Full wwPDB X-ray Structure Validation Report (i)

Jul 28, 2016 – 02:09 PM EDT

PDB ID	:	5FYJ
Title	:	Crystal Structure at 3.4 A Resolution of Fully Glycosylated HIV-1 Clade G X1193.c1 SOSIP.664 Prefusion Env Trimer in Complex with Broadly Neutralizing Antibodies PGT122, 35O22 and VRC01
Authors	:	Stewart-Jones, G.B.E.; Zhou, T.; Thomas, P.V.; Kwong, P.D.
Deposited on	:	2016-03-08
Resolution	:	3.11 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:

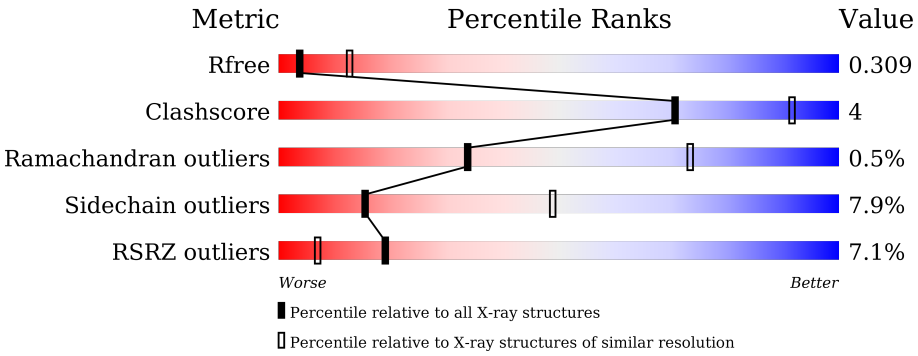
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 3.11 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	1112 (3.16-3.08)
Clashscore	102246	1218 (3.16-3.08)
Ramachandran outliers	100387	1175 (3.16-3.08)
Sidechain outliers	100360	1175 (3.16-3.08)
RSRZ outliers	91569	1114 (3.16-3.08)

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	B	161	83% 12%
2	D	243	16% 85% 14%
3	E	216	9% 81% 17%
4	G	484	4% 77% 19%
5	H	244	5% 82% 10% 7%
6	L	213	4% 79% 17%

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Mol	Chain	Length	Quality of chain
7	U	240	3% 41% 8% 50%
7	V	240	6% 37% 59%

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
10	NAG	B	6251	-	-	-	X
10	NAG	B	6252	-	-	-	X
14	MAN	G	1569(A)	X	-	-	-
14	MAN	G	1569(B)	X	-	-	-
14	MAN	G	2629	X	-	-	-
14	MAN	G	2629(A)	X	-	-	-
14	MAN	G	2629(B)	X	-	-	-
15	MAN	G	1609	X	-	-	-
15	MAN	G	1609(A)	X	-	-	-
15	MAN	G	3329(A)	X	-	-	-
16	BMA	G	2343	-	-	X	-
16	MAN	G	2344	-	-	X	-
18	MAN	G	3869(A)	X	-	-	-
18	MAN	G	3869(B)	X	-	-	-
8	CIT	G	1511	-	-	-	X

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 15476 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 GP41 ENV ECTODOMAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	154	Total	C	N	O	S	0	0	0
			1220	770	215	230	5			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	ENGINEERED MUTATION	UNP C6ZIG9
B	605	CYS	THR	ENGINEERED MUTATION	UNP C6ZIG9
B	666	GLY	-	EXPRESSION TAG	UNP C6ZIG9
B	667	GLY	-	EXPRESSION TAG	UNP C6ZIG9
B	668	GLY	-	EXPRESSION TAG	UNP C6ZIG9
B	669	LEU	-	EXPRESSION TAG	UNP C6ZIG9
B	670	VAL	-	EXPRESSION TAG	UNP C6ZIG9
B	671	PRO	-	EXPRESSION TAG	UNP C6ZIG9
B	672	ARG	-	EXPRESSION TAG	UNP C6ZIG9

- Molecule 2 is a protein called 35O22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	243	Total	C	N	O	S	0	0	1
			1833	1165	307	353	8			

- Molecule 3 is a protein called 35O22.

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

- Molecule 4 is a protein called GP120 ENV ECTODOMAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	479	Total	C	N	O	S	0	0	0
			3769	2351	674	716	28			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	29	ALA	-	EXPRESSION TAG	UNP C6ZIG9
G	30	LEU	-	EXPRESSION TAG	UNP C6ZIG9
G	31	ALA	-	EXPRESSION TAG	UNP C6ZIG9
G	32	GLY	-	EXPRESSION TAG	UNP C6ZIG9
G	459	CYS	GLY	ENGINEERED MUTATION	UNP C6ZIG9
G	501	CYS	ALA	ENGINEERED MUTATION	UNP C6ZIG9
G	509	ARG	-	EXPRESSION TAG	UNP C6ZIG9
G	510	ARG	-	EXPRESSION TAG	UNP C6ZIG9
G	511	ARG	-	EXPRESSION TAG	UNP C6ZIG9
G	512	ARG	-	EXPRESSION TAG	UNP C6ZIG9
G	513	ARG	-	EXPRESSION TAG	UNP C6ZIG9

- Molecule 5 is a protein called PGT122.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	228	Total	C	N	O	S	0	0	0
			1742	1109	295	333	5			

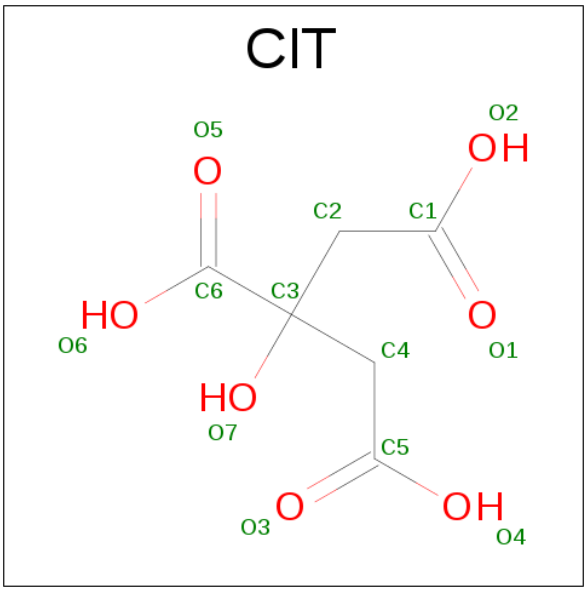
- Molecule 6 is a protein called PGT122.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	L	210	Total	C	N	O	S	0	0	0
			1589	998	267	320	4			

- Molecule 7 is a protein called VRC01.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	U	119	Total	C	N	O	S	0	0	0
			956	603	173	171	9			
7	V	98	Total	C	N	O	S	0	0	0
			758	479	130	147	2			

- Molecule 8 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C O 13 6 7	0	0
8	G	1	Total C O 13 6 7	0	0
8	G	1	Total C O 13 6 7	0	0

- Molecule 9 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 10 is a polymer of unknown type called SUGAR (3-MER).

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

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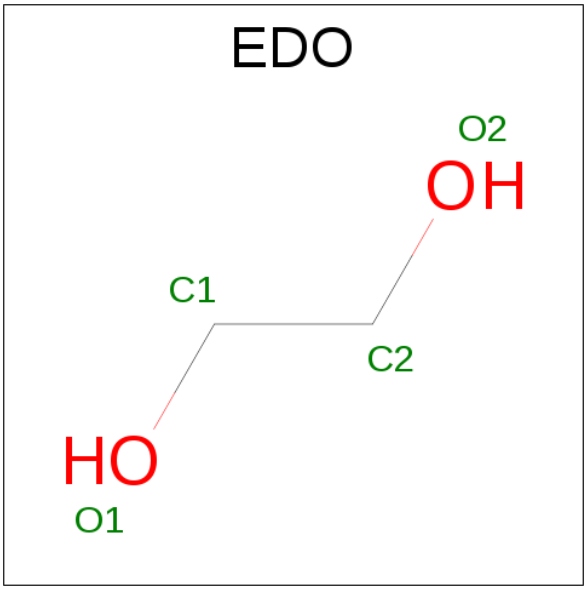
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	G	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 11 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

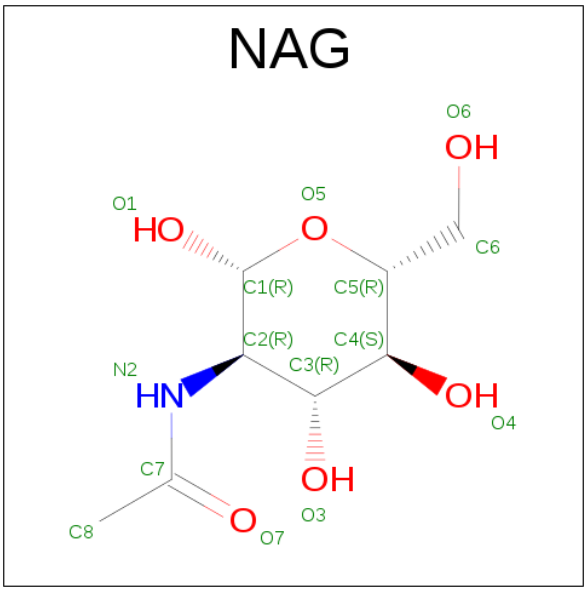


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	D	1	Total	C	O	0	0
			4	2	2		
11	G	1	Total	C	O	0	0
			4	2	2		

- Molecule 12 is a polymer of unknown type called SUGAR (8-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	G	8	Total	C	N	O	0	0
			94	52	2	40		

- Molecule 13 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 14 is a polymer of unknown type called SUGAR (11-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	G	11	Total C N O 127 70 2 55	0	0
14	G	11	Total C N O 127 70 2 55	0	0

- Molecule 15 is a polymer of unknown type called SUGAR (10-MER).

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

- Molecule 16 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	6	Total C N O 72 40 2 30	0	0
16	G	6	Total C N O 72 40 2 30	0	0
16	H	6	Total C N O 72 40 2 30	0	0
16	V	6	Total C N O 72 40 2 30	0	0

- Molecule 17 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	G	7	Total C N O 83 46 2 35	0	0
17	G	7	Total C N O 83 46 2 35	0	0
17	G	7	Total C N O 83 46 2 35	0	0

- Molecule 18 is a polymer of unknown type called SUGAR (9-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	G	9	Total C N O 105 58 2 45	0	0
18	G	9	Total C N O 105 58 2 45	0	0
18	G	9	Total C N O 105 58 2 45	0	0

- Molecule 19 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	B	4	Total O 4 4	0	0
19	D	2	Total O 2 2	0	0
19	E	1	Total O 1 1	0	0
19	G	3	Total O 3 3	0	0
19	H	1	Total O 1 1	0	0

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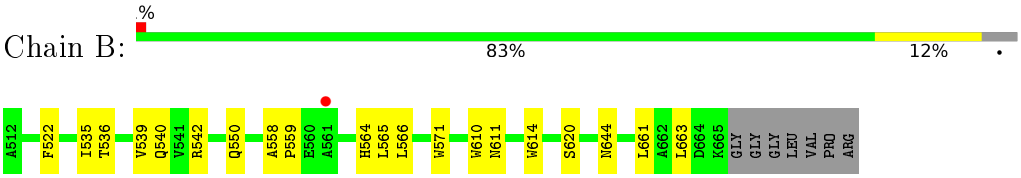
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	L	1	Total O 1 1	0	0

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.

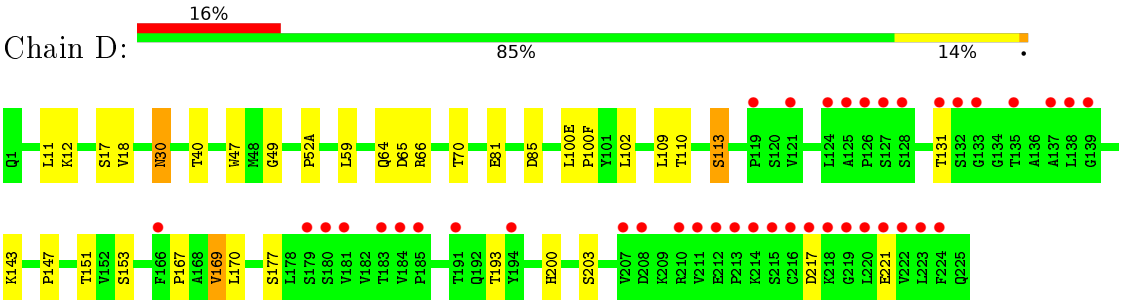
- Molecule 1: GP41 ENV ECTODOMAIN

Chain B:



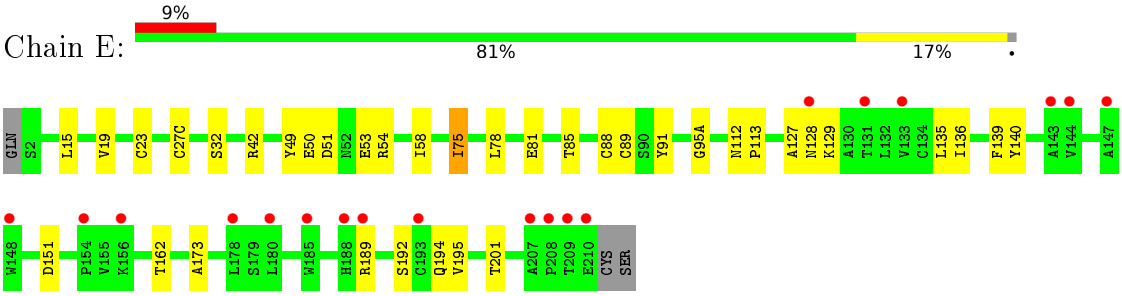
- Molecule 2: 35O22

Chain D:



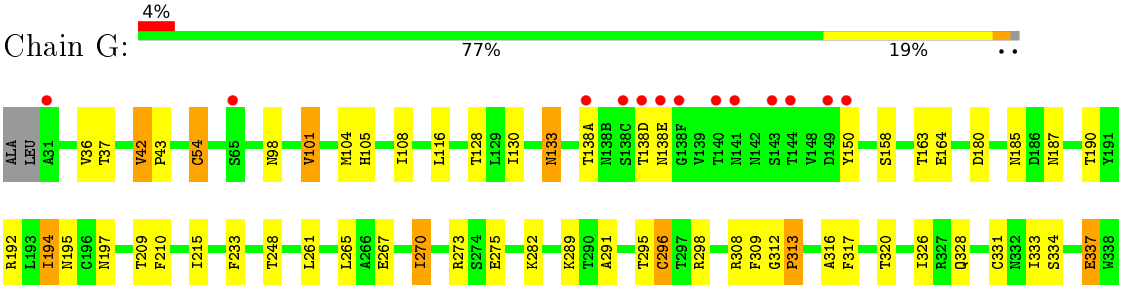
- Molecule 3: 35O22

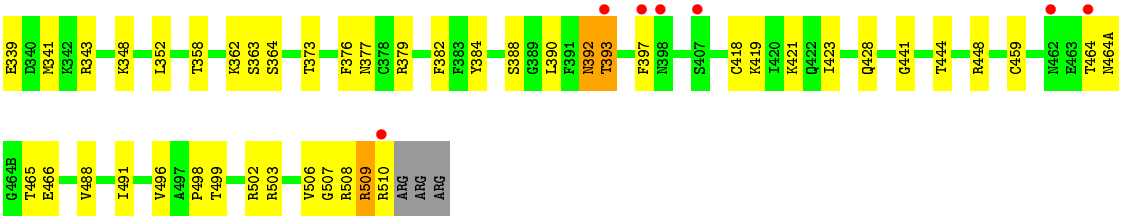
Chain E:



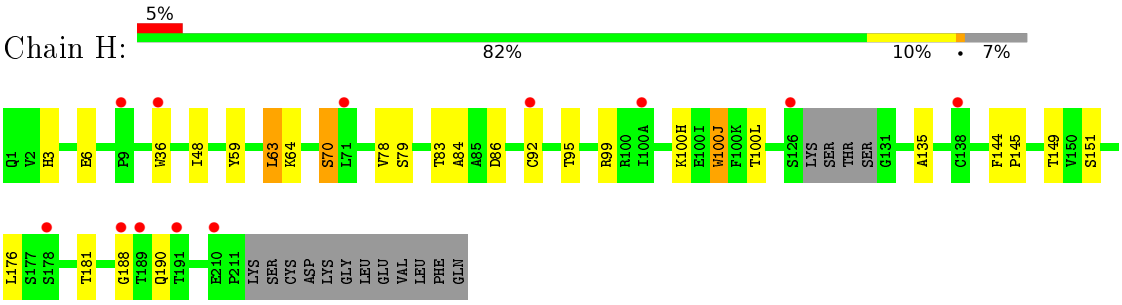
- Molecule 4: GP120 ENV ECTODOMAIN

Chain G:

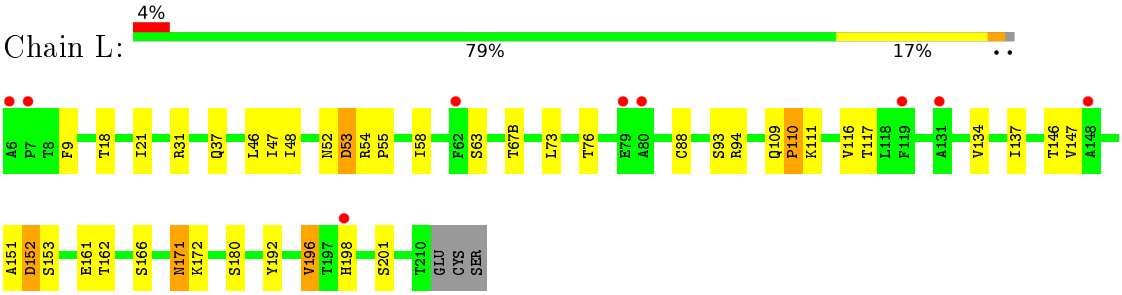




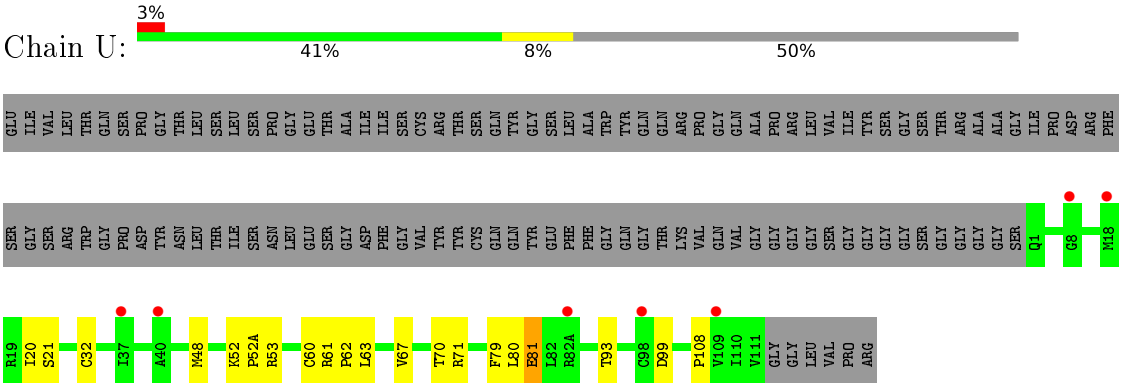
- Molecule 5: PGT122



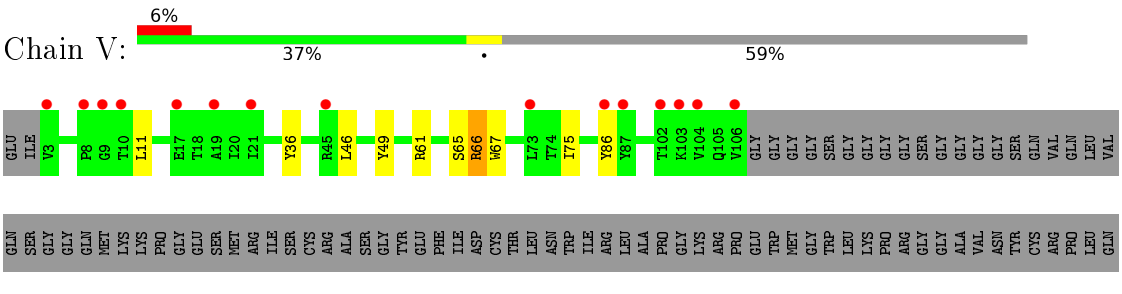
- Molecule 6: PGT122



- Molecule 7: VRC01



- Molecule 7: VRC01



GLY ARG VAL THR MET THR ARG ASP VAL TYR SER ASP THR ALA PHE LEU GLU LEU ARG SER LEU THR VAL ASP ASP THR ALA VAL TYR PHE CYS THR ARG GLY LYS ASN CYS ASP TYR ASN TRP ASP PHE GLU HIS TRP GLY ARG GLY THR PRO VAL ILE VAL GLY GLY LEU VAL PRO ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	127.16Å 127.16Å 313.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.65 – 3.11 44.65 – 3.11	Depositor EDS
% Data completeness (in resolution range)	83.3 (44.65-3.11) 83.3 (44.65-3.11)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.63 (at 3.12Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.9_1692)	Depositor
R, R_{free}	0.214 , 0.273 0.274 , 0.309	Depositor DCC
R_{free} test set	2003 reflections (4.92%)	DCC
Wilson B-factor (Å^2)	74.9	Xtriage
Anisotropy	0.002	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 69.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.114 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	15476	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 2.20% 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, 0.333 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: MAN, BMA, CIT, NAG, EDO

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	B	0.38	1/1242 (0.1%)	0.46	0/1689
2	D	0.27	0/1881	0.44	0/2562
3	E	0.23	0/1659	0.44	0/2269
4	G	0.26	0/3843	0.47	0/5213
5	H	0.22	0/1789	0.43	0/2443
6	L	0.23	0/1632	0.44	0/2236
7	U	0.24	0/981	0.44	0/1328
7	V	0.23	0/778	0.44	0/1058
All	All	0.26	1/13805 (0.0%)	0.45	0/18798

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
14	G	6	0
15	G	3	0
18	G	2	0
All	All	11	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	644	ASN	C-N	8.99	1.54	1.34

There are no bond angle outliers.

All (11) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	G	1569(A)	MAN	C1
14	G	1569(B)	MAN	C1
15	G	1609	MAN	C1
15	G	1609(A)	MAN	C1
14	G	2629	MAN	C1
14	G	2629(A)	MAN	C1,C1
14	G	2629(B)	MAN	C1
15	G	3329(A)	MAN	C1
18	G	3869(A)	MAN	C1
18	G	3869(B)	MAN	C1

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1220	0	1202	7	0
2	D	1833	0	1806	15	1
3	E	1615	0	1542	17	0
4	G	3769	0	3705	45	0
5	H	1742	0	1715	11	0
6	L	1589	0	1530	15	0
7	U	956	0	928	8	0
7	V	758	0	719	5	0
8	B	13	0	5	1	0
8	G	26	0	10	2	0
9	B	84	0	75	1	0
9	G	28	0	25	0	0
10	B	39	0	34	0	0
10	G	78	0	68	0	0
11	D	4	0	6	0	0
11	G	4	0	6	0	0
12	G	94	0	79	1	0
13	G	42	0	39	1	0
14	G	254	0	212	4	0
15	G	464	0	388	5	1
16	G	144	0	122	6	0
16	H	72	0	61	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	V	72	0	61	0	0
17	G	249	0	210	4	0
18	G	315	0	264	0	0
19	B	4	0	0	0	0
19	D	2	0	0	0	0
19	E	1	0	0	0	0
19	G	3	0	0	0	0
19	H	1	0	0	1	0
19	L	1	0	0	0	0
All	All	15476	0	14812	134	2

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 4.

