Full wwPDB X-ray Structure Validation Report (i)

Jun 15, 2024 – 05:06 PM EDT

PDB ID	:	4R0G
Title	:	Crystal structure of Lpg0393 from Legionella pneumophila
Authors	:	Sohn, Y.S.; Shin, H.C.; Oh, B.H.
Deposited on	:	2014-07-31
Resolution	:	2.70 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 (i) 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 (1)) were used in the production of this report:

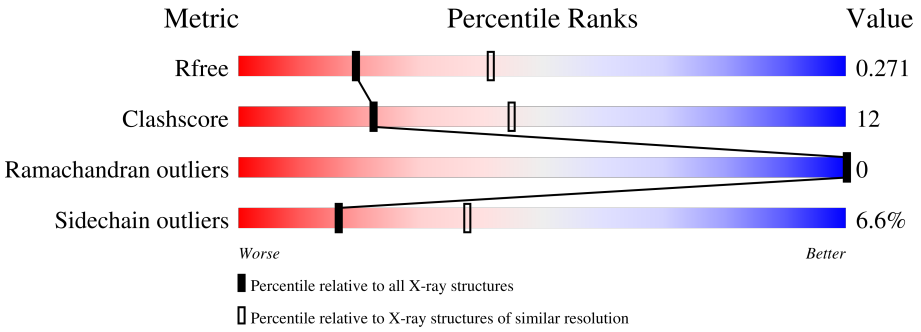
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	287	60% 25% • 12%
1	B	287	56% 25% • 16%
1	C	287	61% 25% • 12%
1	D	287	64% 20% • 13%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 8043 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 Uncharacterized protein.

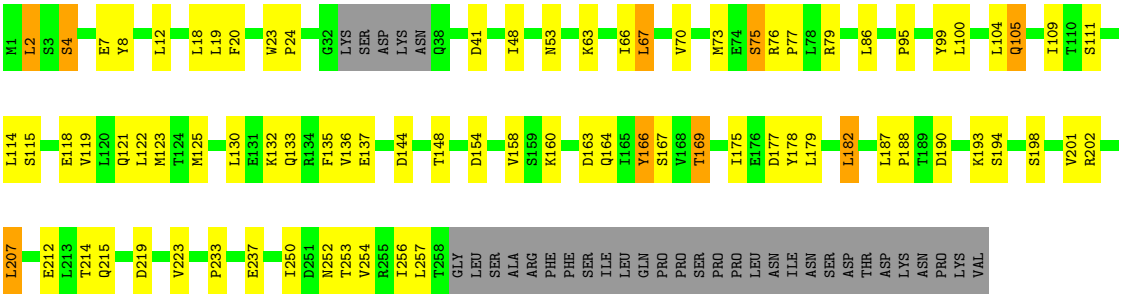
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	253	2064	1348	319	388	9	0	0	0
			Total	C	N	O	S			
1	B	240	1935	1270	296	360	9	0	0	0
			Total	C	N	O	S			
1	C	252	2056	1343	319	385	9	0	0	0
			Total	C	N	O	S			
1	D	250	1988	1294	310	378	6	0	0	0

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. 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. 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.

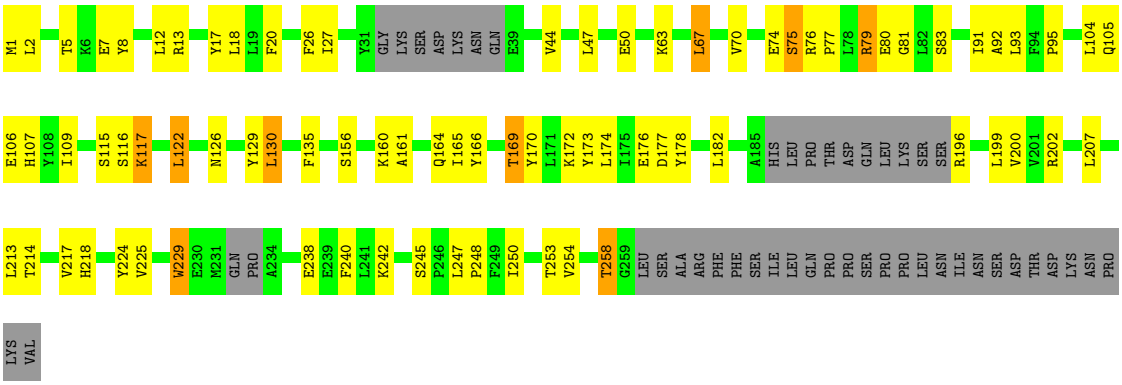
- Molecule 1: Uncharacterized protein

Chain A:



