Full wwPDB X-ray Structure Validation Report (i)

Jul 28, 2016 – 02:38 PM EDT

PDB ID	:	5FYL
Title	:	Crystal Structure at 3.7 A Resolution of Fully Glycosylated HIV-1 Clade A BG505 SOSIP.664 Prefusion Env Trimer in Complex with Broadly Neutralizing Antibodies PGT122 and 35O22
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Deposited on	:	2016-03-08
Resolution	:	3.10 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:

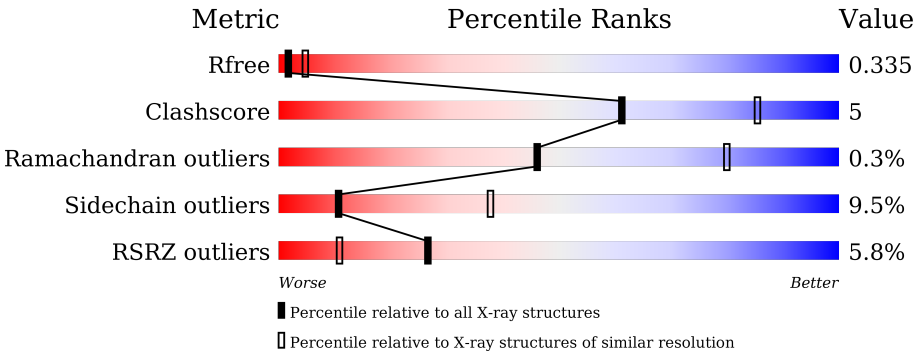
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.10 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	153	59% 20% • 18%
2	D	243	15% 88% 11% •
3	E	216	18% 84% 14% ••
4	G	481	73% 19% • 6%
5	H	244	2% 77% 16% • 7%
6	L	213	2% 72% 24% ••

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 12718 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 BG505 GP120 ENV ECTODOMAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	126	Total	C	N	O	S	0	0	0
			1001	633	172	190	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	ENGINEERED MUTATION	UNP Q2N0S6
B	605	CYS	THR	ENGINEERED MUTATION	UNP Q2N0S6

- Molecule 2 is a protein called 35O22 ANTIBODY FAB HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	242	Total	C	N	O	S	0	0	0
			1832	1165	306	353	8			

- Molecule 3 is a protein called 35O22 ANTIBODY FAB LIGHT CHAIN.

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 BG505 GP120 ENV ECTODOMAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	453	Total	C	N	O	S	0	0	0
			3565	2236	630	671	28			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	332	ASN	THR	ENGINEERED MUTATION	UNP Q2N0S6
G	501	CYS	ALA	ENGINEERED MUTATION	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
G	509	ARG	-	EXPRESSION TAG	UNP Q2N0S6
G	510	ARG	-	EXPRESSION TAG	UNP Q2N0S6
G	511	ARG	-	EXPRESSION TAG	UNP Q2N0S6
G	512	ARG	-	EXPRESSION TAG	UNP Q2N0S6
G	513	ARG	-	EXPRESSION TAG	UNP Q2N0S6

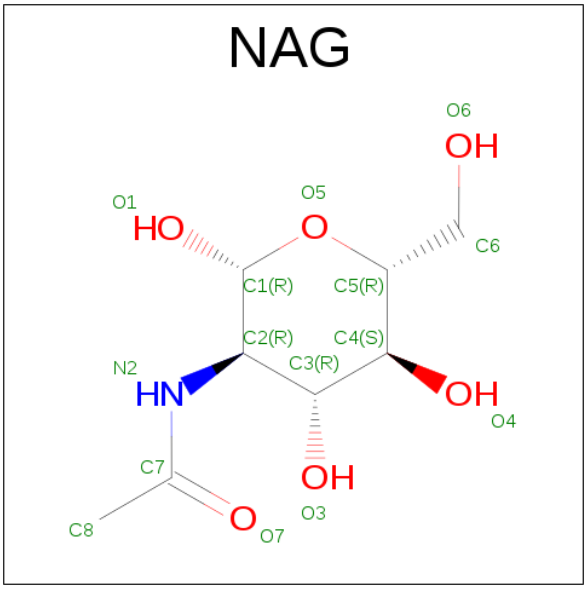
- Molecule 5 is a protein called PGT122 ANTIBODY FAB HEAVY CHAIN.

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 ANTIBODY FAB LIGHT CHAIN.

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



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

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

- 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
8	G	3	Total C N O 39 22 2 15	0	0

- Molecule 9 is a polymer of unknown type called SUGAR (7-MER).

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

- Molecule 10 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 11 is a polymer of unknown type called SUGAR (7-MER).

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

- Molecule 12 is a polymer of unknown type called SUGAR (9-MER).

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

- 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 (6-MER).

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

- Molecule 15 is a polymer of unknown type called SUGAR (5-MER).

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

- Molecule 16 is a polymer of unknown type called SUGAR (10-MER).

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

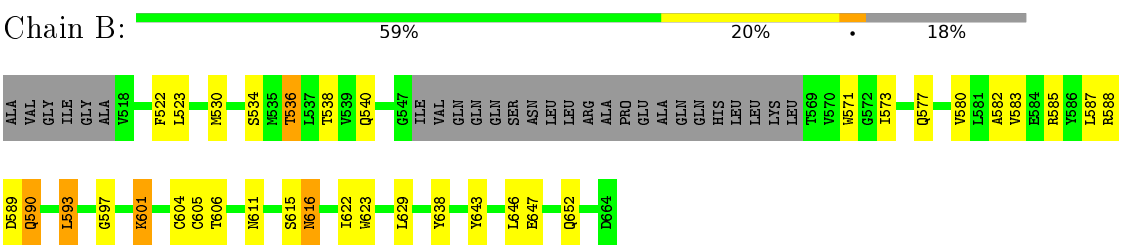
- Molecule 17 is a polymer of unknown type called SUGAR (4-MER).

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

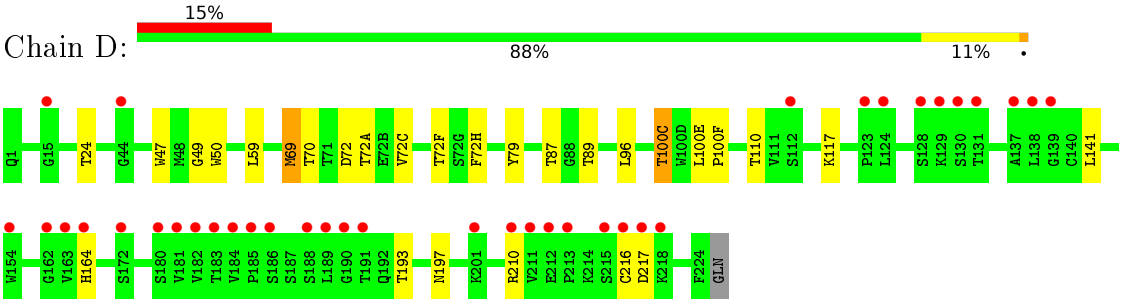
3 Residue-property plots (i)

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.

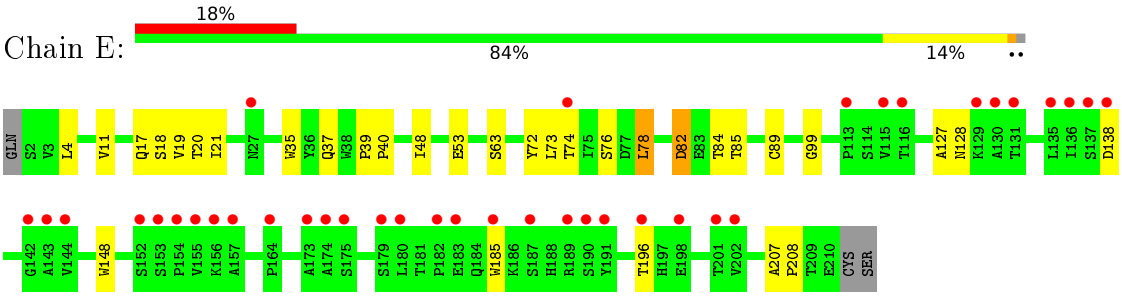
- Molecule 1: BG505 GP120 ENV ECTODOMAIN



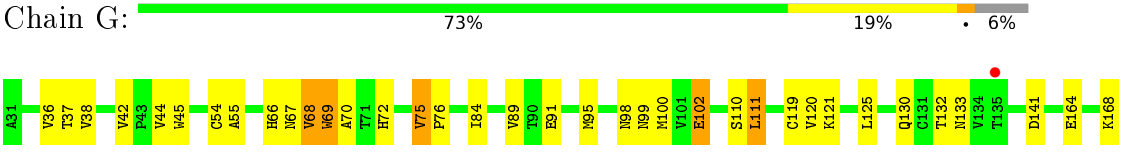
- Molecule 2: 35O22 ANTIBODY FAB HEAVY CHAIN

