



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:22 PM UTC

PDB ID : 4R0G / pdb_00004r0g
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

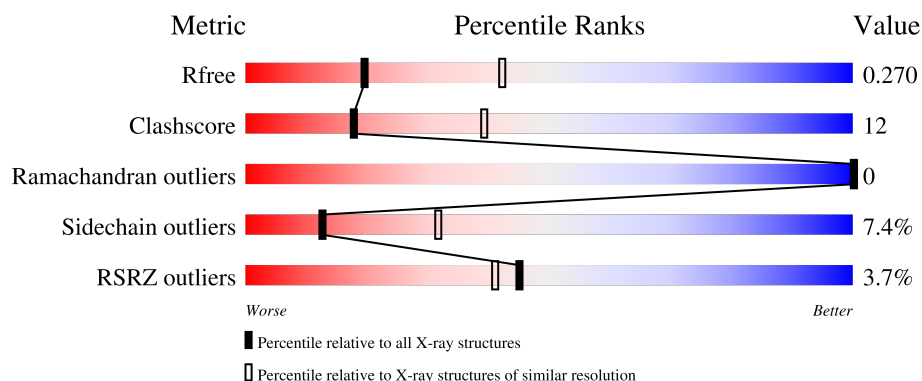
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 $\leq 5\%$. 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	287	
1	B	287	
1	C	287	
1	D	287	

2 Entry composition

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.

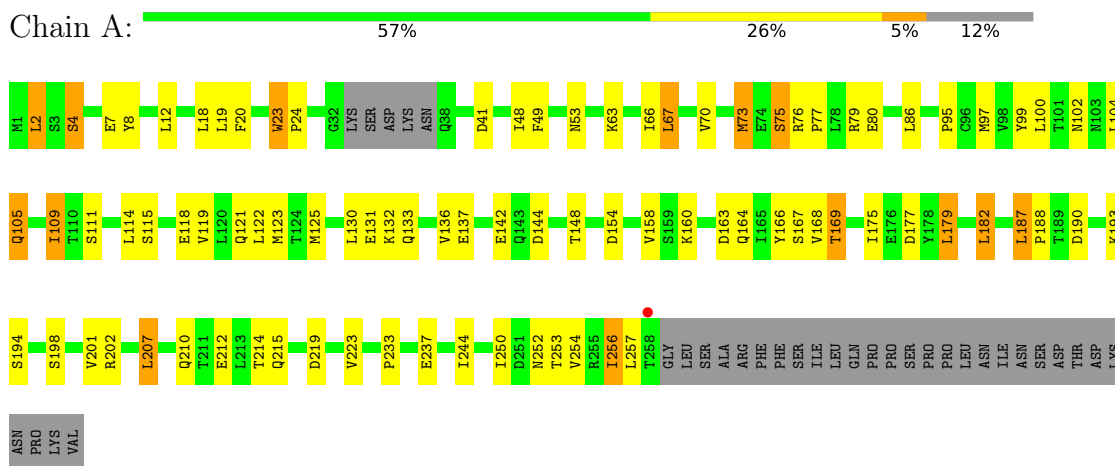
- Molecule 1 is a protein called Uncharacterized protein.