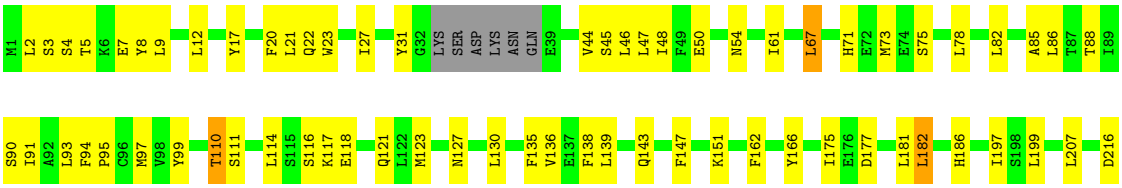
- Molecule 1: Uncharacterized protein

Chain B:



- Molecule 1: Uncharacterized protein

Chain C:



- Molecule 1: Uncharacterized protein

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	79.64Å 111.71Å 167.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.04 – 2.70 34.04 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (34.04-2.70) 80.6 (34.04-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.77 (at 2.39Å)	Xtriage
Refinement program	CNS, PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.222 , 0.269 0.224 , 0.271	Depositor DCC
R_{free} test set	2036 reflections (4.26%)	wwPDB-VP
Wilson B-factor (Å^2)	36.8	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 40.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8043	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.57	0/2111	0.69	0/2862
1	B	0.49	0/1977	0.62	0/2678
1	C	0.49	0/2103	0.63	0/2852
1	D	0.41	0/2033	0.57	0/2764
All	All	0.50	0/8224	0.63	0/11156

There are no bond length outliers.

There are no bond angle outliers.