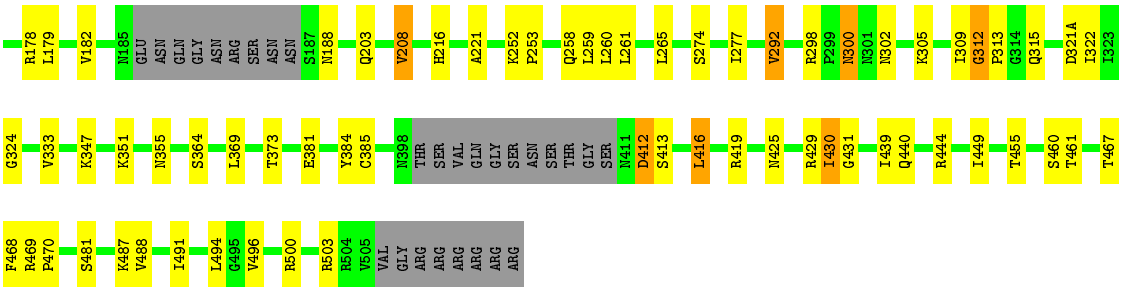


- Molecule 3: 35O22 ANTIBODY FAB LIGHT CHAIN

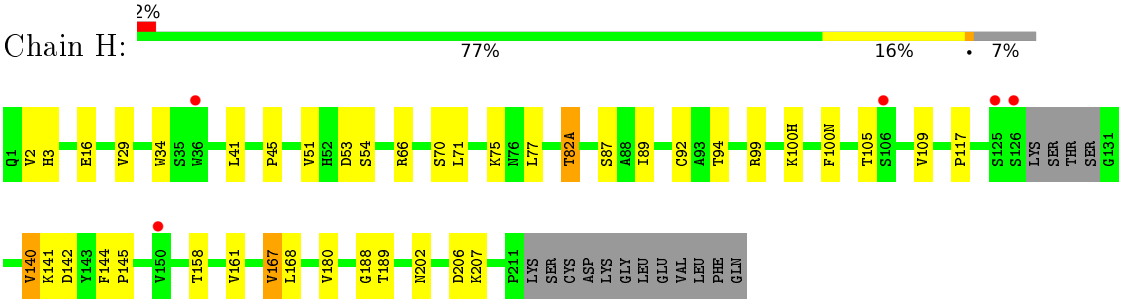


- Molecule 4: BG505 GP120 ENV ECTODOMAIN

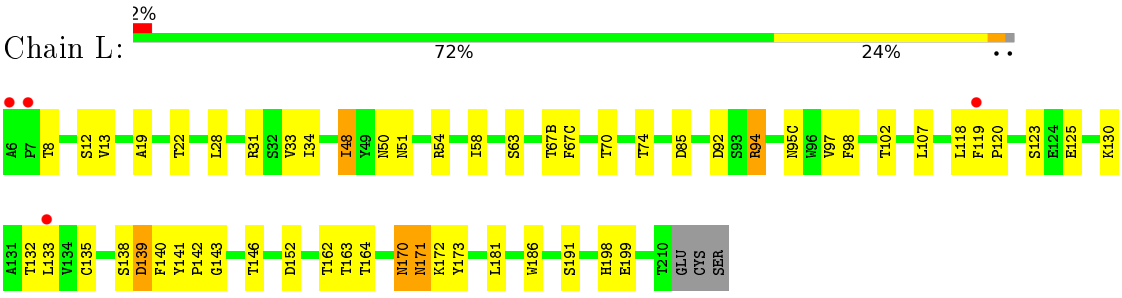




• Molecule 5: PGT122 ANTIBODY FAB HEAVY CHAIN



• Molecule 6: PGT122 ANTIBODY FAB LIGHT CHAIN



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	129.78Å 129.78Å 313.06Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.00 – 3.10 41.00 – 2.91	Depositor EDS
% Data completeness (in resolution range)	58.5 (41.00-3.10) 49.3 (41.00-2.91)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.90 (at 2.90Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.9_1692)	Depositor
R, R_{free}	0.250 , 0.307 0.304 , 0.335	Depositor DCC
R_{free} test set	1594 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	68.8	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 67.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.085 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	12718	wwPDB-VP
Average B, all atoms (Å^2)	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% 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	0.25	0/1019	0.46	0/1382
2	D	0.23	0/1880	0.43	0/2560
3	E	0.23	0/1659	0.42	0/2269
4	G	0.27	0/3639	0.48	1/4941 (0.0%)
5	H	0.23	0/1789	0.45	0/2443
6	L	0.24	0/1632	0.46	0/2236
All	All	0.25	0/11618	0.45	1/15831 (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})
4	G	111	LEU	CA-CB-CG	5.80	128.63	115.30

