80	0.63
2:B:536:THR:O	2:B:540:GLN:NE2	2.27	0.63
1:G:360:ARG:HB2	1:G:467:THR:HG22	1.79	0.63
1:G:179:LEU:HD11	1:G:419:ARG:HD3	1.80	0.62
4:H:22:CYS:HB3	4:H:78:VAL:HB	1.81	0.62
5:I:245:VAL:HG12	5:I:246:ILE:HG13	1.81	0.62
1:A:120:VAL:HG13	1:A:315:GLN:HE21	1.64	0.62
4:F:99:ARG:HG2	4:F:100(L):THR:HG22	1.81	0.62
2:C:536:THR:O	2:C:540:GLN:NE2	2.23	0.62
5:O:245:VAL:HG12	5:O:246:ILE:HG13	1.81	0.62
2:B:523:LEU:H	2:B:540:GLN:HG3	1.64	0.62
1:J:64:GLU:O	1:J:66:HIS:N	2.32	0.61
3:M:146:THR:OG1	3:M:197:THR:OG1	2.18	0.61
4:N:14:PRO:HG3	4:N:111:SER:HB3	1.82	0.61
2:C:523:LEU:HD23	2:C:540:GLN:HG2	1.81	0.61
3:E:133:LEU:HD12	3:E:179:LEU:HD23	1.82	0.61
3:L:24:GLY:HA3	3:L:90:ILE:HD11	1.82	0.61
1:G:201:ILE:HD11	1:G:435:TYR:HB2	1.82	0.61
1:A:350:ARG:NH2	1:A:357:THR:O	2.33	0.61
1:G:136:ASN:ND2	3:L:93:SER:O	2.34	0.60
1:J:260:LEU:HD12	1:J:451:GLY:HA3	1.83	0.60
1:A:297:THR:HG22	1:A:444:ARG:HG2	1.83	0.60
4:H:99:ARG:HG2	4:H:100(L):THR:HG22	1.84	0.60
5:I:96:LYS:HE2	5:I:247:TYR:CZ	2.36	0.60
3:M:83:GLU:HG3	3:M:104:LEU:O	2.02	0.60
1:A:249:HIS:ND1	1:A:486:TYR:OH	2.26	0.60
2:B:591:GLN:NE2	2:K:541:ALA:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:133:LEU:HD12	3:M:179:LEU:HD23	1.83	0.60
1:G:266:ALA:N	1:G:288:PHE:O	2.31	0.60
1:J:101:VAL:HG21	1:J:480:ARG:HG2	1.84	0.59
1:G:64:GLU:O	1:G:66:HIS:N	2.35	0.59
1:G:265:LEU:O	1:G:287:GLN:NE2	2.35	0.59
1:J:297:THR:HG22	1:J:444:ARG:HG2	1.84	0.59
4:N:22:CYS:HB3	4:N:78:VAL:HB	1.82	0.59
1:G:219:ALA:O	1:G:246:GLN:NE2	2.36	0.59
2:B:662:ALA:O	1:J:499:THR:OG1	2.19	0.59
3:E:146:THR:OG1	3:E:197:THR:OG1	2.20	0.59
6:G:608:NAG:O7	4:H:58:ASN:ND2	2.35	0.59
5:O:96:LYS:HE2	5:O:247:TYR:CZ	2.37	0.59
1:A:265:LEU:O	1:A:287:GLN:NE2	2.37	0.58
1:A:466:GLU:HA	5:I:61:ARG:HH21	1.68	0.58
2:B:523:LEU:HD23	2:B:540:GLN:HG2	1.85	0.58
2:B:541:ALA:O	2:C:591:GLN:NE2	2.34	0.58
1:J:179:LEU:HD11	1:J:419:ARG:HD3	1.86	0.58
5:I:287:GLN:NE2	5:I:289:TYR:O	2.34	0.58
1:A:51:THR:HB	2:C:578:ALA:HB2	1.84	0.58
1:J:249:HIS:ND1	1:J:486:TYR:OH	2.31	0.58
2:B:598:CYS:O	2:B:600:GLY:N	2.36	0.58
6:G:602:NAG:H3	6:G:602:NAG:H83	1.84	0.58
6:A:602:NAG:H3	6:A:602:NAG:H83	1.85	0.57
1:G:350:ARG:NH2	1:G:357:THR:O	2.37	0.57
1:G:257:THR:O	1:G:259:LEU:N	2.37	0.57
1:A:257:THR:O	1:A:259:LEU:N	2.37	0.57
6:J:602:NAG:H83	6:J:602:NAG:H3	1.85	0.57
6:A:617:NAG:H3	6:A:617:NAG:H83	1.87	0.57
4:N:148:VAL:HB	4:N:176:LEU:HD21	1.87	0.57
5:I:12:LYS:HB2	5:I:115:VAL:HG12	1.87	0.56
1:A:195:ASN:HD21	1:A:201:ILE:HD12	1.69	0.56
1:A:179:LEU:HD11	1:A:419:ARG:HD3	1.86	0.56
6:J:617:NAG:H3	6:J:617:NAG:H83	1.87	0.56
1:A:174:SER:OG	1:A:175:LEU:N	2.39	0.56
1:J:220:PRO:HG3	2:K:578:ALA:HB1	1.87	0.56
5:O:33:PRO:HG3	5:O:52:LYS:HG2	1.87	0.56
1:G:461:ASN:HD21	5:D:203:VAL:HG22	1.71	0.56
6:G:617:NAG:H3	6:G:617:NAG:H83	1.87	0.56
3:L:61:ARG:HD2	3:L:77:SER:HB2	1.87	0.56
4:F:17:THR:HG22	4:F:82(A):THR:HG22	1.88	0.56
1:J:51:THR:HB	2:K:578:ALA:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:371:VAL:HG21	5:O:54:GLY:HA3	1.86	0.56
1:A:298:ARG:NH1	1:A:302:ASN:OD1	2.38	0.56
1:G:221:ALA:HB3	2:B:582:ALA:HB1	1.88	0.56
4:N:17:THR:HG22	4:N:82(A):THR:HG22	1.88	0.56
1:G:183:GLN:HA	1:G:191:TYR:HA	1.88	0.55
1:G:220:PRO:HG3	2:B:578:ALA:HB1	1.88	0.55
1:J:174:SER:OG	1:J:175:LEU:N	2.40	0.55
1:J:427:TRP:NE1	1:J:475:MET:SD	2.80	0.55
3:E:165:PRO:HA	3:E:174:ALA:O	2.06	0.55
1:A:136:ASN:ND2	3:E:93:SER:O	2.40	0.55
3:E:151:ALA:HB1	3:E:189:HIS:CD2	2.42	0.55
4:H:17:THR:HG22	4:H:82(A):THR:HG22	1.87	0.55
1:J:257:THR:O	1:J:259:LEU:N	2.39	0.54
3:L:83:GLU:HG3	3:L:104:LEU:O	2.08	0.54
1:J:461:ASN:HD21	5:O:203:VAL:HG22	1.73	0.54
5:D:287:GLN:NE2	5:D:289:TYR:O	2.39	0.54
5:I:50:TRP:CZ3	5:I:52:LYS:HG3	2.43	0.54
1:J:350:ARG:NH2	1:J:357:THR:O	2.40	0.54
3:L:80:ALA:HA	3:L:106:VAL:HG21	1.90	0.54
1:A:192:ARG:HE	1:A:196:CYS:HB2	1.73	0.53
1:A:491:ILE:HD11	2:C:523:LEU:HD11	1.88	0.53
2:C:598:CYS:O	2:C:600:GLY:N	2.41	0.53
5:O:50:TRP:CZ3	5:O:52:LYS:HG3	2.43	0.53
5:I:59:TYR:HE1	5:I:69:MET:HG3	1.74	0.53
2:K:598:CYS:O	2:K:600:GLY:N	2.41	0.53
3:M:61:ARG:HD2	3:M:77:SER:HB2	1.90	0.53
1:J:45:TRP:HB3	1:J:491:ILE:HD13	1.91	0.53
3:M:135:CYS:HB3	3:M:177:SER:HB3	1.90	0.53
1:A:64:GLU:C	1:A:66:HIS:H	2.12	0.53
5:D:50:TRP:CZ3	5:D:52:LYS:HG3	2.44	0.53
5:O:12:LYS:HB2	5:O:115:VAL:HG12	1.92	0.53
1:A:370:GLU:O	1:A:375:SER:OG	2.26	0.52
1:J:256:SER:O	1:J:478:ASN:ND2	2.34	0.52
1:G:324:GLY:O	3:L:94:ARG:NH1	2.37	0.52
1:J:491:ILE:HD11	2:K:523:LEU:HD11	1.91	0.52
4:N:121:PRO:HD3	4:N:207:LYS:HE2	1.92	0.52
1:A:490:LYS:HD2	2:C:585:ARG:NH2	2.25	0.52
5:D:12:LYS:HB2	5:D:115:VAL:HG12	1.92	0.52
3:E:112:ALA:HB3	3:E:141:TYR:N	2.25	0.52
4:F:22:CYS:HB3	4:F:78:VAL:HB	1.91	0.52
1:G:174:SER:OG	1:G:175:LEU:N	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:285:LEU:HD21	1:G:477:ASP:HB3	1.92	0.52
5:I:33:PRO:HG3	5:I:52:LYS:HG2	1.91	0.52
1:J:265:LEU:O	1:J:287:GLN:NE2	2.43	0.52
6:J:641:NAG:H83	5:O:229:GLY:HA2	1.92	0.52
3:M:47:ILE:HA	3:M:58:ILE:HD13	1.92	0.52
1:A:280:ASN:HD21	5:I:290:GLU:HG2	1.75	0.52
1:G:101:VAL:HG21	1:G:480:ARG:HG2	1.92	0.51
6:G:601:NAG:O7	2:B:528:SER:OG	2.24	0.51
1:J:370:GLU:O	1:J:375:SER:OG	2.27	0.51
5:O:203:VAL:HG12	5:O:204:LEU:H	1.75	0.51
1:A:266:ALA:N	1:A:288:PHE:O	2.41	0.51
3:E:121:PRO:HB3	3:E:132:THR:H	1.74	0.51
1:J:386:ASN:HB3	1:J:417:PRO:HD2	1.92	0.51
8:J:610:MAN:H4	4:N:99:ARG:HH21	1.74	0.51
1:G:120:VAL:HG13	1:G:315:GLN:HE21	1.76	0.51
5:O:37:ILE:HG12	5:O:47:TRP:HA	1.91	0.51
1:J:121:LYS:O	1:J:315:GLN:NE2	2.44	0.51
3:E:135:CYS:HB3	3:E:177:SER:HB3	1.92	0.51
4:F:121:PRO:HD3	4:F:207:LYS:HE2	1.92	0.51
1:G:195:ASN:HD21	1:G:201:ILE:HD12	1.75	0.51
1:G:350:ARG:NH2	1:G:398:ASN:H	2.09	0.51
1:A:386:ASN:HB3	1:A:417:PRO:HD2	1.93	0.50
5:D:37:ILE:HG12	5:D:47:TRP:HA	1.94	0.50
1:A:211:GLU:OE2	6:A:636:NAG:O3	2.28	0.50
5:D:33:PRO:HG3	5:D:52:LYS:HG2	1.92	0.50
3:M:55:PRO:HG2	3:M:58:ILE:HD12	1.92	0.50
5:O:287:GLN:NE2	5:O:289:TYR:O	2.42	0.50
5:I:203:VAL:HG12	5:I:204:LEU:H	1.76	0.50
1:J:266:ALA:N	1:J:288:PHE:O	2.41	0.50
1:A:350:ARG:NH2	1:A:398:ASN:H	2.09	0.50
2:B:525:ALA:HB1	2:B:528:SER:HB2	1.94	0.50
1:G:136:ASN:HD22	3:L:94:ARG:HA	1.75	0.50
3:M:165:PRO:HA	3:M:174:ALA:O	2.12	0.50
1:J:298:ARG:HE	1:J:443:ILE:HD12	1.76	0.50
1:J:64:GLU:C	1:J:66:HIS:H	2.14	0.50
1:G:294:ILE:HG22	1:G:333:VAL:HG22	1.94	0.50
1:A:260:LEU:HD12	1:A:451:GLY:HA3	1.94	0.49
3:E:55:PRO:HG2	3:E:58:ILE:HD12	1.93	0.49
3:L:112:ALA:HB3	3:L:141:TYR:N	2.27	0.49
1:A:358:ILE:O	1:A:465:THR:OG1	2.28	0.49
1:G:64:GLU:C	1:G:66:HIS:H	2.16	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:THR:OG1	2:K:662:ALA:O	2.31	0.49
1:J:211:GLU:OE2	6:J:636:NAG:O3	2.29	0.49
8:J:621:MAN:O2	5:O:19:ARG:NH1	2.33	0.49
1:G:427:TRP:NE1	1:G:475:MET:SD	2.86	0.49
1:J:204:ALA:HB2	1:J:434:MET:SD	2.53	0.49
1:J:120:VAL:HG13	1:J:315:GLN:HE21	1.78	0.49
4:H:47:TRP:O	4:H:60:ASN:ND2	2.46	0.48
1:G:386:ASN:HB3	1:G:417:PRO:HD2	1.95	0.48
3:L:165:PRO:HA	3:L:174:ALA:O	2.12	0.48
1:A:210:PHE:HB2	1:A:377:ASN:ND2	2.29	0.48
1:J:294:ILE:HG22	1:J:333:VAL:HG22	1.95	0.48
1:A:476:ARG:HA	1:A:479:TRP:CD1	2.49	0.48
1:G:291:PRO:HG3	6:G:667:NAG:H61	1.94	0.48
8:G:610:MAN:H4	4:H:99:ARG:HH21	1.78	0.48
1:J:192:ARG:HE	1:J:196:CYS:HB2	1.78	0.48
4:F:12:VAL:HG21	4:F:18:LEU:HD13	1.93	0.48
1:G:298:ARG:NH1	1:G:302:ASN:OD1	2.47	0.48
1:A:275:GLU:HB3	1:A:282:LYS:HG2	1.94	0.48
5:D:69:MET:HG2	5:D:80:LEU:HD13	1.95	0.48
4:H:153:ASN:HD21	4:H:192:TYR:HA	1.79	0.48
4:N:197:ASN:ND2	4:N:204:LYS:HE2	2.28	0.48
2:C:522:PHE:CD2	2:C:523:LEU:HG	2.48	0.48
5:I:18:MET:HG2	5:I:82(C):LEU:HD21	1.95	0.48
2:K:593:LEU:HD21	2:K:601:LYS:HA	1.96	0.48
2:C:648:GLU:O	2:C:652:GLN:HB3	2.14	0.48
1:G:101:VAL:HG13	1:G:479:TRP:HB2	1.95	0.48
5:O:47:TRP:HZ2	5:O:50:TRP:CD1	2.32	0.48
5:O:59:TYR:HE1	5:O:69:MET:HG3	1.77	0.48
1:A:503:ARG:NH1	2:C:654:GLU:OE1	2.47	0.48
4:F:70:SER:OG	4:F:79:SER:OG	2.32	0.48
1:J:205:CYS:O	1:J:208:VAL:HG22	2.14	0.48
1:J:350:ARG:NH2	1:J:398:ASN:H	2.12	0.48
5:D:47:TRP:CZ2	5:D:49:GLY:HA2	2.49	0.47
2:K:595:ILE:HG13	2:K:596:TRP:CD1	2.49	0.47
3:E:80:ALA:HA	3:E:106:VAL:HG21	1.97	0.47
1:G:270:VAL:HG12	1:G:289:ASN:H	1.79	0.47
1:A:280:ASN:HB2	1:A:456:ARG:O	2.14	0.47
6:A:652:NAG:H2	4:F:100(D):VAL:HA	1.96	0.47
4:F:68:HIS:HB3	4:F:81:ARG:HB2	1.95	0.47
5:I:69:MET:HG2	5:I:80:LEU:HD13	1.95	0.47
1:A:270:VAL:HG12	1:A:289:ASN:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:51:THR:HB	2:B:578:ALA:HB2	1.96	0.47
5:I:37:ILE:HG12	5:I:47:TRP:HA	1.97	0.47
2:B:602:LEU:HD12	2:C:655:LYS:HD2	1.97	0.47
5:I:47:TRP:HZ2	5:I:50:TRP:CD1	2.32	0.47
1:G:98:ASN:ND2	1:G:486:TYR:O	2.47	0.46
2:K:648:GLU:O	2:K:652:GLN:HB3	2.15	0.46
1:J:230:ASP:OD2	1:J:240:PRO:HD2	2.15	0.46
1:J:503:ARG:NH1	2:K:654:GLU:OE1	2.48	0.46
5:I:47:TRP:CZ2	5:I:49:GLY:HA2	2.51	0.46
3:M:83:GLU:HB2	3:M:106:VAL:HG23	1.98	0.46
1:A:219:ALA:O	1:A:246:GLN:NE2	2.49	0.46
1:A:338:TRP:CZ2	1:A:390:LEU:HB3	2.50	0.46
1:A:69:TRP:CE3	1:A:111:LEU:HD21	2.51	0.46
2:C:535:MET:SD	2:K:656:ASN:ND2	2.87	0.46
2:C:603:ILE:HG13	2:K:655:LYS:HD3	1.97	0.46
3:L:163:THR:HG22	4:H:167:VAL:HB	1.96	0.46
5:D:59:TYR:HE1	5:D:69:MET:HG3	1.81	0.46
1:G:298:ARG:NH2	1:G:439:ILE:O	2.48	0.46
1:J:195:ASN:HD21	1:J:201:ILE:HD12	1.81	0.46
1:J:280:ASN:HB3	1:J:456:ARG:NH2	2.31	0.46
3:E:61:ARG:HD2	3:E:77:SER:HB2	1.98	0.46
1:J:219:ALA:O	1:J:246:GLN:NE2	2.49	0.46
1:J:437:PRO:HA	1:J:438:PRO:HD3	1.85	0.46
2:K:646:LEU:O	2:K:650:GLN:HB2	2.16	0.46
1:A:45:TRP:HB3	1:A:491:ILE:HD13	1.98	0.46
1:G:200:ALA:HA	1:J:313:PRO:HG2	1.97	0.46
1:J:298:ARG:NH2	1:J:439:ILE:O	2.48	0.46
1:G:199:SER:HA	1:J:314:GLY:HA3	1.98	0.46
1:J:125:LEU:HG	1:J:193:LEU:HD11	1.97	0.45
2:C:618:ASN:OD1	2:C:619:LEU:N	2.49	0.45
3:E:83:GLU:HG3	3:E:104:LEU:O	2.17	0.45
1:G:298:ARG:HH21	1:G:443:ILE:HG13	1.80	0.45
1:A:259:LEU:HD12	1:A:374:HIS:CD2	2.51	0.45
1:A:461:ASN:HD21	5:I:203:VAL:HG22	1.81	0.45
1:A:50:THR:HG22	1:A:488:VAL:HG11	1.99	0.45
5:D:47:TRP:HZ2	5:D:50:TRP:CD1	2.34	0.45