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

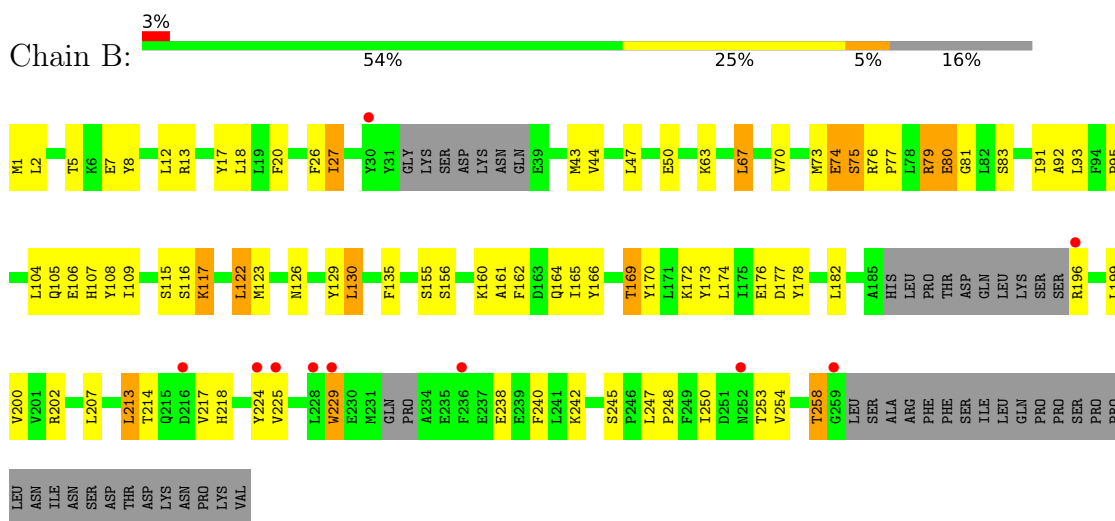
3 Residue-property plots [i](#)

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 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: Uncharacterized protein

