Full wwPDB X-ray Structure Validation Report ⓘ

Jul 28, 2016 – 02:07 PM EDT

PDB ID	:	5FYK
Title	:	Crystal Structure at 3.7 A Resolution of Fully Glycosylated HIV-1 Clade B JR-FL 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 ⓘ symbol.

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

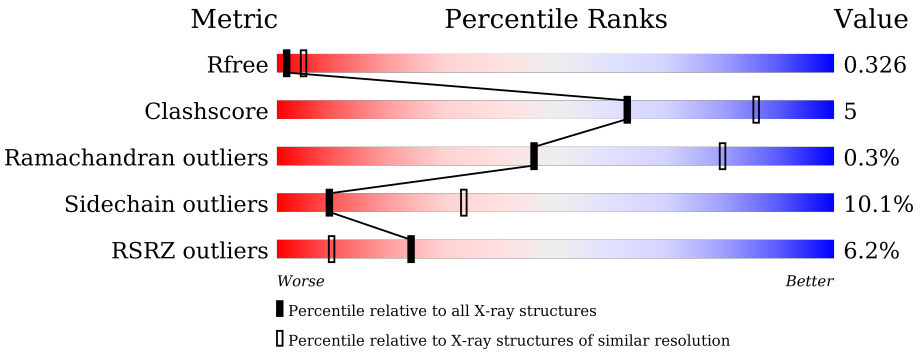
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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	2% 61% 27% 6% 6%
2	D	243	17% 90% 10%
3	E	216	20% 81% 15%
4	G	475	% 69% 23% 5%
5	H	244	% 82% 12% 7%
6	L	213	81% 16%

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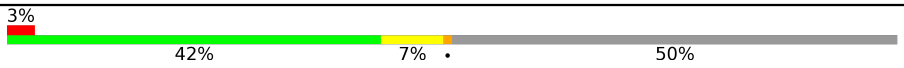
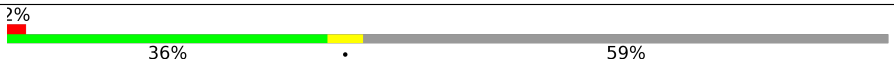
Mol	Chain	Length	Quality of chain
7	U	240	
7	V	240	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 14824 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 JR-FL, GP41 ENV ECTODOMAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	151	Total	C	N	O	S	0	0	0
			1195	753	206	228	8			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	ENGINEERED MUTATION	UNP Q6BC19
B	563	GLU	GLN	CONFLICT	UNP Q6BC19
B	605	CYS	THR	ENGINEERED MUTATION	UNP Q6BC19
B	665	GLY	-	EXPRESSION TAG	UNP Q6BC19
B	666	GLY	-	EXPRESSION TAG	UNP Q6BC19
B	667	LEU	-	EXPRESSION TAG	UNP Q6BC19
B	668	GLU	-	EXPRESSION TAG	UNP Q6BC19
B	669	VAL	-	EXPRESSION TAG	UNP Q6BC19
B	670	LEU	-	EXPRESSION TAG	UNP Q6BC19
B	671	PHE	-	EXPRESSION TAG	UNP Q6BC19
B	672	GLN	-	EXPRESSION TAG	UNP Q6BC19

- 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 JR-FL, GP120 ENV ECTODOMAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	451	Total	C	N	O	S	0	0	0
			3571	2248	627	668	28			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	168	LYS	GLU	ENGINEERED MUTATION	UNP Q75760
G	430	ILE	VAL	CONFLICT	UNP Q75760
G	459	CYS	GLY	ENGINEERED MUTATION	UNP Q75760
G	501	CYS	ALA	ENGINEERED MUTATION	UNP Q75760
G	507	GLY	-	EXPRESSION TAG	UNP Q75760
G	508	ARG	-	EXPRESSION TAG	UNP Q75760
G	509	ARG	-	EXPRESSION TAG	UNP Q75760
G	510	ARG	-	EXPRESSION TAG	UNP Q75760
G	511	ARG	-	EXPRESSION TAG	UNP Q75760
G	512	ARG	-	EXPRESSION TAG	UNP Q75760
G	513	ARG	-	EXPRESSION TAG	UNP Q75760

- 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			

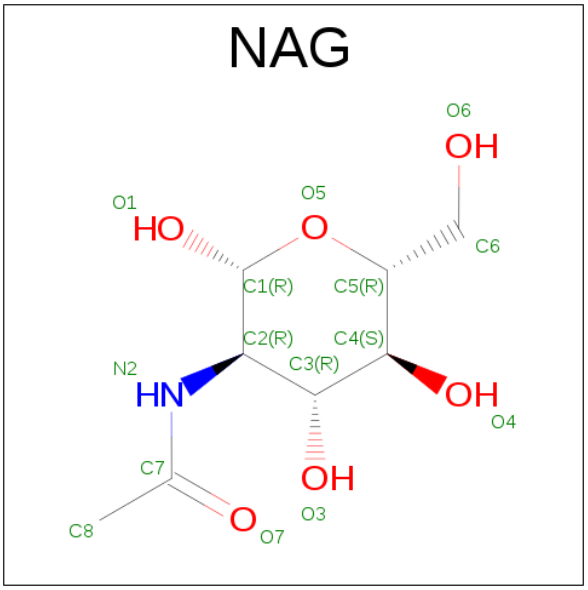
- Molecule 7 is a protein called VRC01.

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

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

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



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

- Molecule 10 is a polymer of unknown type called SUGAR (7-MER).

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

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

- Molecule 11 is a polymer of unknown type called SUGAR (9-MER).

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

- Molecule 12 is a polymer of unknown type called SUGAR (4-MER).

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

- Molecule 13 is a polymer of unknown type called SUGAR (8-MER).

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

- Molecule 14 is a polymer of unknown type called SUGAR (5-MER).

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

- 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	0	0
			116	64	2	50		

- 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	0	0
			72	40	2	30		
16	G	6	Total	C	N	O	0	0
			72	40	2	30		
16	V	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 17 is a polymer of unknown type called SUGAR (2-MER).

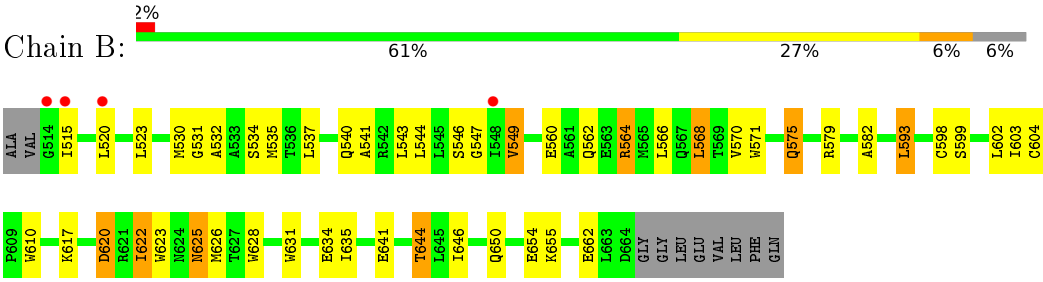
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	G	2	Total	C	N	O	0	0
			28	16	2	10		
17	G	2	Total	C	N	O	0	0
			28	16	2	10		

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.

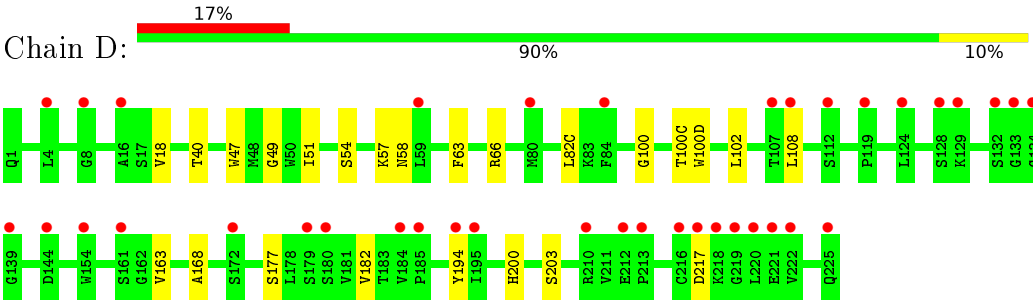
- Molecule 1: JR-FL, GP41 ENV ECTODOMAIN

Chain B:



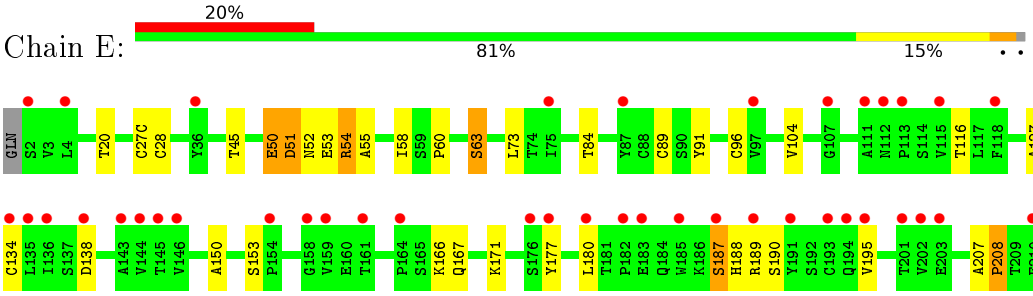
- Molecule 2: 35O22

Chain D:



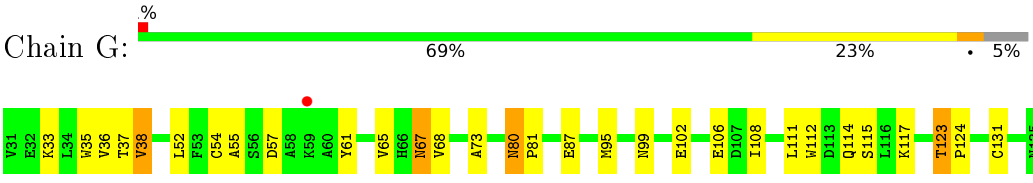
- Molecule 3: 35O22

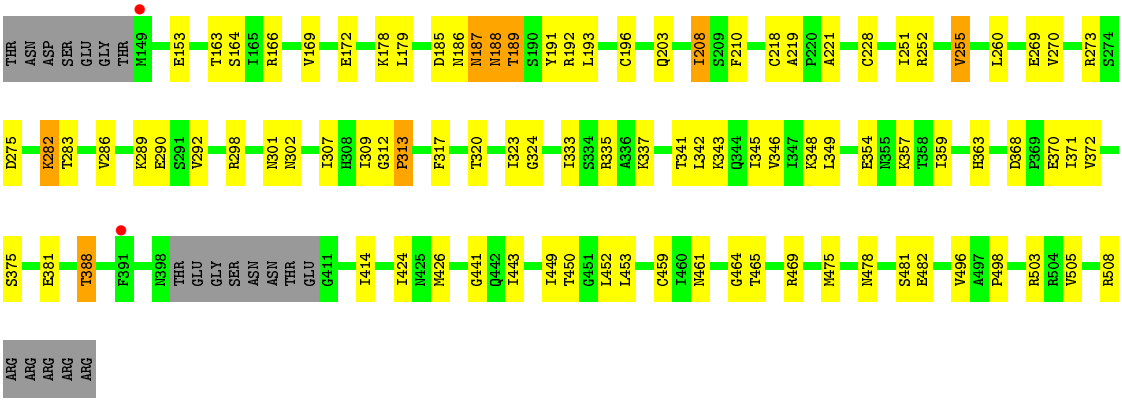
Chain E:



- Molecule 4: JR-FL, GP120 ENV ECTODOMAIN

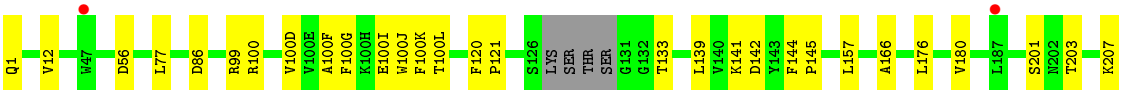
Chain G:





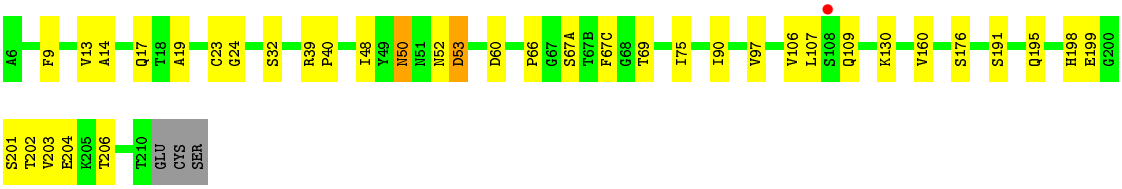
- Molecule 5: PGT122

Chain H:



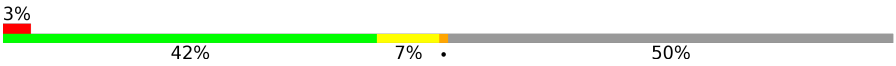
- Molecule 6: PGT122

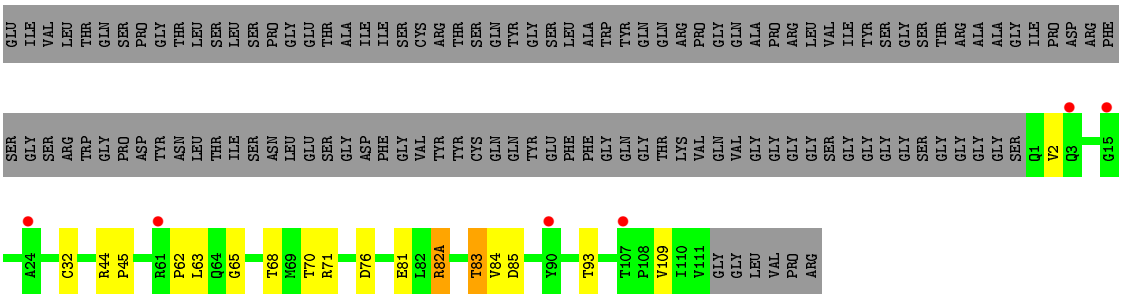
Chain L:



- Molecule 7: VRC01

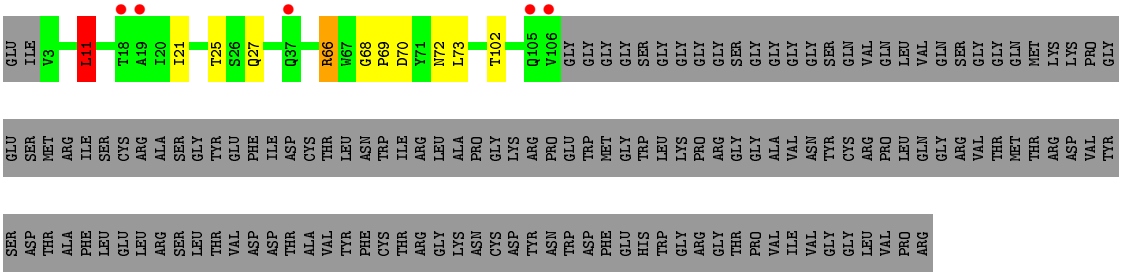
Chain U:





- Molecule 7: VRC01

Chain V:


GLU ILE V3 L11 T18 A19 I20 I21 T25 S26 Q27 Q37 R66 W67 G68 P69 D70 Y71 N72 L73 T102 Q105 V106 GLY GLY GLY GLY SER GLY GLY GLY GLY SER GLY GLY GLY GLY SER GLN VAL GLN LEU VAL GLN SER GLY GLY GLN MET LYS LYS PRO GLY
GLU SER MET ARG ILE SER CYS ARG ALA SER GLY TYR GLU PHE ILE ASP CYS THR LEU ASN TRP ILE ARG LEU ALA PRO GLY LYS ARG PRO GLU TRP MET GLY TRP LEU LYS PRO ARG GLY GLY ALA VAL ASN TYR CYS ARG PRO LEU GLN GLY 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	130.78Å 130.78Å 314.62Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.81 – 3.11 42.81 – 3.11	Depositor EDS
% Data completeness (in resolution range)	58.3 (42.81-3.11) 58.3 (42.81-3.11)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.04 (at 3.12Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.9_1692)	Depositor
R, R_{free}	0.246 , 0.303 0.265 , 0.326	Depositor DCC
R_{free} test set	1583 reflections (4.97%)	DCC
Wilson B-factor (Å^2)	93.3	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 105.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.146 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	14824	wwPDB-VP
Average B, all atoms (Å^2)	162.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% 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: 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	B	0.29	0/1215	0.50	0/1647
2	D	0.25	0/1881	0.43	0/2562
3	E	0.26	0/1658	0.48	0/2266
4	G	0.29	0/3645	0.47	0/4946
5	H	0.24	0/1789	0.47	0/2443
6	L	0.26	0/1632	0.47	0/2236
7	U	0.22	0/981	0.40	0/1328
7	V	0.31	0/778	0.57	1/1058 (0.1%)
All	All	0.27	0/13579	0.47	1/18486 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	V	11	LEU	CB-CG-CD1	5.30	120.02	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1195	0	1176	30	0
2	D	1833	0	1806	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1615	0	1541	21	0
4	G	3571	0	3513	60	0
5	H	1742	0	1715	11	0
6	L	1589	0	1530	18	0
7	U	956	0	928	6	0
7	V	758	0	719	4	0
8	B	39	0	34	0	0
9	B	42	0	39	1	0
9	G	14	0	13	0	0
9	H	14	0	13	0	0
10	D	83	0	70	2	0
10	G	332	0	280	4	0
11	G	210	0	176	1	0
12	G	100	0	86	2	0
13	G	282	0	237	3	0
14	G	61	0	52	2	0
15	G	116	0	97	1	0
16	G	144	0	122	0	0
16	V	72	0	61	0	0
17	G	56	0	50	3	0
All	All	14824	0	14258	155	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (155) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:50:GLU:HB2	3:E:53:GLU:HB2	1.60	0.83
6:L:106:VAL:HG13	6:L:109:GLN:HE21	1.49	0.76
1:B:546:SER:HA	1:B:549:VAL:HG22	1.72	0.71
1:B:617:LYS:HA	9:B:1668:NAG:H82	1.73	0.71
6:L:106:VAL:O	6:L:109:GLN:NE2	2.28	0.66
4:G:292:VAL:HG12	4:G:337:LYS:HE3	1.78	0.65
1:B:605:CYS:HA	4:G:37:THR:HG22	1.80	0.64
4:G:186:ASN:O	4:G:188:ASN:ND2	2.31	0.63
3:E:50:GLU:HB3	3:E:53:GLU:H	1.65	0.61
4:G:342:LEU:HA	4:G:345:ILE:HD12	1.82	0.60
14:G:1554:NAG:H62	14:G:1555:NAG:HN2	1.67	0.59
4:G:298:ARG:NH1	4:G:302:ASN:OD1	2.35	0.59
3:E:127:ALA:N	3:E:128:ASN:HA	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:1579:BMA:H3	10:G:1580:MAN:H5	1.84	0.59
1:B:540:GLN:O	1:B:544:LEU:HD21	2.03	0.58
5:H:100(D):VAL:N	5:H:100(I):GLU:OE1	2.36	0.58
4:G:153:GLU:HA	4:G:178:LYS:HB2	1.85	0.57
4:G:478:ASN:O	4:G:481:SER:OG	2.23	0.57
13:G:1550:MAN:H62	7:V:69:PRO:HD3	1.87	0.56
3:E:189:ARG:O	3:E:190:SER:OG	2.24	0.56
6:L:13:VAL:HG21	6:L:19:ALA:HB2	1.88	0.56
4:G:164:SER:HB3	4:G:313:PRO:HA	1.87	0.56
4:G:251:ILE:HD12	4:G:482:GLU:HB3	1.87	0.55
3:E:150:ALA:HB1	3:E:188:HIS:NE2	2.21	0.54
4:G:357:LYS:HB3	17:G:1610:NAG:H3	1.88	0.54
3:E:50:GLU:CB	3:E:53:GLU:H	2.19	0.54
1:B:575:GLN:O	1:B:579:ARG:N	2.35	0.54
6:L:198:HIS:HB3	6:L:201:SER:H	1.72	0.54
5:H:120:PHE:CE1	5:H:141:LYS:HE3	2.43	0.53
6:L:14:ALA:HB3	6:L:17:GLN:HG3	1.89	0.53
4:G:324:GLY:HA2	6:L:67(C):PHE:CD1	2.43	0.53
4:G:335:ARG:HB3	4:G:414:ILE:HG13	1.90	0.53
1:B:537:LEU:O	1:B:541:ALA:N	2.41	0.53
4:G:123:THR:HG23	4:G:124:PRO:HD3	1.91	0.53
6:L:13:VAL:O	6:L:107:LEU:N	2.42	0.52
3:E:150:ALA:HB1	3:E:188:HIS:CD2	2.44	0.52
1:B:564:ARG:HG3	1:B:568:LEU:CD2	2.41	0.51
6:L:198:HIS:N	6:L:199:GLU:HA	2.26	0.51
7:U:62:PRO:HG2	7:U:63:LEU:HD12	1.93	0.51
5:H:166:ALA:HA	5:H:176:LEU:HB3	1.92	0.51
1:B:610:TRP:CD2	4:G:498:PRO:HB3	2.46	0.51
4:G:131:CYS:N	4:G:189:THR:O	2.44	0.50
1:B:571:TRP:HD1	4:G:73:ALA:HB3	1.76	0.50
3:E:50:GLU:OE1	3:E:52:ASN:ND2	2.45	0.49
12:G:1594:MAN:O3	7:U:82(A):ARG:NH2	2.45	0.49
4:G:187:ASN:N	4:G:187:ASN:OD1	2.44	0.49
1:B:570:VAL:HG21	4:G:111:LEU:HD22	1.95	0.49
6:L:106:VAL:C	6:L:109:GLN:HE22	2.16	0.49
7:U:65:GLY:O	7:U:82(A):ARG:NH1	2.46	0.49
17:G:1617:NAG:H62	17:G:1618:NAG:C7	2.43	0.49
7:U:83:THR:HG22	7:U:84:VAL:H	1.78	0.49
1:B:650:GLN:O	1:B:654:GLU:HG2	2.13	0.48
7:U:68:THR:HB	7:U:81:GLU:HB3	1.94	0.48
4:G:164:SER:HA	4:G:312:GLY:HA3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:167:GLN:N	3:E:171:LYS:O	2.35	0.48
4:G:102:GLU:O	4:G:106:GLU:CD	2.51	0.48
7:U:44:ARG:HG2	7:U:45:PRO:HD2	1.95	0.48
17:G:1609:NAG:H62	17:G:1610:NAG:C7	2.43	0.48
4:G:33:LYS:HE2	4:G:35:TRP:CZ2	2.49	0.48
3:E:187:SER:O	3:E:189:ARG:NH1	2.47	0.47
3:E:50:GLU:N	3:E:51:ASP:HA	2.29	0.47
4:G:346:VAL:HG13	4:G:359:ILE:HD12	1.97	0.47
6:L:39:ARG:HG3	6:L:40:PRO:HD2	1.97	0.47
3:E:27(C):CYS:HA	3:E:28:CYS:HA	1.77	0.47
7:V:11:LEU:HD11	7:V:21:ILE:CD1	2.45	0.47
1:B:631:TRP:O	1:B:635:ILE:HG12	2.15	0.47
1:B:622:ILE:HG22	1:B:623:TRP:CD1	2.50	0.47
4:G:424:ILE:HD12	4:G:426:MET:HG3	1.96	0.46
6:L:195:GLN:HG2	6:L:204:GLU:HB3	1.97	0.46
2:D:18:VAL:HG12	2:D:82(C):LEU:HD11	1.97	0.46
4:G:185:ASP:OD1	4:G:186:ASN:N	2.48	0.46
4:G:95:MET:HE1	4:G:273:ARG:HD3	1.98	0.46
6:L:106:VAL:C	6:L:109:GLN:NE2	2.69	0.46
1:B:631:TRP:CE2	1:B:635:ILE:HG13	2.50	0.46
4:G:131:CYS:HB2	4:G:191:TYR:CD1	2.51	0.46
2:D:47:TRP:CZ2	2:D:49:GLY:HA2	2.50	0.46
4:G:55:ALA:HB2	4:G:218:CYS:SG	2.55	0.45
7:V:11:LEU:HD11	7:V:21:ILE:HD11	1.98	0.45
4:G:357:LYS:HB2	4:G:465:THR:HG21	1.98	0.45
7:V:66:ARG:NH1	7:V:68:GLY:HA3	2.31	0.45
5:H:100(D):VAL:HG12	5:H:100(F):ALA:H	1.82	0.45
4:G:302:ASN:HB3	4:G:320:THR:HG22	1.98	0.45
4:G:464:GLY:HA3	4:G:465:THR:HA	1.62	0.45
1:B:608:VAL:O	4:G:36:VAL:HG12	2.17	0.44
4:G:270:VAL:HG12	4:G:289:LYS:H	1.81	0.44
12:G:1533:NAG:H61	12:G:1534:NAG:N2	2.32	0.44
14:G:1556:BMA:H3	14:G:1557:MAN:H2	1.71	0.44
1:B:543:LEU:HD23	1:B:547:GLY:HA2	1.98	0.44
2:D:168:ALA:HB1	2:D:177:SER:H	1.83	0.44
1:B:531:GLY:O	1:B:534:SER:OG	2.16	0.44
1:B:532:ALA:O	1:B:535:MET:HG2	2.17	0.44
4:G:52:LEU:HD23	4:G:219:ALA:HA	1.99	0.44
4:G:67:ASN:OD1	4:G:67:ASN:N	2.51	0.44
1:B:593:LEU:HB3	1:B:599:SER:HA	2.00	0.44
3:E:190:SER:HA	3:E:208:PRO:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:54:ARG:NE	3:E:60:PRO:HA	2.33	0.44
4:G:323:ILE:HD13	13:G:1559:NAG:H61	2.00	0.43
15:G:1572:MAN:H5	5:H:100:ARG:NH2	2.32	0.43
4:G:193:LEU:HD23	4:G:193:LEU:HA	1.77	0.43
4:G:208:ILE:HD11	4:G:210:PHE:CE1	2.53	0.43
1:B:530:MET:HE3	1:B:622:ILE:HG23	1.99	0.43
1:B:625:ASN:OD1	1:B:626:MET:N	2.51	0.43
4:G:80:ASN:HA	4:G:81:PRO:HD3	1.89	0.43
4:G:324:GLY:HA2	6:L:67(C):PHE:CG	2.53	0.43
4:G:301:ASN:OD1	4:G:441:GLY:HA2	2.18	0.43
4:G:95:MET:CE	4:G:273:ARG:HD3	2.48	0.43
4:G:368:ASP:O	4:G:372:VAL:HG22	2.18	0.43
5:H:100:ARG:HG2	5:H:100(K):PHE:CZ	2.54	0.43
5:H:201:SER:HG	5:H:203:THR:HG1	1.66	0.43
11:G:1539:BMA:H61	11:G:1541:MAN:H2	1.68	0.42
5:H:121:PRO:HD3	5:H:207:LYS:HG2	2.02	0.42
6:L:66:PRO:O	6:L:67(A):SER:N	2.52	0.42
2:D:51:ILE:HG13	2:D:57:LYS:HG2	2.01	0.42
4:G:38:VAL:HB	4:G:496:VAL:HG12	2.01	0.42
3:E:20:THR:HA	3:E:73:LEU:O	2.20	0.42
6:L:23:CYS:SG	6:L:24:GLY:N	2.93	0.42
2:D:100:GLY:HA2	10:D:1229:MAN:H62	2.02	0.42
4:G:270:VAL:O	4:G:348:LYS:HE3	2.20	0.42
2:D:200:HIS:HB3	2:D:203:SER:HG	1.84	0.42
4:G:323:ILE:HD13	13:G:1559:NAG:O5	2.19	0.42
1:B:564:ARG:HG3	1:B:568:LEU:HD21	2.02	0.41
5:H:157:LEU:HD21	5:H:180:VAL:HG11	2.03	0.41
3:E:55:ALA:HB3	3:E:58:ILE:HD13	2.02	0.41
6:L:50:ASN:OD1	6:L:50:ASN:N	2.53	0.41
1:B:641:GLU:O	1:B:644:THR:HG22	2.20	0.41
1:B:544:LEU:O	4:G:221:ALA:HB1	2.21	0.41
4:G:354:GLU:C	4:G:357:LYS:H	2.24	0.41
10:G:1577:NAG:H61	10:G:1578:NAG:N2	2.36	0.41
4:G:67:ASN:HB2	4:G:208:ILE:HG22	2.02	0.41
4:G:363:HIS:HB3	4:G:388:THR:HG22	2.03	0.41
1:B:604:CYS:SG	4:G:38:VAL:HG22	2.61	0.41
4:G:67:ASN:HB2	4:G:208:ILE:HA	2.03	0.41
4:G:99:ASN:HA	4:G:102:GLU:HG2	2.02	0.41
6:L:53:ASP:N	6:L:53:ASP:OD1	2.54	0.41
1:B:564:ARG:HG3	1:B:568:LEU:HD22	2.03	0.41
1:B:530:MET:HA	1:B:628:TRP:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:275:ASP:HB3	4:G:282:LYS:HG2	2.03	0.41
10:G:1579:BMA:H3	10:G:1580:MAN:C5	2.47	0.41
1:B:582:ALA:HB1	4:G:221:ALA:HB3	2.03	0.41
1:B:606:THR:HA	4:G:503:ARG:HD2	2.03	0.41
4:G:255:VAL:HG23	4:G:475:MET:SD	2.61	0.41
4:G:114:GLN:O	4:G:117:LYS:HB2	2.21	0.40
4:G:189:THR:OG1	4:G:189:THR:O	2.39	0.40
6:L:60:ASP:N	6:L:60:ASP:OD1	2.54	0.40
10:D:1226:NAG:H82	4:G:87:GLU:HG2	2.03	0.40
5:H:144:PHE:HA	5:H:145:PRO:HA	1.88	0.40
1:B:620:ASP:OD1	1:B:620:ASP:N	2.51	0.40
2:D:100(D):TRP:HZ2	3:E:91:TYR:HB2	1.86	0.40
10:G:1580:MAN:H2	10:G:1582:MAN:H2	1.79	0.40
3:E:54:ARG:HB2	3:E:54:ARG:HH11	1.87	0.40
4:G:292:VAL:HG23	4:G:449:ILE:HB	2.02	0.40
5:H:100(D):VAL:O	5:H:100(I):GLU:HB2	2.22	0.40
3:E:207:ALA:HA	3:E:208:PRO:HD3	1.92	0.40
3:E:63:SER:O	3:E:73:LEU:HD12	2.22	0.40
3:E:84:THR:O	3:E:104:VAL:HG22	2.22	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	B	149/161 (92%)	135 (91%)	14 (9%)	0	100	100
2	D	241/243 (99%)	217 (90%)	24 (10%)	0	100	100
3	E	209/216 (97%)	188 (90%)	19 (9%)	2 (1%)	19	58
4	G	445/475 (94%)	397 (89%)	45 (10%)	3 (1%)	26	65
5	H	224/244 (92%)	202 (90%)	22 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
6	L	208/213 (98%)	191 (92%)	17 (8%)	0	100 100
7	U	117/240 (49%)	105 (90%)	12 (10%)	0	100 100
7	V	96/240 (40%)	81 (84%)	15 (16%)	0	100 100
All	All	1689/2032 (83%)	1516 (90%)	168 (10%)	5 (0%)	46 80

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	187	SER
4	G	313	PRO
4	G	188	ASN
3	E	208	PRO
4	G	65	VAL

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	127/134 (95%)	104 (82%)	23 (18%)	2 9
2	D	205/206 (100%)	192 (94%)	13 (6%)	22 58
3	E	186/189 (98%)	171 (92%)	15 (8%)	15 47
4	G	406/427 (95%)	354 (87%)	52 (13%)	5 21
5	H	198/213 (93%)	186 (94%)	12 (6%)	23 59
6	L	178/181 (98%)	161 (90%)	17 (10%)	10 37
7	U	102/192 (53%)	92 (90%)	10 (10%)	10 36
7	V	81/192 (42%)	73 (90%)	8 (10%)	10 34
All	All	1483/1734 (86%)	1333 (90%)	150 (10%)	9 33

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	515	ILE

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Mol	Chain	Res	Type
1	B	520	LEU
1	B	523	LEU
1	B	549	VAL
1	B	560	GLU
1	B	562	GLN
1	B	564	ARG
1	B	566	LEU
1	B	568	LEU
1	B	575	GLN
1	B	593	LEU
1	B	598	CYS
1	B	602	LEU
1	B	603	ILE
1	B	606	THR
1	B	620	ASP
1	B	622	ILE
1	B	625	ASN
1	B	634	GLU
1	B	644	THR
1	B	646	ILE
1	B	655	LYS
1	B	662	GLU
2	D	40	THR
2	D	54	SER
2	D	58	ASN
2	D	63	PHE
2	D	66	ARG
2	D	100(C)	THR
2	D	102	LEU
2	D	108	LEU
2	D	138	LEU
2	D	163	VAL
2	D	182	VAL
2	D	194	TYR
2	D	217	ASP
3	E	45	THR
3	E	50	GLU
3	E	51	ASP
3	E	54	ARG
3	E	63	SER
3	E	89	CYS
3	E	96	CYS