1:G:298:ARG:HE	1:G:443:ILE:HD12	1.81	0.45
1:G:258:GLN:HG2	1:G:470:PRO:HB2	1.96	0.45
1:J:298:ARG:NH1	1:J:302:ASN:OD1	2.49	0.45
2:K:570:VAL:C	2:K:572:GLY:H	2.20	0.45
4:N:144:PHE:HA	4:N:145:PRO:HA	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:522:PHE:CD2	2:B:523:LEU:HG	2.51	0.45
1:J:324:GLY:O	3:M:94:ARG:NH1	2.43	0.45
4:N:100(P):MET:N	4:N:100(P):MET:SD	2.89	0.45
1:A:502:LYS:HG2	1:A:503:ARG:N	2.32	0.45
2:B:618:ASN:OD1	2:B:619:LEU:N	2.48	0.45
2:C:646:LEU:O	2:C:650:GLN:HB2	2.17	0.45
1:G:502:LYS:HG2	1:G:503:ARG:N	2.30	0.45
8:G:624:MAN:O2	5:D:82(A):ARG:NH2	2.46	0.45
2:B:570:VAL:C	2:B:572:GLY:H	2.20	0.45
3:E:112:ALA:HB3	3:E:141:TYR:H	1.81	0.45
3:L:116:VAL:HG12	3:L:137:ILE:HG12	1.98	0.45
3:L:97:VAL:HG22	4:H:46:GLU:HG3	1.98	0.45
3:M:121:PRO:HB3	3:M:132:THR:H	1.82	0.45
1:A:183:GLN:HA	1:A:191:TYR:HA	1.99	0.45
6:A:663:NAG:H61	6:A:664:NAG:N2	2.32	0.45
1:G:249:HIS:CE1	1:G:486:TYR:HH	2.29	0.45
1:J:98:ASN:ND2	1:J:486:TYR:O	2.50	0.45
4:H:12:VAL:HG21	4:H:18:LEU:HD13	1.99	0.45
5:I:63:PHE:O	5:I:67:VAL:HG12	2.17	0.45
2:K:522:PHE:CD2	2:K:523:LEU:HG	2.52	0.45
3:L:47:ILE:HA	3:L:58:ILE:HD13	1.99	0.45
1:G:490:LYS:HD2	2:B:585:ARG:NH2	2.31	0.44
5:I:2:VAL:HB	5:I:106:HIS:CE1	2.51	0.44
3:L:135:CYS:HB3	3:L:177:SER:HB3	1.98	0.44
6:A:608:NAG:O7	4:F:58:ASN:ND2	2.50	0.44
1:G:292:VAL:HB	1:G:449:ILE:HB	1.99	0.44
1:G:338:TRP:CZ2	1:G:390:LEU:HB3	2.52	0.44
1:G:416:LEU:HA	1:G:417:PRO:HD3	1.85	0.44
2:C:596:TRP:HE1	2:C:647:GLU:HB3	1.82	0.44
1:J:285:LEU:HD21	1:J:477:ASP:HB3	1.99	0.44
4:H:121:PRO:HD3	4:H:207:LYS:HE2	1.99	0.44
5:D:12:LYS:HE3	5:D:16:GLU:OE2	2.18	0.44
1:J:490:LYS:HD2	2:K:585:ARG:NH2	2.32	0.44
4:N:14:PRO:CG	4:N:111:SER:HB3	2.46	0.44
5:O:47:TRP:CZ2	5:O:49:GLY:HA2	2.53	0.44
5:O:63:PHE:O	5:O:67:VAL:HG12	2.17	0.44
1:G:346:VAL:HG13	1:G:359:ILE:HD12	1.98	0.44
1:A:259:LEU:HB2	1:A:374:HIS:CE1	2.52	0.44
1:A:466:GLU:HA	5:I:61:ARG:NH2	2.32	0.44
1:G:371:VAL:HG21	5:D:54:GLY:HA3	2.00	0.44
1:J:338:TRP:CZ2	1:J:390:LEU:HB3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:111:LEU:HD12	1:G:111:LEU:O	2.18	0.44
1:G:137:ASN:OD1	3:L:95(A):PRO:HA	2.18	0.44
3:L:112:ALA:HB3	3:L:141:TYR:H	1.82	0.44
3:E:120:PRO:HB3	3:E:207:VAL:HG21	2.00	0.43
1:G:36:VAL:CG2	2:B:608:VAL:HB	2.48	0.43
5:D:39:LEU:HD12	5:D:91:PHE:CE2	2.53	0.43
1:J:275:GLU:HB3	1:J:282:LYS:HG2	1.99	0.43
1:J:502:LYS:HG2	1:J:503:ARG:N	2.32	0.43
5:O:39:LEU:HD12	5:O:91:PHE:CE2	2.53	0.43
5:D:50:TRP:CE2	5:D:58:ASN:HB3	2.54	0.43
3:E:116:VAL:HG12	3:E:137:ILE:HG12	2.00	0.43
1:G:358:ILE:O	1:G:465:THR:OG1	2.34	0.43
1:G:95:MET:SD	1:G:273:ARG:HD3	2.58	0.43
1:J:503:ARG:NH2	2:K:597:GLY:O	2.51	0.43
3:L:121:PRO:HB3	3:L:132:THR:H	1.83	0.43
5:I:61:ARG:HG2	5:I:61:ARG:HH11	1.83	0.43
2:B:635:ILE:O	2:B:639:THR:HG23	2.18	0.43
2:C:570:VAL:HG12	2:C:571:TRP:H	1.83	0.43
5:D:2:VAL:HB	5:D:106:HIS:CE1	2.53	0.43
1:G:50:THR:HG22	1:G:488:VAL:HG11	2.01	0.43
4:H:16:GLU:HG2	4:H:17:THR:H	1.82	0.43
1:J:416:LEU:HA	1:J:417:PRO:HD3	1.86	0.43
4:N:12:VAL:HG12	4:N:13:LYS:O	2.18	0.43
4:N:16:GLU:HG2	4:N:17:THR:H	1.83	0.43
4:F:30:ARG:HA	4:F:53:ASP:HB2	2.01	0.43
4:H:12:VAL:HG12	4:H:13:LYS:O	2.19	0.43
3:L:14:ALA:HA	3:L:107:LEU:HB2	2.01	0.43
3:E:121:PRO:HD3	3:E:133:LEU:HD23	2.01	0.43
4:F:12:VAL:HG12	4:F:13:LYS:O	2.19	0.43
1:G:42:VAL:HG22	1:G:493:PRO:O	2.17	0.43
1:A:467:THR:H	5:I:61:ARG:HH21	1.66	0.43
3:L:151:ALA:HB1	3:L:189:HIS:CD2	2.53	0.43
2:B:595:ILE:HG13	2:B:596:TRP:CD1	2.54	0.43
1:A:36:VAL:HG12	2:C:610:TRP:HE3	1.84	0.43
1:J:95:MET:SD	1:J:273:ARG:HD3	2.59	0.43
6:J:608:NAG:O7	4:N:58:ASN:ND2	2.52	0.43
3:M:14:ALA:HB3	3:M:17:GLN:HG3	2.01	0.43
4:N:63:LEU:HD22	4:N:66:ARG:HH21	1.84	0.43
1:A:299:PRO:HB2	1:A:327:ARG:HB2	2.01	0.43
1:A:342:LEU:O	1:A:346:VAL:HG23	2.18	0.43
1:A:426:MET:O	1:A:429:ARG:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:595:ILE:HG13	2:C:596:TRP:CD1	2.53	0.43
1:G:198:THR:OG1	1:G:199:SER:N	2.52	0.43
1:G:342:LEU:O	1:G:346:VAL:HG23	2.18	0.43
4:H:144:PHE:HA	4:H:145:PRO:HA	1.82	0.43
6:J:663:NAG:H61	6:J:664:NAG:N2	2.34	0.43
1:A:416:LEU:HA	1:A:417:PRO:HD3	1.87	0.42
1:G:45:TRP:HB3	1:G:491:ILE:HD13	2.00	0.42
5:I:60:ALA:O	5:I:64:GLN:HG3	2.19	0.42
3:L:19:ALA:HB3	3:L:75:ILE:HB	2.01	0.42
5:O:102:TRP:CD1	5:O:289:TYR:HD1	2.37	0.42
1:A:101:VAL:HG21	1:A:480:ARG:HG2	2.01	0.42
3:E:14:ALA:HA	3:E:107:LEU:HB2	2.00	0.42
4:F:16:GLU:HG2	4:F:17:THR:H	1.84	0.42
1:G:183:GLN:HB3	1:G:191:TYR:CE2	2.54	0.42
1:J:299:PRO:HB2	1:J:327:ARG:HB2	2.01	0.42
4:N:12:VAL:HG21	4:N:18:LEU:HD13	2.00	0.42
1:A:205:CYS:O	1:A:208:VAL:HG22	2.19	0.42
1:A:36:VAL:CG2	2:C:608:VAL:HB	2.49	0.42
1:G:294:ILE:CG2	1:G:333:VAL:HG22	2.49	0.42
1:J:298:ARG:HH21	1:J:443:ILE:HG13	1.85	0.42
1:A:101:VAL:HG13	1:A:479:TRP:HB2	2.02	0.42
6:G:663:NAG:H61	6:G:664:NAG:N2	2.34	0.42
5:I:29:PHE:CD2	5:I:52(A):PRO:HB3	2.54	0.42
2:C:570:VAL:C	2:C:572:GLY:H	2.23	0.42
5:D:38:ARG:HG3	5:D:46:GLU:HB2	2.01	0.42
3:E:60:ASP:N	3:E:60:ASP:OD1	2.52	0.42
2:B:648:GLU:O	2:B:652:GLN:HB3	2.20	0.42
1:J:231:LYS:HD3	1:J:231:LYS:HA	1.84	0.42
2:K:593:LEU:O	2:K:598:CYS:HB2	2.19	0.42
1:A:226:LEU:HD12	1:A:487:LYS:HE2	2.02	0.42
5:D:29:PHE:CD2	5:D:52(A):PRO:HB3	2.54	0.42
1:J:155:LYS:O	1:J:175:LEU:HD12	2.19	0.42
3:M:60:ASP:N	3:M:60:ASP:OD1	2.53	0.42
2:C:525:ALA:HB1	2:C:528:SER:HB2	2.01	0.42
5:D:18:MET:HG2	5:D:82(C):LEU:HD21	2.01	0.42
5:D:23:ARG:HG2	5:D:77:THR:OG1	2.19	0.42
1:J:466:GLU:HA	5:O:61:ARG:NH2	2.35	0.42
1:A:111:LEU:HD12	1:A:111:LEU:O	2.20	0.42
6:A:616:NAG:H62	6:A:617:NAG:H82	2.02	0.42
1:A:491:ILE:HD12	2:C:523:LEU:HD21	2.01	0.42
1:J:258:GLN:HG2	1:J:470:PRO:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:226:LEU:HD12	1:J:487:LYS:HE2	2.01	0.42
1:J:50:THR:OG1	1:J:51:THR:N	2.53	0.42
3:M:112:ALA:HB3	3:M:141:TYR:N	2.34	0.42
1:A:113:ASP:OD1	1:A:429:ARG:NH1	2.43	0.42
4:H:100(B):TYR:CE1	4:H:100(I):GLU:HB3	2.55	0.42
4:H:210:GLU:HA	4:H:211:PRO:HD3	1.91	0.42
5:I:38:ARG:HG3	5:I:46:GLU:HB2	2.02	0.42
3:M:163:THR:HG22	4:N:167:VAL:HB	2.02	0.42
1:A:121:LYS:O	1:A:315:GLN:NE2	2.52	0.41
5:O:60:ALA:O	5:O:64:GLN:HG3	2.20	0.41
1:A:137:ASN:OD1	3:E:95(A):PRO:HA	2.20	0.41
1:G:313:PRO:HG2	1:A:200:ALA:HA	2.02	0.41
2:K:635:ILE:O	2:K:639:THR:HG23	2.19	0.41
4:N:143:TYR:OH	4:N:176:LEU:HD23	2.20	0.41
6:G:641:NAG:H83	5:D:229:GLY:HA2	2.01	0.41
4:H:100(D):VAL:HB	4:H:100(G):PHE:HD2	1.85	0.41
2:B:655:LYS:HD3	2:K:603:ILE:HG13	2.01	0.41
5:I:39:LEU:HD12	5:I:91:PHE:CE2	2.56	0.41
1:J:151:ARG:O	1:J:153:GLU:N	2.53	0.41
1:J:292:VAL:HB	1:J:449:ILE:HB	2.02	0.41
1:J:63:THR:HB	1:J:65:LYS:HE3	2.02	0.41
2:K:618:ASN:OD1	2:K:619:LEU:N	2.51	0.41
3:M:112:ALA:HB3	3:M:141:TYR:H	1.85	0.41
4:N:153:ASN:ND2	4:N:193:ILE:H	2.18	0.41
4:N:210:GLU:HA	4:N:211:PRO:HD3	1.90	0.41
1:A:198:THR:OG1	1:A:199:SER:N	2.53	0.41
1:G:426:MET:O	1:G:429:ARG:HG2	2.21	0.41
8:G:621:MAN:O2	5:D:19:ARG:NH1	2.34	0.41
1:J:270:VAL:HG12	1:J:289:ASN:H	1.85	0.41
5:D:203:VAL:HG12	5:D:204:LEU:H	1.85	0.41
1:G:164:GLU:HA	1:G:312:GLY:HA3	2.01	0.41
1:G:205:CYS:O	1:G:208:VAL:HG22	2.21	0.41
1:J:111:LEU:HD12	1:J:111:LEU:O	2.20	0.41
1:J:294:ILE:CG2	1:J:333:VAL:HG22	2.51	0.41
1:J:342:LEU:O	1:J:346:VAL:HG23	2.19	0.41
2:C:602:LEU:HD12	2:K:655:LYS:HZ2	1.86	0.41
4:H:148:VAL:HB	4:H:176:LEU:HD21	2.02	0.41
1:J:136:ASN:ND2	3:M:93:SER:O	2.54	0.41
3:M:208:ALA:HA	3:M:209:PRO:HD3	1.93	0.41
5:O:69:MET:HG2	5:O:80:LEU:HD13	2.03	0.41
1:A:122:LEU:HD11	1:A:203:GLN:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:VAL:HG13	1:A:359:ILE:HD12	2.03	0.41
4:F:34:TRP:CZ3	4:F:94:THR:HG22	2.56	0.41
1:J:36:VAL:HG22	2:K:608:VAL:HB	2.02	0.41
1:A:292:VAL:HB	1:A:449:ILE:HB	2.03	0.41
3:E:114:PRO:HA	3:E:140:PHE:HB3	2.03	0.41
4:F:197:ASN:ND2	4:F:204:LYS:HE2	2.36	0.41
5:I:67:VAL:HA	5:I:81:GLU:O	2.21	0.41
1:J:272:ILE:HD13	1:J:349:LEU:HD23	2.02	0.41
1:J:426:MET:O	1:J:429:ARG:HG2	2.20	0.41
3:M:107:LEU:HD23	3:M:107:LEU:HA	1.92	0.41
1:A:95:MET:SD	1:A:273:ARG:HD3	2.61	0.41
1:G:136:ASN:HB2	1:G:326:ILE:HD12	2.02	0.41
1:J:123:THR:OG1	1:J:124:PRO:HD3	2.21	0.41
1:A:170:GLN:HG2	1:A:172:VAL:HG13	2.03	0.41
5:O:38:ARG:HG3	5:O:46:GLU:HB2	2.02	0.41
1:A:285:LEU:HD23	1:A:453:ILE:HG23	2.03	0.40
1:A:298:ARG:NH2	1:A:439:ILE:O	2.54	0.40
2:C:523:LEU:H	2:C:540:GLN:CG	2.30	0.40
1:J:249:HIS:CE1	1:J:486:TYR:HH	2.30	0.40
1:J:461:ASN:HB2	5:O:291:PHE:CE1	2.56	0.40
1:G:261:LEU:HD23	1:G:261:LEU:HA	1.77	0.40
1:G:63:THR:HB	1:G:65:LYS:HE3	2.03	0.40
1:J:68:VAL:O	1:J:69:TRP:HB2	2.22	0.40
2:K:570:VAL:HG12	2:K:571:TRP:H	1.86	0.40
3:M:62:PHE:CD1	3:M:75:ILE:HG12	2.56	0.40
1:A:270:VAL:HG12	1:A:289:ASN:N	2.36	0.40
1:A:98:ASN:ND2	1:A:486:TYR:O	2.54	0.40
2:C:596:TRP:O	2:C:651:ASN:ND2	2.55	0.40
1:A:167:ASP:OD2	1:J:128:THR:HG23	2.21	0.40
1:J:122:LEU:HB2	1:J:201:ILE:HG23	2.03	0.40
6:G:607:NAG:H83	3:L:91:TRP:HE3	1.86	0.40
1:A:152:GLY:O	1:A:154:LEU:N	2.49	0.40
1:A:201:ILE:HD11	1:A:435:TYR:HB2	2.03	0.40
1:G:231:LYS:HD3	1:G:231:LYS:HA	1.82	0.40
5:I:233:TRP:HB2	5:I:246:ILE:HB	2.04	0.40
5:O:2:VAL:HB	5:O:106:HIS:CE1	2.55	0.40
4:H:197:ASN:ND2	4:H:204:LYS:HE2	2.36	0.40
1:J:50:THR:HG22	1:J:488:VAL:HG11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	442/472 (94%)	409 (92%)	29 (7%)	4 (1%)	20	63
1	G	442/472 (94%)	410 (93%)	28 (6%)	4 (1%)	20	63
1	J	442/472 (94%)	409 (92%)	29 (7%)	4 (1%)	20	63
2	B	117/152 (77%)	105 (90%)	10 (8%)	2 (2%)	11	52
2	C	117/152 (77%)	105 (90%)	10 (8%)	2 (2%)	11	52
2	K	117/152 (77%)	105 (90%)	10 (8%)	2 (2%)	11	52
3	E	206/211 (98%)	191 (93%)	14 (7%)	1 (0%)	32	74
3	L	206/211 (98%)	191 (93%)	14 (7%)	1 (0%)	32	74
3	M	206/211 (98%)	191 (93%)	14 (7%)	1 (0%)	32	74
4	F	223/235 (95%)	214 (96%)	9 (4%)	0	100	100
4	H	223/235 (95%)	213 (96%)	10 (4%)	0	100	100
4	N	223/235 (95%)	212 (95%)	11 (5%)	0	100	100
5	D	218/241 (90%)	205 (94%)	11 (5%)	2 (1%)	20	63
5	I	218/241 (90%)	206 (94%)	9 (4%)	3 (1%)	13	54
5	O	218/241 (90%)	205 (94%)	10 (5%)	3 (1%)	13	54
All	All	3618/3933 (92%)	3371 (93%)	218 (6%)	29 (1%)	22	67

