Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:08 AM GMT

PDB ID	:	1ZUJ
Title	:	The crystal structure of the Lactococcus lactis MG1363 DpsA protein
Authors	:	Stillman, T.J.; Upadhyay, M.; Norte, V.A.; Sedelnikova, S.E.; Carradus, M.; Tzokov, S.; Bullough, P.A.; Shearman, C.A.; Gasson, M.J.; Williams, C.H.; Artymiuk, P.J.; Green, J.
Deposited on	:	2005-05-31
Resolution	:	2.90 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:

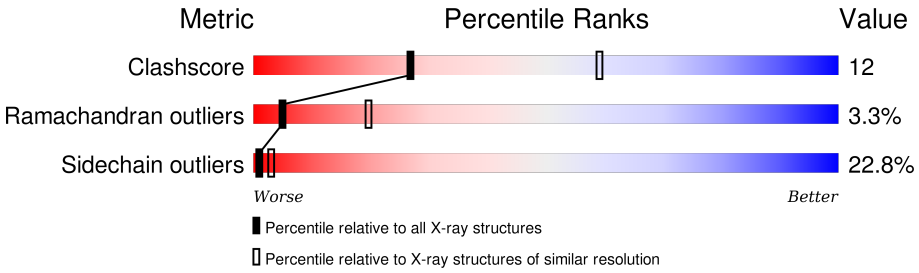
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.90 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	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)

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	179	49% 39% • • 6%
1	B	179	46% 37% 9% • 6%
1	C	179	51% 35% 8% 6%
1	D	179	59% 30% 5% • 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5589 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 hypothetical protein Llacc01001955.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	168	Total	C	N	O	S	0	0	0
			1386	900	221	263	2			
1	B	168	Total	C	N	O	S	0	0	0
			1386	900	221	263	2			
1	C	168	Total	C	N	O	S	0	0	0
			1386	900	221	263	2			
1	D	168	Total	C	N	O	S	0	0	0
			1386	900	221	263	2			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	O	0	0
			3	3		
2	B	6	Total	O	0	0
			6	6		
2	C	19	Total	O	0	0
			19	19		
2	D	17	Total	O	0	0
			17	17		

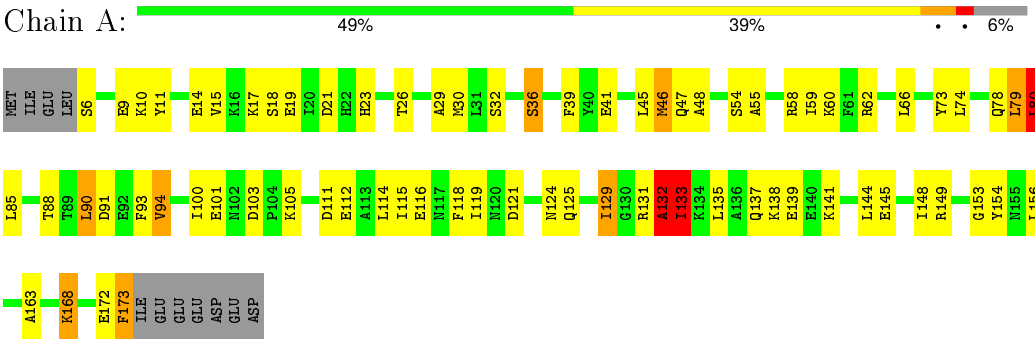
3 Residue-property plots (i)

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.

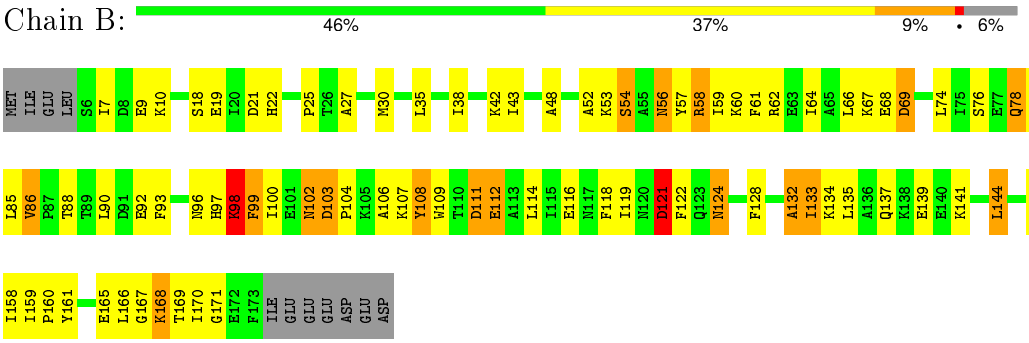
- Molecule 1: hypothetical protein Llacc01001955

