W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 12:43 pm GMT

PDB ID	:	1DJR
Title	:	HEAT-LABILE ENTEROTOXIN B-PENTAMER COMPLEXED WITH M-CARBOXYPHENYL-ALPHA-D-GALACTOSE
Authors	:	Minke, W.E.; Pickens, J.; Merritt, E.A.; Fan, E.; Verlinde, C.L.M.J.; Hol, W.G.J.
Deposited on	:	1999-12-03
Resolution	:	1.30 Å(reported)

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)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	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 1.30 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.
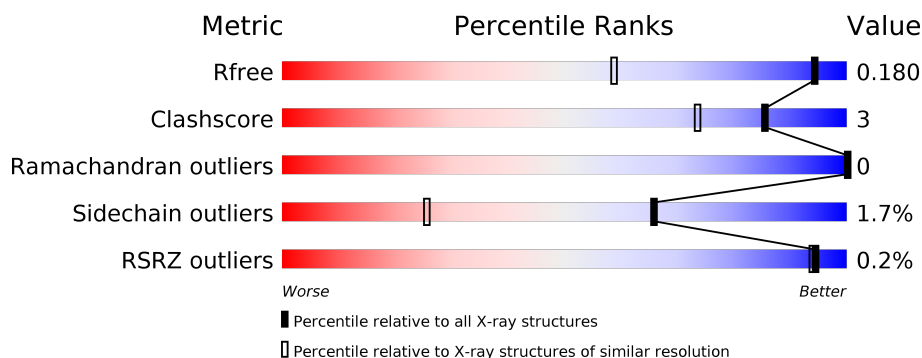
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1131 (1.32-1.28)
Clashscore	112137	1185 (1.32-1.28)
Ramachandran outliers	110173	1138 (1.32-1.28)
Sidechain outliers	110143	1138 (1.32-1.28)
RSRZ outliers	101464	1133 (1.32-1.28)

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

Mol	Chain	Length	Quality of chain
1	D	103	87% 12% •
1	E	103	% 83% 13% • •
1	F	103	83% 14% • •
1	G	103	89% 10% •
1	H	103	84% 11% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLA	D	1104	-	-	-	X
2	GLA	E	1204	-	-	-	X
4	GOL	D	902	-	-	-	X

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 5099 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	103	Total	C	N	O	S	0	3	0
			831	521	140	163	7			
1	E	103	Total	C	N	O	S	0	4	0
			835	525	139	165	6			
1	F	103	Total	C	N	O	S	0	4	0
			839	525	140	168	6			
1	G	103	Total	C	N	O	S	0	4	0
			836	526	139	164	7			
1	H	103	Total	C	N	O	S	0	5	0
			846	531	143	165	7			

- Molecule 2 is D-GALACTOSE (three-letter code: GLA) (formula: $C_6H_{12}O_6$).
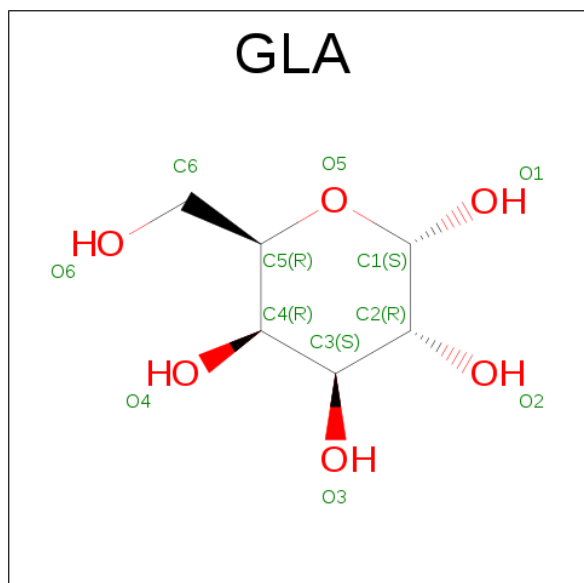
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			12	6	6		

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

- Molecule 3 is BENZOIC ACID (three-letter code: BEZ) (formula: $C_7H_6O_2$).

