Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:21 AM GMT

PDB ID	:	2GQQ
Title	:	Crystal Structure of E. coli Leucine-responsive regulatory protein (Lrp)
Authors	:	de los Rios, S.; Perona, J.J.
Deposited on	:	2006-04-21
Resolution	:	3.20 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

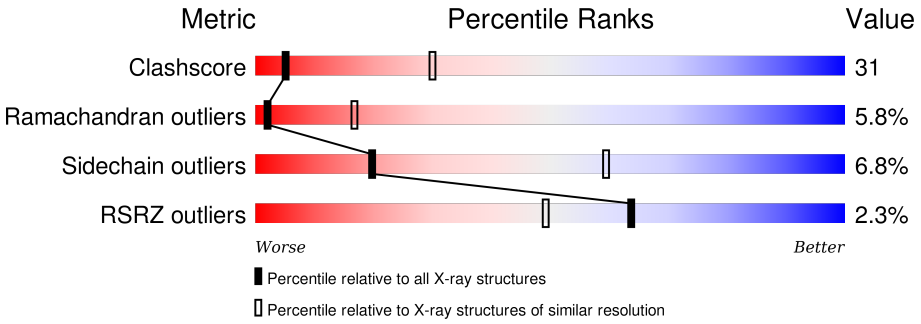
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	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 3.20 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	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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	A	163	2% 56% 35% 6%
1	B	163	2% 53% 35% 7%
1	C	163	4% 44% 47% 6%
1	D	163	% 53% 36% 5% 6%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 4342 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 Leucine-responsive regulatory protein.

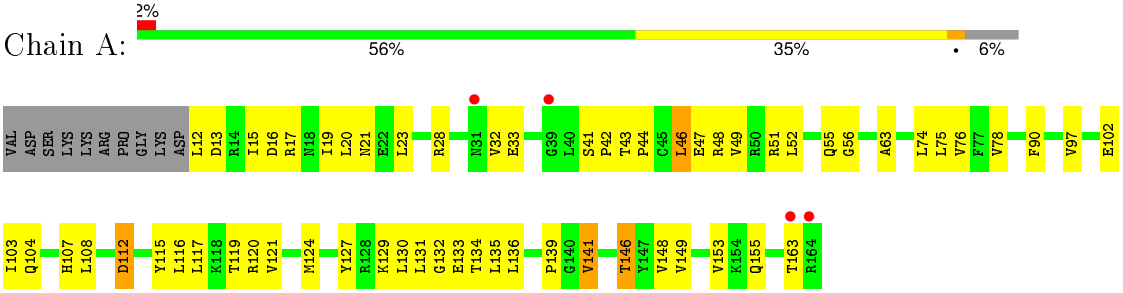
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	153	Total	C	N	O	S	0	0	0
			1053	666	172	211	4			
1	B	151	Total	C	N	O	S	0	0	0
			1050	663	179	204	4			
1	C	157	Total	C	N	O	S	0	0	0
			1156	734	200	218	4			
1	D	153	Total	C	N	O	S	0	0	0
			1083	687	175	217	4			

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.

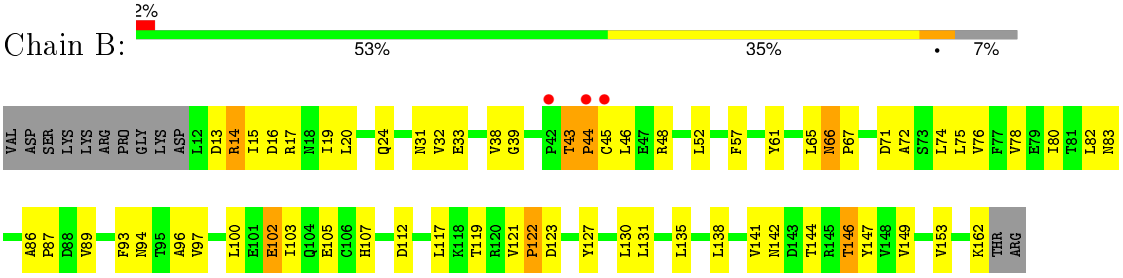
- Molecule 1: Leucine-responsive regulatory protein

Chain A:



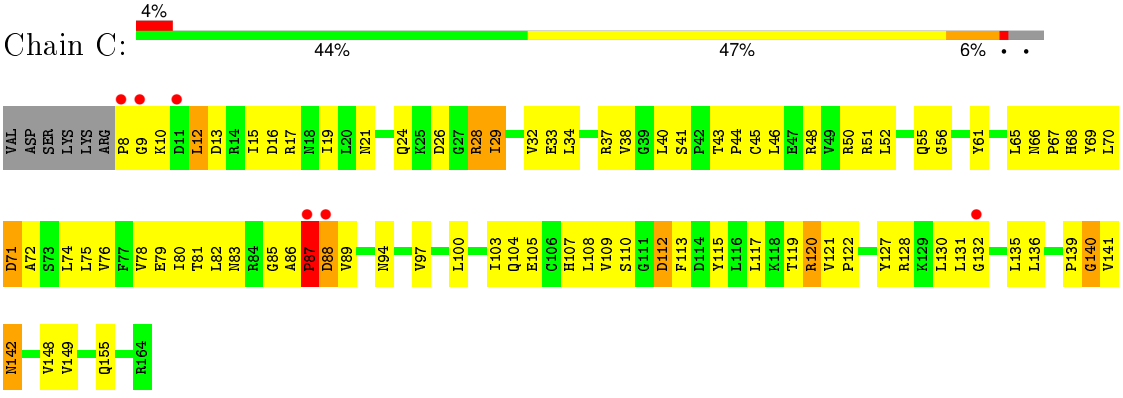
- Molecule 1: Leucine-responsive regulatory protein

Chain B:



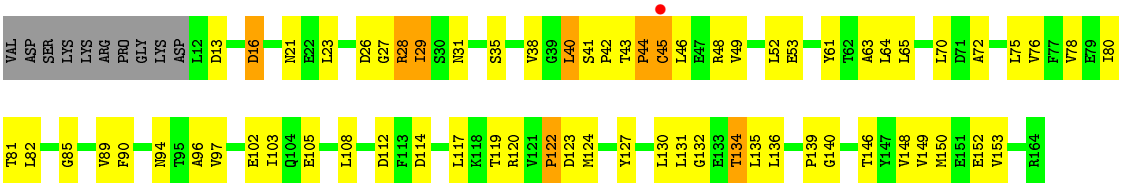
- Molecule 1: Leucine-responsive regulatory protein

Chain C:



- Molecule 1: Leucine-responsive regulatory protein

Chain D:


VAL ASP SER LYS LYS ARG PRO GLY LYS ASP L12 D13 D16 N21 E22 L23 D26 G27 R28 I29 S30 N31 S35 V38 G39 L40 S41 P42 T43 P44 C45 L46 E47 R48 V49 L52 E53 Y61 T62 A63 L64 L65 L70 D71 A72 L75 V76 F77 V78 E79 I80
T81 L82 G85 V89 F90 N94 T95 A96 V97 E102 I103 Q104 E105 L108 D112 F113 D114 L117 K118 T119 R120 V121 P122 D123 M124 Y127 L130 L131 G132 E133 T134 L135 L136 P139 G140 T146 Y147 V148 V149 M150 E151 E152 V153 R164

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	100.10Å 237.00Å 75.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.20 19.95 – 3.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-3.20) 90.8 (19.95-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.77 (at 3.22Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.267 , 0.322 0.266 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	60.4	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 53.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Outliers	0 of 15203 reflections	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	4342	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

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	0.34	0/1069	0.60	2/1469 (0.1%)
1	B	0.32	0/1066	0.52	0/1464
1	C	0.33	0/1173	0.65	3/1598 (0.2%)
1	D	0.33	0/1099	0.57	0/1508
All	All	0.33	0/4407	0.59	5/6039 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	17	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	C	17	ARG	NE-CZ-NH1	-6.84	116.88	120.30
1	A	17	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	C	17	ARG	NE-CZ-NH2	6.41	123.50	120.30
1	C	8	PRO	N-CA-CB	5.55	109.95	103.30

There are no chirality outliers.

There are no planarity outliers.

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	1053	0	882	58	0
1	B	1050	0	891	64	0
1	C	1156	0	1081	86	0
1	D	1083	0	956	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4342	0	3810	250	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 31.

