



Full wwPDB X-ray Structure Validation Report

Feb 18, 2018 – 06:07 am GMT

PDB ID : 1LGC
Title : INTERACTION OF A LEGUME LECTIN WITH THE N2 FRAGMENT OF HUMAN LACTOTRANSFERRIN OR WITH THE ISOLATED BIAN-TEN-NARY GLYCOPEPTIDE: ROLE OF THE FUCOSE MOIETY
Authors : Bourne, Y.; Cambillau, C.
Deposited on : 1994-01-07
Resolution : 2.80 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the  symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

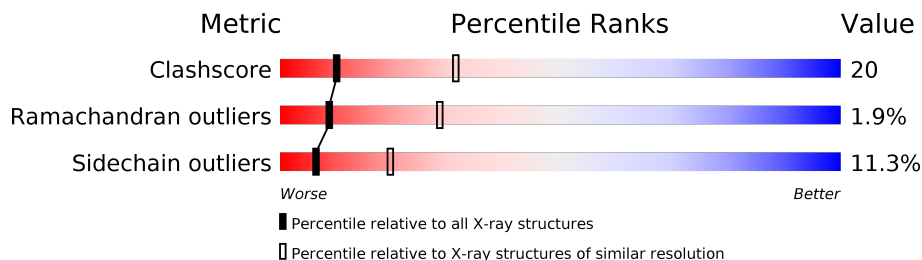
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	122078	3207 (2.80-2.80)
Ramachandran outliers	120005	3156 (2.80-2.80)
Sidechain outliers	119972	3158 (2.80-2.80)



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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	181	
1	C	181	
1	E	181	
2	H	2	
2	I	2	
2	J	2	
3	B	53	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	D	53	 58% 28% 8% 9%
3	F	53	 42% 40% 8% 11%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 6044 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 LEGUME ISOLECTIN II (ALPHA CHAIN).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
1	A	181	1407	896	232	279	0	0	0
1	C	181	1407	896	232	279	0	0	0
1	E	181	1397	889	231	277	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	PRO	GLN	CONFLICT	UNP P04122
A	168	GLY	ALA	CONFLICT	UNP P04122
C	16	PRO	GLN	CONFLICT	UNP P04122
C	168	GLY	ALA	CONFLICT	UNP P04122
E	16	PRO	GLN	CONFLICT	UNP P04122
E	168	GLY	ALA	CONFLICT	UNP P04122

- Molecule 2 is a protein called DIPEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	H	1	9	4	2	3	0	0	0
2	I	1	9	4	2	3	0	0	0
2	J	2	18	9	4	5	0	0	0

- Molecule 3 is a protein called LEGUME ISOLECTIN II (BETA CHAIN).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	B	51	401	261	61	79	0	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	48	Total	C	N	O	0	0	1
			380	249	58	73			
3	F	47	Total	C	N	O	0	0	1
			371	244	57	70			

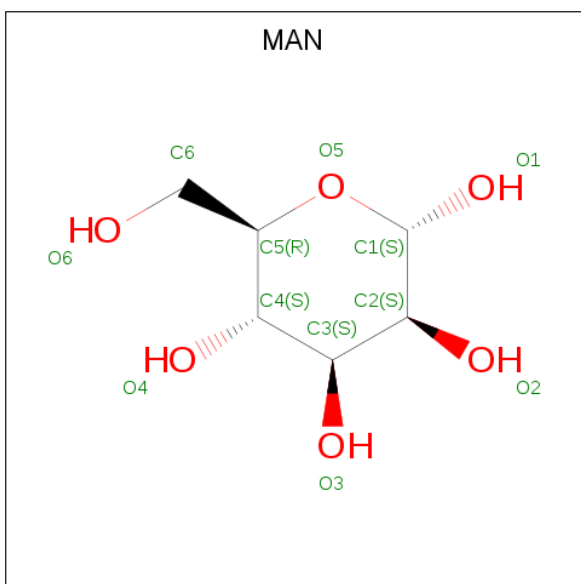
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	C	1	Total	Ca	0	0
			1	1		
4	E	1	Total	Ca	0	0
			1	1		

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

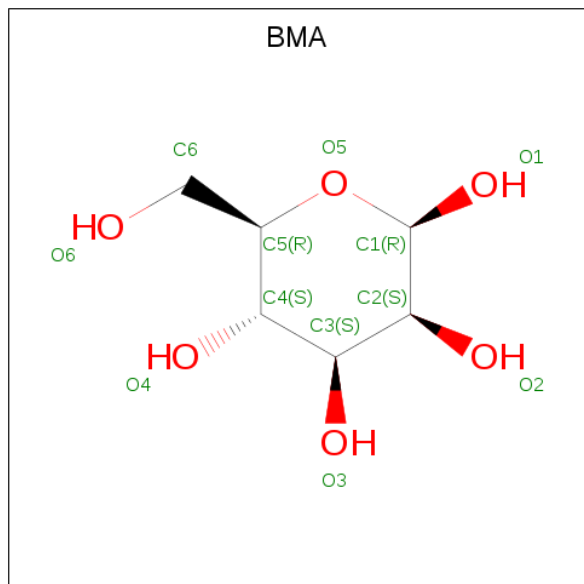
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mn	0	0
			1	1		
5	C	1	Total	Mn	0	0
			1	1		
5	E	1	Total	Mn	0	0
			1	1		

- Molecule 6 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).