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	140	ASP
5	D	53	ARG
1	A	140	ASP
5	I	53	ARG
1	J	140	ASP
5	O	53	ARG
2	B	599	SER
2	B	602	LEU

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Mol	Chain	Res	Type
1	A	258	GLN
1	A	461	ASN
2	C	602	LEU
1	J	461	ASN
2	K	599	SER
2	K	602	LEU
1	G	258	GLN
1	G	461	ASN
3	L	199	GLU
2	C	599	SER
3	E	199	GLU
1	J	258	GLN
3	M	199	GLU
1	J	152	GLY
5	O	230	SER
5	I	230	SER
1	G	152	GLY
1	A	152	GLY
5	D	238	PRO
5	O	238	PRO
5	I	238	PRO

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	399/419 (95%)	393 (98%)	6 (2%)	70	86
1	G	399/419 (95%)	394 (99%)	5 (1%)	73	87
1	J	399/419 (95%)	394 (99%)	5 (1%)	73	87
2	B	104/128 (81%)	100 (96%)	4 (4%)	38	68
2	C	104/128 (81%)	100 (96%)	4 (4%)	38	68
2	K	104/128 (81%)	100 (96%)	4 (4%)	38	68
3	E	177/180 (98%)	175 (99%)	2 (1%)	78	89
3	L	177/180 (98%)	175 (99%)	2 (1%)	78	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	M	177/180 (98%)	175 (99%)	2 (1%)	78	89
4	F	197/205 (96%)	196 (100%)	1 (0%)	91	95
4	H	197/205 (96%)	196 (100%)	1 (0%)	91	95
4	N	197/205 (96%)	196 (100%)	1 (0%)	91	95
5	D	183/190 (96%)	179 (98%)	4 (2%)	57	79
5	I	183/190 (96%)	179 (98%)	4 (2%)	57	79
5	O	183/190 (96%)	178 (97%)	5 (3%)	50	75
All	All	3180/3366 (94%)	3130 (98%)	50 (2%)	68	85

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	61	TYR
1	G	126	CYS
1	G	236	THR
1	G	261	LEU
1	G	320	THR
2	B	536	THR
2	B	544	LEU
2	B	570	VAL
2	B	571	TRP
3	L	54	ARG
3	L	111	LYS
4	H	108	THR
5	D	71	ARG
5	D	203	VAL
5	D	283	VAL
5	D	290	GLU
1	A	61	TYR
1	A	126	CYS
1	A	167	ASP
1	A	236	THR
1	A	261	LEU
1	A	320	THR
2	C	536	THR
2	C	544	LEU
2	C	570	VAL
2	C	571	TRP
3	E	54	ARG
3	E	111	LYS

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Mol	Chain	Res	Type
4	F	108	THR
5	I	71	ARG
5	I	203	VAL
5	I	283	VAL
5	I	290	GLU
1	J	61	TYR
1	J	126	CYS
1	J	236	THR
1	J	261	LEU
1	J	320	THR
2	K	536	THR
2	K	544	LEU
2	K	570	VAL
2	K	571	TRP
3	M	54	ARG
3	M	111	LYS
4	N	108	THR
5	O	57	VAL
5	O	71	ARG
5	O	203	VAL
5	O	283	VAL
5	O	290	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	85	HIS
1	G	136	ASN
1	G	170	GLN
1	G	283	ASN
1	G	352	HIS
1	G	422	GLN
1	G	428	GLN
1	G	461	ASN
4	H	76	ASN
4	H	153	ASN
4	H	197	ASN
5	D	106	HIS
5	D	288	GLN
1	A	85	HIS
1	A	136	ASN
1	A	170	GLN

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Mol	Chain	Res	Type
1	A	280	ASN
1	A	283	ASN
1	A	352	HIS
1	A	422	GLN
1	A	428	GLN
1	A	461	ASN
4	F	76	ASN
4	F	153	ASN
4	F	197	ASN
5	I	106	HIS
5	I	288	GLN
1	J	85	HIS
1	J	99	ASN
1	J	170	GLN
1	J	283	ASN
1	J	352	HIS
1	J	422	GLN
1	J	461	ASN
3	M	51	ASN
4	N	76	ASN
4	N	153	ASN
4	N	197	ASN
5	O	106	HIS
5	O	288	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
5	PCA	D	1	5	8,8,9	1.65	1 (12%)	9,10,12	2.17	6 (66%)
5	PCA	I	1	5	8,8,9	1.67	1 (12%)	9,10,12	2.23	6 (66%)
5	PCA	O	1	5	8,8,9	1.67	1 (12%)	9,10,12	2.21	6 (66%)

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	PCA	D	1	5	-	0/0/11/13	0/1/1/1
5	PCA	I	1	5	-	0/0/11/13	0/1/1/1
5	PCA	O	1	5	-	0/0/11/13	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1	PCA	CD-N	4.25	1.46	1.34
5	O	1	PCA	CD-N	4.27	1.46	1.34
5	I	1	PCA	CD-N	4.30	1.47	1.34

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	1	PCA	CB-CA-C	-3.20	108.30	112.70
5	O	1	PCA	CB-CA-C	-3.11	108.42	112.70
5	O	1	PCA	OE-CD-CG	-3.02	121.29	126.86
5	I	1	PCA	OE-CD-CG	-2.99	121.36	126.86
5	D	1	PCA	OE-CD-CG	-2.97	121.40	126.86
5	D	1	PCA	CB-CA-C	-2.86	108.77	112.70
5	O	1	PCA	CA-N-CD	-2.86	103.79	113.58
5	I	1	PCA	CA-N-CD	-2.85	103.81	113.58
5	D	1	PCA	CA-N-CD	-2.85	103.82	113.58
5	I	1	PCA	O-C-CA	-2.13	120.17	125.15
5	D	1	PCA	O-C-CA	-2.08	120.30	125.15
5	O	1	PCA	O-C-CA	-2.05	120.37	125.15
5	I	1	PCA	CG-CD-N	2.21	114.61	108.33
5	O	1	PCA	CG-CD-N	2.21	114.61	108.33
5	D	1	PCA	CG-CD-N	2.23	114.66	108.33
5	I	1	PCA	CB-CA-N	2.54	110.59	103.30
5	O	1	PCA	CB-CA-N	2.55	110.61	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1	PCA	CB-CA-N	2.60	110.77	103.30