Chain A:



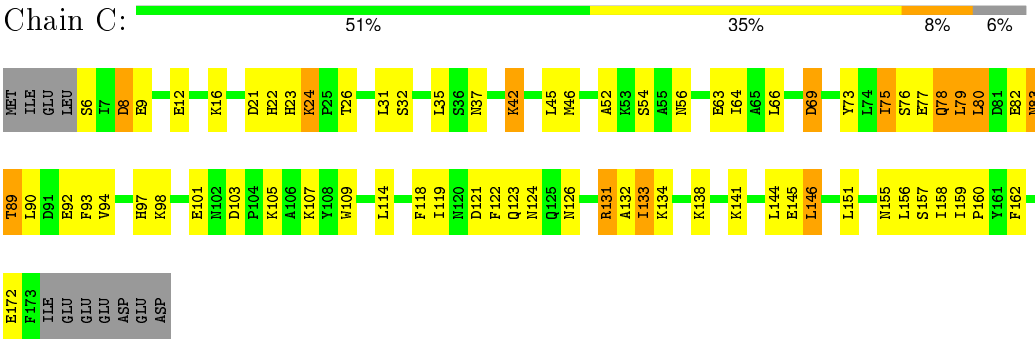
- Molecule 1: hypothetical protein Llacc01001955

Chain B:



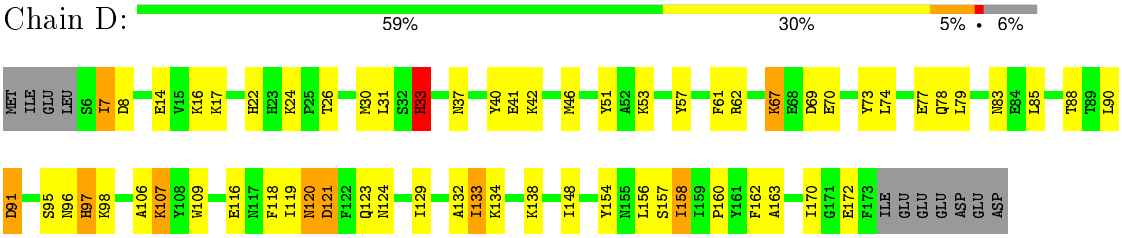
- Molecule 1: hypothetical protein Llacc01001955

Chain C:



• Molecule 1: hypothetical protein Llacc01001955

Chain D:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	131.84Å 131.84Å 325.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.90	Depositor
% Data completeness (in resolution range)	87.1 (15.00-2.90)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.253 , 0.322	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5589	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.56	0/1417	0.76	5/1909 (0.3%)
1	B	0.54	0/1417	0.79	4/1909 (0.2%)
1	C	0.65	0/1417	0.85	5/1909 (0.3%)
1	D	0.77	0/1417	0.93	3/1909 (0.2%)
All	All	0.64	0/5668	0.84	17/7636 (0.2%)

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	A	0	1
1	B	0	1
1	C	0	3
1	D	0	2
All	All	0	7

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	91	ASP	CB-CG-OD2	7.11	124.70	118.30
1	B	21	ASP	CB-CG-OD2	6.68	124.32	118.30
1	A	111	ASP	CB-CG-OD2	6.35	124.02	118.30
1	B	121	ASP	CB-CG-OD2	6.11	123.80	118.30
1	C	103	ASP	CB-CG-OD2	5.84	123.55	118.30
1	A	91	ASP	CB-CG-OD2	5.68	123.41	118.30
1	A	103	ASP	CB-CG-OD2	5.68	123.41	118.30
1	A	133	ILE	N-CA-C	-5.46	96.26	111.00
1	D	33	HIS	N-CA-CB	5.31	120.16	110.60
1	C	121	ASP	CB-CG-OD2	5.30	123.07	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	121	ASP	CB-CG-OD2	5.26	123.04	118.30
1	B	111	ASP	CB-CG-OD2	5.22	123.00	118.30
1	C	69	ASP	CB-CG-OD2	5.20	122.98	118.30
1	C	21	ASP	CB-CG-OD2	5.19	122.97	118.30
1	C	8	ASP	CB-CG-OD2	5.14	122.92	118.30
1	A	21	ASP	CB-CG-OD2	5.10	122.89	118.30
1	B	69	ASP	CB-CG-OD2	5.09	122.88	118.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	132	ALA	Peptide
1	B	132	ALA	Peptide
1	C	131	ARG	Peptide
1	C	132	ALA	Peptide
1	C	24	LYS	Peptide
1	D	132	ALA	Peptide
1	D	24	LYS	Peptide

