



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2024 – 11:22 AM EDT

PDB ID : 1LTA
Title : 2.2 ANGSTROMS CRYSTAL STRUCTURE OF E. COLI HEAT-LABILE ENTEROTOXIN (LT) WITH BOUND GALACTOSE
Authors : Merritt, E.A.; Sixma, T.K.; Kalk, K.H.; Van Zanten, B.A.M.; Hol, W.G.J.
Deposited on : 1993-09-15
Resolution : 2.20 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

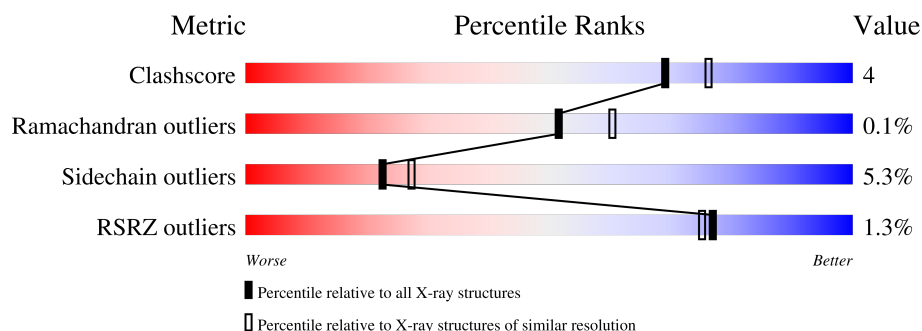
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 2.20 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	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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.

Mol	Chain	Length	Quality of chain
1	D	103	 82% 17% .
1	E	103	 80% 18% .
1	F	103	 80% 17% .
1	G	103	 81% 16% .
1	H	103	 82% 12% 7%
2	A	188	 3% 82% 16% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	49	<div> <div>10%</div> <div>71%</div> <div>14%</div> <div>• • 8%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6390 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			

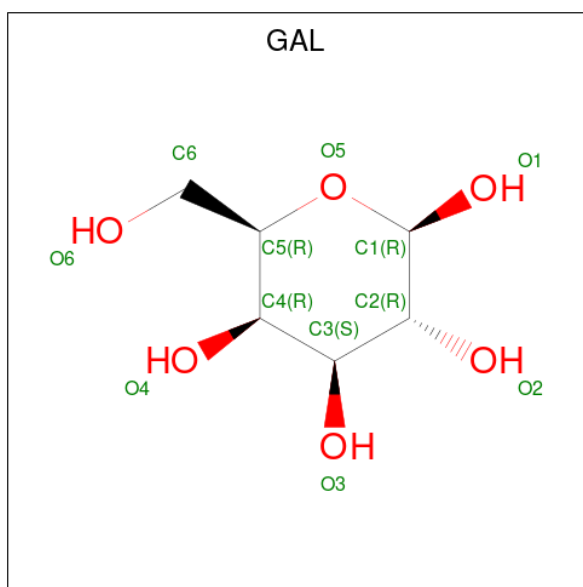
- Molecule 2 is a protein called HEAT-LABILE ENTEROTOXIN, SUBUNIT A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	188	Total	C	N	O	S	0	0	0
			1531	963	280	284	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	45	Total	C	N	O	S	0	0	0
			384	235	66	82	1			

- Molecule 4 is beta-D-galactopyranose (three-letter code: GAL) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			12	6	6		
4	E	1	Total	C	O	0	0
			12	6	6		
4	F	1	Total	C	O	0	0
			12	6	6		
4	G	1	Total	C	O	0	0
			12	6	6		
4	H	1	Total	C	O	0	0
			12	6	6		


- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	52	Total	O	0	0
			52	52		
5	E	44	Total	O	0	0
			44	44		
5	F	29	Total	O	0	0
			29	29		
5	G	52	Total	O	0	0
			52	52		
5	H	39	Total	O	0	0
			39	39		
5	A	58	Total	O	0	0
			58	58		
5	C	21	Total	O	0	0
			21	21		

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

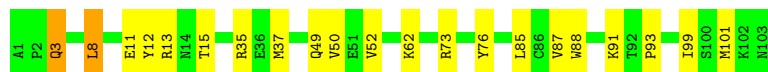
- Molecule 1: HEAT-LABILE ENTEROTOXIN, SUBUNIT B

Chain D:  82% 17% .




