



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:44 PM GMT

PDB ID : 1LTT  
Title : LACTOSE BINDING TO HEAT-LABILE ENTEROTOXIN REVEALED BY  
X-RAY CRYSTALLOGRAPHY  
Authors : Sixma, T.K.; Hol, W.G.J.  
Deposited on : 1992-07-15  
Resolution : 2.30 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

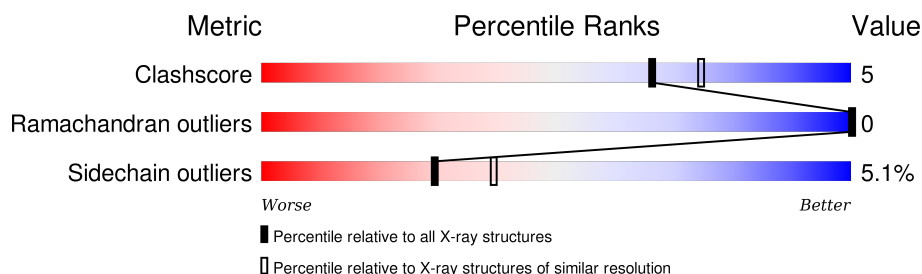
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)

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	D	103	<div> <div>77%</div> <div>21%</div> <div>.</div> </div>
1	E	103	<div> <div>85%</div> <div>13%</div> <div>.</div> </div>
1	F	103	<div> <div>81%</div> <div>13%</div> <div>6%</div> <div>.</div> </div>
1	G	103	<div> <div>83%</div> <div>15%</div> <div>.</div> </div>
1	H	103	<div> <div>81%</div> <div>18%</div> <div>.</div> </div>
2	A	185	<div> <div>75%</div> <div>21%</div> <div>.</div> </div>
3	C	41	<div> <div>68%</div> <div>29%</div> <div>.</div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6427 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 HEAT-LABILE ENTEROTOXIN, SUBUNIT B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	103	Total	C	N	O	S	0	0	0
			824	516	139	163	6			
1	E	103	Total	C	N	O	S	0	0	0
			824	516	139	163	6			
1	F	103	Total	C	N	O	S	0	0	0
			824	516	139	163	6			
1	G	103	Total	C	N	O	S	0	0	0
			824	516	139	163	6			
1	H	103	Total	C	N	O	S	0	0	0
			824	516	139	163	6			

- Molecule 2 is a protein called HEAT-LABILE ENTEROTOXIN, SUBUNIT A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	185	Total	C	N	O	S	0	0	0
			1511	953	276	278	4			

- Molecule 3 is a protein called HEAT-LABILE ENTEROTOXIN, SUBUNIT A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	41	Total	C	N	O	S	0	0	0
			347	214	59	73	1			

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	2	Total	C	O	0	0
			23	12	11		
4	E	2	Total	C	O	0	0
			23	12	11		
4	F	2	Total	C	O	0	0
			23	12	11		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	G	2	Total	C	O	0	0
			23	12	11		
4	H	2	Total	C	O	0	0
			23	12	11		

- Molecule 5 is water.


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	65	Total	O		0	0
			65	65			
5	E	56	Total	O		0	0
			56	56			
5	F	37	Total	O		0	0
			37	37			
5	G	53	Total	O		0	0
			53	53			
5	H	51	Total	O		0	0
			51	51			
5	A	43	Total	O		0	0
			43	43			
5	C	29	Total	O		0	0
			29	29			

### 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.


Note EDS was not executed.

