



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 08:15 AM BST

PDB ID : 7BWK  
Title : Structure of DotL(656-783)-IcmS-IcmW-LvgA-VpdB(461-590) derived from Legionella pneumophila  
Authors : Kim, H.; Kwak, M.J.; Oh, B.H.  
Deposited on : 2020-04-14  
Resolution : 2.80 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](mailto: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.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
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)	:	2.13.1

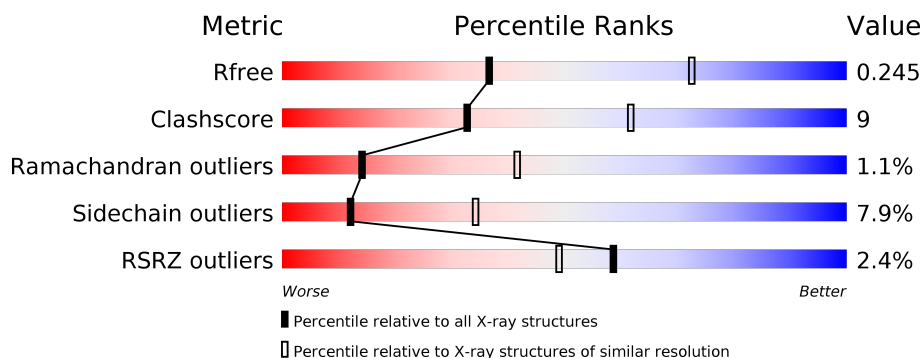
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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  $\geq 3$ , 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	128	<div> <div>7%</div> <div> <div></div> <div>62%</div> <div>22%</div> <div>• •</div> <div>12%</div> </div> </div>
1	F	128	<div> <div>5%</div> <div> <div></div> <div>64%</div> <div>21%</div> <div>•</div> <div>13%</div> </div> </div>
2	B	114	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>20%</div> <div>• •</div> </div> </div>
2	G	114	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>17%</div> <div>• •</div> </div> </div>
3	C	151	<div> <div>%</div> <div> <div></div> <div>79%</div> <div>19%</div> <div>• •</div> </div> </div>
3	H	151	<div> <div>%</div> <div> <div></div> <div>64%</div> <div>29%</div> <div>6%</div> <div>•</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	D	208	
4	I	208	
5	E	130	
5	J	130	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10645 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 IcmO (DotL).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	113	Total	C	N	O	S	0	0	0
			880	555	148	176	1			
1	F	111	Total	C	N	O	S	0	0	0
			864	545	146	172	1			

- Molecule 2 is a protein called IcmS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	113	Total	C	N	O	S	0	0	0
			875	552	141	173	9			
2	G	113	Total	C	N	O	S	0	0	0
			875	552	141	173	9			

- Molecule 3 is a protein called IcmW.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	149	Total	C	N	O	S	0	0	0
			1202	767	205	226	4			
3	H	149	Total	C	N	O	S	0	0	0
			1202	767	205	226	4			

- Molecule 4 is a protein called Hypothetical virulence protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	181	Total	C	N	O	S	0	0	0
			1443	933	237	266	7			
4	I	181	Total	C	N	O	S	0	0	0
			1446	936	237	266	7			

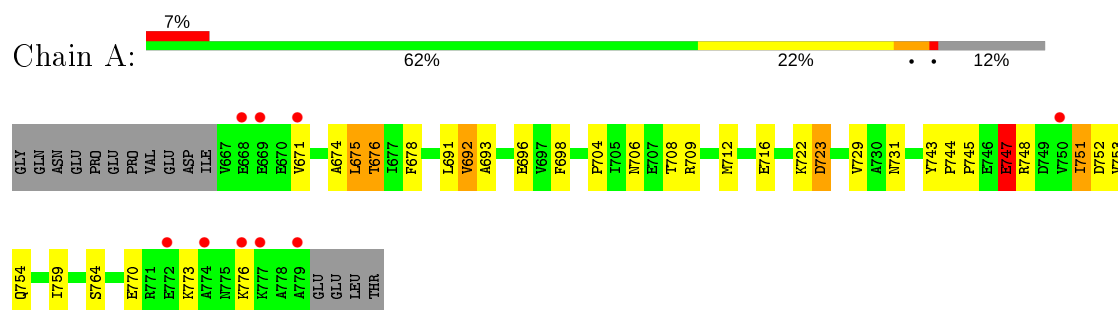
- Molecule 5 is a protein called PNPLA domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	116	Total	C	N	O	S	0	0	0
			929	586	165	176	2			
5	J	116	Total	C	N	O	S	0	0	0
			929	586	165	176	2			