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	2064	0	2028	47	0
1	B	1935	0	1879	54	0
1	C	2056	0	2023	54	0
1	D	1988	0	1892	44	0
All	All	8043	0	7822	185	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 (185) 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:130:LEU:HD13	1:C:135:PHE:HA	1.59	0.84
1:D:31:TYR:HB3	1:D:116:SER:HB3	1.60	0.83
1:A:76:ARG:O	1:A:79:ARG:NH1	2.14	0.81
1:C:182:LEU:HD13	1:C:197:ILE:HG12	1.61	0.80
1:D:3:SER:HB2	1:D:7:GLU:HG3	1.63	0.80
1:D:166:TYR:HA	1:D:169:THR:HG22	1.63	0.79
1:A:256:ILE:HG12	1:C:136:VAL:HG13	1.63	0.79
1:C:5:THR:HG23	1:C:23:TRP:HE1	1.48	0.78
1:C:2:LEU:HD23	1:C:7:GLU:HB3	1.67	0.77
1:C:114:LEU:HB3	1:C:118:GLU:HB2	1.73	0.71
1:B:122:LEU:O	1:B:126:ASN:ND2	2.18	0.69
1:B:225:VAL:HG12	1:B:229:TRP:HZ3	1.57	0.69
1:A:105:GLN:H	1:A:105:GLN:NE2	1.92	0.67
1:A:166:TYR:HA	1:A:169:THR:HG22	1.76	0.67
1:A:166:TYR:HD1	1:A:169:THR:HG22	1.62	0.65
1:C:44:VAL:HG11	1:C:91:ILE:HG22	1.80	0.62
1:D:5:THR:HG21	1:D:50:GLU:HG3	1.79	0.62
1:B:2:LEU:HD23	1:B:7:GLU:HB3	1.81	0.62
1:C:110:THR:OG1	1:C:111:SER:N	2.31	0.62
1:D:76:ARG:O	1:D:79:ARG:HD3	2.00	0.61
1:D:1:MET:HA	1:D:8:TYR:OH	2.01	0.61
1:B:17:TYR:CD1	1:B:67:LEU:HG	2.35	0.60
1:A:250:ILE:HD13	1:B:247:LEU:HD11	1.82	0.60
1:D:156:SER:HB3	1:D:160:LYS:HE3	1.83	0.60
1:D:163:ASP:O	1:D:167:SER:OG	2.19	0.59
1:C:5:THR:HG21	1:C:50:GLU:HG3	1.84	0.59
1:B:225:VAL:HG21	1:B:245:SER:HB2	1.85	0.59
1:B:166:TYR:HD1	1:B:169:THR:HG22	1.67	0.58
1:C:229:TRP:HH2	1:C:238:GLU:HG3	1.68	0.58
1:B:105:GLN:NE2	1:B:106:GLU:OE1	2.35	0.58
1:B:202:ARG:HG2	1:B:224:TYR:OH	2.04	0.58
1:C:114:LEU:HD13	1:C:118:GLU:HB3	1.86	0.57
1:B:238:GLU:HG2	1:B:242:LYS:HE2	1.86	0.57
1:D:115:SER:O	1:D:119:VAL:HG23	2.05	0.57
1:D:114:LEU:HB2	1:D:119:VAL:HG22	1.85	0.57
1:A:252:ASN:O	1:A:256:ILE:HG13	2.04	0.57
1:A:70:VAL:O	1:A:73:MET:HG3	2.05	0.57
1:B:166:TYR:CD1	1:B:169:THR:HG22	2.40	0.57
1:C:253:THR:HA	1:C:256:ILE:HD11	1.85	0.57
1:C:225:VAL:HG21	1:C:245:SER:HB2	1.86	0.57
1:D:175:ILE:HD12	1:D:207:LEU:HD12	1.88	0.56
1:B:115:SER:HB2	1:B:117:LYS:HE2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ASN:OD1	1:A:109:ILE:HA	2.05	0.56
1:B:76:ARG:O	1:B:79:ARG:NH1	2.39	0.55
1:B:214:THR:HB	1:B:217:VAL:HG23	1.88	0.54
1:A:77:PRO:O	1:A:169:THR:HG21	2.07	0.54
1:C:94:PHE:HB2	1:C:95:PRO:HD3	1.90	0.54
1:C:5:THR:HG23	1:C:23:TRP:NE1	2.20	0.54
1:A:177:ASP:OD2	1:B:75:SER:OG	2.26	0.54
1:C:44:VAL:O	1:C:48:ILE:HG13	2.09	0.53
1:B:105:GLN:O	1:B:109:ILE:HG13	2.09	0.53
1:D:50:GLU:O	1:D:54:ASN:ND2	2.38	0.53
1:D:79:ARG:HG2	1:D:173:TYR:CZ	2.44	0.53
1:C:50:GLU:O	1:C:54:ASN:ND2	2.42	0.53
1:C:135:PHE:CE1	1:C:139:LEU:HD22	2.43	0.53
1:B:172:LYS:O	1:B:176:GLU:HB2	2.09	0.53
1:B:5:THR:HG21	1:B:50:GLU:HG3	1.91	0.52
1:C:175:ILE:HD12	1:C:207:LEU:HD13	1.92	0.51
1:C:12:LEU:HB2	1:C:20:PHE:CD1	2.45	0.51
1:D:70:VAL:HG12	1:D:77:PRO:HG2	1.91	0.51
1:D:59:ASP:HA	1:D:62:LYS:HE2	1.92	0.51
1:A:12:LEU:HB2	1:A:20:PHE:CD1	2.45	0.51
