Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 10:13 PM GMT

PDB ID	:	5CEZ
Title	:	Crystal Structure of the BG505 SOSIP gp140 HIV-1 Env trimer in Complex with an early putative precursor of the PGT121 family at 3.0 Angstrom
Authors	:	Wilson, I.A.; Garces, F.
Deposited on	:	2015-07-08
Resolution	:	3.03 Å(reported)

This is a 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

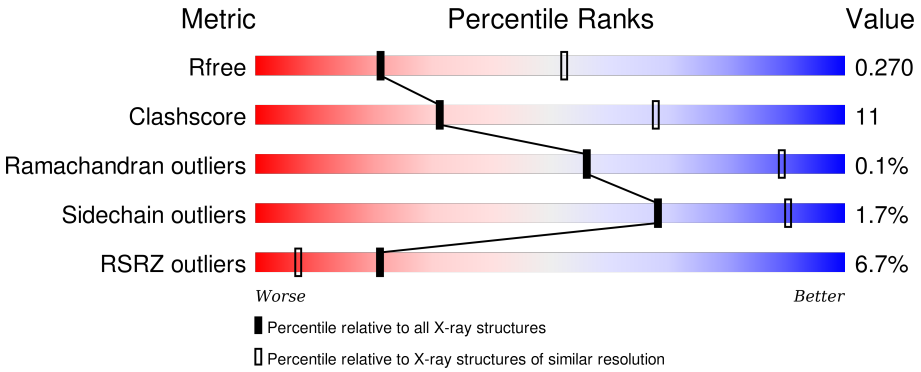
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.03 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1995 (3.08-3.00)
Clashscore	102246	2351 (3.08-3.00)
Ramachandran outliers	100387	2272 (3.08-3.00)
Sidechain outliers	100360	2275 (3.08-3.00)
RSRZ outliers	91569	2013 (3.08-3.00)

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

Mol	Chain	Length	Quality of chain
1	G	480	73% 21% 6%
2	B	153	3% 75% 20%
3	L	218	78% 17%
4	H	236	2% 74% 22%
5	D	240	25% 86% 14%

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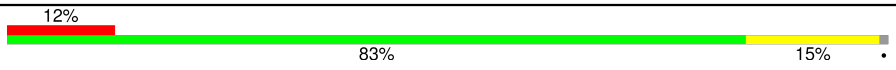
Mol	Chain	Length	Quality of chain
6	E	216	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	MAN	L	309	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 12135 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Envelope glycoprotein gp160.

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

There are 7 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called Envelope glycoprotein gp160.

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

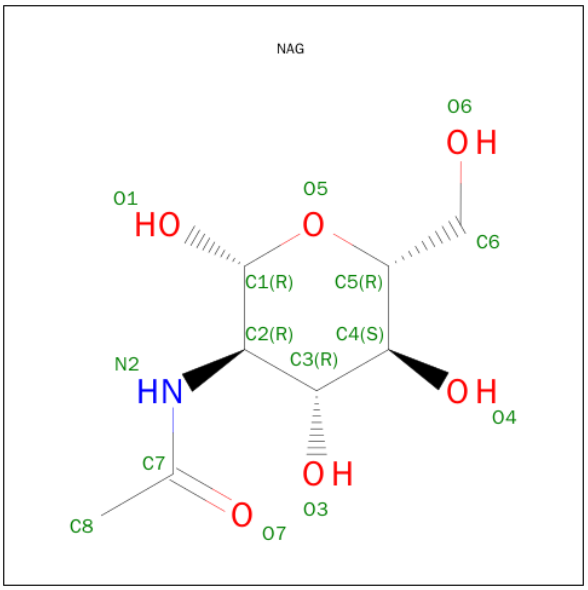
- Molecule 5 is a protein called 35022 Fab Heavy Chain.

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

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

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

- Molecule 7 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

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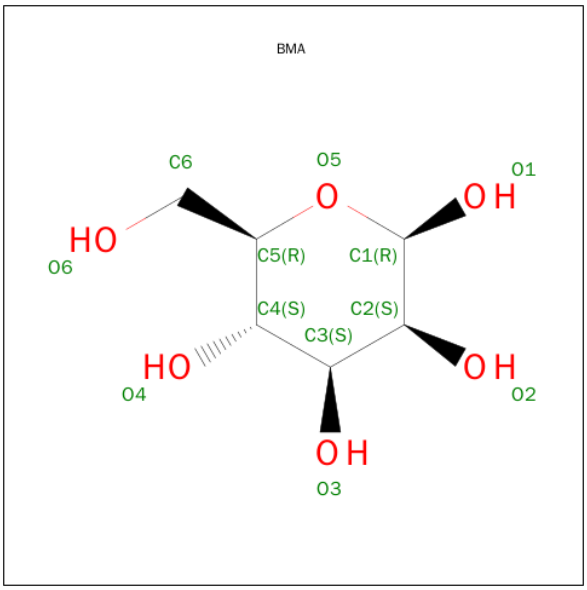
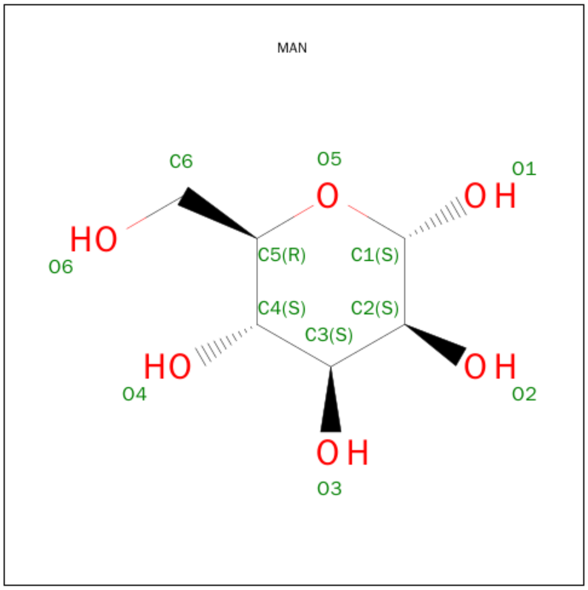
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C N O 14 8 1 5	0	0
7	B	1	Total C N O 14 8 1 5	0	0
7	L	1	Total C N O 14 8 1 5	0	0
7	L	1	Total C N O 14 8 1 5	0	0

