Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:59 PM GMT

PDB ID	:	1DIW
Title	:	THE HC FRAGMENT OF TETANUS TOXIN COMPLEXED WITH GALACTOSE
Authors	:	Emsley, P.; Fotinou, C.; Black, I.; Fairweather, N.F.; Charles, I.G.; Watts, C.; Hewitt, E.; Isaacs, N.W.
Deposited on	:	1999-11-30
Resolution	:	2.00 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

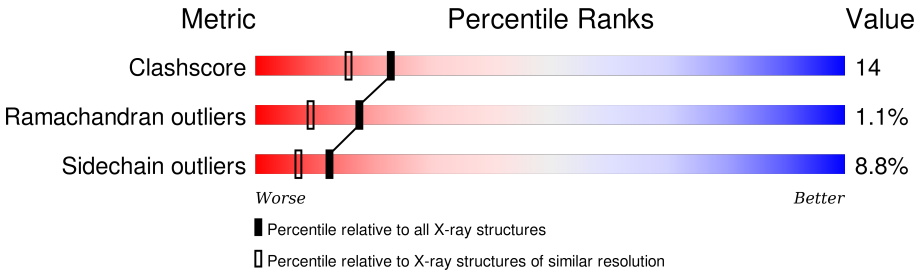
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	441	69% 22% 7% •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3924 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.

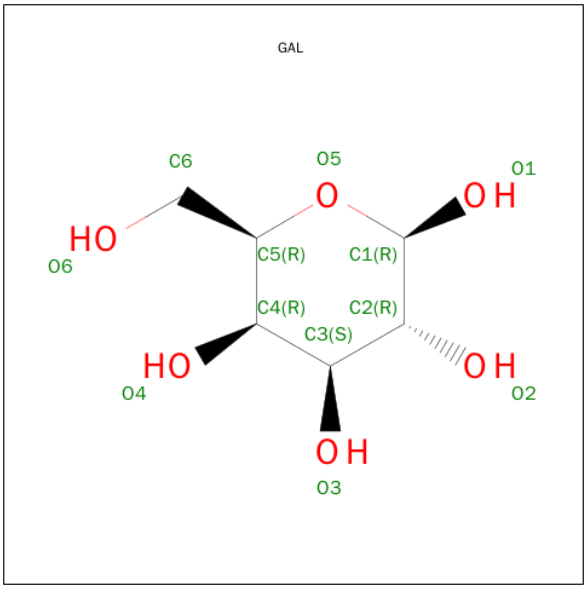
- Molecule 1 is a protein called TETANUS TOXIN HC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	441	Total	C	N	O	S	0	0	0
			3566	2284	597	676	9			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	930	GLU	SER	CONFLICT	UNP P04958

- Molecule 2 is D-GALACTOSE (three-letter code: GAL) (formula: $C_6H_{12}O_6$).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	346	Total	O	0	0
			346	346		

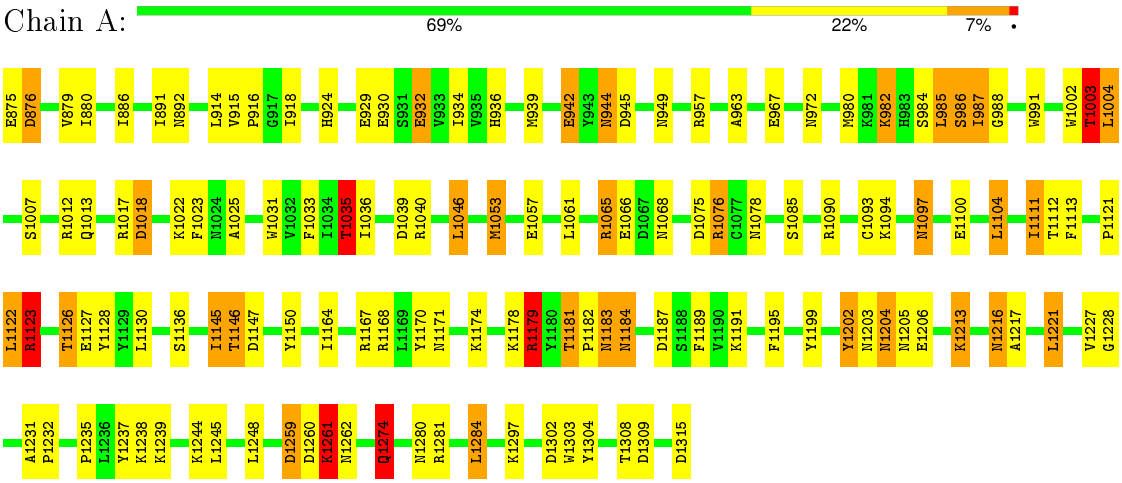
3 Residue-property plots (i)