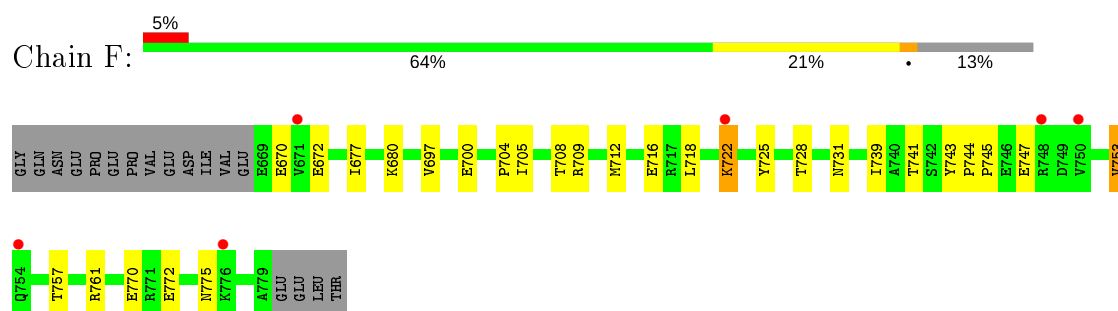
### 3 Residue-property plots [i](#)

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.

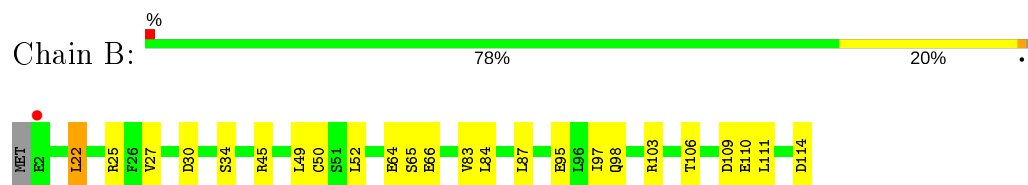
- Molecule 1: IcmO (DotL)



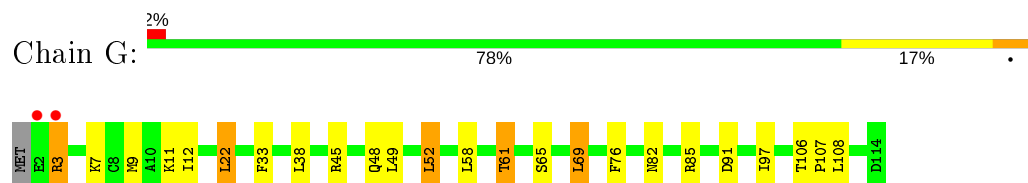
- Molecule 1: IcmO (DotL)