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

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



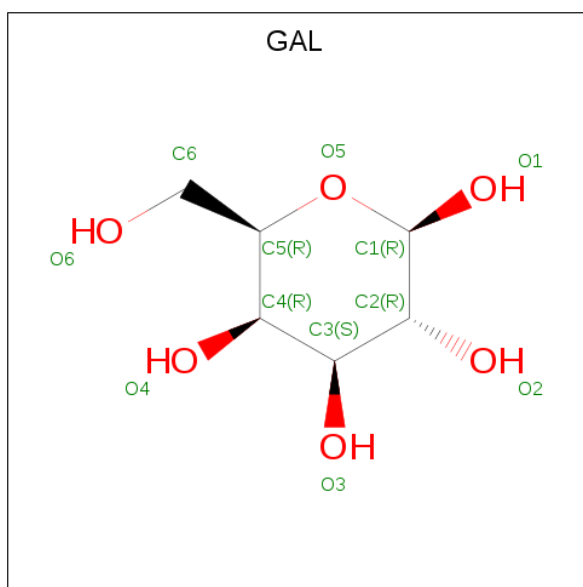
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	H	1	Total C O 11 6 5	0	0
7	I	1	Total C O 11 6 5	0	0
7	J	1	Total C O 11 6 5	0	0

- Molecule 8 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



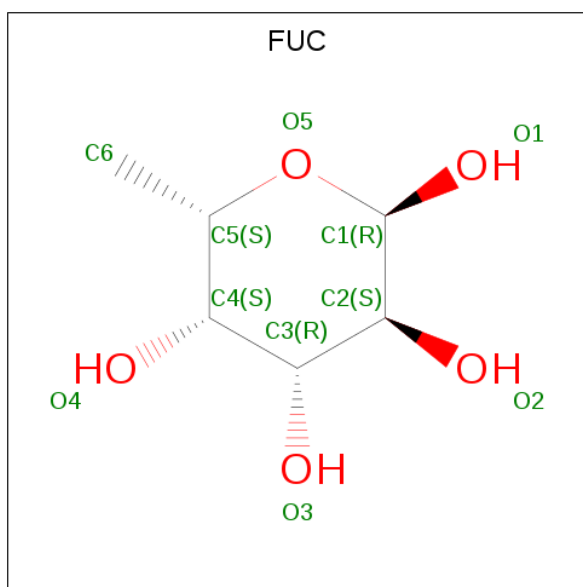
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
8	H	1	14	8	1	5	0	0
8	H	1	14	8	1	5	0	0
8	H	1	14	8	1	5	0	0
8	H	1	14	8	1	5	0	0
8	I	1	14	8	1	5	0	0
8	I	1	14	8	1	5	0	0
8	I	1	14	8	1	5	0	0
8	J	1	14	8	1	5	0	0
8	J	1	14	8	1	5	0	0
8	J	1	14	8	1	5	0	0

- Molecule 9 is BETA-D-GALACTOSE (three-letter code: GAL) (formula: C₆H₁₂O₆).



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

- Molecule 10 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: C₆H₁₂O₅).



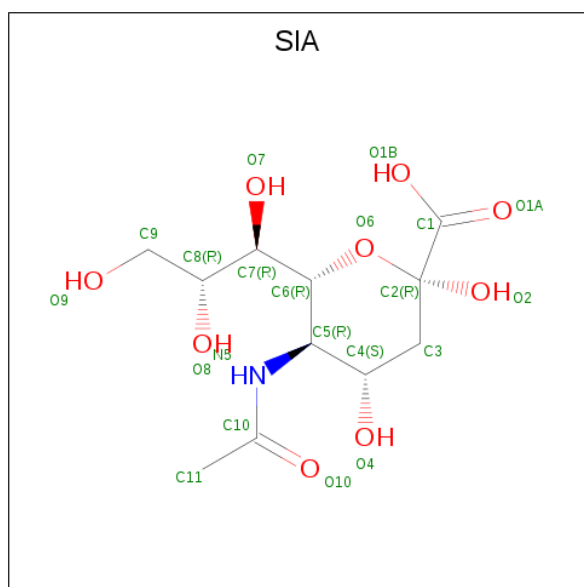
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	H	1	Total	C	O	0	0
			10	6	4		

Continued on next page...

Continued from previous page...

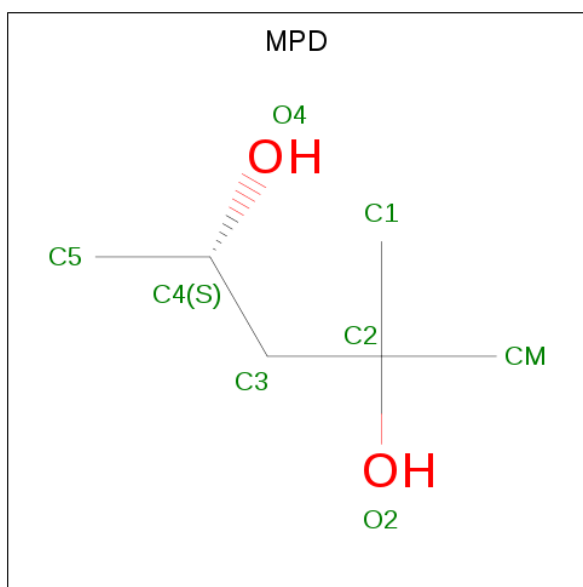
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	H	1	Total	C	O	0	0
			10	6	4		
10	I	1	Total	C	O	0	0
			10	6	4		
10	J	1	Total	C	O	0	0
			10	6	4		

- Molecule 11 is O-SIALIC ACID (three-letter code: SIA) (formula: $C_{11}H_{19}NO_9$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	I	1	Total	C	N	O	0	0
			20	11	1	8		
11	J	1	Total	C	N	O	0	0
			20	11	1	8		

- Molecule 12 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	E	1	Total C O 8 6 2	0	0

- Molecule 13 is water.