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: TETANUS TOXIN HC

Chain A:



4 Data and refinement statistics (i)

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, α, β, γ	67.08Å 70.88Å 122.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.90 – 2.00	Depositor
% Data completeness (in resolution range)	98.8 (27.90-2.00)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.216 , 0.267	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3924	wwPDB-VP
Average B, all atoms (Å^2)	36.0	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: 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	A	0.52	0/3647	1.52	58/4949 (1.2%)

There are no bond length outliers.

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1065	ARG	NE-CZ-NH1	22.68	131.64	120.30
1	A	1179	ARG	NE-CZ-NH1	16.98	128.79	120.30
1	A	1090	ARG	NE-CZ-NH1	14.62	127.61	120.30
1	A	1123	ARG	NE-CZ-NH2	13.45	127.03	120.30
1	A	1065	ARG	CD-NE-CZ	13.36	142.30	123.60
1	A	1179	ARG	NH1-CZ-NH2	-13.05	105.04	119.40
1	A	1179	ARG	NE-CZ-NH2	11.67	126.14	120.30
1	A	1221	LEU	CA-CB-CG	11.62	142.02	115.30
1	A	1145	ILE	C-N-CA	11.38	150.16	121.70
1	A	985	LEU	N-CA-CB	10.86	132.12	110.40
1	A	1145	ILE	CA-C-O	9.49	140.02	120.10
1	A	1065	ARG	NE-CZ-NH2	-9.19	115.71	120.30
1	A	957	ARG	NE-CZ-NH2	-9.13	115.74	120.30
1	A	1168	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	A	1259	ASP	CB-CG-OD2	-7.65	111.42	118.30
1	A	1046	LEU	CA-CB-CG	7.63	132.85	115.30
1	A	1202	TYR	CB-CG-CD1	7.61	125.57	121.00
1	A	1145	ILE	CA-C-N	-7.58	100.53	117.20
1	A	985	LEU	CA-C-O	7.35	135.54	120.10
1	A	957	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	A	1274	GLN	CA-CB-CG	7.09	128.99	113.40
1	A	1145	ILE	N-CA-CB	7.04	126.98	110.80
1	A	1122	LEU	CA-CB-CG	7.03	131.47	115.30
1	A	1090	ARG	NE-CZ-NH2	-6.91	116.85	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1123	ARG	NH1-CZ-NH2	-6.72	112.01	119.40
1	A	1123	ARG	CA-CB-CG	6.69	128.12	113.40
1	A	1039	ASP	CB-CG-OD1	6.68	124.31	118.30
1	A	985	LEU	CA-C-N	-6.51	102.88	117.20
1	A	1284	LEU	CB-CG-CD2	6.51	122.06	111.00
1	A	1123	ARG	CD-NE-CZ	6.50	132.69	123.60
1	A	1004	LEU	CA-CB-CG	6.45	130.14	115.30
1	A	1146	THR	N-CA-CB	6.41	122.47	110.30
1	A	1309	ASP	CB-CG-OD1	6.36	124.03	118.30
1	A	1065	ARG	NH1-CZ-NH2	-6.13	112.66	119.40
1	A	1259	ASP	CB-CG-OD1	6.11	123.80	118.30
1	A	1035	THR	CA-CB-CG2	5.97	120.76	112.40
1	A	1304	TYR	CA-CB-CG	5.97	124.75	113.40
1	A	930	GLU	OE1-CD-OE2	-5.89	116.23	123.30
1	A	1076	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	A	1284	LEU	CA-CB-CG	5.66	128.31	115.30
1	A	1128	TYR	CB-CG-CD2	-5.65	117.61	121.00
1	A	942	GLU	CA-CB-CG	5.62	125.76	113.40
1	A	1261	LYS	CA-CB-CG	5.49	125.47	113.40
1	A	1202	TYR	CA-CB-CG	5.48	123.80	113.40
1	A	1090	ARG	CD-NE-CZ	5.47	131.27	123.60
1	A	1202	TYR	CB-CG-CD2	-5.47	117.72	121.00
1	A	1003	THR	N-CA-CB	5.44	120.63	110.30
1	A	1018	ASP	CB-CG-OD1	5.43	123.19	118.30
1	A	1076	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	A	932	GLU	N-CA-CB	-5.37	100.94	110.60
1	A	1126	THR	N-CA-CB	5.30	120.36	110.30
1	A	1128	TYR	CB-CG-CD1	5.25	124.15	121.00
1	A	1302	ASP	CB-CG-OD2	-5.24	113.58	118.30
1	A	1315	ASP	CA-C-O	-5.21	109.16	120.10
1	A	1181	THR	O-C-N	5.13	130.86	121.10
1	A	1066	GLU	OE1-CD-OE2	-5.10	117.18	123.30
1	A	1179	ARG	CD-NE-CZ	5.08	130.72	123.60
1	A	1122	LEU	CB-CG-CD2	5.05	119.59	111.00