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	1001	0	975	18	0
2	D	1832	0	1806	11	0
3	E	1615	0	1542	14	0
4	G	3565	0	3495	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	1742	0	1715	22	0
6	L	1589	0	1530	28	0
7	B	28	0	26	1	0
7	G	28	0	26	1	0
8	B	39	0	34	0	0
8	G	39	0	34	1	0
9	D	83	0	70	2	0
10	G	28	0	25	0	0
11	G	166	0	140	0	0
12	G	105	0	88	0	0
13	G	282	0	237	3	0
14	G	288	0	244	2	0
15	G	122	0	104	0	0
16	G	116	0	97	0	0
17	H	50	0	43	3	0
All	All	12718	0	12231	137	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 (137) 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)
13:G:1527:BMA:H3	13:G:1528:MAN:H5	1.23	1.14
13:G:1527:BMA:H3	13:G:1528:MAN:C5	2.00	0.92
5:H:77:LEU:HD22	17:H:1213:NAG:H83	1.62	0.82
1:B:615:SER:O	1:B:616:ASN:ND2	2.17	0.75
6:L:139:ASP:H	6:L:172:LYS:HE3	1.57	0.69
4:G:274:SER:HB3	4:G:277:ILE:HG13	1.75	0.68
3:E:127:ALA:H	3:E:128:ASN:HA	1.59	0.67
4:G:412:ASP:OD1	4:G:412:ASP:N	2.29	0.65
5:H:29:VAL:HA	5:H:34:TRP:CZ2	2.33	0.63
5:H:77:LEU:HD22	17:H:1213:NAG:C8	2.29	0.62
4:G:132:THR:OG1	4:G:133:ASN:N	2.31	0.62
4:G:258:GLN:HG3	4:G:470:PRO:HB2	1.81	0.62
4:G:292:VAL:HG13	4:G:449:ILE:HB	1.81	0.61
4:G:75:VAL:HG22	4:G:76:PRO:HD2	1.83	0.59
4:G:67:ASN:HA	4:G:208:VAL:HA	1.85	0.59
4:G:322:ILE:O	6:L:94:ARG:NH2	2.35	0.59
4:G:309:ILE:HB	4:G:315:GLN:HB2	1.85	0.59
6:L:118:LEU:HD13	6:L:135:CYS:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:167:VAL:HB	6:L:163:THR:HG22	1.84	0.58
7:B:1666:NAG:H62	3:E:53:GLU:HA	1.83	0.58
5:H:141:LYS:HZ1	6:L:130:LYS:HD3	1.68	0.58
3:E:17:GLN:HG3	3:E:18:SER:H	1.69	0.57
4:G:55:ALA:HB3	4:G:216:HIS:HB2	1.84	0.57
6:L:170:ASN:O	6:L:172:LYS:N	2.38	0.57
4:G:351:LYS:HA	7:G:1583:NAG:H82	1.86	0.57
3:E:82:ASP:OD1	3:E:82:ASP:N	2.37	0.57
4:G:430:ILE:HD12	4:G:431:GLY:H	1.71	0.56
9:D:1226:BMA:H61	9:D:1228:MAN:H3	1.88	0.56
4:G:258:GLN:HE21	4:G:470:PRO:HB2	1.71	0.56
5:H:34:TRP:CZ3	5:H:94:THR:HG22	2.41	0.56
1:B:643:TYR:HA	1:B:646:LEU:HD12	1.88	0.55
5:H:45:PRO:HD2	6:L:98:PHE:HB2	1.88	0.55
6:L:171:ASN:N	6:L:171:ASN:OD1	2.38	0.55
2:D:87:THR:HG23	2:D:110:THR:HA	1.89	0.54
4:G:164:GLU:HA	4:G:312:GLY:HA3	1.88	0.54
6:L:198:HIS:CG	6:L:199:GLU:H	2.25	0.54
4:G:430:ILE:HD12	4:G:431:GLY:N	2.23	0.54
4:G:119:CYS:HB3	4:G:203:GLN:O	2.07	0.54
3:E:84:THR:OG1	3:E:85:THR:N	2.39	0.53
4:G:373:THR:HG21	4:G:384:TYR:HB3	1.91	0.53
4:G:369:LEU:O	4:G:373:THR:HG22	2.08	0.53
1:B:605:CYS:HA	4:G:37:THR:HG22	1.91	0.53
6:L:152:ASP:OD1	6:L:191:SER:N	2.39	0.52
17:H:1213:NAG:O3	17:H:1214:BMA:O5	2.23	0.52
4:G:460:SER:O	4:G:461:THR:OG1	2.28	0.51
2:D:100(C):THR:HG21	9:D:1225:NAG:H3	1.91	0.51
5:H:29:VAL:HA	5:H:34:TRP:HZ2	1.75	0.51
6:L:33:VAL:HG12	6:L:51:ASN:ND2	2.26	0.51
1:B:590:GLN:OE1	1:B:601:LYS:NZ	2.44	0.50
2:D:96:LEU:HD22	2:D:100(E):LEU:HD23	1.93	0.50
5:H:34:TRP:HB2	5:H:51:VAL:HG13	1.95	0.48
4:G:460:SER:OG	4:G:461:THR:N	2.44	0.48
5:H:117:PRO:HA	5:H:142:ASP:O	2.12	0.48
1:B:582:ALA:HB1	4:G:221:ALA:HB3	1.95	0.48
4:G:385:CYS:HB3	4:G:416:LEU:HD12	1.95	0.48
4:G:69:TRP:CE3	4:G:111:LEU:HD21	2.48	0.48
4:G:425:ASN:HA	4:G:429:ARG:HD2	1.94	0.48
4:G:98:ASN:OD1	4:G:100:MET:N	2.47	0.48
1:B:604:CYS:SG	4:G:503:ARG:NH2	2.87	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:63:SER:HB2	6:L:74:THR:HB	1.96	0.47
4:G:455:THR:N	4:G:469:ARG:O	2.48	0.47
3:E:4:LEU:HB3	3:E:99:GLY:HA2	1.96	0.47
6:L:143:GLY:HA3	6:L:173:TYR:CD2	2.50	0.47
1:B:530:MET:O	1:B:534:SER:OG	2.21	0.47
4:G:120:VAL:HG23	4:G:315:GLN:NE2	2.30	0.46
4:G:381:GLU:HB2	4:G:439:ILE:HD11	1.97	0.46
4:G:300:ASN:OD1	4:G:300:ASN:N	2.49	0.46
1:B:536:THR:O	1:B:540:GLN:NE2	2.45	0.46
3:E:20:THR:HG22	3:E:74:THR:HG22	1.97	0.46
1:B:571:TRP:CD1	4:G:70:ALA:HB1	2.51	0.46
4:G:69:TRP:CD2	4:G:111:LEU:HD21	2.50	0.46
4:G:252:LYS:HA	4:G:253:PRO:HD3	1.69	0.46
4:G:321(A):ASP:OD1	4:G:322:ILE:N	2.49	0.46
5:H:141:LYS:NZ	6:L:130:LYS:HD3	2.31	0.45
1:B:589:ASP:O	1:B:593:LEU:HD22	2.17	0.45
5:H:53:ASP:O	5:H:54:SER:OG	2.25	0.45
4:G:324:GLY:HA2	6:L:67(C):PHE:CD1	2.52	0.45
4:G:298:ARG:NH2	4:G:439:ILE:O	2.48	0.45
6:L:140:PHE:CE2	6:L:143:GLY:HA2	2.51	0.45
6:L:139:ASP:N	6:L:172:LYS:HE3	2.27	0.45
1:B:629:LEU:HA	4:G:44:VAL:HG23	1.99	0.45
1:B:522:PHE:N	4:G:84:ILE:HD13	2.32	0.44
6:L:13:VAL:HG21	6:L:19:ALA:HB2	1.98	0.44
1:B:577:GLN:HA	1:B:580:VAL:HG22	1.99	0.44
2:D:47:TRP:CZ2	2:D:49:GLY:HA2	2.52	0.44
4:G:42:VAL:HG12	4:G:44:VAL:HG12	1.99	0.44
2:D:100(E):LEU:HD12	2:D:100(F):PRO:HD2	2.00	0.44
3:E:19:VAL:HG12	3:E:78:LEU:HD21	1.99	0.44
1:B:571:TRP:NE1	4:G:70:ALA:HB1	2.33	0.44
14:G:1588:NAG:H82	14:G:1593:NAG:H83	1.99	0.44
5:H:141:LYS:HZ1	6:L:130:LYS:CD	2.30	0.44
3:E:35:TRP:HB2	3:E:48:ILE:HG22	2.00	0.43
2:D:216:CYS:SG	2:D:217:ASP:N	2.92	0.43
3:E:78:LEU:HA	3:E:78:LEU:HD13	1.90	0.43
6:L:13:VAL:O	6:L:107:LEU:N	2.51	0.43
6:L:31:ARG:HG2	6:L:92:ASP:HA	2.00	0.43
3:E:35:TRP:CE2	3:E:73:LEU:HB2	2.54	0.43
5:H:117:PRO:HB3	5:H:140:VAL:HG23	2.00	0.43
2:D:193:THR:HG23	2:D:210:ARG:HH12	1.83	0.42
6:L:170:ASN:OD1	6:L:172:LYS:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:207:ALA:HA	3:E:208:PRO:HD3	1.92	0.42
1:B:522:PHE:O	1:B:523:LEU:HB2	2.18	0.42
2:D:59:LEU:HD11	2:D:69:MET:HG3	2.00	0.42
6:L:48:ILE:HG23	6:L:50:ASN:O	2.20	0.42
4:G:67:ASN:OD1	4:G:68:VAL:HG22	2.19	0.42
5:H:89:ILE:O	5:H:89:ILE:HG13	2.20	0.42
2:D:70:THR:HB	2:D:79:TYR:HB2	2.02	0.42
6:L:125:GLU:OE2	6:L:132:THR:N	2.53	0.42
6:L:141:TYR:HA	6:L:142:PRO:HA	1.85	0.42
6:L:199:GLU:HA	6:L:199:GLU:OE1	2.20	0.42
4:G:99:ASN:O	4:G:102:GLU:N	2.53	0.42
2:D:72(F):THR:HG23	2:D:72(H):PHE:H	1.85	0.42
4:G:130:GLN:HG3	13:G:1525:NAG:H82	2.01	0.41
4:G:45:TRP:HB3	4:G:491:ILE:HD13	2.02	0.41
4:G:300:ASN:HB2	4:G:302:ASN:OD1	2.20	0.41
5:H:75:LYS:O	5:H:77:LEU:HD12	2.20	0.41
5:H:141:LYS:NZ	6:L:130:LYS:CD	2.83	0.41
4:G:91:GLU:HG3	4:G:487:LYS:HZ2	1.86	0.41
2:D:47:TRP:HZ2	2:D:50:TRP:CD1	2.38	0.41
5:H:144:PHE:HA	5:H:145:PRO:HA	1.83	0.41
5:H:70:SER:OG	5:H:71:LEU:N	2.53	0.41
3:E:127:ALA:N	3:E:128:ASN:HA	2.25	0.41
3:E:39:PRO:HA	3:E:40:PRO:HD3	1.94	0.41
4:G:261:LEU:HD23	4:G:449:ILE:HA	2.03	0.41
6:L:119:PHE:HA	6:L:120:PRO:HD3	1.88	0.41
5:H:161:VAL:HG12	5:H:180:VAL:HG12	2.03	0.41
4:G:179:LEU:HD21	4:G:419:ARG:HD3	2.01	0.41
8:G:1585:NAG:O4	14:G:1588:NAG:H61	2.21	0.41
4:G:385:CYS:HB3	4:G:416:LEU:CD1	2.51	0.41
4:G:98:ASN:OD1	4:G:99:ASN:N	2.54	0.41
1:B:622:ILE:HG13	1:B:623:TRP:N	2.36	0.40
5:H:188:GLY:HA3	5:H:189:THR:HA	1.88	0.40
4:G:54:CYS:SG	4:G:55:ALA:N	2.94	0.40
5:H:66:ARG:HB2	5:H:82(A):THR:O	2.22	0.40
4:G:467:THR:OG1	4:G:468:PHE:N	2.55	0.40
1:B:536:THR:OG1	1:B:536:THR:O	2.36	0.40
1:B:597:GLY:HA3	4:G:503:ARG:HH12	1.87	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	122/153 (80%)	109 (89%)	13 (11%)	0	100	100
2	D	240/243 (99%)	212 (88%)	27 (11%)	1 (0%)	39	75
3	E	211/216 (98%)	189 (90%)	22 (10%)	0	100	100
4	G	447/481 (93%)	406 (91%)	39 (9%)	2 (0%)	39	75
5	H	224/244 (92%)	203 (91%)	20 (9%)	1 (0%)	39	75
6	L	208/213 (98%)	183 (88%)	24 (12%)	1 (0%)	34	72
All	All	1452/1550 (94%)	1302 (90%)	145 (10%)	5 (0%)	46	80

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	H	202	ASN
6	L	171	ASN
4	G	500	ARG
2	D	197	ASN
4	G	312	GLY

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	108/129 (84%)	92 (85%)	16 (15%)	4	16
2	D	205/206 (100%)	195 (95%)	10 (5%)	31	68
3	E	186/189 (98%)	173 (93%)	13 (7%)	19	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	G	404/428 (94%)	364 (90%)	40 (10%)	10 34
5	H	198/213 (93%)	180 (91%)	18 (9%)	12 40
6	L	178/181 (98%)	153 (86%)	25 (14%)	4 18
All	All	1279/1346 (95%)	1157 (90%)	122 (10%)	11 38

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	536	THR
1	B	538	THR
1	B	573	ILE
1	B	583	VAL
1	B	585	ARG
1	B	587	LEU
1	B	588	ARG
1	B	590	GLN
1	B	593	LEU
1	B	601	LYS
1	B	606	THR
1	B	611	ASN
1	B	616	ASN
1	B	638	TYR
1	B	647	GLU
1	B	652	GLN
2	D	24	THR
2	D	69	MET
2	D	72	ASP
2	D	72(A)	THR
2	D	72(C)	VAL
2	D	89	THR
2	D	100(C)	THR
2	D	117	LYS
2	D	141	LEU
2	D	164	HIS
3	E	11	VAL
3	E	21	ILE
3	E	37	GLN
3	E	63	SER
3	E	72	TYR
3	E	76	SER
3	E	78	LEU