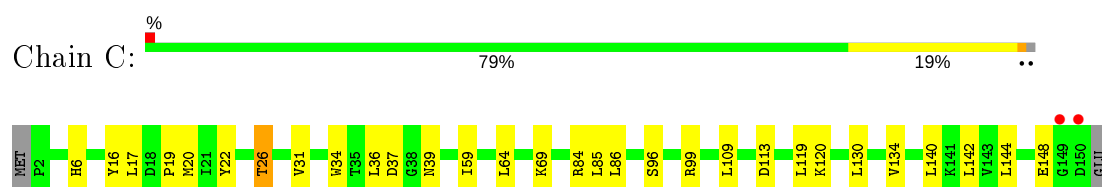
- Molecule 2: IcmS



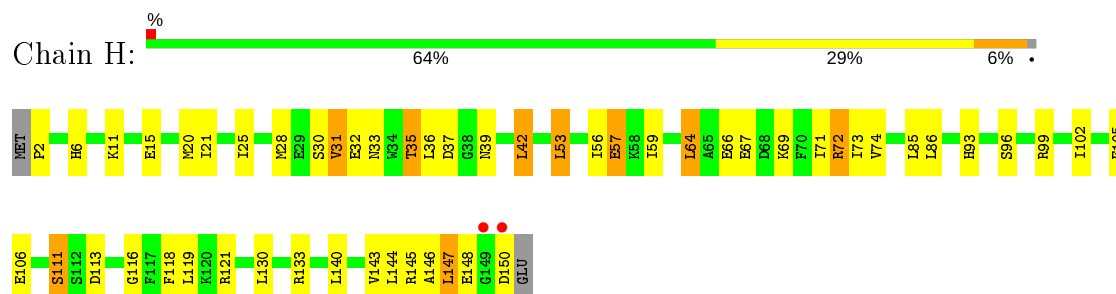
- Molecule 2: IcmS



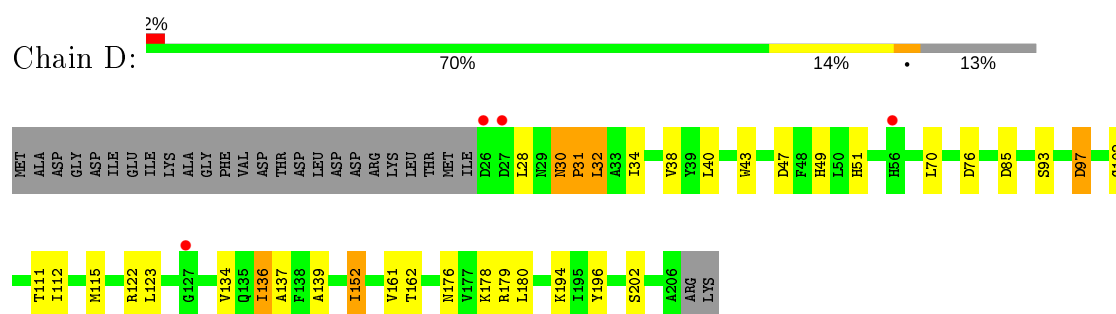
- Molecule 3: IcmW



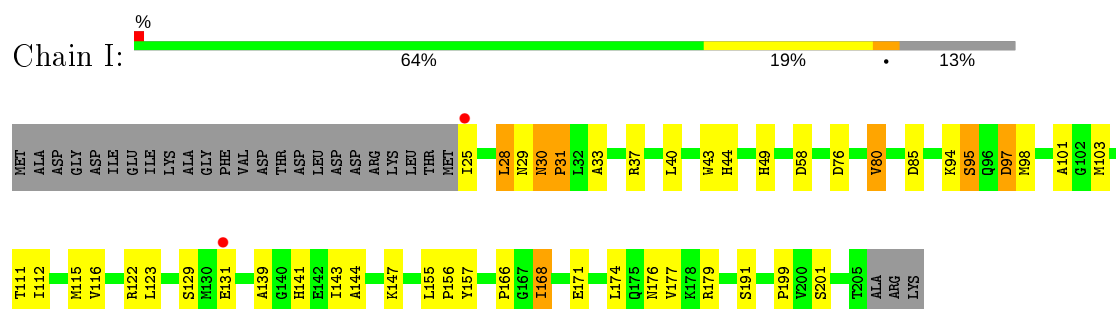
- Molecule 3: IcmW



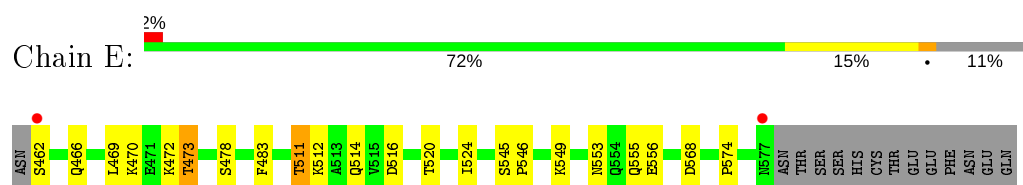
- Molecule 4: Hypothetical virulence protein



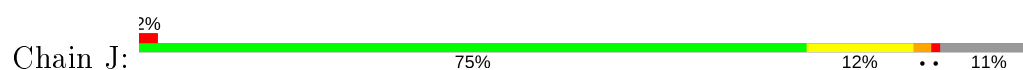
- Molecule 4: Hypothetical virulence protein

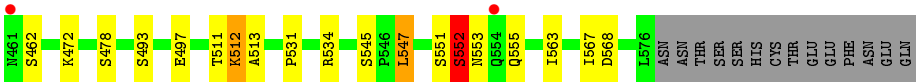


- Molecule 5: PNPLA domain-containing protein



- Molecule 5: PNPLA domain-containing protein







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	188.99Å 188.99Å 170.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.25 – 2.80 47.25 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.25-2.80) 99.5 (47.25-2.80)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.07 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.199 , 0.245 0.200 , 0.245	Depositor DCC
$R_{free}$ test set	3841 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.0	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 36.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	10645	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.72% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.49	0/891	0.56	0/1206
1	F	0.44	0/875	0.52	0/1184
2	B	0.49	0/888	0.66	0/1198
2	G	0.45	0/888	0.64	0/1198
3	C	0.43	0/1224	0.57	0/1650
3	H	0.45	0/1224	0.57	0/1650
4	D	0.46	0/1485	0.59	0/2020
4	I	0.48	0/1488	0.60	0/2024
5	E	0.45	0/944	0.51	0/1264
5	J	0.42	0/944	0.54	0/1264
All	All	0.46	0/10851	0.58	0/14658

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	880	0	901	25	0
1	F	864	0	886	19	0
2	B	875	0	862	14	0
2	G	875	0	862	19	0
3	C	1202	0	1206	18	0
3	H	1202	0	1206	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1443	0	1414	24	0
4	I	1446	0	1420	48	0
5	E	929	0	948	12	0
5	J	929	0	948	13	0
All	All	10645	0	10653	186	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 9.