- Molecule 1: HEAT-LABILE ENTEROTOXIN, SUBUNIT B

Chain E:  80% 18% .




- Molecule 1: HEAT-LABILE ENTEROTOXIN, SUBUNIT B

Chain F:  80% 17% .




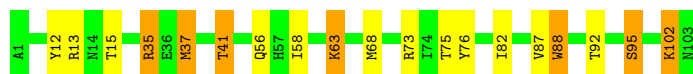
- Molecule 1: HEAT-LABILE ENTEROTOXIN, SUBUNIT B

Chain G:  81% 16% .




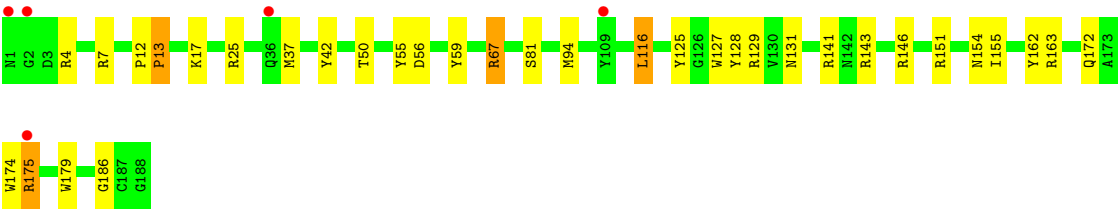
- Molecule 1: HEAT-LABILE ENTEROTOXIN, SUBUNIT B

Chain H:  82% 12% 7% .



- Molecule 2: HEAT-LABILE ENTEROTOXIN, SUBUNIT A

Chain A:  3% 82% 16% .



● Molecule 3: HEAT-LABILE ENTEROTOXIN, SUBUNIT A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.70Å 73.50Å 163.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.20 48.64 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.20) 87.7 (48.64-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.74 (at 2.20Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.175 , (Not available) 0.162 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	23.8	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 62.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6390	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: 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	1.39	5/1124 (0.4%)
1	E	0.82	0/835	1.51	13/1124 (1.2%)
1	F	0.79	0/835	1.45	9/1124 (0.8%)
1	G	0.84	0/835	1.58	15/1124 (1.3%)
1	H	0.85	0/835	1.60	17/1124 (1.5%)
2	A	0.87	0/1579	1.60	31/2147 (1.4%)
3	C	0.79	0/388	1.68	9/520 (1.7%)
All	All	0.83	0/6142	1.54	99/8287 (1.2%)

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	D	0	1
1	E	0	1
1	H	0	1
All	All	0	3

There are no bond length outliers.