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Mol	Chain	Res	Type
3	E	82	ASP
3	E	89	CYS
3	E	138	ASP
3	E	148	TRP
3	E	185	TRP
3	E	196	THR
4	G	36	VAL
4	G	38	VAL
4	G	66	HIS
4	G	68	VAL
4	G	69	TRP
4	G	72	HIS
4	G	75	VAL
4	G	89	VAL
4	G	95	MET
4	G	102	GLU
4	G	110	SER
4	G	121	LYS
4	G	125	LEU
4	G	141	ASP
4	G	168	LYS
4	G	178	ARG
4	G	182	VAL
4	G	188	ASN
4	G	208	VAL
4	G	259	LEU
4	G	260	LEU
4	G	265	LEU
4	G	292	VAL
4	G	300	ASN
4	G	305	LYS
4	G	313	PRO
4	G	333	VAL
4	G	347	LYS
4	G	355	ASN
4	G	364	SER
4	G	412	ASP
4	G	413	SER
4	G	416	LEU
4	G	430	ILE
4	G	440	GLN
4	G	444	ARG

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Mol	Chain	Res	Type
4	G	481	SER
4	G	488	VAL
4	G	494	LEU
4	G	496	VAL
5	H	2	VAL
5	H	3	HIS
5	H	16	GLU
5	H	41	LEU
5	H	82(A)	THR
5	H	87	SER
5	H	92	CYS
5	H	99	ARG
5	H	100(H)	LYS
5	H	100(N)	PHE
5	H	105	THR
5	H	109	VAL
5	H	140	VAL
5	H	158	THR
5	H	167	VAL
5	H	168	LEU
5	H	206	ASP
5	H	207	LYS
6	L	8	THR
6	L	12	SER
6	L	22	THR
6	L	28	LEU
6	L	34	ILE
6	L	48	ILE
6	L	54	ARG
6	L	58	ILE
6	L	67(B)	THR
6	L	70	THR
6	L	85	ASP
6	L	94	ARG
6	L	95(C)	ASN
6	L	97	VAL
6	L	102	THR
6	L	123	SER
6	L	133	LEU
6	L	138	SER
6	L	139	ASP
6	L	146	THR

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Mol	Chain	Res	Type
6	L	162	THR
6	L	164	THR
6	L	170	ASN
6	L	181	LEU
6	L	186	TRP

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
4	G	258	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