All (134) 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)
17:G:3445:MAN:H3	17:G:3447:MAN:H5	1.19	1.13
16:G:2343:BMA:H3	16:G:2344:MAN:H5	1.44	0.96
4:G:459:CYS:HB2	7:U:61:ARG:HG2	1.47	0.93
17:G:3445:MAN:H3	17:G:3447:MAN:C5	2.02	0.89
15:G:1883:BMA:H3	15:G:1884:MAN:H3	1.56	0.86
6:L:109:GLN:OE1	6:L:171:ASN:ND2	2.13	0.80
4:G:105:HIS:HE2	8:G:1513:CIT:H22	1.47	0.79
16:G:2343:BMA:H3	16:G:2344:MAN:C5	2.16	0.76
4:G:233:PHE:O	4:G:273:ARG:NH1	2.19	0.75
17:G:3445:MAN:C3	17:G:3447:MAN:H5	2.11	0.74
16:G:2343:BMA:C3	16:G:2344:MAN:H5	2.18	0.72
15:G:1883:BMA:C3	15:G:1884:MAN:H3	2.24	0.68
7:V:66:ARG:NE	7:V:67:TRP:O	2.30	0.65
9:B:6161:NAG:H4	9:B:6162:NAG:N2	2.10	0.64
4:G:428:GLN:NE2	7:U:53:ARG:O	2.26	0.63
2:D:30:ASN:HA	2:D:52(A):PRO:HB2	1.82	0.62
3:E:127:ALA:HB3	3:E:129:LYS:N	2.17	0.59
3:E:54:ARG:NH1	3:E:58:ILE:O	2.35	0.59
8:B:1666:CIT:O7	8:B:1666:CIT:O3	2.17	0.58
15:G:1883:BMA:O4	15:G:1884:MAN:H5	2.03	0.58
7:V:61:ARG:HB3	7:V:75:ILE:HG13	1.85	0.58
4:G:308:ARG:HG2	4:G:316:ALA:HB2	1.85	0.57
4:G:333:ILE:HD13	4:G:390:LEU:HD21	1.86	0.57
4:G:105:HIS:NE2	8:G:1513:CIT:H22	2.16	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:343:ARG:HB2	4:G:397:PHE:CE1	2.39	0.57
5:H:83:THR:N	5:H:86:ASP:OD2	2.24	0.56
2:D:143:LYS:HD2	2:D:177:SER:HB3	1.88	0.55
15:G:1883:BMA:H3	15:G:1884:MAN:C3	2.18	0.55
4:G:194:ILE:HG13	4:G:423:ILE:HD11	1.87	0.55
4:G:334:SER:HB3	4:G:337:GLU:HB3	1.88	0.55
5:H:59:TYR:HB2	5:H:64:LYS:HG3	1.89	0.55
3:E:151:ASP:HB2	3:E:189:ARG:HB2	1.90	0.54
4:G:506:VAL:HG22	4:G:508:ARG:H	1.73	0.54
1:B:611:ASN:HB3	1:B:614:TRP:CD2	2.43	0.53
3:E:50:GLU:HB2	3:E:53:GLU:HB2	1.90	0.53
4:G:358:THR:O	4:G:465:THR:OG1	2.18	0.53
6:L:37:GLN:HB3	6:L:47:ILE:HD11	1.90	0.53
4:G:379:ARG:NH1	14:G:2623:BMA:H3	2.24	0.53
4:G:377:ASN:HB3	4:G:382:PHE:CD1	2.43	0.53
4:G:133:ASN:HB3	13:G:1331:NAG:O5	2.09	0.53
4:G:373:THR:HG21	4:G:384:TYR:HB3	1.90	0.52
16:G:2343:BMA:H3	16:G:2344:MAN:H3	1.91	0.52
4:G:36:VAL:HG13	4:G:496:VAL:HG13	1.92	0.52
4:G:265:LEU:HD11	4:G:291:ALA:HB2	1.92	0.51
3:E:49:TYR:O	3:E:91:TYR:OH	2.21	0.51
4:G:298:ARG:NH2	4:G:441:GLY:O	2.43	0.51
4:G:180:ASP:HA	4:G:194:ILE:HD11	1.91	0.51
16:G:2343:BMA:C3	16:G:2344:MAN:C5	2.85	0.51
4:G:379:ARG:HG2	4:G:379:ARG:HH11	1.76	0.51
2:D:11:LEU:HD13	2:D:147:PRO:HG3	1.92	0.51
2:D:12:LYS:NZ	2:D:17:SER:O	2.43	0.51
1:B:610:TRP:CG	4:G:498:PRO:HB3	2.46	0.50
5:H:70:SER:HB2	5:H:79:SER:HB2	1.93	0.50
4:G:502:ARG:HB3	4:G:506:VAL:HG13	1.93	0.50
7:V:46:LEU:HD11	7:V:49:TYR:HB3	1.94	0.50
3:E:19:VAL:HG13	3:E:75:ILE:HG23	1.93	0.49
1:B:550:GLN:N	1:B:550:GLN:OE1	2.45	0.49
4:G:507:GLY:O	4:G:510:ARG:NH2	2.44	0.49
4:G:270:ILE:HG22	4:G:289:LYS:H	1.76	0.49
4:G:163:THR:OG1	4:G:164:GLU:N	2.45	0.49
4:G:392:ASN:O	4:G:393:THR:OG1	2.22	0.48
4:G:37:THR:OG1	4:G:499:THR:HB	2.14	0.48
4:G:295:THR:HG21	15:G:4132:NAG:H82	1.97	0.47
2:D:47:TRP:CZ3	3:E:95(A):GLY:HA3	2.49	0.47
3:E:49:TYR:CD2	3:E:50:GLU:HG3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:194:GLN:HG2	3:E:201:THR:HG22	1.96	0.47
3:E:127:ALA:HB3	3:E:129:LYS:H	1.76	0.47
5:H:48:ILE:HG23	5:H:63:LEU:HD11	1.97	0.46
17:G:3445:MAN:H2	17:G:3447:MAN:H3	1.96	0.46
3:E:136:ILE:HG21	3:E:195:VAL:HG21	1.97	0.46
4:G:312:GLY:HA2	4:G:313:PRO:C	2.36	0.46
5:H:188:GLY:HA3	5:H:190:GLN:N	2.31	0.46
4:G:130:ILE:HG13	4:G:158:SER:HB3	1.97	0.46
4:G:42:VAL:HA	4:G:43:PRO:HD3	1.77	0.45
1:B:535:ILE:HG23	1:B:536:THR:HG23	1.98	0.45
4:G:379:ARG:HH12	14:G:2623:BMA:H3	1.81	0.45
6:L:21:ILE:HD11	6:L:73:LEU:HD23	1.99	0.45
6:L:53:ASP:OD1	6:L:53:ASP:N	2.49	0.45
7:U:60:CYS:SG	7:U:62:PRO:HD2	2.57	0.45
7:U:67:VAL:HG23	7:U:80:LEU:HD11	1.98	0.45
5:H:100(H):LYS:HA	5:H:100(J):TRP:CZ3	2.52	0.44
4:G:464:THR:HA	4:G:464(A):ASN:HA	1.67	0.44
4:G:296:CYS:SG	4:G:376:PHE:HZ	2.40	0.44
7:U:80:LEU:HD12	7:U:81:GLU:N	2.33	0.44
14:G:1566:MAN:C2	14:G:1569:MAN:H5	2.47	0.44
6:L:55:PRO:HD2	6:L:58:ILE:HD13	1.99	0.44
6:L:18:THR:HG23	6:L:76:THR:HA	1.99	0.43
4:G:98:ASN:O	4:G:101:VAL:HG13	2.19	0.43
4:G:275:GLU:HB3	4:G:282:LYS:HD3	1.99	0.43
5:H:84:ALA:N	19:H:2001:HOH:O	2.41	0.43
6:L:54:ARG:HA	6:L:55:PRO:HD3	1.84	0.43
2:D:102:LEU:HD12	2:D:102:LEU:HA	1.90	0.43
5:H:135:ALA:HB2	5:H:181:THR:HG22	1.99	0.43
6:L:151:ALA:HA	6:L:192:TYR:CE1	2.53	0.43
2:D:59:LEU:HD23	2:D:64:GLN:HA	1.99	0.43
14:G:1565:MAN:O5	14:G:1568:MAN:C1	2.67	0.43
7:V:65:SER:OG	7:V:66:ARG:N	2.51	0.43
2:D:169:VAL:HG22	3:E:162:THR:HG22	1.99	0.43
4:G:185:ASN:OD1	4:G:185:ASN:N	2.35	0.43
1:B:558:ALA:HB1	1:B:559:PRO:HD2	2.01	0.43
2:D:217:ASP:N	2:D:221:GLU:OE2	2.51	0.43
2:D:18:VAL:O	2:D:81:GLU:HA	2.19	0.42
1:B:571:TRP:CD2	4:G:54:CYS:HB3	2.54	0.42
6:L:46:LEU:HD23	6:L:47:ILE:N	2.35	0.42
4:G:138(D):THR:OG1	4:G:138(E):ASN:HA	2.20	0.42
16:G:2343:BMA:H3	16:G:2344:MAN:C3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:152:ASP:O	6:L:153:SER:OG	2.24	0.42
4:G:343:ARG:HB2	4:G:397:PHE:CZ	2.55	0.42
2:D:100(E):LEU:HA	2:D:100(F):PRO:HD3	1.89	0.42
2:D:47:TRP:CH2	3:E:95(A):GLY:HA3	2.55	0.41
6:L:109:GLN:HE22	6:L:172:LYS:HG3	1.85	0.41
4:G:104:MET:O	4:G:108:ILE:HG12	2.20	0.41
7:U:52:LYS:HA	7:U:52(A):PRO:HD3	1.84	0.41
2:D:11:LEU:HD12	2:D:110:THR:O	2.21	0.41
6:L:137:ILE:HG21	6:L:196:VAL:HG21	2.03	0.41
3:E:139:PHE:CE2	3:E:173:ALA:HA	2.56	0.41
5:H:100(H):LYS:HA	5:H:100(J):TRP:CE3	2.56	0.41
7:V:36:TYR:O	7:V:86:TYR:HA	2.21	0.41
3:E:112:ASN:HA	3:E:113:PRO:HD3	1.84	0.41
2:D:47:TRP:CZ2	2:D:49:GLY:HA2	2.55	0.41
5:H:36:TRP:HB3	5:H:48:ILE:HD12	2.01	0.41
6:L:110:PRO:O	6:L:111:LYS:HG3	2.21	0.41
4:G:362:LYS:HG3	4:G:363:SER:H	1.86	0.41
5:H:144:PHE:HA	5:H:145:PRO:HA	1.85	0.41
6:L:109:GLN:HB3	6:L:110:PRO:C	2.42	0.41
2:D:200:HIS:ND1	2:D:203:SER:OG	2.29	0.40
1:B:522:PHE:HZ	4:G:491:ILE:HG12	1.86	0.40
3:E:15:LEU:HA	3:E:78:LEU:HB2	2.03	0.40
7:U:21:SER:HB3	7:U:79:PHE:CE1	2.56	0.40
3:E:127:ALA:N	3:E:128:ASN:HA	2.36	0.40
4:G:195:ASN:C	4:G:197:ASN:N	2.75	0.40
12:G:884:MAN:H2	12:G:886:MAN:H2	1.82	0.40
7:U:48:MET:HE3	7:U:63:LEU:HD22	2.04	0.40
6:L:198:HIS:O	6:L:201:SER:HB3	2.20	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:65:ASP:OD1	2:D:113:SER:OG[2_555]	2.14	0.06
15:G:1606:MAN:O6	15:G:1607:MAN:O3[2_655]	2.18	0.02

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	B	152/161 (94%)	141 (93%)	11 (7%)	0	100	100
2	D	241/243 (99%)	213 (88%)	26 (11%)	2 (1%)	24	64
3	E	211/216 (98%)	187 (89%)	24 (11%)	0	100	100
4	G	477/484 (99%)	434 (91%)	40 (8%)	3 (1%)	30	70
5	H	224/244 (92%)	210 (94%)	14 (6%)	0	100	100
6	L	208/213 (98%)	185 (89%)	21 (10%)	2 (1%)	19	59
7	U	117/240 (49%)	108 (92%)	8 (7%)	1 (1%)	21	62
7	V	96/240 (40%)	87 (91%)	8 (8%)	1 (1%)	19	59
All	All	1726/2041 (85%)	1565 (91%)	152 (9%)	9 (0%)	34	73

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	G	393	THR
2	D	85	ASP
4	G	509	ARG
2	D	167	PRO
6	L	152	ASP
7	V	66	ARG
7	U	108	PRO
6	L	110	PRO
4	G	313	PRO

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	B	131/135 (97%)	122 (93%)	9 (7%)	19 55
2	D	205/206 (100%)	193 (94%)	12 (6%)	24 60
3	E	186/189 (98%)	173 (93%)	13 (7%)	19 54
4	G	428/432 (99%)	385 (90%)	43 (10%)	9 34
5	H	198/213 (93%)	185 (93%)	13 (7%)	21 57
6	L	178/181 (98%)	157 (88%)	21 (12%)	6 26
7	U	102/192 (53%)	95 (93%)	7 (7%)	19 55
7	V	81/192 (42%)	80 (99%)	1 (1%)	78 92
All	All	1509/1740 (87%)	1390 (92%)	119 (8%)	15 49

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	539	VAL
1	B	540	GLN
1	B	542	ARG
1	B	564	HIS
1	B	565	LEU
1	B	566	LEU
1	B	620	SER
1	B	661	LEU
1	B	663	LEU
2	D	30	ASN
2	D	40	THR
2	D	66	ARG
2	D	70	THR
2	D	109	LEU
2	D	113	SER
2	D	131	THR
2	D	151	THR
2	D	153	SER
2	D	169	VAL
2	D	170	LEU
2	D	193	THR
3	E	23	CYS
3	E	27(C)	CYS
3	E	32	SER
3	E	42	ARG

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Mol	Chain	Res	Type
3	E	51	ASP
3	E	75	ILE
3	E	81	GLU
3	E	85	THR
3	E	88	CYS
3	E	89	CYS
3	E	135	LEU
3	E	140	TYR
3	E	192	SER
4	G	42	VAL
4	G	54	CYS
4	G	101	VAL
4	G	116	LEU
4	G	128	THR
4	G	133	ASN
4	G	138(A)	THR
4	G	150	TYR
4	G	187	ASN
4	G	190	THR
4	G	192	ARG
4	G	194	ILE
4	G	209	THR
4	G	210	PHE
4	G	215	ILE
4	G	248	THR
4	G	261	LEU
4	G	267	GLU
4	G	270	ILE
4	G	296	CYS
4	G	309	PHE
4	G	317	PHE
4	G	320	THR
4	G	326	ILE
4	G	328	GLN
4	G	331	CYS
4	G	337	GLU
4	G	339	GLU
4	G	341	MET
4	G	348	LYS
4	G	352	LEU
4	G	364	SER
4	G	388	SER

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Mol	Chain	Res	Type
4	G	392	ASN
4	G	418	CYS
4	G	419	LYS
4	G	421	LYS
4	G	444	THR
4	G	448	ARG
4	G	466	GLU
4	G	488	VAL
4	G	503	ARG
4	G	509	ARG
5	H	3	HIS
5	H	6	GLU
5	H	63	LEU
5	H	70	SER
5	H	78	VAL
5	H	92	CYS
5	H	95	THR
5	H	99	ARG
5	H	100(J)	TRP
5	H	100(L)	THR
5	H	149	THR
5	H	151	SER
5	H	176	LEU
6	L	9	PHE
6	L	31	ARG
6	L	48	ILE
6	L	52	ASN
6	L	53	ASP
6	L	63	SER
6	L	67(B)	THR
6	L	88	CYS
6	L	93	SER
6	L	94	ARG
6	L	116	VAL
6	L	117	THR
6	L	134	VAL
6	L	146	THR
6	L	147	VAL
6	L	161	GLU
6	L	162	THR
6	L	166	SER
6	L	171	ASN

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Mol	Chain	Res	Type
6	L	180	SER
6	L	196	VAL
7	U	20	ILE
7	U	32	CYS
7	U	70	THR
7	U	71	ARG
7	U	81	GLU
7	U	93	THR
7	U	99	ASP
7	V	11	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