All (250) 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:63:ALA:H	1:B:24:GLN:HA	1.40	0.86
1:B:83:ASN:H	1:B:142:ASN:ND2	1.75	0.85
1:B:83:ASN:H	1:B:142:ASN:HD22	1.21	0.84
1:D:41:SER:HB3	1:D:44:PRO:HG2	1.60	0.84
1:C:40:LEU:H	1:C:40:LEU:HD23	1.47	0.79
1:C:103:ILE:HG22	1:C:119:THR:HG22	1.65	0.76
1:C:34:LEU:HD12	1:C:45:CYS:SG	2.25	0.76
1:C:29:ILE:HG13	1:C:34:LEU:HD23	1.67	0.75
1:C:81:THR:HG23	1:C:113:PHE:HA	1.71	0.72
1:B:121:VAL:HB	1:B:122:PRO:HD2	1.73	0.71
1:A:48:ARG:O	1:A:51:ARG:HG2	1.91	0.71
1:C:130:LEU:CD2	1:C:135:LEU:HD13	2.22	0.70
1:C:46:LEU:HD11	1:C:50:ARG:HH11	1.56	0.70
1:C:104:GLN:HE22	1:C:120:ARG:HD2	1.55	0.70
1:C:104:GLN:NE2	1:C:120:ARG:HD2	2.07	0.70
1:D:26:ASP:O	1:D:29:ILE:HD12	1.91	0.69
1:C:46:LEU:HD11	1:C:50:ARG:NH1	2.07	0.68
1:D:132:GLY:HA2	1:D:136:LEU:HB2	1.77	0.67
1:B:66:ASN:HD22	1:B:66:ASN:H	1.40	0.67
1:D:41:SER:O	1:D:44:PRO:HD2	1.95	0.67
1:B:13:ASP:HB3	1:B:16:ASP:OD2	1.95	0.67
1:C:43:THR:HB	1:C:44:PRO:HD3	1.77	0.66
1:C:19:ILE:HD13	1:C:38:VAL:HG11	1.78	0.65
1:B:48:ARG:O	1:B:52:LEU:HD13	1.97	0.64
1:C:80:ILE:HB	1:C:115:TYR:HB2	1.79	0.64
1:B:103:ILE:HG22	1:B:119:THR:HB	1.79	0.64
1:C:32:VAL:HG13	1:C:33:GLU:H	1.62	0.64
1:A:148:VAL:HG21	1:D:148:VAL:HG21	1.80	0.63
1:C:121:VAL:HG21	1:C:127:TYR:HB2	1.79	0.63
1:D:131:LEU:HA	1:D:135:LEU:HB3	1.78	0.63
1:C:132:GLY:HA2	1:C:136:LEU:HB2	1.81	0.63
1:C:67:PRO:HB3	1:C:120:ARG:HE	1.64	0.63
1:B:131:LEU:HA	1:B:135:LEU:HB3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:78:VAL:HG22	1:D:117:LEU:HB2	1.81	0.63
1:B:66:ASN:H	1:B:66:ASN:ND2	1.97	0.62
1:A:74:LEU:HB3	1:A:121:VAL:O	1.99	0.62
1:B:32:VAL:HG23	1:B:33:GLU:H	1.64	0.61
1:D:108:LEU:HD12	1:D:114:ASP:O	2.01	0.61
1:C:40:LEU:N	1:C:40:LEU:HD23	2.16	0.61
1:D:89:VAL:HG23	1:D:90:PHE:N	2.16	0.60
1:C:131:LEU:HA	1:C:135:LEU:HB2	1.83	0.60
1:D:76:VAL:HG13	1:D:119:THR:HG23	1.83	0.60
1:D:64:LEU:C	1:D:65:LEU:HD12	2.22	0.60
1:B:46:LEU:HD13	1:B:46:LEU:O	2.02	0.60
1:D:49:VAL:O	1:D:53:GLU:HG3	2.02	0.60
1:B:78:VAL:CG2	1:B:117:LEU:HB2	2.32	0.59
1:D:94:ASN:O	1:D:97:VAL:HG12	2.02	0.59
1:A:117:LEU:N	1:A:117:LEU:HD12	2.17	0.59
1:C:51:ARG:O	1:C:55:GLN:HG2	2.02	0.59
1:C:80:ILE:HD12	1:C:117:LEU:HD13	1.83	0.59