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

216 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	NAG	A	601	1,6	14,14,15	0.27	0	15,19,21	0.50	0
6	NAG	A	602	7,6	14,14,15	0.54	0	15,19,21	1.32	1 (6%)
7	BMA	A	603	8,6	11,11,12	0.64	0	13,15,17	0.61	0
8	MAN	A	604	7	11,11,12	0.90	1 (9%)	13,15,17	1.47	3 (23%)
8	MAN	A	605	7	11,11,12	0.92	0	13,15,17	1.08	1 (7%)
6	NAG	A	606	1	14,14,15	0.22	0	15,19,21	0.47	0
6	NAG	A	607	1,6	14,14,15	0.46	0	15,19,21	0.50	0
6	NAG	A	608	7,6	14,14,15	0.27	0	15,19,21	0.41	0
7	BMA	A	609	8,6	11,11,12	0.64	0	13,15,17	0.70	0
8	MAN	A	610	7	11,11,12	0.76	1 (9%)	13,15,17	1.04	1 (7%)
6	NAG	A	611	1,6	14,14,15	0.20	0	15,19,21	0.54	0
6	NAG	A	612	7,6	14,14,15	0.25	0	15,19,21	0.39	0
7	BMA	A	613	8,6	11,11,12	0.61	0	13,15,17	0.44	0
8	MAN	A	614	7	11,11,12	0.81	0	13,15,17	1.05	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	MAN	A	615	7	11,11,12	0.66	0	13,15,17	1.07	2 (15%)
6	NAG	A	616	1,6	14,14,15	0.26	0	15,19,21	0.55	0
6	NAG	A	617	6	14,14,15	0.47	0	15,19,21	1.28	1 (6%)
6	NAG	A	618	1,6	14,14,15	0.53	0	15,19,21	0.67	0
6	NAG	A	619	7,6	14,14,15	0.28	0	15,19,21	0.49	0
7	BMA	A	620	8,6	11,11,12	0.66	0	13,15,17	1.73	2 (15%)
8	MAN	A	621	7	11,11,12	0.72	0	13,15,17	1.47	3 (23%)
8	MAN	A	622	8,7	11,11,12	1.19	1 (9%)	13,15,17	1.47	3 (23%)
8	MAN	A	623	8	11,11,12	0.81	0	13,15,17	1.44	2 (15%)
8	MAN	A	624	8	11,11,12	0.73	0	13,15,17	1.59	3 (23%)
6	NAG	A	625	1,6	14,14,15	0.80	1 (7%)	15,19,21	0.76	0
6	NAG	A	626	7,6	14,14,15	0.42	0	15,19,21	0.49	0
7	BMA	A	627	8,6	11,11,12	0.66	0	13,15,17	1.26	2 (15%)
8	MAN	A	628	8,7	11,11,12	0.64	0	13,15,17	1.48	2 (15%)
8	MAN	A	629	8	11,11,12	0.87	0	13,15,17	1.23	1 (7%)
8	MAN	A	630	8	11,11,12	0.95	0	13,15,17	1.11	1 (7%)
8	MAN	A	631	8,7	11,11,12	1.14	2 (18%)	13,15,17	1.40	2 (15%)
8	MAN	A	632	8	11,11,12	0.96	0	13,15,17	1.36	1 (7%)
8	MAN	A	633	8	11,11,12	0.83	0	13,15,17	1.26	2 (15%)
8	MAN	A	634	8	11,11,12	0.61	0	13,15,17	1.46	2 (15%)
8	MAN	A	635	8	11,11,12	0.69	0	13,15,17	1.28	2 (15%)
6	NAG	A	636	1,6	14,14,15	0.69	1 (7%)	15,19,21	0.72	0
6	NAG	A	637	7,6	14,14,15	0.29	0	15,19,21	0.51	0
7	BMA	A	638	8,6	11,11,12	0.65	0	13,15,17	1.01	1 (7%)
8	MAN	A	639	7	11,11,12	0.72	0	13,15,17	1.42	2 (15%)
8	MAN	A	640	7	11,11,12	0.80	0	13,15,17	1.15	2 (15%)
6	NAG	A	641	1	14,14,15	0.21	0	15,19,21	0.42	0
6	NAG	A	642	1,6	14,14,15	0.31	0	15,19,21	0.55	0
6	NAG	A	643	6	14,14,15	0.25	0	15,19,21	0.45	0
6	NAG	A	644	1,6	14,14,15	0.59	1 (7%)	15,19,21	0.82	0
6	NAG	A	645	7,6	14,14,15	0.48	0	15,19,21	0.38	0
7	BMA	A	646	8,6	11,11,12	0.63	0	13,15,17	0.91	0
8	MAN	A	647	7	11,11,12	0.69	0	13,15,17	1.31	2 (15%)
8	MAN	A	648	8,7	11,11,12	1.00	0	13,15,17	1.38	2 (15%)
8	MAN	A	649	8	11,11,12	0.66	0	13,15,17	1.31	2 (15%)
8	MAN	A	650	8	11,11,12	0.73	0	13,15,17	1.49	3 (23%)
6	NAG	A	651	1,6	14,14,15	0.39	0	15,19,21	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	A	652	7,6	14,14,15	0.34	0	15,19,21	0.55	0
7	BMA	A	653	8,6	11,11,12	0.75	0	13,15,17	1.20	2 (15%)
8	MAN	A	654	8,7	11,11,12	0.81	0	13,15,17	1.07	2 (15%)
8	MAN	A	655	8	11,11,12	0.71	0	13,15,17	1.13	2 (15%)
8	MAN	A	656	8	11,11,12	0.69	0	13,15,17	1.08	2 (15%)
8	MAN	A	657	8,7	11,11,12	0.75	0	13,15,17	1.45	3 (23%)
8	MAN	A	658	8	11,11,12	0.83	1 (9%)	13,15,17	0.91	1 (7%)
8	MAN	A	659	8	11,11,12	0.62	0	13,15,17	1.28	2 (15%)
8	MAN	A	660	8	11,11,12	0.75	0	13,15,17	1.25	2 (15%)
6	NAG	A	661	1	14,14,15	0.21	0	15,19,21	0.45	0
6	NAG	A	662	1	14,14,15	0.32	0	15,19,21	0.51	0
6	NAG	A	663	1,6	14,14,15	0.27	0	15,19,21	0.69	0
6	NAG	A	664	6	14,14,15	0.22	0	15,19,21	0.45	0
6	NAG	A	665	1,6	14,14,15	0.26	0	15,19,21	0.45	0
6	NAG	A	666	6	14,14,15	0.36	0	15,19,21	0.52	0
6	NAG	A	667	1,6	14,14,15	0.20	0	15,19,21	0.60	0
6	NAG	A	668	6	14,14,15	0.27	0	15,19,21	0.45	0
6	NAG	A	669	1,6	14,14,15	0.70	1 (7%)	15,19,21	0.73	0
6	NAG	A	670	6	14,14,15	0.27	0	15,19,21	0.45	0
6	NAG	B	701	2	14,14,15	0.17	0	15,19,21	0.57	0
6	NAG	B	702	2	14,14,15	0.18	0	15,19,21	0.49	0
6	NAG	C	701	2	14,14,15	0.20	0	15,19,21	0.52	0
6	NAG	C	702	2	14,14,15	0.19	0	15,19,21	0.46	0
6	NAG	G	601	1,6	14,14,15	0.31	0	15,19,21	0.50	0
6	NAG	G	602	7,6	14,14,15	0.58	0	15,19,21	1.34	2 (13%)
7	BMA	G	603	8,6	11,11,12	0.60	0	13,15,17	0.59	0
8	MAN	G	604	7	11,11,12	0.81	0	13,15,17	1.38	3 (23%)
8	MAN	G	605	7	11,11,12	0.93	0	13,15,17	1.11	1 (7%)
6	NAG	G	606	1	14,14,15	0.23	0	15,19,21	0.48	0
6	NAG	G	607	1,6	14,14,15	0.52	0	15,19,21	0.46	0
6	NAG	G	608	7,6	14,14,15	0.28	0	15,19,21	0.42	0
7	BMA	G	609	8,6	11,11,12	0.62	0	13,15,17	0.67	0
8	MAN	G	610	7	11,11,12	0.91	1 (9%)	13,15,17	0.96	1 (7%)
6	NAG	G	611	1,6	14,14,15	0.22	0	15,19,21	0.55	0
6	NAG	G	612	7,6	14,14,15	0.23	0	15,19,21	0.41	0
7	BMA	G	613	8,6	11,11,12	0.62	0	13,15,17	0.55	0
8	MAN	G	614	7	11,11,12	0.73	0	13,15,17	1.14	2 (15%)
8	MAN	G	615	7	11,11,12	0.68	0	13,15,17	1.09	2 (15%)
6	NAG	G	616	1,6	14,14,15	0.25	0	15,19,21	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	G	617	6	14,14,15	0.51	0	15,19,21	1.29	1 (6%)
6	NAG	G	618	1,6	14,14,15	0.48	0	15,19,21	0.70	0
6	NAG	G	619	7,6	14,14,15	0.35	0	15,19,21	0.48	0
7	BMA	G	620	8,6	11,11,12	0.65	0	13,15,17	1.55	3 (23%)
8	MAN	G	621	7	11,11,12	0.69	0	13,15,17	1.38	3 (23%)
8	MAN	G	622	8,7	11,11,12	1.25	2 (18%)	13,15,17	1.43	3 (23%)
8	MAN	G	623	8	11,11,12	0.77	0	13,15,17	1.45	2 (15%)
8	MAN	G	624	8	11,11,12	0.67	0	13,15,17	1.45	3 (23%)
6	NAG	G	625	1,6	14,14,15	0.64	0	15,19,21	0.73	0
6	NAG	G	626	7,6	14,14,15	0.38	0	15,19,21	0.47	0
7	BMA	G	627	8,6	11,11,12	0.68	0	13,15,17	1.33	2 (15%)
8	MAN	G	628	8,7	11,11,12	0.65	0	13,15,17	1.43	2 (15%)
8	MAN	G	629	8	11,11,12	0.89	1 (9%)	13,15,17	1.17	2 (15%)
8	MAN	G	630	8	11,11,12	0.91	0	13,15,17	1.16	2 (15%)
8	MAN	G	631	8,7	11,11,12	1.21	2 (18%)	13,15,17	1.47	3 (23%)
8	MAN	G	632	8	11,11,12	1.05	1 (9%)	13,15,17	1.30	1 (7%)
8	MAN	G	633	8	11,11,12	0.80	0	13,15,17	1.28	2 (15%)
8	MAN	G	634	8	11,11,12	0.63	0	13,15,17	1.52	2 (15%)
8	MAN	G	635	8	11,11,12	0.75	0	13,15,17	1.34	2 (15%)
6	NAG	G	636	1,6	14,14,15	0.77	1 (7%)	15,19,21	0.70	0
6	NAG	G	637	7,6	14,14,15	0.32	0	15,19,21	0.54	0
7	BMA	G	638	8,6	11,11,12	0.65	0	13,15,17	1.10	1 (7%)
8	MAN	G	639	7	11,11,12	0.73	0	13,15,17	1.33	2 (15%)
8	MAN	G	640	7	11,11,12	0.88	0	13,15,17	1.11	1 (7%)
6	NAG	G	641	1	14,14,15	0.25	0	15,19,21	0.45	0
6	NAG	G	642	1,6	14,14,15	0.39	0	15,19,21	0.50	0
6	NAG	G	643	6	14,14,15	0.21	0	15,19,21	0.44	0
6	NAG	G	644	1,6	14,14,15	0.67	1 (7%)	15,19,21	0.84	1 (6%)
6	NAG	G	645	7,6	14,14,15	0.43	0	15,19,21	0.38	0
7	BMA	G	646	8,6	11,11,12	0.63	0	13,15,17	0.85	0
8	MAN	G	647	7	11,11,12	0.73	0	13,15,17	1.36	2 (15%)
8	MAN	G	648	8,7	11,11,12	1.06	1 (9%)	13,15,17	1.29	2 (15%)
8	MAN	G	649	8	11,11,12	0.67	0	13,15,17	1.26	2 (15%)
8	MAN	G	650	8	11,11,12	0.70	0	13,15,17	1.49	3 (23%)
6	NAG	G	651	1,6	14,14,15	0.30	0	15,19,21	0.48	0
6	NAG	G	652	7,6	14,14,15	0.27	0	15,19,21	0.58	0
7	BMA	G	653	8,6	11,11,12	0.71	0	13,15,17	1.28	2 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	MAN	G	654	8,7	11,11,12	0.85	1 (9%)	13,15,17	1.16	2 (15%)
8	MAN	G	655	8	11,11,12	0.71	0	13,15,17	1.11	1 (7%)
8	MAN	G	656	8	11,11,12	0.70	0	13,15,17	1.12	2 (15%)
8	MAN	G	657	8,7	11,11,12	0.67	0	13,15,17	1.41	3 (23%)
8	MAN	G	658	8	11,11,12	0.71	1 (9%)	13,15,17	0.97	1 (7%)
8	MAN	G	659	8	11,11,12	0.54	0	13,15,17	1.38	3 (23%)
8	MAN	G	660	8	11,11,12	0.73	0	13,15,17	1.25	2 (15%)
6	NAG	G	661	1	14,14,15	0.21	0	15,19,21	0.46	0
6	NAG	G	662	1	14,14,15	0.34	0	15,19,21	0.55	0
6	NAG	G	663	1,6	14,14,15	0.24	0	15,19,21	0.68	0
6	NAG	G	664	6	14,14,15	0.23	0	15,19,21	0.45	0
6	NAG	G	665	1,6	14,14,15	0.23	0	15,19,21	0.47	0
6	NAG	G	666	6	14,14,15	0.44	0	15,19,21	0.53	0
6	NAG	G	667	1,6	14,14,15	0.17	0	15,19,21	0.57	0
6	NAG	G	668	6	14,14,15	0.26	0	15,19,21	0.41	0
6	NAG	G	669	1,6	14,14,15	0.80	1 (7%)	15,19,21	0.73	0
6	NAG	G	670	6	14,14,15	0.24	0	15,19,21	0.46	0
6	NAG	J	601	1,6	14,14,15	0.34	0	15,19,21	0.51	0
6	NAG	J	602	7,6	14,14,15	0.56	0	15,19,21	1.34	1 (6%)
7	BMA	J	603	8,6	11,11,12	0.59	0	13,15,17	0.45	0
8	MAN	J	604	7	11,11,12	0.87	0	13,15,17	1.35	3 (23%)
8	MAN	J	605	7	11,11,12	0.92	1 (9%)	13,15,17	1.05	1 (7%)
6	NAG	J	606	1	14,14,15	0.21	0	15,19,21	0.46	0
6	NAG	J	607	1,6	14,14,15	0.45	0	15,19,21	0.53	0
6	NAG	J	608	7,6	14,14,15	0.27	0	15,19,21	0.42	0
7	BMA	J	609	8,6	11,11,12	0.65	0	13,15,17	0.66	0
8	MAN	J	610	7	11,11,12	0.78	1 (9%)	13,15,17	1.02	1 (7%)
6	NAG	J	611	1,6	14,14,15	0.14	0	15,19,21	0.55	0
6	NAG	J	612	7,6	14,14,15	0.19	0	15,19,21	0.44	0
7	BMA	J	613	8,6	11,11,12	0.61	0	13,15,17	0.50	0
8	MAN	J	614	7	11,11,12	0.80	0	13,15,17	1.11	2 (15%)
8	MAN	J	615	7	11,11,12	0.63	0	13,15,17	1.10	2 (15%)
6	NAG	J	616	1,6	14,14,15	0.25	0	15,19,21	0.54	0
6	NAG	J	617	6	14,14,15	0.53	0	15,19,21	1.32	2 (13%)
6	NAG	J	618	1,6	14,14,15	0.51	0	15,19,21	0.67	0
6	NAG	J	619	7,6	14,14,15	0.36	0	15,19,21	0.47	0
7	BMA	J	620	8,6	11,11,12	0.64	0	13,15,17	1.44	1 (7%)
8	MAN	J	621	7	11,11,12	0.68	0	13,15,17	1.39	3 (23%)
8	MAN	J	622	8,7	11,11,12	1.29	1 (9%)	13,15,17	1.38	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	MAN	J	623	8	11,11,12	0.80	0	13,15,17	1.35	2 (15%)
8	MAN	J	624	8	11,11,12	0.63	0	13,15,17	1.49	3 (23%)
6	NAG	J	625	1,6	14,14,15	0.68	1 (7%)	15,19,21	0.77	0
6	NAG	J	626	7,6	14,14,15	0.38	0	15,19,21	0.45	0
7	BMA	J	627	8,6	11,11,12	0.68	0	13,15,17	1.40	3 (23%)
8	MAN	J	628	8,7	11,11,12	0.67	0	13,15,17	1.43	2 (15%)
8	MAN	J	629	8	11,11,12	0.90	0	13,15,17	1.23	1 (7%)
8	MAN	J	630	8	11,11,12	0.95	0	13,15,17	1.14	1 (7%)
8	MAN	J	631	8,7	11,11,12	1.15	2 (18%)	13,15,17	1.35	2 (15%)
8	MAN	J	632	8	11,11,12	0.92	0	13,15,17	1.36	1 (7%)
8	MAN	J	633	8	11,11,12	0.77	0	13,15,17	1.20	2 (15%)
8	MAN	J	634	8	11,11,12	0.61	0	13,15,17	1.54	2 (15%)
8	MAN	J	635	8	11,11,12	0.67	0	13,15,17	1.17	2 (15%)
6	NAG	J	636	1,6	14,14,15	0.85	1 (7%)	15,19,21	0.69	0
6	NAG	J	637	7,6	14,14,15	0.35	0	15,19,21	0.55	0
7	BMA	J	638	8,6	11,11,12	0.65	0	13,15,17	1.12	1 (7%)
8	MAN	J	639	7	11,11,12	0.79	0	13,15,17	1.33	2 (15%)
8	MAN	J	640	7	11,11,12	0.85	0	13,15,17	1.10	1 (7%)