159 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	NAG	B	6111	1,9	14,14,15	0.47	0	15,19,21	0.64	0
9	NAG	B	6112	9	14,14,15	0.40	0	15,19,21	0.23	0
9	NAG	B	6161	1,9	14,14,15	0.74	1 (7%)	15,19,21	1.03	1 (6%)
9	NAG	B	6162	9	14,14,15	0.59	0	15,19,21	0.40	0
10	NAG	B	6251	1,10	14,14,15	0.22	0	15,19,21	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	NAG	B	6252	10	14,14,15	0.27	0	15,19,21	1.07	2 (13%)
10	BMA	B	6253	10	11,11,12	0.44	0	15,15,17	1.02	1 (6%)
9	NAG	B	6371	1,9	14,14,15	0.46	0	15,19,21	0.34	0
9	NAG	B	6372	9	14,14,15	0.62	0	15,19,21	0.36	0
14	NAG	G	1561	4,14	14,14,15	0.28	0	15,19,21	0.35	0
14	NAG	G	1562	14	14,14,15	0.40	0	15,19,21	0.92	1 (6%)
14	BMA	G	1563	14	11,11,12	0.78	0	15,15,17	1.23	1 (6%)
14	MAN	G	1564	14	11,11,12	0.68	0	15,15,17	0.90	1 (6%)
14	MAN	G	1565	14	11,11,12	0.80	0	15,15,17	1.36	2 (13%)
14	MAN	G	1566	14	11,11,12	0.74	0	15,15,17	1.36	2 (13%)
14	MAN	G	1567	14	11,11,12	0.62	0	15,15,17	1.15	2 (13%)
14	MAN	G	1568	14	11,11,12	0.77	0	15,15,17	0.98	1 (6%)
14	MAN	G	1569	14	11,11,12	0.24	0	15,15,17	0.52	0
14	MAN	G	1569(A)	14	11,11,12	0.61	0	15,15,17	0.91	2 (13%)
14	MAN	G	1569(B)	14	11,11,12	0.61	0	15,15,17	0.93	2 (13%)
15	NAG	G	1601	15,4	14,14,15	0.29	0	15,19,21	0.62	0
15	NAG	G	1602	15	14,14,15	0.34	0	15,19,21	0.36	0
15	BMA	G	1603	15	11,11,12	0.85	1 (9%)	15,15,17	1.08	0
15	MAN	G	1604	15	11,11,12	0.91	0	15,15,17	1.12	1 (6%)
15	MAN	G	1605	15	11,11,12	0.82	0	15,15,17	1.17	3 (20%)
15	MAN	G	1606	15	11,11,12	0.82	0	15,15,17	1.30	2 (13%)
15	MAN	G	1607	15	11,11,12	0.53	0	15,15,17	1.04	1 (6%)
15	MAN	G	1608	15	11,11,12	0.63	0	15,15,17	1.03	2 (13%)
15	MAN	G	1609	15	11,11,12	0.68	0	15,15,17	1.00	2 (13%)
15	MAN	G	1609(A)	15	11,11,12	0.63	0	15,15,17	0.99	2 (13%)
15	NAG	G	1881	15,4	14,14,15	0.19	0	15,19,21	0.48	0
15	NAG	G	1882	15	14,14,15	0.23	0	15,19,21	0.34	0
15	BMA	G	1883	15	11,11,12	0.89	1 (9%)	15,15,17	1.21	1 (6%)
15	MAN	G	1884	15	11,11,12	0.67	0	15,15,17	1.21	1 (6%)
15	MAN	G	1885	15	11,11,12	0.66	0	15,15,17	1.13	2 (13%)
15	MAN	G	1886	15	11,11,12	0.57	0	15,15,17	1.27	2 (13%)
15	MAN	G	1887	15	11,11,12	0.54	0	15,15,17	1.09	2 (13%)
15	MAN	G	1888	15	11,11,12	0.76	0	15,15,17	1.02	2 (13%)
15	MAN	G	1889	15	11,11,12	0.65	0	15,15,17	1.01	2 (13%)
15	MAN	G	1889(A)	15	11,11,12	0.72	0	15,15,17	0.88	1 (6%)
10	NAG	G	1971	10,4	14,14,15	1.39	1 (7%)	15,19,21	0.83	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	NAG	G	1972	10	14,14,15	0.24	0	15,19,21	0.44	0
10	BMA	G	1973	10	11,11,12	0.85	1 (9%)	15,15,17	0.83	0
16	NAG	G	2341	4,16	14,14,15	0.26	0	15,19,21	0.44	0
16	NAG	G	2342	16	14,14,15	0.44	0	15,19,21	0.28	0
16	BMA	G	2343	16	11,11,12	0.43	0	15,15,17	1.20	1 (6%)
16	MAN	G	2344	16	11,11,12	0.29	0	15,15,17	0.94	1 (6%)
16	MAN	G	2345	16	11,11,12	0.71	0	15,15,17	1.15	2 (13%)
16	MAN	G	2346	16	11,11,12	0.79	0	15,15,17	0.78	1 (6%)
17	NAG	G	2411	4,17	14,14,15	0.39	0	15,19,21	0.47	0
17	NAG	G	2412	17	14,14,15	0.44	0	15,19,21	0.67	0
17	BMA	G	2413	17	11,11,12	0.97	0	15,15,17	1.01	1 (6%)
17	MAN	G	2414	17	11,11,12	0.70	0	15,15,17	1.08	1 (6%)
17	MAN	G	2415	17	11,11,12	0.67	0	15,15,17	0.97	2 (13%)
17	MAN	G	2416	17	11,11,12	0.77	0	15,15,17	0.89	1 (6%)
17	MAN	G	2417	17	11,11,12	0.70	0	15,15,17	0.94	1 (6%)
14	NAG	G	2621	4,14	14,14,15	0.41	0	15,19,21	0.36	0
14	NAG	G	2622	14	14,14,15	0.29	0	15,19,21	0.29	0
14	BMA	G	2623	14	11,11,12	0.64	0	15,15,17	0.85	0
14	MAN	G	2624	14	11,11,12	0.78	0	15,15,17	1.24	2 (13%)
14	MAN	G	2625	14	11,11,12	0.66	0	15,15,17	1.06	2 (13%)
14	MAN	G	2626	14	11,11,12	0.67	0	15,15,17	1.39	2 (13%)
14	MAN	G	2627	14	11,11,12	0.66	0	15,15,17	1.26	3 (20%)
14	MAN	G	2628	14	11,11,12	0.60	0	15,15,17	1.05	2 (13%)
14	MAN	G	2629	14	11,11,12	0.86	1 (9%)	15,15,17	0.87	1 (6%)
14	MAN	G	2629(A)	14	11,11,12	0.75	0	15,15,17	0.88	1 (6%)
14	MAN	G	2629(B)	14	11,11,12	0.65	0	15,15,17	0.90	1 (6%)
18	NAG	G	2761	18,4	14,14,15	0.56	0	15,19,21	0.56	0
18	NAG	G	2762	18	14,14,15	0.25	0	15,19,21	0.65	0
18	BMA	G	2763	18	11,11,12	0.69	0	15,15,17	0.78	0
18	MAN	G	2764	18	11,11,12	0.61	0	15,15,17	0.92	2 (13%)
18	MAN	G	2765	18	11,11,12	0.97	0	15,15,17	1.07	2 (13%)
18	MAN	G	2766	18	11,11,12	0.59	0	15,15,17	1.35	3 (20%)
18	MAN	G	2767	18	11,11,12	0.63	0	15,15,17	1.41	2 (13%)
18	MAN	G	2769	18	11,11,12	0.49	0	15,15,17	1.06	2 (13%)
18	MAN	G	2769(A)	18	11,11,12	0.57	0	15,15,17	1.13	2 (13%)
18	NAG	G	2931	18,4	14,14,15	0.27	0	15,19,21	0.44	0
18	NAG	G	2932	18	14,14,15	0.56	0	15,19,21	1.26	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	BMA	G	2933	18	11,11,12	0.60	0	15,15,17	1.39	2 (13%)
18	MAN	G	2934	18	11,11,12	1.38	3 (27%)	15,15,17	1.33	2 (13%)
18	MAN	G	2935	18	11,11,12	1.18	2 (18%)	15,15,17	1.53	3 (20%)
18	MAN	G	2936	18	11,11,12	0.70	0	15,15,17	1.03	2 (13%)
18	MAN	G	2937	18	11,11,12	0.64	0	15,15,17	1.00	2 (13%)
18	MAN	G	2938	18	11,11,12	0.69	0	15,15,17	1.23	3 (20%)
18	MAN	G	2939(A)	18	11,11,12	0.64	0	15,15,17	0.88	1 (6%)
16	NAG	G	3011	4,16	14,14,15	0.48	0	15,19,21	0.61	0
16	NAG	G	3012	16	14,14,15	0.38	0	15,19,21	0.62	0
16	BMA	G	3013	16	11,11,12	1.07	2 (18%)	15,15,17	1.14	1 (6%)
16	MAN	G	3014	16	11,11,12	0.72	1 (9%)	15,15,17	1.24	2 (13%)
16	MAN	G	3015	16	11,11,12	0.81	1 (9%)	15,15,17	1.31	2 (13%)
16	MAN	G	3018	16	11,11,12	0.75	0	15,15,17	0.93	1 (6%)
15	NAG	G	3321	15,4	14,14,15	0.49	0	15,19,21	0.33	0
15	NAG	G	3322	15	14,14,15	0.26	0	15,19,21	0.63	0
15	BMA	G	3323	15	11,11,12	1.19	2 (18%)	15,15,17	1.41	2 (13%)
15	MAN	G	3324	15	11,11,12	0.77	1 (9%)	15,15,17	1.39	2 (13%)
15	MAN	G	3325	15	11,11,12	0.62	0	15,15,17	1.08	2 (13%)
15	MAN	G	3326	15	11,11,12	0.84	0	15,15,17	1.36	3 (20%)
15	MAN	G	3327	15	11,11,12	0.81	1 (9%)	15,15,17	1.14	1 (6%)
15	MAN	G	3328	15	11,11,12	0.75	0	15,15,17	0.88	1 (6%)
15	MAN	G	3329	15	11,11,12	0.99	1 (9%)	15,15,17	1.60	4 (26%)
15	MAN	G	3329(A)	15	11,11,12	0.77	0	15,15,17	1.02	2 (13%)
17	NAG	G	3441	4,17	14,14,15	0.28	0	15,19,21	0.35	0
17	NAG	G	3442	17	14,14,15	0.19	0	15,19,21	0.31	0
17	BMA	G	3443	17	11,11,12	0.93	1 (9%)	15,15,17	0.87	1 (6%)
17	MAN	G	3444	17	11,11,12	0.60	0	15,15,17	0.97	2 (13%)
17	MAN	G	3445	17	11,11,12	0.69	0	15,15,17	1.06	2 (13%)
17	MAN	G	3447	17	11,11,12	1.04	1 (9%)	15,15,17	1.67	2 (13%)
17	MAN	G	3449(A)	17	11,11,12	0.62	0	15,15,17	1.15	2 (13%)
10	NAG	G	3551	10,4	14,14,15	0.26	0	15,19,21	0.38	0
10	NAG	G	3552	10	14,14,15	0.22	0	15,19,21	0.33	0
10	BMA	G	3553	10	11,11,12	0.54	0	15,15,17	0.98	1 (6%)
18	NAG	G	3861	18,4	14,14,15	0.35	0	15,19,21	0.57	0
18	NAG	G	3862	18	14,14,15	0.29	0	15,19,21	0.39	0
18	BMA	G	3863	18	11,11,12	1.07	2 (18%)	15,15,17	1.20	1 (6%)
18	MAN	G	3864	18	11,11,12	0.84	1 (9%)	15,15,17	1.20	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	MAN	G	3865	18	11,11,12	0.89	0	15,15,17	0.85	1 (6%)
18	MAN	G	3867	18	11,11,12	0.58	0	15,15,17	1.13	2 (13%)
18	MAN	G	3868	18	11,11,12	0.63	0	15,15,17	1.20	2 (13%)
18	MAN	G	3869(A)	18	11,11,12	0.61	0	15,15,17	0.96	2 (13%)
18	MAN	G	3869(B)	18	11,11,12	0.63	0	15,15,17	0.91	2 (13%)
15	NAG	G	4131	15,4	14,14,15	0.32	0	15,19,21	0.33	0
15	NAG	G	4132	15	14,14,15	0.19	0	15,19,21	0.42	0
15	BMA	G	4133	15	11,11,12	0.67	0	15,15,17	0.98	1 (6%)
15	MAN	G	4134	15	11,11,12	1.10	2 (18%)	15,15,17	1.32	2 (13%)
15	MAN	G	4135	15	11,11,12	0.83	0	15,15,17	1.64	3 (20%)
15	MAN	G	4136	15	11,11,12	0.68	0	15,15,17	1.11	2 (13%)
15	MAN	G	4137	15	11,11,12	0.74	0	15,15,17	0.89	0
15	MAN	G	4138	15	11,11,12	0.71	0	15,15,17	0.94	1 (6%)
15	MAN	G	4139(A)	15	11,11,12	0.71	0	15,15,17	1.23	2 (13%)
15	MAN	G	4140(B)	15	11,11,12	0.70	0	15,15,17	1.03	2 (13%)
17	NAG	G	4421	4,17	14,14,15	0.28	0	15,19,21	0.41	0
17	NAG	G	4422	17	14,14,15	0.25	0	15,19,21	0.60	0
17	BMA	G	4423	17	11,11,12	0.73	0	15,15,17	1.50	3 (20%)
17	MAN	G	4424	17	11,11,12	1.88	4 (36%)	15,15,17	1.40	3 (20%)
17	MAN	G	4425	17	11,11,12	0.66	0	15,15,17	1.02	2 (13%)
17	MAN	G	4426	17	11,11,12	0.94	1 (9%)	15,15,17	0.86	0
17	MAN	G	4429	17	11,11,12	0.68	1 (9%)	15,15,17	1.19	2 (13%)
9	NAG	G	4641(A)	9,4	14,14,15	0.21	0	15,19,21	0.29	0
9	NAG	G	4642(A)	9	14,14,15	0.43	0	15,19,21	0.23	0
12	NAG	G	881	12,4	14,14,15	0.35	0	15,19,21	0.64	0
12	NAG	G	882	12	14,14,15	0.35	0	15,19,21	0.37	0
12	BMA	G	883	12	11,11,12	0.67	0	15,15,17	0.85	0
12	MAN	G	884	12	11,11,12	0.84	1 (9%)	15,15,17	1.32	2 (13%)
12	MAN	G	885	12	11,11,12	1.04	0	15,15,17	1.35	2 (13%)
12	MAN	G	886	12	11,11,12	0.75	0	15,15,17	0.94	1 (6%)
12	MAN	G	887	12	11,11,12	0.96	1 (9%)	15,15,17	0.86	1 (6%)
12	MAN	G	888	12	11,11,12	0.64	0	15,15,17	1.03	1 (6%)
16	NAG	H	231	5,16	14,14,15	0.54	0	15,19,21	0.61	0
16	NAG	H	232	16	14,14,15	0.40	0	15,19,21	0.66	1 (6%)
16	BMA	H	233	16	11,11,12	1.07	1 (9%)	15,15,17	0.90	0
16	MAN	H	234	16	11,11,12	0.72	0	15,15,17	1.04	2 (13%)
16	MAN	H	235	16	11,11,12	0.73	0	15,15,17	0.86	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	MAN	H	238	16	11,11,12	0.91	1 (9%)	15,15,17	1.36	3 (20%)
16	NAG	V	721	7,16	14,14,15	0.38	0	15,19,21	0.49	0
16	NAG	V	722	16	14,14,15	0.39	0	15,19,21	0.48	0
16	BMA	V	723	16	11,11,12	0.90	1 (9%)	15,15,17	0.85	1 (6%)
16	MAN	V	724	16	11,11,12	0.64	0	15,15,17	1.07	2 (13%)
16	MAN	V	725	16	11,11,12	0.86	1 (9%)	15,15,17	1.30	2 (13%)
16	MAN	V	728	16	11,11,12	0.70	0	15,15,17	1.07	2 (13%)