110 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	1667	1,8	14,14,15	0.26	0	15,19,21	0.26	0
8	NAG	B	1668	8	14,14,15	0.31	0	15,19,21	0.47	0
8	BMA	B	1669	8	11,11,12	0.63	0	15,15,17	0.78	0
9	NAG	D	1225	9	14,14,15	0.39	0	15,19,21	0.50	0
9	BMA	D	1226	9	11,11,12	0.54	0	15,15,17	0.68	0
9	MAN	D	1227	9	11,11,12	0.63	0	15,15,17	1.03	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	MAN	D	1228	9	11,11,12	0.85	0	15,15,17	1.46	2 (13%)
9	MAN	D	1229	9	11,11,12	0.62	0	15,15,17	0.90	1 (6%)
9	MAN	D	1230	9	11,11,12	0.59	0	15,15,17	0.89	1 (6%)
9	NAG	D	1506	-	14,14,15	0.20	0	15,19,21	0.39	0
10	NAG	G	1507	10,4	14,14,15	0.32	0	15,19,21	0.54	0
10	NAG	G	1508	10	14,14,15	0.36	0	15,19,21	0.25	0
11	NAG	G	1509	11,4	14,14,15	0.38	0	15,19,21	0.40	0
11	NAG	G	1510	11	14,14,15	0.32	0	15,19,21	0.62	0
11	BMA	G	1511	11	11,11,12	1.09	1 (9%)	15,15,17	0.96	1 (6%)
11	MAN	G	1512	11	11,11,12	0.64	0	15,15,17	1.13	2 (13%)
11	MAN	G	1513	11	11,11,12	1.17	1 (9%)	15,15,17	1.47	2 (13%)
11	MAN	G	1514	11	11,11,12	0.55	0	15,15,17	1.10	2 (13%)
11	MAN	G	1515	11	11,11,12	0.65	0	15,15,17	0.90	1 (6%)
12	NAG	G	1516	12,4	14,14,15	0.25	0	15,19,21	0.36	0
12	NAG	G	1517	12	14,14,15	0.17	0	15,19,21	0.38	0
12	BMA	G	1518	12	11,11,12	0.62	0	15,15,17	0.78	0
12	MAN	G	1519	12	11,11,12	0.60	0	15,15,17	1.16	2 (13%)
12	MAN	G	1520	12	11,11,12	0.54	0	15,15,17	1.20	2 (13%)
12	MAN	G	1521	12	11,11,12	0.62	0	15,15,17	0.93	2 (13%)
12	MAN	G	1522	12	11,11,12	0.65	0	15,15,17	0.97	2 (13%)
12	MAN	G	1523	12	11,11,12	0.52	0	15,15,17	1.06	1 (6%)
12	MAN	G	1524(B)	12	11,11,12	0.68	0	15,15,17	1.23	2 (13%)
13	NAG	G	1525	13,4	14,14,15	0.31	0	15,19,21	0.45	0
13	NAG	G	1526	13	14,14,15	0.24	0	15,19,21	0.30	0
13	BMA	G	1527	13	11,11,12	0.55	0	15,15,17	0.88	0
13	MAN	G	1528	13	11,11,12	0.42	0	15,15,17	1.14	2 (13%)
13	MAN	G	1529	13	11,11,12	1.04	1 (9%)	15,15,17	0.93	1 (6%)
13	MAN	G	1530	13	11,11,12	0.73	0	15,15,17	1.07	1 (6%)
13	MAN	G	1531	13	11,11,12	0.90	1 (9%)	15,15,17	1.49	2 (13%)
13	MAN	G	1532	13	11,11,12	0.67	0	15,15,17	1.12	2 (13%)
14	NAG	G	1533	4,14	14,14,15	0.23	0	15,19,21	0.40	0
14	NAG	G	1534	14	14,14,15	0.32	0	15,19,21	0.64	0
14	BMA	G	1535	14	11,11,12	1.09	1 (9%)	15,15,17	1.19	2 (13%)
14	MAN	G	1536	14	11,11,12	0.79	1 (9%)	15,15,17	1.22	1 (6%)
14	MAN	G	1537	14	11,11,12	0.91	1 (9%)	15,15,17	1.17	2 (13%)
14	MAN	G	1538	14	11,11,12	0.77	0	15,15,17	0.83	1 (6%)
15	NAG	G	1539	15,4	14,14,15	0.32	0	15,19,21	0.52	0
15	NAG	G	1540	15	14,14,15	0.19	0	15,19,21	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	BMA	G	1541	15	11,11,12	0.70	0	15,15,17	0.99	1 (6%)
15	MAN	G	1542	15	11,11,12	0.64	0	15,15,17	0.97	2 (13%)
15	MAN	G	1543	15	11,11,12	0.60	0	15,15,17	1.09	2 (13%)
13	NAG	G	1544	13,4	14,14,15	0.32	0	15,19,21	0.31	0
13	NAG	G	1545	13	14,14,15	0.29	0	15,19,21	0.28	0
13	BMA	G	1546	13	11,11,12	1.02	1 (9%)	15,15,17	0.88	0
13	MAN	G	1547	13	11,11,12	0.78	0	15,15,17	1.14	3 (20%)
13	MAN	G	1548	13	11,11,12	1.27	2 (18%)	15,15,17	1.37	3 (20%)
13	MAN	G	1549	13	11,11,12	0.81	1 (9%)	15,15,17	1.37	2 (13%)
13	MAN	G	1550	13	11,11,12	0.78	0	15,15,17	0.89	1 (6%)
13	MAN	G	1551(A)	13	11,11,12	0.73	1 (9%)	15,15,17	1.20	2 (13%)
15	NAG	G	1552	15,4	14,14,15	0.32	0	15,19,21	0.42	0
15	NAG	G	1553	15	14,14,15	0.23	0	15,19,21	0.49	0
15	BMA	G	1554	15	11,11,12	1.05	0	15,15,17	1.19	2 (13%)
15	MAN	G	1555	15	11,11,12	0.66	0	15,15,17	1.15	2 (13%)
15	MAN	G	1556	15	11,11,12	0.67	0	15,15,17	1.10	2 (13%)
11	NAG	G	1557	11,4	14,14,15	0.40	0	15,19,21	0.41	0
11	NAG	G	1558	11	14,14,15	0.21	0	15,19,21	0.29	0
11	BMA	G	1559	11	11,11,12	1.03	0	15,15,17	0.86	0
11	MAN	G	1560	11	11,11,12	0.71	0	15,15,17	1.04	2 (13%)
11	MAN	G	1561	11	11,11,12	0.87	1 (9%)	15,15,17	1.14	2 (13%)
11	MAN	G	1562	11	11,11,12	0.82	1 (9%)	15,15,17	1.12	1 (6%)
11	MAN	G	1563	11	11,11,12	0.67	0	15,15,17	1.14	2 (13%)
13	NAG	G	1564	13,4	14,14,15	0.33	0	15,19,21	0.46	0
13	NAG	G	1565	13	14,14,15	0.38	0	15,19,21	1.32	2 (13%)
13	BMA	G	1566	13	11,11,12	1.01	0	15,15,17	1.67	2 (13%)
13	MAN	G	1567	13	11,11,12	0.63	0	15,15,17	1.04	2 (13%)
13	MAN	G	1568	13	11,11,12	1.01	0	15,15,17	1.30	1 (6%)
13	MAN	G	1569	13	11,11,12	0.58	0	15,15,17	0.99	2 (13%)
13	MAN	G	1570	13	11,11,12	0.59	0	15,15,17	0.96	2 (13%)
13	MAN	G	1571	13	11,11,12	0.85	1 (9%)	15,15,17	1.32	2 (13%)
16	NAG	G	1572	4,16	14,14,15	0.31	0	15,19,21	0.35	0
16	NAG	G	1573	16	14,14,15	0.37	0	15,19,21	0.54	0
16	BMA	G	1574	16	11,11,12	0.61	0	15,15,17	0.86	0
16	MAN	G	1575	16	11,11,12	0.62	0	15,15,17	1.33	2 (13%)
16	MAN	G	1576	16	11,11,12	0.70	0	15,15,17	0.98	2 (13%)
16	MAN	G	1577	16	11,11,12	0.62	0	15,15,17	1.09	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	MAN	G	1578	16	11,11,12	0.76	0	15,15,17	1.12	1 (6%)
16	MAN	G	1579	16	11,11,12	0.65	0	15,15,17	1.02	2 (13%)
16	MAN	G	1580(A)	16	11,11,12	0.66	0	15,15,17	0.85	1 (6%)
16	MAN	G	1581	16	11,11,12	0.70	0	15,15,17	1.11	2 (13%)
8	NAG	G	1584	8,4	14,14,15	0.23	0	15,19,21	0.32	0
8	NAG	G	1585	8	14,14,15	0.27	0	15,19,21	0.46	0
8	BMA	G	1586	8	11,11,12	0.76	0	15,15,17	1.08	1 (6%)
14	NAG	G	1587	4,14	14,14,15	0.52	0	15,19,21	0.66	0
14	NAG	G	1588	14	14,14,15	0.24	0	15,19,21	0.61	0
14	BMA	G	1589	14	11,11,12	0.62	0	15,15,17	0.80	0
14	MAN	G	1590	14	11,11,12	1.22	1 (9%)	15,15,17	1.34	2 (13%)
14	MAN	G	1591	14	11,11,12	0.61	0	15,15,17	0.95	2 (13%)
14	MAN	G	1592	14	11,11,12	0.60	0	15,15,17	0.99	2 (13%)
14	NAG	G	1593	4,14	14,14,15	0.50	0	15,19,21	0.56	0
14	NAG	G	1594	14	14,14,15	0.32	0	15,19,21	0.89	1 (6%)
14	BMA	G	1595	14	11,11,12	0.96	1 (9%)	15,15,17	1.03	1 (6%)
14	MAN	G	1596	14	11,11,12	0.88	0	15,15,17	1.09	1 (6%)
14	MAN	G	1597	14	11,11,12	0.69	0	15,15,17	1.01	2 (13%)
14	MAN	G	1598	14	11,11,12	0.64	0	15,15,17	1.12	2 (13%)
14	NAG	G	1599	4,14	14,14,15	0.26	0	15,19,21	0.45	0
14	NAG	G	1600	14	14,14,15	0.31	0	15,19,21	0.40	0
14	BMA	G	1601	14	11,11,12	0.60	0	15,15,17	1.12	1 (6%)
14	MAN	G	1602	14	11,11,12	0.91	1 (9%)	15,15,17	1.52	2 (13%)
14	MAN	G	1603	14	11,11,12	0.80	0	15,15,17	1.08	1 (6%)
14	MAN	G	1604(B)	14	11,11,12	0.65	0	15,15,17	1.08	2 (13%)
17	NAG	H	1212	5,17	14,14,15	0.64	1 (7%)	15,19,21	0.64	0
17	NAG	H	1213	17	14,14,15	0.41	0	15,19,21	0.64	1 (6%)
17	BMA	H	1214	17	11,11,12	0.92	1 (9%)	15,15,17	1.01	1 (6%)
17	MAN	H	1215	17	11,11,12	0.67	0	15,15,17	0.84	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	1667	1,8	-	0/6/23/26	0/1/1/1
8	NAG	B	1668	8	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BMA	B	1669	8	-	0/2/19/22	0/1/1/1
9	NAG	D	1225	9	-	0/6/23/26	0/1/1/1
9	BMA	D	1226	9	-	0/2/19/22	0/1/1/1
9	MAN	D	1227	9	-	0/2/19/22	0/1/1/1
9	MAN	D	1228	9	-	0/2/19/22	0/1/1/1
9	MAN	D	1229	9	-	0/2/19/22	0/1/1/1
9	MAN	D	1230	9	-	0/2/19/22	0/1/1/1
9	NAG	D	1506	-	-	0/6/23/26	0/1/1/1
10	NAG	G	1507	10,4	-	0/6/23/26	0/1/1/1
10	NAG	G	1508	10	-	0/6/23/26	0/1/1/1
11	NAG	G	1509	11,4	-	0/6/23/26	0/1/1/1
11	NAG	G	1510	11	-	0/6/23/26	0/1/1/1
11	BMA	G	1511	11	-	0/2/19/22	0/1/1/1
11	MAN	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
12	NAG	G	1516	12,4	-	0/6/23/26	0/1/1/1
12	NAG	G	1517	12	-	0/6/23/26	0/1/1/1
12	BMA	G	1518	12	-	0/2/19/22	0/1/1/1
12	MAN	G	1519	12	-	0/2/19/22	0/1/1/1
12	MAN	G	1520	12	-	0/2/19/22	0/1/1/1
12	MAN	G	1521	12	-	0/2/19/22	0/1/1/1
12	MAN	G	1522	12	-	0/2/19/22	0/1/1/1
12	MAN	G	1523	12	-	0/2/19/22	0/1/1/1
12	MAN	G	1524(B)	12	-	0/2/19/22	0/1/1/1
13	NAG	G	1525	13,4	-	0/6/23/26	0/1/1/1
13	NAG	G	1526	13	-	0/6/23/26	0/1/1/1
13	BMA	G	1527	13	-	0/2/19/22	0/1/1/1
13	MAN	G	1528	13	-	0/2/19/22	0/1/1/1
13	MAN	G	1529	13	-	0/2/19/22	0/1/1/1
13	MAN	G	1530	13	-	0/2/19/22	0/1/1/1
13	MAN	G	1531	13	-	0/2/19/22	0/1/1/1
13	MAN	G	1532	13	-	0/2/19/22	0/1/1/1
14	NAG	G	1533	4,14	-	0/6/23/26	0/1/1/1
14	NAG	G	1534	14	-	0/6/23/26	0/1/1/1
14	BMA	G	1535	14	-	0/2/19/22	0/1/1/1
14	MAN	G	1536	14	-	0/2/19/22	0/1/1/1
14	MAN	G	1537	14	-	0/2/19/22	0/1/1/1
14	MAN	G	1538	14	-	0/2/19/22	0/1/1/1
15	NAG	G	1539	15,4	-	0/6/23/26	0/1/1/1
15	NAG	G	1540	15	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BMA	G	1541	15	-	0/2/19/22	0/1/1/1
15	MAN	G	1542	15	-	0/2/19/22	0/1/1/1
15	MAN	G	1543	15	-	0/2/19/22	0/1/1/1
13	NAG	G	1544	13,4	-	0/6/23/26	0/1/1/1
13	NAG	G	1545	13	-	0/6/23/26	0/1/1/1
13	BMA	G	1546	13	-	0/2/19/22	0/1/1/1
13	MAN	G	1547	13	-	0/2/19/22	0/1/1/1
13	MAN	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(A)	13	-	0/2/19/22	0/1/1/1
15	NAG	G	1552	15,4	-	0/6/23/26	0/1/1/1
15	NAG	G	1553	15	-	0/6/23/26	0/1/1/1
15	BMA	G	1554	15	-	0/2/19/22	0/1/1/1
15	MAN	G	1555	15	-	0/2/19/22	0/1/1/1
15	MAN	G	1556	15	-	0/2/19/22	0/1/1/1
11	NAG	G	1557	11,4	-	0/6/23/26	0/1/1/1
11	NAG	G	1558	11	-	0/6/23/26	0/1/1/1
11	BMA	G	1559	11	-	0/2/19/22	0/1/1/1
11	MAN	G	1560	11	-	0/2/19/22	0/1/1/1
11	MAN	G	1561	11	-	0/2/19/22	0/1/1/1
11	MAN	G	1562	11	-	0/2/19/22	0/1/1/1
11	MAN	G	1563	11	-	0/2/19/22	0/1/1/1
13	NAG	G	1564	13,4	-	0/6/23/26	0/1/1/1
13	NAG	G	1565	13	-	0/6/23/26	0/1/1/1
13	BMA	G	1566	13	-	0/2/19/22	0/1/1/1
13	MAN	G	1567	13	-	0/2/19/22	0/1/1/1
13	MAN	G	1568	13	-	0/2/19/22	0/1/1/1
13	MAN	G	1569	13	-	0/2/19/22	0/1/1/1
13	MAN	G	1570	13	-	0/2/19/22	0/1/1/1
13	MAN	G	1571	13	-	0/2/19/22	0/1/1/1
16	NAG	G	1572	4,16	-	0/6/23/26	0/1/1/1
16	NAG	G	1573	16	-	0/6/23/26	0/1/1/1
16	BMA	G	1574	16	-	0/2/19/22	0/1/1/1
16	MAN	G	1575	16	-	0/2/19/22	0/1/1/1
16	MAN	G	1576	16	-	0/2/19/22	0/1/1/1
16	MAN	G	1577	16	-	0/2/19/22	0/1/1/1
16	MAN	G	1578	16	-	0/2/19/22	0/1/1/1
16	MAN	G	1579	16	-	0/2/19/22	0/1/1/1
16	MAN	G	1580(A)	16	-	0/2/19/22	0/1/1/1
16	MAN	G	1581	16	-	0/2/19/22	0/1/1/1
8	NAG	G	1584	8,4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	G	1585	8	-	0/6/23/26	0/1/1/1
8	BMA	G	1586	8	-	0/2/19/22	0/1/1/1
14	NAG	G	1587	4,14	-	0/6/23/26	0/1/1/1
14	NAG	G	1588	14	-	0/6/23/26	0/1/1/1
14	BMA	G	1589	14	-	0/2/19/22	0/1/1/1
14	MAN	G	1590	14	-	0/2/19/22	0/1/1/1
14	MAN	G	1591	14	-	0/2/19/22	0/1/1/1
14	MAN	G	1592	14	-	0/2/19/22	0/1/1/1
14	NAG	G	1593	4,14	-	0/6/23/26	0/1/1/1
14	NAG	G	1594	14	-	0/6/23/26	0/1/1/1
14	BMA	G	1595	14	-	0/2/19/22	0/1/1/1
14	MAN	G	1596	14	-	0/2/19/22	0/1/1/1
14	MAN	G	1597	14	-	0/2/19/22	0/1/1/1
14	MAN	G	1598	14	-	0/2/19/22	0/1/1/1
14	NAG	G	1599	4,14	-	0/6/23/26	0/1/1/1
14	NAG	G	1600	14	-	0/6/23/26	0/1/1/1
14	BMA	G	1601	14	-	0/2/19/22	0/1/1/1
14	MAN	G	1602	14	-	0/2/19/22	0/1/1/1
14	MAN	G	1603	14	-	0/2/19/22	0/1/1/1
14	MAN	G	1604(B)	14	-	0/2/19/22	0/1/1/1
17	NAG	H	1212	5,17	-	0/6/23/26	0/1/1/1
17	NAG	H	1213	17	-	0/6/23/26	0/1/1/1
17	BMA	H	1214	17	-	0/2/19/22	0/1/1/1
17	MAN	H	1215	17	-	0/2/19/22	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	G	1548	MAN	C1-C2	2.01	1.57	1.52
14	G	1537	MAN	C1-C2	2.05	1.57	1.52
13	G	1551(A)	MAN	C1-C2	2.05	1.57	1.52
13	G	1546	BMA	C4-C5	2.06	1.57	1.53
11	G	1562	MAN	C1-C2	2.08	1.57	1.52
13	G	1529	MAN	C4-C3	2.09	1.57	1.52
13	G	1549	MAN	C1-C2	2.13	1.57	1.52
17	H	1212	NAG	C1-C2	2.15	1.55	1.52
14	G	1536	MAN	C1-C2	2.22	1.57	1.52
11	G	1561	MAN	C1-C2	2.28	1.57	1.52
14	G	1590	MAN	O2-C2	2.33	1.48	1.43
14	G	1535	BMA	C2-C3	2.37	1.55	1.52
17	H	1214	BMA	C2-C3	2.37	1.55	1.52
11	G	1513	MAN	C2-C3	2.47	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	G	1531	MAN	C1-C2	2.55	1.58	1.52
13	G	1571	MAN	C1-C2	2.57	1.58	1.52
11	G	1511	BMA	C1-C2	2.58	1.58	1.52
14	G	1602	MAN	C1-C2	2.58	1.58	1.52
13	G	1548	MAN	C2-C3	2.59	1.56	1.52
14	G	1595	BMA	C1-C2	2.62	1.58	1.52