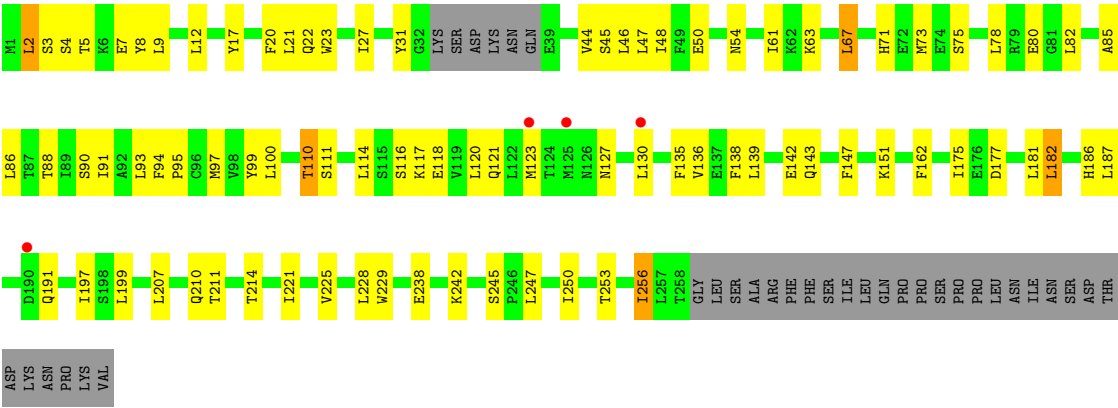


- Molecule 1: Uncharacterized protein

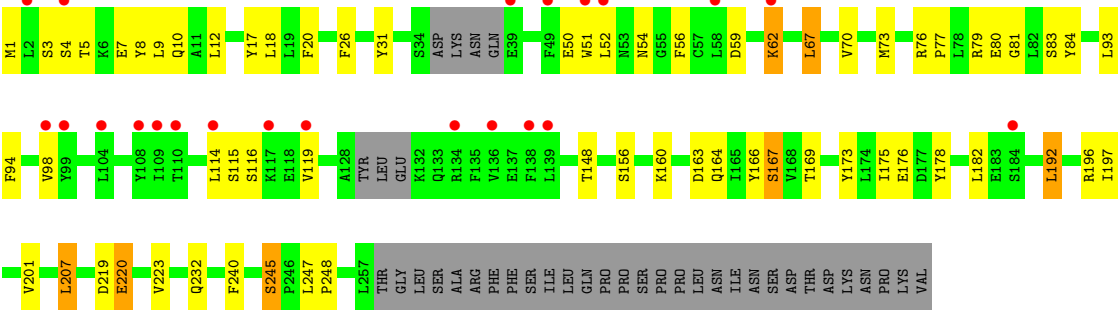


- Molecule 1: Uncharacterized protein





• Molecule 1: Uncharacterized protein



4 Data and refinement statistics

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 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (34.04-2.70) 88.2 (34.04-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 2.39Å)	Xtriage
Refinement program	CNS, PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.222 , 0.269 0.223 , 0.270	Depositor DCC
R_{free} test set	2036 reflections (3.86%)	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)	0.30 , 37.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.68	0/2111	1.01	11/2862 (0.4%)
1	B	0.56	0/1977	0.94	0/2678
1	C	0.60	0/2103	0.99	8/2852 (0.3%)
1	D	0.54	0/2033	0.93	3/2764 (0.1%)
All	All	0.60	0/8224	0.97	22/11156 (0.2%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	191	GLN	N-CA-C	-7.37	104.29	113.28
1	C	187	LEU	CA-C-N	6.67	128.18	119.84
1	C	187	LEU	C-N-CA	6.67	128.18	119.84
1	A	256	ILE	CB-CA-C	-6.49	103.57	111.88
1	C	80	GLU	CB-CA-C	-6.28	109.32	116.54
1	C	247	LEU	CA-C-N	6.13	126.24	119.87
1	C	247	LEU	C-N-CA	6.13	126.24	119.87
1	D	245	SER	CA-C-N	6.08	125.80	119.05
1	D	245	SER	C-N-CA	6.08	125.80	119.05
1	A	80	GLU	CB-CA-C	-6.07	109.56	116.54
1	A	244	ILE	N-CA-C	5.92	116.58	110.36
1	A	168	VAL	CB-CA-C	-5.86	104.39	112.24
1	A	23	TRP	CA-C-N	-5.85	113.66	119.56
1	A	23	TRP	C-N-CA	-5.85	113.66	119.56
1	A	80	GLU	N-CA-C	5.63	116.87	108.31
1	A	102	ASN	N-CA-C	5.59	119.80	112.92
1	C	214	THR	N-CA-C	-5.57	101.76	110.17
1	A	187	LEU	CA-C-N	5.54	126.77	119.84
1	A	187	LEU	C-N-CA	5.54	126.77	119.84
1	C	221	ILE	CB-CA-C	-5.32	105.07	111.88
1	A	109	ILE	N-CA-C	5.18	115.56	107.99
1	D	80	GLU	CB-CA-C	-5.04	110.38	117.23

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	2064	0	2028	50	0
1	B	1935	0	1879	61	0
1	C	2056	0	2023	54	0
1	D	1988	0	1892	43	0
All	All	8043	0	7822	195	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 (195) 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:73:MET:HE2	1:C:162:PHE:CD1	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:49:PHE:HB2	1:A:123:MET:HE3	1.85	0.59
1:B:225:VAL:HG21	1:B:245:SER:HB2	1.85	0.59
1:B:43:MET:HE3	1:B:47:LEU:HD11	1.86	0.58
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:B:108:TYR:CE1	1:B:123:MET:HE3	2.39	0.56
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:THR:HG21	1:B:50:GLU:HG3	1.91	0.52
1:C:97:MET:HE2	1:C:142:GLU:OE2	2.10	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:B:1:MET:HE1	1:B:26:PHE:HD1	1.75	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:97:MET:HE2	1:A:142:GLU:OE1	2.11	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:C:73:MET:HE2	1:C:162:PHE:CG	2.46	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:1:MET:HE1	1:B:26:PHE:HA	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: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:B:73:MET:HE2	1:B:162:PHE:CG	2.50	0.47
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:LYS:O	1:A:164:GLN:HG2	2.17	0.43
1:B:1:MET:HE3	1:B:1:MET:HB3	1.93	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:B:108:TYR:HE1	1:B:123:MET:HE3	1.81	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:A:177:ASP:CG	1:B:74:GLU:H	2.26	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: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
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:D:1:MET:HE2	1:D:26:PHE:HA	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	206 (92%)	19 (8%)	10	26
1	B	204/265 (77%)	183 (90%)	21 (10%)	7	18
1	C	224/265 (84%)	209 (93%)	15 (7%)	15	36
1	D	209/265 (79%)	200 (96%)	9 (4%)	26	54
All	All	862/1060 (81%)	798 (93%)	64 (7%)	13	32