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Mol	Chain	Res	Type
3	E	116	THR
3	E	134	CYS
3	E	138	ASP
3	E	153	SER
3	E	166	LYS
3	E	177	TYR
3	E	180	LEU
3	E	195	VAL
4	G	38	VAL
4	G	54	CYS
4	G	57	ASP
4	G	61	TYR
4	G	67	ASN
4	G	68	VAL
4	G	80	ASN
4	G	108	ILE
4	G	112	TRP
4	G	115	SER
4	G	123	THR
4	G	163	THR
4	G	166	ARG
4	G	169	VAL
4	G	172	GLU
4	G	179	LEU
4	G	187	ASN
4	G	189	THR
4	G	192	ARG
4	G	196	CYS
4	G	203	GLN
4	G	208	ILE
4	G	228	CYS
4	G	252	ARG
4	G	255	VAL
4	G	260	LEU
4	G	269	GLU
4	G	282	LYS
4	G	283	THR
4	G	286	VAL
4	G	290	GLU
4	G	307	ILE
4	G	309	ILE
4	G	317	PHE

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Mol	Chain	Res	Type
4	G	333	ILE
4	G	341	THR
4	G	343	LYS
4	G	349	LEU
4	G	370	GLU
4	G	371	ILE
4	G	375	SER
4	G	381	GLU
4	G	388	THR
4	G	443	ILE
4	G	450	THR
4	G	452	LEU
4	G	453	LEU
4	G	459	CYS
4	G	461	ASN
4	G	469	ARG
4	G	505	VAL
4	G	508	ARG
5	H	1	GLN
5	H	12	VAL
5	H	56	ASP
5	H	77	LEU
5	H	86	ASP
5	H	99	ARG
5	H	100(G)	PHE
5	H	100(J)	TRP
5	H	100(L)	THR
5	H	133	THR
5	H	139	LEU
5	H	142	ASP
6	L	9	PHE
6	L	32	SER
6	L	48	ILE
6	L	50	ASN
6	L	52	ASN
6	L	53	ASP
6	L	69	THR
6	L	75	ILE
6	L	90	ILE
6	L	97	VAL
6	L	130	LYS
6	L	160	VAL

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Mol	Chain	Res	Type
6	L	176	SER
6	L	191	SER
6	L	202	THR
6	L	203	VAL
6	L	206	THR
7	U	2	VAL
7	U	32	CYS
7	U	70	THR
7	U	71	ARG
7	U	76	ASP
7	U	82(A)	ARG
7	U	83	THR
7	U	85	ASP
7	U	93	THR
7	U	109	VAL
7	V	11	LEU
7	V	25	THR
7	V	27	GLN
7	V	66	ARG
7	V	70	ASP
7	V	72	ASN
7	V	73	LEU
7	V	102	THR

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

Mol	Chain	Res	Type
4	G	188	ASN
6	L	109	GLN

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 (i)

125 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	$\#\|Z\| > 2$
8	NAG	B	1665	1,8	14,14,15	0.38	0	15,19,21	0.42	0
8	NAG	B	1666	8	14,14,15	0.41	0	15,19,21	1.17	3 (20%)
8	BMA	B	1667	8	11,11,12	1.06	1 (9%)	15,15,17	1.30	3 (20%)
10	NAG	D	1226	10,4	14,14,15	0.43	0	15,19,21	0.40	0
10	NAG	D	1227	10	14,14,15	0.29	0	15,19,21	0.30	0
10	BMA	D	1228	10	11,11,12	0.47	0	15,15,17	0.82	0
10	MAN	D	1229	10	11,11,12	0.91	1 (9%)	15,15,17	0.87	1 (6%)
10	MAN	D	1230	10	11,11,12	0.56	0	15,15,17	1.12	1 (6%)
10	MAN	D	1231	10	11,11,12	0.77	0	15,15,17	0.95	1 (6%)
10	MAN	D	1232	10	11,11,12	0.56	0	15,15,17	1.06	2 (13%)
11	NAG	G	1510	11,4	14,14,15	0.43	0	15,19,21	0.45	0
11	NAG	G	1511	11	14,14,15	0.38	0	15,19,21	0.79	1 (6%)
11	BMA	G	1512	11	11,11,12	1.08	0	15,15,17	1.20	2 (13%)
11	MAN	G	1513	11	11,11,12	0.59	0	15,15,17	1.03	2 (13%)
11	MAN	G	1514	11	11,11,12	0.91	1 (9%)	15,15,17	1.30	3 (20%)
11	MAN	G	1515	11	11,11,12	0.78	0	15,15,17	1.40	2 (13%)
11	MAN	G	1516	11	11,11,12	0.73	0	15,15,17	0.91	1 (6%)
11	MAN	G	1517	11	11,11,12	0.58	0	15,15,17	0.93	2 (13%)
11	MAN	G	1518	11	11,11,12	0.63	0	15,15,17	0.95	2 (13%)
10	NAG	G	1519	10,4	14,14,15	0.31	0	15,19,21	0.79	0
10	NAG	G	1520	10	14,14,15	0.26	0	15,19,21	0.61	0
10	BMA	G	1521	10	11,11,12	0.64	0	15,15,17	0.80	0
10	MAN	G	1522	10	11,11,12	0.87	0	15,15,17	1.62	3 (20%)
10	MAN	G	1523	10	11,11,12	0.81	0	15,15,17	0.90	1 (6%)
10	MAN	G	1524	10	11,11,12	0.69	0	15,15,17	0.91	1 (6%)
10	MAN	G	1525(A)	10	11,11,12	0.91	1 (9%)	15,15,17	1.50	2 (13%)
10	NAG	G	1526	10,4	14,14,15	0.86	1 (7%)	15,19,21	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	NAG	G	1527	10	14,14,15	0.39	0	15,19,21	0.94	1 (6%)
10	BMA	G	1528	10	11,11,12	0.49	0	15,15,17	0.95	1 (6%)
10	MAN	G	1529	10	11,11,12	0.77	0	15,15,17	1.01	2 (13%)
10	MAN	G	1530	10	11,11,12	0.66	0	15,15,17	1.14	2 (13%)
10	MAN	G	1531	10	11,11,12	0.57	0	15,15,17	1.01	2 (13%)
10	MAN	G	1532(B)	10	11,11,12	0.63	0	15,15,17	1.00	2 (13%)
12	NAG	G	1533	12,4	14,14,15	0.35	0	15,19,21	0.26	0
12	NAG	G	1534	12	14,14,15	0.17	0	15,19,21	0.40	0
12	BMA	G	1535	12	11,11,12	0.59	0	15,15,17	0.70	0
12	MAN	G	1536	12	11,11,12	0.64	0	15,15,17	0.89	1 (6%)
11	NAG	G	1537	11,4	14,14,15	0.21	0	15,19,21	0.55	0
11	NAG	G	1538	11	14,14,15	0.33	0	15,19,21	0.41	0
11	BMA	G	1539	11	11,11,12	0.60	0	15,15,17	0.71	1 (6%)
11	MAN	G	1540	11	11,11,12	0.60	0	15,15,17	1.15	1 (6%)
11	MAN	G	1541	11	11,11,12	1.04	1 (9%)	15,15,17	1.40	2 (13%)
11	MAN	G	1542	11	11,11,12	0.76	1 (9%)	15,15,17	1.36	1 (6%)
11	MAN	G	1543	11	11,11,12	0.68	0	15,15,17	0.98	2 (13%)
11	MAN	G	1544	11	11,11,12	0.68	0	15,15,17	1.02	2 (13%)
11	MAN	G	1545	11	11,11,12	0.85	1 (9%)	15,15,17	0.99	1 (6%)
13	NAG	G	1546	13,4	14,14,15	0.58	0	15,19,21	0.64	0
13	NAG	G	1547	13	14,14,15	0.19	0	15,19,21	0.80	0
13	BMA	G	1548	13	11,11,12	1.18	1 (9%)	15,15,17	1.78	3 (20%)
13	MAN	G	1549	13	11,11,12	0.71	0	15,15,17	0.95	1 (6%)
13	MAN	G	1550	13	11,11,12	1.30	2 (18%)	15,15,17	1.20	2 (13%)
13	MAN	G	1551	13	11,11,12	0.87	1 (9%)	15,15,17	1.13	1 (6%)
13	MAN	G	1552	13	11,11,12	0.62	0	15,15,17	1.26	2 (13%)
13	MAN	G	1553	13	11,11,12	0.69	0	15,15,17	0.91	1 (6%)
14	NAG	G	1554	4,14	14,14,15	0.39	0	15,19,21	0.42	0
14	NAG	G	1555	14	14,14,15	0.21	0	15,19,21	0.47	0
14	BMA	G	1556	14	11,11,12	1.36	1 (9%)	15,15,17	1.02	1 (6%)
14	MAN	G	1557	14	11,11,12	0.73	0	15,15,17	1.05	2 (13%)
14	MAN	G	1558	14	11,11,12	0.80	1 (9%)	15,15,17	1.12	2 (13%)
13	NAG	G	1559	13,4	14,14,15	0.64	1 (7%)	15,19,21	0.83	1 (6%)
13	NAG	G	1560	13	14,14,15	0.27	0	15,19,21	0.58	0
13	BMA	G	1561	13	11,11,12	0.87	1 (9%)	15,15,17	1.11	1 (6%)
13	MAN	G	1562	13	11,11,12	0.68	0	15,15,17	1.29	2 (13%)
13	MAN	G	1563	13	11,11,12	1.23	1 (9%)	15,15,17	1.11	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	MAN	G	1564	13	11,11,12	0.89	0	15,15,17	1.01	1 (6%)
13	MAN	G	1565	13	11,11,12	1.80	3 (27%)	15,15,17	1.19	3 (20%)
13	MAN	G	1566(A)	13	11,11,12	0.74	0	15,15,17	1.01	1 (6%)
15	NAG	G	1567	15,4	14,14,15	0.30	0	15,19,21	0.38	0
15	NAG	G	1568	15	14,14,15	0.20	0	15,19,21	0.62	0
15	BMA	G	1569	15	11,11,12	0.90	1 (9%)	15,15,17	0.87	0
15	MAN	G	1570	15	11,11,12	0.68	0	15,15,17	1.33	2 (13%)
15	MAN	G	1571	15	11,11,12	0.64	0	15,15,17	1.05	2 (13%)
15	MAN	G	1572	15	11,11,12	0.65	0	15,15,17	0.90	2 (13%)
15	MAN	G	1573	15	11,11,12	0.64	0	15,15,17	1.09	2 (13%)
15	MAN	G	1574	15	11,11,12	0.64	0	15,15,17	1.02	2 (13%)
15	MAN	G	1575	15	11,11,12	0.69	0	15,15,17	1.00	2 (13%)
15	MAN	G	1576(A)	15	11,11,12	0.63	0	15,15,17	0.90	1 (6%)
10	NAG	G	1577	10,4	14,14,15	0.74	1 (7%)	15,19,21	0.73	0
10	NAG	G	1578	10	14,14,15	0.17	0	15,19,21	0.28	0
10	BMA	G	1579	10	11,11,12	0.90	1 (9%)	15,15,17	1.17	1 (6%)
10	MAN	G	1580	10	11,11,12	1.32	2 (18%)	15,15,17	1.80	2 (13%)
10	MAN	G	1581	10	11,11,12	0.56	0	15,15,17	1.18	2 (13%)
10	MAN	G	1582	10	11,11,12	0.83	1 (9%)	15,15,17	1.05	2 (13%)
10	MAN	G	1583	10	11,11,12	0.68	0	15,15,17	1.10	2 (13%)
10	NAG	G	1584	10,4	14,14,15	0.23	0	15,19,21	0.27	0
10	NAG	G	1585	10	14,14,15	0.27	0	15,19,21	0.68	0
10	BMA	G	1586	10	11,11,12	0.77	0	15,15,17	0.94	0
10	MAN	G	1587	10	11,11,12	0.61	0	15,15,17	1.05	2 (13%)
10	MAN	G	1588	10	11,11,12	0.49	0	15,15,17	1.00	2 (13%)
10	MAN	G	1589	10	11,11,12	0.71	0	15,15,17	1.03	2 (13%)
10	MAN	G	1590	10	11,11,12	0.66	0	15,15,17	0.98	2 (13%)
12	NAG	G	1591	12,4	14,14,15	0.36	0	15,19,21	0.81	1 (6%)
12	NAG	G	1592	12	14,14,15	0.47	0	15,19,21	0.83	0
12	BMA	G	1593	12	11,11,12	0.98	1 (9%)	15,15,17	1.02	1 (6%)
12	MAN	G	1594	12	11,11,12	0.69	0	15,15,17	1.24	2 (13%)
13	NAG	G	1595	13,4	14,14,15	0.33	0	15,19,21	0.55	0
13	NAG	G	1596	13	14,14,15	0.56	0	15,19,21	0.68	1 (6%)
13	BMA	G	1597	13	11,11,12	0.65	0	15,15,17	0.81	0
13	MAN	G	1598	13	11,11,12	0.73	0	15,15,17	1.19	2 (13%)
13	MAN	G	1599	13	11,11,12	0.86	0	15,15,17	1.19	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	MAN	G	1600	13	11,11,12	0.64	0	15,15,17	0.89	1 (6%)
13	MAN	G	1601	13	11,11,12	0.66	0	15,15,17	1.15	2 (13%)
13	MAN	G	1602(B)	13	11,11,12	0.71	0	15,15,17	0.95	1 (6%)
16	NAG	G	1603	4,16	14,14,15	0.37	0	15,19,21	0.45	0
16	NAG	G	1604	16	14,14,15	0.42	0	15,19,21	1.44	2 (13%)
16	BMA	G	1605	16	11,11,12	0.93	0	15,15,17	1.40	1 (6%)
16	MAN	G	1606	16	11,11,12	0.81	0	15,15,17	0.94	1 (6%)
16	MAN	G	1607	16	11,11,12	0.62	0	15,15,17	1.12	2 (13%)
16	MAN	G	1608	16	11,11,12	0.67	0	15,15,17	0.91	1 (6%)
17	NAG	G	1609	4,17	14,14,15	0.24	0	15,19,21	0.35	0
17	NAG	G	1610	17	14,14,15	0.26	0	15,19,21	0.32	0
16	NAG	G	1611	4,16	14,14,15	0.29	0	15,19,21	0.33	0
16	NAG	G	1612	16	14,14,15	0.24	0	15,19,21	0.34	0
16	BMA	G	1613	16	11,11,12	0.91	0	15,15,17	1.20	2 (13%)
16	MAN	G	1614	16	11,11,12	0.69	0	15,15,17	1.42	2 (13%)
16	MAN	G	1615	16	11,11,12	1.92	4 (36%)	15,15,17	1.17	2 (13%)
16	MAN	G	1616(A)	16	11,11,12	0.66	0	15,15,17	1.08	2 (13%)
17	NAG	G	1617	4,17	14,14,15	0.73	1 (7%)	15,19,21	0.67	0
17	NAG	G	1618	17	14,14,15	0.37	0	15,19,21	0.57	0
16	NAG	V	1107	7,16	14,14,15	0.43	0	15,19,21	0.55	0
16	NAG	V	1108	16	14,14,15	0.52	0	15,19,21	1.34	2 (13%)
16	BMA	V	1109	16	11,11,12	0.53	0	15,15,17	1.28	2 (13%)
16	MAN	V	1110	16	11,11,12	0.84	0	15,15,17	1.52	2 (13%)
16	MAN	V	1111	16	11,11,12	0.93	1 (9%)	15,15,17	1.37	3 (20%)
16	MAN	V	1112	16	11,11,12	0.95	1 (9%)	15,15,17	0.83	1 (6%)