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	73	ARG	NE-CZ-NH2	-13.89	113.36	120.30
1	G	73	ARG	NE-CZ-NH1	11.87	126.23	120.30
3	C	235	ARG	NE-CZ-NH2	-11.85	114.38	120.30
1	H	73	ARG	NE-CZ-NH2	-9.87	115.36	120.30
1	E	73	ARG	NE-CZ-NH1	9.69	125.15	120.30
1	H	73	ARG	NE-CZ-NH1	9.56	125.08	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	25	ARG	NE-CZ-NH1	9.40	125.00	120.30
1	E	88	TRP	CD1-CG-CD2	9.07	113.56	106.30
2	A	146	ARG	NE-CZ-NH2	-9.01	115.80	120.30
2	A	174	TRP	CD1-CG-CD2	8.97	113.47	106.30
2	A	146	ARG	NE-CZ-NH1	8.69	124.64	120.30
1	E	73	ARG	NE-CZ-NH2	-8.69	115.96	120.30
1	H	88	TRP	CD1-CG-CD2	8.66	113.23	106.30
1	G	88	TRP	CD1-CG-CD2	8.60	113.18	106.30
2	A	127	TRP	CD1-CG-CD2	8.37	112.99	106.30
2	A	163	ARG	NE-CZ-NH1	8.21	124.40	120.30
2	A	174	TRP	CE2-CD2-CG	-8.12	100.80	107.30
1	F	18	TYR	CB-CG-CD2	-8.06	116.17	121.00
1	E	8	LEU	CA-CB-CG	7.89	133.46	115.30
1	D	88	TRP	CD1-CG-CD2	7.87	112.60	106.30
1	F	88	TRP	CD1-CG-CD2	7.86	112.59	106.30
3	C	237	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	E	88	TRP	CE2-CD2-CG	-7.59	101.23	107.30
1	H	88	TRP	CE2-CD2-CG	-7.57	101.25	107.30
3	C	235	ARG	NE-CZ-NH1	7.52	124.06	120.30
2	A	179	TRP	CD1-CG-CD2	7.45	112.26	106.30
3	C	237	ARG	CA-CB-CG	7.23	129.30	113.40
2	A	179	TRP	CE2-CD2-CG	-7.16	101.57	107.30
2	A	127	TRP	CE2-CD2-CG	-7.08	101.63	107.30
1	D	88	TRP	CE2-CD2-CG	-7.01	101.69	107.30
1	G	88	TRP	CE2-CD2-CG	-7.00	101.70	107.30
1	F	35	ARG	NE-CZ-NH1	6.91	123.75	120.30
2	A	4	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	E	88	TRP	CB-CG-CD1	-6.75	118.22	127.00
3	C	212	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	H	35	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	H	88	TRP	CG-CD2-CE3	6.47	139.72	133.90
2	A	143	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	F	88	TRP	CE2-CD2-CG	-6.38	102.20	107.30
2	A	7	ARG	NE-CZ-NH2	-6.35	117.12	120.30
2	A	25	ARG	NE-CZ-NH2	-6.34	117.13	120.30
2	A	174	TRP	CG-CD2-CE3	6.33	139.60	133.90
1	D	18	TYR	CB-CG-CD2	-6.33	117.20	121.00
1	H	37	MET	CG-SD-CE	-6.27	90.17	100.20
1	G	102	LYS	O-C-N	6.25	132.70	122.70
2	A	128	TYR	CB-CG-CD2	-6.20	117.28	121.00
1	H	13	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	E	88	TRP	CG-CD2-CE3	6.13	139.41	133.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	E	12	TYR	CB-CG-CD1	-6.02	117.39	121.00
1	E	3	GLN	CA-CB-CG	-6.00	100.21	113.40
1	H	95	SER	N-CA-CB	5.99	119.49	110.50
1	G	99	ILE	CB-CG1-CD1	-5.99	97.13	113.90
1	G	22	ASP	CB-CG-OD1	5.98	123.68	118.30
1	G	13	ARG	NE-CZ-NH1	5.96	123.28	120.30