1:C:16:ASP:OD2	1:C:48:ARG:HD2	2.02	0.59
1:B:122:PRO:HG2	1:B:123:ASP:H	1.66	0.59
1:D:75:LEU:O	1:D:149:VAL:HG12	2.02	0.59
1:A:78:VAL:CG2	1:A:117:LEU:HB2	2.33	0.59
1:B:17:ARG:NH2	1:B:162:LYS:H	2.01	0.59
1:B:100:LEU:HB2	1:B:103:ILE:HD11	1.84	0.59
1:D:75:LEU:HD22	1:D:120:ARG:HH12	1.68	0.58
1:C:86:ALA:O	1:C:88:ASP:N	2.36	0.58
1:C:41:SER:O	1:C:44:PRO:HD2	2.04	0.58
1:D:46:LEU:O	1:D:46:LEU:HD13	2.04	0.58
1:D:43:THR:HB	1:D:44:PRO:HD3	1.86	0.58
1:A:51:ARG:HG3	1:A:52:LEU:HD12	1.85	0.58
1:B:66:ASN:HD22	1:B:66:ASN:N	1.99	0.57
1:A:103:ILE:HG22	1:A:119:THR:HB	1.85	0.57
1:A:75:LEU:HD12	1:A:119:THR:O	2.05	0.57
1:B:80:ILE:HG23	1:B:141:VAL:HG23	1.87	0.56
1:C:34:LEU:O	1:C:38:VAL:HG22	2.03	0.56
1:A:124:MET:CE	1:D:150:MET:HG2	2.35	0.56
1:B:78:VAL:HG23	1:B:117:LEU:HB2	1.88	0.56
1:D:122:PRO:HG2	1:D:123:ASP:H	1.70	0.56
1:C:32:VAL:HG13	1:C:33:GLU:N	2.21	0.56
1:C:100:LEU:O	1:C:103:ILE:HG12	2.06	0.55
1:C:13:ASP:OD1	1:C:15:ILE:HG22	2.06	0.55
1:C:33:GLU:O	1:C:37:ARG:HG2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:103:ILE:HD13	1:D:117:LEU:HD23	1.89	0.54
1:A:153:VAL:CB	1:B:94:ASN:HD22	2.20	0.54
1:D:78:VAL:CG2	1:D:117:LEU:HB2	2.37	0.54
1:C:130:LEU:O	1:C:130:LEU:HD23	2.08	0.54
1:C:100:LEU:HD12	1:C:100:LEU:N	2.23	0.53
1:B:16:ASP:HB3	1:B:52:LEU:HD21	1.89	0.53
1:C:28:ARG:HG3	1:D:61:TYR:CG	2.43	0.53
1:D:41:SER:C	1:D:44:PRO:HD2	2.29	0.53
1:C:51:ARG:HH11	1:C:52:LEU:HD12	1.73	0.53
1:B:117:LEU:HD12	1:B:117:LEU:N	2.23	0.53
1:D:130:LEU:HD23	1:D:134:THR:HG23	1.91	0.53
1:C:29:ILE:N	1:C:29:ILE:HD13	2.24	0.53
1:A:75:LEU:O	1:A:149:VAL:HG12	2.09	0.53
1:A:46:LEU:HD13	1:A:47:GLU:N	2.23	0.53
1:D:153:VAL:O	1:D:153:VAL:HG22	2.09	0.53
1:A:153:VAL:HB	1:B:94:ASN:HD22	1.74	0.52
1:B:75:LEU:O	1:B:149:VAL:HG12	2.09	0.52
1:A:155:GLN:HA	1:B:105:GLU:HG2	1.90	0.52
1:C:79:GLU:HG2	1:C:113:PHE:CE1	2.45	0.52
1:B:82:LEU:O	1:B:82:LEU:HD12	2.09	0.52
1:B:93:PHE:CZ	1:B:138:LEU:HD13	2.45	0.52
1:A:153:VAL:HG21	1:B:94:ASN:HD22	1.75	0.52
1:B:14:ARG:CZ	1:B:15:ILE:HA	2.40	0.51
1:C:40:LEU:H	1:C:40:LEU:CD2	2.18	0.51
1:C:75:LEU:HG	1:C:149:VAL:HG21	1.91	0.51
1:A:131:LEU:HD13	1:A:135:LEU:HD23	1.92	0.51
1:A:132:GLY:HA2	1:A:136:LEU:HB2	1.92	0.51