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	A	1386	0	1366	43	0
1	B	1386	0	1366	36	0
1	C	1386	0	1366	30	0
1	D	1386	0	1366	32	0
2	A	3	0	0	0	0
2	B	6	0	0	0	0
2	C	19	0	0	0	0
2	D	17	0	0	1	0
All	All	5589	0	5464	133	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 12.

All (133) 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:156:LEU:O	1:C:160:PRO:CD	2.15	0.94
1:A:154:TYR:CE2	1:A:158:ILE:HD11	2.07	0.90
1:C:156:LEU:O	1:C:160:PRO:HD3	1.71	0.88
1:A:41:GLU:OE1	1:A:121:ASP:HB3	1.81	0.80
1:C:107:LYS:NZ	1:D:14:GLU:OE2	2.15	0.79
1:B:106:ALA:HA	1:B:109:TRP:CD1	2.21	0.75
1:D:119:ILE:HD11	1:D:162:PHE:HB3	1.69	0.74
1:A:90:LEU:HD12	1:B:102:ASN:HD21	1.52	0.74
1:C:156:LEU:O	1:C:160:PRO:HD2	1.87	0.73
1:D:33:HIS:O	1:D:37:ASN:ND2	2.25	0.70
1:A:32:SER:O	1:A:36:SER:HB2	1.94	0.68
1:C:118:PHE:O	1:C:122:PHE:HD1	1.75	0.67
1:B:97:HIS:O	1:B:98:LYS:HD2	1.93	0.67
1:D:156:LEU:O	1:D:160:PRO:CD	2.43	0.67
1:C:73:TYR:O	1:C:77:GLU:HG2	1.96	0.66
1:D:22:HIS:HE1	1:D:96:ASN:HD21	1.46	0.64
1:C:78:GLN:HB3	1:C:144:LEU:HD12	1.79	0.63
1:D:22:HIS:HE1	1:D:96:ASN:ND2	1.97	0.62
1:A:14:GLU:OE2	1:B:108:TYR:OH	2.15	0.62
1:C:37:ASN:HD21	1:C:98:LYS:H	1.48	0.61
1:B:27:ALA:HB3	1:B:139:GLU:OE2	2.01	0.60
1:B:92:GLU:O	1:B:96:ASN:HB2	2.01	0.60
1:D:156:LEU:O	1:D:160:PRO:HD2	2.02	0.59
1:A:154:TYR:CZ	1:A:158:ILE:HD11	2.36	0.59
1:B:121:ASP:HA	1:B:124:ASN:HB2	1.85	0.59
1:B:159:ILE:HB	1:B:160:PRO:HD3	1.85	0.58
1:D:119:ILE:CD1	1:D:162:PHE:HB3	2.34	0.58
1:A:154:TYR:CE2	1:A:158:ILE:CD1	2.84	0.57
1:A:58:ARG:O	1:A:62:ARG:HG3	2.05	0.56
1:B:85:LEU:HD22	1:B:86:VAL:N	2.20	0.56
1:C:79:LEU:HD13	1:C:144:LEU:HD11	1.87	0.56
1:C:83:ASN:ND2	1:C:83:ASN:O	2.39	0.56
1:B:27:ALA:CB	1:B:139:GLU:OE2	2.54	0.55
1:A:131:ARG:O	1:A:133:ILE:N	2.38	0.55
1:B:132:ALA:HB3	1:B:133:ILE:HB	1.87	0.55
1:B:102:ASN:O	1:B:103:ASP:HB2	2.07	0.55
1:B:42:LYS:NZ	1:B:69:ASP:OD1	2.25	0.54
1:A:41:GLU:HG3	1:A:125:GLN:OE1	2.06	0.54
1:D:154:TYR:CZ	1:D:158:ILE:CD1	2.91	0.54
1:A:145:GLU:O	1:A:149:ARG:HG3	2.08	0.54
1:A:125:GLN:O	1:A:129:ILE:HG13	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:LYS:HE2	1:D:42:LYS:HZ3	1.73	0.53