All (186) 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)
4:I:155:LEU:HD23	4:I:191:SER:CB	1.91	1.00
4:I:155:LEU:CD2	4:I:191:SER:CB	2.41	0.99
4:I:155:LEU:HD23	4:I:191:SER:HB2	1.47	0.96
4:I:155:LEU:CD2	4:I:191:SER:HB3	2.00	0.91
4:I:155:LEU:HD21	4:I:191:SER:HB3	1.52	0.88
2:B:97:ILE:HA	2:B:106:THR:HG21	1.58	0.84
4:I:155:LEU:CD2	4:I:191:SER:HB2	2.06	0.83
5:E:472:LYS:HE2	2:G:61:THR:HB	1.62	0.82
5:J:511:THR:HG22	5:J:513:ALA:H	1.45	0.81
1:A:676:THR:HG23	1:A:678:PHE:H	1.46	0.80
2:G:97:ILE:HA	2:G:106:THR:HG21	1.67	0.75
4:D:161:VAL:H	5:E:473:THR:HG21	1.54	0.72
4:I:168:ILE:HD12	4:I:168:ILE:H	1.54	0.71
3:H:111:SER:OG	4:I:30:ASN:ND2	2.24	0.71
4:I:85:ASP:OD2	4:I:122:ARG:NH2	2.24	0.71
4:I:95:SER:HA	4:I:98:MET:HG3	1.73	0.71
2:B:45:ARG:HD2	2:B:114:ASP:OD2	1.90	0.70
4:I:116:VAL:CG1	4:I:155:LEU:HD11	2.21	0.70
4:D:28:LEU:HD13	5:J:462:SER:HB3	1.74	0.68
5:E:553:ASN:HB3	5:E:556:GLU:HB2	1.76	0.67
4:I:155:LEU:HD23	4:I:191:SER:C	2.15	0.66
5:E:469:LEU:O	5:E:473:THR:HG22	1.95	0.66
1:A:745:PRO:HB2	1:A:747:GLU:HG2	1.76	0.65
4:I:85:ASP:CG	4:I:122:ARG:HH22	2.00	0.65
5:E:511:THR:HB	5:E:514:GLN:H	1.62	0.64
4:I:111:THR:HG22	4:I:115:MET:HE2	1.80	0.64
4:I:80:VAL:HG22	4:I:111:THR:HA	1.78	0.64
1:A:722:LYS:HD3	1:A:723:ASP:H	1.63	0.63
4:D:123:LEU:HD11	4:D:134:VAL:HG11	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:28:LEU:O	4:I:37:ARG:NH2	2.31	0.63
1:F:718:LEU:HB3	3:H:147:LEU:HD22	1.81	0.62
1:A:709:ARG:HD2	1:A:731:ASN:OD1	1.99	0.62
4:I:116:VAL:HG13	4:I:155:LEU:HD11	1.81	0.62
4:I:97:ASP:HB2	4:I:101:ALA:HB2	1.82	0.61
2:G:12:ILE:HD13	3:H:143:VAL:HG22	1.83	0.60
4:I:112:ILE:HA	4:I:115:MET:HE3	1.83	0.60
4:I:166:PRO:HD2	5:J:472:LYS:HD3	1.83	0.60
1:F:680:LYS:HD2	1:F:680:LYS:H	1.66	0.59
2:B:45:ARG:NH2	2:B:110:GLU:OE1	2.34	0.59
4:D:49:HIS:HB2	4:D:139:ALA:HB3	1.85	0.59
4:I:30:ASN:N	4:I:31:PRO:HD3	2.18	0.58
4:I:28:LEU:HD22	4:I:31:PRO:HG2	1.85	0.58
1:F:677:ILE:HB	1:F:741:THR:HG21	1.84	0.57
1:F:722:LYS:HE2	1:F:725:TYR:HB2	1.86	0.57
2:G:58:LEU:O	2:G:85:ARG:NH1	2.38	0.56
1:A:704:PRO:O	1:A:708:THR:HG23	2.05	0.56
2:B:49:LEU:HD12	3:C:130:LEU:HD13	1.88	0.56
4:D:112:ILE:HA	4:D:115:MET:HE3	1.87	0.55
1:A:751:ILE:HG12	1:A:752:ASP:H	1.71	0.55
1:A:745:PRO:O	1:A:748:ARG:HG3	2.07	0.55
4:D:178:LYS:HG2	5:E:483:PHE:CE1	2.41	0.55
5:J:511:THR:HG22	5:J:513:ALA:N	2.20	0.55
5:J:497:GLU:HG3	5:J:534:ARG:HH12	1.70	0.55
1:A:744:PRO:HD3	3:C:31:VAL:HG11	1.88	0.54
1:F:772:GLU:HA	1:F:775:ASN:HB2	1.89	0.54
1:A:753:VAL:HG12	3:C:39:ASN:HD22	1.72	0.54
4:I:174:LEU:HA	4:I:177:VAL:HG13	1.90	0.54
2:B:98:GLN:OE1	2:B:103:ARG:NH1	2.41	0.54
3:C:22:TYR:O	3:C:26:THR:HG23	2.07	0.53
4:I:155:LEU:CG	4:I:191:SER:HB2	2.38	0.53
3:H:105:GLU:HA	3:H:119:LEU:HD11	1.91	0.52
3:H:74:VAL:O	3:H:121:ARG:NH2	2.42	0.52
2:G:91:ASP:OD1	3:H:133:ARG:NH1	2.43	0.52
1:A:753:VAL:HA	3:C:36:LEU:HD13	1.91	0.52
4:I:49:HIS:HB2	4:I:139:ALA:HB3	1.91	0.52