1:B:80:ILE:HG12	1:B:144:THR:HG22	1.92	0.51
1:A:46:LEU:C	1:A:46:LEU:HD22	2.31	0.51
1:D:131:LEU:HA	1:D:135:LEU:CB	2.41	0.51
1:B:83:ASN:N	1:B:142:ASN:HD22	2.00	0.51
1:A:146:THR:O	1:C:110:SER:HB2	2.11	0.51
1:A:124:MET:HE2	1:D:150:MET:HG2	1.93	0.50
1:C:61:TYR:O	1:D:26:ASP:HA	2.11	0.50
1:A:153:VAL:CG2	1:B:94:ASN:HD22	2.25	0.50
1:A:130:LEU:HD22	1:A:135:LEU:HD22	1.93	0.50
1:C:26:ASP:O	1:C:29:ILE:HD12	2.12	0.50
1:B:32:VAL:HG23	1:B:33:GLU:N	2.25	0.50
1:C:51:ARG:HG3	1:C:52:LEU:HD12	1.94	0.49
1:C:45:CYS:O	1:C:48:ARG:HB3	2.11	0.49
1:D:82:LEU:HG	1:D:140:GLY:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:VAL:CG2	1:C:117:LEU:HB2	2.43	0.49
1:A:131:LEU:HA	1:A:135:LEU:HB3	1.94	0.49
1:C:48:ARG:O	1:C:52:LEU:HD13	2.12	0.49
1:B:131:LEU:HA	1:B:135:LEU:CB	2.42	0.49
1:B:130:LEU:O	1:B:130:LEU:HD23	2.13	0.49
1:A:130:LEU:CD2	1:A:135:LEU:HD22	2.43	0.48
1:D:81:THR:C	1:D:82:LEU:HD12	2.33	0.48
1:A:108:LEU:HD13	1:A:115:TYR:CZ	2.47	0.48
1:A:51:ARG:CG	1:A:52:LEU:HD12	2.42	0.48
1:C:130:LEU:O	1:C:135:LEU:HB2	2.12	0.48
1:B:38:VAL:HG23	1:B:39:GLY:H	1.78	0.48
1:C:24:GLN:HA	1:D:63:ALA:H	1.78	0.48
1:D:41:SER:HB3	1:D:44:PRO:CG	2.39	0.48
1:B:14:ARG:O	1:B:17:ARG:HG3	2.14	0.47
1:C:97:VAL:O	1:C:103:ILE:HD11	2.15	0.47
1:C:86:ALA:HB3	1:C:89:VAL:HG22	1.97	0.47
1:C:12:LEU:HA	1:C:12:LEU:HD22	1.77	0.47
1:D:23:LEU:HD12	1:D:27:GLY:HA2	1.96	0.47
1:D:28:ARG:HG3	1:D:28:ARG:HH11	1.79	0.47
1:C:82:LEU:HB2	1:C:140:GLY:O	2.14	0.47
1:A:104:GLN:HE22	1:A:120:ARG:HD2	1.78	0.47
1:B:127:TYR:OH	1:B:146:THR:HB	2.14	0.47
1:C:65:LEU:O	1:C:67:PRO:HD3	2.14	0.47
1:C:109:VAL:HG12	1:D:149:VAL:HA	1.96	0.47
1:B:105:GLU:HB3	1:B:107:HIS:HE1	1.79	0.47
1:A:78:VAL:O	1:A:78:VAL:HG23	2.15	0.47
1:B:20:LEU:HD21	1:B:52:LEU:HD23	1.96	0.47
1:C:103:ILE:O	1:C:103:ILE:HG13	2.15	0.46
1:B:46:LEU:HD13	1:B:46:LEU:C	2.36	0.46
1:A:76:VAL:HG23	1:A:148:VAL:HA	1.98	0.46
1:A:129:LYS:O	1:A:133:GLU:HB3	2.15	0.46
1:D:46:LEU:O	1:D:49:VAL:HG22	2.16	0.46
1:D:13:ASP:HB3	1:D:16:ASP:HB2	1.97	0.46
1:A:78:VAL:HG22	1:A:117:LEU:HB2	1.98	0.46
1:A:153:VAL:HG21	1:B:94:ASN:HB3	1.97	0.46
1:C:132:GLY:HA2	1:C:136:LEU:CB	2.46	0.46
1:C:107:HIS:HB3	1:D:149:VAL:CG2	2.46	0.46
1:D:40:LEU:HD13	1:D:45:CYS:HB2	1.98	0.46