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	NAG	B	1665	1,8	-	0/6/23/26	0/1/1/1
8	NAG	B	1666	8	-	0/6/23/26	0/1/1/1
8	BMA	B	1667	8	-	0/2/19/22	0/1/1/1
10	NAG	D	1226	10,4	-	0/6/23/26	0/1/1/1
10	NAG	D	1227	10	-	0/6/23/26	0/1/1/1
10	BMA	D	1228	10	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	MAN	D	1229	10	-	0/2/19/22	0/1/1/1
10	MAN	D	1230	10	-	0/2/19/22	0/1/1/1
10	MAN	D	1231	10	-	0/2/19/22	0/1/1/1
10	MAN	D	1232	10	-	0/2/19/22	0/1/1/1
11	NAG	G	1510	11,4	-	0/6/23/26	0/1/1/1
11	NAG	G	1511	11	-	0/6/23/26	0/1/1/1
11	BMA	G	1512	11	-	0/2/19/22	0/1/1/1
11	MAN	G	1513	11	-	0/2/19/22	0/1/1/1
11	MAN	G	1514	11	-	0/2/19/22	0/1/1/1
11	MAN	G	1515	11	-	0/2/19/22	0/1/1/1
11	MAN	G	1516	11	-	0/2/19/22	0/1/1/1
11	MAN	G	1517	11	-	0/2/19/22	0/1/1/1
11	MAN	G	1518	11	-	0/2/19/22	0/1/1/1
10	NAG	G	1519	10,4	-	0/6/23/26	0/1/1/1
10	NAG	G	1520	10	-	0/6/23/26	0/1/1/1
10	BMA	G	1521	10	-	0/2/19/22	0/1/1/1
10	MAN	G	1522	10	-	0/2/19/22	0/1/1/1
10	MAN	G	1523	10	-	0/2/19/22	0/1/1/1
10	MAN	G	1524	10	-	0/2/19/22	0/1/1/1
10	MAN	G	1525(A)	10	-	0/2/19/22	0/1/1/1
10	NAG	G	1526	10,4	-	0/6/23/26	0/1/1/1
10	NAG	G	1527	10	-	0/6/23/26	0/1/1/1
10	BMA	G	1528	10	-	0/2/19/22	0/1/1/1
10	MAN	G	1529	10	-	0/2/19/22	0/1/1/1
10	MAN	G	1530	10	-	0/2/19/22	0/1/1/1
10	MAN	G	1531	10	-	0/2/19/22	0/1/1/1
10	MAN	G	1532(B)	10	-	0/2/19/22	0/1/1/1
12	NAG	G	1533	12,4	-	0/6/23/26	0/1/1/1
12	NAG	G	1534	12	-	0/6/23/26	0/1/1/1
12	BMA	G	1535	12	-	0/2/19/22	0/1/1/1
12	MAN	G	1536	12	-	0/2/19/22	0/1/1/1
11	NAG	G	1537	11,4	-	0/6/23/26	0/1/1/1
11	NAG	G	1538	11	-	0/6/23/26	0/1/1/1
11	BMA	G	1539	11	-	0/2/19/22	0/1/1/1
11	MAN	G	1540	11	-	0/2/19/22	0/1/1/1
11	MAN	G	1541	11	-	0/2/19/22	0/1/1/1
11	MAN	G	1542	11	-	0/2/19/22	0/1/1/1
11	MAN	G	1543	11	-	0/2/19/22	0/1/1/1
11	MAN	G	1544	11	-	0/2/19/22	0/1/1/1
11	MAN	G	1545	11	-	0/2/19/22	0/1/1/1
13	NAG	G	1546	13,4	-	0/6/23/26	0/1/1/1
13	NAG	G	1547	13	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	BMA	G	1548	13	-	0/2/19/22	0/1/1/1
13	MAN	G	1549	13	-	0/2/19/22	0/1/1/1
13	MAN	G	1550	13	-	0/2/19/22	0/1/1/1
13	MAN	G	1551	13	-	0/2/19/22	0/1/1/1
13	MAN	G	1552	13	-	0/2/19/22	0/1/1/1
13	MAN	G	1553	13	-	0/2/19/22	0/1/1/1
14	NAG	G	1554	4,14	-	0/6/23/26	0/1/1/1
14	NAG	G	1555	14	-	0/6/23/26	0/1/1/1
14	BMA	G	1556	14	-	0/2/19/22	0/1/1/1
14	MAN	G	1557	14	-	0/2/19/22	0/1/1/1
14	MAN	G	1558	14	-	0/2/19/22	0/1/1/1
13	NAG	G	1559	13,4	-	0/6/23/26	0/1/1/1
13	NAG	G	1560	13	-	0/6/23/26	0/1/1/1
13	BMA	G	1561	13	-	0/2/19/22	0/1/1/1
13	MAN	G	1562	13	-	0/2/19/22	0/1/1/1
13	MAN	G	1563	13	-	0/2/19/22	0/1/1/1
13	MAN	G	1564	13	-	0/2/19/22	0/1/1/1
13	MAN	G	1565	13	-	0/2/19/22	0/1/1/1
13	MAN	G	1566(A)	13	-	0/2/19/22	0/1/1/1
15	NAG	G	1567	15,4	-	0/6/23/26	0/1/1/1
15	NAG	G	1568	15	-	0/6/23/26	0/1/1/1
15	BMA	G	1569	15	-	0/2/19/22	0/1/1/1
15	MAN	G	1570	15	-	0/2/19/22	0/1/1/1
15	MAN	G	1571	15	-	0/2/19/22	0/1/1/1
15	MAN	G	1572	15	-	0/2/19/22	0/1/1/1
15	MAN	G	1573	15	-	0/2/19/22	0/1/1/1
15	MAN	G	1574	15	-	0/2/19/22	0/1/1/1
15	MAN	G	1575	15	-	0/2/19/22	0/1/1/1
15	MAN	G	1576(A)	15	-	0/2/19/22	0/1/1/1
10	NAG	G	1577	10,4	-	0/6/23/26	0/1/1/1
10	NAG	G	1578	10	-	0/6/23/26	0/1/1/1
10	BMA	G	1579	10	-	0/2/19/22	0/1/1/1
10	MAN	G	1580	10	-	0/2/19/22	0/1/1/1
10	MAN	G	1581	10	-	0/2/19/22	0/1/1/1
10	MAN	G	1582	10	-	0/2/19/22	0/1/1/1
10	MAN	G	1583	10	-	0/2/19/22	0/1/1/1
10	NAG	G	1584	10,4	-	0/6/23/26	0/1/1/1
10	NAG	G	1585	10	-	0/6/23/26	0/1/1/1
10	BMA	G	1586	10	-	0/2/19/22	0/1/1/1
10	MAN	G	1587	10	-	0/2/19/22	0/1/1/1
10	MAN	G	1588	10	-	0/2/19/22	0/1/1/1
10	MAN	G	1589	10	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	MAN	G	1590	10	-	0/2/19/22	0/1/1/1
12	NAG	G	1591	12,4	-	0/6/23/26	0/1/1/1
12	NAG	G	1592	12	-	0/6/23/26	0/1/1/1
12	BMA	G	1593	12	-	0/2/19/22	0/1/1/1
12	MAN	G	1594	12	-	0/2/19/22	0/1/1/1
13	NAG	G	1595	13,4	-	0/6/23/26	0/1/1/1
13	NAG	G	1596	13	-	0/6/23/26	0/1/1/1
13	BMA	G	1597	13	-	0/2/19/22	0/1/1/1
13	MAN	G	1598	13	-	0/2/19/22	0/1/1/1
13	MAN	G	1599	13	-	0/2/19/22	0/1/1/1
13	MAN	G	1600	13	-	0/2/19/22	0/1/1/1
13	MAN	G	1601	13	-	0/2/19/22	0/1/1/1
13	MAN	G	1602(B)	13	-	0/2/19/22	0/1/1/1
16	NAG	G	1603	4,16	-	0/6/23/26	0/1/1/1
16	NAG	G	1604	16	-	0/6/23/26	0/1/1/1
16	BMA	G	1605	16	-	0/2/19/22	0/1/1/1
16	MAN	G	1606	16	-	0/2/19/22	0/1/1/1
16	MAN	G	1607	16	-	0/2/19/22	0/1/1/1
16	MAN	G	1608	16	-	0/2/19/22	0/1/1/1
17	NAG	G	1609	4,17	-	0/6/23/26	0/1/1/1
17	NAG	G	1610	17	-	0/6/23/26	0/1/1/1
16	NAG	G	1611	4,16	-	0/6/23/26	0/1/1/1
16	NAG	G	1612	16	-	0/6/23/26	0/1/1/1
16	BMA	G	1613	16	-	0/2/19/22	0/1/1/1
16	MAN	G	1614	16	-	0/2/19/22	0/1/1/1
16	MAN	G	1615	16	-	0/2/19/22	0/1/1/1
16	MAN	G	1616(A)	16	-	0/2/19/22	0/1/1/1
17	NAG	G	1617	4,17	-	0/6/23/26	0/1/1/1
17	NAG	G	1618	17	-	0/6/23/26	0/1/1/1
16	NAG	V	1107	7,16	-	0/6/23/26	0/1/1/1
16	NAG	V	1108	16	-	0/6/23/26	0/1/1/1
16	BMA	V	1109	16	-	0/2/19/22	0/1/1/1
16	MAN	V	1110	16	-	0/2/19/22	0/1/1/1
16	MAN	V	1111	16	-	0/2/19/22	0/1/1/1
16	MAN	V	1112	16	-	0/2/19/22	0/1/1/1