- Molecule 1: HEAT-LABILE ENTEROTOXIN, SUBUNIT B

Chain D: 




- Molecule 1: HEAT-LABILE ENTEROTOXIN, SUBUNIT B

Chain E: 




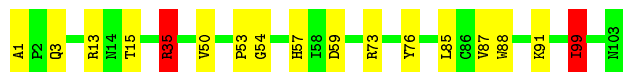
- Molecule 1: HEAT-LABILE ENTEROTOXIN, SUBUNIT B

Chain F: 




- Molecule 1: HEAT-LABILE ENTEROTOXIN, SUBUNIT B

Chain G: 



- Molecule 1: HEAT-LABILE ENTEROTOXIN, SUBUNIT B

Chain H: 

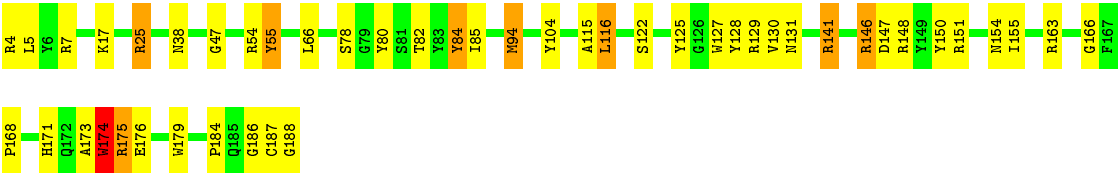


- Molecule 2: HEAT-LABILE ENTEROTOXIN, SUBUNIT A

Chain A: 

75%

21%



● Molecule 3: HEAT-LABILE ENTEROTOXIN, SUBUNIT A

Chain C: 

68%

29%



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.80 Å 101.20 Å 64.20 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.30)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.182 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6427	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BGC, GAL

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	D	0.82	0/835	1.44	9/1124 (0.8%)
1	E	0.79	0/835	1.50	13/1124 (1.2%)
1	F	0.84	0/835	1.57	15/1124 (1.3%)
1	G	0.85	0/835	1.62	10/1124 (0.9%)
1	H	0.80	0/835	1.57	13/1124 (1.2%)
2	A	0.78	0/1559	1.53	29/2120 (1.4%)
3	C	0.73	0/351	1.60	5/472 (1.1%)
All	All	0.80	0/6085	1.54	94/8212 (1.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
1	G	0	1
All	All	0	2

There are no bond length outliers.