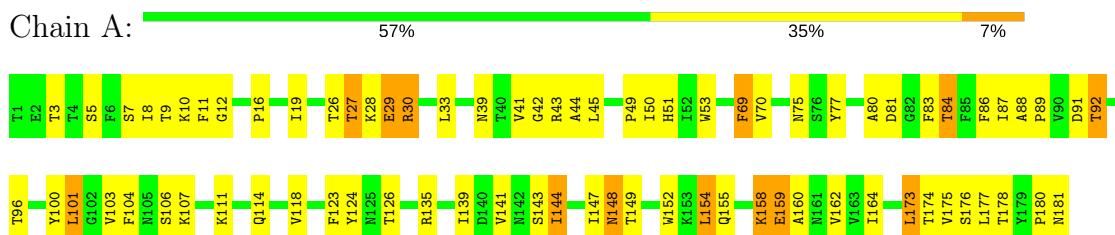
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	74	Total O 74 74	0	0
13	H	15	Total O 15 15	0	0
13	B	22	Total O 22 22	0	0
13	C	74	Total O 74 74	0	0
13	I	8	Total O 8 8	0	0
13	D	21	Total O 21 21	0	0
13	E	48	Total O 48 48	0	0
13	J	6	Total O 6 6	0	0
13	F	11	Total O 11 11	0	0

3 Residue-property plots i

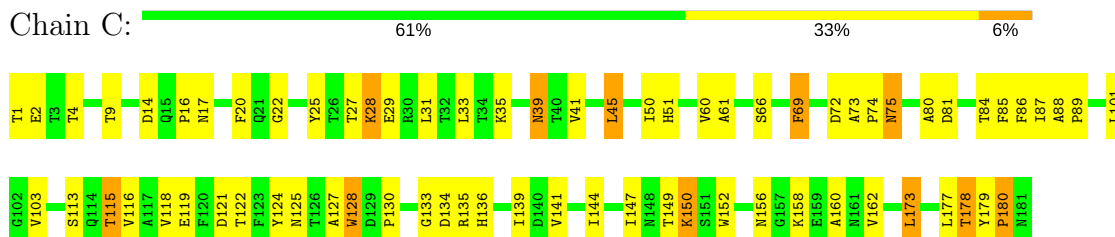
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

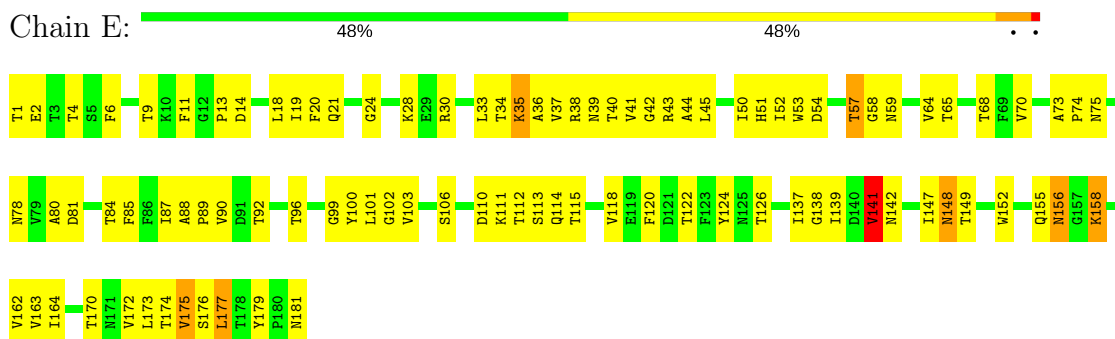
- Molecule 1: LEGUME ISOLECTIN II (ALPHA CHAIN)



- Molecule 1: LEGUME ISOLECTIN II (ALPHA CHAIN)



- Molecule 1: LEGUME ISOLECTIN II (ALPHA CHAIN)



- Molecule 2: DIPEPTIDE



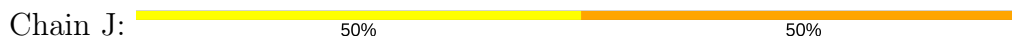
NE12
GLN

- Molecule 2: DIPEPTIDE



NE12
GLN

- Molecule 2: DIPEPTIDE



NE12
QS13

- Molecule 3: LEGUME ISOLECTIN II (BETA CHAIN)



E1 T2 S9 Y4 T5 L6 N7 P11 E14 F15 V16 F17 E18 W19 V20 F24 S25 A26 T27 F32 E36 V37 L38 Y41 F42 M43 S44 V48 S51 SER ASN

- Molecule 3: LEGUME ISOLECTIN II (BETA CHAIN)



E1 Y4 L6 N7 K13 M19 V20 R21 L22 G23 F24 S25 E31 V37 L38 F42 M43 S44 E45 L46 S47 V48 THR SER SER SER ASN

- Molecule 3: LEGUME ISOLECTIN II (BETA CHAIN)



GLU T2 S3 Y4 T5 L6 N7 E8 V9 P11 V16 P17 E18 W19 V20 R21 L22 G23 F24 S25 A26 T27 E31 F32 H35 L38 S39 W40 Y41 F42 L46 S47 V48 THR SER SER SER ASN

4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	117.00Å 117.00Å 120.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.185 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	6044	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, BMA, NAG, CA, MN, SIA, GAL, FUC, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.44	0/1442	0.76	1/1967 (0.1%)
1	C	0.44	0/1442	0.74	0/1967
1	E	0.44	0/1431	0.74	0/1952
2	H	0.93	0/8	0.72	0/8
2	I	0.74	0/8	0.66	0/8
2	J	0.65	0/17	0.56	0/20
3	B	0.47	0/413	0.66	0/566
3	D	0.50	0/392	0.70	0/537
3	F	0.50	0/383	0.65	0/525
All	All	0.45	0/5536	0.73	1/7550 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	154	LEU	CA-CB-CG	5.12	127.08	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1407	0	1357	61	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1407	0	1357	51	0
1	E	1397	0	1346	83	0
2	H	9	0	4	1	0
2	I	9	0	4	0	0
2	J	18	0	11	2	0
3	B	401	0	377	23	0
3	D	380	0	353	18	0
3	F	371	0	344	41	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	E	1	0	0	0	0
6	H	22	0	18	1	0
6	I	22	0	19	3	0
6	J	22	0	19	0	0
7	H	11	0	8	0	0
7	I	11	0	8	2	0
7	J	11	0	8	0	0
8	H	56	0	47	3	0
8	I	42	0	35	2	0
8	J	42	0	35	3	0
9	H	11	0	10	1	0
9	I	11	0	9	0	0
9	J	11	0	9	0	0
10	H	20	0	20	3	0
10	I	10	0	10	0	0
10	J	10	0	10	0	0
11	I	20	0	17	1	0
11	J	20	0	17	0	0
12	E	8	0	14	1	0
13	A	74	0	0	2	0
13	B	22	0	0	1	0
13	C	74	0	0	2	0
13	D	21	0	0	0	0
13	E	48	0	0	4	0
13	F	11	0	0	1	0
13	H	15	0	0	1	0
13	I	8	0	0	0	0
13	J	6	0	0	0	0
All	All	6044	0	5466	228	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 20.