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	G	1526	NAG	O5-C1	-3.13	1.38	1.43
16	G	1615	MAN	O5-C1	-2.94	1.38	1.43
10	G	1577	NAG	O5-C1	-2.60	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	1229	MAN	O5-C1	-2.43	1.39	1.43
17	G	1617	NAG	O5-C1	-2.40	1.39	1.43
15	G	1569	BMA	O5-C1	-2.36	1.39	1.43
13	G	1565	MAN	O5-C1	-2.19	1.40	1.43
13	G	1559	NAG	O5-C1	-2.19	1.40	1.43
13	G	1551	MAN	O5-C1	-2.12	1.40	1.43
11	G	1541	MAN	C2-C3	2.05	1.55	1.52
13	G	1550	MAN	O3-C3	2.05	1.47	1.43
10	G	1579	BMA	C4-C3	2.05	1.57	1.52
10	G	1582	MAN	C1-C2	2.06	1.57	1.52
16	V	1112	MAN	C1-C2	2.07	1.57	1.52
14	G	1558	MAN	C1-C2	2.13	1.57	1.52
11	G	1514	MAN	C1-C2	2.17	1.57	1.52
13	G	1561	BMA	C1-C2	2.19	1.57	1.52
11	G	1545	MAN	C1-C2	2.19	1.57	1.52
11	G	1542	MAN	C1-C2	2.21	1.57	1.52
16	G	1615	MAN	C4-C3	2.29	1.58	1.52
10	G	1525(A)	MAN	C1-C2	2.32	1.57	1.52
16	V	1111	MAN	C1-C2	2.48	1.58	1.52
10	G	1580	MAN	O5-C1	2.51	1.47	1.43
13	G	1563	MAN	C2-C3	2.58	1.56	1.52
13	G	1565	MAN	O2-C2	2.60	1.49	1.43
8	B	1667	BMA	O5-C5	2.63	1.49	1.43
12	G	1593	BMA	C1-C2	2.69	1.58	1.52
16	G	1615	MAN	O2-C2	2.86	1.49	1.43
13	G	1548	BMA	O5-C5	3.00	1.50	1.43
13	G	1550	MAN	C2-C3	3.12	1.56	1.52
10	G	1580	MAN	C1-C2	3.13	1.59	1.52
14	G	1556	BMA	C1-C2	3.31	1.60	1.52
16	G	1615	MAN	C2-C3	4.04	1.58	1.52
13	G	1565	MAN	C2-C3	4.17	1.58	1.52

All (147) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	G	1551	MAN	O2-C2-C3	-3.59	102.95	110.19
13	G	1562	MAN	O2-C2-C3	-3.23	103.68	110.19
13	G	1601	MAN	O2-C2-C3	-2.54	105.07	110.19
13	G	1548	BMA	C3-C4-C5	-2.53	105.72	110.23
10	G	1579	BMA	C1-C2-C3	-2.52	106.50	109.55
12	G	1593	BMA	O2-C2-C3	-2.48	105.20	110.19
10	G	1522	MAN	C1-C2-C3	-2.45	106.58	109.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	G	1549	MAN	O2-C2-C3	-2.45	105.26	110.19
15	G	1573	MAN	O2-C2-C3	-2.44	105.27	110.19
16	G	1613	BMA	C1-C2-C3	-2.43	106.61	109.55
16	G	1613	BMA	O2-C2-C3	-2.42	105.31	110.19
16	G	1606	MAN	O2-C2-C3	-2.37	105.41	110.19
10	G	1587	MAN	O2-C2-C3	-2.37	105.41	110.19
10	G	1531	MAN	O2-C2-C3	-2.35	105.45	110.19
14	G	1557	MAN	O2-C2-C3	-2.35	105.45	110.19
10	G	1525(A)	MAN	O2-C2-C3	-2.34	105.46	110.19
15	G	1574	MAN	O2-C2-C3	-2.34	105.47	110.19
10	G	1530	MAN	O2-C2-C3	-2.34	105.47	110.19
15	G	1570	MAN	O2-C2-C3	-2.33	105.49	110.19
10	D	1232	MAN	O2-C2-C3	-2.33	105.50	110.19
11	G	1516	MAN	O2-C2-C3	-2.32	105.50	110.19
16	G	1616(A)	MAN	O2-C2-C3	-2.29	105.56	110.19
13	G	1600	MAN	O2-C2-C3	-2.29	105.57	110.19
13	G	1566(A)	MAN	O2-C2-C3	-2.29	105.57	110.19
13	G	1552	MAN	O2-C2-C3	-2.29	105.58	110.19
10	G	1581	MAN	O2-C2-C3	-2.28	105.58	110.19
10	G	1590	MAN	O2-C2-C3	-2.28	105.58	110.19
13	G	1602(B)	MAN	O2-C2-C3	-2.27	105.61	110.19
15	G	1576(A)	MAN	O2-C2-C3	-2.27	105.62	110.19
10	G	1583	MAN	O2-C2-C3	-2.25	105.64	110.19
11	G	1513	MAN	O2-C2-C3	-2.25	105.65	110.19
11	G	1517	MAN	O2-C2-C3	-2.25	105.66	110.19
11	G	1544	MAN	O2-C2-C3	-2.25	105.66	110.19
14	G	1558	MAN	O2-C2-C3	-2.24	105.67	110.19
10	G	1529	MAN	O2-C2-C3	-2.24	105.68	110.19
16	G	1608	MAN	O2-C2-C3	-2.23	105.68	110.19
12	G	1536	MAN	O2-C2-C3	-2.23	105.69	110.19
16	V	1110	MAN	O2-C2-C3	-2.23	105.70	110.19
10	G	1532(B)	MAN	O2-C2-C3	-2.22	105.71	110.19
10	G	1524	MAN	O2-C2-C3	-2.21	105.73	110.19
13	G	1598	MAN	O2-C2-C3	-2.19	105.77	110.19
13	G	1559	NAG	O4-C4-C3	-2.19	105.42	110.36
11	G	1518	MAN	O2-C2-C3	-2.19	105.78	110.19
10	G	1582	MAN	O2-C2-C3	-2.17	105.80	110.19
15	G	1571	MAN	O2-C2-C3	-2.17	105.81	110.19
10	D	1231	MAN	O2-C2-C3	-2.17	105.81	110.19
15	G	1575	MAN	O2-C2-C3	-2.17	105.82	110.19
10	D	1229	MAN	O2-C2-C3	-2.16	105.83	110.19
16	V	1112	MAN	O2-C2-C3	-2.16	105.84	110.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	G	1545	MAN	O2-C2-C3	-2.15	105.85	110.19
13	G	1553	MAN	O2-C2-C3	-2.15	105.86	110.19
12	G	1594	MAN	O2-C2-C3	-2.13	105.90	110.19
16	V	1111	MAN	O2-C2-C3	-2.10	105.95	110.19
11	G	1543	MAN	O2-C2-C3	-2.10	105.96	110.19
16	G	1607	MAN	O2-C2-C3	-2.10	105.96	110.19
13	G	1596	NAG	O4-C4-C3	-2.09	105.64	110.36
15	G	1572	MAN	O2-C2-C3	-2.09	105.98	110.19
8	B	1667	BMA	O5-C1-C2	-2.09	107.56	110.89
10	G	1588	MAN	O2-C2-C3	-2.09	105.98	110.19
10	G	1589	MAN	O2-C2-C3	-2.08	105.99	110.19
11	G	1514	MAN	O2-C2-C3	-2.08	106.00	110.19
8	B	1667	BMA	O2-C2-C3	-2.07	106.02	110.19
13	G	1564	MAN	O2-C2-C3	-2.06	106.04	110.19
11	G	1515	MAN	O2-C2-C3	-2.04	106.08	110.19
14	G	1556	BMA	O2-C2-C3	-2.03	106.09	110.19
11	G	1539	BMA	O2-C2-C3	-2.01	106.14	110.19
15	G	1572	MAN	C1-O5-C5	2.02	115.12	112.14
11	G	1518	MAN	C1-O5-C5	2.04	115.14	112.14
11	G	1544	MAN	C1-O5-C5	2.07	115.18	112.14
13	G	1565	MAN	C2-C3-C4	2.07	114.67	111.05
16	V	1108	NAG	O4-C4-C5	2.08	114.71	109.23
11	G	1511	NAG	O4-C4-C3	2.08	115.06	110.36
10	G	1590	MAN	C1-O5-C5	2.10	115.23	112.14
13	G	1563	MAN	C1-C2-C3	2.10	112.10	109.55
13	G	1565	MAN	C1-C2-C3	2.11	112.11	109.55
11	G	1512	BMA	C1-O5-C5	2.12	115.25	112.14
12	G	1591	NAG	O4-C4-C3	2.14	115.18	110.36
16	V	1109	BMA	C1-C2-C3	2.14	112.14	109.55
10	G	1523	MAN	C1-O5-C5	2.16	115.31	112.14
11	G	1517	MAN	C1-O5-C5	2.18	115.34	112.14
14	G	1557	MAN	C1-O5-C5	2.23	115.41	112.14
16	V	1111	MAN	C1-C2-C3	2.24	112.26	109.55
16	G	1615	MAN	C2-C3-C4	2.25	114.97	111.05
10	G	1529	MAN	C1-O5-C5	2.29	115.51	112.14
13	G	1550	MAN	C1-O5-C5	2.31	115.54	112.14
15	G	1573	MAN	C1-O5-C5	2.32	115.56	112.14
8	B	1666	NAG	O4-C4-C5	2.33	115.36	109.23
10	G	1532(B)	MAN	C1-O5-C5	2.33	115.57	112.14
14	G	1558	MAN	C1-O5-C5	2.33	115.57	112.14
10	G	1528	BMA	C1-O5-C5	2.35	115.59	112.14
8	B	1666	NAG	O4-C4-C3	2.37	115.71	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	1666	NAG	C1-O5-C5	2.40	115.67	112.14
16	G	1616(A)	MAN	C1-O5-C5	2.44	115.73	112.14
10	G	1588	MAN	C1-O5-C5	2.46	115.76	112.14
10	G	1527	NAG	C3-C4-C5	2.49	114.66	110.23
10	G	1589	MAN	C1-O5-C5	2.52	115.85	112.14
11	G	1514	MAN	C1-O5-C5	2.53	115.86	112.14
10	G	1582	MAN	C1-O5-C5	2.58	115.93	112.14
15	G	1574	MAN	C1-O5-C5	2.58	115.93	112.14
11	G	1543	MAN	C1-O5-C5	2.59	115.94	112.14
15	G	1575	MAN	C1-O5-C5	2.60	115.96	112.14
15	G	1571	MAN	C1-O5-C5	2.61	115.97	112.14
13	G	1565	MAN	O2-C2-C1	2.64	114.52	109.23
16	G	1604	NAG	O4-C4-C5	2.64	116.18	109.23
11	G	1513	MAN	C1-O5-C5	2.66	116.06	112.14
10	G	1531	MAN	C1-O5-C5	2.67	116.06	112.14
13	G	1599	MAN	C1-O5-C5	2.76	116.19	112.14
10	G	1587	MAN	C1-O5-C5	2.76	116.20	112.14
13	G	1599	MAN	O3-C3-C2	2.78	115.11	110.01
10	G	1583	MAN	C1-O5-C5	2.81	116.27	112.14
13	G	1601	MAN	C1-O5-C5	2.83	116.30	112.14
16	G	1615	MAN	O2-C2-C1	2.83	114.90	109.23
13	G	1561	BMA	C1-C2-C3	2.88	113.04	109.55
11	G	1512	BMA	O3-C3-C4	2.89	116.88	110.36
11	G	1514	MAN	C1-C2-C3	2.91	113.08	109.55
10	D	1232	MAN	C1-O5-C5	2.92	116.44	112.14
10	G	1530	MAN	C1-O5-C5	2.97	116.51	112.14
16	V	1111	MAN	C1-O5-C5	3.07	116.66	112.14
10	G	1580	MAN	C1-C2-C3	3.08	113.29	109.55
10	D	1230	MAN	C1-O5-C5	3.14	116.75	112.14
11	G	1541	MAN	O3-C3-C2	3.19	115.85	110.01
16	G	1607	MAN	C1-O5-C5	3.21	116.86	112.14
13	G	1562	MAN	C1-O5-C5	3.21	116.87	112.14
13	G	1598	MAN	C1-O5-C5	3.22	116.87	112.14
16	V	1108	NAG	C1-O5-C5	3.35	117.07	112.14
11	G	1540	MAN	C1-O5-C5	3.39	117.13	112.14
16	G	1614	MAN	O3-C3-C2	3.40	116.24	110.01
16	G	1614	MAN	C1-O5-C5	3.42	117.17	112.14
10	G	1522	MAN	C1-O5-C5	3.43	117.19	112.14
10	G	1581	MAN	C1-O5-C5	3.48	117.26	112.14
13	G	1550	MAN	O3-C3-C2	3.52	116.45	110.01
16	V	1109	BMA	C1-O5-C5	3.56	117.38	112.14
8	B	1667	BMA	C1-O5-C5	3.59	117.42	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	G	1570	MAN	C1-O5-C5	3.66	117.52	112.14
13	G	1552	MAN	C1-O5-C5	3.69	117.56	112.14
11	G	1541	MAN	C1-O5-C5	3.74	117.64	112.14
12	G	1594	MAN	C1-O5-C5	3.74	117.64	112.14
13	G	1548	BMA	O3-C3-C2	3.84	117.04	110.01
16	G	1604	NAG	C1-O5-C5	3.92	117.91	112.14
10	G	1522	MAN	O3-C3-C2	4.07	117.46	110.01
16	G	1605	BMA	C1-O5-C5	4.17	118.28	112.14
11	G	1542	MAN	C1-O5-C5	4.19	118.30	112.14
13	G	1548	BMA	C1-O5-C5	4.21	118.33	112.14
11	G	1515	MAN	C1-O5-C5	4.56	118.84	112.14
10	G	1525(A)	MAN	C1-O5-C5	4.71	119.06	112.14
16	V	1110	MAN	C1-O5-C5	4.91	119.36	112.14
10	G	1580	MAN	C1-O5-C5	5.51	120.25	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