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
9	NAG	B	6111	1,9	-	0/6/23/26	0/1/1/1
9	NAG	B	6112	9	-	0/6/23/26	0/1/1/1
9	NAG	B	6161	1,9	-	0/6/23/26	0/1/1/1
9	NAG	B	6162	9	-	0/6/23/26	0/1/1/1
10	NAG	B	6251	1,10	-	0/6/23/26	0/1/1/1
10	NAG	B	6252	10	-	0/6/23/26	0/1/1/1
10	BMA	B	6253	10	-	0/2/19/22	0/1/1/1
9	NAG	B	6371	1,9	-	0/6/23/26	0/1/1/1
9	NAG	B	6372	9	-	0/6/23/26	0/1/1/1
14	NAG	G	1561	4,14	-	0/6/23/26	0/1/1/1
14	NAG	G	1562	14	-	0/6/23/26	0/1/1/1
14	BMA	G	1563	14	-	0/2/19/22	0/1/1/1
14	MAN	G	1564	14	-	0/2/19/22	0/1/1/1
14	MAN	G	1565	14	-	0/2/19/22	0/1/1/1
14	MAN	G	1566	14	-	0/2/19/22	0/1/1/1
14	MAN	G	1567	14	-	0/2/19/22	0/1/1/1
14	MAN	G	1568	14	-	0/2/19/22	0/1/1/1
14	MAN	G	1569	14	-	0/2/19/22	0/1/1/1
14	MAN	G	1569(A)	14	1/1/4/5	0/2/19/22	0/1/1/1
14	MAN	G	1569(B)	14	1/1/4/5	0/2/19/22	0/1/1/1
15	NAG	G	1601	15,4	-	0/6/23/26	0/1/1/1
15	NAG	G	1602	15	-	0/6/23/26	0/1/1/1
15	BMA	G	1603	15	-	0/2/19/22	0/1/1/1
15	MAN	G	1604	15	-	0/2/19/22	0/1/1/1
15	MAN	G	1605	15	-	0/2/19/22	0/1/1/1
15	MAN	G	1606	15	-	0/2/19/22	0/1/1/1
15	MAN	G	1607	15	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	MAN	G	1608	15	-	0/2/19/22	0/1/1/1
15	MAN	G	1609	15	1/1/4/5	0/2/19/22	0/1/1/1
15	MAN	G	1609(A)	15	1/1/4/5	0/2/19/22	0/1/1/1
15	NAG	G	1881	15,4	-	0/6/23/26	0/1/1/1
15	NAG	G	1882	15	-	0/6/23/26	0/1/1/1
15	BMA	G	1883	15	-	0/2/19/22	0/1/1/1
15	MAN	G	1884	15	-	0/2/19/22	0/1/1/1
15	MAN	G	1885	15	-	0/2/19/22	0/1/1/1
15	MAN	G	1886	15	-	0/2/19/22	0/1/1/1
15	MAN	G	1887	15	-	0/2/19/22	0/1/1/1
15	MAN	G	1888	15	-	0/2/19/22	0/1/1/1
15	MAN	G	1889	15	-	0/2/19/22	0/1/1/1
15	MAN	G	1889(A)	15	-	0/2/19/22	0/1/1/1
10	NAG	G	1971	10,4	-	0/6/23/26	0/1/1/1
10	NAG	G	1972	10	-	0/6/23/26	0/1/1/1
10	BMA	G	1973	10	-	0/2/19/22	0/1/1/1
16	NAG	G	2341	4,16	-	0/6/23/26	0/1/1/1
16	NAG	G	2342	16	-	0/6/23/26	0/1/1/1
16	BMA	G	2343	16	-	0/2/19/22	0/1/1/1
16	MAN	G	2344	16	-	0/2/19/22	0/1/1/1
16	MAN	G	2345	16	-	0/2/19/22	0/1/1/1
16	MAN	G	2346	16	-	0/2/19/22	0/1/1/1
17	NAG	G	2411	4,17	-	0/6/23/26	0/1/1/1
17	NAG	G	2412	17	-	0/6/23/26	0/1/1/1
17	BMA	G	2413	17	-	0/2/19/22	0/1/1/1
17	MAN	G	2414	17	-	0/2/19/22	0/1/1/1
17	MAN	G	2415	17	-	0/2/19/22	0/1/1/1
17	MAN	G	2416	17	-	0/2/19/22	0/1/1/1
17	MAN	G	2417	17	-	0/2/19/22	0/1/1/1
14	NAG	G	2621	4,14	-	0/6/23/26	0/1/1/1
14	NAG	G	2622	14	-	0/6/23/26	0/1/1/1
14	BMA	G	2623	14	-	0/2/19/22	0/1/1/1
14	MAN	G	2624	14	-	0/2/19/22	0/1/1/1
14	MAN	G	2625	14	-	0/2/19/22	0/1/1/1
14	MAN	G	2626	14	-	0/2/19/22	0/1/1/1
14	MAN	G	2627	14	-	0/2/19/22	0/1/1/1
14	MAN	G	2628	14	-	0/2/19/22	0/1/1/1
14	MAN	G	2629	14	1/1/4/5	0/2/19/22	0/1/1/1
14	MAN	G	2629(A)	14	2/2/4/5	0/2/19/22	0/1/1/1
14	MAN	G	2629(B)	14	1/1/4/5	0/2/19/22	0/1/1/1
18	NAG	G	2761	18,4	-	0/6/23/26	0/1/1/1
18	NAG	G	2762	18	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	BMA	G	2763	18	-	0/2/19/22	0/1/1/1
18	MAN	G	2764	18	-	0/2/19/22	0/1/1/1
18	MAN	G	2765	18	-	0/2/19/22	0/1/1/1
18	MAN	G	2766	18	-	0/2/19/22	0/1/1/1
18	MAN	G	2767	18	-	0/2/19/22	0/1/1/1
18	MAN	G	2769	18	-	0/2/19/22	0/1/1/1
18	MAN	G	2769(A)	18	-	0/2/19/22	0/1/1/1
18	NAG	G	2931	18,4	-	0/6/23/26	0/1/1/1
18	NAG	G	2932	18	-	0/6/23/26	0/1/1/1
18	BMA	G	2933	18	-	0/2/19/22	0/1/1/1
18	MAN	G	2934	18	-	0/2/19/22	0/1/1/1
18	MAN	G	2935	18	-	0/2/19/22	0/1/1/1
18	MAN	G	2936	18	-	0/2/19/22	0/1/1/1
18	MAN	G	2937	18	-	0/2/19/22	0/1/1/1
18	MAN	G	2938	18	-	0/2/19/22	0/1/1/1
18	MAN	G	2939(A)	18	-	0/2/19/22	0/1/1/1
16	NAG	G	3011	4,16	-	0/6/23/26	0/1/1/1
16	NAG	G	3012	16	-	0/6/23/26	0/1/1/1
16	BMA	G	3013	16	-	0/2/19/22	0/1/1/1
16	MAN	G	3014	16	-	0/2/19/22	0/1/1/1
16	MAN	G	3015	16	-	0/2/19/22	0/1/1/1
16	MAN	G	3018	16	-	0/2/19/22	0/1/1/1
15	NAG	G	3321	15,4	-	0/6/23/26	0/1/1/1
15	NAG	G	3322	15	-	0/6/23/26	0/1/1/1
15	BMA	G	3323	15	-	0/2/19/22	0/1/1/1
15	MAN	G	3324	15	-	0/2/19/22	0/1/1/1
15	MAN	G	3325	15	-	0/2/19/22	0/1/1/1
15	MAN	G	3326	15	-	0/2/19/22	0/1/1/1
15	MAN	G	3327	15	-	0/2/19/22	0/1/1/1
15	MAN	G	3328	15	-	0/2/19/22	0/1/1/1
15	MAN	G	3329	15	-	0/2/19/22	0/1/1/1
15	MAN	G	3329(A)	15	1/1/4/5	0/2/19/22	0/1/1/1
17	NAG	G	3441	4,17	-	0/6/23/26	0/1/1/1
17	NAG	G	3442	17	-	0/6/23/26	0/1/1/1
17	BMA	G	3443	17	-	0/2/19/22	0/1/1/1
17	MAN	G	3444	17	-	0/2/19/22	0/1/1/1
17	MAN	G	3445	17	-	0/2/19/22	0/1/1/1
17	MAN	G	3447	17	-	0/2/19/22	0/1/1/1
17	MAN	G	3449(A)	17	-	0/2/19/22	0/1/1/1
10	NAG	G	3551	10,4	-	0/6/23/26	0/1/1/1
10	NAG	G	3552	10	-	0/6/23/26	0/1/1/1
10	BMA	G	3553	10	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	NAG	G	3861	18,4	-	0/6/23/26	0/1/1/1
18	NAG	G	3862	18	-	0/6/23/26	0/1/1/1
18	BMA	G	3863	18	-	0/2/19/22	0/1/1/1
18	MAN	G	3864	18	-	0/2/19/22	0/1/1/1
18	MAN	G	3865	18	-	0/2/19/22	0/1/1/1
18	MAN	G	3867	18	-	0/2/19/22	0/1/1/1
18	MAN	G	3868	18	-	0/2/19/22	0/1/1/1
18	MAN	G	3869(A)	18	1/1/4/5	0/2/19/22	0/1/1/1
18	MAN	G	3869(B)	18	1/1/4/5	0/2/19/22	0/1/1/1
15	NAG	G	4131	15,4	-	0/6/23/26	0/1/1/1
15	NAG	G	4132	15	-	0/6/23/26	0/1/1/1
15	BMA	G	4133	15	-	0/2/19/22	0/1/1/1
15	MAN	G	4134	15	-	0/2/19/22	0/1/1/1
15	MAN	G	4135	15	-	0/2/19/22	0/1/1/1
15	MAN	G	4136	15	-	0/2/19/22	0/1/1/1
15	MAN	G	4137	15	-	0/2/19/22	0/1/1/1
15	MAN	G	4138	15	-	0/2/19/22	0/1/1/1
15	MAN	G	4139(A)	15	-	0/2/19/22	0/1/1/1
15	MAN	G	4140(B)	15	-	0/2/19/22	0/1/1/1
17	NAG	G	4421	4,17	-	0/6/23/26	0/1/1/1
17	NAG	G	4422	17	-	0/6/23/26	0/1/1/1
17	BMA	G	4423	17	-	0/2/19/22	0/1/1/1
17	MAN	G	4424	17	-	0/2/19/22	0/1/1/1
17	MAN	G	4425	17	-	0/2/19/22	0/1/1/1
17	MAN	G	4426	17	-	0/2/19/22	0/1/1/1
17	MAN	G	4429	17	-	0/2/19/22	0/1/1/1
9	NAG	G	4641(A)	9,4	-	0/6/23/26	0/1/1/1
9	NAG	G	4642(A)	9	-	0/6/23/26	0/1/1/1
12	NAG	G	881	12,4	-	0/6/23/26	0/1/1/1
12	NAG	G	882	12	-	0/6/23/26	0/1/1/1
12	BMA	G	883	12	-	0/2/19/22	0/1/1/1
12	MAN	G	884	12	-	0/2/19/22	0/1/1/1
12	MAN	G	885	12	-	0/2/19/22	0/1/1/1
12	MAN	G	886	12	-	0/2/19/22	0/1/1/1
12	MAN	G	887	12	-	0/2/19/22	0/1/1/1
12	MAN	G	888	12	-	0/2/19/22	0/1/1/1
16	NAG	H	231	5,16	-	0/6/23/26	0/1/1/1
16	NAG	H	232	16	-	0/6/23/26	0/1/1/1
16	BMA	H	233	16	-	0/2/19/22	0/1/1/1
16	MAN	H	234	16	-	0/2/19/22	0/1/1/1
16	MAN	H	235	16	-	0/2/19/22	0/1/1/1
16	MAN	H	238	16	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	NAG	V	721	7,16	-	0/6/23/26	0/1/1/1
16	NAG	V	722	16	-	0/6/23/26	0/1/1/1
16	BMA	V	723	16	-	0/2/19/22	0/1/1/1
16	MAN	V	724	16	-	0/2/19/22	0/1/1/1
16	MAN	V	725	16	-	0/2/19/22	0/1/1/1
16	MAN	V	728	16	-	0/2/19/22	0/1/1/1