All (228) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:ALA:HB1	1:C:177:LEU:HD11	1.38	1.04
1:E:54:ASP:HB2	3:F:46:LEU:HD21	1.62	0.82
1:C:14:ASP:HA	13:C:306:HOH:O	1.80	0.79
3:F:16:VAL:HG22	3:F:17:PRO:HD2	1.66	0.77
1:A:33:LEU:O	1:A:42:GLY:HA3	1.86	0.76
1:A:45:LEU:HD21	1:A:86:PHE:CZ	2.26	0.71
1:C:160:ALA:HB1	1:C:177:LEU:CD1	2.19	0.69
1:E:4:THR:HG21	1:E:50:ILE:HG22	1.74	0.68
1:A:118:VAL:HG11	1:A:164:ILE:HD13	1.75	0.68
1:E:162:VAL:HG22	1:E:177:LEU:HD22	1.76	0.68
3:F:17:PRO:HB2	13:F:163:HOH:O	1.93	0.68
1:E:87:ILE:HG22	3:F:16:VAL:HG21	1.75	0.67
3:D:43:ASN:HD22	3:D:44:SER:N	1.93	0.66
1:C:88:ALA:HB1	1:C:89:PRO:HD2	1.79	0.65
1:C:150:LYS:HD2	3:D:5:THR:O	1.96	0.65
1:A:107:LYS:HB3	1:A:107:LYS:NZ	2.13	0.64
1:E:57:THR:HB	1:E:59:ASN:OD1	1.98	0.64
13:E:347:HOH:O	3:F:22:ILE:HD13	1.96	0.64
1:E:68:THR:HG23	3:F:38:LEU:HB2	1.80	0.64
1:C:113:SER:O	1:C:115:THR:HG22	1.97	0.63
1:E:52:ILE:HG22	3:F:18:GLU:O	1.99	0.63
1:A:88:ALA:HB1	1:A:89:PRO:HD2	1.80	0.63
1:E:84:THR:HG21	1:E:103:VAL:HG21	1.79	0.63
1:E:158:LYS:HB2	1:E:179:TYR:CE2	2.34	0.62
1:E:33:LEU:O	1:E:42:GLY:HA3	2.00	0.61
1:E:33:LEU:HD11	3:F:24:PHE:HB2	1.82	0.61
3:D:13:LYS:NZ	3:D:13:LYS:HB2	2.15	0.61
1:E:137:ILE:HD11	1:E:177:LEU:HB2	1.82	0.61
1:E:147:ILE:O	1:E:148:ASN:HB2	2.00	0.61
1:C:173:LEU:O	3:D:7:ASN:HA	2.02	0.60
1:A:111:LYS:NZ	1:A:111:LYS:HB3	2.17	0.59
1:E:111:LYS:HD3	13:E:320:HOH:O	2.02	0.59
1:E:155:GLN:HB2	1:E:179:TYR:CE2	2.38	0.59
7:I:502:BMA:H4	6:I:503:MAN:C2	2.31	0.59
1:E:148:ASN:OD1	3:F:6:LEU:HD21	2.03	0.58
1:C:122:THR:HA	1:C:135:ARG:HG2	1.85	0.58
1:E:35:LYS:O	1:E:37:VAL:N	2.37	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:90:VAL:HG13	3:F:21:ARG:NH2	2.18	0.58
1:A:12:GLY:O	1:A:26:THR:HG21	2.04	0.57
1:C:84:THR:HB	3:D:25:SER:HB3	1.87	0.57
1:C:160:ALA:CB	1:C:177:LEU:HD11	2.26	0.57
1:A:49:PRO:HD2	1:C:17:ASN:HA	1.87	0.57
3:B:38:LEU:N	3:B:38:LEU:HD12	2.20	0.57
7:I:502:BMA:H4	6:I:503:MAN:C1	2.35	0.57
1:A:152:TRP:CZ2	1:A:154:LEU:HD23	2.40	0.56
1:A:80:ALA:HB2	1:A:123:PHE:CD2	2.40	0.56
1:E:73:ALA:HB3	1:E:156:ASN:OD1	2.04	0.56
3:B:16:VAL:HG13	3:B:20:VAL:HG11	1.87	0.56
8:H:516:NAG:N2	10:H:518:FUC:O5	2.39	0.56
1:E:118:VAL:HG21	1:E:164:ILE:HD13	1.86	0.56
1:A:80:ALA:HB2	1:A:123:PHE:HD2	1.71	0.56
3:B:11:PRO:HG2	3:B:15:PHE:HE2	1.71	0.56
1:E:38:ARG:O	1:E:40:THR:HG23	2.06	0.56
1:C:136:HIS:HA	1:C:152:TRP:HB3	1.87	0.55
1:E:173:LEU:O	3:F:7:ASN:HA	2.06	0.55
1:E:120:PHE:CE2	1:E:177:LEU:HD23	2.42	0.55
1:A:148:ASN:HD22	1:A:149:THR:H	1.54	0.55
3:D:22:ILE:HD13	3:D:42:PHE:CE1	2.42	0.55
3:B:48:VAL:HG21	1:C:9:THR:OG1	2.07	0.55
8:H:516:NAG:N2	10:H:518:FUC:C1	2.69	0.55
1:C:87:ILE:HB	1:C:116:VAL:HG22	1.89	0.54
1:E:158:LYS:HB2	1:E:179:TYR:HE2	1.70	0.54
1:E:176:SER:HA	3:F:4:TYR:O	2.07	0.54
1:E:33:LEU:HD11	3:F:24:PHE:CB	2.37	0.54
1:E:152:TRP:HE1	1:E:179:TYR:HE1	1.54	0.54
1:E:84:THR:HB	3:F:25:SER:OG	2.07	0.54
1:E:110:ASP:OD2	1:E:112:THR:HB	2.09	0.53
1:C:80:ALA:CB	3:D:31:GLU:HB2	2.38	0.53
1:E:92:THR:HA	13:E:336:HOH:O	2.09	0.53
1:E:148:ASN:ND2	3:F:8:GLU:HG2	2.24	0.53
1:E:139:ILE:HD12	3:F:8:GLU:HB2	1.90	0.52
1:C:14:ASP:O	1:C:16:PRO:HD3	2.10	0.52
1:C:45:LEU:HD12	3:D:21:ARG:HD3	1.90	0.52
1:E:19:ILE:O	1:E:44:ALA:HA	2.09	0.52
1:E:162:VAL:CG2	1:E:177:LEU:HD22	2.39	0.52
1:A:160:ALA:HB1	1:A:177:LEU:HG	1.92	0.52
1:A:87:ILE:HG22	3:B:16:VAL:HG21	1.91	0.52
1:C:101:LEU:HD23	1:C:144:ILE:HD11	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:VAL:HA	1:A:176:SER:O	2.10	0.52
1:E:51:HIS:HB2	3:F:19:TRP:CZ3	2.45	0.52
1:E:51:HIS:HB2	3:F:19:TRP:CH2	2.45	0.51
1:C:28:LYS:HG2	13:C:362:HOH:O	2.11	0.51
1:E:87:ILE:O	1:E:115:THR:HG23	2.11	0.50
1:A:43:ARG:HH22	1:A:92:THR:CG2	2.23	0.50
1:C:150:LYS:HB2	1:C:150:LYS:NZ	2.26	0.50
1:C:22:GLY:HA3	1:C:41:VAL:O	2.11	0.50
3:F:16:VAL:CG2	3:F:17:PRO:HD2	2.37	0.50
3:B:11:PRO:HG2	3:B:15:PHE:CE2	2.45	0.50
1:C:84:THR:HG21	1:C:103:VAL:HG21	1.93	0.50
1:A:164:ILE:HA	1:A:174:THR:O	2.12	0.50
1:C:4:THR:HG21	1:C:50:ILE:CD1	2.41	0.50
1:E:81:ASP:OD1	1:E:99:GLY:HA2	2.11	0.50
1:E:122:THR:HG22	1:E:152:TRP:CZ3	2.47	0.50
1:A:124:TYR:CE2	1:A:126:THR:HG22	2.47	0.49
1:E:70:VAL:HG23	3:F:38:LEU:HD11	1.94	0.49
1:C:80:ALA:HB3	3:D:31:GLU:HB2	1.94	0.49
1:E:30:ARG:HE	3:F:38:LEU:HD21	1.75	0.49
1:A:75:ASN:OD1	1:A:77:TYR:HD2	1.95	0.49
8:H:516:NAG:H61	9:H:517:GAL:O2	2.13	0.49
8:J:508:NAG:O7	8:J:508:NAG:C1	2.60	0.49
1:A:144:ILE:O	1:A:144:ILE:HD13	2.12	0.49
1:C:75:ASN:HD22	1:C:75:ASN:H	1.58	0.49
3:F:22:ILE:H	3:F:22:ILE:HD13	1.78	0.49
1:E:1:THR:HA	3:F:46:LEU:O	2.13	0.49
1:E:149:THR:HG23	12:E:303:MPD:H53	1.95	0.48
1:E:148:ASN:HD22	3:F:8:GLU:HG2	1.78	0.48
1:C:25:TYR:OH	1:C:35:LYS:HD3	2.13	0.48
1:E:101:LEU:O	1:E:103:VAL:HG23	2.14	0.48
1:E:37:VAL:HG12	1:E:38:ARG:N	2.29	0.48
1:E:74:PRO:HG3	3:F:32:PHE:CE2	2.49	0.48
1:A:155:GLN:HB3	1:A:158:LYS:HB2	1.96	0.47
1:E:164:ILE:HG12	1:E:175:VAL:HB	1.96	0.47
1:A:96:THR:HG23	10:H:518:FUC:H63	1.96	0.47
1:A:101:LEU:HA	3:B:27:THR:OG1	2.15	0.47
1:A:100:TYR:CE1	1:A:106:SER:HA	2.49	0.47
1:A:100:TYR:HA	1:A:144:ILE:HG13	1.97	0.47
1:C:141:VAL:HG23	1:C:141:VAL:O	2.14	0.47