1:C:74:LEU:HD13	1:C:75:LEU:N	2.31	0.45
1:D:48:ARG:O	1:D:52:LEU:HB2	2.15	0.45
1:A:130:LEU:HD21	1:A:135:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:TYR:OH	1:A:146:THR:HB	2.16	0.45
1:B:94:ASN:HA	1:B:97:VAL:HG12	1.98	0.45
1:D:38:VAL:HG12	1:D:38:VAL:O	2.17	0.45
1:D:65:LEU:HD12	1:D:65:LEU:N	2.32	0.45
1:C:46:LEU:HD13	1:C:46:LEU:C	2.36	0.45
1:B:86:ALA:O	1:B:89:VAL:N	2.50	0.45
1:C:76:VAL:HG23	1:C:148:VAL:HA	1.99	0.45
1:B:121:VAL:HG21	1:B:127:TYR:HB2	1.98	0.45
1:C:41:SER:C	1:C:44:PRO:HD2	2.37	0.45
1:D:31:ASN:OD1	1:D:46:LEU:HB2	2.17	0.45
1:D:94:ASN:N	1:D:94:ASN:HD22	2.13	0.45
1:C:82:LEU:HB3	1:C:141:VAL:HG12	1.99	0.45
1:B:65:LEU:O	1:B:67:PRO:HD3	2.17	0.45
1:B:66:ASN:O	1:B:66:ASN:ND2	2.50	0.44
1:A:131:LEU:HA	1:A:135:LEU:CB	2.46	0.44
1:C:127:TYR:O	1:C:128:ARG:C	2.56	0.44
1:B:65:LEU:HD12	1:B:65:LEU:N	2.33	0.44
1:C:108:LEU:HD13	1:C:115:TYR:CZ	2.52	0.44
1:A:75:LEU:HD13	1:A:120:ARG:HG3	1.99	0.44
1:B:76:VAL:HG23	1:B:147:TYR:O	2.17	0.44
1:D:76:VAL:HG11	1:D:127:TYR:CD1	2.52	0.44
1:A:107:HIS:O	1:A:115:TYR:HA	2.17	0.44
1:D:40:LEU:O	1:D:40:LEU:HD12	2.17	0.44
1:A:13:ASP:HB2	1:A:16:ASP:HB2	1.99	0.44
1:D:46:LEU:C	1:D:46:LEU:HD13	2.37	0.44
1:A:146:THR:HG23	1:C:110:SER:HB2	2.00	0.44
1:C:82:LEU:HA	1:C:142:ASN:H	1.82	0.44
1:A:43:THR:N	1:A:44:PRO:CD	2.81	0.44
1:C:74:LEU:HB3	1:C:121:VAL:O	2.18	0.44
1:A:49:VAL:HA	1:A:52:LEU:HD13	1.99	0.43
1:B:153:VAL:O	1:B:153:VAL:HG22	2.18	0.43
1:B:93:PHE:CE1	1:B:138:LEU:HD13	2.52	0.43
1:A:130:LEU:O	1:A:135:LEU:HB2	2.18	0.43
1:B:43:THR:H	1:B:44:PRO:HD2	1.83	0.43
1:C:12:LEU:HD13	1:C:13:ASP:N	2.34	0.43
1:C:15:ILE:O	1:C:19:ILE:HG12	2.19	0.43
1:D:130:LEU:CD2	1:D:135:LEU:HB2	2.49	0.43
1:D:75:LEU:HD22	1:D:120:ARG:NH1	2.33	0.43
1:A:130:LEU:CD2	1:A:135:LEU:HD13	2.49	0.43
1:D:89:VAL:HG23	1:D:90:PHE:H	1.81	0.43
1:A:41:SER:CB	1:A:44:PRO:HG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:VAL:HG13	1:A:33:GLU:N	2.34	0.43
1:C:131:LEU:HA	1:C:135:LEU:CB	2.48	0.43
1:B:16:ASP:O	1:B:19:ILE:N	2.52	0.43
1:B:135:LEU:HD12	1:B:135:LEU:HA	1.89	0.43
1:B:105:GLU:HB3	1:B:107:HIS:CE1	2.54	0.43
1:A:16:ASP:O	1:A:19:ILE:HB	2.18	0.43
1:C:79:GLU:HG2	1:C:113:PHE:CZ	2.53	0.43
1:C:15:ILE:HD11	1:C:38:VAL:HB	2.01	0.42