- Molecule 8 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



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

- Molecule 9 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



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

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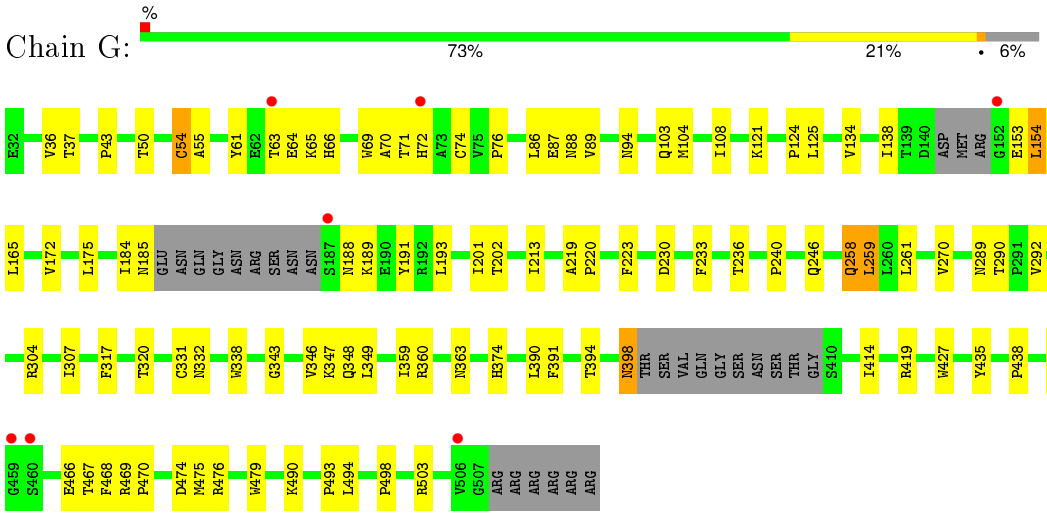
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	L	1	Total	C	O	0	0
			11	6	5		
9	L	1	Total	C	O	0	0
			11	6	5		
9	H	1	Total	C	O	0	0
			11	6	5		
9	D	1	Total	C	O	0	0
			11	6	5		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

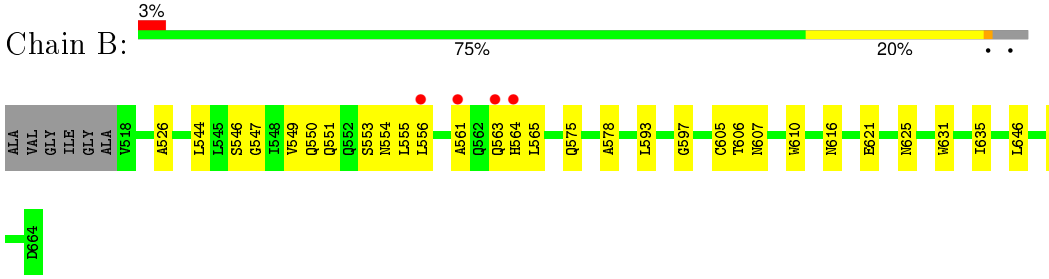
- Molecule 1: Envelope glycoprotein gp160

Chain G:



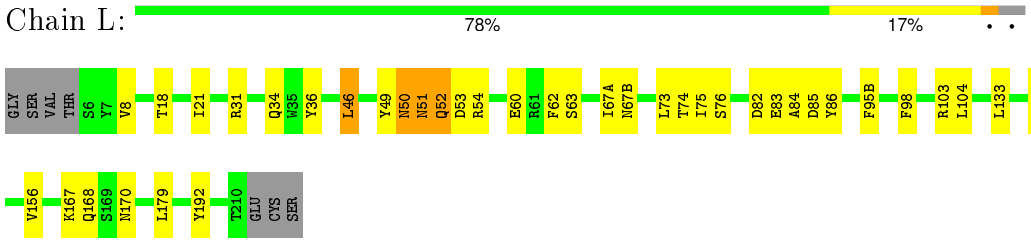
- Molecule 2: Envelope glycoprotein gp160

Chain B:



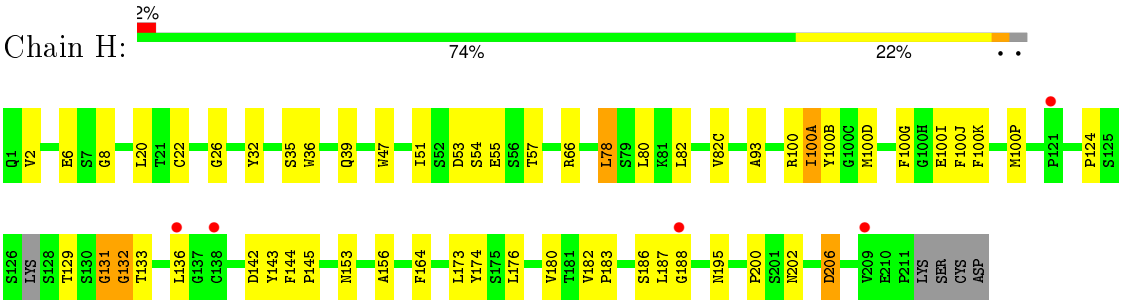
- Molecule 3: 3H+109L Fab Light Chain

Chain L:



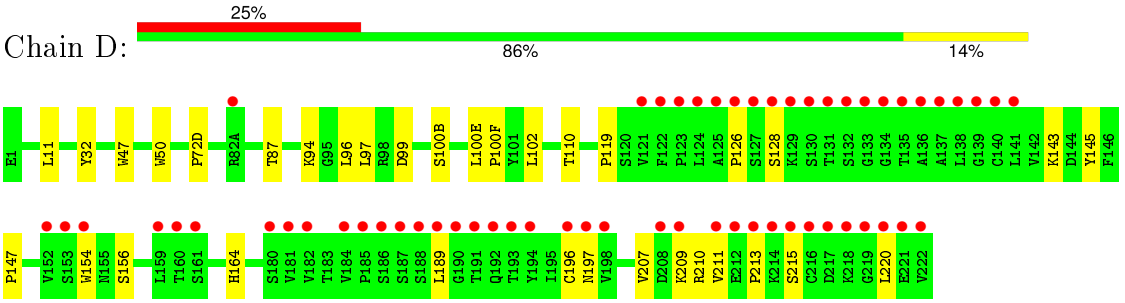
- Molecule 4: 3H+109L Fab Heavy Chain

Chain H:



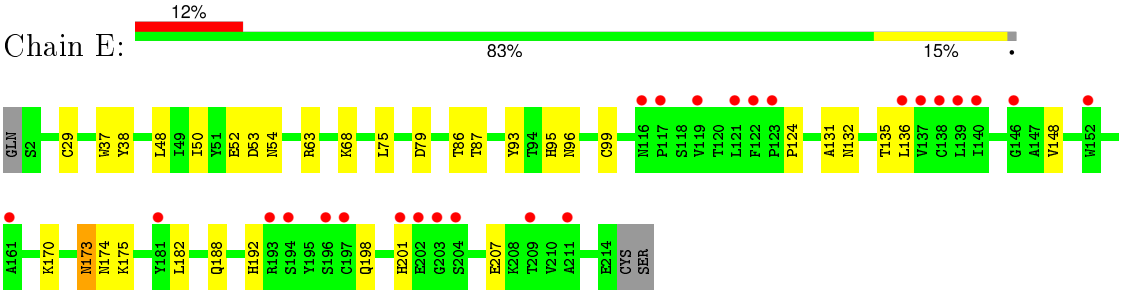
- Molecule 5: 35022 Fab Heavy Chain

Chain D:



- Molecule 6: 35022 Fab Light Chain

Chain E:



4 Data and refinement statistics (i)

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

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

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	G	0.26	0/3617	0.46	0/4911
2	B	0.24	0/1192	0.42	0/1618
3	L	0.25	0/1646	0.45	1/2247 (0.0%)
4	H	0.25	0/1787	0.45	0/2436
5	D	0.25	0/1860	0.45	0/2533
6	E	0.25	0/1659	0.47	0/2269
All	All	0.25	0/11761	0.45	1/16014 (0.0%)

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

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

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

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	E	29	CYS	Peptide
4	H	131	GLY	Peptide
4	H	132	GLY	Peptide
3	L	150	LYS	Peptide
3	L	50	ASN	Peptide
3	L	52	GLN	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	3544	0	3474	106	0
2	B	1171	0	1158	48	0
3	L	1603	0	1545	39	0
4	H	1744	0	1710	39	0
5	D	1813	0	1784	21	0
6	E	1615	0	1544	24	0
7	B	42	0	38	1	0
7	G	322	0	285	3	0
7	L	28	0	24	5	0
8	G	44	0	33	1	0
8	L	11	0	7	0	0
9	D	11	0	10	0	0
9	G	110	0	95	7	0
9	H	11	0	10	4	0
9	L	66	0	54	12	0
All	All	12135	0	11771	257	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (257) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:259:LEU:HD13	1:G:449:ILE:CD1	1.74	1.16
1:G:259:LEU:CD1	1:G:449:ILE:HD12	1.75	1.14
1:G:65:LYS:HD2	2:B:563:GLN:NE2	1.65	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:259:LEU:HD13	1:G:449:ILE:HD12	1.31	1.06
1:G:71:THR:HG22	1:G:72:HIS:H	1.21	1.03
1:G:259:LEU:CD1	1:G:449:ILE:CD1	2.37	1.00
1:G:259:LEU:CB	1:G:449:ILE:HD11	1.95	0.96
1:G:332:ASN:ND2	7:L:301:NAG:H82	1.79	0.95
3:L:52:GLN:NE2	9:L:308:MAN:O2	1.98	0.95
1:G:71:THR:HG22	1:G:72:HIS:N	1.80	0.95
3:L:50:ASN:O	3:L:53:ASP:N	2.03	0.90
3:L:52:GLN:N	3:L:52:GLN:OE1	2.05	0.89
1:G:259:LEU:HD12	1:G:449:ILE:HD12	1.55	0.87
2:B:553:SER:H	2:B:554:ASN:HA	1.40	0.86
1:G:153:GLU:OE2	1:G:419:ARG:NE	2.10	0.85
1:G:65:LYS:HD2	2:B:563:GLN:HE21	1.44	0.82
1:G:259:LEU:HB2	1:G:449:ILE:HD11	1.60	0.81
1:G:154:LEU:HD23	1:G:154:LEU:H	1.45	0.81
1:G:71:THR:CG2	1:G:72:HIS:H	1.94	0.80
3:L:52:GLN:HB2	3:L:53:ASP:OD1	1.82	0.79
2:B:607:ASN:N	2:B:650:GLN:OE1	2.16	0.78
3:L:52:GLN:HG2	9:L:309:MAN:C3	2.14	0.77
1:G:64:GLU:HB2	9:G:607:MAN:H62	1.66	0.77
3:L:52:GLN:HG2	9:L:309:MAN:H2	1.67	0.77
2:B:550:GLN:HG3	2:B:551:GLN:HG2	1.68	0.75
1:G:134:VAL:HG13	7:G:623:NAG:H81	1.68	0.75
1:G:155:LYS:NZ	1:G:191:TYR:OH	2.20	0.75
1:G:65:LYS:CD	2:B:563:GLN:NE2	2.47	0.74
1:G:64:GLU:HG2	9:G:605:MAN:O4	1.87	0.74
1:G:65:LYS:HE3	1:G:66:HIS:CE1	2.23	0.73
1:G:230:ASP:HB3	1:G:233:PHE:HB2	1.70	0.73
1:G:332:ASN:CG	7:L:301:NAG:H82	2.08	0.72
1:G:154:LEU:CD2	1:G:154:LEU:H	2.04	0.71
1:G:219:ALA:O	1:G:246:GLN:NE2	2.23	0.71
4:H:142:ASP:HB2	4:H:173:LEU:HB2	1.73	0.70
1:G:65:LYS:CD	2:B:563:GLN:HE21	2.02	0.70
6:E:136:LEU:HD12	6:E:182:LEU:HD23	1.72	0.70
3:L:83:GLU:HG3	3:L:104:LEU:O	1.91	0.69
1:G:259:LEU:HD13	1:G:449:ILE:HD11	1.74	0.69
1:G:503:ARG:NH2	2:B:650:GLN:NE2	2.41	0.68
1:G:72:HIS:HD2	2:B:563:GLN:HB2	1.59	0.68
5:D:143:LYS:HE3	6:E:135:THR:HG21	1.77	0.67
1:G:259:LEU:HB3	1:G:449:ILE:HD11	1.76	0.67
3:L:52:GLN:HG2	9:L:309:MAN:C2	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:259:LEU:HB2	1:G:449:ILE:CD1	2.24	0.67
4:H:129:THR:OG1	4:H:133:THR:OG1	2.10	0.67
4:H:2:VAL:HA	4:H:26:GLY:HA3	1.77	0.67
1:G:493:PRO:HG3	2:B:544:LEU:HD21	1.77	0.67
5:D:119:PRO:HB3	5:D:145:TYR:HB3	1.76	0.66
1:G:494:LEU:HD21	2:B:593:LEU:HD11	1.78	0.66
2:B:547:GLY:H	2:B:550:GLN:CD	1.99	0.66
1:G:259:LEU:CD1	1:G:449:ILE:HD11	2.25	0.66
1:G:37:THR:HG22	2:B:605:CYS:HA	1.78	0.65
1:G:86:LEU:HB3	1:G:89:VAL:HG21	1.76	0.65
1:G:188:ASN:N	1:G:189:LYS:HA	2.11	0.65
1:G:298:ARG:NH2	1:G:441:GLY:O	2.30	0.64
3:L:52:GLN:HG2	9:L:309:MAN:H3	1.78	0.64
1:G:72:HIS:HB2	2:B:564:HIS:HD2	1.63	0.64
2:B:606:THR:HG22	2:B:650:GLN:HE22	1.62	0.63
6:E:173:ASN:O	6:E:175:LYS:NZ	2.30	0.63
5:D:128:SER:HB2	5:D:220:LEU:HB2	1.80	0.63
1:G:363:ASN:O	1:G:469:ARG:NH1	2.31	0.63
3:L:52:GLN:CG	9:L:309:MAN:H2	2.29	0.63
3:L:54:ARG:NH2	3:L:62:PHE:O	2.28	0.63
3:L:152:ASP:OD1	3:L:152:ASP:N	2.31	0.62
1:G:503:ARG:NH2	2:B:650:GLN:HE22	1.97	0.62
6:E:148:VAL:HG12	6:E:201:HIS:HE1	1.65	0.62