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	G	1577	MAN	O2-C2-C3	-2.81	104.53	110.19
14	G	1595	BMA	O2-C2-C3	-2.64	104.86	110.19
12	G	1519	MAN	O2-C2-C3	-2.60	104.94	110.19
11	G	1560	MAN	O2-C2-C3	-2.59	104.98	110.19
16	G	1575	MAN	O2-C2-C3	-2.38	105.39	110.19
12	G	1520	MAN	O2-C2-C3	-2.38	105.39	110.19
13	G	1529	MAN	O2-C2-C3	-2.37	105.41	110.19
13	G	1550	MAN	O2-C2-C3	-2.30	105.55	110.19
15	G	1555	MAN	O2-C2-C3	-2.29	105.56	110.19
16	G	1581	MAN	O2-C2-C3	-2.29	105.57	110.19
9	D	1227	MAN	O2-C2-C3	-2.28	105.59	110.19
14	G	1592	MAN	O2-C2-C3	-2.28	105.59	110.19
15	G	1542	MAN	O2-C2-C3	-2.28	105.59	110.19
14	G	1598	MAN	O2-C2-C3	-2.27	105.61	110.19
16	G	1579	MAN	O2-C2-C3	-2.26	105.62	110.19
14	G	1597	MAN	O2-C2-C3	-2.26	105.63	110.19
13	G	1569	MAN	O2-C2-C3	-2.26	105.63	110.19
16	G	1576	MAN	O2-C2-C3	-2.25	105.64	110.19
11	G	1515	MAN	O2-C2-C3	-2.25	105.64	110.19
15	G	1543	MAN	O2-C2-C3	-2.25	105.64	110.19
14	G	1538	MAN	O2-C2-C3	-2.25	105.65	110.19
11	G	1514	MAN	O2-C2-C3	-2.24	105.66	110.19
14	G	1537	MAN	O2-C2-C3	-2.24	105.67	110.19
12	G	1522	MAN	O2-C2-C3	-2.23	105.69	110.19
14	G	1591	MAN	O2-C2-C3	-2.23	105.69	110.19
11	G	1563	MAN	O2-C2-C3	-2.23	105.70	110.19
13	G	1570	MAN	O2-C2-C3	-2.22	105.71	110.19
8	G	1586	BMA	O2-C2-C3	-2.22	105.72	110.19
9	D	1230	MAN	O2-C2-C3	-2.21	105.72	110.19
9	D	1229	MAN	O2-C2-C3	-2.21	105.72	110.19
16	G	1580(A)	MAN	O2-C2-C3	-2.21	105.73	110.19
13	G	1571	MAN	O2-C2-C3	-2.21	105.74	110.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	G	1524(B)	MAN	O2-C2-C3	-2.20	105.76	110.19
13	G	1532	MAN	O2-C2-C3	-2.19	105.77	110.19
11	G	1561	MAN	O2-C2-C3	-2.17	105.81	110.19
11	G	1512	MAN	O2-C2-C3	-2.17	105.81	110.19
12	G	1521	MAN	O2-C2-C3	-2.17	105.82	110.19
15	G	1556	MAN	O2-C2-C3	-2.16	105.83	110.19
14	G	1602	MAN	O2-C2-C3	-2.15	105.85	110.19
11	G	1562	MAN	O2-C2-C3	-2.15	105.86	110.19
17	H	1215	MAN	O2-C2-C3	-2.14	105.86	110.19
13	G	1531	MAN	O2-C2-C3	-2.12	105.91	110.19
14	G	1604(B)	MAN	O2-C2-C3	-2.12	105.92	110.19
13	G	1551(A)	MAN	O2-C2-C3	-2.12	105.92	110.19
11	G	1511	BMA	O2-C2-C3	-2.11	105.93	110.19
13	G	1549	MAN	O2-C2-C3	-2.10	105.96	110.19
16	G	1578	MAN	O2-C2-C3	-2.09	105.97	110.19
13	G	1547	MAN	C1-C2-C3	-2.06	107.06	109.55
13	G	1567	MAN	O2-C2-C3	-2.05	106.05	110.19
17	H	1213	NAG	C1-O5-C5	2.03	115.13	112.14
15	G	1541	BMA	C1-O5-C5	2.04	115.14	112.14
14	G	1590	MAN	C1-O5-C5	2.11	115.24	112.14
15	G	1542	MAN	C1-O5-C5	2.13	115.27	112.14
17	H	1214	BMA	C1-O5-C5	2.14	115.28	112.14
13	G	1548	MAN	O3-C3-C4	2.14	115.19	110.36
13	G	1528	MAN	O5-C1-C2	2.16	114.35	110.89
12	G	1521	MAN	C1-O5-C5	2.16	115.32	112.14
11	G	1560	MAN	C1-O5-C5	2.24	115.43	112.14
16	G	1579	MAN	C1-O5-C5	2.24	115.44	112.14
14	G	1591	MAN	C1-O5-C5	2.26	115.47	112.14
13	G	1570	MAN	C1-O5-C5	2.29	115.51	112.14
13	G	1547	MAN	C1-O5-C5	2.35	115.59	112.14
16	G	1576	MAN	C1-O5-C5	2.35	115.59	112.14
13	G	1569	MAN	C1-O5-C5	2.35	115.60	112.14
11	G	1561	MAN	C1-O5-C5	2.36	115.61	112.14
14	G	1596	MAN	C1-O5-C5	2.36	115.61	112.14
14	G	1592	MAN	C1-O5-C5	2.37	115.62	112.14
12	G	1522	MAN	C1-O5-C5	2.41	115.68	112.14
13	G	1547	MAN	O3-C3-C2	2.42	114.44	110.01
9	D	1227	MAN	C1-O5-C5	2.42	115.71	112.14
14	G	1597	MAN	C1-O5-C5	2.43	115.72	112.14
14	G	1603	MAN	C1-O5-C5	2.53	115.86	112.14
14	G	1537	MAN	C1-C2-C3	2.63	112.73	109.55
13	G	1567	MAN	C1-O5-C5	2.63	116.01	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	G	1581	MAN	C1-O5-C5	2.64	116.03	112.14
14	G	1535	BMA	O3-C3-C2	2.65	114.86	110.01
14	G	1594	NAG	C1-O5-C5	2.65	116.04	112.14
16	G	1577	MAN	C1-O5-C5	2.70	116.11	112.14
14	G	1604(B)	MAN	C1-O5-C5	2.71	116.12	112.14
13	G	1532	MAN	C1-O5-C5	2.75	116.19	112.14
13	G	1548	MAN	C1-C2-C3	2.76	112.89	109.55
15	G	1554	BMA	C1-O5-C5	2.85	116.33	112.14
13	G	1528	MAN	C1-C2-C3	2.86	113.02	109.55
15	G	1556	MAN	C1-O5-C5	2.87	116.36	112.14
13	G	1565	NAG	O4-C4-C5	2.89	116.84	109.23
14	G	1598	MAN	C1-O5-C5	2.97	116.50	112.14
15	G	1543	MAN	C1-O5-C5	2.97	116.51	112.14
13	G	1548	MAN	C1-O5-C5	3.00	116.55	112.14
13	G	1551(A)	MAN	C1-O5-C5	3.00	116.56	112.14
13	G	1530	MAN	C1-O5-C5	3.02	116.58	112.14
9	D	1228	MAN	O3-C3-C2	3.04	115.58	110.01
11	G	1514	MAN	C1-O5-C5	3.06	116.63	112.14
11	G	1563	MAN	C1-O5-C5	3.06	116.64	112.14
12	G	1519	MAN	C1-O5-C5	3.09	116.68	112.14
12	G	1520	MAN	C1-O5-C5	3.13	116.75	112.14
12	G	1523	MAN	C1-O5-C5	3.13	116.75	112.14
13	G	1566	BMA	O3-C3-C2	3.20	115.88	110.01
15	G	1554	BMA	O3-C3-C2	3.22	115.91	110.01
11	G	1512	MAN	C1-O5-C5	3.25	116.91	112.14
14	G	1536	MAN	C1-O5-C5	3.27	116.95	112.14
15	G	1555	MAN	C1-O5-C5	3.27	116.95	112.14
13	G	1571	MAN	C1-O5-C5	3.36	117.08	112.14
11	G	1513	MAN	C1-O5-C5	3.37	117.10	112.14
14	G	1535	BMA	C1-O5-C5	3.50	117.29	112.14
12	G	1524(B)	MAN	C1-O5-C5	3.54	117.35	112.14
14	G	1601	BMA	C1-O5-C5	3.59	117.42	112.14
13	G	1565	NAG	C1-O5-C5	3.64	117.50	112.14
11	G	1513	MAN	O3-C3-C2	3.69	116.76	110.01
14	G	1590	MAN	O2-C2-C1	3.89	117.02	109.23
13	G	1568	MAN	C1-O5-C5	3.99	118.01	112.14
13	G	1531	MAN	C1-O5-C5	4.04	118.08	112.14
16	G	1575	MAN	C1-O5-C5	4.07	118.13	112.14
9	D	1228	MAN	C1-C2-C3	4.13	114.55	109.55
13	G	1549	MAN	C1-O5-C5	4.25	118.38	112.14
14	G	1602	MAN	C1-O5-C5	4.35	118.53	112.14
13	G	1566	BMA	C1-O5-C5	4.95	119.42	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	1225	NAG	1	0
9	D	1226	BMA	1	0
9	D	1228	MAN	1	0
13	G	1525	NAG	1	0
13	G	1527	BMA	2	0
13	G	1528	MAN	2	0
8	G	1585	NAG	1	0
14	G	1588	NAG	2	0
14	G	1593	NAG	1	0
17	H	1213	NAG	3	0
17	H	1214	BMA	1	0