2	A	127	TRP	CG-CD1-NE1	-5.90	104.20	110.10
1	E	88	TRP	CG-CD1-NE1	-5.88	104.22	110.10
1	F	13	ARG	CA-CB-CG	5.82	126.21	113.40
1	H	88	TRP	CG-CD1-NE1	-5.82	104.28	110.10
2	A	127	TRP	CG-CD2-CE3	5.80	139.12	133.90
1	H	95	SER	CB-CA-C	-5.80	99.09	110.10
1	G	99	ILE	CB-CA-C	-5.77	100.06	111.60
1	H	88	TRP	CB-CG-CD1	-5.76	119.51	127.00
3	C	236	ILE	CA-CB-CG1	-5.74	100.09	111.00
3	C	235	ARG	CG-CD-NE	-5.74	99.75	111.80
2	A	42	TYR	CB-CG-CD2	-5.73	117.56	121.00
1	G	35	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	H	68	MET	CG-SD-CE	-5.66	91.14	100.20
1	F	51	GLU	CA-CB-CG	5.61	125.74	113.40
2	A	116	LEU	CA-CB-CG	5.59	128.16	115.30
1	G	67	ARG	NE-CZ-NH1	5.56	123.08	120.30
2	A	56	ASP	CB-CG-OD1	5.52	123.27	118.30
2	A	174	TRP	CG-CD1-NE1	-5.52	104.58	110.10
1	G	1	ALA	CA-C-N	5.45	132.37	117.10
2	A	179	TRP	CG-CD2-CE3	5.41	138.77	133.90
2	A	37	MET	N-CA-CB	-5.34	101.00	110.60
2	A	162	TYR	CB-CG-CD2	-5.33	117.80	121.00
1	D	88	TRP	CG-CD1-NE1	-5.30	104.80	110.10
2	A	37	MET	CA-CB-CG	5.30	122.31	113.30
1	G	50	VAL	N-CA-C	-5.29	96.72	111.00
1	E	13	ARG	NE-CZ-NH1	5.23	122.92	120.30
2	A	67	ARG	NE-CZ-NH2	-5.22	117.69	120.30
2	A	174	TRP	CB-CG-CD1	-5.22	120.22	127.00
1	E	50	VAL	N-CA-C	-5.20	96.97	111.00
2	A	163	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	F	88	TRP	CG-CD1-NE1	-5.16	104.94	110.10
3	C	214	TYR	CB-CG-CD2	-5.15	117.91	121.00
2	A	59	TYR	CB-CG-CD2	-5.12	117.93	121.00
1	D	13	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	G	88	TRP	CG-CD1-NE1	-5.11	104.99	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	95	SER	N-CA-CB	-5.08	102.88	110.50
3	C	226	TYR	CB-CG-CD2	-5.07	117.96	121.00
1	G	88	TRP	CB-CG-CD1	-5.07	120.41	127.00
1	H	13	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	E	101	MET	CG-SD-CE	-5.04	92.14	100.20
1	F	52	VAL	CG1-CB-CG2	-5.04	102.84	110.90
1	H	102	LYS	C-N-CA	5.02	134.25	121.70
1	H	12	TYR	CB-CG-CD2	-5.02	117.99	121.00
1	H	41	THR	N-CA-CB	-5.01	100.77	110.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	76	TYR	Sidechain
1	E	76	TYR	Sidechain
1	H	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	9	0
1	E	824	0	841	10	0
1	F	824	0	841	8	0
1	G	824	0	841	5	0
1	H	824	0	841	7	0
2	A	1531	0	1423	12	0
3	C	384	0	361	3	0
4	D	12	0	12	0	0
4	E	12	0	12	0	0
4	F	12	0	12	1	0
4	G	12	0	12	0	0
4	H	12	0	12	0	0
5	A	58	0	0	0	0
5	C	21	0	0	0	0
5	D	52	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	44	0	0	0	0
5	F	29	0	0	0	0
5	G	52	0	0	0	0
5	H	39	0	0	1	0
All	All	6390	0	6049	45	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 4.