1:A:4:SER:HB2	1:A:7:GLU:H	1.75	0.51
1:C:130:LEU:HD11	1:C:138:PHE:HD2	1.76	0.50
1:B:92:ALA:O	1:B:95:PRO:HD2	2.10	0.50
1:C:229:TRP:CH2	1:C:238:GLU:HG3	2.45	0.50
1:B:196:ARG:O	1:B:200:VAL:HG23	2.11	0.50
1:A:48:ILE:HD11	1:A:95:PRO:HG2	1.94	0.50
1:A:121:GLN:O	1:A:125:MET:HG2	2.12	0.50
1:A:154:ASP:O	1:A:158:VAL:HG23	2.12	0.50
1:B:13:ARG:HA	1:B:63:LYS:HD2	1.94	0.49
1:B:258:THR:HA	1:C:151:LYS:HE2	1.94	0.49
1:B:178:TYR:HD1	1:B:240:PHE:HD2	1.60	0.49
1:D:196:ARG:NH1	1:D:232:GLN:O	2.46	0.49
1:C:73:MET:HE2	1:C:162:PHE:CG	2.48	0.48
1:C:99:TYR:CE1	1:C:135:PHE:HE2	2.32	0.48
1:D:81:GLY:O	1:D:84:TYR:HB3	2.14	0.48
1:D:94:PHE:O	1:D:98:VAL:HG23	2.13	0.48
1:B:245:SER:O	1:B:248:PRO:HD2	2.14	0.48
1:A:253:THR:HA	1:A:256:ILE:HD12	1.96	0.47
1:A:18:LEU:HD23	1:A:18:LEU:HA	1.73	0.47
1:A:114:LEU:HD22	1:A:118:GLU:HB3	1.96	0.47
1:C:73:MET:HE1	1:D:177:ASP:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:TYR:CD2	1:C:67:LEU:HG	2.50	0.47
1:D:51:TRP:CH2	1:D:93:LEU:HD13	2.50	0.47
1:B:44:VAL:HG11	1:B:91:ILE:HG22	1.97	0.47
1:D:160:LYS:O	1:D:164:GLN:HG2	2.15	0.47
1:A:256:ILE:HD11	1:C:139:LEU:HD23	1.97	0.47
1:C:45:SER:HB2	1:C:123:MET:HG3	1.97	0.47
1:D:12:LEU:HB2	1:D:20:PHE:CD1	2.51	0.46
1:D:178:TYR:HB2	1:D:240:PHE:CD1	2.51	0.46
1:D:166:TYR:HA	1:D:169:THR:CG2	2.41	0.46
1:A:250:ILE:O	1:A:254:VAL:HG23	2.14	0.46
1:B:80:GLU:O	1:B:83:SER:N	2.48	0.46
1:C:118:GLU:O	1:C:121:GLN:HB3	2.16	0.46
1:D:7:GLU:O	1:D:10:GLN:HG2	2.15	0.46
1:D:17:TYR:CD1	1:D:67:LEU:HG	2.51	0.46
1:A:212:GLU:HG3	1:A:214:THR:HG23	1.98	0.46
1:B:160:LYS:O	1:B:164:GLN:HG3	2.15	0.46
1:D:77:PRO:O	1:D:169:THR:HG21	2.15	0.46
1:A:187:LEU:HB3	1:A:190:ASP:HB3	1.97	0.46
1:B:170:TYR:CE2	1:B:174:LEU:HD22	2.50	0.45
1:A:175:ILE:HD12	1:A:207:LEU:HD12	1.98	0.45
1:A:179:LEU:HD21	1:A:201:VAL:HG22	1.99	0.45
1:B:12:LEU:HB2	1:B:20:PHE:CD1	2.51	0.45
1:C:177:ASP:HB3	1:D:73:MET:CE	2.47	0.45
1:A:219:ASP:O	1:A:223:VAL:HG23	2.16	0.45
1:B:70:VAL:HG11	1:B:165:ILE:HD12	1.99	0.45
1:B:77:PRO:O	1:B:169:THR:HG21	2.16	0.45
1:D:51:TRP:CD1	1:D:56:PHE:HB2	2.51	0.45
1:D:52:LEU:HD23	1:D:56:PHE:HB3	1.98	0.45
1:A:2:LEU:HD21	1:A:19:LEU:HD21	1.99	0.45
1:B:1:MET:HE1	1:B:26:PHE:HA	1.99	0.45
1:B:130:LEU:HD12	1:B:135:PHE:HB2	1.97	0.45
1:B:166:TYR:HD1	1:B:169:THR:CG2	2.28	0.45
1:B:169:THR:HG23	1:B:173:TYR:CE2	2.51	0.45
1:C:71:HIS:ND1	1:C:86:LEU:HD12	2.32	0.45
1:C:85:ALA:HA	1:C:88:THR:HG22	1.99	0.45
1:C:117:LYS:HE3	1:C:117:LYS:HB2	1.71	0.45
1:B:27:ILE:HD12	1:B:47:LEU:HD12	1.99	0.45
1:B:79:ARG:HA	1:B:83:SER:HB2	1.98	0.45
1:B:107:HIS:CD2	1:B:129:TYR:CZ	3.05	0.45
1:C:250:ILE:HD13	1:D:247:LEU:HD11	1.98	0.45
1:D:197:ILE:O	1:D:201:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:245:SER:O	1:D:248:PRO:HD2	2.17	0.44
1:A:215:GLN:NE2	1:A:219:ASP:OD1	2.51	0.44
1:A:144:ASP:O	1:A:148:THR:HG23	2.18	0.44
1:B:80:GLU:HB3	1:B:81:GLY:H	1.61	0.44
1:C:139:LEU:O	1:C:143:GLN:HG3	2.17	0.44