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	A	3566	0	3516	96	1
2	A	12	0	12	0	0
3	A	346	0	0	22	1
All	All	3924	0	3528	96	1

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 14.

All (96) 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:A:918:ILE:HD12	1:A:918:ILE:H	1.47	0.80
1:A:1111:ILE:HG22	1:A:1248:LEU:HD11	1.64	0.78
1:A:918:ILE:HG23	3:A:42:HOH:O	1.84	0.77
1:A:1260:ASP:HB3	3:A:49:HOH:O	1.85	0.76
1:A:1003:THR:HB	1:A:1013:GLN:HG2	1.66	0.75
1:A:1097:ASN:ND2	1:A:1100:GLU:H	1.83	0.75
1:A:1274:GLN:NE2	1:A:1280:ASN:HD22	1.86	0.73
1:A:1111:ILE:H	1:A:1111:ILE:HD13	1.55	0.71
1:A:1203:ASN:O	1:A:1204:ASN:HB2	1.90	0.71
1:A:1274:GLN:HE22	1:A:1280:ASN:HD22	1.39	0.70
1:A:1053:MET:SD	3:A:239:HOH:O	2.51	0.67
1:A:1123:ARG:HH21	1:A:1189:PHE:HE2	1.43	0.67
1:A:1179:ARG:NH2	1:A:1187:ASP:O	2.28	0.65
1:A:1274:GLN:NE2	3:A:43:HOH:O	2.31	0.64
1:A:1178:LYS:HE2	3:A:349:HOH:O	1.98	0.64
1:A:1195:PHE:CD1	1:A:1239:LYS:HE3	2.34	0.62
1:A:1022:LYS:HZ1	1:A:1164:ILE:HG22	1.64	0.62
1:A:1003:THR:HG23	3:A:23:HOH:O	1.99	0.61
1:A:918:ILE:CD1	1:A:918:ILE:H	2.14	0.61
1:A:1113:PHE:HB3	3:A:157:HOH:O	1.99	0.61
1:A:891:ILE:HD13	1:A:914:LEU:HD22	1.83	0.59
1:A:949:ASN:ND2	1:A:1040:ARG:H	2.00	0.59
1:A:1213:LYS:HD2	1:A:1235:PRO:HG2	1.84	0.59
1:A:1187:ASP:OD2	1:A:1191:LYS:NZ	2.36	0.58
1:A:980:MET:HB3	1:A:988:GLY:HA2	1.86	0.57
1:A:1259:ASP:OD2	1:A:1261:LYS:HD2	2.05	0.56
1:A:939:MET:HA	1:A:942:GLU:HG3	1.87	0.56
1:A:991:TRP:HB3	1:A:1004:LEU:HD23	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:918:ILE:N	1:A:918:ILE:HD12	2.18	0.56
1:A:982:LYS:HD2	1:A:1076:ARG:NH2	2.21	0.55
1:A:1178:LYS:HD2	1:A:1199:TYR:CE1	2.42	0.55
1:A:1203:ASN:O	1:A:1204:ASN:CB	2.51	0.55
1:A:1171:ASN:HB2	3:A:67:HOH:O	2.07	0.55
1:A:1003:THR:HG21	1:A:1013:GLN:HE21	1.72	0.54
1:A:963:ALA:O	1:A:967:GLU:HG3	2.08	0.53
1:A:936:HIS:HB3	3:A:25:HOH:O	2.09	0.52
1:A:1093:CYS:HB2	3:A:62:HOH:O	2.07	0.52
1:A:929:GLU:HG2	3:A:111:HOH:O	2.10	0.51
1:A:932:GLU:OE2	1:A:934:ILE:HD11	2.11	0.51
1:A:918:ILE:HD11	1:A:1031:TRP:CE3	2.46	0.51
1:A:1111:ILE:HG22	1:A:1248:LEU:CD1	2.36	0.50
1:A:985:LEU:HD12	1:A:986:SER:H	1.76	0.50
1:A:1183:ASN:O	1:A:1184:ASN:HB2	2.11	0.50
1:A:924:HIS:HE1	3:A:135:HOH:O	1.95	0.50
1:A:1261:LYS:O	1:A:1262:ASN:HB2	2.11	0.50
1:A:880:ILE:HD13	1:A:1100:GLU:OE2	2.11	0.49