All (64) 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	73	MET
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	131	GLU
1	A	169	THR
1	A	179	LEU
1	A	182	LEU
1	A	194	SER
1	A	207	LEU
1	A	210	GLN
1	B	27	ILE
1	B	67	LEU
1	B	74	GLU
1	B	75	SER
1	B	79	ARG
1	B	80	GLU
1	B	93	LEU
1	B	104	LEU
1	B	116	SER

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Mol	Chain	Res	Type
1	B	117	LYS
1	B	122	LEU
1	B	130	LEU
1	B	155	SER
1	B	156	SER
1	B	169	THR
1	B	182	LEU
1	B	199	LEU
1	B	207	LEU
1	B	213	LEU
1	B	229	TRP
1	B	258	THR
1	C	2	LEU
1	C	3	SER
1	C	4	SER
1	C	63	LYS
1	C	67	LEU
1	C	100	LEU
1	C	110	THR
1	C	116	SER
1	C	120	LEU
1	C	181	LEU
1	C	182	LEU
1	C	186	HIS
1	C	210	GLN
1	C	211	THR
1	C	256	ILE
1	D	62	LYS
1	D	67	LEU
1	D	148	THR
1	D	167	SER
1	D	176	GLU
1	D	182	LEU
1	D	192	LEU
1	D	207	LEU
1	D	220	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	GLN
1	A	210	GLN

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Mol	Chain	Res	Type
1	B	107	HIS
1	B	164	GLN
1	C	121	GLN
1	C	210	GLN
1	C	232	GLN
1	D	127	ASN
1	D	186	HIS
1	D	218	HIS
1	D	252	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 oligosaccharides 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

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	A	253/287 (88%)	-0.28	1 (0%) 88 87	37, 56, 94, 118	0
1	B	240/287 (83%)	0.22	10 (4%) 40 37	48, 80, 114, 124	0
1	C	252/287 (87%)	0.08	4 (1%) 70 68	45, 75, 102, 113	0
1	D	250/287 (87%)	0.54	22 (8%) 15 13	57, 99, 155, 163	0
All	All	995/1148 (86%)	0.14	37 (3%) 45 41	37, 75, 136, 163	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	49	PHE	4.9
1	D	119	VAL	4.4
1	D	134	ARG	3.8
1	D	99	TYR	3.4
1	D	114	LEU	3.4
1	D	98	VAL	3.1
1	D	39	GLU	3.0
1	B	259	GLY	2.8
1	D	108	TYR	2.8
1	D	138	PHE	2.8
1	B	225	VAL	2.7
1	A	258	THR	2.7
1	D	184	SER	2.6
1	B	252	ASN	2.6
1	B	229	TRP	2.5
1	D	104	LEU	2.4
1	B	224	TYR	2.4
1	D	58	LEU	2.4
1	D	51	TRP	2.4
1	D	117	LYS	2.3
1	D	136	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	196	ARG	2.3
1	D	109	ILE	2.2
1	C	130	LEU	2.2
1	D	52	LEU	2.1
1	D	139	LEU	2.1
1	D	62	LYS	2.1
1	B	236	PHE	2.1
1	B	228	LEU	2.1
1	D	2	LEU	2.1
1	B	30	TYR	2.1
1	D	4	SER	2.1
1	C	123	MET	2.1
1	C	125	MET	2.1
1	B	216	ASP	2.0
1	C	190	ASP	2.0
1	D	110	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.