BEZ
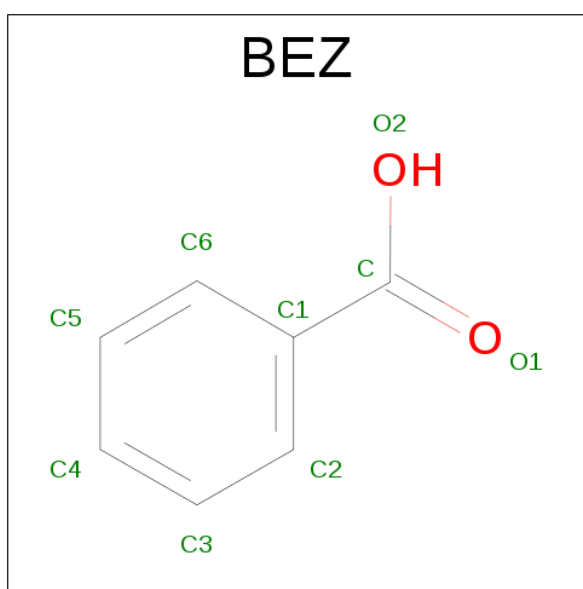
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total 9	C 7	O 2	0	0
3	G	1	Total 9	C 7	O 2	0	0
3	H	1	Total 9	C 7	O 2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total 6	C 3	O 3	0	0
4	D	1	Total 6	C 3	O 3	0	0
4	G	1	Total 6	C 3	O 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	154	Total 154	O 154	0	0
5	E	163	Total 163	O 163	0	0
5	F	150	Total 150	O 150	0	0
5	G	173	Total 173	O 173	0	0
5	H	167	Total 167	O 167	0	0

3 Residue-property plots ⓘ

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.

• Molecule 1: HEAT-LABILE ENTEROTOXIN

Chain D:

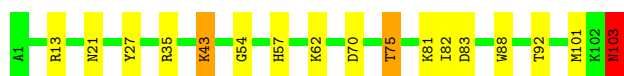• Molecule 1: HEAT-LABILE ENTEROTOXIN

Chain E:

• Molecule 1: HEAT-LABILE ENTEROTOXIN

Chain F:

• Molecule 1: HEAT-LABILE ENTEROTOXIN

Chain G:

• Molecule 1: HEAT-LABILE ENTEROTOXIN

Chain H:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	42.37Å　95.04Å　67.51Å 90.00°　100.71°　90.00°	Depositor
Resolution (Å)	20.00　–　1.30 19.38　–　1.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-1.30) 93.8 (19.38-1.30)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.60 (at 1.30Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.134　,　0.189 0.137　,　0.180	Depositor DCC
R_{free} test set	6479 reflections (5.65%)	DCC
Wilson B-factor (Å^2)	7.9	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 67.2	EDS
L-test for twinning[2]	$< |L| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	5099	wwPDB-VP
Average B, all atoms (Å^2)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.15% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BEZ, GOL, GLA

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	1.04	3/858 (0.3%)	1.55	13/1153 (1.1%)
1	E	1.05	3/865 (0.3%)	1.66	23/1163 (2.0%)
1	F	1.08	3/868 (0.3%)	1.64	19/1169 (1.6%)
1	G	1.03	1/864 (0.1%)	1.44	13/1158 (1.1%)
1	H	1.02	5/880 (0.6%)	2.23	15/1182 (1.3%)
All	All	1.05	15/4335 (0.3%)	1.73	83/5825 (1.4%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	44	SER	CB-OG	6.78	1.51	1.42
1	H	54	GLY	N-CA	-6.48	1.36	1.46
1	D	26	SER	CB-OG	-6.43	1.33	1.42
1	F	83	ASP	CG-OD2	-6.30	1.10	1.25
1	H	46	GLU	CG-CD	-6.08	1.42	1.51
1	F	54	GLY	N-CA	-6.03	1.37	1.46
1	E	46	GLU	CG-CD	-5.85	1.43	1.51
1	G	46	GLU	CD-OE1	-5.82	1.19	1.25
1	D	79	GLU	CD-OE2	-5.71	1.19	1.25
1	H	79	GLU	CD-OE2	-5.53	1.19	1.25
1	D	54	GLY	N-CA	-5.50	1.37	1.46
1	F	101	MET	CG-SD	5.37	1.95	1.81
1	E	102[A]	LYS	C-O	5.13	1.33	1.23
1	E	102[B]	LYS	C-O	5.13	1.33	1.23
1	H	83	ASP	CG-OD2	-5.11	1.13	1.25