1:C:16:ASP:HB3	1:C:52:LEU:HD21	2.01	0.42
1:A:20:LEU:HD21	1:A:52:LEU:HD23	2.01	0.42
1:B:43:THR:H	1:B:44:PRO:CD	2.32	0.42
1:A:116:LEU:C	1:A:117:LEU:HD12	2.40	0.42
1:D:152:GLU:O	1:D:152:GLU:HG3	2.19	0.42
1:C:15:ILE:HD11	1:C:38:VAL:O	2.20	0.42
1:C:94:ASN:CB	1:D:153:VAL:HG21	2.50	0.42
1:D:35:SER:HB2	1:D:40:LEU:O	2.19	0.42
1:C:103:ILE:HG22	1:C:119:THR:CG2	2.44	0.42
1:B:117:LEU:N	1:B:117:LEU:CD1	2.82	0.42
1:D:27:GLY:O	1:D:29:ILE:HD13	2.20	0.42
1:C:105:GLU:O	1:C:117:LEU:HA	2.19	0.42
1:D:75:LEU:HD13	1:D:120:ARG:HG2	2.01	0.42
1:A:131:LEU:CD1	1:A:135:LEU:HD23	2.50	0.42
1:D:82:LEU:N	1:D:82:LEU:HD12	2.35	0.42
1:B:74:LEU:HB2	1:B:122:PRO:O	2.19	0.41
1:C:46:LEU:O	1:C:50:ARG:HB2	2.19	0.41
1:D:89:VAL:CG2	1:D:90:PHE:N	2.83	0.41
1:C:9:GLY:O	1:C:10:LYS:HB3	2.20	0.41
1:B:20:LEU:CD2	1:B:52:LEU:HD23	2.50	0.41
1:C:86:ALA:O	1:C:87:PRO:C	2.59	0.41
1:A:28:ARG:H	1:B:61:TYR:HB2	1.86	0.41
1:D:117:LEU:HD12	1:D:117:LEU:N	2.36	0.41
1:C:69:TYR:O	1:C:70:LEU:HD23	2.20	0.41
1:C:71:ASP:HB3	1:C:122:PRO:CG	2.50	0.41
1:B:76:VAL:HG11	1:B:127:TYR:CD1	2.56	0.41
1:C:155:GLN:HA	1:D:105:GLU:HG2	2.01	0.41
1:A:141:VAL:HG13	1:A:141:VAL:O	2.21	0.41
1:B:121:VAL:HB	1:B:122:PRO:CD	2.46	0.41
1:A:19:ILE:O	1:A:23:LEU:HD13	2.21	0.41
1:D:102:GLU:H	1:D:102:GLU:CD	2.22	0.41
1:C:16:ASP:OD1	1:C:52:LEU:HD11	2.21	0.41
1:A:74:LEU:HD22	1:A:75:LEU:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:MET:HE3	1:D:127:TYR:HB3	2.03	0.41
1:B:102:GLU:H	1:B:102:GLU:HG2	1.73	0.41
1:C:61:TYR:CG	1:D:28:ARG:HB2	2.56	0.40
1:D:80:ILE:HD12	1:D:117:LEU:HD13	2.04	0.40
1:A:97:VAL:HG22	1:A:103:ILE:HD11	2.03	0.40
1:A:90:PHE:CE2	1:A:108:LEU:HD11	2.56	0.40
1:B:31:ASN:CB	1:B:46:LEU:HG	2.50	0.40
1:C:29:ILE:N	1:C:29:ILE:CD1	2.84	0.40
1:C:51:ARG:NH1	1:C:52:LEU:HD12	2.36	0.40
1:A:15:ILE:O	1:A:19:ILE:HG12	2.21	0.40
1:C:66:ASN:C	1:C:68:HIS:H	2.24	0.40
1:A:102:GLU:OE1	1:A:102:GLU:N	2.54	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	151/163 (93%)	122 (81%)	21 (14%)	8 (5%)	2	19
1	B	149/163 (91%)	119 (80%)	21 (14%)	9 (6%)	2	16
1	C	155/163 (95%)	130 (84%)	15 (10%)	10 (6%)	1	13
1	D	151/163 (93%)	127 (84%)	16 (11%)	8 (5%)	2	19
All	All	606/652 (93%)	498 (82%)	73 (12%)	35 (6%)	2	17