1:A:770:GLU:HG3	3:C:64:LEU:HD12	1.92	0.51
1:F:743:TYR:CD1	1:F:744:PRO:HA	2.46	0.51
2:G:52:LEU:HD23	4:I:37:ARG:HD3	1.91	0.51
1:A:692:VAL:HG21	1:A:698:PHE:CD2	2.46	0.50
5:E:546:PRO:HA	5:E:549:LYS:HE3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:739:ILE:HD13	4:I:25:ILE:HA	1.94	0.50
1:F:709:ARG:HD2	1:F:731:ASN:OD1	2.11	0.50
3:C:119:LEU:HD13	4:D:34:ILE:HD11	1.93	0.49
1:F:716:GLU:OE2	2:G:82:ASN:N	2.44	0.49
1:A:747:GLU:HG3	3:C:120:LYS:NZ	2.27	0.49
4:D:134:VAL:HG12	4:D:136:ILE:HD13	1.94	0.49
4:D:123:LEU:HD13	4:D:134:VAL:HG21	1.95	0.49
4:D:176:ASN:OD1	4:D:179:ARG:NH1	2.46	0.49
3:H:69:LYS:O	3:H:73:ILE:HG13	2.13	0.48
2:B:95:GLU:OE2	4:D:102:GLY:HA3	2.13	0.48
3:H:72:ARG:HD2	3:H:72:ARG:HA	1.60	0.48
1:A:743:TYR:CD1	1:A:744:PRO:HA	2.48	0.48
1:A:744:PRO:HD3	3:C:31:VAL:CG1	2.43	0.48
1:A:759:ILE:HG23	3:C:69:LYS:HD3	1.95	0.48
4:D:161:VAL:N	5:E:473:THR:HG21	2.27	0.47
4:I:76:ASP:HB3	4:I:199:PRO:HB2	1.96	0.47
3:H:56:ILE:O	3:H:59:ILE:HG22	2.15	0.47
4:D:34:ILE:O	4:D:38:VAL:HG23	2.14	0.47
2:G:48:GLN:HB2	4:I:103:MET:HE1	1.96	0.47
5:E:470:LYS:O	5:E:473:THR:HG23	2.14	0.47
1:A:674:ALA:HA	3:C:31:VAL:HG11	1.97	0.47
2:B:64:GLU:HG3	4:I:171:GLU:O	2.15	0.46
1:F:770:GLU:HB3	3:H:59:ILE:HD11	1.95	0.46
2:G:45:ARG:HA	4:I:103:MET:HE1	1.98	0.46
3:H:11:LYS:O	3:H:15:GLU:HG3	2.15	0.46
4:I:40:LEU:O	4:I:43:TRP:HB3	2.15	0.46
4:I:155:LEU:HD23	4:I:191:SER:CA	2.42	0.46
4:I:129:SER:OG	4:I:131:GLU:HG2	2.15	0.46
4:D:40:LEU:O	4:D:43:TRP:HB3	2.15	0.46
3:C:120:LYS:HB2	3:C:120:LYS:HE3	1.82	0.46
2:G:69:LEU:O	4:I:179:ARG:HD2	2.15	0.46
5:J:547:LEU:HA	5:J:547:LEU:HD12	1.69	0.46
4:D:152:ILE:HD11	4:D:161:VAL:HG23	1.98	0.45
3:H:33:ASN:N	3:H:33:ASN:OD1	2.49	0.45
4:D:194:LYS:HB3	4:D:196:TYR:CE2	2.52	0.45
1:F:718:LEU:HD11	3:H:148:GLU:HG3	1.99	0.45
5:J:563:ILE:O	5:J:567:ILE:HG13	2.16	0.45
5:E:462:SER:O	5:E:466:GLN:HG3	2.16	0.45
3:H:21:ILE:O	3:H:25:ILE:HG13	2.16	0.45
5:J:497:GLU:HG3	5:J:534:ARG:NH1	2.32	0.45
4:D:47:ASP:HA	4:D:93:SER:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:28:MET:O	3:H:32:GLU:HG3	2.17	0.45
4:I:95:SER:O	4:I:98:MET:HG3	2.17	0.44
2:G:3:ARG:HD3	2:G:7:LYS:HD2	1.98	0.44
2:B:97:ILE:HA	2:B:106:THR:CG2	2.40	0.44
4:D:111:THR:HG22	4:D:115:MET:HE2	1.99	0.44
3:H:32:GLU:O	3:H:35:THR:HB	2.18	0.44
4:D:30:ASN:N	4:D:31:PRO:HD3	2.32	0.44
3:H:2:PRO:HD2	3:H:53:LEU:HB3	2.00	0.44
1:F:745:PRO:C	1:F:747:GLU:H	2.20	0.44
1:F:712:MET:HE2	1:F:712:MET:HB2	1.94	0.44
4:I:176:ASN:OD1	4:I:179:ARG:NH1	2.50	0.43
1:A:712:MET:HG2	2:B:83:VAL:HG21	1.99	0.43
1:F:708:THR:O	1:F:712:MET:HG3	2.19	0.43
1:A:743:TYR:CG	1:A:744:PRO:HA	2.53	0.43
3:H:67:GLU:O	3:H:71:ILE:HG13	2.18	0.43
2:G:3:ARG:HB2	2:G:7:LYS:HB2	2.00	0.43
4:I:147:LYS:HD2	4:I:147:LYS:HA	1.75	0.43
4:I:155:LEU:CD2	4:I:191:SER:C	2.86	0.43
5:J:552:SER:HB3	5:J:553:ASN:H	1.57	0.43
2:B:22:LEU:HB2	2:B:27:VAL:CG2	2.49	0.43
4:D:85:ASP:OD2	4:D:122:ARG:NH2	2.31	0.43