1:G:36:VAL:HG12	2:B:610:TRP:HE3	1.63	0.62
1:G:50:THR:O	1:G:103:GLN:NE2	2.33	0.62
1:G:63:THR:O	9:G:607:MAN:O6	2.17	0.61
1:G:360:ARG:HG2	1:G:467:THR:HG22	1.83	0.61
1:G:61:TYR:HB3	1:G:64:GLU:O	2.00	0.61
1:G:154:LEU:HD23	1:G:154:LEU:N	2.11	0.61
1:G:138:ILE:HG23	1:G:138:ILE:O	2.01	0.60
1:G:65:LYS:HB3	1:G:66:HIS:CD2	2.36	0.60
4:H:187:LEU:HD22	4:H:188:GLY:HA3	1.83	0.60
4:H:82:LEU:HD22	4:H:82(C):VAL:HG12	1.83	0.60
3:L:50:ASN:OD1	3:L:51:ASN:N	2.33	0.60
1:G:72:HIS:HB2	2:B:564:HIS:CD2	2.37	0.59
7:L:301:NAG:O3	7:L:302:NAG:O5	2.17	0.59
2:B:553:SER:N	2:B:554:ASN:HA	2.13	0.59
3:L:85:ASP:OD1	3:L:103:ARG:HD3	2.03	0.59
4:H:131:GLY:HA2	4:H:133:THR:N	2.18	0.58
1:G:94:ASN:HA	1:G:236:THR:HG22	1.84	0.58
1:G:72:HIS:CD2	2:B:563:GLN:HB2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:63:THR:OG1	9:G:607:MAN:H61	2.04	0.57
6:E:52:GLU:O	6:E:53:ASP:HB2	2.03	0.57
1:G:87:GLU:O	1:G:88:ASN:HB2	2.05	0.57
3:L:51:ASN:N	3:L:51:ASN:OD1	2.34	0.57
3:L:18:THR:HG22	3:L:76:SER:HA	1.86	0.57
9:L:308:MAN:O4	4:H:100:ARG:NH1	2.38	0.56
7:G:633:NAG:H83	7:G:633:NAG:H3	1.87	0.56
3:L:52:GLN:H	3:L:52:GLN:CD	2.03	0.56
6:E:131:ALA:N	6:E:132:ASN:HA	2.20	0.56
9:G:635:MAN:O6	5:D:99:ASP:OD1	2.21	0.55
2:B:553:SER:O	2:B:575:GLN:NE2	2.38	0.55
1:G:201:ILE:HD11	1:G:435:TYR:HB2	1.89	0.55
7:L:302:NAG:H2	4:H:100(D):MET:HA	1.88	0.55
2:B:547:GLY:O	2:B:550:GLN:HG2	2.06	0.55
1:G:184:ILE:HG13	1:G:185:ASN:H	1.72	0.55
1:G:188:ASN:H	1:G:189:LYS:HA	1.71	0.54
6:E:37:TRP:HB2	6:E:50:ILE:HB	1.89	0.54
2:B:547:GLY:N	2:B:550:GLN:HG2	2.23	0.54
5:D:126:PRO:HB2	5:D:215:SER:HB2	1.90	0.54
3:L:98:PHE:HE1	4:H:47:TRP:HB2	1.72	0.53
3:L:63:SER:OG	3:L:74:THR:OG1	2.23	0.53
2:B:606:THR:HB	2:B:650:GLN:OE1	2.08	0.53
1:G:153:GLU:OE2	1:G:419:ARG:CZ	2.56	0.53
4:H:195:ASN:ND2	4:H:206:ASP:OD2	2.40	0.53
1:G:503:ARG:HH12	2:B:651:ASN:ND2	2.06	0.53
4:H:22:CYS:HB3	4:H:78:LEU:HG	1.89	0.53
3:L:52:GLN:HE21	9:L:309:MAN:C1	2.21	0.53
1:G:474:ASP:OD1	1:G:475:MET:N	2.42	0.53
6:E:148:VAL:HG12	6:E:201:HIS:CE1	2.43	0.52
3:L:21:ILE:HD12	3:L:73:LEU:HD23	1.91	0.52
1:G:220:PRO:HB3	2:B:578:ALA:HB1	1.90	0.52
1:G:70:ALA:HB2	1:G:213:ILE:HD11	1.91	0.52
3:L:34:GLN:NE2	3:L:49:TYR:O	2.41	0.52
6:E:170:LYS:HE2	6:E:174:ASN:HA	1.90	0.52
3:L:168:GLN:HG3	3:L:170:ASN:HD22	1.75	0.52
6:E:124:PRO:HD3	6:E:136:LEU:HD23	1.92	0.52
1:G:449:ILE:O	1:G:449:ILE:HG23	2.10	0.51
1:G:261:LEU:HD11	1:G:374:HIS:HE1	1.74	0.51
1:G:175:LEU:HB2	1:G:320:THR:HB	1.92	0.51
1:G:332:ASN:HA	1:G:414:ILE:O	2.10	0.51
2:B:547:GLY:H	2:B:550:GLN:CG	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:104:MET:O	1:G:108:ILE:HG12	2.10	0.51
4:H:131:GLY:HA2	4:H:133:THR:H	1.76	0.51
1:G:270:VAL:HG12	1:G:289:ASN:H	1.76	0.51
4:H:131:GLY:HA2	4:H:132:GLY:C	2.32	0.51
4:H:124:PRO:HG3	4:H:136:LEU:HB3	1.92	0.51
2:B:546:SER:HB2	2:B:549:VAL:HG23	1.93	0.50
3:L:63:SER:HG	3:L:74:THR:HG1	1.57	0.50
1:G:474:ASP:OD2	1:G:476:ARG:NH1	2.44	0.50
1:G:295:ASN:O	1:G:331:CYS:HA	2.11	0.50
6:E:198:GLN:HG2	6:E:207:GLU:HG3	1.94	0.50
5:D:207:VAL:HG12	5:D:209:LYS:HG2	1.94	0.50
4:H:51:ILE:HD13	4:H:57:THR:HG22	1.94	0.50
4:H:183:PRO:HG2	4:H:186:SER:HB2	1.94	0.50
3:L:98:PHE:CE1	4:H:47:TRP:HB2	2.47	0.50
2:B:547:GLY:H	2:B:550:GLN:HG2	1.77	0.50
5:D:11:LEU:HB2	5:D:147:PRO:HG3	1.92	0.50
6:E:95:HIS:CE1	6:E:96:ASN:HD22	2.30	0.49
6:E:188:GLN:O	6:E:192:HIS:ND1	2.42	0.49
1:G:69:TRP:HE1	1:G:108:ILE:HD12	1.77	0.49
1:G:261:LEU:HD11	1:G:374:HIS:CE1	2.47	0.49
1:G:121:LYS:HA	1:G:202:THR:HA	1.93	0.49
5:D:100(B):SER:HB3	6:E:93:TYR:HE2	1.77	0.49
4:H:8:GLY:HA3	4:H:20:LEU:HD23	1.95	0.48
3:L:136:LEU:HD23	4:H:164:PHE:CE1	2.48	0.48
1:G:76:PRO:HG3	2:B:556:LEU:HB3	1.94	0.48
1:G:476:ARG:HA	1:G:479:TRP:CD1	2.48	0.48
9:L:304:MAN:C3	9:H:301:MAN:H5	2.40	0.48
5:D:100(B):SER:HB3	6:E:93:TYR:CE2	2.48	0.48
2:B:650:GLN:O	2:B:654:GLU:N	2.36	0.48
2:B:546:SER:HA	2:B:547:GLY:HA3	1.55	0.48
1:G:292:VAL:HB	1:G:449:ILE:CG2	2.43	0.48
3:L:156:VAL:HG11	3:L:179:LEU:HD11	1.96	0.48
1:G:240:PRO:HG3	5:D:72(D):PRO:HG2	1.95	0.48
1:G:304:ARG:NH2	1:G:438:PRO:O	2.44	0.47
2:B:631:TRP:CE2	2:B:635:ILE:HG13	2.49	0.47
2:B:597:GLY:HA3	2:B:651:ASN:HD21	1.79	0.47
2:B:561:ALA:HB1	2:B:563:GLN:HG3	1.96	0.47