1:E:114:GLN:O	3:F:16:VAL:HG23	2.14	0.47
1:E:13:PRO:HB3	13:E:328:HOH:O	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:VAL:HG22	1:A:159:GLU:HB3	1.97	0.47
1:C:119:GLU:OE2	1:C:121:ASP:HB2	2.14	0.47
1:A:9:THR:O	1:A:10:LYS:HG3	2.15	0.47
1:A:26:THR:HG22	13:A:336:HOH:O	2.14	0.47
1:A:173:LEU:O	3:B:7:ASN:HB2	2.15	0.47
1:C:149:THR:CG2	1:C:150:LYS:N	2.77	0.47
1:E:80:ALA:HB3	3:F:31:GLU:HB2	1.97	0.47
6:H:519:MAN:O4	13:H:265:HOH:O	2.20	0.47
1:A:11:PHE:O	1:A:29:GLU:HA	2.15	0.46
1:E:21:GLN:HE22	1:E:43:ARG:HH21	1.63	0.46
1:E:141:VAL:O	1:E:142:ASN:HB2	2.15	0.46
1:A:180:PRO:O	1:A:181:ASN:HB2	2.16	0.46
1:A:26:THR:O	1:A:26:THR:HG23	2.16	0.46
1:A:43:ARG:HH22	1:A:92:THR:HG22	1.80	0.46
1:E:89:PRO:O	1:E:92:THR:HG22	2.16	0.46
1:E:80:ALA:CB	3:F:31:GLU:HB2	2.46	0.46
1:A:69:PHE:CE1	1:A:160:ALA:HB3	2.51	0.45
1:C:25:TYR:CE2	1:C:27:THR:OG1	2.69	0.45
1:C:69:PHE:HA	3:D:37:VAL:HA	1.98	0.45
1:E:137:ILE:HG22	1:E:138:GLY:N	2.31	0.45
1:E:88:ALA:HB1	1:E:89:PRO:HD2	1.98	0.45
3:B:14:GLU:HB2	13:B:75:HOH:O	2.16	0.45
1:A:139:ILE:O	1:A:147:ILE:HG12	2.16	0.45
1:A:111:LYS:HZ2	1:A:111:LYS:HB3	1.81	0.45
1:A:80:ALA:O	3:B:32:PHE:HA	2.17	0.45
1:E:96:THR:O	1:E:102:GLY:HA2	2.17	0.45
11:I:511:SIA:C9	11:I:511:SIA:O6	2.64	0.45
1:C:51:HIS:CD2	3:D:46:LEU:HD23	2.51	0.45
1:E:78:ASN:HD21	2:J:512:ASN:ND2	2.14	0.45
1:C:152:TRP:HA	3:D:4:TYR:CE2	2.52	0.45
3:D:13:LYS:HB2	3:D:13:LYS:HZ3	1.82	0.44
1:A:83:PHE:CZ	3:B:24:PHE:CD1	3.05	0.44
1:C:60:VAL:HG12	1:C:61:ALA:N	2.33	0.44
1:E:20:PHE:HB3	1:E:24:GLY:O	2.18	0.44
1:E:122:THR:HG22	1:E:152:TRP:HZ3	1.83	0.44
1:A:159:GLU:HG2	1:A:159:GLU:H	1.70	0.44
1:E:102:GLY:N	3:F:27:THR:HG21	2.33	0.44
1:A:148:ASN:HD22	1:A:149:THR:N	2.14	0.44
1:A:5:SER:OG	3:B:43:ASN:ND2	2.50	0.44
1:E:100:TYR:HE2	1:E:106:SER:HA	1.83	0.44
1:A:70:VAL:CG2	1:A:159:GLU:HB3	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:VAL:HA	3:B:27:THR:HG22	2.00	0.44
1:C:69:PHE:HD1	1:C:69:PHE:H	1.66	0.44
1:C:84:THR:CG2	1:C:85:PHE:N	2.80	0.44
1:C:45:LEU:HD22	1:C:86:PHE:CZ	2.53	0.44
1:E:52:ILE:HG23	1:E:53:TRP:HD1	1.83	0.44
1:A:27:THR:O	1:A:30:ARG:HG2	2.17	0.44
1:C:125:ASN:HB2	1:C:128:TRP:NE1	2.33	0.43
1:C:130:PRO:HG2	1:C:149:THR:HG21	1.99	0.43
1:E:11:PHE:HE1	3:F:39:SER:HA	1.84	0.43
1:A:114:GLN:HA	3:B:15:PHE:O	2.19	0.43
1:C:177:LEU:HD12	1:C:178:THR:N	2.32	0.43
1:E:162:VAL:HG12	1:E:163:VAL:N	2.33	0.43
1:E:41:VAL:HG13	3:F:27:THR:HG22	1.99	0.43
1:E:174:THR:HA	3:F:6:LEU:O	2.18	0.43
1:E:84:THR:CG2	1:E:85:PHE:N	2.82	0.43
1:A:51:HIS:HB3	13:A:305:HOH:O	2.19	0.43
3:B:6:LEU:HD12	3:B:7:ASN:H	1.84	0.43
1:E:9:THR:O	1:E:9:THR:HG22	2.18	0.43
1:A:19:ILE:O	1:A:44:ALA:HA	2.19	0.43
1:E:65:THR:HB	3:F:42:PHE:HD2	1.83	0.43
1:A:107:LYS:HB3	1:A:107:LYS:HZ3	1.81	0.42
1:A:9:THR:O	1:A:9:THR:HG22	2.19	0.42
1:A:53:TRP:O	3:B:18:GLU:HG2	2.19	0.42
1:E:34:THR:HG23	1:E:40:THR:OG1	2.19	0.42
1:A:178:THR:O	1:A:180:PRO:HD3	2.19	0.42
3:F:17:PRO:HG2	3:F:20:VAL:HG12	2.00	0.42
1:C:124:TYR:CD1	1:C:133:GLY:HA2	2.53	0.42
1:E:30:ARG:HE	3:F:38:LEU:CD2	2.33	0.42
1:A:3:THR:HG23	3:B:44:SER:O	2.19	0.42
3:D:5:THR:CG2	3:D:6:LEU:N	2.83	0.42
1:C:139:ILE:O	1:C:147:ILE:HG22	2.19	0.42
2:H:512:ASN:OD1	2:H:512:ASN:N	2.52	0.42
2:J:512:ASN:ND2	8:J:509:NAG:O7	2.52	0.42
1:A:80:ALA:HA	1:A:81:ASP:HA	1.64	0.42
1:C:179:TYR:HA	1:C:180:PRO:HD2	1.83	0.42
3:D:5:THR:HG22	3:D:6:LEU:N	2.34	0.42
1:E:90:VAL:HG13	3:F:21:ARG:HH21	1.83	0.42
1:A:7:SER:HB2	1:C:1:THR:O	2.20	0.42
8:I:508:NAG:O7	8:I:509:NAG:H61	2.20	0.42
3:F:6:LEU:HD23	3:F:6:LEU:HA	1.82	0.42
1:C:20:PHE:HE1	1:C:31:LEU:CD1	2.33	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:ILE:HG21	1:A:11:PHE:CE2	2.55	0.41
1:E:148:ASN:HD22	3:F:8:GLU:CG	2.33	0.41
1:E:78:ASN:HD21	8:J:509:NAG:H2	1.84	0.41
1:A:16:PRO:HD2	3:D:19:TRP:CE2	2.55	0.41
1:E:33:LEU:HD23	1:E:33:LEU:HA	1.84	0.41
1:A:103:VAL:HG23	1:A:104:PHE:CD2	2.56	0.41
1:E:124:TYR:CE2	1:E:126:THR:HG22	2.56	0.41
1:E:172:VAL:O	1:E:172:VAL:HG13	2.21	0.41
1:E:28:LYS:HD3	1:E:30:ARG:HH11	1.86	0.41
6:I:501:MAN:H2	8:I:505:NAG:H2	1.77	0.41
1:E:34:THR:HB	3:F:35:HIS:HD2	1.84	0.41
1:A:5:SER:HA	3:B:42:PHE:O	2.21	0.41
3:B:16:VAL:HG13	3:B:20:VAL:CG1	2.50	0.41
3:B:41:TYR:OH	3:B:43:ASN:HB2	2.21	0.41
1:A:181:ASN:O	3:B:1:GLU:N	2.53	0.41
1:C:136:HIS:HB2	1:C:149:THR:HG23	2.04	0.40
1:C:45:LEU:HA	3:D:23:GLY:HA3	2.03	0.40
1:A:84:THR:HG22	3:B:25:SER:HB3	2.04	0.40
1:C:4:THR:HG21	1:C:50:ILE:HD13	2.03	0.40
3:D:43:ASN:HD22	3:D:43:ASN:C	2.23	0.40
1:E:88:ALA:HB2	1:E:115:THR:HG23	2.04	0.40
1:E:6:PHE:HZ	3:F:40:TRP:CZ2	2.39	0.40
1:A:152:TRP:HA	3:B:4:TYR:CE2	2.57	0.40
1:C:14:ASP:C	1:C:16:PRO:HD3	2.42	0.40
1:C:73:ALA:HB3	1:C:156:ASN:ND2	2.36	0.40
3:F:9:VAL:O	3:F:11:PRO:HD3	2.21	0.40
1:C:73:ALA:HA	1:C:74:PRO:HD3	1.92	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	A	179/181 (99%)	164 (92%)	14 (8%)	1 (1%)	27	60
1	C	179/181 (99%)	145 (81%)	29 (16%)	5 (3%)	5	18
1	E	179/181 (99%)	147 (82%)	25 (14%)	7 (4%)	3	11
3	B	49/53 (92%)	44 (90%)	5 (10%)	0	100	100
3	D	46/53 (87%)	41 (89%)	5 (11%)	0	100	100
3	F	45/53 (85%)	39 (87%)	6 (13%)	0	100	100
All	All	677/702 (96%)	580 (86%)	84 (12%)	13 (2%)	9	28