3:C:16:TYR:OH	4:D:97:ASP:HA	2.19	0.43
4:D:32:LEU:H	4:D:32:LEU:HD23	1.82	0.43
4:I:141:HIS:CE1	4:I:143:ILE:HG13	2.53	0.43
4:D:51:HIS:HB2	4:D:137:ALA:HB3	2.01	0.43
1:A:676:THR:CG2	1:A:678:PHE:H	2.25	0.42
1:F:704:PRO:HG2	1:F:708:THR:HG23	2.00	0.42
3:H:145:ARG:HG3	3:H:146:ALA:N	2.34	0.42
4:I:122:ARG:HD3	4:I:122:ARG:HA	1.88	0.42
2:G:11:LYS:NZ	3:H:150:ASP:HB3	2.34	0.42
1:F:753:VAL:HG11	3:H:39:ASN:ND2	2.34	0.42
4:I:112:ILE:HD11	4:I:144:ALA:HB1	2.00	0.42
3:C:99:ARG:HA	3:C:99:ARG:HD3	1.88	0.42
5:J:493:SER:HA	5:J:531:PRO:HB3	2.00	0.42
5:E:520:THR:O	5:E:524:ILE:HG13	2.19	0.42
5:E:546:PRO:O	5:E:549:LYS:HG2	2.19	0.42
1:A:773:LYS:O	1:A:776:LYS:HB3	2.20	0.42
4:I:155:LEU:HG	4:I:191:SER:HB2	2.01	0.42
1:A:745:PRO:CB	1:A:747:GLU:HG2	2.49	0.42
2:G:49:LEU:HD12	3:H:130:LEU:HD13	2.02	0.41
3:C:17:LEU:O	3:C:19:PRO:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:512:LYS:H	5:J:512:LYS:HD2	1.85	0.41
5:J:545:SER:C	5:J:547:LEU:H	2.22	0.41
3:C:31:VAL:O	3:C:31:VAL:HG12	2.20	0.41
2:B:87:LEU:HD12	3:C:134:VAL:O	2.20	0.41
3:H:57:GLU:HG2	3:H:57:GLU:H	1.55	0.41
3:H:71:ILE:HG23	3:H:118:PHE:HB2	2.01	0.41
1:A:675:LEU:HD23	1:A:743:TYR:O	2.19	0.41
3:H:93:HIS:O	3:H:96:SER:HB2	2.20	0.41
5:J:512:LYS:H	5:J:512:LYS:CD	2.33	0.41
2:B:50:CYS:SG	2:B:84:LEU:HD21	2.61	0.41
2:G:108:LEU:HD23	2:G:108:LEU:HA	1.78	0.41
3:H:99:ARG:HA	3:H:99:ARG:HD3	1.93	0.41
4:I:156:PRO:HG2	4:I:157:TYR:CD1	2.55	0.41
1:F:718:LEU:HD23	1:F:718:LEU:HA	1.89	0.41
2:G:9:MET:HB3	2:G:33:PHE:CD1	2.56	0.41
3:H:102:ILE:O	3:H:106:GLU:HG2	2.20	0.41
1:F:757:THR:HG23	3:H:42:LEU:HA	2.02	0.41
1:F:697:VAL:HA	1:F:700:GLU:OE1	2.21	0.41
3:H:35:THR:HG23	3:H:37:ASP:OD1	2.20	0.41
4:I:44:HIS:O	4:I:94:LYS:HE3	2.20	0.41
1:A:716:GLU:OE1	2:B:83:VAL:HG12	2.19	0.41
3:C:144:LEU:O	3:C:148:GLU:HG2	2.20	0.41
2:G:22:LEU:HA	2:G:22:LEU:HD12	1.78	0.41
4:I:156:PRO:HG2	4:I:157:TYR:HD1	1.84	0.41
4:D:112:ILE:HA	4:D:115:MET:CE	2.49	0.41
2:B:30:ASP:O	2:B:34:SER:HB2	2.21	0.41
2:G:106:THR:HA	2:G:107:PRO:HD3	1.90	0.41
4:I:33:ALA:O	4:I:37:ARG:HG3	2.21	0.41
2:G:76:PHE:CD2	2:G:85:ARG:HD3	2.56	0.40
3:H:113:ASP:HB3	3:H:116:GLY:H	1.86	0.40
3:H:53:LEU:HA	3:H:53:LEU:HD12	1.80	0.40
1:A:752:ASP:OD2	1:A:754:GLN:HG2	2.20	0.40
3:H:64:LEU:HD13	3:H:66:GLU:HB2	2.03	0.40
4:I:112:ILE:HA	4:I:115:MET:CE	2.52	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	111/128 (87%)	105 (95%)	3 (3%)	3 (3%)	5	17
1	F	109/128 (85%)	99 (91%)	8 (7%)	2 (2%)	8	28
2	B	111/114 (97%)	108 (97%)	3 (3%)	0	100	100
2	G	111/114 (97%)	107 (96%)	4 (4%)	0	100	100
3	C	147/151 (97%)	142 (97%)	4 (3%)	1 (1%)	22	53
3	H	147/151 (97%)	138 (94%)	7 (5%)	2 (1%)	11	34
4	D	179/208 (86%)	171 (96%)	6 (3%)	2 (1%)	14	41
4	I	179/208 (86%)	164 (92%)	12 (7%)	3 (2%)	9	29
5	E	114/130 (88%)	112 (98%)	2 (2%)	0	100	100
5	J	114/130 (88%)	108 (95%)	5 (4%)	1 (1%)	17	46
All	All	1322/1462 (90%)	1254 (95%)	54 (4%)	14 (1%)	14	41