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	G	1971	NAG	O5-C1	-4.89	1.35	1.43
17	G	3447	MAN	O2-C2	-3.25	1.36	1.43
12	G	887	MAN	O5-C1	-2.47	1.39	1.43
12	G	884	MAN	O5-C1	-2.26	1.40	1.43
17	G	4426	MAN	O5-C1	-2.20	1.40	1.43
17	G	4424	MAN	O5-C1	-2.04	1.40	1.43
14	G	2629	MAN	O5-C1	-2.03	1.40	1.43
17	G	3443	BMA	C2-C3	2.03	1.55	1.52
16	H	233	BMA	O3-C3	2.03	1.47	1.43
17	G	4429	MAN	C1-C2	2.03	1.57	1.52
15	G	1603	BMA	C1-C2	2.09	1.57	1.52
17	G	4424	MAN	C1-C2	2.11	1.57	1.52
15	G	3327	MAN	C1-C2	2.12	1.57	1.52
18	G	2934	MAN	C1-C2	2.12	1.57	1.52
15	G	3324	MAN	C1-C2	2.13	1.57	1.52
16	G	3013	BMA	C2-C3	2.14	1.55	1.52
18	G	2934	MAN	O2-C2	2.15	1.48	1.43
16	G	3013	BMA	O3-C3	2.16	1.48	1.43
16	V	723	BMA	C1-C2	2.23	1.57	1.52
16	G	3014	MAN	C1-C2	2.25	1.57	1.52
18	G	3863	BMA	C1-C2	2.26	1.57	1.52
18	G	2935	MAN	C2-C3	2.27	1.55	1.52
9	B	6161	NAG	C1-C2	2.28	1.55	1.52
18	G	3863	BMA	C2-C3	2.30	1.55	1.52
10	G	1973	BMA	C1-C2	2.30	1.57	1.52
15	G	3323	BMA	C1-C2	2.33	1.57	1.52
15	G	1883	BMA	C1-C2	2.36	1.58	1.52
16	G	3015	MAN	C1-C2	2.38	1.58	1.52
16	V	725	MAN	C1-C2	2.39	1.58	1.52
15	G	4134	MAN	C2-C3	2.41	1.55	1.52
17	G	4424	MAN	O2-C2	2.42	1.48	1.43
18	G	3864	MAN	C1-C2	2.52	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	G	4134	MAN	C1-C2	2.58	1.58	1.52
16	H	238	MAN	C1-C2	2.68	1.58	1.52
18	G	2935	MAN	C1-C2	2.77	1.59	1.52
15	G	3323	BMA	C2-C3	2.78	1.56	1.52
15	G	3329	MAN	C1-C2	2.92	1.59	1.52
18	G	2934	MAN	C2-C3	2.95	1.56	1.52
17	G	4424	MAN	C2-C3	4.66	1.58	1.52

All (189) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	G	3447	MAN	O2-C2-C3	-4.70	100.71	110.19
14	G	2626	MAN	O2-C2-C3	-3.88	102.37	110.19
15	G	1604	MAN	O2-C2-C3	-3.69	102.75	110.19
12	G	884	MAN	O2-C2-C3	-3.59	102.95	110.19
14	G	2624	MAN	O2-C2-C3	-3.33	103.48	110.19
15	G	3326	MAN	C1-C2-C3	-3.14	105.74	109.55
15	G	1606	MAN	O2-C2-C3	-3.14	103.86	110.19
18	G	2938	MAN	O2-C2-C3	-2.93	104.29	110.19
15	G	1887	MAN	O2-C2-C3	-2.90	104.35	110.19
17	G	2414	MAN	O2-C2-C3	-2.86	104.42	110.19
15	G	3324	MAN	O2-C2-C3	-2.85	104.45	110.19
14	G	2627	MAN	O2-C2-C3	-2.58	104.99	110.19
15	G	3325	MAN	O2-C2-C3	-2.55	105.04	110.19
14	G	1567	MAN	O2-C2-C3	-2.53	105.08	110.19
18	G	3868	MAN	O2-C2-C3	-2.52	105.11	110.19
18	G	3867	MAN	O2-C2-C3	-2.50	105.14	110.19
15	G	4138	MAN	O2-C2-C3	-2.48	105.19	110.19
14	G	2627	MAN	C1-C2-C3	-2.48	106.55	109.55
15	G	1886	MAN	O2-C2-C3	-2.47	105.20	110.19
12	G	885	MAN	O2-C2-C3	-2.45	105.24	110.19
14	G	1568	MAN	O2-C2-C3	-2.45	105.25	110.19
14	G	2628	MAN	O2-C2-C3	-2.41	105.33	110.19
18	G	2937	MAN	O2-C2-C3	-2.39	105.38	110.19
17	G	4429	MAN	O2-C2-C3	-2.38	105.39	110.19
15	G	1605	MAN	O2-C2-C3	-2.37	105.42	110.19
16	V	723	BMA	O2-C2-C3	-2.36	105.44	110.19
15	G	1885	MAN	O2-C2-C3	-2.34	105.46	110.19
14	G	1569(B)	MAN	O2-C2-C3	-2.31	105.53	110.19
15	G	4140(B)	MAN	O2-C2-C3	-2.31	105.53	110.19
12	G	887	MAN	O2-C2-C3	-2.30	105.54	110.19
16	H	234	MAN	O2-C2-C3	-2.30	105.55	110.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	G	2765	MAN	O2-C2-C3	-2.30	105.56	110.19
14	G	2629(B)	MAN	O2-C2-C3	-2.30	105.56	110.19
16	V	725	MAN	O2-C2-C3	-2.30	105.56	110.19
17	G	3445	MAN	O2-C2-C3	-2.29	105.57	110.19
15	G	1609(A)	MAN	O2-C2-C3	-2.28	105.59	110.19
18	G	2935	MAN	O2-C2-C3	-2.27	105.62	110.19
15	G	1609	MAN	O2-C2-C3	-2.27	105.62	110.19
18	G	3869(B)	MAN	O2-C2-C3	-2.26	105.63	110.19
15	G	4135	MAN	O2-C2-C3	-2.26	105.64	110.19
16	G	3015	MAN	O2-C2-C3	-2.25	105.66	110.19
18	G	2936	MAN	O2-C2-C3	-2.24	105.67	110.19
15	G	3328	MAN	O2-C2-C3	-2.23	105.69	110.19
17	G	4425	MAN	O2-C2-C3	-2.23	105.70	110.19
16	V	728	MAN	O2-C2-C3	-2.22	105.71	110.19
15	G	1608	MAN	O2-C2-C3	-2.22	105.72	110.19
18	G	3864	MAN	O2-C2-C3	-2.21	105.72	110.19
12	G	886	MAN	O2-C2-C3	-2.21	105.74	110.19
16	V	724	MAN	O2-C2-C3	-2.20	105.76	110.19
16	G	2345	MAN	O2-C2-C3	-2.20	105.76	110.19
18	G	2939(A)	MAN	O2-C2-C3	-2.20	105.76	110.19
15	G	1888	MAN	O2-C2-C3	-2.19	105.77	110.19
17	G	2415	MAN	O2-C2-C3	-2.19	105.77	110.19
18	G	3869(A)	MAN	O2-C2-C3	-2.19	105.78	110.19
16	H	235	MAN	O2-C2-C3	-2.18	105.79	110.19
18	G	2766	MAN	O2-C2-C3	-2.18	105.79	110.19
16	H	238	MAN	O2-C2-C3	-2.18	105.79	110.19
15	G	1889(A)	MAN	O2-C2-C3	-2.18	105.80	110.19
17	G	3449(A)	MAN	O2-C2-C3	-2.18	105.80	110.19
14	G	2629	MAN	O2-C2-C3	-2.17	105.82	110.19
16	G	3014	MAN	O2-C2-C3	-2.15	105.86	110.19
14	G	1569(A)	MAN	O2-C2-C3	-2.13	105.89	110.19
16	G	3018	MAN	O2-C2-C3	-2.13	105.89	110.19
17	G	2417	MAN	O2-C2-C3	-2.13	105.89	110.19
15	G	3329(A)	MAN	O2-C2-C3	-2.13	105.89	110.19
14	G	2625	MAN	O2-C2-C3	-2.13	105.90	110.19
17	G	3444	MAN	O2-C2-C3	-2.12	105.91	110.19
18	G	2769(A)	MAN	O2-C2-C3	-2.11	105.92	110.19
15	G	4136	MAN	O2-C2-C3	-2.11	105.94	110.19
15	G	1883	BMA	O5-C5-C4	-2.11	106.64	110.13
17	G	4423	BMA	O2-C2-C3	-2.10	105.95	110.19
15	G	4139(A)	MAN	O2-C2-C3	-2.09	105.97	110.19
15	G	3329	MAN	O2-C2-C3	-2.09	105.98	110.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	2629(A)	MAN	O2-C2-C3	-2.09	105.98	110.19
18	G	3865	MAN	O2-C2-C3	-2.08	105.99	110.19
17	G	2416	MAN	O2-C2-C3	-2.08	106.00	110.19
18	G	2769	MAN	O2-C2-C3	-2.07	106.01	110.19
16	G	2346	MAN	O2-C2-C3	-2.06	106.03	110.19
15	G	1889	MAN	O2-C2-C3	-2.06	106.04	110.19
18	G	2767	MAN	O2-C2-C3	-2.02	106.12	110.19
18	G	2764	MAN	O2-C2-C3	-2.01	106.14	110.19
18	G	3869(B)	MAN	C1-O5-C5	2.00	115.08	112.14
15	G	1605	MAN	C1-O5-C5	2.01	115.09	112.14
14	G	1569(B)	MAN	C1-O5-C5	2.01	115.10	112.14
15	G	1888	MAN	C1-O5-C5	2.04	115.13	112.14
12	G	884	MAN	O2-C2-C1	2.04	113.32	109.23
18	G	2766	MAN	O3-C3-C2	2.04	113.75	110.01
17	G	4424	MAN	O3-C3-C2	2.06	113.78	110.01
17	G	3443	BMA	O3-C3-C2	2.09	113.84	110.01
10	G	1971	NAG	C3-C4-C5	2.10	113.98	110.23
12	G	888	MAN	C1-O5-C5	2.12	115.25	112.14
14	G	1569(A)	MAN	C1-O5-C5	2.13	115.27	112.14
17	G	2415	MAN	C1-O5-C5	2.13	115.28	112.14
15	G	3323	BMA	C1-O5-C5	2.14	115.28	112.14
14	G	1562	NAG	C1-O5-C5	2.15	115.30	112.14
16	H	232	NAG	C1-O5-C5	2.17	115.32	112.14
15	G	3329(A)	MAN	C1-O5-C5	2.17	115.33	112.14
18	G	2938	MAN	O2-C2-C1	2.17	113.58	109.23
10	G	3553	BMA	C1-O5-C5	2.17	115.33	112.14
15	G	1609	MAN	C1-O5-C5	2.17	115.33	112.14
17	G	2413	BMA	O3-C3-C4	2.17	115.26	110.36
15	G	1605	MAN	C1-C2-C3	2.18	112.19	109.55
15	G	3329	MAN	O5-C1-C2	2.19	114.41	110.89
14	G	2628	MAN	C1-O5-C5	2.20	115.38	112.14
9	B	6161	NAG	C1-O5-C5	2.23	115.42	112.14
15	G	4135	MAN	C3-C4-C5	2.23	114.20	110.23
17	G	4423	BMA	C1-O5-C5	2.23	115.42	112.14
16	H	238	MAN	C1-C2-C3	2.23	112.26	109.55
15	G	1609(A)	MAN	C1-O5-C5	2.26	115.46	112.14
16	H	234	MAN	C1-O5-C5	2.28	115.49	112.14
14	G	1564	MAN	C1-O5-C5	2.28	115.49	112.14
15	G	3329	MAN	C1-C2-C3	2.30	112.34	109.55
18	G	2933	BMA	O3-C3-C2	2.30	114.23	110.01
14	G	2626	MAN	C1-O5-C5	2.31	115.54	112.14
18	G	2932	NAG	O4-C4-C5	2.34	115.39	109.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	G	2764	MAN	C1-O5-C5	2.34	115.58	112.14
18	G	2936	MAN	C1-O5-C5	2.35	115.60	112.14
14	G	2625	MAN	C1-O5-C5	2.38	115.64	112.14
15	G	4134	MAN	C1-O5-C5	2.39	115.65	112.14
18	G	2934	MAN	C1-C2-C3	2.39	112.44	109.55
15	G	1887	MAN	C1-O5-C5	2.39	115.65	112.14
18	G	3869(A)	MAN	C1-O5-C5	2.39	115.65	112.14
16	G	2344	MAN	C1-O5-C5	2.40	115.67	112.14
18	G	2765	MAN	C1-C2-C3	2.41	112.47	109.55
14	G	1566	MAN	C1-C2-C3	2.44	112.51	109.55
14	G	2627	MAN	C1-O5-C5	2.45	115.74	112.14
15	G	4140(B)	MAN	C1-O5-C5	2.46	115.76	112.14
15	G	3326	MAN	C1-O5-C5	2.49	115.81	112.14
18	G	2937	MAN	C1-O5-C5	2.50	115.81	112.14
15	G	1889	MAN	C1-O5-C5	2.52	115.84	112.14
17	G	4425	MAN	C1-O5-C5	2.52	115.85	112.14
17	G	4424	MAN	O2-C2-C1	2.52	114.29	109.23
10	B	6252	NAG	O4-C4-C5	2.53	115.89	109.23
18	G	2938	MAN	C1-O5-C5	2.54	115.88	112.14
14	G	2624	MAN	C1-O5-C5	2.55	115.89	112.14
16	V	728	MAN	C1-O5-C5	2.55	115.90	112.14
17	G	3444	MAN	C1-O5-C5	2.56	115.91	112.14
15	G	4133	BMA	C1-O5-C5	2.57	115.92	112.14
15	G	1608	MAN	C1-O5-C5	2.60	115.97	112.14
14	G	1565	MAN	C1-C2-C3	2.61	112.72	109.55
17	G	3445	MAN	C1-O5-C5	2.62	116.00	112.14
18	G	3867	MAN	C1-O5-C5	2.67	116.06	112.14
18	G	3863	BMA	C1-O5-C5	2.67	116.07	112.14
15	G	4136	MAN	C1-O5-C5	2.68	116.09	112.14
15	G	3325	MAN	C1-O5-C5	2.71	116.13	112.14
15	G	1885	MAN	C1-O5-C5	2.75	116.19	112.14
18	G	3864	MAN	C1-O5-C5	2.76	116.20	112.14
15	G	1606	MAN	C1-O5-C5	2.77	116.21	112.14
18	G	2769	MAN	C1-O5-C5	2.84	116.32	112.14
18	G	2935	MAN	C1-O5-C5	2.86	116.34	112.14
16	V	724	MAN	C1-O5-C5	2.88	116.37	112.14
17	G	4424	MAN	C1-C2-C3	2.88	113.04	109.55
15	G	1607	MAN	C1-O5-C5	2.88	116.38	112.14
18	G	2932	NAG	C1-O5-C5	2.92	116.43	112.14
15	G	3327	MAN	C1-O5-C5	2.93	116.44	112.14
10	B	6252	NAG	C1-O5-C5	2.93	116.44	112.14
15	G	3326	MAN	O3-C3-C2	2.97	115.44	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	G	3015	MAN	C1-O5-C5	2.99	116.53	112.14
15	G	4134	MAN	C1-C2-C3	3.02	113.22	109.55
10	B	6253	BMA	C1-O5-C5	3.03	116.60	112.14
17	G	4429	MAN	C1-O5-C5	3.04	116.60	112.14
14	G	1567	MAN	C1-O5-C5	3.05	116.62	112.14
16	G	2345	MAN	C1-O5-C5	3.10	116.70	112.14
18	G	2934	MAN	O2-C2-C1	3.11	115.47	109.23
16	V	725	MAN	C1-O5-C5	3.15	116.77	112.14
18	G	2769(A)	MAN	C1-O5-C5	3.18	116.81	112.14
15	G	1886	MAN	C1-O5-C5	3.19	116.83	112.14
18	G	3868	MAN	C1-O5-C5	3.19	116.84	112.14
15	G	3323	BMA	C1-C2-C3	3.20	113.42	109.55
16	H	238	MAN	C1-O5-C5	3.24	116.90	112.14
16	G	2343	BMA	C1-C2-C3	3.26	113.50	109.55
16	G	3014	MAN	C1-O5-C5	3.31	117.00	112.14
17	G	3449(A)	MAN	C1-O5-C5	3.31	117.01	112.14
18	G	2766	MAN	C1-O5-C5	3.34	117.06	112.14
12	G	885	MAN	C1-C2-C3	3.35	113.61	109.55
16	G	3013	BMA	O3-C3-C2	3.37	116.18	110.01
14	G	1565	MAN	O3-C3-C2	3.49	116.40	110.01
17	G	4423	BMA	C1-C2-C3	3.53	113.83	109.55
14	G	1563	BMA	C1-O5-C5	3.57	117.39	112.14
15	G	4139(A)	MAN	C1-O5-C5	3.69	117.57	112.14
15	G	1884	MAN	O2-C2-C1	3.71	116.66	109.23
17	G	3447	MAN	O2-C2-C1	3.72	116.68	109.23
14	G	1566	MAN	C1-O5-C5	3.75	117.65	112.14
15	G	3324	MAN	C1-O5-C5	3.94	117.93	112.14
18	G	2767	MAN	C1-O5-C5	3.97	117.98	112.14
18	G	2935	MAN	C1-C2-C3	4.08	114.49	109.55
15	G	3329	MAN	C1-O5-C5	4.28	118.44	112.14
18	G	2933	BMA	C1-O5-C5	4.31	118.47	112.14
15	G	4135	MAN	C1-O5-C5	4.43	118.66	112.14