1:B:78:GLN:HG2	1:B:144:LEU:HA	1.89	0.53
1:B:161:TYR:O	1:B:165:GLU:HG2	2.09	0.53
1:D:129:ILE:O	1:D:133:ILE:HG13	2.09	0.53
1:C:158:ILE:HG23	1:C:162:PHE:CE1	2.44	0.52
1:D:51:TYR:CE1	1:D:107:LYS:HD3	2.44	0.52
1:A:26:THR:HG22	1:A:29:ALA:HB2	1.92	0.52
1:D:156:LEU:O	1:D:160:PRO:HD3	2.08	0.52
1:A:157:SER:C	1:A:160:PRO:HD2	2.30	0.52
1:A:135:LEU:O	1:A:139:GLU:HG3	2.09	0.52
1:D:97:HIS:O	1:D:98:LYS:HD2	2.10	0.52
1:C:6:SER:N	1:C:9:GLU:OE2	2.44	0.51
1:C:119:ILE:HG23	1:C:159:ILE:HG23	1.92	0.51
1:A:114:LEU:O	1:A:118:PHE:CD2	2.64	0.51
1:C:126:ASN:HD21	1:C:155:ASN:HB3	1.76	0.51
1:A:79:LEU:O	1:A:80:LEU:C	2.48	0.51
1:C:45:LEU:HD13	1:C:64:ILE:HG22	1.93	0.51
1:A:41:GLU:OE1	1:A:121:ASP:CB	2.57	0.51
1:D:106:ALA:HA	1:D:109:TRP:CD1	2.46	0.50
1:A:55:ALA:O	1:A:59:ILE:HG22	2.11	0.50
1:A:36:SER:OG	1:A:93:PHE:HA	2.12	0.49
1:D:41:GLU:OE1	1:D:121:ASP:HB3	2.12	0.49
1:D:40:TYR:CZ	1:D:97:HIS:ND1	2.81	0.49
1:A:90:LEU:O	1:A:94:VAL:HG23	2.13	0.49
1:C:89:THR:HG23	1:C:92:GLU:HG3	1.95	0.49
1:D:73:TYR:O	1:D:77:GLU:HG3	2.14	0.48
1:A:153:GLY:O	1:A:154:TYR:C	2.50	0.48
1:A:115:ILE:O	1:A:119:ILE:HG13	2.12	0.48
1:A:173:PHE:N	1:A:173:PHE:CD1	2.82	0.48
1:B:64:ILE:O	1:B:68:GLU:HG2	2.14	0.48
1:D:118:PHE:O	1:D:119:ILE:C	2.53	0.48
1:B:93:PHE:O	1:B:97:HIS:HB3	2.14	0.47
1:A:144:LEU:HG	1:A:148:ILE:HD11	1.96	0.47
1:C:76:SER:O	1:C:80:LEU:HD22	2.15	0.47
1:A:132:ALA:HB3	1:A:148:ILE:HG21	1.96	0.47
1:B:18:SER:O	1:B:22:HIS:HD2	1.97	0.47
1:C:93:PHE:O	1:C:97:HIS:HB3	2.15	0.47
1:C:133:ILE:HG22	1:C:134:LYS:N	2.30	0.47
1:D:116:GLU:HA	1:D:119:ILE:HD13	1.98	0.46
1:C:90:LEU:O	1:C:94:VAL:HG13	2.16	0.45
1:B:133:ILE:HG22	1:B:134:LYS:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:TYR:CZ	1:D:97:HIS:CE1	3.05	0.45
1:C:73:TYR:CE1	1:D:62:ARG:HD3	2.51	0.45
1:B:54:SER:O	1:B:58:ARG:HB2	2.17	0.44
1:A:168:LYS:HD2	1:A:168:LYS:HA	1.85	0.44
1:C:145:GLU:O	1:C:146:LEU:C	2.56	0.44
1:C:31:LEU:O	1:C:32:SER:C	2.55	0.44
1:D:57:TYR:O	1:D:61:PHE:CD2	2.70	0.44
1:B:106:ALA:HA	1:B:109:TRP:NE1	2.32	0.44
1:B:103:ASP:O	1:B:104:PRO:C	2.55	0.44