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	692	VAL
1	A	693	ALA
3	H	31	VAL
5	J	552	SER
1	A	747	GLU
3	C	34	TRP
4	I	201	SER
1	F	670	GLU
4	I	31	PRO
4	D	31	PRO
3	H	30	SER
1	F	753	VAL
4	D	30	ASN
4	I	30	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	96/110 (87%)	85 (88%)	11 (12%)	5	17
1	F	94/110 (86%)	89 (95%)	5 (5%)	22	54
2	B	96/97 (99%)	89 (93%)	7 (7%)	14	38
2	G	96/97 (99%)	89 (93%)	7 (7%)	14	38
3	C	131/133 (98%)	118 (90%)	13 (10%)	8	23
3	H	131/133 (98%)	115 (88%)	16 (12%)	5	15
4	D	159/182 (87%)	150 (94%)	9 (6%)	20	50
4	I	160/182 (88%)	152 (95%)	8 (5%)	24	56
5	E	103/117 (88%)	94 (91%)	9 (9%)	10	30
5	J	103/117 (88%)	96 (93%)	7 (7%)	16	42
All	All	1169/1278 (92%)	1077 (92%)	92 (8%)	12	34

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	671	VAL
1	A	675	LEU
1	A	676	THR
1	A	691	LEU
1	A	696	GLU
1	A	706	ASN
1	A	723	ASP
1	A	729	VAL
1	A	747	GLU
1	A	751	ILE
1	A	764	SER
2	B	22	LEU
2	B	25	ARG
2	B	52	LEU
2	B	65	SER
2	B	66	GLU