23 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	1226	NAG	1	0
10	D	1229	MAN	1	0
12	G	1533	NAG	1	0
12	G	1534	NAG	1	0
11	G	1539	BMA	1	0
11	G	1541	MAN	1	0
13	G	1550	MAN	1	0
14	G	1554	NAG	1	0
14	G	1555	NAG	1	0
14	G	1556	BMA	1	0
14	G	1557	MAN	1	0
13	G	1559	NAG	2	0
15	G	1572	MAN	1	0
10	G	1577	NAG	1	0
10	G	1578	NAG	1	0
10	G	1579	BMA	2	0
10	G	1580	MAN	3	0
10	G	1582	MAN	1	0
12	G	1594	MAN	1	0
17	G	1609	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	G	1610	NAG	2	0
17	G	1617	NAG	1	0
17	G	1618	NAG	1	0

5.6 Ligand geometry (i)

5 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	$\#\|Z\| > 2$
9	NAG	B	1668	1	14,14,15	0.42	0	15,19,21	0.54	0
9	NAG	B	1669	1	14,14,15	0.34	0	15,19,21	0.43	0
9	NAG	B	1670	1	14,14,15	0.39	0	15,19,21	0.36	0
9	NAG	G	1509	4	14,14,15	0.38	0	15,19,21	0.35	0
9	NAG	H	1212	5	14,14,15	0.25	0	15,19,21	0.31	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
9	NAG	B	1668	1	-	0/6/23/26	0/1/1/1
9	NAG	B	1669	1	-	0/6/23/26	0/1/1/1
9	NAG	B	1670	1	-	0/6/23/26	0/1/1/1
9	NAG	G	1509	4	-	0/6/23/26	0/1/1/1
9	NAG	H	1212	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	1668	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	151/161 (93%)	0.07	4 (2%) 59 35	39, 104, 223, 254	0
2	D	243/243 (100%)	0.67	42 (17%) 2 1	133, 213, 281, 315	0
3	E	213/216 (98%)	0.78	43 (20%) 1 0	131, 210, 284, 309	0
4	G	451/475 (94%)	-0.07	3 (0%) 89 78	43, 110, 187, 295	0
5	H	228/244 (93%)	-0.14	3 (1%) 79 62	105, 156, 197, 247	0
6	L	210/213 (98%)	-0.28	1 (0%) 91 83	85, 136, 179, 212	0
7	U	119/240 (49%)	-0.04	6 (5%) 32 13	130, 167, 232, 248	0
7	V	98/240 (40%)	0.08	5 (5%) 32 13	136, 204, 240, 342	0
All	All	1713/2032 (84%)	0.13	107 (6%) 24 10	39, 154, 264, 342	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	146	VAL	10.4
2	D	194	TYR	9.4
2	D	138	LEU	9.2
1	B	514	GLY	9.1
3	E	161	THR	8.3
3	E	144	VAL	7.8
2	D	195	ILE	6.9
2	D	221	GLU	6.7
7	V	18	THR	6.6
3	E	115	VAL	6.1
4	G	149	MET	6.0
3	E	159	VAL	5.8
2	D	108	LEU	5.7
5	H	187	LEU	5.5
2	D	172	SER	5.3
7	V	19	ALA	5.3

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Mol	Chain	Res	Type	RSRZ
2	D	134	GLY	5.3
3	E	180	LEU	5.2
2	D	137	ALA	5.1
3	E	118	PHE	5.0
2	D	222	VAL	5.0
3	E	164	PRO	4.9
3	E	183	GLU	4.8
3	E	176	SER	4.7
2	D	124	LEU	4.7
2	D	112	SER	4.7
2	D	219	GLY	4.6
2	D	16	ALA	4.5
3	E	189	ARG	4.5
3	E	201	THR	4.5
3	E	145	THR	4.2
7	V	105	GLN	4.2
5	H	209	VAL	4.1
3	E	203	GLU	4.1
2	D	212	GLU	4.1
2	D	213	PRO	3.8
2	D	119	PRO	3.8
2	D	154	TRP	3.7
2	D	210	ARG	3.7
2	D	185	PRO	3.7
1	B	515	ILE	3.7
2	D	217	ASP	3.7
3	E	36	TYR	3.7
2	D	144	ASP	3.5
3	E	182	PRO	3.4
2	D	132	SER	3.4
3	E	143	ALA	3.4
2	D	218	LYS	3.4
3	E	112	ASN	3.3
7	U	3	GLN	3.3
2	D	139	GLY	3.2
3	E	191	TYR	3.1
3	E	177	TYR	3.1
2	D	133	GLY	3.1
7	U	24	ALA	3.0
2	D	216	CYS	3.0
3	E	158	GLY	3.0
3	E	195	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
3	E	113	PRO	2.9
3	E	2	SER	2.9
3	E	136	ILE	2.9
3	E	135	LEU	2.9
2	D	136	ALA	2.8
3	E	111	ALA	2.8
3	E	133	VAL	2.8
3	E	138	ASP	2.8
3	E	187	SER	2.8
3	E	107	GLY	2.7
3	E	193	CYS	2.7
1	B	520	LEU	2.6
2	D	225	GLN	2.6
2	D	84	PHE	2.6
2	D	180	SER	2.5
3	E	202	VAL	2.5
3	E	210	GLU	2.5
2	D	220	LEU	2.5
7	U	107	THR	2.5
2	D	107	THR	2.5
3	E	194	GLN	2.5
2	D	4	LEU	2.4
3	E	185	TRP	2.4
7	U	90	TYR	2.4
2	D	8	GLY	2.4
2	D	129	LYS	2.4
2	D	184	VAL	2.4
3	E	97	VAL	2.4
3	E	154	PRO	2.3
2	D	128	SER	2.3
2	D	161	SER	2.3
4	G	59	LYS	2.3
2	D	80	MET	2.3
4	G	391	PHE	2.3
7	U	61	ARG	2.3
3	E	87	TYR	2.3
7	U	15	GLY	2.3
2	D	59	LEU	2.2
2	D	179	SER	2.2
7	V	37	GLN	2.2
2	D	135	THR	2.2
3	E	132	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	548	ILE	2.1
3	E	75	ILE	2.1
3	E	4	LEU	2.1
6	L	108	SER	2.1
7	V	106	VAL	2.1
3	E	134	CYS	2.1
5	H	47	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)