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	235	ARG	NE-CZ-NH2	-13.72	113.44	120.30
1	H	35	ARG	NE-CZ-NH2	-12.29	114.15	120.30
1	E	67	ARG	NE-CZ-NH1	11.96	126.28	120.30
1	G	73	ARG	NE-CZ-NH1	11.87	126.24	120.30
1	G	13	ARG	NE-CZ-NH2	-11.61	114.50	120.30
1	H	35	ARG	NE-CZ-NH1	10.98	125.79	120.30
1	H	88	TRP	CD1-CG-CD2	9.04	113.53	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	127	TRP	CD1-CG-CD2	8.95	113.46	106.30
3	C	235	ARG	NE-CZ-NH1	8.88	124.74	120.30
1	G	73	ARG	NE-CZ-NH2	-8.87	115.86	120.30
1	H	67	ARG	NE-CZ-NH2	-8.75	115.93	120.30
1	D	73	ARG	NE-CZ-NH1	8.45	124.53	120.30
1	E	88	TRP	CD1-CG-CD2	8.45	113.06	106.30
2	A	25	ARG	NE-CZ-NH1	8.11	124.35	120.30
1	D	88	TRP	CD1-CG-CD2	7.95	112.66	106.30
2	A	174	TRP	CD1-CG-CD2	7.93	112.64	106.30
1	E	88	TRP	CE2-CD2-CG	-7.86	101.02	107.30
1	F	13	ARG	NE-CZ-NH1	7.81	124.20	120.30
1	E	35	ARG	NE-CZ-NH1	7.79	124.20	120.30
1	G	13	ARG	NE-CZ-NH1	7.78	124.19	120.30
2	A	174	TRP	CE2-CD2-CG	-7.78	101.08	107.30
1	H	73	ARG	NE-CZ-NH1	7.58	124.09	120.30
2	A	127	TRP	CE2-CD2-CG	-7.57	101.25	107.30
1	H	88	TRP	CE2-CD2-CG	-7.53	101.27	107.30
1	E	67	ARG	NE-CZ-NH2	-7.52	116.54	120.30
1	G	88	TRP	CD1-CG-CD2	7.44	112.25	106.30
1	G	88	TRP	CE2-CD2-CG	-7.41	101.37	107.30
1	F	88	TRP	CD1-CG-CD2	7.38	112.21	106.30
1	D	12	TYR	CB-CG-CD2	-7.29	116.62	121.00
1	F	88	TRP	CE2-CD2-CG	-7.23	101.52	107.30
2	A	163	ARG	NE-CZ-NH1	7.20	123.90	120.30
2	A	116	LEU	CA-CB-CG	7.15	131.75	115.30
2	A	179	TRP	CE2-CD2-CG	-7.07	101.65	107.30
1	E	73	ARG	NE-CZ-NH1	7.06	123.83	120.30
2	A	128	TYR	CB-CG-CD2	-7.04	116.77	121.00
2	A	25	ARG	NE-CZ-NH2	-6.99	116.80	120.30
2	A	179	TRP	CD1-CG-CD2	6.99	111.89	106.30
1	D	88	TRP	CE2-CD2-CG	-6.96	101.73	107.30
1	E	101	MET	CG-SD-CE	-6.64	89.58	100.20
1	D	27	TYR	CB-CG-CD2	-6.59	117.04	121.00
1	H	73	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	G	35	ARG	NE-CZ-NH1	6.55	123.57	120.30
2	A	174	TRP	CG-CD2-CE3	6.54	139.78	133.90
2	A	174	TRP	CB-CG-CD1	-6.47	118.59	127.00
2	A	127	TRP	CG-CD2-CE3	6.47	139.72	133.90
2	A	175	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	H	88	TRP	CG-CD2-CE3	6.30	139.57	133.90
2	A	55	TYR	CB-CG-CD2	-6.30	117.22	121.00