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Mol	Chain	Res	Type
2	B	109	ASP
2	B	111	LEU
3	C	6	HIS
3	C	20	MET
3	C	26	THR
3	C	37	ASP
3	C	59	ILE
3	C	84	ARG
3	C	85	LEU
3	C	86	LEU
3	C	96	SER
3	C	109	LEU
3	C	113	ASP
3	C	140	LEU
3	C	142	LEU
4	D	32	LEU
4	D	70	LEU
4	D	76	ASP
4	D	97	ASP
4	D	136	ILE
4	D	152	ILE
4	D	162	THR
4	D	180	LEU
4	D	202	SER
5	E	473	THR
5	E	478	SER
5	E	511	THR
5	E	512	LYS
5	E	516	ASP
5	E	545	SER
5	E	555	GLN
5	E	568	ASP
5	E	574	PRO
1	F	672	GLU
1	F	705	ILE
1	F	722	LYS
1	F	728	THR
1	F	761	ARG
2	G	3	ARG
2	G	22	LEU
2	G	38	LEU
2	G	52	LEU

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Mol	Chain	Res	Type
2	G	61	THR
2	G	65	SER
2	G	69	LEU
3	H	6	HIS
3	H	20	MET
3	H	31	VAL
3	H	35	THR
3	H	36	LEU
3	H	42	LEU
3	H	53	LEU
3	H	57	GLU
3	H	64	LEU
3	H	72	ARG
3	H	85	LEU
3	H	86	LEU
3	H	111	SER
3	H	140	LEU
3	H	144	LEU
3	H	147	LEU
4	I	28	LEU
4	I	29	ASN
4	I	58	ASP
4	I	80	VAL
4	I	95	SER
4	I	97	ASP
4	I	123	LEU
4	I	168	ILE
5	J	478	SER
5	J	512	LYS
5	J	547	LEU
5	J	551	SER
5	J	552	SER
5	J	555	GLN
5	J	568	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	H	137	GLN
4	I	30	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 ⓘ

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	113/128 (88%)	0.19	9 (7%) 12 6	19, 36, 76, 92	0
1	F	111/128 (86%)	0.25	6 (5%) 25 17	15, 34, 75, 107	0
2	B	113/114 (99%)	-0.55	1 (0%) 84 80	6, 14, 28, 59	0
2	G	113/114 (99%)	-0.50	2 (1%) 68 61	8, 14, 30, 70	0
3	C	149/151 (98%)	-0.42	2 (1%) 77 72	12, 27, 47, 94	0
3	H	149/151 (98%)	-0.42	2 (1%) 77 72	11, 23, 44, 88	0
4	D	181/208 (87%)	-0.34	4 (2%) 62 52	8, 16, 49, 105	0
4	I	181/208 (87%)	-0.43	2 (1%) 80 75	7, 16, 46, 89	0
5	E	116/130 (89%)	-0.29	2 (1%) 70 63	9, 24, 51, 60	0
5	J	116/130 (89%)	-0.17	2 (1%) 70 63	9, 26, 56, 65	0
All	All	1342/1462 (91%)	-0.29	32 (2%) 59 49	6, 23, 58, 107	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	748	ARG	6.5
4	I	25	ILE	5.7
1	F	750	VAL	4.9
4	D	26	ASP	4.2
2	G	2	GLU	3.8
3	H	150	ASP	3.6
3	C	149	GLY	3.5
4	D	27	ASP	3.3
2	G	3	ARG	3.3
1	A	776	LYS	3.2
1	A	671	VAL	3.1
1	A	777	LYS	3.1
1	A	669	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	2	GLU	2.9
3	H	149	GLY	2.7
5	E	577	ASN	2.7
1	A	750	VAL	2.7
1	A	668	GLU	2.7
3	C	150	ASP	2.6
4	D	127	GLY	2.5
5	E	462	SER	2.4
1	F	776	LYS	2.4
5	J	554	GLN	2.4
5	J	461	ASN	2.3
1	F	722	LYS	2.3
1	A	779	ALA	2.2
1	A	772	GLU	2.2
1	A	774	ALA	2.2
4	I	131	GLU	2.1
1	F	754	GLN	2.1
4	D	56	HIS	2.0
1	F	671	VAL	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 monosaccharides 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.