



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 12:01 am GMT

PDB ID : 1LGC  
Title : INTERACTION OF A LEGUME LECTIN WITH THE N2 FRAGMENT OF  
HUMAN LACTOTRANSFERRIN OR WITH THE ISOLATED BIAN-  
TENNARY 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

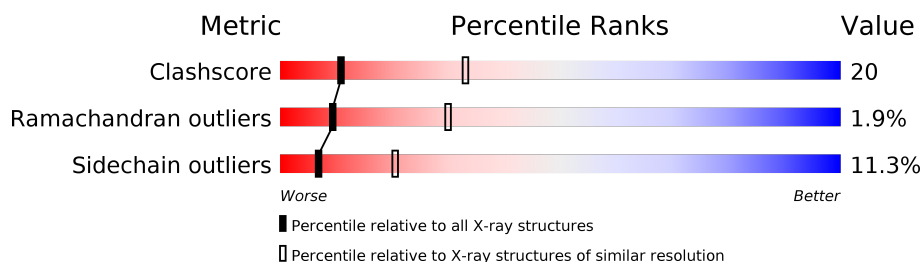
# 1 Overall quality at a glance

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	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (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  $\geq 3$ , 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	

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

## 2 Entry composition

There are 10 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
1	A	181	Total	C	N	O	0	0	0
			1407	896	232	279			
1	C	181	Total	C	N	O	0	0	0
			1407	896	232	279			
1	E	181	Total	C	N	O	0	0	0
			1397	889	231	277			

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
2	H	1	Total	C	N	O	0	0	0
			9	4	2	3			
2	I	1	Total	C	N	O	0	0	0
			9	4	2	3			
2	J	2	Total	C	N	O	0	0	0
			18	9	4	5			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	10	Total	C	N	O	0	0
			120	68	4	48		

- Molecule 5 is a polymer of unknown type called SUGAR (9-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	I	9	Total	C	N	O	0	0
			116	65	4	47		

- Molecule 6 is a polymer of unknown type called SUGAR (9-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	J	9	Total	C	N	O	0	0
			116	65	4	47		

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 8 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

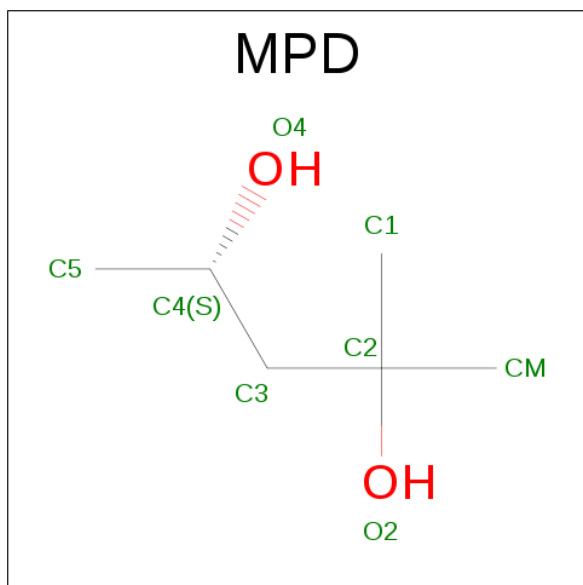
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Mn	0	0
			1	1		
8	C	1	Total	Mn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	E	1	Total	Mn	0	0
			1	1		

- Molecule 9 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



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

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	74	Total	O	0	0
			74	74		
10	B	22	Total	O	0	0
			22	22		
10	C	74	Total	O	0	0
			74	74		
10	D	21	Total	O	0	0
			21	21		
10	E	48	Total	O	0	0
			48	48		
10	F	11	Total	O	0	0
			11	11		
10	H	15	Total	O	0	0
			15	15		

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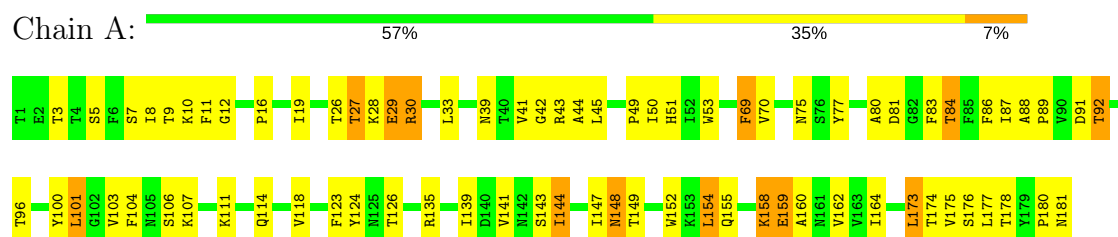
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	I	8	Total	O	0	0
			8	8		
10	J	6	Total	O	0	0
			6	6		