All (45) 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:3:GLN:HE22	1:H:92:THR:HG22	1.43	0.83
1:E:85:LEU:HD23	1:E:99:ILE:HG22	1.64	0.80
1:F:103:ASN:HB2	2:A:151:ARG:HH12	1.64	0.63
2:A:94:MET:HB2	2:A:155:ILE:HD12	1.81	0.61
1:H:35:ARG:HD2	1:H:37:MET:HE1	1.84	0.60
1:D:44:SER:OG	1:D:46:GLU:HG3	2.01	0.60
1:F:25:LEU:HB2	1:F:43:LYS:HD2	1.85	0.59
1:H:75:THR:HG21	1:H:82:ILE:HD11	1.83	0.59
1:E:85:LEU:CD2	1:E:99:ILE:HG22	2.33	0.57
1:E:49:GLN:HB3	1:E:93:PRO:HG2	1.86	0.57
1:G:20:ILE:HG21	1:G:42:PHE:CE1	2.42	0.54
1:G:3:GLN:NE2	1:H:92:THR:HG22	2.18	0.53
1:F:91:LYS:HD3	4:F:104:GAL:O3	2.09	0.53
1:D:11:GLU:OE1	1:E:35:ARG:HD2	2.08	0.53
1:H:63:LYS:HG3	5:H:130:HOH:O	2.09	0.52
1:E:3:GLN:HG2	1:F:93:PRO:HD3	1.91	0.52
1:D:90:ASN:O	1:D:91:LYS:HD2	2.10	0.51
1:F:82:ILE:HD12	1:F:99:ILE:HD11	1.94	0.50
1:G:15:THR:HA	1:G:87:VAL:O	2.13	0.48
2:A:125:TYR:CZ	2:A:141:ARG:HD3	2.47	0.48
1:E:62:LYS:HE3	3:C:240:LEU:HA	1.94	0.48
1:F:14:ASN:O	1:F:88:TRP:HA	2.13	0.48
2:A:172:GLN:HA	2:A:175:ARG:HE	1.79	0.48
1:E:15:THR:HA	1:E:87:VAL:O	2.14	0.48
1:H:88:TRP:HE3	1:H:95:SER:HB2	1.79	0.47
1:H:15:THR:HA	1:H:87:VAL:O	2.15	0.47
2:A:129:ARG:HH12	2:A:131:ASN:HD21	1.63	0.47
2:A:94:MET:CB	2:A:155:ILE:HD12	2.46	0.46
1:D:4:THR:HB	5:D:143:HOH:O	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:99:ILE:HD13	1:E:99:ILE:HG21	1.75	0.45
1:D:2:PRO:HA	1:D:7:GLU:OE2	2.17	0.45
1:F:15:THR:HA	1:F:87:VAL:O	2.16	0.44
1:D:12:TYR:OH	1:E:35:ARG:HG3	2.18	0.44
2:A:129:ARG:NH1	2:A:131:ASN:HD21	2.16	0.44
2:A:186:GLY:O	3:C:199:CYS:HB2	2.18	0.43
1:D:15:THR:HA	1:D:87:VAL:O	2.18	0.42
1:G:102:LYS:O	1:G:103:ASN:HB2	2.19	0.42
2:A:155:ILE:HD13	2:A:155:ILE:HA	1.75	0.42
1:F:71:THR:O	1:F:75:THR:HG23	2.20	0.42
2:A:172:GLN:HA	2:A:175:ARG:NE	2.35	0.42
2:A:125:TYR:O	2:A:141:ARG:HD2	2.20	0.42
1:D:34:LYS:HE2	1:D:34:LYS:HB2	1.84	0.41
1:D:59:ASP:HB3	3:C:239:GLU:HG2	2.01	0.41
2:A:12:PRO:HA	2:A:13:PRO:HD3	1.86	0.41
1:E:37:MET:HE3	1:E:52:VAL:HG23	2.03	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	D	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
1	E	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
1	F	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
1	G	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
1	H	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
2	A	186/188 (99%)	179 (96%)	7 (4%)	0	100	100
3	C	43/49 (88%)	41 (95%)	1 (2%)	1 (2%)	6	3
All	All	734/752 (98%)	716 (98%)	17 (2%)	1 (0%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	237	ARG