1:A:945:ASP:HB3	3:A:257:HOH:O	2.12	0.49
1:A:1111:ILE:H	1:A:1111:ILE:CD1	2.24	0.49
1:A:924:HIS:HD2	1:A:1085:SER:OG	1.95	0.49
1:A:1068:ASN:HB2	3:A:318:HOH:O	2.12	0.49
1:A:1127:GLU:CD	1:A:1174:LYS:HE2	2.32	0.49
1:A:980:MET:HB3	1:A:988:GLY:CA	2.43	0.48
1:A:876:ASP:HB2	1:A:879:VAL:HG23	1.96	0.48
1:A:1112:THR:HG23	3:A:290:HOH:O	2.14	0.48
1:A:1022:LYS:NZ	3:A:28:HOH:O	2.21	0.48
1:A:1097:ASN:HD21	1:A:1100:GLU:HG3	1.77	0.48
1:A:972:ASN:ND2	1:A:1078:ASN:H	2.12	0.48
1:A:1097:ASN:HD22	1:A:1100:GLU:H	1.61	0.47
1:A:1178:LYS:NZ	1:A:1206:GLU:OE1	2.41	0.47
1:A:1057:GLU:HG2	3:A:299:HOH:O	2.14	0.47
1:A:1033:PHE:CZ	1:A:1104:LEU:HD13	2.49	0.47
1:A:1017:ARG:HH11	1:A:1017:ARG:HB3	1.78	0.47
1:A:1121:PRO:HB2	1:A:1189:PHE:CE2	2.50	0.47
1:A:1022:LYS:HE3	1:A:1164:ILE:HB	1.97	0.47
1:A:1205:ASN:HB2	3:A:326:HOH:O	2.15	0.47
1:A:1146:THR:HA	1:A:1227:VAL:O	2.14	0.47
1:A:944:ASN:HD22	1:A:944:ASN:N	2.14	0.46
1:A:1213:LYS:HG3	1:A:1237:TYR:OH	2.16	0.46
1:A:1130:LEU:HD22	1:A:1303:TRP:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1260:ASP:HB3	3:A:303:HOH:O	2.16	0.46
1:A:1121:PRO:HB2	1:A:1189:PHE:CD2	2.50	0.45
1:A:1123:ARG:NH2	1:A:1189:PHE:CE2	2.83	0.45
1:A:1097:ASN:ND2	1:A:1100:GLU:HG3	2.32	0.45
1:A:876:ASP:CB	1:A:879:VAL:HG23	2.47	0.45
1:A:1146:THR:HG22	1:A:1228:GLY:O	2.17	0.45
1:A:915:VAL:HB	1:A:916:PRO:CD	2.47	0.45
1:A:1170:TYR:CE1	1:A:1308:THR:HA	2.52	0.44
1:A:986:SER:O	1:A:987:ILE:HG22	2.17	0.44
1:A:1035:THR:HG23	3:A:35:HOH:O	2.17	0.44
1:A:1012:ARG:HG2	1:A:1061:LEU:HD21	2.00	0.44
1:A:1002:TRP:CE3	1:A:1036:ILE:HD13	2.53	0.44
1:A:1123:ARG:NH2	1:A:1189:PHE:HE2	2.13	0.44
1:A:1213:LYS:HA	1:A:1237:TYR:CE2	2.52	0.44
1:A:1007:SER:OG	1:A:1065:ARG:NH1	2.51	0.44
1:A:1097:ASN:C	1:A:1097:ASN:HD22	2.22	0.43
1:A:987:ILE:HG23	1:A:987:ILE:O	2.19	0.42
1:A:1018:ASP:OD2	1:A:1025:ALA:HB1	2.20	0.42
1:A:1274:GLN:HB2	3:A:43:HOH:O	2.18	0.42
1:A:1150:TYR:CG	1:A:1281:ARG:HD3	2.54	0.42
1:A:1216:ASN:HD22	1:A:1217:ALA:H	1.67	0.42
1:A:1231:ALA:HA	1:A:1232:PRO:HD3	1.86	0.41
1:A:1033:PHE:HZ	1:A:1104:LEU:HD13	1.85	0.41
1:A:1123:ARG:NH2	3:A:10:HOH:O	2.54	0.41
1:A:1097:ASN:HD21	1:A:1100:GLU:H	1.63	0.40
1:A:1023:PHE:CE2	1:A:1136:SER:HB2	2.56	0.40
1:A:1075:ASP:O	1:A:1076:ARG:HB2	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1179:ARG:NH1	3:A:108:HOH:O[4_456]	2.15	0.05