All (11) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	G	3869(B)	MAN	C1
14	G	1569(B)	MAN	C1
14	G	2629	MAN	C1
14	G	2629(B)	MAN	C1
14	G	1569(A)	MAN	C1
15	G	1609(A)	MAN	C1

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Mol	Chain	Res	Type	Atom
18	G	3869(A)	MAN	C1
15	G	1609	MAN	C1
14	G	2629(A)	MAN	C1
14	G	2629(A)	MAN	C1
15	G	3329(A)	MAN	C1

There are no torsion outliers.

There are no ring outliers.

18 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	6161	NAG	1	0
9	B	6162	NAG	1	0
14	G	1565	MAN	1	0
14	G	1566	MAN	1	0
14	G	1568	MAN	1	0
14	G	1569	MAN	1	0
15	G	1606	MAN	0	1
15	G	1607	MAN	0	1
15	G	1883	BMA	4	0
15	G	1884	MAN	4	0
16	G	2343	BMA	6	0
16	G	2344	MAN	6	0
14	G	2623	BMA	2	0
17	G	3445	MAN	4	0
17	G	3447	MAN	4	0
15	G	4132	NAG	1	0
12	G	884	MAN	1	0
12	G	886	MAN	1	0

5.6 Ligand geometry (i)

8 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	$\#\|Z\|>2$
8	CIT	B	1666	-	3,12,12	1.09	0	3,17,17	1.71	1 (33%)
11	EDO	D	1225	-	3,3,3	0.46	0	2,2,2	0.43	0
13	NAG	G	1331	4	14,14,15	0.36	0	15,19,21	0.27	0
13	NAG	G	1421	4	14,14,15	0.24	0	15,19,21	0.35	0
8	CIT	G	1511	-	3,12,12	1.15	0	3,17,17	1.18	0
11	EDO	G	1512	-	3,3,3	0.46	0	2,2,2	0.37	0
8	CIT	G	1513	-	3,12,12	1.21	0	3,17,17	1.17	0
13	NAG	G	3921	4	14,14,15	0.33	0	15,19,21	0.42	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
8	CIT	B	1666	-	-	0/6/16/16	0/0/0/0
11	EDO	D	1225	-	-	0/1/1/1	0/0/0/0
13	NAG	G	1331	4	-	0/6/23/26	0/1/1/1
13	NAG	G	1421	4	-	0/6/23/26	0/1/1/1
8	CIT	G	1511	-	-	0/6/16/16	0/0/0/0
11	EDO	G	1512	-	-	0/1/1/1	0/0/0/0
8	CIT	G	1513	-	-	0/6/16/16	0/0/0/0
13	NAG	G	3921	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	1666	CIT	C3-C4-C5	-2.86	110.48	114.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	1666	CIT	1	0
13	G	1331	NAG	1	0
8	G	1513	CIT	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	B	154/161 (95%)	0.15	1 (0%) 90 81	24, 57, 163, 187	0
2	D	243/243 (100%)	0.71	40 (16%) 2 1	54, 108, 222, 242	0
3	E	213/216 (98%)	0.50	19 (8%) 12 4	70, 134, 195, 262	0
4	G	479/484 (98%)	0.18	20 (4%) 40 19	25, 86, 171, 260	0
5	H	228/244 (93%)	0.47	12 (5%) 30 12	88, 140, 189, 225	0
6	L	210/213 (98%)	0.27	9 (4%) 39 18	82, 137, 183, 216	0
7	U	119/240 (49%)	0.35	7 (5%) 26 10	84, 130, 179, 215	0
7	V	98/240 (40%)	0.74	15 (15%) 3 1	112, 158, 225, 247	0
All	All	1744/2041 (85%)	0.38	123 (7%) 19 7	24, 118, 195, 262	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	209	THR	9.7
2	D	184	VAL	8.5
7	V	9	GLY	7.1
2	D	222	VAL	6.9
3	E	185	TRP	6.8
2	D	223	LEU	6.7
2	D	219	GLY	6.7
2	D	137	ALA	6.6
5	H	126	SER	6.5
2	D	210	ARG	6.5
2	D	119	PRO	6.0
5	H	189	THR	5.9
7	V	3	VAL	5.9
4	G	138(C)	SER	5.7
4	G	140	THR	5.4
6	L	148	ALA	5.3

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Mol	Chain	Res	Type	RSRZ
3	E	143	ALA	5.3
3	E	207	ALA	5.1
4	G	138(E)	ASN	4.9
5	H	138	CYS	4.8
4	G	138(A)	THR	4.8
2	D	138	LEU	4.8
2	D	218	LYS	4.5
5	H	191	THR	4.5
3	E	133	VAL	4.4
2	D	194	TYR	4.3
2	D	131	THR	4.2
7	V	8	PRO	4.1
7	V	106	VAL	4.0
2	D	208	ASP	4.0
2	D	127	SER	3.9
2	D	207	VAL	3.9
7	V	17	GLU	3.9
2	D	224	PHE	3.8
4	G	144	THR	3.8
7	U	40	ALA	3.8
5	H	210	GLU	3.8
6	L	79	GLU	3.7
2	D	221	GLU	3.7
4	G	138(F)	GLY	3.6
7	V	103	LYS	3.6
1	B	561	ALA	3.5
7	V	104	VAL	3.5
2	D	133	GLY	3.5
2	D	185	PRO	3.5
2	D	217	ASP	3.5
4	G	138(D)	THR	3.5
2	D	124	LEU	3.4
3	E	189	ARG	3.4
5	H	188	GLY	3.3
3	E	148	TRP	3.3
2	D	216	CYS	3.3
6	L	119	PHE	3.3
3	E	210	GLU	3.3
5	H	9	PRO	3.2
3	E	188	HIS	3.2
4	G	31	ALA	3.2
4	G	65	SER	3.1

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Mol	Chain	Res	Type	RSRZ
2	D	135	THR	3.1
7	V	45	ARG	3.1
6	L	6	ALA	3.1
2	D	139	GLY	3.1
7	V	19	ALA	3.0
4	G	464	THR	3.0
2	D	212	GLU	3.0
3	E	208	PRO	3.0
5	H	36	TRP	3.0
2	D	121	VAL	3.0
4	G	397	PHE	2.9
2	D	191	THR	2.8
4	G	150	TYR	2.8
2	D	166	PHE	2.8
2	D	180	SER	2.8
5	H	71	LEU	2.8
7	U	18	MET	2.8
4	G	141	ASN	2.8
7	V	86	TYR	2.8
7	V	87	TYR	2.8
3	E	156	LYS	2.7
2	D	128	SER	2.7
2	D	220	LEU	2.7
7	U	109	VAL	2.7
3	E	178	LEU	2.6
5	H	92	CYS	2.6
4	G	510	ARG	2.6
2	D	214	LYS	2.6
6	L	80	ALA	2.6
2	D	215	SER	2.5
3	E	147	ALA	2.4
2	D	132	SER	2.4
4	G	149	ASP	2.4
3	E	154	PRO	2.4
3	E	131	THR	2.4
3	E	180	LEU	2.4
5	H	178	SER	2.4
2	D	125	ALA	2.4
3	E	128	ASN	2.3
4	G	143	SER	2.3
4	G	407	SER	2.3
6	L	198	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
6	L	62	PHE	2.3
7	U	82(A)	ARG	2.3
2	D	183	THR	2.2
4	G	393	THR	2.2
3	E	144	VAL	2.2
6	L	7	PRO	2.2
2	D	213	PRO	2.2
7	V	102	THR	2.2
6	L	131	ALA	2.2
5	H	100(A)	ILE	2.2
2	D	126	PRO	2.1
7	U	37	ILE	2.1
7	U	8	GLY	2.1
2	D	179	SER	2.1
7	V	21	ILE	2.1
7	V	73	LEU	2.1
2	D	211	VAL	2.1
3	E	193	CYS	2.0
4	G	398	ASN	2.0
4	G	462	ASN	2.0
7	U	98	CYS	2.0
7	V	10	THR	2.0
2	D	181	VAL	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)