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	13[A]	ARG	CD-NE-CZ	39.33	178.66	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	13[B]	ARG	CD-NE-CZ	39.33	178.66	123.60
1	F	13	ARG	NE-CZ-NH1	14.87	127.73	120.30
1	D	35	ARG	NE-CZ-NH1	12.63	126.61	120.30
1	F	101	MET	CG-SD-CE	-12.14	80.77	100.20
1	H	73	ARG	NE-CZ-NH2	10.91	125.75	120.30
1	E	73	ARG	NE-CZ-NH1	10.75	125.67	120.30
1	F	43	LYS	CA-CB-CG	10.32	136.10	113.40
1	H	83	ASP	CB-CG-OD2	10.03	127.32	118.30
1	E	57	HIS	CG-ND1-CE1	10.02	122.23	108.20
1	E	18	TYR	CB-CG-CD1	9.93	126.96	121.00
1	G	34	LYS	CD-CE-NZ	9.91	134.49	111.70
1	D	57	HIS	CG-ND1-CE1	9.89	122.04	108.20
1	F	35	ARG	NE-CZ-NH2	-9.56	115.52	120.30
1	D	53	PRO	C-N-CA	9.25	141.73	122.30
1	H	57	HIS	CG-ND1-CE1	9.17	121.04	108.20
1	F	83	ASP	CB-CG-OD2	9.04	126.44	118.30
1	D	35	ARG	NE-CZ-NH2	-9.02	115.79	120.30
1	D	53	PRO	O-C-N	-8.82	108.21	123.20
1	E	101	MET	CG-SD-CE	-8.57	86.49	100.20
1	F	57	HIS	CG-ND1-CE1	8.17	119.64	108.20
1	G	57	HIS	CG-ND1-CE1	7.92	119.29	108.20
1	F	13	ARG	CD-NE-CZ	7.77	134.48	123.60
1	E	35	ARG	NE-CZ-NH2	-7.75	116.42	120.30
1	D	103	ASN	CA-CB-CG	7.46	129.81	113.40
1	F	75	THR	CA-CB-CG2	-7.30	102.18	112.40
1	F	70	ASP	CB-CG-OD1	7.01	124.61	118.30
1	E	35	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	G	83	ASP	CB-CG-OD2	6.91	124.52	118.30
1	G	18	TYR	CB-CG-CD1	6.86	125.11	121.00
1	G	35	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	D	18	TYR	CB-CG-CD1	6.53	124.92	121.00
1	F	13	ARG	NH1-CZ-NH2	-6.46	112.30	119.40
1	E	102[A]	LYS	CA-CB-CG	6.45	127.59	113.40
1	E	102[B]	LYS	CA-CB-CG	6.45	127.59	113.40
1	E	102[A]	LYS	C-N-CA	6.32	137.50	121.70
1	E	102[B]	LYS	C-N-CA	6.32	137.50	121.70
1	E	103	ASN	N-CA-CB	-6.28	99.29	110.60
1	G	53	PRO	O-C-N	-6.28	112.52	123.20
1	G	73	ARG	CD-NE-CZ	6.26	132.37	123.60
1	H	35	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	E	53	PRO	C-N-CA	6.20	135.32	122.30