6	NAG	J	641	1	14,14,15	0.22	0	15,19,21	0.45	0
6	NAG	J	642	1,6	14,14,15	0.36	0	15,19,21	0.52	0
6	NAG	J	643	6	14,14,15	0.24	0	15,19,21	0.42	0
6	NAG	J	644	1,6	14,14,15	0.68	1 (7%)	15,19,21	0.86	1 (6%)
6	NAG	J	645	7,6	14,14,15	0.42	0	15,19,21	0.41	0
7	BMA	J	646	8,6	11,11,12	0.63	0	13,15,17	0.95	0
8	MAN	J	647	7	11,11,12	0.68	0	13,15,17	1.31	1 (7%)
8	MAN	J	648	8,7	11,11,12	1.07	1 (9%)	13,15,17	1.34	2 (15%)
8	MAN	J	649	8	11,11,12	0.69	0	13,15,17	1.27	2 (15%)
8	MAN	J	650	8	11,11,12	0.70	0	13,15,17	1.50	3 (23%)
6	NAG	J	651	1,6	14,14,15	0.24	0	15,19,21	0.47	0
6	NAG	J	652	7,6	14,14,15	0.32	0	15,19,21	0.58	0
7	BMA	J	653	8,6	11,11,12	0.72	0	13,15,17	1.29	1 (7%)
8	MAN	J	654	8,7	11,11,12	0.85	1 (9%)	13,15,17	1.09	2 (15%)
8	MAN	J	655	8	11,11,12	0.75	1 (9%)	13,15,17	1.11	1 (7%)
8	MAN	J	656	8	11,11,12	0.73	0	13,15,17	1.08	1 (7%)
8	MAN	J	657	8,7	11,11,12	0.71	0	13,15,17	1.42	3 (23%)
8	MAN	J	658	8	11,11,12	0.73	1 (9%)	13,15,17	0.97	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	MAN	J	659	8	11,11,12	0.55	0	13,15,17	1.34	3 (23%)
8	MAN	J	660	8	11,11,12	0.78	0	13,15,17	1.25	2 (15%)
6	NAG	J	661	1	14,14,15	0.23	0	15,19,21	0.47	0
6	NAG	J	662	1	14,14,15	0.28	0	15,19,21	0.50	0
6	NAG	J	663	1,6	14,14,15	0.25	0	15,19,21	0.64	0
6	NAG	J	664	6	14,14,15	0.23	0	15,19,21	0.46	0
6	NAG	J	665	1,6	14,14,15	0.24	0	15,19,21	0.48	0
6	NAG	J	666	6	14,14,15	0.39	0	15,19,21	0.53	0
6	NAG	J	667	1,6	14,14,15	0.20	0	15,19,21	0.61	0
6	NAG	J	668	6	14,14,15	0.27	0	15,19,21	0.45	0
6	NAG	J	669	1,6	14,14,15	0.69	1 (7%)	15,19,21	0.71	0
6	NAG	J	670	6	14,14,15	0.22	0	15,19,21	0.51	0
6	NAG	K	701	2	14,14,15	0.24	0	15,19,21	0.54	0
6	NAG	K	702	2	14,14,15	0.19	0	15,19,21	0.46	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	601	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	602	7,6	-	0/6/23/26	0/1/1/1
7	BMA	A	603	8,6	-	0/2/19/22	0/1/1/1
8	MAN	A	604	7	-	0/2/19/22	0/1/1/1
8	MAN	A	605	7	-	0/2/19/22	0/1/1/1
6	NAG	A	606	1	-	0/6/23/26	0/1/1/1
6	NAG	A	607	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	608	7,6	-	0/6/23/26	0/1/1/1
7	BMA	A	609	8,6	-	0/2/19/22	0/1/1/1
8	MAN	A	610	7	-	0/2/19/22	0/1/1/1
6	NAG	A	611	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	612	7,6	-	0/6/23/26	0/1/1/1
7	BMA	A	613	8,6	-	0/2/19/22	0/1/1/1
8	MAN	A	614	7	-	0/2/19/22	0/1/1/1
8	MAN	A	615	7	-	0/2/19/22	0/1/1/1
6	NAG	A	616	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	617	6	-	0/6/23/26	0/1/1/1
6	NAG	A	618	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	619	7,6	-	0/6/23/26	0/1/1/1
7	BMA	A	620	8,6	-	0/2/19/22	0/1/1/1
8	MAN	A	621	7	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	MAN	A	622	8,7	-	0/2/19/22	0/1/1/1
8	MAN	A	623	8	-	0/2/19/22	0/1/1/1
8	MAN	A	624	8	-	0/2/19/22	0/1/1/1
6	NAG	A	625	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	626	7,6	-	0/6/23/26	0/1/1/1
7	BMA	A	627	8,6	-	0/2/19/22	0/1/1/1
8	MAN	A	628	8,7	-	0/2/19/22	0/1/1/1
8	MAN	A	629	8	-	0/2/19/22	0/1/1/1
8	MAN	A	630	8	-	0/2/19/22	0/1/1/1
8	MAN	A	631	8,7	-	0/2/19/22	0/1/1/1
8	MAN	A	632	8	-	0/2/19/22	0/1/1/1
8	MAN	A	633	8	-	0/2/19/22	0/1/1/1
8	MAN	A	634	8	-	0/2/19/22	0/1/1/1
8	MAN	A	635	8	-	0/2/19/22	0/1/1/1
6	NAG	A	636	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	637	7,6	-	0/6/23/26	0/1/1/1
7	BMA	A	638	8,6	-	0/2/19/22	0/1/1/1
8	MAN	A	639	7	-	0/2/19/22	0/1/1/1
8	MAN	A	640	7	-	0/2/19/22	0/1/1/1
6	NAG	A	641	1	-	0/6/23/26	0/1/1/1
6	NAG	A	642	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	643	6	-	0/6/23/26	0/1/1/1
6	NAG	A	644	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	645	7,6	-	0/6/23/26	0/1/1/1
7	BMA	A	646	8,6	-	0/2/19/22	0/1/1/1
8	MAN	A	647	7	-	0/2/19/22	0/1/1/1
8	MAN	A	648	8,7	-	0/2/19/22	0/1/1/1
8	MAN	A	649	8	-	0/2/19/22	0/1/1/1
8	MAN	A	650	8	-	0/2/19/22	0/1/1/1
6	NAG	A	651	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	652	7,6	-	0/6/23/26	0/1/1/1
7	BMA	A	653	8,6	-	0/2/19/22	0/1/1/1
8	MAN	A	654	8,7	-	0/2/19/22	0/1/1/1
8	MAN	A	655	8	-	0/2/19/22	0/1/1/1
8	MAN	A	656	8	-	0/2/19/22	0/1/1/1
8	MAN	A	657	8,7	-	0/2/19/22	0/1/1/1
8	MAN	A	658	8	-	0/2/19/22	0/1/1/1
8	MAN	A	659	8	-	0/2/19/22	0/1/1/1
8	MAN	A	660	8	-	0/2/19/22	1/1/1/1
6	NAG	A	661	1	-	0/6/23/26	0/1/1/1
6	NAG	A	662	1	-	0/6/23/26	0/1/1/1
6	NAG	A	663	1,6	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	664	6	-	0/6/23/26	0/1/1/1
6	NAG	A	665	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	666	6	-	0/6/23/26	0/1/1/1
6	NAG	A	667	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	668	6	-	0/6/23/26	0/1/1/1
6	NAG	A	669	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	670	6	-	0/6/23/26	0/1/1/1
6	NAG	B	701	2	-	0/6/23/26	0/1/1/1
6	NAG	B	702	2	-	0/6/23/26	0/1/1/1
6	NAG	C	701	2	-	0/6/23/26	0/1/1/1
6	NAG	C	702	2	-	0/6/23/26	0/1/1/1
6	NAG	G	601	1,6	-	0/6/23/26	0/1/1/1
6	NAG	G	602	7,6	-	0/6/23/26	0/1/1/1
7	BMA	G	603	8,6	-	0/2/19/22	0/1/1/1
8	MAN	G	604	7	-	0/2/19/22	0/1/1/1
8	MAN	G	605	7	-	0/2/19/22	0/1/1/1
6	NAG	G	606	1	-	0/6/23/26	0/1/1/1
6	NAG	G	607	1,6	-	0/6/23/26	0/1/1/1
6	NAG	G	608	7,6	-	0/6/23/26	0/1/1/1
7	BMA	G	609	8,6	-	0/2/19/22	0/1/1/1
8	MAN	G	610	7	-	0/2/19/22	0/1/1/1
6	NAG	G	611	1,6	-	0/6/23/26	0/1/1/1
6	NAG	G	612	7,6	-	0/6/23/26	0/1/1/1
7	BMA	G	613	8,6	-	0/2/19/22	0/1/1/1
8	MAN	G	614	7	-	0/2/19/22	0/1/1/1
8	MAN	G	615	7	-	0/2/19/22	0/1/1/1
6	NAG	G	616	1,6	-	0/6/23/26	0/1/1/1
6	NAG	G	617	6	-	0/6/23/26	0/1/1/1
6	NAG	G	618	1,6	-	0/6/23/26	0/1/1/1
6	NAG	G	619	7,6	-	0/6/23/26	0/1/1/1
7	BMA	G	620	8,6	-	0/2/19/22	0/1/1/1
8	MAN	G	621	7	-	0/2/19/22	0/1/1/1
8	MAN	G	622	8,7	-	0/2/19/22	0/1/1/1
8	MAN	G	623	8	-	0/2/19/22	0/1/1/1
8	MAN	G	624	8	-	0/2/19/22	0/1/1/1
6	NAG	G	625	1,6	-	0/6/23/26	0/1/1/1
6	NAG	G	626	7,6	-	0/6/23/26	0/1/1/1
7	BMA	G	627	8,6	-	0/2/19/22	0/1/1/1
8	MAN	G	628	8,7	-	0/2/19/22	0/1/1/1
8	MAN	G	629	8	-	0/2/19/22	0/1/1/1
8	MAN	G	630	8	-	0/2/19/22	0/1/1/1
8	MAN	G	631	8,7	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	MAN	G	632	8	-	0/2/19/22	0/1/1/1
8	MAN	G	633	8	-	0/2/19/22	0/1/1/1
8	MAN	G	634	8	-	0/2/19/22	0/1/1/1
8	MAN	G	635	8	-	0/2/19/22	0/1/1/1
6	NAG	G	636	1,6	-	0/6/23/26	0/1/1/1
6	NAG	G	637	7,6	-	0/6/23/26	0/1/1/1
7	BMA	G	638	8,6	-	0/2/19/22	0/1/1/1
8	MAN	G	639	7	-	0/2/19/22	0/1/1/1
8	MAN	G	640	7	-	0/2/19/22	0/1/1/1
6	NAG	G	641	1	-	0/6/23/26	0/1/1/1
6	NAG	G	642	1,6	-	0/6/23/26	0/1/1/1
6	NAG	G	643	6	-	0/6/23/26	0/1/1/1
6	NAG	G	644	1,6	-	0/6/23/26	0/1/1/1
6	NAG	G	645	7,6	-	0/6/23/26	0/1/1/1
7	BMA	G	646	8,6	-	0/2/19/22	0/1/1/1
8	MAN	G	647	7	-	0/2/19/22	0/1/1/1
8	MAN	G	648	8,7	-	0/2/19/22	0/1/1/1
8	MAN	G	649	8	-	0/2/19/22	0/1/1/1
8	MAN	G	650	8	-	0/2/19/22	0/1/1/1
6	NAG	G	651	1,6	-	0/6/23/26	0/1/1/1
6	NAG	G	652	7,6	-	0/6/23/26	0/1/1/1
7	BMA	G	653	8,6	-	0/2/19/22	0/1/1/1
8	MAN	G	654	8,7	-	0/2/19/22	0/1/1/1
8	MAN	G	655	8	-	0/2/19/22	0/1/1/1
8	MAN	G	656	8	-	0/2/19/22	0/1/1/1
8	MAN	G	657	8,7	-	0/2/19/22	0/1/1/1
8	MAN	G	658	8	-	0/2/19/22	0/1/1/1
8	MAN	G	659	8	-	0/2/19/22	0/1/1/1
8	MAN	G	660	8	-	0/2/19/22	1/1/1/1
6	NAG	G	661	1	-	0/6/23/26	0/1/1/1
6	NAG	G	662	1	-	0/6/23/26	0/1/1/1
6	NAG	G	663	1,6	-	0/6/23/26	0/1/1/1
6	NAG	G	664	6	-	0/6/23/26	0/1/1/1
6	NAG	G	665	1,6	-	0/6/23/26	0/1/1/1
6	NAG	G	666	6	-	0/6/23/26	0/1/1/1
6	NAG	G	667	1,6	-	0/6/23/26	0/1/1/1
6	NAG	G	668	6	-	0/6/23/26	0/1/1/1
6	NAG	G	669	1,6	-	0/6/23/26	0/1/1/1
6	NAG	G	670	6	-	0/6/23/26	0/1/1/1
6	NAG	J	601	1,6	-	0/6/23/26	0/1/1/1
6	NAG	J	602	7,6	-	0/6/23/26	0/1/1/1
7	BMA	J	603	8,6	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	MAN	J	604	7	-	0/2/19/22	0/1/1/1
8	MAN	J	605	7	-	0/2/19/22	0/1/1/1
6	NAG	J	606	1	-	0/6/23/26	0/1/1/1
6	NAG	J	607	1,6	-	0/6/23/26	0/1/1/1
6	NAG	J	608	7,6	-	0/6/23/26	0/1/1/1
7	BMA	J	609	8,6	-	0/2/19/22	0/1/1/1
8	MAN	J	610	7	-	0/2/19/22	0/1/1/1
6	NAG	J	611	1,6	-	0/6/23/26	0/1/1/1
6	NAG	J	612	7,6	-	0/6/23/26	0/1/1/1
7	BMA	J	613	8,6	-	0/2/19/22	0/1/1/1
8	MAN	J	614	7	-	0/2/19/22	0/1/1/1
8	MAN	J	615	7	-	0/2/19/22	0/1/1/1
6	NAG	J	616	1,6	-	0/6/23/26	0/1/1/1
6	NAG	J	617	6	-	0/6/23/26	0/1/1/1
6	NAG	J	618	1,6	-	0/6/23/26	0/1/1/1
6	NAG	J	619	7,6	-	0/6/23/26	0/1/1/1
7	BMA	J	620	8,6	-	0/2/19/22	0/1/1/1
8	MAN	J	621	7	-	0/2/19/22	0/1/1/1
8	MAN	J	622	8,7	-	0/2/19/22	0/1/1/1
8	MAN	J	623	8	-	0/2/19/22	0/1/1/1
8	MAN	J	624	8	-	0/2/19/22	0/1/1/1
6	NAG	J	625	1,6	-	0/6/23/26	0/1/1/1
6	NAG	J	626	7,6	-	0/6/23/26	0/1/1/1
7	BMA	J	627	8,6	-	0/2/19/22	0/1/1/1
8	MAN	J	628	8,7	-	0/2/19/22	0/1/1/1
8	MAN	J	629	8	-	0/2/19/22	0/1/1/1
8	MAN	J	630	8	-	0/2/19/22	0/1/1/1
8	MAN	J	631	8,7	-	0/2/19/22	0/1/1/1
8	MAN	J	632	8	-	0/2/19/22	0/1/1/1
8	MAN	J	633	8	-	0/2/19/22	0/1/1/1
8	MAN	J	634	8	-	0/2/19/22	0/1/1/1
8	MAN	J	635	8	-	0/2/19/22	0/1/1/1
6	NAG	J	636	1,6	-	0/6/23/26	0/1/1/1
6	NAG	J	637	7,6	-	0/6/23/26	0/1/1/1
7	BMA	J	638	8,6	-	0/2/19/22	0/1/1/1
8	MAN	J	639	7	-	0/2/19/22	0/1/1/1
8	MAN	J	640	7	-	0/2/19/22	0/1/1/1
6	NAG	J	641	1	-	0/6/23/26	0/1/1/1
6	NAG	J	642	1,6	-	0/6/23/26	0/1/1/1
6	NAG	J	643	6	-	0/6/23/26	0/1/1/1
6	NAG	J	644	1,6	-	0/6/23/26	0/1/1/1
6	NAG	J	645	7,6	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BMA	J	646	8,6	-	0/2/19/22	0/1/1/1
8	MAN	J	647	7	-	0/2/19/22	0/1/1/1
8	MAN	J	648	8,7	-	0/2/19/22	0/1/1/1
8	MAN	J	649	8	-	0/2/19/22	0/1/1/1
8	MAN	J	650	8	-	0/2/19/22	0/1/1/1
6	NAG	J	651	1,6	-	0/6/23/26	0/1/1/1
6	NAG	J	652	7,6	-	0/6/23/26	0/1/1/1
7	BMA	J	653	8,6	-	0/2/19/22	0/1/1/1
8	MAN	J	654	8,7	-	0/2/19/22	0/1/1/1
8	MAN	J	655	8	-	0/2/19/22	0/1/1/1
8	MAN	J	656	8	-	0/2/19/22	0/1/1/1
8	MAN	J	657	8,7	-	0/2/19/22	0/1/1/1
8	MAN	J	658	8	-	0/2/19/22	0/1/1/1
8	MAN	J	659	8	-	0/2/19/22	0/1/1/1
8	MAN	J	660	8	-	0/2/19/22	1/1/1/1
6	NAG	J	661	1	-	0/6/23/26	0/1/1/1
6	NAG	J	662	1	-	0/6/23/26	0/1/1/1
6	NAG	J	663	1,6	-	0/6/23/26	0/1/1/1
6	NAG	J	664	6	-	0/6/23/26	0/1/1/1
6	NAG	J	665	1,6	-	0/6/23/26	0/1/1/1
6	NAG	J	666	6	-	0/6/23/26	0/1/1/1
6	NAG	J	667	1,6	-	0/6/23/26	0/1/1/1
6	NAG	J	668	6	-	0/6/23/26	0/1/1/1
6	NAG	J	669	1,6	-	0/6/23/26	0/1/1/1
6	NAG	J	670	6	-	0/6/23/26	0/1/1/1
6	NAG	K	701	2	-	0/6/23/26	0/1/1/1
6	NAG	K	702	2	-	0/6/23/26	0/1/1/1