1:G:270:VAL:HG22	1:G:348:GLN:HG3	1.96	0.47
1:G:125:LEU:HD23	1:G:193:LEU:HD11	1.96	0.47
9:L:304:MAN:C2	9:H:301:MAN:H5	2.44	0.47
6:E:53:ASP:OD2	6:E:68:LYS:HE2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:35:SER:OG	4:H:47:TRP:NE1	2.42	0.47
3:L:85:ASP:OD2	3:L:103:ARG:NH1	2.48	0.47
6:E:86:THR:OG1	6:E:87:THR:N	2.47	0.47
9:L:304:MAN:H2	9:H:301:MAN:H5	1.96	0.47
1:G:343:GLY:O	1:G:347:LYS:HG2	2.14	0.47
1:G:258:GLN:HG3	1:G:470:PRO:HB2	1.96	0.47
4:H:142:ASP:HB2	4:H:173:LEU:CB	2.45	0.46
2:B:553:SER:HB3	2:B:555:LEU:HG	1.97	0.46
4:H:142:ASP:HA	4:H:174:TYR:O	2.15	0.46
4:H:180:VAL:HG12	4:H:182:VAL:HG13	1.98	0.46
4:H:51:ILE:HD11	4:H:55:GLU:HA	1.96	0.46
4:H:100(B):TYR:CZ	4:H:100(I):GLU:HA	2.51	0.46
2:B:621:GLU:O	2:B:625:ASN:HB3	2.16	0.46
7:L:301:NAG:C1	7:L:301:NAG:H82	2.42	0.46
1:G:36:VAL:HG12	2:B:610:TRP:CE3	2.48	0.46
1:G:63:THR:C	9:G:607:MAN:HO6	2.19	0.46
2:B:547:GLY:C	2:B:550:GLN:HG2	2.36	0.46
2:B:625:ASN:HB2	5:D:97:LEU:HD22	1.98	0.46
5:D:189:LEU:HD22	5:D:213:PRO:HB2	1.97	0.46
1:G:64:GLU:HG3	1:G:65:LYS:N	2.30	0.46
4:H:100:ARG:HG2	4:H:100(K):PHE:CZ	2.51	0.46
1:G:360:ARG:NH1	1:G:394:THR:OG1	2.49	0.46
8:G:634:BMA:H61	9:G:636:MAN:H2	1.29	0.45
3:L:21:ILE:HB	3:L:73:LEU:HB3	1.99	0.45
4:H:93:ALA:HB1	4:H:100(P):MET:HB3	1.97	0.45
4:H:143:TYR:OH	4:H:176:LEU:HD23	2.17	0.45
4:H:36:TRP:CE2	4:H:80:LEU:HB2	2.51	0.45
1:G:54:CYS:SG	1:G:55:ALA:N	2.90	0.45
2:B:616:ASN:OD1	7:B:702:NAG:H61	2.17	0.45
2:B:547:GLY:O	2:B:550:GLN:CG	2.65	0.45
1:G:503:ARG:HH22	2:B:650:GLN:NE2	2.13	0.44
4:H:131:GLY:CA	4:H:132:GLY:C	2.86	0.44
1:G:63:THR:HG23	1:G:64:GLU:N	2.33	0.44
5:D:156:SER:H	5:D:197:ASN:HD21	1.66	0.44
1:G:343:GLY:O	1:G:346:VAL:HG12	2.17	0.44
5:D:210:ARG:NH1	5:D:211:VAL:O	2.51	0.43
5:D:87:THR:HG23	5:D:110:THR:HA	1.99	0.43
1:G:349:LEU:HD13	1:G:468:PHE:CE2	2.54	0.43
4:H:100(A):ILE:HG23	4:H:100(J):PHE:HB3	2.00	0.43
5:D:102:LEU:HD23	5:D:102:LEU:HA	1.84	0.43
1:G:124:PRO:HB2	1:G:161:MET:HE1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:259:LEU:CG	1:G:449:ILE:HD11	2.46	0.43
1:G:494:LEU:HD23	1:G:494:LEU:HA	1.67	0.43
4:H:6:GLU:N	4:H:6:GLU:OE1	2.51	0.43
4:H:145:PRO:HD2	4:H:200:PRO:HG2	2.00	0.43
6:E:132:ASN:N	6:E:132:ASN:OD1	2.52	0.43
1:G:391:PHE:CD2	1:G:470:PRO:HG3	2.53	0.42
4:H:53:ASP:OD1	4:H:54:SER:N	2.52	0.42
5:D:154:TRP:CH2	5:D:196:CYS:HB3	2.54	0.42
7:G:601:NAG:H61	7:G:602:NAG:N2	2.34	0.42
3:L:133:LEU:HD12	3:L:179:LEU:HD23	2.00	0.42
4:H:100(P):MET:SD	4:H:100(P):MET:N	2.92	0.42
1:G:498:PRO:HB3	2:B:610:TRP:CD2	2.53	0.42
4:H:144:PHE:HA	4:H:145:PRO:HA	1.76	0.42
1:G:172:VAL:HG21	1:G:307:ILE:HD12	2.01	0.42
3:L:36:TYR:HA	3:L:46:LEU:HA	2.01	0.42
1:G:289:ASN:OD1	1:G:290:THR:N	2.53	0.42
5:D:47:TRP:HZ2	5:D:50:TRP:CD1	2.38	0.42
3:L:8:VAL:HG11	3:L:103:ARG:HB2	2.02	0.42
3:L:151:ALA:HB2	3:L:192:TYR:CE1	2.55	0.42
2:B:650:GLN:O	2:B:654:GLU:HG3	2.20	0.42
1:G:223:PHE:CE2	1:G:490:LYS:HB3	2.55	0.42
1:G:43:PRO:HB2	2:B:526:ALA:HA	2.02	0.42
9:L:304:MAN:C3	9:H:301:MAN:C5	2.92	0.41
3:L:82:ASP:O	3:L:86:TYR:OH	2.28	0.41
5:D:100(E):LEU:HD12	5:D:100(F):PRO:HD2	2.01	0.41
3:L:54:ARG:HD3	3:L:62:PHE:O	2.21	0.41
6:E:37:TRP:CE2	6:E:75:LEU:HB2	2.56	0.41
3:L:67(A):ILE:HG13	3:L:67(B):ASN:N	2.35	0.41
6:E:53:ASP:OD2	6:E:68:LYS:CE	2.69	0.41
5:D:96:LEU:HG	5:D:97:LEU:HG	2.03	0.41
1:G:346:VAL:HA	1:G:349:LEU:HB2	2.02	0.41
1:G:398:ASN:OD1	1:G:398:ASN:N	2.54	0.41
1:G:359:ILE:HD13	1:G:466:GLU:HB3	2.03	0.41
4:H:100(D):MET:HG3	4:H:100(G):PHE:HD1	1.85	0.41
3:L:62:PHE:CD1	3:L:75:ILE:HG12	2.56	0.41
6:E:38:TYR:CZ	6:E:48:LEU:HD13	2.56	0.41
3:L:167:LYS:HB2	3:L:167:LYS:HE3	1.93	0.41
6:E:63:ARG:HD2	6:E:79:ASP:HB3	2.02	0.41
2:B:607:ASN:HB2	2:B:650:GLN:HB3	2.02	0.40
6:E:50:ILE:HG23	6:E:53:ASP:O	2.21	0.40
1:G:427:TRP:CD1	1:G:475:MET:HG2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:307:ILE:HD11	1:G:317:PHE:HD2	1.86	0.40
2:B:646:LEU:HA	2:B:646:LEU:HD12	1.80	0.40
4:H:153:ASN:HB2	4:H:156:ALA:HB3	2.03	0.40
4:H:66:ARG:NH1	4:H:82:LEU:HD21	2.36	0.40
6:E:54:ASN:OD1	6:E:54:ASN:N	2.51	0.40
3:L:54:ARG:NH2	3:L:60:GLU:O	2.54	0.40
5:D:32:TYR:CD2	5:D:94:LYS:HE3	2.56	0.40
1:G:338:TRP:CE2	1:G:390:LEU:HD22	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