1:C:199:LEU:HD12	1:C:228:LEU:HD23	1.99	0.44
1:C:90:SER:O	1:C:93:LEU:HB3	2.18	0.44
1:D:219:ASP:O	1:D:223:VAL:HG23	2.18	0.43
1:A:2:LEU:HB2	1:A:8:TYR:CZ	2.53	0.43
1:D:79:ARG:HA	1:D:83:SER:HB3	2.00	0.43
1:A:67:LEU:HD13	1:A:86:LEU:HD12	2.00	0.43
1:A:160:LYS:O	1:A:164:GLN:HG2	2.17	0.43
1:A:132:LYS:O	1:A:136:VAL:HG23	2.18	0.43
1:C:78:LEU:HD22	1:C:82:LEU:HB3	1.99	0.43
1:D:166:TYR:CA	1:D:169:THR:HG22	2.43	0.43
1:A:182:LEU:O	1:A:193:LYS:HE3	2.19	0.43
1:C:9:LEU:HD23	1:C:9:LEU:HA	1.87	0.43
1:C:238:GLU:O	1:C:242:LYS:HG3	2.18	0.43
1:C:75:SER:HA	1:D:79:ARG:HH21	1.84	0.43
1:A:23:TRP:HB3	1:A:24:PRO:HD3	2.01	0.43
1:B:254:VAL:HG13	1:C:147:PHE:CE1	2.54	0.43
1:C:253:THR:O	1:C:256:ILE:HD12	2.19	0.43
1:D:192:LEU:O	1:D:196:ARG:HB2	2.19	0.43
1:B:169:THR:O	1:B:172:LYS:HB3	2.19	0.42
1:B:8:TYR:HE2	1:B:26:PHE:HB2	1.84	0.42
1:B:18:LEU:HD23	1:B:18:LEU:HA	1.82	0.42
1:A:99:TYR:O	1:A:105:GLN:NE2	2.52	0.42
1:C:228:LEU:HD23	1:C:228:LEU:HA	1.82	0.42
1:A:119:VAL:O	1:A:123:MET:HG2	2.19	0.42
1:A:133:GLN:O	1:A:137:GLU:HG3	2.19	0.42
1:B:225:VAL:HG21	1:B:245:SER:CB	2.48	0.42
1:D:9:LEU:HD13	1:D:54:ASN:HB2	2.01	0.42
1:C:177:ASP:HB3	1:D:73:MET:HE3	2.00	0.42
1:C:2:LEU:HB2	1:C:8:TYR:CE2	2.55	0.42
1:D:76:ARG:HB2	1:D:79:ARG:HH11	1.85	0.42
1:B:218:HIS:O	1:B:218:HIS:ND1	2.51	0.42
1:C:61:ILE:HD13	1:C:97:MET:HG2	2.01	0.42
1:B:178:TYR:CD1	1:B:240:PHE:HD2	2.37	0.42
1:B:178:TYR:HD1	1:B:240:PHE:CD2	2.37	0.41
1:A:115:SER:H	1:A:118:GLU:HB2	1.85	0.41
1:B:250:ILE:HD12	1:C:91:ILE:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:LEU:HA	1:A:188:PRO:HD2	1.86	0.41
1:B:170:TYR:HE2	1:B:174:LEU:HD22	1.86	0.41
1:C:27:ILE:HG13	1:C:47:LEU:HD23	2.01	0.41
1:A:63:LYS:HA	1:A:66:ILE:HD12	2.02	0.41
1:A:198:SER:O	1:A:202:ARG:HD3	2.21	0.41
1:C:31:TYR:CE2	1:C:46:LEU:HD22	2.55	0.41
1:A:233:PRO:HB2	1:A:237:GLU:HB2	2.03	0.41
1:A:257:LEU:HG	1:B:253:THR:HG21	2.03	0.41
1:A:163:ASP:O	1:A:167:SER:HB2	2.20	0.41
1:A:2:LEU:HD22	1:A:8:TYR:CE1	2.56	0.41
1:D:4:SER:HA	1:D:26:PHE:CZ	2.56	0.41
1:D:18:LEU:HD12	1:D:18:LEU:HA	1.88	0.41
1:D:220:GLU:O	1:D:223:VAL:HB	2.20	0.40
1:B:161:ALA:O	1:B:164:GLN:HB2	2.22	0.40
1:C:8:TYR:HE1	1:C:22:GLN:HB2	1.86	0.40
1:B:225:VAL:HG12	1:B:229:TRP:CZ3	2.47	0.40
1:C:123:MET:O	1:C:127:ASN:HB2	2.21	0.40
1:A:75:SER:OG	1:B:177:ASP:OD2	2.32	0.40
1:B:213:LEU:HD23	1:B:213:LEU:HA	1.94	0.40
1:C:21:LEU:HD23	1:C:21:LEU:HA	1.90	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	249/287 (87%)	244 (98%)	5 (2%)	0	100	100
1	B	232/287 (81%)	225 (97%)	7 (3%)	0	100	100
1	C	248/287 (86%)	236 (95%)	12 (5%)	0	100	100
1	D	244/287 (85%)	229 (94%)	15 (6%)	0	100	100
All	All	973/1148 (85%)	934 (96%)	39 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	225/265 (85%)	207 (92%)	18 (8%)	12	27
1	B	204/265 (77%)	187 (92%)	17 (8%)	11	25
1	C	224/265 (84%)	213 (95%)	11 (5%)	25	52
1	D	209/265 (79%)	198 (95%)	11 (5%)	22	48
All	All	862/1060 (81%)	805 (93%)	57 (7%)	16	38