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%)	92 (97%)	3 (3%)	39	50
1	E	95/95 (100%)	92 (97%)	3 (3%)	39	50
1	F	95/95 (100%)	90 (95%)	5 (5%)	22	27
1	G	95/95 (100%)	88 (93%)	7 (7%)	13	14
1	H	95/95 (100%)	90 (95%)	5 (5%)	22	27
2	A	157/157 (100%)	148 (94%)	9 (6%)	20	24
3	C	44/48 (92%)	40 (91%)	4 (9%)	9	9
All	All	676/680 (99%)	640 (95%)	36 (5%)	22	27

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	21	ASN
1	D	91	LYS
1	D	101	MET
1	E	8	LEU
1	E	11	GLU
1	E	91	LYS
1	F	6	THR
1	F	43	LYS
1	F	59	ASP
1	F	91	LYS
1	F	103	ASN
1	G	11	GLU
1	G	35	ARG
1	G	55	SER
1	G	91	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	99	ILE
1	G	100	SER
1	G	103	ASN
1	H	41	THR
1	H	56	GLN
1	H	58	ILE
1	H	63	LYS
1	H	102	LYS
2	A	13	PRO
2	A	17	LYS
2	A	50	THR
2	A	55	TYR
2	A	67	ARG
2	A	81	SER
2	A	116	LEU
2	A	154	ASN
2	A	175	ARG
3	C	234	ASN
3	C	235	ARG
3	C	237	ARG
3	C	239	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	16	GLN
1	D	21	ASN
1	F	94	ASN
1	G	3	GLN
1	H	56	GLN
2	A	1	ASN
2	A	38	ASN
2	A	131	ASN

5.3.3 RNA ⓘ

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GAL	F	104	-	12,12,12	1.02	1 (8%)	17,17,17	0.88	1 (5%)
4	GAL	E	104	-	12,12,12	0.66	0	17,17,17	0.54	0
4	GAL	G	104	-	12,12,12	0.88	0	17,17,17	0.68	0
4	GAL	D	104	-	12,12,12	0.71	0	17,17,17	0.66	0
4	GAL	H	104	-	12,12,12	0.74	0	17,17,17	0.91	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	F	104	-	-	2/2/22/22	0/1/1/1
4	GAL	E	104	-	-	0/2/22/22	0/1/1/1
4	GAL	G	104	-	-	0/2/22/22	0/1/1/1
4	GAL	D	104	-	-	0/2/22/22	0/1/1/1
4	GAL	H	104	-	-	0/2/22/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	104	GAL	C4-C3	2.13	1.57	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	104	GAL	O5-C5-C6	2.01	111.44	106.44

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	104	GAL	O5-C5-C6-O6
4	F	104	GAL	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	104	GAL	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 [i](#)

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

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, 95th 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	D	103/103 (100%)	-0.93	0	100	100	6, 16, 33, 52	0
1	E	103/103 (100%)	-0.93	0	100	100	8, 16, 32, 49	0
1	F	103/103 (100%)	-0.81	0	100	100	9, 21, 40, 52	0
1	G	103/103 (100%)	-0.91	0	100	100	8, 19, 36, 48	0
1	H	103/103 (100%)	-0.94	0	100	100	9, 18, 36, 53	0
2	A	188/188 (100%)	-0.37	5 (2%)	54	52	10, 24, 56, 109	0
3	C	45/49 (91%)	0.20	5 (11%)	5	4	11, 23, 90, 99	0
All	All	748/752 (99%)	-0.70	10 (1%)	77	75	6, 20, 47, 109	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	1	ASN	19.2
3	C	240	LEU	12.6
2	A	2	GLY	6.7
3	C	196	GLY	6.5
3	C	239	GLU	6.3
3	C	238	ASP	3.6
3	C	197	ASP	3.2
2	A	175	ARG	3.1
2	A	109	TYR	2.9
2	A	36	GLN	2.3

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](#)

There are no monosaccharides in this entry.

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. 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	B-factors(\AA^2)	Q<0.9
4	GAL	G	104	12/12	0.92	0.17	31,37,43,45	0
4	GAL	F	104	12/12	0.93	0.17	39,40,42,43	0
4	GAL	D	104	12/12	0.94	0.09	25,27,33,40	0
4	GAL	E	104	12/12	0.94	0.13	26,34,38,40	0
4	GAL	H	104	12/12	0.94	0.09	32,34,40,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.