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
8	NAG	B	1665	14/15	0.69	0.32	0.38	190,199,211,214	0
15	NAG	G	1567	14/15	0.91	0.19	-0.05	126,131,134,135	0
11	NAG	G	1510	14/15	0.94	0.19	-0.30	97,110,125,135	0
15	MAN	G	1570	11/12	0.88	0.20	-0.37	101,105,114,122	0
12	NAG	G	1591	14/15	0.90	0.18	-0.41	144,155,163,169	0
10	NAG	D	1227	14/15	0.94	0.15	-0.44	101,103,108,112	0
14	NAG	G	1554	14/15	0.89	0.21	-0.54	168,170,185,189	0
10	BMA	D	1228	11/12	0.95	0.14	-0.64	110,116,128,134	0
11	NAG	G	1538	14/15	0.92	0.18	-0.85	101,105,113,123	0
15	MAN	G	1572	11/12	0.94	0.14	-0.91	129,132,135,138	0
10	NAG	D	1226	14/15	0.96	0.17	-1.00	95,98,101,102	0
11	NAG	G	1537	14/15	0.96	0.17	-1.12	69,75,81,93	0
13	NAG	G	1546	14/15	0.90	0.14	-1.22	133,143,150,153	0
8	NAG	B	1666	14/15	0.83	0.15	-1.24	197,200,201,202	0
15	NAG	G	1568	14/15	0.92	0.15	-1.31	106,117,119,122	0
17	NAG	G	1609	14/15	0.81	0.12	-1.68	145,150,154,156	0
10	MAN	D	1230	11/12	0.90	0.09	-1.85	137,140,142,143	0
13	BMA	G	1548	11/12	0.88	0.10	-	166,168,169,172	0
11	MAN	G	1543	11/12	0.66	0.45	-	196,201,203,203	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
13	MAN	G	1600	11/12	0.92	0.18	-	231,234,234,234	0
13	NAG	G	1547	14/15	0.90	0.22	-	156,161,164,165	0
10	MAN	G	1532(B)	11/12	0.77	0.21	-	242,245,248,248	0
13	MAN	G	1563	11/12	0.64	0.15	-	190,193,220,221	0
13	MAN	G	1553	11/12	0.84	0.21	-	201,203,204,204	0
10	NAG	G	1519	14/15	0.90	0.13	-	134,146,157,172	0
12	MAN	G	1594	11/12	0.83	0.32	-	214,215,216,216	0
13	MAN	G	1552	11/12	0.92	0.10	-	163,164,164,165	0
16	MAN	G	1606	11/12	0.86	0.15	-	193,194,197,198	0
10	MAN	G	1581	11/12	0.65	0.19	-	211,212,215,216	0
13	MAN	G	1601	11/12	0.70	0.21	-	242,248,250,250	0
11	NAG	G	1511	14/15	0.93	0.14	-	148,154,163,172	0
13	MAN	G	1599	11/12	0.82	0.13	-	225,235,237,240	0
16	MAN	G	1607	11/12	0.92	0.11	-	198,200,202,203	0
11	MAN	G	1514	11/12	0.78	0.12	-	204,215,219,222	0
10	MAN	D	1231	11/12	0.94	0.11	-	135,137,139,141	0
10	MAN	D	1232	11/12	0.93	0.09	-	140,144,145,146	0
14	MAN	G	1558	11/12	0.84	0.43	-	198,201,203,204	0
16	BMA	G	1605	11/12	0.62	0.20	-	198,199,199,200	0
11	BMA	G	1539	11/12	0.96	0.12	-	131,133,154,162	0
10	MAN	D	1229	11/12	0.95	0.17	-	122,125,125,126	0
16	BMA	G	1613	11/12	0.83	0.15	-	167,179,247,247	0
10	NAG	G	1520	14/15	0.81	0.19	-	186,195,198,203	0
15	MAN	G	1573	11/12	0.94	0.10	-	146,148,153,155	0
10	MAN	G	1589	11/12	0.77	0.62	-	257,261,265,265	0
16	MAN	G	1616(A)	11/12	0.77	0.17	-	203,204,205,205	0
13	MAN	G	1551	11/12	0.88	0.28	-	192,197,198,200	0
13	NAG	G	1559	14/15	0.89	0.29	-	177,182,192,202	0
10	MAN	G	1530	11/12	0.73	0.22	-	242,244,247,248	0
12	NAG	G	1534	14/15	0.93	0.13	-	133,140,149,156	0
11	MAN	G	1515	11/12	0.83	0.17	-	210,212,217,218	0
16	MAN	G	1614	11/12	0.92	0.10	-	180,183,191,194	0
16	NAG	G	1604	14/15	0.73	0.18	-	189,193,195,197	0
14	NAG	G	1555	14/15	0.86	0.20	-	171,173,177,180	0
13	MAN	G	1549	11/12	0.91	0.12	-	172,174,178,185	0
10	MAN	G	1583	11/12	0.76	0.25	-	214,215,217,217	0
12	BMA	G	1593	11/12	0.79	0.12	-	187,190,214,215	0
16	MAN	V	1111	11/12	0.76	0.26	-	258,261,263,263	0
16	NAG	V	1108	14/15	0.79	0.20	-	241,247,250,252	0
16	MAN	G	1615	11/12	0.91	0.10	-	195,197,203,203	0
10	MAN	G	1523	11/12	0.81	0.21	-	223,225,227,228	0
10	NAG	G	1577	14/15	0.85	0.22	-	188,193,196,198	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
10	NAG	G	1585	14/15	0.88	0.13	-	188,192,200,206	0
10	MAN	G	1588	11/12	0.87	0.15	-	199,199,200,200	0
17	NAG	G	1618	14/15	0.77	0.21	-	194,199,200,200	0
11	MAN	G	1541	11/12	0.87	0.11	-	170,176,181,189	0
8	BMA	B	1667	11/12	0.73	0.27	-	200,201,204,205	0
10	MAN	G	1522	11/12	0.85	0.11	-	220,221,223,225	0
10	MAN	G	1582	11/12	0.68	0.46	-	214,216,219,219	0
10	MAN	G	1587	11/12	0.91	0.21	-	245,248,250,254	0
15	MAN	G	1574	11/12	0.90	0.15	-	144,146,147,148	0
14	MAN	G	1557	11/12	0.85	0.16	-	194,197,201,204	0
10	MAN	G	1524	11/12	0.77	0.26	-	226,228,229,229	0
13	MAN	G	1564	11/12	0.80	0.23	-	198,199,203,203	0
10	BMA	G	1521	11/12	0.76	0.25	-	207,215,218,219	0
10	BMA	G	1528	11/12	0.74	0.27	-	230,233,238,240	0
16	NAG	G	1603	14/15	0.89	0.22	-	183,189,193,193	0
16	NAG	G	1611	14/15	0.89	0.13	-	113,125,132,141	0
11	MAN	G	1517	11/12	0.89	0.22	-	211,212,214,214	0
14	BMA	G	1556	11/12	0.74	0.20	-	183,195,211,211	0
11	MAN	G	1518	11/12	0.76	0.38	-	217,220,220,220	0
12	BMA	G	1535	11/12	0.79	0.15	-	163,166,172,173	0
10	MAN	G	1580	11/12	0.82	0.15	-	206,207,210,212	0
10	MAN	G	1529	11/12	0.58	0.16	-	241,244,248,249	0
13	MAN	G	1566(A)	11/12	0.89	0.18	-	222,223,225,225	0
13	MAN	G	1602(B)	11/12	0.63	0.34	-	244,245,248,249	0
16	MAN	G	1608	11/12	0.70	0.34	-	202,205,206,206	0
16	MAN	V	1110	11/12	0.79	0.15	-	241,242,247,249	0
15	MAN	G	1576(A)	11/12	0.79	0.24	-	157,157,158,158	0
10	NAG	G	1584	14/15	0.91	0.09	-	159,165,172,180	0
15	BMA	G	1569	11/12	0.96	0.17	-	112,117,124,130	0
11	MAN	G	1540	11/12	0.93	0.12	-	144,146,149,151	0
16	NAG	G	1612	14/15	0.88	0.13	-	151,155,159,163	0
12	NAG	G	1533	14/15	0.94	0.17	-	85,91,104,119	0
17	NAG	G	1617	14/15	0.85	0.31	-	160,178,183,188	0
11	MAN	G	1513	11/12	0.93	0.14	-	196,200,206,208	0
13	BMA	G	1561	11/12	0.81	0.11	-	184,188,191,192	0
12	NAG	G	1592	14/15	0.82	0.12	-	178,182,186,189	0
13	NAG	G	1560	14/15	0.77	0.22	-	170,179,181,183	0
10	NAG	G	1527	14/15	0.79	0.16	-	206,212,217,224	0
10	BMA	G	1579	11/12	0.80	0.13	-	206,208,212,213	0
16	NAG	V	1107	14/15	0.81	0.27	-	235,241,244,245	0
10	NAG	G	1526	14/15	0.81	0.15	-	183,195,198,203	0
16	BMA	V	1109	11/12	0.81	0.15	-	252,254,257,258	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
12	MAN	G	1536	11/12	0.87	0.23	-	171,174,174,175	0
11	MAN	G	1516	11/12	0.72	0.32	-	223,224,225,225	0
11	MAN	G	1544	11/12	0.91	0.10	-	177,179,181,181	0
13	NAG	G	1596	14/15	0.83	0.21	-	156,166,175,187	0
11	MAN	G	1545	11/12	0.74	0.39	-	178,184,190,190	0
11	BMA	G	1512	11/12	0.84	0.12	-	181,189,197,200	0
13	MAN	G	1598	11/12	0.69	0.45	-	219,226,230,230	0
13	MAN	G	1565	11/12	0.83	0.15	-	220,221,245,245	0
15	MAN	G	1571	11/12	0.86	0.15	-	134,141,145,148	0
11	MAN	G	1542	11/12	0.94	0.12	-	155,162,170,174	0
10	NAG	G	1578	14/15	0.83	0.27	-	203,206,207,207	0
13	NAG	G	1595	14/15	0.92	0.22	-	110,117,127,140	0
10	MAN	G	1531	11/12	0.80	0.25	-	242,244,245,245	0
13	MAN	G	1550	11/12	0.89	0.09	-	163,167,172,172	0
17	NAG	G	1610	14/15	0.85	0.19	-	161,163,165,165	0
10	MAN	G	1525(A)	11/12	0.80	0.17	-	226,226,227,228	0
10	BMA	G	1586	11/12	0.82	0.11	-	201,213,232,237	0
10	MAN	G	1590	11/12	0.87	0.17	-	201,203,204,204	0
13	BMA	G	1597	11/12	0.61	0.16	-	199,207,214,220	0
16	MAN	V	1112	11/12	0.50	0.39	-	246,250,254,256	0
15	MAN	G	1575	11/12	0.90	0.24	-	143,151,152,152	0
13	MAN	G	1562	11/12	0.78	0.16	-	193,194,196,197	0

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
9	NAG	G	1509	14/15	0.85	0.26	0.90	135,144,144,146	0
9	NAG	B	1669	14/15	0.85	0.19	-0.53	123,136,154,157	0
9	NAG	B	1668	14/15	0.84	0.31	-	147,156,161,162	0
9	NAG	H	1212	14/15	0.91	0.21	-	121,132,140,149	0
9	NAG	B	1670	14/15	0.48	0.54	-	170,182,187,189	0

6.5 Other polymers (i)

There are no such residues in this entry.