1:D:53:LYS:N	1:D:53:LYS:HD2	2.32	0.44
1:B:154:TYR:O	1:B:158:ILE:HG12	2.17	0.44
1:B:56:ASN:O	1:B:59:ILE:HG13	2.17	0.44
1:C:159:ILE:N	1:C:160:PRO:HD2	2.33	0.44
1:A:45:LEU:O	1:A:48:ALA:N	2.51	0.44
1:A:11:TYR:O	1:A:15:VAL:HG23	2.18	0.43
1:A:47:GLN:HG3	1:B:88:THR:OG1	2.17	0.43
1:A:156:LEU:HA	1:A:159:ILE:HD12	2.00	0.43
1:A:156:LEU:O	1:A:160:PRO:HD3	2.18	0.43
1:A:6:SER:N	1:A:9:GLU:CD	2.72	0.43
1:A:90:LEU:HD12	1:B:102:ASN:ND2	2.29	0.43
1:D:22:HIS:CE1	1:D:96:ASN:HD21	2.32	0.43
1:C:35:LEU:HD21	1:C:75:ILE:CG2	2.49	0.43
1:A:39:PHE:HE2	1:B:43:ILE:HD12	1.84	0.43
1:A:133:ILE:HG13	1:A:148:ILE:HG22	2.00	0.42
1:B:166:LEU:O	1:B:168:LYS:N	2.53	0.42
1:B:102:ASN:O	1:B:103:ASP:CB	2.67	0.42
1:A:144:LEU:HG	1:A:148:ILE:CD1	2.48	0.42
1:A:131:ARG:O	1:A:132:ALA:C	2.57	0.42
1:D:41:GLU:OE1	1:D:121:ASP:CB	2.67	0.42
1:B:48:ALA:O	1:B:52:ALA:HB3	2.19	0.42
1:C:31:LEU:HD23	1:C:31:LEU:HA	1.92	0.42
1:A:83:ASN:C	1:A:83:ASN:HD22	2.22	0.42
1:D:160:PRO:HA	1:D:163:ALA:HB3	2.02	0.41
1:A:124:ASN:O	1:A:125:GLN:C	2.56	0.41
1:D:120:ASN:O	1:D:124:ASN:OD1	2.38	0.41
1:C:124:ASN:N	1:C:124:ASN:HD22	2.18	0.41
1:B:118:PHE:HA	1:B:121:ASP:OD1	2.20	0.41
1:D:154:TYR:CZ	1:D:158:ILE:HD12	2.54	0.41
1:C:6:SER:HA	1:C:9:GLU:CD	2.41	0.41
1:A:79:LEU:O	1:A:82:GLU:N	2.53	0.41
1:D:134:LYS:HE3	2:D:197:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:ILE:O	1:B:137:GLN:HG3	2.21	0.40
1:A:45:LEU:HD23	1:A:118:PHE:CZ	2.56	0.40
1:B:169:THR:HG22	1:B:171:GLY:H	1.87	0.40
1:A:160:PRO:HA	1:A:163:ALA:HB3	2.04	0.40
1:B:116:GLU:HA	1:B:119:ILE:HD12	2.03	0.40
1:C:168:LYS:HD2	1:C:172:GLU:CB	2.52	0.40
1:B:57:TYR:O	1:B:61:PHE:CD2	2.75	0.40
1:D:67:LYS:HE2	1:D:70:GLU:OE2	2.21	0.40
1:D:31:LEU:HD11	1:D:148:ILE:HD11	2.04	0.40
1:B:111:ASP:O	1:B:112:GLU:C	2.59	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	A	166/179 (93%)	136 (82%)	25 (15%)	5 (3%)	5 22
1	B	166/179 (93%)	133 (80%)	25 (15%)	8 (5%)	3 10
1	C	166/179 (93%)	140 (84%)	19 (11%)	7 (4%)	3 13
1	D	166/179 (93%)	153 (92%)	11 (7%)	2 (1%)	16 48
All	All	664/716 (93%)	562 (85%)	80 (12%)	22 (3%)	5 20