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	39	ASN
1	C	134	ASP
1	E	36	ALA
1	E	39	ASN
1	A	101	LEU
1	E	148	ASN
1	C	127	ALA
1	E	75	ASN
1	E	156	ASN
1	C	128	TRP
1	E	58	GLY
1	E	141	VAL
1	C	180	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	156/156 (100%)	137 (88%)	19 (12%)	5	16
1	C	156/156 (100%)	138 (88%)	18 (12%)	6	19
1	E	154/156 (99%)	140 (91%)	14 (9%)	10	30
2	H	1/2 (50%)	0	1 (100%)	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	I	1/2 (50%)	1 (100%)	0	100	100
2	J	2/2 (100%)	0	2 (100%)	0	0
3	B	44/47 (94%)	39 (89%)	5 (11%)	6	19
3	D	40/47 (85%)	37 (92%)	3 (8%)	15	39
3	F	39/47 (83%)	34 (87%)	5 (13%)	5	14
All	All	593/615 (96%)	526 (89%)	67 (11%)	6	20

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	THR
1	A	28	LYS
1	A	29	GLU
1	A	30	ARG
1	A	39	ASN
1	A	50	ILE
1	A	69	PHE
1	A	84	THR
1	A	91	ASP
1	A	92	THR
1	A	135	ARG
1	A	141	VAL
1	A	143	SER
1	A	144	ILE
1	A	148	ASN
1	A	158	LYS
1	A	159	GLU
1	A	173	LEU
1	A	175	VAL
2	H	512	ASN
3	B	2	THR
3	B	16	VAL
3	B	36	GLU
3	B	43	ASN
3	B	48	VAL
1	C	2	GLU
1	C	28	LYS
1	C	29	GLU
1	C	33	LEU
1	C	39	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	45	LEU
1	C	66	SER
1	C	69	PHE
1	C	72	ASP
1	C	75	ASN
1	C	81	ASP
1	C	115	THR
1	C	118	VAL
1	C	150	LYS
1	C	158	LYS
1	C	162	VAL
1	C	173	LEU
1	C	178	THR
3	D	21	ARG
3	D	38	LEU
3	D	43	ASN
1	E	2	GLU
1	E	14	ASP
1	E	18	LEU
1	E	35	LYS
1	E	45	LEU
1	E	57	THR
1	E	64	VAL
1	E	113	SER
1	E	141	VAL
1	E	158	LYS
1	E	170	THR
1	E	175	VAL
1	E	177	LEU
1	E	181	ASN
2	J	512	ASN
2	J	513	GLN
3	F	2	THR
3	F	6	LEU
3	F	16	VAL
3	F	22	ILE
3	F	39	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	148	ASN
1	A	155	GLN
3	B	35	HIS
3	B	43	ASN
1	C	21	GLN
1	C	51	HIS
1	C	59	ASN
1	C	75	ASN
1	C	114	GLN
3	D	43	ASN
1	E	21	GLN
1	E	78	ASN
1	E	181	ASN
3	F	35	HIS
3	F	43	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 35 ligands modelled in this entry, 6 are monoatomic - leaving 29 for Mogul analysis.