2	A	127	TRP	CG-CD1-NE1	-6.22	103.88	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	73	ARG	NE-CZ-NH1	6.17	123.38	120.30
1	F	88	TRP	CB-CG-CD1	-6.16	119.00	127.00
2	A	150	TYR	CB-CG-CD1	-6.13	117.32	121.00
1	D	67	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	H	88	TRP	CB-CG-CD1	-6.12	119.05	127.00
1	H	88	TRP	CG-CD1-NE1	-6.10	104.00	110.10
1	G	99	ILE	CB-CA-C	-6.09	99.41	111.60
1	F	101	MET	CA-CB-CG	6.06	123.61	113.30
1	E	88	TRP	CG-CD2-CE3	6.05	139.35	133.90
1	F	67	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	F	67	ARG	NE-CZ-NH2	-6.00	117.30	120.30
3	C	213	GLU	CA-CB-CG	-5.96	100.30	113.40
1	F	23	LYS	CA-CB-CG	5.92	126.41	113.40
1	E	88	TRP	CB-CG-CD1	-5.86	119.38	127.00
1	H	12	TYR	CB-CG-CD2	-5.83	117.50	121.00
1	F	50	VAL	N-CA-C	-5.82	95.29	111.00
3	C	210	TYR	CB-CG-CD2	-5.74	117.56	121.00
1	G	50	VAL	N-CA-C	-5.70	95.60	111.00
2	A	7	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	D	13	ARG	NE-CZ-NH2	-5.69	117.46	120.30
1	H	35	ARG	CG-CD-NE	-5.68	99.86	111.80
2	A	7	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	E	18	TYR	CB-CG-CD1	-5.61	117.63	121.00
2	A	175	ARG	NE-CZ-NH2	-5.57	117.52	120.30
2	A	80	TYR	N-CA-C	-5.52	96.10	111.00
1	D	18	TYR	CB-CG-CD2	-5.50	117.70	121.00
1	D	73	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	E	50	VAL	N-CA-C	-5.46	96.26	111.00
1	E	35	ARG	NE-CZ-NH2	-5.43	117.59	120.30
2	A	84	TYR	CB-CG-CD2	-5.42	117.75	121.00
1	G	88	TRP	CB-CG-CD1	-5.41	119.97	127.00
2	A	127	TRP	CB-CG-CD1	-5.40	119.98	127.00
1	F	69	LYS	CG-CD-CE	5.36	127.99	111.90
1	F	88	TRP	CG-CD2-CE3	5.36	138.72	133.90
2	A	4	ARG	NE-CZ-NH2	-5.32	117.64	120.30
3	C	236	ILE	CA-CB-CG1	-5.26	101.01	111.00
2	A	148	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	H	50	VAL	N-CA-C	-5.21	96.93	111.00
1	F	3	GLN	CA-CB-CG	-5.20	101.96	113.40
1	F	91	LYS	CA-CB-CG	-5.20	101.97	113.40
2	A	146	ARG	NE-CZ-NH2	-5.20	117.70	120.30
2	A	94	MET	CA-CB-CG	5.19	122.12	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	174	TRP	CG-CD1-NE1	-5.17	104.93	110.10
1	F	13	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	E	88	TRP	CG-CD1-NE1	-5.08	105.03	110.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	76	TYR	Sidechain
1	G	76	TYR	Sidechain