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

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	84	ALA

5.3.2 Protein sidechains (i)

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

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

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

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	54	CYS
1	G	74	CYS
1	G	154	LEU
1	G	165	LEU
1	G	258	GLN
1	G	259	LEU
1	G	398	ASN
2	B	565	LEU
2	B	651	ASN
3	L	31	ARG
3	L	51	ASN
3	L	95(B)	PHE
3	L	152	ASP
4	H	32	TYR
4	H	39	GLN
4	H	78	LEU
4	H	100(A)	ILE
4	H	202	ASN
4	H	206	ASP
5	D	164	HIS
6	E	99	CYS
6	E	173	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	72	HIS
1	G	356	ASN
2	B	552	GLN
2	B	563	GLN
2	B	564	HIS
2	B	607	ASN
3	L	127	GLN
3	L	170	ASN
4	H	31	ASN
4	H	76	ASN
4	H	97	GLN
5	D	197	ASN
6	E	95	HIS
6	E	112	GLN
6	E	201	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

51 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	NAG	B	701	2	14,14,15	2.64	3 (21%)	15,19,21	0.55	0
7	NAG	B	702	2	14,14,15	2.05	2 (14%)	15,19,21	1.33	1 (6%)
7	NAG	B	703	2	14,14,15	0.18	0	15,19,21	0.31	0
9	MAN	D	301	-	11,11,12	0.63	0	15,15,17	1.08	2 (13%)
7	NAG	G	601	1,7	14,14,15	0.25	0	15,19,21	0.41	0
7	NAG	G	602	8,7	14,14,15	0.32	0	15,19,21	0.31	0
8	BMA	G	603	9,7	11,11,12	0.65	0	15,15,17	0.69	0
9	MAN	G	604	8	11,11,12	0.65	0	15,15,17	1.09	2 (13%)
9	MAN	G	605	9,8	11,11,12	0.67	0	15,15,17	1.02	2 (13%)
9	MAN	G	606	9	11,11,12	0.52	0	15,15,17	0.68	0
9	MAN	G	607	9	11,11,12	0.62	0	15,15,17	0.60	0
7	NAG	G	608	1,7	14,14,15	0.18	0	15,19,21	0.42	0
7	NAG	G	609	7	14,14,15	0.26	0	15,19,21	0.25	0
7	NAG	G	610	1	14,14,15	0.16	0	15,19,21	0.32	0
7	NAG	G	611	1	14,14,15	0.16	0	15,19,21	0.33	0
7	NAG	G	612	1,7	14,14,15	0.26	0	15,19,21	0.40	0
7	NAG	G	613	7	14,14,15	0.17	0	15,19,21	0.30	0
7	NAG	G	614	1,7	14,14,15	0.24	0	15,19,21	0.55	0
7	NAG	G	615	7	14,14,15	1.37	1 (7%)	15,19,21	0.31	0
7	NAG	G	616	1	14,14,15	0.20	0	15,19,21	0.23	0
7	NAG	G	617	1,7	14,14,15	0.16	0	15,19,21	0.34	0
7	NAG	G	618	7	14,14,15	2.66	3 (21%)	15,19,21	0.81	1 (6%)
7	NAG	G	619	1,7	14,14,15	0.22	0	15,19,21	0.26	0
7	NAG	G	620	7	14,14,15	0.18	0	15,19,21	0.34	0
7	NAG	G	621	1,7	14,14,15	0.21	0	15,19,21	0.26	0
7	NAG	G	622	7	14,14,15	0.22	0	15,19,21	0.35	0
7	NAG	G	623	1,7	14,14,15	0.25	0	15,19,21	0.26	0
7	NAG	G	624	8,7	14,14,15	0.20	0	15,19,21	0.26	0
8	BMA	G	625	9,7	11,11,12	0.59	0	15,15,17	0.78	0
9	MAN	G	626	8	11,11,12	0.68	0	15,15,17	1.09	2 (13%)
9	MAN	G	627	8	11,11,12	0.68	0	15,15,17	1.04	2 (13%)
7	NAG	G	628	1,7	14,14,15	0.26	0	15,19,21	0.26	0
7	NAG	G	629	8,7	14,14,15	0.23	0	15,19,21	0.26	0
8	BMA	G	630	9,7	11,11,12	0.61	0	15,15,17	0.78	0
9	MAN	G	631	8	11,11,12	0.67	0	15,15,17	1.04	2 (13%)
7	NAG	G	632	1,7	14,14,15	0.30	0	15,19,21	0.31	0
7	NAG	G	633	8,7	14,14,15	0.90	1 (7%)	15,19,21	1.29	1 (6%)
8	BMA	G	634	9,7	11,11,12	0.67	0	15,15,17	0.75	0
9	MAN	G	635	8	11,11,12	0.62	0	15,15,17	1.17	2 (13%)
9	MAN	G	636	9,8	11,11,12	0.81	1 (9%)	15,15,17	1.29	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	MAN	G	637	9	11,11,12	0.69	0	15,15,17	1.01	1 (6%)
9	MAN	H	301	-	11,11,12	0.25	0	15,15,17	0.64	0
7	NAG	L	301	1,7	14,14,15	0.34	0	15,19,21	0.80	0
7	NAG	L	302	8,7	14,14,15	0.37	0	15,19,21	0.88	0
8	BMA	L	303	9,7	11,11,12	1.44	2 (18%)	15,15,17	4.41	4 (26%)
9	MAN	L	304	9,8	11,11,12	0.23	0	15,15,17	0.77	0
9	MAN	L	305	9	11,11,12	0.27	0	15,15,17	0.76	0
9	MAN	L	306	9	11,11,12	0.23	0	15,15,17	0.64	0
9	MAN	L	307	9,8	11,11,12	0.22	0	15,15,17	0.69	0
9	MAN	L	308	9,3	11,11,12	0.29	0	15,15,17	0.70	0
9	MAN	L	309	9	11,11,12	0.35	0	15,15,17	0.68	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	B	701	2	-	0/6/23/26	0/1/1/1
7	NAG	B	702	2	-	0/6/23/26	0/1/1/1
7	NAG	B	703	2	-	0/6/23/26	0/1/1/1
9	MAN	D	301	-	-	0/2/19/22	0/1/1/1
7	NAG	G	601	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	602	8,7	-	0/6/23/26	0/1/1/1
8	BMA	G	603	9,7	-	0/2/19/22	0/1/1/1
9	MAN	G	604	8	-	0/2/19/22	0/1/1/1
9	MAN	G	605	9,8	-	0/2/19/22	0/1/1/1
9	MAN	G	606	9	-	0/2/19/22	0/1/1/1
9	MAN	G	607	9	-	0/2/19/22	0/1/1/1
7	NAG	G	608	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	609	7	-	0/6/23/26	0/1/1/1
7	NAG	G	610	1	-	0/6/23/26	0/1/1/1
7	NAG	G	611	1	-	0/6/23/26	0/1/1/1
7	NAG	G	612	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	613	7	-	0/6/23/26	0/1/1/1
7	NAG	G	614	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	615	7	-	0/6/23/26	0/1/1/1
7	NAG	G	616	1	-	0/6/23/26	0/1/1/1
7	NAG	G	617	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	618	7	-	0/6/23/26	0/1/1/1
7	NAG	G	619	1,7	-	0/6/23/26	0/1/1/1
7	NAG	G	620	7	-	0/6/23/26	0/1/1/1