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	4	SER
1	A	41	ASP
1	A	67	LEU
1	A	75	SER
1	A	100	LEU
1	A	104	LEU
1	A	105	GLN
1	A	111	SER
1	A	122	LEU
1	A	130	LEU
1	A	135	PHE
1	A	166	TYR
1	A	169	THR
1	A	178	TYR
1	A	182	LEU
1	A	194	SER
1	A	207	LEU
1	B	67	LEU
1	B	74	GLU
1	B	75	SER
1	B	79	ARG

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Mol	Chain	Res	Type
1	B	93	LEU
1	B	104	LEU
1	B	116	SER
1	B	117	LYS
1	B	122	LEU
1	B	130	LEU
1	B	156	SER
1	B	169	THR
1	B	182	LEU
1	B	199	LEU
1	B	207	LEU
1	B	229	TRP
1	B	258	THR
1	C	3	SER
1	C	4	SER
1	C	67	LEU
1	C	110	THR
1	C	116	SER
1	C	166	TYR
1	C	181	LEU
1	C	182	LEU
1	C	186	HIS
1	C	216	ASP
1	C	256	ILE
1	D	60	ASP
1	D	62	LYS
1	D	67	LEU
1	D	79	ARG
1	D	148	THR
1	D	166	TYR
1	D	167	SER
1	D	176	GLU
1	D	182	LEU
1	D	192	LEU
1	D	207	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	GLN
1	A	215	GLN
1	B	54	ASN

5.3.3 RNA (i)

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)

There are no ligands in this entry.

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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.