1	G	45	GLY	O-C-N	-6.09	112.96	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	13	ARG	CD-NE-CZ	6.04	132.06	123.60
1	G	18	TYR	CZ-CE2-CD2	6.01	125.21	119.80
1	H	13[A]	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	H	13[B]	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	D	53	PRO	CA-C-N	5.96	128.12	116.20
1	E	12	TYR	CG-CD1-CE1	-5.94	116.55	121.30
1	E	18	TYR	CB-CG-CD2	-5.91	117.45	121.00
1	F	35	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	E	73	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	E	53	PRO	O-C-N	-5.88	113.19	123.20
1	H	53	PRO	O-C-N	-5.83	113.30	123.20
1	H	73	ARG	CD-NE-CZ	5.79	131.70	123.60
1	D	42	PHE	CB-CG-CD2	5.74	124.82	120.80
1	D	62	LYS	CD-CE-NZ	5.69	124.79	111.70
1	H	18	TYR	CG-CD1-CE1	5.68	125.84	121.30
1	E	103	ASN	CB-CG-OD1	-5.66	110.28	121.60
1	D	62	LYS	CG-CD-CE	5.66	128.88	111.90
1	H	44	SER	CA-CB-OG	-5.62	96.02	111.20
1	F	27	TYR	CG-CD1-CE1	5.61	125.79	121.30
1	F	88	TRP	CE2-CD2-CG	5.61	111.79	107.30
1	F	92	THR	CA-CB-CG2	-5.59	104.57	112.40
1	G	79	GLU	OE1-CD-OE2	-5.57	116.62	123.30
1	H	57	HIS	ND1-CG-CD2	-5.50	98.30	106.00
1	D	42	PHE	CB-CG-CD1	-5.45	116.99	120.80
1	H	42	PHE	CB-CG-CD2	5.37	124.56	120.80
1	H	53	PRO	C-N-CA	5.33	133.50	122.30
1	F	103	ASN	CB-CG-OD1	-5.32	110.97	121.60
1	E	57	HIS	ND1-CE1-NE2	-5.23	98.39	109.90
1	F	43	LYS	CD-CE-NZ	-5.20	99.74	111.70
1	F	35	ARG	CG-CD-NE	-5.16	100.96	111.80
1	E	60	SER	N-CA-CB	-5.16	102.76	110.50
1	G	27	TYR	CB-CG-CD1	5.12	124.07	121.00
1	E	46	GLU	CA-CB-CG	-5.07	102.24	113.40
1	F	62	LYS	CB-CG-CD	5.07	124.78	111.60
1	E	12	TYR	CD1-CE1-CZ	5.07	124.36	119.80
1	G	18	TYR	CD1-CE1-CZ	5.06	124.35	119.80
1	G	27	TYR	CG-CD1-CE1	5.05	125.34	121.30
1	E	43[A]	LYS	CA-CB-CG	5.04	124.49	113.40
1	E	43[B]	LYS	CA-CB-CG	5.04	124.49	113.40
1	F	57	HIS	ND1-CG-CD2	-5.03	98.96	106.00