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	PRO
1	B	72	ALA
1	C	71	ASP

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Mol	Chain	Res	Type
1	C	72	ALA
1	C	87	PRO
1	C	88	ASP
1	D	96	ALA
1	A	112	ASP
1	A	134	THR
1	A	163	THR
1	B	71	ASP
1	C	140	GLY
1	C	142	ASN
1	D	70	LEU
1	B	122	PRO
1	C	139	PRO
1	A	56	GLY
1	A	139	PRO
1	B	96	ALA
1	D	85	GLY
1	A	141	VAL
1	B	43	THR
1	B	57	PHE
1	B	102	GLU
1	C	85	GLY
1	C	112	ASP
1	D	44	PRO
1	D	72	ALA
1	D	122	PRO
1	A	55	GLN
1	D	42	PRO
1	B	44	PRO
1	B	87	PRO
1	D	139	PRO
1	C	56	GLY

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	91/149 (61%)	86 (94%)	5 (6%)	27	68
1	B	90/149 (60%)	85 (94%)	5 (6%)	26	68
1	C	112/149 (75%)	104 (93%)	8 (7%)	18	57
1	D	102/149 (68%)	93 (91%)	9 (9%)	12	45
All	All	395/596 (66%)	368 (93%)	27 (7%)	20	59

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	21	ASN
1	A	46	LEU
1	A	112	ASP
1	A	146	THR
1	B	14	ARG
1	B	45	CYS
1	B	66	ASN
1	B	112	ASP
1	B	146	THR
1	C	12	LEU
1	C	21	ASN
1	C	28	ARG
1	C	29	ILE
1	C	83	ASN
1	C	87	PRO
1	C	112	ASP
1	C	120	ARG
1	D	16	ASP
1	D	21	ASN
1	D	28	ARG
1	D	29	ILE
1	D	40	LEU
1	D	45	CYS
1	D	112	ASP
1	D	134	THR
1	D	146	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN

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Mol	Chain	Res	Type
1	A	24	GLN
1	A	104	GLN
1	B	24	GLN
1	B	55	GLN
1	B	66	ASN
1	B	92	GLN
1	B	94	ASN
1	B	104	GLN
1	B	142	ASN
1	C	21	ASN
1	C	24	GLN
1	C	31	ASN
1	C	55	GLN
1	C	83	ASN
1	C	104	GLN
1	D	21	ASN
1	D	94	ASN
1	D	98	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

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

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, 95^{th} 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	A	153/163 (93%)	-0.27	4 (2%)	59	45	11, 47, 89, 99	0
1	B	151/163 (92%)	-0.26	3 (1%)	68	54	6, 45, 87, 96	0
1	C	157/163 (96%)	-0.33	6 (3%)	44	29	4, 33, 69, 95	0
1	D	153/163 (93%)	-0.44	1 (0%)	89	83	3, 32, 74, 91	0
All	All	614/652 (94%)	-0.33	14 (2%)	64	49	3, 40, 82, 99	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	9	GLY	5.4
1	B	42	PRO	4.4
1	C	8	PRO	3.7
1	C	87	PRO	3.7
1	A	39	GLY	3.2
1	A	164	ARG	2.7
1	B	45	CYS	2.7
1	C	132	GLY	2.7
1	A	31	ASN	2.7
1	D	45	CYS	2.3
1	C	11	ASP	2.2
1	B	44	PRO	2.2
1	A	163	THR	2.1
1	C	88	ASP	2.0

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 (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.