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	132	ALA
1	B	103	ASP
1	B	167	GLY
1	C	133	ILE

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Mol	Chain	Res	Type
1	D	133	ILE
1	A	46	MET
1	C	52	ALA
1	C	78	GLN
1	A	133	ILE
1	B	99	PHE
1	B	112	GLU
1	C	83	ASN
1	D	7	ILE
1	B	25	PRO
1	B	98	LYS
1	B	102	ASN
1	A	80	LEU
1	C	24	LYS
1	B	121	ASP
1	C	171	GLY
1	C	75	ILE

5.3.2 Protein sidechains (i)

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	148/159 (93%)	113 (76%)	35 (24%)	1	2
1	B	148/159 (93%)	108 (73%)	40 (27%)	0	2
1	C	148/159 (93%)	116 (78%)	32 (22%)	1	3
1	D	148/159 (93%)	120 (81%)	28 (19%)	2	6
All	All	592/636 (93%)	457 (77%)	135 (23%)	1	3

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LYS
1	A	17	LYS
1	A	18	SER
1	A	19	GLU

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Mol	Chain	Res	Type
1	A	23	HIS
1	A	30	MET
1	A	36	SER
1	A	46	MET
1	A	54	SER
1	A	60	LYS
1	A	66	LEU
1	A	73	TYR
1	A	74	LEU
1	A	78	GLN
1	A	79	LEU
1	A	80	LEU
1	A	83	ASN
1	A	84	GLU
1	A	85	LEU
1	A	88	THR
1	A	90	LEU
1	A	94	VAL
1	A	100	ILE
1	A	101	GLU
1	A	105	LYS
1	A	112	GLU
1	A	116	GLU
1	A	129	ILE
1	A	133	ILE
1	A	137	GLN
1	A	138	LYS
1	A	141	LYS
1	A	168	LYS
1	A	172	GLU
1	A	173	PHE
1	B	7	ILE
1	B	9	GLU
1	B	10	LYS
1	B	19	GLU
1	B	30	MET
1	B	35	LEU
1	B	38	ILE
1	B	53	LYS
1	B	54	SER
1	B	56	ASN
1	B	58	ARG

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Mol	Chain	Res	Type
1	B	60	LYS
1	B	62	ARG
1	B	66	LEU
1	B	67	LYS
1	B	74	LEU
1	B	76	SER
1	B	78	GLN
1	B	79	LEU
1	B	82	GLU
1	B	84	GLU
1	B	86	VAL
1	B	90	LEU
1	B	98	LYS
1	B	99	PHE
1	B	100	ILE
1	B	107	LYS
1	B	108	TYR
1	B	114	LEU
1	B	122	PHE
1	B	124	ASN
1	B	128	PHE
1	B	133	ILE
1	B	135	LEU
1	B	141	LYS
1	B	144	LEU
1	B	151	LEU
1	B	152	TYR
1	B	168	LYS
1	B	170	ILE
1	C	8	ASP
1	C	12	GLU
1	C	16	LYS
1	C	22	HIS
1	C	23	HIS
1	C	26	THR
1	C	42	LYS
1	C	46	MET
1	C	54	SER
1	C	56	ASN
1	C	63	GLU
1	C	66	LEU
1	C	69	ASP

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Mol	Chain	Res	Type
1	C	79	LEU
1	C	80	LEU
1	C	82	GLU
1	C	85	LEU
1	C	88	THR
1	C	89	THR
1	C	101	GLU
1	C	105	LYS
1	C	109	TRP
1	C	114	LEU
1	C	123	GLN
1	C	131	ARG
1	C	138	LYS
1	C	141	LYS
1	C	146	LEU
1	C	151	LEU
1	C	157	SER
1	C	168	LYS
1	C	169	THR
1	D	7	ILE
1	D	8	ASP
1	D	16	LYS
1	D	17	LYS
1	D	26	THR
1	D	30	MET
1	D	33	HIS
1	D	46	MET
1	D	67	LYS
1	D	69	ASP
1	D	74	LEU
1	D	78	GLN
1	D	79	LEU
1	D	83	ASN
1	D	85	LEU
1	D	88	THR
1	D	90	LEU
1	D	91	ASP
1	D	95	SER
1	D	97	HIS
1	D	107	LYS
1	D	120	ASN
1	D	123	GLN

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Mol	Chain	Res	Type
1	D	138	LYS
1	D	157	SER
1	D	158	ILE
1	D	170	ILE
1	D	172	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	37	ASN
1	A	96	ASN
1	A	117	ASN
1	A	124	ASN
1	A	137	GLN
1	A	155	ASN
1	B	22	HIS
1	B	96	ASN
1	B	102	ASN
1	B	125	GLN
1	C	22	HIS
1	C	37	ASN
1	C	117	ASN
1	C	126	ASN
1	D	22	HIS
1	D	78	GLN
1	D	96	ASN
1	D	120	ASN
1	D	123	GLN
1	D	124	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

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

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.