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	439/441 (100%)	410 (93%)	24 (6%)	5 (1%)	17 9

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	987	ILE
1	A	1182	PRO
1	A	1183	ASN
1	A	1213	LYS
1	A	1184	ASN

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	397/397 (100%)	362 (91%)	35 (9%)	12 7

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	875	GLU
1	A	876	ASP
1	A	886	ILE
1	A	892	ASN
1	A	944	ASN
1	A	982	LYS
1	A	984	SER
1	A	986	SER
1	A	1003	THR
1	A	1035	THR
1	A	1046	LEU
1	A	1053	MET

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Mol	Chain	Res	Type
1	A	1094	LYS
1	A	1097	ASN
1	A	1104	LEU
1	A	1111	ILE
1	A	1122	LEU
1	A	1123	ARG
1	A	1126	THR
1	A	1145	ILE
1	A	1147	ASP
1	A	1167	ARG
1	A	1179	ARG
1	A	1181	THR
1	A	1202	TYR
1	A	1204	ASN
1	A	1216	ASN
1	A	1221	LEU
1	A	1238	LYS
1	A	1244	LYS
1	A	1245	LEU
1	A	1261	LYS
1	A	1274	GLN
1	A	1284	LEU
1	A	1297	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	924	HIS
1	A	936	HIS
1	A	944	ASN
1	A	949	ASN
1	A	972	ASN
1	A	1013	GLN
1	A	1082	GLN
1	A	1097	ASN
1	A	1184	ASN
1	A	1216	ASN
1	A	1271	HIS
1	A	1274	GLN

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

1 ligand is 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	GAL	A	1400	-	12,12,12	0.43	0	17,17,17	1.35	3 (17%)

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	GAL	A	1400	-	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1400	GAL	O5-C5-C4	-2.07	105.81	109.68
2	A	1400	GAL	O5-C1-C2	2.70	114.10	109.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1400	GAL	O2-C2-C3	2.78	116.60	110.34

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 (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

6.1 Protein, DNA and RNA chains

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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