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	636	NAG	O5-C1	-2.96	1.38	1.43
6	G	669	NAG	O5-C1	-2.85	1.39	1.43
6	G	636	NAG	O5-C1	-2.73	1.39	1.43
6	A	625	NAG	O5-C1	-2.63	1.39	1.43
8	A	658	MAN	O5-C1	-2.56	1.39	1.43
6	A	636	NAG	O5-C1	-2.46	1.39	1.43
6	J	644	NAG	O5-C1	-2.42	1.39	1.43
8	G	610	MAN	O5-C1	-2.42	1.39	1.43
6	A	669	NAG	O5-C1	-2.41	1.39	1.43
6	G	644	NAG	O5-C1	-2.40	1.39	1.43
6	J	669	NAG	O5-C1	-2.38	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	654	MAN	O5-C1	-2.23	1.40	1.43
8	J	610	MAN	O5-C1	-2.22	1.40	1.43
8	G	654	MAN	O5-C1	-2.21	1.40	1.43
8	J	658	MAN	O5-C1	-2.19	1.40	1.43
6	A	644	NAG	O5-C1	-2.12	1.40	1.43
8	G	658	MAN	O5-C1	-2.09	1.40	1.43
6	J	625	NAG	O5-C1	-2.06	1.40	1.43
8	G	629	MAN	O5-C1	-2.06	1.40	1.43
8	J	605	MAN	O5-C1	-2.04	1.40	1.43
8	J	655	MAN	O5-C1	-2.03	1.40	1.43
8	A	610	MAN	O5-C1	-2.01	1.40	1.43
8	G	622	MAN	C1-C2	2.12	1.57	1.52
8	J	648	MAN	C2-C3	2.14	1.55	1.52
8	G	632	MAN	C2-C3	2.16	1.55	1.52
8	J	631	MAN	C1-C2	2.16	1.57	1.52
8	G	648	MAN	C2-C3	2.17	1.55	1.52
8	A	631	MAN	C1-C2	2.26	1.57	1.52
8	A	631	MAN	C2-C3	2.33	1.55	1.52
8	A	604	MAN	C1-C2	2.34	1.57	1.52
8	G	631	MAN	C2-C3	2.36	1.55	1.52
8	J	631	MAN	C2-C3	2.40	1.55	1.52
8	G	622	MAN	C2-C3	2.47	1.55	1.52
8	A	622	MAN	C2-C3	2.48	1.55	1.52
8	G	631	MAN	C1-C2	2.55	1.58	1.52
8	J	622	MAN	C2-C3	2.89	1.56	1.52

All (207) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	657	MAN	O2-C2-C3	-3.29	103.71	110.17
8	A	624	MAN	O2-C2-C3	-3.05	104.18	110.17
8	J	657	MAN	O2-C2-C3	-2.97	104.33	110.17
8	J	628	MAN	O2-C2-C3	-2.95	104.38	110.17
8	G	628	MAN	O2-C2-C3	-2.91	104.47	110.17
8	A	635	MAN	O2-C2-C3	-2.87	104.53	110.17
8	A	628	MAN	O2-C2-C3	-2.84	104.59	110.17
8	G	635	MAN	O2-C2-C3	-2.80	104.67	110.17
8	J	610	MAN	O2-C2-C3	-2.69	104.89	110.17
7	A	620	BMA	O3-C3-C2	-2.69	105.13	110.02
8	G	634	MAN	O2-C2-C3	-2.65	104.96	110.17
8	J	634	MAN	O2-C2-C3	-2.65	104.98	110.17
8	G	657	MAN	O2-C2-C3	-2.64	104.99	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	610	MAN	O2-C2-C3	-2.58	105.10	110.17
8	A	634	MAN	O2-C2-C3	-2.54	105.18	110.17
8	J	639	MAN	O2-C2-C3	-2.53	105.20	110.17
8	J	655	MAN	O2-C2-C3	-2.53	105.21	110.17
8	A	659	MAN	O2-C2-C3	-2.53	105.21	110.17
8	G	655	MAN	O2-C2-C3	-2.52	105.22	110.17
8	A	655	MAN	O2-C2-C3	-2.52	105.22	110.17
8	A	615	MAN	O2-C2-C3	-2.48	105.30	110.17
8	G	610	MAN	O2-C2-C3	-2.48	105.30	110.17
8	J	659	MAN	O2-C2-C3	-2.44	105.39	110.17
8	J	615	MAN	O2-C2-C3	-2.43	105.39	110.17
8	G	659	MAN	O2-C2-C3	-2.43	105.39	110.17
8	A	623	MAN	O2-C2-C3	-2.43	105.40	110.17
8	G	639	MAN	O2-C2-C3	-2.41	105.44	110.17
8	A	604	MAN	O2-C2-C3	-2.40	105.47	110.17
8	J	635	MAN	O2-C2-C3	-2.39	105.47	110.17
8	J	624	MAN	O2-C2-C3	-2.37	105.51	110.17
8	G	654	MAN	O2-C2-C3	-2.37	105.52	110.17
8	G	623	MAN	O2-C2-C3	-2.37	105.53	110.17
8	A	633	MAN	O2-C2-C3	-2.36	105.53	110.17
8	G	660	MAN	O2-C2-C3	-2.35	105.56	110.17
8	J	654	MAN	O2-C2-C3	-2.35	105.57	110.17
8	J	660	MAN	O2-C2-C3	-2.32	105.61	110.17
8	G	604	MAN	O2-C2-C3	-2.32	105.61	110.17
8	J	623	MAN	O2-C2-C3	-2.32	105.62	110.17
6	J	644	NAG	O4-C4-C5	-2.30	103.48	109.28
8	J	649	MAN	O2-C2-C3	-2.28	105.70	110.17
8	A	660	MAN	O2-C2-C3	-2.27	105.72	110.17
8	G	615	MAN	O2-C2-C3	-2.26	105.73	110.17
8	G	629	MAN	O2-C2-C3	-2.26	105.74	110.17
8	G	614	MAN	O2-C2-C3	-2.25	105.75	110.17
8	A	639	MAN	O2-C2-C3	-2.25	105.75	110.17
8	G	624	MAN	O2-C2-C3	-2.25	105.76	110.17
8	J	605	MAN	O2-C2-C3	-2.23	105.79	110.17
8	G	649	MAN	O2-C2-C3	-2.23	105.79	110.17
8	G	631	MAN	O2-C2-C3	-2.23	105.79	110.17
8	G	656	MAN	O2-C2-C3	-2.23	105.80	110.17
8	A	631	MAN	O2-C2-C3	-2.22	105.81	110.17
8	A	621	MAN	O2-C2-C3	-2.19	105.88	110.17
8	A	648	MAN	O2-C2-C3	-2.18	105.89	110.17
8	A	654	MAN	O2-C2-C3	-2.17	105.91	110.17
8	G	605	MAN	O2-C2-C3	-2.17	105.91	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	656	MAN	O2-C2-C3	-2.14	105.97	110.17
8	J	658	MAN	O2-C2-C3	-2.13	105.98	110.17
8	J	604	MAN	O2-C2-C3	-2.12	106.01	110.17
8	G	658	MAN	O2-C2-C3	-2.12	106.01	110.17
8	J	631	MAN	O2-C2-C3	-2.12	106.01	110.17
8	A	614	MAN	O2-C2-C3	-2.12	106.02	110.17
8	J	650	MAN	O2-C2-C3	-2.11	106.02	110.17
8	J	621	MAN	O2-C2-C3	-2.10	106.04	110.17
8	G	621	MAN	O2-C2-C3	-2.09	106.06	110.17
8	G	647	MAN	O2-C2-C3	-2.09	106.07	110.17
8	A	640	MAN	O2-C2-C3	-2.09	106.07	110.17
8	J	614	MAN	O2-C2-C3	-2.08	106.09	110.17
8	A	658	MAN	O2-C2-C3	-2.07	106.10	110.17
6	G	644	NAG	O4-C4-C5	-2.07	104.06	109.28
8	J	648	MAN	O2-C2-C3	-2.06	106.12	110.17
8	J	633	MAN	O2-C2-C3	-2.05	106.14	110.17
8	A	649	MAN	O2-C2-C3	-2.05	106.14	110.17
8	G	648	MAN	O2-C2-C3	-2.03	106.18	110.17
8	A	605	MAN	O2-C2-C3	-2.03	106.18	110.17
8	A	647	MAN	O2-C2-C3	-2.03	106.19	110.17
7	G	620	BMA	O3-C3-C2	-2.02	106.34	110.02
8	G	650	MAN	O2-C2-C3	-2.02	106.21	110.17
8	A	650	MAN	O2-C2-C3	-2.01	106.22	110.17
8	G	633	MAN	O2-C2-C3	-2.01	106.23	110.17
8	G	630	MAN	O2-C2-C3	-2.00	106.24	110.17
8	J	659	MAN	O5-C1-C2	2.01	113.94	110.79
7	G	620	BMA	C1-O5-C5	2.01	114.94	112.17
8	G	604	MAN	O5-C1-C2	2.01	113.95	110.79
8	A	615	MAN	C1-O5-C5	2.02	114.95	112.17
8	A	657	MAN	O5-C1-C2	2.03	113.97	110.79
6	G	602	NAG	C1-C2-N2	2.03	113.96	110.49
8	G	650	MAN	O5-C1-C2	2.04	113.98	110.79
8	J	604	MAN	O5-C1-C2	2.04	113.99	110.79
8	G	624	MAN	O5-C1-C2	2.04	113.99	110.79
8	G	622	MAN	O5-C1-C2	2.05	114.00	110.79
7	A	627	BMA	C3-C4-C5	2.05	113.83	110.22
6	J	617	NAG	C1-C2-N2	2.06	114.00	110.49
8	G	659	MAN	O5-C1-C2	2.06	114.02	110.79
8	G	614	MAN	C1-O5-C5	2.06	115.01	112.17
7	J	627	BMA	C3-C4-C5	2.07	113.86	110.22
8	A	622	MAN	C1-C2-C3	2.07	112.28	109.65
8	G	631	MAN	C1-C2-C3	2.09	112.30	109.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	J	627	BMA	C1-O5-C5	2.10	115.06	112.17
8	J	654	MAN	C1-O5-C5	2.10	115.06	112.17
8	J	657	MAN	O5-C1-C2	2.10	114.08	110.79
7	G	653	BMA	C1-O5-C5	2.10	115.06	112.17
8	A	622	MAN	O5-C1-C2	2.10	114.08	110.79
8	A	654	MAN	C1-O5-C5	2.13	115.10	112.17
8	A	650	MAN	O5-C1-C2	2.14	114.14	110.79
8	G	657	MAN	O5-C1-C2	2.14	114.14	110.79
8	J	624	MAN	O5-C1-C2	2.15	114.16	110.79
8	G	615	MAN	C1-O5-C5	2.16	115.14	112.17
8	J	615	MAN	C1-O5-C5	2.16	115.14	112.17
7	A	653	BMA	C1-O5-C5	2.16	115.15	112.17
8	J	650	MAN	O5-C1-C2	2.17	114.19	110.79
8	A	655	MAN	C1-O5-C5	2.17	115.16	112.17
8	G	622	MAN	C1-C2-C3	2.18	112.42	109.65
8	G	654	MAN	C1-O5-C5	2.19	115.18	112.17
8	J	621	MAN	O5-C1-C2	2.19	114.22	110.79
8	A	604	MAN	O5-C1-C2	2.19	114.22	110.79
8	J	614	MAN	C1-O5-C5	2.19	115.19	112.17
8	J	631	MAN	C1-O5-C5	2.20	115.20	112.17
8	A	624	MAN	O5-C1-C2	2.21	114.25	110.79
7	A	638	BMA	C1-C2-C3	2.23	112.48	109.65
8	G	648	MAN	C1-O5-C5	2.23	115.25	112.17
8	J	640	MAN	C1-O5-C5	2.24	115.26	112.17
7	G	627	BMA	C1-O5-C5	2.26	115.28	112.17
8	G	640	MAN	C1-O5-C5	2.27	115.30	112.17
8	A	656	MAN	C1-O5-C5	2.28	115.31	112.17
8	A	621	MAN	O5-C1-C2	2.33	114.43	110.79
8	A	631	MAN	C1-O5-C5	2.34	115.39	112.17
8	J	656	MAN	C1-O5-C5	2.37	115.44	112.17
8	G	629	MAN	C1-O5-C5	2.40	115.48	112.17
7	G	638	BMA	C1-C2-C3	2.41	112.70	109.65
8	G	656	MAN	C1-O5-C5	2.41	115.49	112.17
8	G	621	MAN	O5-C1-C2	2.41	114.57	110.79
8	G	631	MAN	C1-O5-C5	2.42	115.50	112.17
8	A	640	MAN	C1-O5-C5	2.48	115.59	112.17
8	J	648	MAN	C1-O5-C5	2.49	115.59	112.17
8	A	630	MAN	C1-O5-C5	2.53	115.65	112.17
7	J	638	BMA	C1-C2-C3	2.59	112.93	109.65
8	A	648	MAN	C1-O5-C5	2.59	115.74	112.17
8	A	657	MAN	C1-O5-C5	2.59	115.74	112.17
8	G	630	MAN	C1-O5-C5	2.71	115.90	112.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	J	630	MAN	C1-O5-C5	2.73	115.93	112.17
7	A	627	BMA	C1-C2-C3	2.76	113.15	109.65
8	J	657	MAN	C1-O5-C5	2.79	116.02	112.17
8	A	633	MAN	C1-O5-C5	2.84	116.08	112.17
8	G	622	MAN	C1-O5-C5	2.87	116.12	112.17
8	G	657	MAN	C1-O5-C5	2.89	116.15	112.17
8	J	635	MAN	C1-O5-C5	2.90	116.17	112.17
8	A	629	MAN	C1-O5-C5	2.95	116.23	112.17
7	G	627	BMA	C1-C2-C3	2.97	113.41	109.65
8	J	629	MAN	C1-O5-C5	2.98	116.27	112.17
8	J	622	MAN	C1-O5-C5	2.98	116.28	112.17
8	J	633	MAN	C1-O5-C5	2.98	116.28	112.17
8	A	659	MAN	C1-O5-C5	2.99	116.29	112.17
7	J	627	BMA	C1-C2-C3	3.00	113.46	109.65
8	J	604	MAN	C1-O5-C5	3.02	116.32	112.17
7	A	653	BMA	C1-C2-C3	3.04	113.50	109.65
8	G	621	MAN	C1-O5-C5	3.08	116.41	112.17
8	G	649	MAN	C1-O5-C5	3.08	116.41	112.17
8	G	660	MAN	C1-O5-C5	3.10	116.44	112.17
8	J	660	MAN	C1-O5-C5	3.10	116.44	112.17
8	G	604	MAN	C1-O5-C5	3.12	116.46	112.17
8	G	633	MAN	C1-O5-C5	3.12	116.47	112.17
8	A	635	MAN	C1-O5-C5	3.14	116.50	112.17
8	A	660	MAN	C1-O5-C5	3.15	116.50	112.17
8	A	622	MAN	C1-O5-C5	3.15	116.51	112.17
7	G	653	BMA	C1-C2-C3	3.16	113.66	109.65
8	A	604	MAN	C1-O5-C5	3.20	116.58	112.17
8	J	649	MAN	C1-O5-C5	3.22	116.60	112.17
8	J	659	MAN	C1-O5-C5	3.22	116.61	112.17
8	J	639	MAN	C1-O5-C5	3.27	116.68	112.17
8	J	621	MAN	C1-O5-C5	3.35	116.78	112.17
8	G	639	MAN	C1-O5-C5	3.35	116.78	112.17
7	J	653	BMA	C1-C2-C3	3.38	113.94	109.65
8	A	621	MAN	C1-O5-C5	3.40	116.85	112.17
8	J	647	MAN	C1-O5-C5	3.40	116.86	112.17
8	G	628	MAN	C1-O5-C5	3.40	116.86	112.17
8	J	628	MAN	C1-O5-C5	3.41	116.86	112.17
8	G	659	MAN	C1-O5-C5	3.42	116.88	112.17
8	G	632	MAN	C1-O5-C5	3.47	116.94	112.17
8	G	635	MAN	C1-O5-C5	3.47	116.95	112.17
7	J	620	BMA	C1-C2-C3	3.48	114.06	109.65
8	A	649	MAN	C1-O5-C5	3.50	116.99	112.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	647	MAN	C1-O5-C5	3.50	117.00	112.17
7	G	620	BMA	C1-C2-C3	3.52	114.11	109.65
8	J	623	MAN	C1-O5-C5	3.54	117.04	112.17
8	G	647	MAN	C1-O5-C5	3.60	117.13	112.17
8	A	632	MAN	C1-O5-C5	3.61	117.15	112.17
8	A	639	MAN	C1-O5-C5	3.67	117.22	112.17
8	J	632	MAN	C1-O5-C5	3.72	117.29	112.17
8	A	623	MAN	C1-O5-C5	3.81	117.41	112.17
8	G	623	MAN	C1-O5-C5	3.83	117.44	112.17
8	A	628	MAN	C1-O5-C5	3.83	117.45	112.17
8	A	624	MAN	C1-O5-C5	3.84	117.46	112.17
8	G	624	MAN	C1-O5-C5	3.93	117.58	112.17
8	A	634	MAN	C1-O5-C5	3.97	117.64	112.17
8	J	624	MAN	C1-O5-C5	3.99	117.67	112.17
8	J	650	MAN	C1-O5-C5	4.06	117.77	112.17
8	A	650	MAN	C1-O5-C5	4.09	117.81	112.17
6	G	617	NAG	C2-N2-C7	4.10	128.92	122.94
8	G	634	MAN	C1-O5-C5	4.11	117.83	112.17
6	A	617	NAG	C2-N2-C7	4.14	128.98	122.94
7	A	620	BMA	C1-C2-C3	4.14	114.90	109.65
8	J	634	MAN	C1-O5-C5	4.15	117.89	112.17
6	J	617	NAG	C2-N2-C7	4.18	129.04	122.94
6	A	602	NAG	C2-N2-C7	4.19	129.06	122.94
6	G	602	NAG	C2-N2-C7	4.20	129.07	122.94
6	J	602	NAG	C2-N2-C7	4.21	129.08	122.94
8	G	650	MAN	C1-O5-C5	4.23	117.99	112.17