## 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	D	824	0	841	8	0
1	E	824	0	841	5	0
1	F	824	0	841	8	0
1	G	824	0	841	11	0
1	H	824	0	841	9	0
2	A	1511	0	1407	26	0
3	C	347	0	327	6	0
4	D	23	0	21	0	0
4	E	23	0	21	0	0
4	F	23	0	21	0	0
4	G	23	0	21	0	0
4	H	23	0	21	0	0
5	A	43	0	0	1	0
5	C	29	0	0	0	0
5	D	65	0	0	0	0
5	E	56	0	0	0	0
5	F	37	0	0	1	0
5	G	53	0	0	0	0
5	H	51	0	0	0	0
All	All	6427	0	6044	59	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 (59) 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:G:54:GLY:H	1:G:57:HIS:HD2	1.32	0.77
2:A:174:TRP:HB3	2:A:188:GLY:HA2	1.66	0.76
1:D:93:PRO:HG3	1:H:3:GLN:HG2	1.70	0.73
1:H:59:ASP:HA	1:H:62:LYS:HD3	1.75	0.69
3:C:198:THR:HA	3:C:201:GLU:HG2	1.75	0.68
1:G:3:GLN:HG2	1:H:93:PRO:HG3	1.76	0.68
1:G:1:ALA:HA	1:H:92:THR:O	1.93	0.68
1:F:82:ILE:HD12	1:F:99:ILE:HD11	1.78	0.66
1:F:61:GLN:O	1:F:65:ILE:HG13	1.98	0.64
2:A:84:TYR:CE2	2:A:129:ARG:HG2	2.33	0.63
1:G:53:PRO:HA	1:G:57:HIS:CD2	2.35	0.61
2:A:125:TYR:O	2:A:141:ARG:HD2	2.04	0.57
1:F:25:LEU:HB2	1:F:43:LYS:HD2	1.89	0.55
2:A:84:TYR:HE2	2:A:129:ARG:HG2	1.72	0.55
1:G:15:THR:HA	1:G:87:VAL:O	2.07	0.54
2:A:147:ASP:O	2:A:151:ARG:HB2	2.08	0.53
2:A:54:ARG:HG2	5:A:217:HOH:O	2.08	0.53
2:A:82:THR:HA	2:A:130:VAL:O	2.10	0.51
2:A:122:SER:HB2	2:A:146:ARG:HG2	1.92	0.51
2:A:168:PRO:HG2	2:A:171:HIS:HB2	1.93	0.51
1:G:54:GLY:N	1:G:57:HIS:HD2	2.05	0.51
1:D:12:TYR:OH	1:E:35:ARG:HG3	2.12	0.50
2:A:94:MET:SD	2:A:115:ALA:HB2	2.53	0.49
1:G:99:ILE:HD12	1:H:29:GLU:HB3	1.94	0.49
2:A:125:TYR:CE1	2:A:141:ARG:HD3	2.48	0.49
2:A:129:ARG:NH2	2:A:131:ASN:HD21	2.12	0.48
1:H:15:THR:HA	1:H:87:VAL:O	2.14	0.48
2:A:104:TYR:CD1	2:A:171:HIS:HE1	2.32	0.47
1:F:103:ASN:HB2	2:A:151:ARG:HH12	1.78	0.47
1:F:65:ILE:HG22	1:F:69:LYS:HE2	1.97	0.46
1:D:3:GLN:HG3	1:E:47:THR:HG21	1.98	0.46
1:H:88:TRP:HB3	1:H:90:ASN:OD1	2.15	0.46
2:A:184:PRO:HB3	3:C:202:GLU:HB3	1.99	0.45
1:G:85:LEU:HD23	1:G:99:ILE:HG23	1.98	0.45
1:D:86:CYS:HB3	1:D:98:ALA:HB3	1.98	0.45
1:G:54:GLY:H	1:G:57:HIS:CD2	2.23	0.45
2:A:25:ARG:HH11	2:A:25:ARG:HG2	1.82	0.45
3:C:217:LYS:HA	3:C:217:LYS:HD3	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:20:ILE:HG21	1:H:42:PHE:CE1	2.53	0.43
1:H:88:TRP:HE3	1:H:95:SER:HB2	1.83	0.43
2:A:25:ARG:NH1	2:A:25:ARG:HG2	2.33	0.43
2:A:38:ASN:HA	3:C:204:GLN:OE1	2.19	0.43
1:F:12:TYR:OH	1:G:35:ARG:HB2	2.19	0.43
2:A:174:TRP:CD1	2:A:187:CYS:HB3	2.54	0.42
2:A:174:TRP:HB3	2:A:188:GLY:CA	2.43	0.42
1:D:61:GLN:HG2	1:E:31:MET:O	2.19	0.42
1:F:23:LYS:HD3	5:F:113:HOH:O	2.20	0.42
1:D:15:THR:HA	1:D:87:VAL:O	2.20	0.42
2:A:47:GLY:O	2:A:54:ARG:NH1	2.49	0.41
1:G:85:LEU:CD2	1:G:99:ILE:HG23	2.50	0.41
2:A:186:GLY:O	3:C:199:CYS:HB2	2.20	0.41
2:A:173:ALA:HA	2:A:176:GLU:HG2	2.02	0.41
1:E:99:ILE:HD13	1:E:101:MET:HE2	2.02	0.41
1:D:65:ILE:HG22	1:D:69:LYS:HE2	2.03	0.41
2:A:66:LEU:HD12	2:A:85:ILE:HG21	2.02	0.41
1:D:58:ILE:HD12	1:E:34:LYS:HE2	2.03	0.40
2:A:166:GLY:HA2	3:C:203:THR:HG21	2.04	0.40
1:F:4:THR:HB	1:F:7:GLU:HG3	2.02	0.40
2:A:5:LEU:HD11	2:A:155:ILE:HD11	2.01	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	D	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
1	E	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
1	F	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
1	G	101/103 (98%)	96 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
2	A	183/185 (99%)	175 (96%)	8 (4%)	0	100	100
3	C	39/41 (95%)	39 (100%)	0	0	100	100
All	All	727/741 (98%)	701 (96%)	26 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	D	95/95 (100%)	87 (92%)	8 (8%)	14	16
1	E	95/95 (100%)	92 (97%)	3 (3%)	46	62
1	F	95/95 (100%)	89 (94%)	6 (6%)	22	29
1	G	95/95 (100%)	91 (96%)	4 (4%)	36	49
1	H	95/95 (100%)	93 (98%)	2 (2%)	61	78
2	A	155/155 (100%)	147 (95%)	8 (5%)	29	38
3	C	40/40 (100%)	37 (92%)	3 (8%)	17	21
All	All	670/670 (100%)	636 (95%)	34 (5%)	29	39