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

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	701	NAG	O6-C6	-7.90	1.08	1.42
7	G	615	NAG	C8-C7	-5.04	1.40	1.50
7	G	618	NAG	C2-N2	-4.84	1.37	1.46
7	B	702	NAG	C1-C2	-4.83	1.45	1.52
7	G	618	NAG	C3-C2	-2.09	1.47	1.52
8	L	303	BMA	O2-C2	-2.01	1.38	1.43
9	G	636	MAN	C1-C2	2.15	1.57	1.52
8	L	303	BMA	O5-C1	2.61	1.48	1.43
7	G	633	NAG	O6-C6	3.01	1.55	1.42
7	B	701	NAG	O5-C1	3.17	1.48	1.43
7	B	701	NAG	C1-C2	4.95	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	702	NAG	O5-C1	5.95	1.53	1.43
7	G	618	NAG	C1-C2	8.45	1.64	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	L	303	BMA	O3-C3-C2	-13.11	85.99	110.01
9	G	605	MAN	O2-C2-C3	-2.72	104.71	110.19
8	L	303	BMA	O2-C2-C3	-2.71	104.73	110.19
9	D	301	MAN	O2-C2-C3	-2.33	105.50	110.19
9	G	635	MAN	O2-C2-C3	-2.31	105.53	110.19
9	G	604	MAN	O2-C2-C3	-2.27	105.61	110.19
9	G	626	MAN	O2-C2-C3	-2.25	105.65	110.19
9	G	637	MAN	O2-C2-C3	-2.25	105.65	110.19
9	G	631	MAN	O2-C2-C3	-2.24	105.68	110.19
9	G	627	MAN	O2-C2-C3	-2.23	105.68	110.19
9	G	636	MAN	O2-C2-C3	-2.22	105.72	110.19
9	G	627	MAN	C1-O5-C5	2.09	115.22	112.14
9	G	631	MAN	C1-O5-C5	2.09	115.22	112.14
9	G	636	MAN	C1-C2-C3	2.13	112.13	109.55
9	G	605	MAN	C1-O5-C5	2.20	115.38	112.14
9	G	626	MAN	C1-O5-C5	2.25	115.45	112.14
7	G	618	NAG	C4-C3-C2	2.36	115.00	111.34
9	D	301	MAN	C1-O5-C5	2.37	115.62	112.14
9	G	604	MAN	C1-O5-C5	2.42	115.70	112.14
9	G	635	MAN	C1-O5-C5	2.54	115.87	112.14
9	G	636	MAN	C1-O5-C5	2.68	116.07	112.14
8	L	303	BMA	C1-O5-C5	2.72	116.14	112.14
7	G	633	NAG	C2-N2-C7	4.66	129.17	123.11
7	B	702	NAG	C1-O5-C5	5.08	119.60	112.14
8	L	303	BMA	O3-C3-C4	9.72	132.27	110.36

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

There are no ring outliers.

16 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	702	NAG	1	0
7	G	601	NAG	1	0
7	G	602	NAG	1	0
9	G	605	MAN	1	0
9	G	607	MAN	4	0
7	G	623	NAG	1	0
7	G	633	NAG	1	0
8	G	634	BMA	1	0
9	G	635	MAN	1	0
9	G	636	MAN	1	0
9	H	301	MAN	4	0
7	L	301	NAG	4	0
7	L	302	NAG	2	0
9	L	304	MAN	4	0
9	L	308	MAN	2	0
9	L	309	MAN	6	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	G	452/480 (94%)	0.01	7 (1%) 76 49	58, 95, 164, 244	0
2	B	147/153 (96%)	0.09	4 (2%) 58 28	61, 95, 200, 230	0
3	L	211/218 (96%)	-0.26	0 100 100	77, 113, 140, 169	0
4	H	231/236 (97%)	-0.06	5 (2%) 65 35	81, 118, 171, 189	0
5	D	240/240 (100%)	1.12	59 (24%) 1 0	71, 143, 294, 323	0
6	E	213/216 (98%)	0.55	25 (11%) 6 2	74, 145, 223, 240	0
All	All	1494/1543 (96%)	0.22	100 (6%) 21 7	58, 111, 217, 323	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	D	213	PRO	12.5
5	D	214	LYS	11.0
5	D	132	SER	10.5
5	D	215	SER	9.8
5	D	212	GLU	9.7
5	D	138	LEU	9.2
5	D	126	PRO	8.5
5	D	139	GLY	7.8
5	D	216	CYS	7.8
5	D	127	SER	6.8
6	E	121	LEU	6.8
5	D	194	TYR	6.4
5	D	129	LYS	6.2
5	D	188	SER	6.0
5	D	123	PRO	6.0
5	D	130	SER	5.9
5	D	122	PHE	5.8
5	D	193	THR	5.5
5	D	181	VAL	5.5