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
12	MPD	E	303	-	7,7,7	0.52	0	9,10,10	0.36	0
6	MAN	H	514	8,7	11,11,12	0.61	0	15,15,17	0.78	0
7	BMA	H	515	8,6	11,11,12	0.44	0	15,15,17	1.10	2 (13%)
8	NAG	H	516	9,10,6	14,14,15	1.01	0	17,19,21	0.91	1 (5%)
9	GAL	H	517	8	11,11,12	0.50	0	15,15,17	0.79	0
10	FUC	H	518	8	9,10,11	0.66	0	13,14,16	1.06	0
6	MAN	H	519	8,7	11,11,12	0.67	0	15,15,17	0.69	0
8	NAG	H	520	8,7	14,14,15	0.41	0	17,19,21	0.82	1 (5%)
8	NAG	H	521	8,2,10	14,14,15	0.58	0	17,19,21	0.62	0
10	FUC	H	522	8	9,10,11	0.50	0	13,14,16	0.61	0
8	NAG	H	523	6	14,14,15	0.55	0	17,19,21	0.56	0
6	MAN	I	501	8,7	11,11,12	0.38	0	15,15,17	0.81	0
7	BMA	I	502	8,6	11,11,12	0.68	0	15,15,17	0.60	0
6	MAN	I	503	7	11,11,12	0.57	0	15,15,17	1.04	1 (6%)
8	NAG	I	505	9,6	14,14,15	0.55	0	17,19,21	0.56	0
9	GAL	I	507	11,8	11,11,12	0.43	0	15,15,17	0.55	0
8	NAG	I	508	8,7	14,14,15	0.51	0	17,19,21	1.25	2 (11%)
8	NAG	I	509	8,2,10	14,14,15	0.57	0	17,19,21	0.78	1 (5%)
10	FUC	I	510	8	9,10,11	0.37	0	13,14,16	0.61	0
11	SIA	I	511	9	17,20,21	0.70	0	19,28,31	0.77	0
6	MAN	J	501	8,7	11,11,12	0.55	0	15,15,17	0.79	0
7	BMA	J	502	8,6	11,11,12	0.59	0	15,15,17	0.50	0
6	MAN	J	503	7	11,11,12	0.53	0	15,15,17	0.52	0
8	NAG	J	505	9,6	14,14,15	0.44	0	17,19,21	0.53	0
9	GAL	J	507	11,8	11,11,12	0.37	0	15,15,17	0.77	0
8	NAG	J	508	8,7	14,14,15	0.62	0	17,19,21	1.11	3 (17%)
8	NAG	J	509	8,2,10	14,14,15	0.54	0	17,19,21	0.89	0
10	FUC	J	510	8	9,10,11	0.29	0	13,14,16	0.43	0
11	SIA	J	511	9	17,20,21	0.66	0	19,28,31	0.77	1 (5%)