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	3	GLN
1	D	16	GLN
1	D	55	SER
1	D	63	LYS
1	D	81	LYS
1	D	91	LYS
1	D	101	MET
1	D	103	ASN
1	E	23	LYS

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Mol	Chain	Res	Type
1	E	91	LYS
1	E	95	SER
1	F	4	THR
1	F	23	LYS
1	F	43	LYS
1	F	91	LYS
1	F	101	MET
1	F	103	ASN
1	G	35	ARG
1	G	59	ASP
1	G	91	LYS
1	G	99	ILE
1	H	56	GLN
1	H	102	LYS
2	A	17	LYS
2	A	55	TYR
2	A	78	SER
2	A	116	LEU
2	A	141	ARG
2	A	154	ASN
2	A	174	TRP
2	A	175	ARG
3	C	200	ASN
3	C	234	ASN
3	C	235	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	3	GLN
1	D	16	GLN
1	D	21	ASN
1	E	3	GLN
1	F	103	ASN
1	G	16	GLN
1	G	57	HIS
1	G	103	ASN
1	H	3	GLN
2	A	131	ASN
2	A	171	HIS

### 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 ⓘ

10 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	GAL	D	104	4	11,11,12	0.83	0	14,15,17	0.76	0
4	BGC	D	105	4	12,12,12	0.44	0	17,17,17	0.84	1 (5%)
4	GAL	E	104	4	11,11,12	0.96	1 (9%)	14,15,17	1.59	2 (14%)
4	BGC	E	105	4	12,12,12	0.70	0	17,17,17	1.39	2 (11%)
4	GAL	F	104	4	11,11,12	0.69	0	14,15,17	1.33	2 (14%)
4	BGC	F	105	4	12,12,12	1.10	0	17,17,17	1.45	3 (17%)
4	GAL	G	104	4	11,11,12	1.05	1 (9%)	14,15,17	0.92	0
4	BGC	G	105	4	12,12,12	0.97	1 (8%)	17,17,17	1.00	1 (5%)
4	GAL	H	104	4	11,11,12	0.88	0	14,15,17	1.09	2 (14%)
4	BGC	H	105	4	12,12,12	0.88	0	17,17,17	0.98	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
4	GAL	D	104	4	-	0/2/19/22	0/1/1/1
4	BGC	D	105	4	-	0/2/22/22	0/1/1/1
4	GAL	E	104	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BGC	E	105	4	-	0/2/22/22	0/1/1/1
4	GAL	F	104	4	-	0/2/19/22	0/1/1/1
4	BGC	F	105	4	-	0/2/22/22	0/1/1/1
4	GAL	G	104	4	-	0/2/19/22	0/1/1/1
4	BGC	G	105	4	-	0/2/22/22	0/1/1/1
4	GAL	H	104	4	-	0/2/19/22	0/1/1/1
4	BGC	H	105	4	-	0/2/22/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	105	BGC	C4-C5	2.22	1.57	1.53
4	G	104	GAL	C4-C5	2.56	1.58	1.53
4	E	104	GAL	C2-C3	2.74	1.56	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	104	GAL	C1-C2-C3	-4.12	104.67	109.54
4	F	105	BGC	C4-C3-C2	-3.69	103.91	110.79
4	F	104	GAL	O3-C3-C2	-2.59	105.32	110.00
4	E	105	BGC	O4-C4-C5	-2.14	103.58	109.24
4	H	104	GAL	C2-C3-C4	-2.12	107.43	111.04
4	H	104	GAL	C1-O5-C5	2.01	114.80	112.25
4	G	105	BGC	O5-C1-C2	2.05	113.07	109.80
4	E	104	GAL	O2-C2-C3	2.13	114.41	110.12
4	F	105	BGC	O3-C3-C4	2.19	115.27	110.34
4	F	105	BGC	O4-C4-C3	2.50	115.96	110.34
4	D	105	BGC	C3-C4-C5	2.51	114.56	110.20
4	F	104	GAL	C1-O5-C5	3.73	116.98	112.25
4	E	105	BGC	C3-C4-C5	3.99	117.16	110.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 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 [i](#)

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.