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	D	831	0	846	3	0
1	E	835	0	852	9	0
1	F	839	0	846	5	0
1	G	836	0	857	1	0
1	H	846	0	869	7	0
2	D	12	0	12	0	0
2	E	12	0	12	0	0
2	F	12	0	11	0	0
2	G	12	0	11	0	0
2	H	12	0	11	0	0
3	F	9	0	4	0	0
3	G	9	0	4	0	0
3	H	9	0	4	0	0
4	D	6	0	8	0	0
4	G	6	0	8	0	0
4	H	6	0	8	0	0
5	D	154	0	0	0	0
5	E	163	0	0	5	0
5	F	150	0	0	1	0
5	G	173	0	0	1	0
5	H	167	0	0	5	0
All	All	5099	0	4363	23	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 3.

All (23) 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:H:102:LYS:HD3	5:H:1667:HOH:O	1.84	0.77
1:E:43[A]:LYS:HG3	5:E:1219:HOH:O	1.97	0.64
1:F:103:ASN:ND2	1:F:103:ASN:OXT	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:83:ASP:OD2	1:E:102[A]:LYS:HE3	2.04	0.57
1:F:75:THR:HG21	1:F:82[B]:ILE:HD11	1.89	0.54
1:H:13[B]:ARG:HD3	5:H:1593:HOH:O	2.10	0.52
1:H:81[B]:LYS:HE3	5:H:1605:HOH:O	2.10	0.51
1:D:58:ILE:CD1	1:E:34:LYS:HE2	2.41	0.51
1:E:46:GLU:HG2	5:E:1341:HOH:O	2.11	0.50
1:F:21:ASN:OD1	1:F:81:LYS:HD3	2.14	0.47
1:E:103:ASN:N	5:E:1279:HOH:O	2.47	0.46
1:H:21:ASN:HB2	5:H:1642:HOH:O	2.16	0.46
1:G:34:LYS:NZ	5:G:1532:HOH:O	2.49	0.45
1:F:81:LYS:NZ	5:F:1435:HOH:O	2.50	0.44
1:E:81:LYS:NZ	5:E:1367:HOH:O	2.52	0.42
1:D:101[B]:MET:HG3	1:E:76:TYR:CE2	2.54	0.42
1:H:83:ASP:OD1	5:H:1642:HOH:O	2.22	0.42
1:H:44:SER:OG	1:H:46:GLU:OE1	2.26	0.42
1:E:63:LYS:NZ	5:E:1273:HOH:O	2.46	0.42
1:D:103:ASN:OXT	1:D:103:ASN:ND2	2.54	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	104/103 (101%)	103 (99%)	1 (1%)	0	100	100
1	E	105/103 (102%)	104 (99%)	1 (1%)	0	100	100
1	F	105/103 (102%)	104 (99%)	1 (1%)	0	100	100
1	G	104/103 (101%)	102 (98%)	2 (2%)	0	100	100
1	H	106/103 (103%)	105 (99%)	1 (1%)	0	100	100
All	All	524/515 (102%)	518 (99%)	6 (1%)	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	97/95 (102%)	96 (99%)	1 (1%)	80	47
1	E	98/95 (103%)	95 (97%)	3 (3%)	45	7
1	F	99/95 (104%)	97 (98%)	2 (2%)	60	18
1	G	98/95 (103%)	98 (100%)	0	100	100
1	H	100/95 (105%)	96 (96%)	4 (4%)	36	3
All	All	492/475 (104%)	482 (98%)	10 (2%)	66	18

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	103	ASN
1	E	26	SER
1	E	101	MET
1	E	103	ASN
1	F	43	LYS
1	F	103	ASN
1	H	13[A]	ARG
1	H	13[B]	ARG
1	H	101[A]	MET
1	H	101[B]	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	94	ASN
1	E	16	GLN
1	E	94	ASN
1	E	103	ASN
1	H	94	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