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	NAG	B	1665	1	14,14,15	0.23	0	15,19,21	0.33	0
7	NAG	B	1666	1	14,14,15	0.21	0	15,19,21	0.25	0
7	NAG	G	1582	4	14,14,15	0.74	1 (7%)	15,19,21	0.99	1 (6%)
7	NAG	G	1583	4	14,14,15	0.22	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
7	NAG	B	1665	1	-	0/6/23/26	0/1/1/1
7	NAG	B	1666	1	-	0/6/23/26	0/1/1/1
7	NAG	G	1582	4	-	0/6/23/26	0/1/1/1
7	NAG	G	1583	4	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	1582	NAG	C1-C2	2.32	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	1582	NAG	C1-O5-C5	3.17	116.80	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	1666	NAG	1	0
7	G	1583	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	126/153 (82%)	-0.13	0 100 100	27, 78, 122, 155	0
2	D	242/243 (99%)	0.73	37 (15%) 3 1	107, 168, 258, 273	0
3	E	213/216 (98%)	0.71	38 (17%) 2 1	127, 183, 238, 258	0
4	G	453/481 (94%)	-0.24	1 (0%) 95 91	37, 71, 126, 176	0
5	H	228/244 (93%)	0.04	5 (2%) 65 42	86, 136, 180, 205	0
6	L	210/213 (98%)	-0.26	4 (1%) 70 48	66, 108, 147, 173	0
All	All	1472/1550 (94%)	0.11	85 (5%) 26 11	27, 118, 229, 273	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	189	ARG	15.1
2	D	185	PRO	12.1
3	E	143	ALA	10.2
5	H	126	SER	9.7
3	E	153	SER	8.2
3	E	136	ILE	8.2
3	E	130	ALA	7.7
2	D	215	SER	7.6
2	D	183	THR	7.6
2	D	137	ALA	7.4
3	E	156	LYS	7.2
2	D	216	CYS	7.0
2	D	184	VAL	6.9
3	E	154	PRO	6.3
2	D	131	THR	6.0
2	D	217	ASP	5.9
2	D	180	SER	5.8
2	D	212	GLU	5.6
2	D	128	SER	5.5