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
10	NAG	B	6251	14/15	0.78	0.51	5.95	148,159,164,166	0
10	NAG	B	6252	14/15	0.79	0.35	2.16	146,159,167,179	0
15	NAG	G	3321	14/15	0.92	0.24	0.07	56,80,89,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
15	NAG	G	1601	14/15	0.85	0.24	-0.03	120,140,157,171	0
12	NAG	G	881	14/15	0.96	0.21	-0.18	11,43,63,82	0
9	NAG	B	6111	14/15	0.72	0.37	-0.25	107,130,146,147	0
10	NAG	G	1971	14/15	0.86	0.22	-0.35	90,112,117,127	0
18	NAG	G	2761	14/15	0.92	0.20	-0.42	86,106,119,126	0
15	MAN	G	3324	11/12	0.87	0.20	-0.60	77,81,93,94	0
14	NAG	G	2621	14/15	0.97	0.19	-0.72	20,38,69,70	0
15	MAN	G	3326	11/12	0.90	0.16	-0.75	66,68,86,98	0
18	NAG	G	3861	14/15	0.90	0.19	-0.84	75,97,107,111	0
14	NAG	G	1561	14/15	0.89	0.20	-0.89	66,82,119,126	0
12	BMA	G	883	11/12	0.93	0.15	-0.96	71,89,112,125	0
15	NAG	G	3322	14/15	0.84	0.23	-1.03	79,87,90,90	0
17	NAG	G	3441	14/15	0.88	0.20	-1.06	110,138,156,158	0
14	NAG	G	2622	14/15	0.93	0.17	-1.07	46,55,63,69	0
12	NAG	G	882	14/15	0.93	0.19	-1.13	43,53,61,72	0
9	NAG	B	6112	14/15	0.86	0.16	-1.73	125,153,161,166	0
14	MAN	G	2626	11/12	0.92	0.16	-2.32	98,107,107,108	0
14	BMA	G	1563	11/12	0.63	0.28	-	168,183,193,196	0
14	MAN	G	2624	11/12	0.93	0.12	-	86,92,95,104	0
15	MAN	G	4139(A)	11/12	0.49	0.42	-	178,182,188,191	0
18	MAN	G	2934	11/12	0.84	0.12	-	174,179,184,184	0
18	BMA	G	3863	11/12	0.64	0.32	-	163,172,179,184	0
14	MAN	G	2627	11/12	0.84	0.16	-	119,130,135,146	0
18	MAN	G	3869(B)	11/12	0.90	0.24	-	183,186,187,188	0
14	MAN	G	1569(B)	11/12	0.81	0.36	-	200,204,206,206	0
16	NAG	G	2342	14/15	0.84	0.23	-	170,176,182,182	0
9	NAG	B	6162	14/15	0.68	0.28	-	167,180,189,191	0
17	MAN	G	4425	11/12	0.75	0.21	-	168,181,192,194	0
16	BMA	G	3013	11/12	0.55	0.33	-	153,164,169,172	0
9	NAG	B	6372	14/15	0.75	0.28	-	135,140,148,149	0
16	NAG	V	721	14/15	0.62	0.42	-	196,213,219,221	0
16	BMA	G	2343	11/12	0.71	0.14	-	171,174,183,192	0
18	MAN	G	2767	11/12	0.81	0.14	-	143,145,146,146	0
10	NAG	G	1972	14/15	0.85	0.24	-	124,133,139,140	0
15	MAN	G	3329	11/12	0.89	0.21	-	113,136,141,149	0
14	MAN	G	2629	11/12	0.91	0.17	-	95,109,116,120	0
18	MAN	G	2764	11/12	0.90	0.16	-	124,132,134,137	0
17	MAN	G	2414	11/12	0.69	0.23	-	137,150,167,174	0
15	MAN	G	1889(A)	11/12	0.18	0.43	-	193,195,196,197	0
18	BMA	G	2763	11/12	0.74	0.21	-	120,131,143,151	0
14	BMA	G	2623	11/12	0.92	0.14	-	66,70,80,83	0
14	MAN	G	2629(B)	11/12	0.77	0.31	-	151,154,157,157	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
16	MAN	G	3018	11/12	0.69	0.29	-	152,158,167,169	0
10	BMA	G	1973	11/12	0.85	0.17	-	118,122,134,138	0
17	NAG	G	4422	14/15	0.72	0.25	-	158,176,183,189	0
15	MAN	G	1886	11/12	0.53	0.30	-	163,175,181,187	0
14	MAN	G	1568	11/12	0.76	0.29	-	199,203,206,206	0
18	NAG	G	2762	14/15	0.85	0.18	-	92,131,140,142	0
17	MAN	G	2417	11/12	0.65	0.54	-	186,191,194,194	0
18	MAN	G	3864	11/12	0.74	0.43	-	162,167,171,172	0
17	MAN	G	3447	11/12	0.38	0.47	-	171,184,195,195	0
16	MAN	G	2346	11/12	0.84	0.13	-	148,150,152,152	0
14	MAN	G	1569(A)	11/12	0.52	0.32	-	204,207,212,212	0
18	MAN	G	3865	11/12	0.55	0.21	-	186,192,207,209	0
18	MAN	G	2938	11/12	0.53	0.39	-	190,196,202,203	0
17	MAN	G	3445	11/12	0.75	0.31	-	183,185,188,188	0
17	MAN	G	2415	11/12	0.45	0.42	-	172,177,182,186	0
16	MAN	H	238	11/12	0.60	0.49	-	188,191,199,201	0
17	MAN	G	4426	11/12	0.69	0.21	-	191,193,199,202	0
16	MAN	G	2345	11/12	0.76	0.39	-	201,225,228,228	0
15	NAG	G	1881	14/15	0.82	0.27	-	141,156,167,179	0
18	NAG	G	2932	14/15	0.89	0.15	-	123,137,149,156	0
9	NAG	G	4641(A)	14/15	0.73	0.34	-	149,174,185,196	0
16	NAG	G	3011	14/15	0.92	0.14	-	76,100,120,125	0
14	MAN	G	2628	11/12	0.89	0.24	-	121,125,139,146	0
18	MAN	G	3868	11/12	0.88	0.19	-	175,183,185,187	0
16	BMA	H	233	11/12	0.55	0.25	-	183,185,188,190	0
17	NAG	G	3442	14/15	0.82	0.17	-	150,157,171,172	0
16	NAG	G	3012	14/15	0.80	0.20	-	128,139,142,147	0
14	MAN	G	1564	11/12	0.51	0.32	-	182,184,187,188	0
18	MAN	G	2765	11/12	0.66	0.19	-	127,130,142,150	0
15	NAG	G	4131	14/15	0.89	0.21	-	53,73,96,99	0
16	MAN	V	728	11/12	0.69	0.32	-	181,186,191,193	0
15	MAN	G	1609(A)	11/12	0.74	0.16	-	167,173,175,178	0
18	MAN	G	2935	11/12	0.62	0.22	-	181,192,203,205	0
12	MAN	G	887	11/12	0.80	0.22	-	137,142,146,147	0
16	MAN	G	3015	11/12	0.70	0.20	-	160,172,174,174	0
15	NAG	G	1882	14/15	0.68	0.23	-	188,198,201,202	0
12	MAN	G	885	11/12	0.77	0.18	-	119,126,161,163	0
17	NAG	G	4421	14/15	0.89	0.26	-	115,130,148,154	0
16	NAG	G	2341	14/15	0.81	0.24	-	119,147,158,167	0
15	MAN	G	4138	11/12	0.37	0.22	-	202,207,213,215	0
10	NAG	G	3551	14/15	0.59	0.23	-	147,167,177,188	0
16	NAG	H	232	14/15	0.70	0.35	-	170,185,192,193	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
12	MAN	G	884	11/12	0.89	0.18	-	77,91,104,109	0
16	BMA	V	723	11/12	0.10	0.29	-	199,204,233,235	0
17	NAG	G	2412	14/15	0.91	0.18	-	105,120,131,135	0
16	MAN	H	234	11/12	0.42	0.63	-	189,191,193,193	0
16	MAN	H	235	11/12	0.53	0.31	-	190,191,198,201	0
16	MAN	V	724	11/12	0.60	0.20	-	204,211,214,220	0
9	NAG	B	6161	14/15	0.84	0.19	-	111,139,152,165	0
18	MAN	G	2937	11/12	0.62	0.21	-	168,174,177,178	0
17	MAN	G	3444	11/12	0.69	0.36	-	189,194,196,196	0
17	BMA	G	4423	11/12	0.57	0.18	-	181,183,193,196	0
18	MAN	G	2766	11/12	0.85	0.19	-	137,139,143,144	0
15	MAN	G	4134	11/12	0.65	0.34	-	169,173,174,176	0
15	BMA	G	4133	11/12	0.61	0.19	-	147,160,172,178	0
15	MAN	G	4135	11/12	0.62	0.20	-	183,196,198,202	0
18	MAN	G	2939(A)	11/12	0.72	0.27	-	192,192,195,195	0
16	NAG	H	231	14/15	0.64	0.27	-	145,155,161,174	0
15	MAN	G	1889	11/12	0.47	0.49	-	189,191,197,198	0
15	MAN	G	4137	11/12	0.70	0.28	-	181,188,192,193	0
9	NAG	B	6371	14/15	0.89	0.14	-	92,101,115,126	0
15	MAN	G	3325	11/12	0.72	0.18	-	148,150,151,153	0
15	MAN	G	4136	11/12	0.64	0.56	-	170,173,176,176	0
14	MAN	G	2625	11/12	0.84	0.15	-	92,115,123,124	0
9	NAG	G	4642(A)	14/15	0.50	0.26	-	187,194,196,196	0
15	MAN	G	1604	11/12	0.39	0.35	-	196,205,210,215	0
15	MAN	G	1608	11/12	0.68	0.55	-	195,199,203,206	0
18	BMA	G	2933	11/12	0.68	0.15	-	163,167,178,185	0
15	BMA	G	1603	11/12	0.51	0.38	-	205,211,211,211	0
15	BMA	G	3323	11/12	0.88	0.23	-	74,108,134,144	0
15	MAN	G	3328	11/12	0.80	0.20	-	146,151,152,153	0
18	MAN	G	3869(A)	11/12	0.42	0.39	-	168,181,187,188	0
17	MAN	G	4429	11/12	0.82	0.35	-	205,211,220,220	0
17	BMA	G	2413	11/12	0.70	0.20	-	144,152,173,175	0
10	BMA	G	3553	11/12	0.38	0.46	-	186,192,199,201	0
15	NAG	G	4132	14/15	0.89	0.21	-	103,118,123,135	0
10	NAG	G	3552	14/15	0.54	0.47	-	193,201,203,204	0
15	MAN	G	4140(B)	11/12	0.55	0.24	-	163,174,195,203	0
18	NAG	G	3862	14/15	0.64	0.33	-	123,130,142,155	0
16	NAG	V	722	14/15	0.67	0.33	-	191,206,210,210	0
15	MAN	G	1609	11/12	0.65	0.30	-	196,198,205,210	0
17	NAG	G	2411	14/15	0.93	0.20	-	64,74,82,93	0
16	MAN	V	725	11/12	0.75	0.18	-	188,191,195,197	0
18	MAN	G	2769(A)	11/12	0.82	0.27	-	131,139,144,144	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
14	MAN	G	1567	11/12	0.69	0.25	-	176,189,200,200	0
16	MAN	G	2344	11/12	0.75	0.21	-	154,158,167,169	0
18	MAN	G	3867	11/12	0.78	0.23	-	184,190,194,198	0
14	MAN	G	1566	11/12	0.80	0.23	-	152,159,169,177	0
15	MAN	G	1887	11/12	0.76	0.43	-	194,200,201,202	0
14	MAN	G	1569	11/12	0.77	0.25	-	163,167,185,188	0
17	MAN	G	3449(A)	11/12	0.53	0.50	-	193,197,207,209	0
14	MAN	G	2629(A)	11/12	0.45	0.39	-	144,154,158,158	0
15	MAN	G	3329(A)	11/12	0.80	0.28	-	135,151,162,163	0
18	MAN	G	2769	11/12	0.70	0.24	-	134,138,141,147	0
15	MAN	G	1884	11/12	0.72	0.25	-	181,184,194,198	0
15	MAN	G	1605	11/12	0.65	0.27	-	201,211,212,212	0
17	MAN	G	2416	11/12	0.49	0.25	-	181,185,188,191	0
17	BMA	G	3443	11/12	0.42	0.35	-	178,187,191,192	0
14	NAG	G	1562	14/15	0.86	0.20	-	104,117,128,150	0
15	MAN	G	1606	11/12	0.73	0.34	-	213,216,217,217	0
15	NAG	G	1602	14/15	0.78	0.30	-	155,182,190,200	0
15	MAN	G	1888	11/12	0.62	0.34	-	163,173,182,184	0
15	MAN	G	1607	11/12	0.81	0.31	-	183,191,193,194	0
10	BMA	B	6253	11/12	0.36	0.46	-	189,194,199,199	0
12	MAN	G	888	11/12	0.82	0.19	-	96,105,113,118	0
18	MAN	G	2936	11/12	0.63	0.30	-	152,160,174,180	0
17	MAN	G	4424	11/12	0.72	0.21	-	200,207,210,212	0
15	MAN	G	1885	11/12	0.79	0.18	-	177,182,189,189	0
15	MAN	G	3327	11/12	0.84	0.16	-	144,151,165,167	0
12	MAN	G	886	11/12	0.88	0.15	-	113,128,134,134	0
14	MAN	G	1565	11/12	0.54	0.46	-	198,206,211,212	0
15	BMA	G	1883	11/12	0.66	0.19	-	192,197,202,203	0
16	MAN	G	3014	11/12	0.77	0.24	-	164,166,171,173	0
18	NAG	G	2931	14/15	0.92	0.16	-	67,88,96,114	0

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
8	CIT	G	1511	13/13	0.48	0.58	5.81	178,185,196,196	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
13	NAG	G	1331	14/15	0.63	0.24	0.60	114,138,145,148	0
11	EDO	G	1512	4/4	0.84	0.20	-0.01	82,84,87,90	0
8	CIT	G	1513	13/13	0.81	0.22	-0.27	113,123,129,129	0
8	CIT	B	1666	13/13	0.91	0.21	-0.66	77,93,97,101	0
11	EDO	D	1225	4/4	0.86	0.25	-	70,76,83,89	0
13	NAG	G	3921	14/15	0.67	0.55	-	144,164,170,172	0
13	NAG	G	1421	14/15	0.46	0.76	-	164,183,186,188	0

6.5 Other polymers

There are no such residues in this entry.