### 3 Residue-property plots [i](#)

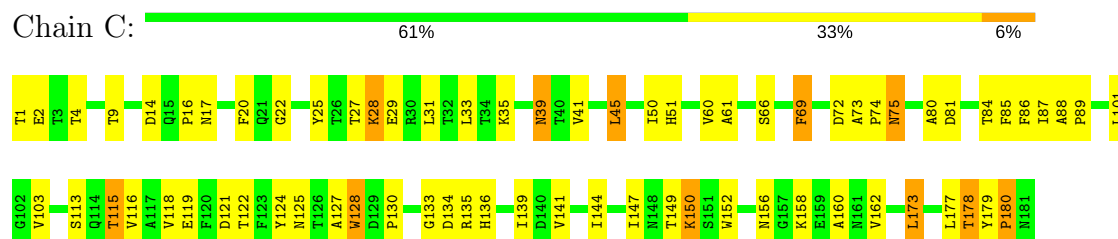
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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







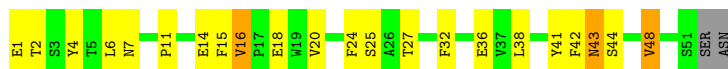
• Molecule 2: DIPEPTIDE



• Molecule 2: DIPEPTIDE



• Molecule 3: LEGUME ISOLECTIN II (BETA CHAIN)



• Molecule 3: LEGUME ISOLECTIN II (BETA CHAIN)



• Molecule 3: LEGUME ISOLECTIN II (BETA CHAIN)



## 4 Data and refinement statistics

Xtriage (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, $\alpha$ , $\beta$ , $\gamma$	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.	Xtriage
Total number of atoms	6044	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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

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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	H	120	0	103	5	0
5	I	116	0	98	5	0
6	J	116	0	98	3	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
7	E	1	0	0	0	0
8	A	1	0	0	0	0
8	C	1	0	0	0	0
8	E	1	0	0	0	0
9	E	8	0	14	1	0
10	A	74	0	0	2	0
10	B	22	0	0	1	0
10	C	74	0	0	2	0
10	D	21	0	0	0	0
10	E	48	0	0	4	0
10	F	11	0	0	1	0
10	H	15	0	0	1	0
10	I	8	0	0	0	0
10	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	10: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	10: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
10: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	10:E:320:HOH:O	2.02	0.59
1:E:155:GLN:HB2	1:E:179:TYR:CE2	2.38	0.59
5:I:502:BMA:H4	5: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
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
5:I:502:BMA:H4	5: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:16:VAL:HG13	3:B:20:VAL:HG11	1.87	0.56
4:H:516:NAG:N2	4: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
4:H:516:NAG:N2	4: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	10: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
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	10: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:H:516:NAG:H61	4:H:517:GAL:O2	2.13	0.49
6:J:508:NAG:O7	6: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	9: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	4: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	10:E:328:HOH:O	2.13	0.47
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	10: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
4:H:519:MAN:O4	10: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	10: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
5:I:511:SIA:C9	5: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	10: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	6: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
5:I:508:NAG:O7	5: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
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	6: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
5:I:501:MAN:H2	5:I:505:NAG:H2	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 ⓘ

### 5.3.1 Protein backbone ⓘ

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%)	28	62
1	C	179/181 (99%)	145 (81%)	29 (16%)	5 (3%)	6	19
1	E	179/181 (99%)	147 (82%)	25 (14%)	7 (4%)	3	12
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	30

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 ⓘ

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%)	6	17
1	C	156/156 (100%)	138 (88%)	18 (12%)	6	20
1	E	154/156 (99%)	140 (91%)	14 (9%)	11	31
2	H	1/2 (50%)	0	1 (100%)	0	0
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%)	7	20
3	D	40/47 (85%)	37 (92%)	3 (8%)	16	41
3	F	39/47 (83%)	34 (87%)	5 (13%)	5	15
All	All	593/615 (96%)	526 (89%)	67 (11%)	7	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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
3	F	35	HIS
3	F	43	ASN