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Mol	Chain	Res	Type	RSRZ
2	D	129	LYS	5.4
6	L	7	PRO	5.3
3	E	157	ALA	5.3
2	D	182	VAL	4.9
2	D	213	PRO	4.8
3	E	201	THR	4.7
3	E	190	SER	4.6
2	D	172	SER	4.5
3	E	182	PRO	4.5
2	D	218	LYS	3.9
2	D	181	VAL	3.9
2	D	138	LEU	3.8
2	D	210	ARG	3.8
2	D	130	SER	3.7
2	D	190	GLY	3.7
3	E	142	GLY	3.7
3	E	152	SER	3.6
3	E	129	LYS	3.5
3	E	179	SER	3.4
3	E	198	GLU	3.4
3	E	183	GLU	3.4
2	D	211	VAL	3.4
6	L	6	ALA	3.3
2	D	124	LEU	3.2
3	E	144	VAL	3.2
2	D	189	LEU	3.2
3	E	155	VAL	3.2
3	E	131	THR	3.1
3	E	115	VAL	3.1
2	D	15	GLY	2.9
2	D	154	TRP	2.8
2	D	186	SER	2.8
3	E	175	SER	2.8
3	E	187	SER	2.7
3	E	135	LEU	2.7
6	L	119	PHE	2.7
5	H	125	SER	2.7
3	E	196	THR	2.7
3	E	116	THR	2.6
2	D	201	LYS	2.6
3	E	180	LEU	2.6
6	L	133	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
3	E	173	ALA	2.5
3	E	138	ASP	2.5
2	D	112	SER	2.4
3	E	174	ALA	2.4
3	E	191	TYR	2.4
2	D	123	PRO	2.4
5	H	150	VAL	2.3
5	H	106	SER	2.3
2	D	139	GLY	2.2
2	D	163	VAL	2.2
3	E	27	ASN	2.2
2	D	162	GLY	2.2
3	E	164	PRO	2.2
2	D	44	GLY	2.1
3	E	202	VAL	2.1
3	E	74	THR	2.1
3	E	137	SER	2.1
2	D	191	THR	2.1
4	G	135	THR	2.1
3	E	113	PRO	2.1
2	D	188	SER	2.1
2	D	164	HIS	2.0
3	E	185	TRP	2.0
5	H	36	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
11	NAG	G	1509	14/15	0.85	0.23	1.19	121,134,144,146	0
9	BMA	D	1226	11/12	0.81	0.17	1.03	104,110,130,134	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
13	NAG	G	1525	14/15	0.90	0.19	0.24	97,107,126,130	0
16	NAG	G	1572	14/15	0.92	0.19	0.20	77,96,101,111	0
10	NAG	G	1507	14/15	0.89	0.18	-0.12	125,145,159,164	0
12	NAG	G	1516	14/15	0.85	0.24	-0.19	59,82,93,93	0
9	NAG	D	1225	14/15	0.87	0.16	-0.40	98,117,124,124	0
13	NAG	G	1544	14/15	0.96	0.19	-0.45	46,67,85,86	0
16	MAN	G	1577	11/12	0.98	0.15	-0.64	30,42,62,63	0
9	MAN	D	1230	11/12	0.82	0.13	-0.76	110,119,139,150	0
11	NAG	G	1557	14/15	0.92	0.17	-0.98	55,85,107,111	0
16	MAN	G	1575	11/12	0.97	0.17	-1.02	37,53,93,120	0
14	NAG	G	1533	14/15	0.90	0.16	-1.24	114,130,143,148	0
9	NAG	D	1506	14/15	0.92	0.14	-1.26	65,78,93,96	0
15	NAG	G	1539	14/15	0.86	0.12	-1.90	106,124,138,140	0
13	BMA	G	1527	11/12	0.64	0.32	-	166,185,192,193	0
14	NAG	G	1594	14/15	0.84	0.19	-	155,161,165,169	0
14	MAN	G	1537	11/12	0.83	0.11	-	169,172,180,187	0
13	NAG	G	1545	14/15	0.94	0.19	-	89,100,124,140	0
14	NAG	G	1588	14/15	0.90	0.14	-	96,113,124,130	0
14	MAN	G	1538	11/12	0.78	0.50	-	181,187,189,191	0
8	NAG	B	1667	14/15	0.85	0.35	-	122,146,158,166	0
14	MAN	G	1596	11/12	0.72	0.20	-	170,187,192,194	0
13	MAN	G	1571	11/12	0.73	0.22	-	177,183,191,194	0
14	MAN	G	1602	11/12	0.72	0.38	-	169,180,186,190	0
14	NAG	G	1599	14/15	0.93	0.12	-	88,105,122,148	0
9	MAN	D	1227	11/12	0.85	0.24	-	117,131,136,137	0
15	MAN	G	1555	11/12	0.63	0.19	-	182,190,203,205	0
13	MAN	G	1528	11/12	0.69	0.37	-	181,190,192,193	0
14	MAN	G	1597	11/12	0.62	0.31	-	156,174,179,180	0
11	MAN	G	1563	11/12	0.67	0.22	-	163,174,181,184	0
15	MAN	G	1556	11/12	0.60	0.36	-	181,189,190,192	0
13	MAN	G	1551(A)	11/12	0.77	0.27	-	150,160,174,177	0
9	MAN	D	1229	11/12	0.94	0.12	-	127,131,141,142	0
14	NAG	G	1600	14/15	0.78	0.20	-	135,153,163,173	0
12	MAN	G	1522	11/12	0.69	0.40	-	183,188,194,195	0
11	MAN	G	1513	11/12	0.55	0.32	-	172,178,197,200	0
12	MAN	G	1521	11/12	0.88	0.14	-	131,140,154,158	0
14	MAN	G	1536	11/12	0.17	0.54	-	183,189,194,195	0
8	NAG	B	1668	14/15	0.65	0.40	-	173,184,193,197	0
14	NAG	G	1587	14/15	0.97	0.14	-	62,83,112,112	0
14	MAN	G	1592	11/12	0.58	0.53	-	175,184,193,197	0
12	NAG	G	1517	14/15	0.84	0.22	-	96,111,126,129	0
15	BMA	G	1541	11/12	0.80	0.14	-	160,167,172,176	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
12	MAN	G	1520	11/12	0.54	0.18	-	174,182,190,200	0
11	MAN	G	1514	11/12	0.86	0.35	-	173,179,184,188	0
14	MAN	G	1603	11/12	0.84	0.33	-	172,182,193,195	0
13	MAN	G	1547	11/12	0.90	0.16	-	125,136,152,156	0
13	MAN	G	1531	11/12	0.80	0.25	-	164,170,180,183	0
13	NAG	G	1565	14/15	0.91	0.17	-	128,145,154,154	0
14	BMA	G	1595	11/12	0.67	0.15	-	171,174,195,195	0
12	MAN	G	1524(B)	11/12	0.54	0.22	-	180,190,196,196	0
13	MAN	G	1549	11/12	0.93	0.16	-	121,135,145,154	0
14	BMA	G	1601	11/12	0.62	0.26	-	162,176,180,185	0
15	BMA	G	1554	11/12	0.58	0.29	-	189,195,203,203	0
15	NAG	G	1553	14/15	0.81	0.37	-	160,169,182,184	0
16	MAN	G	1578	11/12	0.91	0.11	-	132,142,147,166	0
13	MAN	G	1568	11/12	0.73	0.15	-	178,183,193,193	0
9	MAN	D	1228	11/12	0.93	0.12	-	109,132,138,138	0
13	MAN	G	1529	11/12	0.92	0.17	-	180,182,186,188	0
14	MAN	G	1591	11/12	0.67	0.22	-	165,170,174,178	0
16	NAG	G	1573	14/15	0.95	0.16	-	51,80,100,108	0
15	NAG	G	1552	14/15	0.78	0.21	-	126,140,155,158	0
14	MAN	G	1604(B)	11/12	0.61	0.60	-	177,189,199,199	0
16	MAN	G	1579	11/12	0.90	0.19	-	92,105,128,138	0
11	NAG	G	1510	14/15	0.87	0.15	-	110,128,138,146	0
14	MAN	G	1590	11/12	0.74	0.35	-	178,186,190,190	0
14	NAG	G	1593	14/15	0.91	0.11	-	94,111,130,154	0
8	BMA	B	1669	11/12	0.81	0.66	-	184,198,201,206	0
11	MAN	G	1515	11/12	0.54	0.37	-	164,179,186,190	0
11	MAN	G	1560	11/12	0.83	0.14	-	161,171,181,183	0
14	BMA	G	1589	11/12	0.81	0.21	-	152,157,164,172	0
13	MAN	G	1567	11/12	0.80	0.29	-	176,187,192,195	0
16	MAN	G	1576	11/12	0.76	0.18	-	106,120,130,130	0
15	MAN	G	1543	11/12	0.80	0.26	-	157,167,174,174	0
10	NAG	G	1508	14/15	0.69	0.22	-	142,154,157,158	0
16	BMA	G	1574	11/12	0.93	0.16	-	75,92,107,118	0
13	MAN	G	1569	11/12	0.86	0.13	-	184,193,198,198	0
11	BMA	G	1559	11/12	0.88	0.07	-	139,155,196,199	0
17	MAN	H	1215	11/12	0.88	0.13	-	196,207,213,216	0
8	NAG	G	1584	14/15	0.95	0.12	-	97,107,118,118	0
16	MAN	G	1580(A)	11/12	0.80	0.22	-	137,147,159,164	0
17	BMA	H	1214	11/12	0.53	0.24	-	200,203,210,212	0
17	NAG	H	1213	14/15	0.69	0.31	-	197,206,211,213	0
11	MAN	G	1561	11/12	0.81	0.13	-	160,172,181,184	0
12	MAN	G	1519	11/12	0.90	0.14	-	133,146,160,161	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
13	NAG	G	1564	14/15	0.93	0.20	-	96,111,122,127	0
12	MAN	G	1523	11/12	0.67	0.23	-	189,197,201,201	0
13	MAN	G	1548	11/12	0.79	0.12	-	152,157,173,175	0
14	BMA	G	1535	11/12	0.44	0.33	-	162,168,181,186	0
15	NAG	G	1540	14/15	0.82	0.22	-	136,148,158,165	0
14	NAG	G	1534	14/15	0.82	0.15	-	127,141,149,155	0
16	MAN	G	1581	11/12	0.93	0.17	-	70,107,120,133	0
11	NAG	G	1558	14/15	0.89	0.20	-	107,126,141,143	0
14	MAN	G	1598	11/12	0.61	0.19	-	172,183,193,194	0
13	MAN	G	1550	11/12	0.80	0.26	-	164,172,173,173	0
13	BMA	G	1566	11/12	0.58	0.10	-	160,172,177,177	0
13	MAN	G	1532	11/12	0.85	0.12	-	166,174,176,177	0
11	MAN	G	1512	11/12	0.57	0.19	-	147,162,167,175	0
15	MAN	G	1542	11/12	0.70	0.23	-	177,183,187,188	0
13	MAN	G	1570	11/12	0.67	0.24	-	177,185,188,189	0
11	BMA	G	1511	11/12	0.84	0.11	-	144,156,170,176	0
12	BMA	G	1518	11/12	0.79	0.15	-	128,136,154,168	0
8	NAG	G	1585	14/15	0.89	0.13	-	97,108,120,141	0
11	MAN	G	1562	11/12	0.53	0.27	-	171,181,185,186	0
8	BMA	G	1586	11/12	0.67	0.23	-	125,136,147,149	0
13	MAN	G	1530	11/12	0.82	0.42	-	178,185,191,193	0
13	BMA	G	1546	11/12	0.90	0.12	-	124,135,150,157	0
17	NAG	H	1212	14/15	0.82	0.12	-	138,168,180,189	0
13	NAG	G	1526	14/15	0.88	0.15	-	133,147,161,178	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
7	NAG	B	1666	14/15	0.88	0.16	-0.72	100,112,117,117	0
7	NAG	B	1665	14/15	0.66	0.47	-	132,154,161,168	0
7	NAG	G	1583	14/15	0.77	0.31	-	155,171,177,177	0
7	NAG	G	1582	14/15	0.77	0.14	-	107,129,144,146	0

6.5 Other polymers (i)

There are no such residues in this entry.