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Mol	Chain	Res	Type	RSRZ
5	D	137	ALA	5.5
5	D	211	VAL	5.4
5	D	131	THR	5.3
6	E	119	VAL	5.0
5	D	187	SER	5.0
2	B	556	LEU	5.0
5	D	221	GLU	4.9
6	E	152	TRP	4.9
5	D	128	SER	4.8
5	D	182	VAL	4.6
5	D	185	PRO	4.5
5	D	190	GLY	4.3
5	D	140	CYS	4.2
5	D	217	ASP	4.0
5	D	218	LYS	3.9
5	D	192	GLN	3.9
1	G	63	THR	3.8
5	D	219	GLY	3.6
1	G	72	HIS	3.6
5	D	141	LEU	3.6
6	E	209	THR	3.6
5	D	121	VAL	3.5
5	D	133	GLY	3.4
5	D	161	SER	3.4
6	E	201	HIS	3.4
6	E	196	SER	3.4
6	E	140	ILE	3.4
6	E	138	CYS	3.4
5	D	197	ASN	3.3
1	G	459	GLY	3.3
6	E	193	ARG	3.3
6	E	137	VAL	3.2
5	D	124	LEU	3.2
6	E	197	CYS	3.2
5	D	184	VAL	3.2
5	D	191	THR	3.1
5	D	196	CYS	3.1
5	D	160	THR	3.1
5	D	125	ALA	3.1
5	D	180	SER	3.0
6	E	117	PRO	3.0
6	E	161	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
5	D	159	LEU	2.9
5	D	222	VAL	2.9
5	D	134	GLY	2.9
6	E	116	ASN	2.8
4	H	138	CYS	2.8
6	E	123	PRO	2.8
4	H	209	VAL	2.7
2	B	563	GLN	2.7
4	H	136	LEU	2.7
2	B	564	HIS	2.7
6	E	194	SER	2.6
5	D	136	ALA	2.6
6	E	181	TYR	2.6
5	D	220	LEU	2.5
5	D	209	LYS	2.5
6	E	204	SER	2.5
5	D	198	VAL	2.5
4	H	188	GLY	2.5
6	E	146	GLY	2.5
6	E	139	LEU	2.5
1	G	460	SER	2.5
2	B	561	ALA	2.5
6	E	202	GLU	2.5
5	D	208	ASP	2.5
1	G	506	VAL	2.4
4	H	121	PRO	2.4
6	E	211	ALA	2.4
5	D	186	SER	2.4
5	D	189	LEU	2.3
1	G	187	SER	2.3
5	D	135	THR	2.2
5	D	82(A)	ARG	2.2
6	E	122	PHE	2.2
5	D	153	SER	2.2
1	G	152	GLY	2.1
6	E	136	LEU	2.1
5	D	152	VAL	2.1
6	E	203	GLY	2.1
5	D	154	TRP	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
7	NAG	G	617	14/15	0.88	0.25	0.43	132,143,176,177	0
7	NAG	G	621	14/15	0.88	0.29	0.34	136,156,163,166	0
7	NAG	G	619	14/15	0.90	0.20	0.26	120,145,166,169	0
7	NAG	G	610	14/15	0.86	0.23	0.23	104,132,154,161	0
7	NAG	L	301	14/15	0.92	0.22	0.23	92,106,116,116	0
9	MAN	D	301	11/12	0.88	0.20	0.12	118,135,149,151	0
7	NAG	G	632	14/15	0.96	0.21	-0.05	65,79,91,93	0
7	NAG	G	633	14/15	0.96	0.22	-0.24	60,84,92,97	0
7	NAG	G	612	14/15	0.97	0.19	-0.49	83,104,137,143	0
7	NAG	G	601	14/15	0.96	0.23	-0.61	77,92,110,113	0
7	NAG	G	623	14/15	0.94	0.18	-0.65	108,145,179,182	0
9	MAN	L	308	11/12	0.95	0.16	-0.70	88,98,116,118	0
9	MAN	L	307	11/12	0.96	0.14	-1.30	73,78,107,108	0
7	NAG	L	302	14/15	0.94	0.15	-1.58	79,100,119,122	0
9	MAN	G	635	11/12	0.94	0.18	-	74,92,101,105	0
7	NAG	G	609	14/15	0.87	0.23	-	163,176,183,206	0
7	NAG	G	611	14/15	0.93	0.27	-	128,151,164,173	0
7	NAG	G	608	14/15	0.85	0.23	-	118,152,170,174	0
7	NAG	G	614	14/15	0.90	0.17	-	92,142,163,169	0
7	NAG	G	613	14/15	0.91	0.16	-	137,156,165,178	0
8	BMA	G	603	11/12	0.83	0.14	-	176,187,196,202	0
7	NAG	G	628	14/15	0.96	0.19	-	86,118,135,138	0
9	MAN	G	637	11/12	0.94	0.23	-	125,148,163,164	0
9	MAN	G	605	11/12	0.90	0.16	-	173,199,206,215	0
7	NAG	B	701	14/15	0.89	0.12	-	129,150,172,172	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
9	MAN	L	306	11/12	0.90	0.30	-	136,147,157,161	0
7	NAG	G	616	14/15	0.92	0.19	-	101,141,154,157	0
7	NAG	G	618	14/15	0.81	0.27	-	143,184,189,202	0
8	BMA	G	630	11/12	0.75	0.28	-	188,209,222,228	0
7	NAG	G	622	14/15	0.82	0.39	-	157,175,191,195	0
9	MAN	L	305	11/12	0.96	0.11	-	108,123,130,135	0
8	BMA	G	625	11/12	0.61	0.24	-	229,237,248,259	0
9	MAN	G	627	11/12	0.73	0.23	-	195,215,230,234	0
9	MAN	L	304	11/12	0.90	0.12	-	119,124,135,140	0
9	MAN	G	607	11/12	0.68	0.48	-	223,233,240,249	0
7	NAG	G	615	14/15	0.82	0.26	-	129,176,187,190	0
9	MAN	G	636	11/12	0.81	0.17	-	119,129,145,159	0
8	BMA	L	303	11/12	0.94	0.17	-	93,96,121,125	0
7	NAG	B	702	14/15	0.90	0.13	-	116,143,159,164	0
9	MAN	G	631	11/12	0.73	0.38	-	191,222,229,231	0
9	MAN	G	604	11/12	0.69	0.32	-	173,200,215,218	0
8	BMA	G	634	11/12	0.91	0.23	-	78,87,127,130	0
7	NAG	G	624	14/15	0.90	0.25	-	154,200,221,233	0
9	MAN	G	626	11/12	0.74	0.61	-	251,264,271,276	0
9	MAN	H	301	11/12	0.92	0.14	-	134,138,155,160	0
7	NAG	G	629	14/15	0.91	0.14	-	135,146,175,197	0
9	MAN	L	309	11/12	0.96	0.12	-	89,107,112,113	0
7	NAG	G	620	14/15	0.91	0.17	-	134,170,177,179	0
7	NAG	G	602	14/15	0.94	0.16	-	108,133,150,163	0
7	NAG	B	703	14/15	0.85	0.27	-	150,170,188,199	0
9	MAN	G	606	11/12	0.78	0.21	-	171,199,222,235	0

6.5 Other polymers (i)

There are no such residues in this entry.