11 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	#$|Z| > 2$
2	GLA	D	1104	-	12,12,12	0.96	0	17,17,17	1.10	2 (11%)
4	GOL	D	902	-	5,5,5	0.83	0	5,5,5	1.10	0
2	GLA	E	1204	-	12,12,12	0.75	0	17,17,17	1.32	4 (23%)
2	GLA	F	1304	3	12,12,12	0.84	0	17,17,17	1.39	2 (11%)
3	BEZ	F	1305	2	6,9,9	1.11	0	8,11,11	2.63	4 (50%)
2	GLA	G	1404	3	12,12,12	0.83	0	17,17,17	1.21	1 (5%)
3	BEZ	G	1405	2	6,9,9	0.75	0	8,11,11	2.51	2 (25%)
4	GOL	G	903	-	5,5,5	1.02	0	5,5,5	0.66	0
2	GLA	H	1504	3	12,12,12	0.67	0	17,17,17	0.96	1 (5%)
3	BEZ	H	1505	2	6,9,9	0.63	0	8,11,11	2.05	4 (50%)
4	GOL	H	901	-	5,5,5	0.95	0	5,5,5	0.57	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
2	GLA	D	1104	-	-	0/2/22/22	0/1/1/1
4	GOL	D	902	-	-	0/4/4/4	0/0/0/0
2	GLA	E	1204	-	-	0/2/22/22	0/1/1/1
2	GLA	F	1304	3	-	0/2/22/22	0/1/1/1
3	BEZ	F	1305	2	-	0/0/4/4	0/1/1/1
2	GLA	G	1404	3	-	0/2/22/22	0/1/1/1
3	BEZ	G	1405	2	-	0/0/4/4	0/1/1/1
4	GOL	G	903	-	-	0/4/4/4	0/0/0/0
2	GLA	H	1504	3	-	0/2/22/22	0/1/1/1
3	BEZ	H	1505	2	-	0/0/4/4	0/1/1/1
4	GOL	H	901	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	1405	BEZ	C2-C1-C	-5.11	113.58	120.45
3	F	1305	BEZ	C3-C2-C1	-4.34	115.07	120.57
3	F	1305	BEZ	C2-C1-C	-3.96	115.13	120.45
2	F	1304	GLA	O2-C2-C3	-2.43	105.08	110.36
2	G	1404	GLA	O5-C5-C6	-2.40	100.67	106.41
3	H	1505	BEZ	C3-C2-C1	-2.27	117.69	120.57
2	E	1204	GLA	O4-C4-C3	-2.20	105.57	110.36
2	D	1104	GLA	C6-C5-C4	-2.20	107.85	113.00
2	D	1104	GLA	C1-C2-C3	2.05	114.35	110.65
2	E	1204	GLA	C1-C2-C3	2.08	114.40	110.65
3	H	1505	BEZ	C6-C1-C	2.12	123.31	120.45
2	E	1204	GLA	O5-C1-C2	2.17	113.64	110.04
2	E	1204	GLA	O1-C1-C2	2.23	115.70	109.42
2	F	1304	GLA	O5-C5-C4	2.37	114.02	109.66
3	F	1305	BEZ	C6-C1-C2	2.62	122.79	117.59
2	H	1504	GLA	O5-C1-C2	2.64	114.43	110.04
3	H	1505	BEZ	C4-C3-C2	2.94	124.25	120.21
3	F	1305	BEZ	C4-C3-C2	3.05	124.41	120.21
3	H	1505	BEZ	C5-C6-C1	3.30	124.75	120.57
3	G	1405	BEZ	C6-C1-C	4.48	126.48	120.45

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

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%)	-0.48	0	100	100	6, 10, 18, 31	0
1	E	103/103 (100%)	-0.42	1 (0%)	82	82	6, 10, 21, 31	0
1	F	103/103 (100%)	-0.53	0	100	100	6, 9, 17, 35	0
1	G	103/103 (100%)	-0.57	0	100	100	6, 9, 17, 22	0
1	H	103/103 (100%)	-0.58	0	100	100	6, 9, 17, 21	0
All	All	515/515 (100%)	-0.52	1 (0%)	94	94	6, 9, 19, 35	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	103	ASN	3.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	GOL	D	902	6/6	0.94	0.10	5.59	15,24,31,38	0
2	GLA	D	1104	12/12	0.87	0.15	4.95	17,20,23,24	0
2	GLA	E	1204	12/12	0.90	0.13	2.79	15,19,26,33	0
2	GLA	G	1404	12/12	0.95	0.08	1.98	12,15,18,24	0
3	BEZ	H	1505	9/9	0.96	0.12	1.48	15,16,16,18	0
4	GOL	G	903	6/6	0.95	0.07	0.61	13,15,20,25	0
4	GOL	H	901	6/6	0.98	0.06	-0.05	9,10,11,13	0
2	GLA	H	1504	12/12	0.97	0.06	-0.28	9,12,14,15	0
3	BEZ	F	1305	9/9	0.97	0.06	-0.43	10,12,16,23	0
2	GLA	F	1304	12/12	0.98	0.05	-0.64	8,9,11,12	0
3	BEZ	G	1405	9/9	0.72	0.30	-	32,35,39,42	0

6.5 Other polymers ⓘ

There are no such residues in this entry.