There are no chirality outliers.

There are no torsion outliers.

All (3) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	660	MAN	C1-C2-C3-C4-C5-O5
8	G	660	MAN	C1-C2-C3-C4-C5-O5
8	J	660	MAN	C1-C2-C3-C4-C5-O5

29 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	602	NAG	1	0
6	A	608	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	616	NAG	1	0
6	A	617	NAG	2	0
6	A	636	NAG	1	0
6	A	652	NAG	1	0
6	A	663	NAG	1	0
6	A	664	NAG	1	0
6	G	601	NAG	1	0
6	G	602	NAG	1	0
6	G	607	NAG	1	0
6	G	608	NAG	1	0
8	G	610	MAN	1	0
6	G	617	NAG	1	0
8	G	621	MAN	1	0
8	G	624	MAN	1	0
6	G	641	NAG	1	0
6	G	663	NAG	1	0
6	G	664	NAG	1	0
6	G	667	NAG	1	0
6	J	602	NAG	1	0
6	J	608	NAG	1	0
8	J	610	MAN	1	0
6	J	617	NAG	1	0
8	J	621	MAN	1	0
6	J	636	NAG	1	0
6	J	641	NAG	1	0
6	J	663	NAG	1	0
6	J	664	NAG	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	A	448/472 (94%)	0.02	5 (1%) 80 73	138, 198, 269, 365	0
1	G	448/472 (94%)	-0.05	13 (2%) 52 43	133, 193, 262, 390	0
1	J	448/472 (94%)	-0.04	11 (2%) 58 49	113, 193, 270, 367	0
2	B	121/152 (79%)	-0.05	5 (4%) 38 30	140, 200, 245, 279	0
2	C	121/152 (79%)	-0.10	0 100 100	132, 199, 244, 290	0
2	K	121/152 (79%)	-0.06	4 (3%) 47 38	128, 205, 240, 274	0
3	E	208/211 (98%)	0.13	7 (3%) 46 38	159, 212, 241, 269	0
3	L	208/211 (98%)	0.40	14 (6%) 19 16	179, 234, 277, 291	0
3	M	208/211 (98%)	0.17	11 (5%) 27 23	148, 199, 250, 269	0
4	F	227/235 (96%)	0.02	9 (3%) 39 31	135, 192, 242, 301	0
4	H	227/235 (96%)	0.08	12 (5%) 27 23	167, 211, 278, 383	0
4	N	227/235 (96%)	-0.16	4 (1%) 69 61	138, 188, 248, 275	0
5	D	221/241 (91%)	0.26	6 (2%) 55 46	178, 227, 270, 317	0
5	I	221/241 (91%)	0.48	13 (5%) 23 19	200, 267, 312, 339	0
5	O	221/241 (91%)	0.54	20 (9%) 10 10	210, 267, 301, 322	0
All	All	3675/3933 (93%)	0.10	134 (3%) 43 35	113, 208, 284, 390	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	D	8	GLY	8.6
4	H	187	LEU	5.3
4	H	188	GLY	5.3
3	L	204	GLU	5.2
5	D	7	SER	5.0
5	O	7	SER	4.9
4	H	189	THR	4.9