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
12	MPD	E	303	-	-	0/5/5/5	0/0/0/0
6	MAN	H	514	8,7	-	0/2/19/22	0/1/1/1
7	BMA	H	515	8,6	-	0/2/19/22	0/1/1/1
8	NAG	H	516	9,10,6	-	0/6/23/26	0/1/1/1
9	GAL	H	517	8	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	FUC	H	518	8	-	0/0/17/20	0/1/1/1
6	MAN	H	519	8,7	-	0/2/19/22	0/1/1/1
8	NAG	H	520	8,7	-	0/6/23/26	0/1/1/1
8	NAG	H	521	8,2,10	-	0/6/23/26	0/1/1/1
10	FUC	H	522	8	-	0/0/17/20	0/1/1/1
8	NAG	H	523	6	-	0/6/23/26	0/1/1/1
6	MAN	I	501	8,7	-	0/2/19/22	0/1/1/1
7	BMA	I	502	8,6	-	0/2/19/22	0/1/1/1
6	MAN	I	503	7	-	0/2/19/22	0/1/1/1
8	NAG	I	505	9,6	-	0/6/23/26	0/1/1/1
9	GAL	I	507	11,8	-	0/2/19/22	0/1/1/1
8	NAG	I	508	8,7	-	0/6/23/26	0/1/1/1
8	NAG	I	509	8,2,10	-	0/6/23/26	0/1/1/1
10	FUC	I	510	8	-	0/0/17/20	0/1/1/1
11	SIA	I	511	9	-	0/14/34/38	0/1/1/1
6	MAN	J	501	8,7	-	0/2/19/22	0/1/1/1
7	BMA	J	502	8,6	-	0/2/19/22	0/1/1/1
6	MAN	J	503	7	-	0/2/19/22	0/1/1/1
8	NAG	J	505	9,6	-	0/6/23/26	0/1/1/1
9	GAL	J	507	11,8	-	0/2/19/22	0/1/1/1
8	NAG	J	508	8,7	-	0/6/23/26	0/1/1/1
8	NAG	J	509	8,2,10	-	0/6/23/26	0/1/1/1
10	FUC	J	510	8	-	0/0/17/20	0/1/1/1
11	SIA	J	511	9	-	0/14/34/38	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	508	NAG	C4-C3-C2	-3.69	105.61	111.02
7	H	515	BMA	C6-C5-C4	-3.04	105.81	112.99
8	J	508	NAG	O5-C1-C2	-2.87	107.56	111.52
8	I	508	NAG	O5-C1-C2	-2.58	107.96	111.52
8	J	508	NAG	C4-C3-C2	-2.40	107.50	111.02
8	I	509	NAG	C3-C4-C5	-2.04	106.59	110.24
8	H	520	NAG	O5-C1-C2	-2.03	108.72	111.52
7	H	515	BMA	C3-C4-C5	2.11	114.02	110.24
11	J	511	SIA	C4-C3-C2	2.21	113.83	109.78
8	J	508	NAG	C1-C2-N2	2.31	114.44	110.49
8	H	516	NAG	C6-C5-C4	2.35	118.55	112.99
6	I	503	MAN	C1-O5-C5	2.91	116.19	112.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	E	303	MPD	1	0
8	H	516	NAG	3	0
9	H	517	GAL	1	0
10	H	518	FUC	3	0
6	H	519	MAN	1	0
6	I	501	MAN	1	0
7	I	502	BMA	2	0
6	I	503	MAN	2	0
8	I	505	NAG	1	0
8	I	508	NAG	1	0
8	I	509	NAG	1	0
11	I	511	SIA	1	0
8	J	508	NAG	1	0
8	J	509	NAG	2	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.