### 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 ⓘ

28 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	$\# Z  > 2$
4	MAN	H	514	4	11,11,12	0.62	0	13,15,17	0.85	0
4	BMA	H	515	4	11,11,12	0.45	0	13,15,17	1.20	2 (15%)
4	NAG	H	516	4	14,14,15	1.03	0	15,19,21	0.96	1 (6%)
4	GAL	H	517	4	11,11,12	0.50	0	13,15,17	0.85	0
4	FUC	H	518	4	9,10,11	0.66	0	13,14,16	1.06	0
4	MAN	H	519	4	11,11,12	0.69	0	13,15,17	0.71	0
4	NAG	H	520	4	14,14,15	0.41	0	15,19,21	0.86	0
4	NAG	H	521	2,4	14,14,15	0.58	0	15,19,21	0.65	0
4	FUC	H	522	4	9,10,11	0.51	0	13,14,16	0.62	0
4	NAG	H	523	4	14,14,15	0.55	0	15,19,21	0.59	0
5	MAN	I	501	5	11,11,12	0.37	0	13,15,17	0.87	0
5	BMA	I	502	5	11,11,12	0.69	0	13,15,17	0.62	0
5	MAN	I	503	5	11,11,12	0.57	0	13,15,17	1.12	1 (7%)
5	NAG	I	505	5	14,14,15	0.55	0	15,19,21	0.53	0
5	GAL	I	507	5	11,11,12	0.43	0	13,15,17	0.56	0
5	NAG	I	508	5	14,14,15	0.52	0	15,19,21	1.32	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	I	509	2,5	14,14,15	0.58	0	15,19,21	0.82	1 (6%)
5	FUC	I	510	5	9,10,11	0.38	0	13,14,16	0.62	0
5	SIA	I	511	5	17,20,21	0.70	0	19,28,31	0.77	0
6	MAN	J	501	6	11,11,12	0.55	0	13,15,17	0.85	0
6	BMA	J	502	6	11,11,12	0.61	0	13,15,17	0.53	0
6	MAN	J	503	6	11,11,12	0.54	0	13,15,17	0.55	0
6	NAG	J	505	6	14,14,15	0.44	0	15,19,21	0.52	0
6	GAL	J	507	6	11,11,12	0.38	0	13,15,17	0.78	0
6	NAG	J	508	6	14,14,15	0.63	0	15,19,21	1.17	3 (20%)
6	NAG	J	509	2,6	14,14,15	0.55	0	15,19,21	0.94	0
6	FUC	J	510	6	9,10,11	0.29	0	13,14,16	0.43	0
6	SIA	J	511	6	17,20,21	0.65	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
4	MAN	H	514	4	-	0/2/19/22	0/1/1/1
4	BMA	H	515	4	-	0/2/19/22	0/1/1/1
4	NAG	H	516	4	-	0/6/23/26	0/1/1/1
4	GAL	H	517	4	-	0/2/19/22	0/1/1/1
4	FUC	H	518	4	-	0/0/17/20	0/1/1/1
4	MAN	H	519	4	-	0/2/19/22	0/1/1/1
4	NAG	H	520	4	-	0/6/23/26	0/1/1/1
4	NAG	H	521	2,4	-	0/6/23/26	0/1/1/1
4	FUC	H	522	4	-	0/0/17/20	0/1/1/1
4	NAG	H	523	4	-	0/6/23/26	0/1/1/1
5	MAN	I	501	5	-	0/2/19/22	0/1/1/1
5	BMA	I	502	5	-	0/2/19/22	0/1/1/1
5	MAN	I	503	5	-	0/2/19/22	0/1/1/1
5	NAG	I	505	5	-	0/6/23/26	0/1/1/1
5	GAL	I	507	5	-	0/2/19/22	0/1/1/1
5	NAG	I	508	5	-	0/6/23/26	0/1/1/1
5	NAG	I	509	2,5	-	0/6/23/26	0/1/1/1
5	FUC	I	510	5	-	0/0/17/20	0/1/1/1
5	SIA	I	511	5	-	0/14/34/38	0/1/1/1
6	MAN	J	501	6	-	0/2/19/22	0/1/1/1
6	BMA	J	502	6	-	0/2/19/22	0/1/1/1
6	MAN	J	503	6	-	0/2/19/22	0/1/1/1
6	NAG	J	505	6	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GAL	J	507	6	-	0/2/19/22	0/1/1/1
6	NAG	J	508	6	-	0/6/23/26	0/1/1/1
6	NAG	J	509	2,6	-	0/6/23/26	0/1/1/1
6	FUC	J	510	6	-	0/0/17/20	0/1/1/1
6	SIA	J	511	6	-	0/14/34/38	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	508	NAG	C4-C3-C2	-3.69	105.61	111.02
4	H	515	BMA	C6-C5-C4	-3.07	105.81	113.00
6	J	508	NAG	O5-C1-C2	-2.82	107.56	111.47
5	I	508	NAG	O5-C1-C2	-2.53	107.96	111.47
6	J	508	NAG	C4-C3-C2	-2.40	107.50	111.02
5	I	509	NAG	C3-C4-C5	-2.06	106.59	110.22
4	H	515	BMA	C3-C4-C5	2.16	114.02	110.22
6	J	511	SIA	C4-C3-C2	2.17	113.83	109.75
6	J	508	NAG	C1-C2-N2	2.31	114.44	110.49
4	H	516	NAG	C6-C5-C4	2.37	118.55	113.00
5	I	503	MAN	C1-O5-C5	2.92	116.19	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	516	NAG	3	0
4	H	517	GAL	1	0
4	H	518	FUC	3	0
4	H	519	MAN	1	0
5	I	501	MAN	1	0
5	I	502	BMA	2	0
5	I	503	MAN	2	0
5	I	505	NAG	1	0
5	I	508	NAG	1	0
5	I	509	NAG	1	0
5	I	511	SIA	1	0
6	J	508	NAG	1	0

*Continued on next page...*



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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	509	NAG	2	0

## 5.6 Ligand geometry

Of 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 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	$\# Z  > 2$
9	MPD	E	303	-	7,7,7	0.50	0	9,10,10	0.34	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	MPD	E	303	-	-	0/5/5/5	0/0/0/0

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	E	303	MPD	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.