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Mol	Chain	Res	Type	RSRZ
5	D	265	TRP	4.5
3	L	82	ASP	4.2
5	I	249	GLY	4.2
5	I	8	GLY	4.1
4	F	71	LEU	4.0
5	O	249	GLY	4.0
5	O	250	SER	4.0
5	I	265	TRP	3.9
4	F	187	LEU	3.9
4	H	73	LYS	3.9
5	I	3	ARG	3.8
1	A	356	ASN	3.8
5	O	26	GLY	3.8
5	O	265	TRP	3.6
3	E	13	VAL	3.5
4	H	158	THR	3.5
3	M	108	SER	3.4
5	I	7	SER	3.4
1	G	155	LYS	3.4
3	M	32	SER	3.4
5	I	213	LEU	3.4
5	I	2	VAL	3.4
3	E	108	SER	3.3
1	J	495	GLY	3.3
2	B	626	MET	3.2
3	L	108	SER	3.2
3	M	204	GLU	3.2
3	L	203	VAL	3.2
3	L	179	LEU	3.2
1	G	213	ILE	3.2
3	M	192	TYR	3.1
3	M	195	GLN	3.1
5	O	266	GLY	3.1
1	G	496	VAL	3.1
4	H	191	THR	3.1
5	I	18	MET	3.1
4	N	81	ARG	3.0
5	O	288	GLN	3.0
5	O	8	GLY	3.0
5	D	250	SER	3.0
4	H	71	LEU	3.0
1	J	471	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
3	M	133	LEU	2.9
1	A	61	TYR	2.9
1	J	139	THR	2.9
3	L	111	LYS	2.9
5	D	249	GLY	2.9
3	M	207	VAL	2.9
5	O	264	ARG	2.9
5	I	19	ARG	2.8
5	O	3	ARG	2.8
1	G	495	GLY	2.7
4	F	191	THR	2.7
3	L	153	SER	2.7
1	A	496	VAL	2.6
4	N	71	LEU	2.6
2	K	538	THR	2.6
2	K	614	TRP	2.6
4	F	158	THR	2.6
5	I	250	SER	2.6
4	F	29	VAL	2.6
3	L	80	ALA	2.6
1	J	356	ASN	2.6
4	F	185	SER	2.6
2	K	615	SER	2.6
1	A	140	ASP	2.6
3	M	179	LEU	2.6
1	G	59	LYS	2.6
3	L	190	LYS	2.5
1	G	139	THR	2.5
3	L	107	LEU	2.5
3	E	106	VAL	2.5
1	J	59	LYS	2.5
5	O	2	VAL	2.5
5	O	213	LEU	2.4
3	M	121	PRO	2.4
5	O	233	TRP	2.4
5	O	18	MET	2.4
1	G	60	ALA	2.4
3	L	180	SER	2.4
5	O	219	ALA	2.3
5	O	280	ASP	2.3
1	J	61	TYR	2.3
5	I	233	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	614	TRP	2.3
5	O	299	GLN	2.3
5	I	260	PHE	2.2
4	F	188	GLY	2.2
1	J	140	ASP	2.2
5	O	242	PRO	2.2
4	H	66	ARG	2.2
3	L	152	ASP	2.2
3	E	207	VAL	2.2
2	B	538	THR	2.2
1	J	370	GLU	2.2
3	M	180	SER	2.2
3	L	165	PRO	2.2
5	D	3	ARG	2.2
4	H	185	SER	2.1
1	G	61	TYR	2.1
5	O	231	LEU	2.1
1	G	370	GLU	2.1
3	L	145	VAL	2.1
4	H	99	ARG	2.1
1	G	58	ALA	2.1
4	F	72	ASP	2.1
1	J	32	GLU	2.1
1	G	498	PRO	2.1
3	E	114	PRO	2.1
4	H	72	ASP	2.1
1	J	355	ASN	2.1
1	J	496	VAL	2.1
1	G	62	GLU	2.1
4	N	90	TYR	2.1
4	H	75	LYS	2.1
3	E	80	ALA	2.1
2	B	638	TYR	2.1
4	N	38	ARG	2.1
5	I	215	PRO	2.1
1	G	356	ASN	2.1
2	K	527	GLY	2.1
3	M	203	VAL	2.0
5	O	108	GLY	2.0
3	E	204	GLU	2.0
1	A	213	ILE	2.0
2	B	542	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
4	F	73	LYS	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	PCA	I	1	8/9	0.53	0.97	-	267,277,289,294	0
5	PCA	O	1	8/9	0.64	0.80	-	222,231,268,273	0
5	PCA	D	1	8/9	0.83	0.57	-	184,193,214,219	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	NAG	G	641	14/15	0.73	0.42	3.95	261,261,261,261	0
6	NAG	J	667	14/15	0.84	0.38	3.33	259,277,289,292	0
6	NAG	G	616	14/15	0.77	0.54	3.01	252,275,284,297	0
6	NAG	G	662	14/15	0.60	0.54	2.45	267,275,300,318	0
6	NAG	G	625	14/15	0.79	0.30	2.18	261,261,261,261	0
6	NAG	G	601	14/15	0.85	0.34	1.52	221,229,242,243	0
6	NAG	G	669	14/15	0.69	0.39	1.37	261,261,261,261	0
6	NAG	A	662	14/15	0.61	0.52	1.35	267,275,300,318	0
6	NAG	J	669	14/15	0.71	0.50	1.31	261,261,261,261	0
6	NAG	A	616	14/15	0.79	0.49	1.08	252,275,284,297	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	NAG	J	641	14/15	0.71	0.46	1.08	261,261,261,261	0
6	NAG	J	662	14/15	0.61	0.54	1.02	267,275,300,318	0
6	NAG	A	651	14/15	0.84	0.38	0.98	237,248,265,270	0
6	NAG	G	618	14/15	0.71	0.34	0.69	261,261,261,261	0
6	NAG	A	669	14/15	0.72	0.38	0.55	261,261,261,261	0
6	NAG	A	618	14/15	0.71	0.33	0.54	261,261,261,261	0
6	NAG	J	636	14/15	0.92	0.27	0.51	261,261,261,261	0
6	NAG	G	651	14/15	0.91	0.31	0.41	237,248,265,270	0
6	NAG	A	625	14/15	0.83	0.26	0.34	261,261,261,261	0
6	NAG	J	651	14/15	0.90	0.35	0.31	237,248,265,270	0
6	NAG	J	616	14/15	0.84	0.37	0.16	252,275,284,297	0
6	NAG	J	611	14/15	0.91	0.26	0.12	213,259,277,280	0
6	NAG	A	607	14/15	0.89	0.40	0.07	258,284,302,304	0
6	NAG	A	641	14/15	0.79	0.35	0.03	261,261,261,261	0
6	NAG	A	606	14/15	0.72	0.40	-0.03	290,305,316,319	0
6	NAG	G	606	14/15	0.69	0.39	-0.18	290,305,316,319	0
6	NAG	G	611	14/15	0.91	0.26	-0.19	213,259,277,280	0
6	NAG	J	606	14/15	0.78	0.29	-0.20	290,305,316,319	0
6	NAG	J	625	14/15	0.86	0.20	-0.21	261,261,261,261	0
6	NAG	J	607	14/15	0.91	0.33	-0.25	258,284,302,304	0
6	NAG	J	618	14/15	0.83	0.25	-0.33	261,261,261,261	0
6	NAG	G	642	14/15	0.92	0.22	-0.40	245,261,286,296	0
6	NAG	A	611	14/15	0.93	0.23	-0.45	213,259,277,280	0
6	NAG	G	652	14/15	0.85	0.36	-0.48	257,273,294,300	0
6	NAG	G	637	14/15	0.91	0.23	-0.54	261,261,261,261	0
6	NAG	G	607	14/15	0.85	0.31	-0.58	258,284,302,304	0
6	NAG	G	667	14/15	0.84	0.28	-0.69	259,277,289,292	0
8	MAN	A	658	11/12	0.94	0.24	-0.79	262,265,279,286	0
8	MAN	G	657	11/12	0.97	0.28	-0.79	235,240,258,278	0
6	NAG	A	667	14/15	0.87	0.26	-0.81	259,277,289,292	0
6	NAG	G	636	14/15	0.96	0.20	-0.88	261,261,261,261	0
6	NAG	J	642	14/15	0.86	0.19	-0.95	245,261,286,296	0
8	MAN	J	658	11/12	0.88	0.20	-1.00	262,265,279,286	0
8	MAN	G	658	11/12	0.85	0.18	-1.09	262,265,279,286	0
6	NAG	A	636	14/15	0.93	0.26	-1.12	261,261,261,261	0
8	MAN	J	657	11/12	0.96	0.18	-1.16	235,240,258,278	0
8	MAN	A	657	11/12	0.98	0.19	-1.30	235,240,258,278	0
6	NAG	A	642	14/15	0.88	0.17	-1.33	245,261,286,296	0
6	NAG	A	652	14/15	0.86	0.27	-1.38	257,273,294,300	0
6	NAG	J	652	14/15	0.90	0.19	-2.07	257,273,294,300	0
8	MAN	G	655	11/12	0.84	0.23	-	280,295,301,303	0
6	NAG	G	666	14/15	0.61	0.32	-	307,328,330,330	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	NAG	A	601	14/15	0.78	0.36	-	221,229,242,243	0
8	MAN	G	648	11/12	0.80	0.49	-	261,261,261,261	0
6	NAG	J	644	14/15	0.80	0.34	-	261,261,261,261	0
8	MAN	J	605	11/12	0.67	0.36	-	293,300,308,309	0
6	NAG	A	602	14/15	0.91	0.48	-	230,242,258,262	0
6	NAG	A	643	14/15	0.82	0.33	-	303,317,328,336	0
8	MAN	J	630	11/12	0.65	0.74	-	261,261,261,261	0
7	BMA	G	613	11/12	0.64	0.19	-	312,321,331,341	0
6	NAG	G	608	14/15	0.85	0.26	-	295,304,312,313	0
8	MAN	A	655	11/12	0.50	0.40	-	280,295,301,303	0
8	MAN	A	610	11/12	0.82	0.37	-	325,342,352,353	0
8	MAN	A	631	11/12	0.59	0.34	-	261,261,261,261	0
7	BMA	G	609	11/12	0.77	0.35	-	309,319,327,335	0
6	NAG	G	643	14/15	0.85	0.33	-	303,317,328,336	0
8	MAN	J	647	11/12	0.78	0.35	-	261,261,261,261	0
6	NAG	J	619	14/15	0.88	0.23	-	261,261,261,261	0
8	MAN	J	655	11/12	0.71	0.35	-	280,295,301,303	0
6	NAG	B	702	14/15	0.73	0.86	-	285,303,316,317	0
6	NAG	J	663	14/15	0.88	0.23	-	260,297,316,323	0
8	MAN	J	633	11/12	0.67	0.94	-	261,261,261,261	0
6	NAG	A	645	14/15	0.87	0.25	-	261,261,261,261	0
8	MAN	G	654	11/12	0.81	0.23	-	286,303,309,318	0
6	NAG	G	645	14/15	0.88	0.28	-	261,261,261,261	0
8	MAN	J	649	11/12	0.71	0.44	-	261,261,261,261	0
7	BMA	A	613	11/12	0.74	0.33	-	312,321,331,341	0
6	NAG	J	602	14/15	0.85	0.62	-	230,242,258,262	0
7	BMA	J	638	11/12	0.87	0.30	-	261,261,261,261	0
7	BMA	A	646	11/12	0.71	0.25	-	261,261,261,261	0
6	NAG	J	601	14/15	0.88	0.51	-	221,229,242,243	0
6	NAG	G	612	14/15	0.87	0.23	-	277,291,302,313	0
8	MAN	G	650	11/12	0.65	1.00	-	261,261,261,261	0
7	BMA	J	646	11/12	0.74	0.23	-	261,261,261,261	0
6	NAG	G	617	14/15	0.77	0.32	-	279,293,304,311	0
8	MAN	A	647	11/12	0.74	0.39	-	261,261,261,261	0
8	MAN	A	604	11/12	0.77	0.74	-	253,260,277,291	0
8	MAN	J	610	11/12	0.69	0.56	-	325,342,352,353	0
7	BMA	G	638	11/12	0.89	0.16	-	261,261,261,261	0
8	MAN	A	635	11/12	0.65	0.58	-	261,261,261,261	0
8	MAN	G	640	11/12	0.61	0.32	-	261,261,261,261	0
8	MAN	G	615	11/12	0.70	0.62	-	339,341,344,346	0
8	MAN	G	622	11/12	0.47	0.61	-	261,261,261,261	0
8	MAN	A	654	11/12	0.85	0.44	-	286,303,309,318	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
8	MAN	G	631	11/12	0.55	0.28	-	261,261,261,261	0
8	MAN	G	604	11/12	0.84	0.53	-	253,260,277,291	0
6	NAG	G	668	14/15	0.80	0.27	-	288,310,336,363	0
7	BMA	J	620	11/12	0.87	0.15	-	261,261,261,261	0
8	MAN	J	632	11/12	0.86	0.95	-	261,261,261,261	0
7	BMA	G	627	11/12	0.78	0.16	-	261,261,261,261	0
8	MAN	J	654	11/12	0.71	0.22	-	286,303,309,318	0
6	NAG	G	665	14/15	0.87	0.38	-	296,306,323,326	0
8	MAN	G	647	11/12	0.75	0.38	-	261,261,261,261	0
6	NAG	J	608	14/15	0.82	0.31	-	295,304,312,313	0
6	NAG	A	617	14/15	0.72	0.30	-	279,293,304,311	0
6	NAG	A	665	14/15	0.88	0.68	-	296,306,323,326	0
6	NAG	J	664	14/15	0.72	0.37	-	317,335,342,344	0
8	MAN	A	633	11/12	0.67	1.06	-	261,261,261,261	0
8	MAN	J	623	11/12	0.67	1.21	-	261,261,261,261	0
6	NAG	A	668	14/15	0.76	0.28	-	288,310,336,363	0
8	MAN	G	630	11/12	0.66	0.74	-	261,261,261,261	0
8	MAN	A	615	11/12	0.76	0.56	-	339,341,344,346	0
8	MAN	A	628	11/12	0.90	0.27	-	261,261,261,261	0
6	NAG	G	663	14/15	0.88	0.26	-	260,297,316,323	0
7	BMA	J	627	11/12	0.60	0.19	-	261,261,261,261	0
6	NAG	B	701	14/15	0.77	0.25	-	296,313,326,330	0
8	MAN	G	624	11/12	0.56	0.65	-	261,261,261,261	0
8	MAN	J	621	11/12	0.80	0.27	-	261,261,261,261	0
8	MAN	G	632	11/12	0.82	0.90	-	261,261,261,261	0
6	NAG	A	644	14/15	0.84	0.32	-	261,261,261,261	0
8	MAN	J	631	11/12	0.63	0.43	-	261,261,261,261	0
7	BMA	A	609	11/12	0.76	0.41	-	309,319,327,335	0
8	MAN	A	632	11/12	0.72	0.80	-	261,261,261,261	0
6	NAG	G	644	14/15	0.75	0.30	-	261,261,261,261	0
6	NAG	A	663	14/15	0.90	0.25	-	260,297,316,323	0
6	NAG	J	661	14/15	0.77	0.44	-	293,311,318,323	0
6	NAG	A	612	14/15	0.87	0.26	-	277,291,302,313	0
8	MAN	G	659	11/12	0.78	0.39	-	301,306,311,311	0
8	MAN	A	623	11/12	0.72	1.37	-	261,261,261,261	0
6	NAG	J	666	14/15	0.83	0.44	-	307,328,330,330	0
8	MAN	G	635	11/12	0.58	0.67	-	261,261,261,261	0
6	NAG	J	668	14/15	0.82	0.24	-	288,310,336,363	0
6	NAG	J	645	14/15	0.82	0.31	-	261,261,261,261	0
7	BMA	A	627	11/12	0.58	0.25	-	261,261,261,261	0
8	MAN	G	656	11/12	0.78	0.60	-	321,323,332,338	0
6	NAG	A	661	14/15	0.75	0.49	-	293,311,318,323	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	NAG	G	619	14/15	0.91	0.30	-	261,261,261,261	0
8	MAN	G	660	11/12	0.82	0.45	-	327,335,339,340	0
8	MAN	A	656	11/12	0.86	0.60	-	321,323,332,338	0
8	MAN	G	633	11/12	0.68	0.93	-	261,261,261,261	0
7	BMA	A	603	11/12	0.81	0.39	-	252,263,287,290	0
8	MAN	J	640	11/12	0.67	0.36	-	261,261,261,261	0
8	MAN	A	659	11/12	0.85	0.27	-	301,306,311,311	0
7	BMA	J	613	11/12	0.86	0.27	-	312,321,331,341	0
7	BMA	G	603	11/12	0.80	0.30	-	252,263,287,290	0
6	NAG	K	701	14/15	0.76	0.23	-	296,313,326,330	0
8	MAN	G	634	11/12	0.86	0.35	-	261,261,261,261	0
6	NAG	G	670	14/15	0.62	0.64	-	261,261,261,261	0
8	MAN	J	628	11/12	0.87	0.27	-	261,261,261,261	0
6	NAG	J	626	14/15	0.84	0.21	-	261,261,261,261	0
6	NAG	J	617	14/15	0.72	0.36	-	279,293,304,311	0
8	MAN	J	639	11/12	0.87	0.34	-	261,261,261,261	0
6	NAG	C	702	14/15	0.86	0.61	-	285,303,316,317	0
6	NAG	C	701	14/15	0.82	0.21	-	296,313,326,330	0
8	MAN	J	650	11/12	0.82	0.64	-	261,261,261,261	0
8	MAN	G	623	11/12	0.66	1.33	-	261,261,261,261	0
8	MAN	A	640	11/12	0.63	0.28	-	261,261,261,261	0
7	BMA	A	653	11/12	0.87	0.33	-	251,268,283,285	0
8	MAN	A	630	11/12	0.60	0.98	-	261,261,261,261	0
8	MAN	J	656	11/12	0.79	0.50	-	321,323,332,338	0
8	MAN	A	622	11/12	0.68	0.71	-	261,261,261,261	0
6	NAG	A	608	14/15	0.80	0.32	-	295,304,312,313	0
6	NAG	J	665	14/15	0.88	0.37	-	296,306,323,326	0
7	BMA	G	646	11/12	0.73	0.29	-	261,261,261,261	0
6	NAG	K	702	14/15	0.81	0.57	-	285,303,316,317	0
6	NAG	G	661	14/15	0.92	0.46	-	293,311,318,323	0
8	MAN	G	621	11/12	0.68	0.27	-	261,261,261,261	0
8	MAN	J	622	11/12	0.72	0.49	-	261,261,261,261	0
6	NAG	J	637	14/15	0.90	0.28	-	261,261,261,261	0
8	MAN	J	660	11/12	0.81	0.44	-	327,335,339,340	0
7	BMA	J	603	11/12	0.74	0.42	-	252,263,287,290	0
8	MAN	J	635	11/12	0.78	0.46	-	261,261,261,261	0
8	MAN	G	649	11/12	0.74	0.48	-	261,261,261,261	0
8	MAN	J	648	11/12	0.92	0.40	-	261,261,261,261	0
8	MAN	J	659	11/12	0.84	0.25	-	301,306,311,311	0
8	MAN	A	649	11/12	0.74	0.69	-	261,261,261,261	0
7	BMA	A	638	11/12	0.81	0.19	-	261,261,261,261	0
8	MAN	A	639	11/12	0.85	0.36	-	261,261,261,261	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
8	MAN	A	621	11/12	0.54	0.35	-	261,261,261,261	0
7	BMA	J	653	11/12	0.90	0.21	-	251,268,283,285	0
6	NAG	A	666	14/15	0.80	0.44	-	307,328,330,330	0
8	MAN	G	610	11/12	0.61	0.54	-	325,342,352,353	0
8	MAN	A	648	11/12	0.87	0.49	-	261,261,261,261	0
7	BMA	G	620	11/12	0.70	0.20	-	261,261,261,261	0
8	MAN	A	605	11/12	0.79	0.40	-	293,300,308,309	0
8	MAN	G	639	11/12	0.90	0.29	-	261,261,261,261	0
8	MAN	G	629	11/12	0.66	0.38	-	261,261,261,261	0
8	MAN	A	660	11/12	0.87	0.31	-	327,335,339,340	0
8	MAN	J	634	11/12	0.92	0.30	-	261,261,261,261	0
8	MAN	A	650	11/12	0.82	0.79	-	261,261,261,261	0
8	MAN	J	615	11/12	0.62	0.46	-	339,341,344,346	0
6	NAG	G	664	14/15	0.77	0.35	-	317,335,342,344	0
6	NAG	A	637	14/15	0.92	0.17	-	261,261,261,261	0
8	MAN	G	605	11/12	0.84	0.30	-	293,300,308,309	0
8	MAN	J	629	11/12	0.66	0.49	-	261,261,261,261	0
6	NAG	G	626	14/15	0.92	0.15	-	261,261,261,261	0
8	MAN	A	634	11/12	0.82	0.35	-	261,261,261,261	0
8	MAN	A	629	11/12	0.78	0.55	-	261,261,261,261	0
8	MAN	G	628	11/12	0.86	0.23	-	261,261,261,261	0
6	NAG	A	619	14/15	0.90	0.29	-	261,261,261,261	0
8	MAN	J	604	11/12	0.69	0.66	-	253,260,277,291	0
6	NAG	J	643	14/15	0.84	0.27	-	303,317,328,336	0
7	BMA	A	620	11/12	0.82	0.27	-	261,261,261,261	0
6	NAG	A	670	14/15	0.75	0.55	-	261,261,261,261	0
8	MAN	J	614	11/12	0.88	0.22	-	296,308,312,313	0
8	MAN	J	624	11/12	0.74	0.66	-	261,261,261,261	0
7	BMA	G	653	11/12	0.94	0.22	-	251,268,283,285	0
8	MAN	A	614	11/12	0.85	0.19	-	296,308,312,313	0
6	NAG	J	670	14/15	0.65	0.44	-	261,261,261,261	0
8	MAN	A	624	11/12	0.60	0.88	-	261,261,261,261	0
8	MAN	G	614	11/12	0.81	0.21	-	296,308,312,313	0
6	NAG	A	626	14/15	0.89	0.18	-	261,261,261,261	0
7	BMA	J	609	11/12	0.83	0.58	-	309,319,327,335	0
6	NAG	A	664	14/15	0.82	0.33	-	317,335,342,344	0
6	NAG	G	602	14/15	0.81	0.61	-	230,242,258,262	0
6	NAG	J	612	14/15	0.84	0.26	-	277,291,302,313	0

6.5 Other polymers ⓘ

There are no such residues in this entry.