



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 05:22 am BST

PDB ID : 4LP7
Title : Crystal structure of the human metapneumovirus matrix protein
Authors : Leyrat, C.; Harlos, K.; Grimes, J.M.
Deposited on : 2013-07-15
Resolution : 2.83 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 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 : 2.11
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) : 2.11

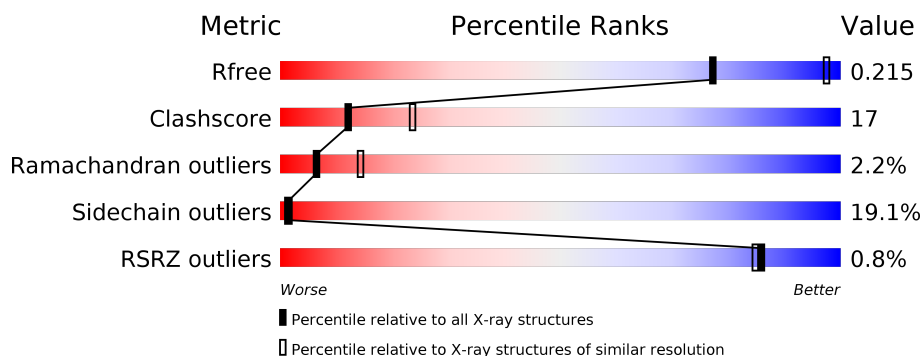
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.83 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	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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 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	254	<div> <div>52%</div> <div>29%</div> <div>• •</div> <div>14%</div> </div>
1	B	254	<div> <div>52%</div> <div>31%</div> <div>• •</div> <div>11%</div> </div>
1	C	254	<div> <div>2%</div> <div>52%</div> <div>35%</div> <div>• •</div> <div>10%</div> </div>
1	D	254	<div> <div>%</div> <div>57%</div> <div>30%</div> <div>•</div> <div>9%</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7114 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 Matrix protein M.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	0	0	0
			1689	1094	267	318	10			
1	B	225	Total	C	N	O	S	0	0	0
			1730	1120	274	325	11			
1	C	229	Total	C	N	O	S	0	0	0
			1756	1135	277	334	10			
1	D	230	Total	C	N	O	S	0	0	0
			1760	1137	278	335	10			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		
2	D	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Cl	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	42	Total	O	0	0
			42	42		

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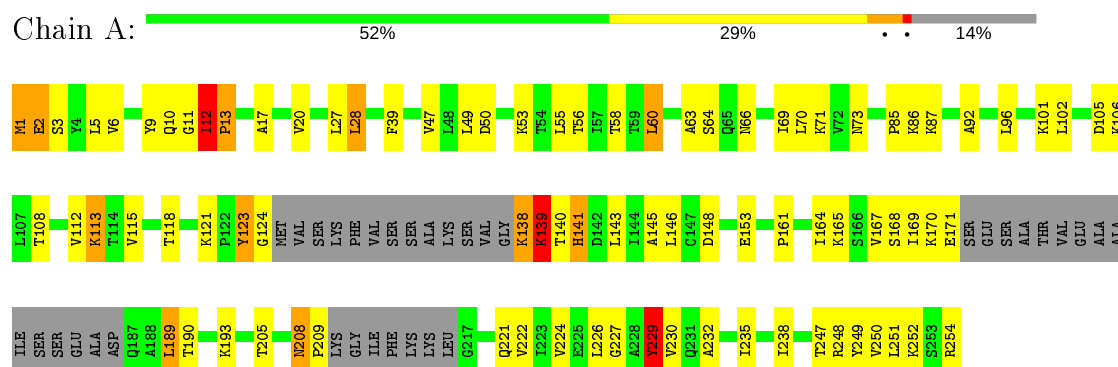
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	37	Total 37	O 37	0	0
4	C	49	Total 49	O 49	0	0
4	D	46	Total 46	O 46	0	0

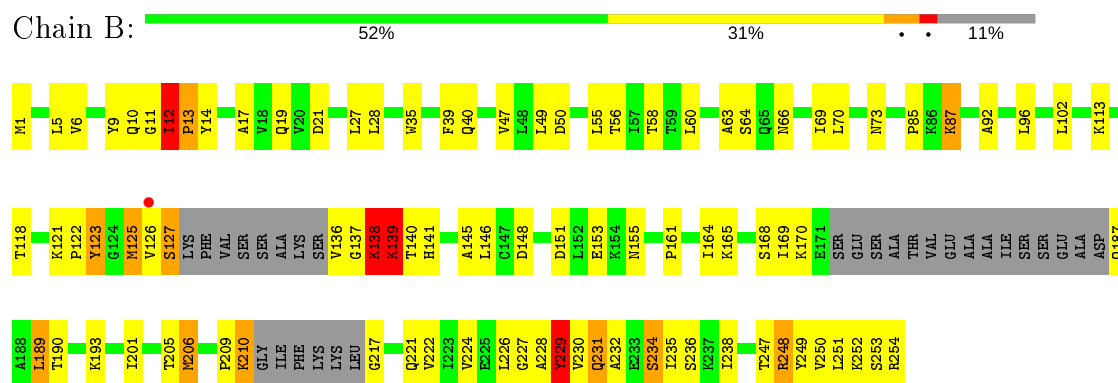
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

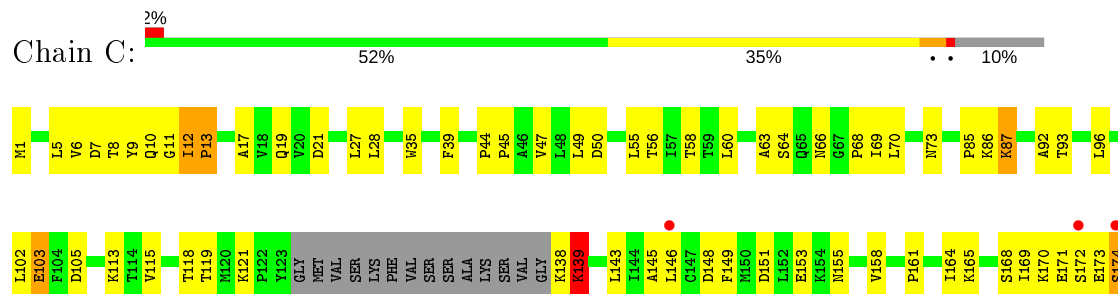
• Molecule 1: Matrix protein M



• Molecule 1: Matrix protein M

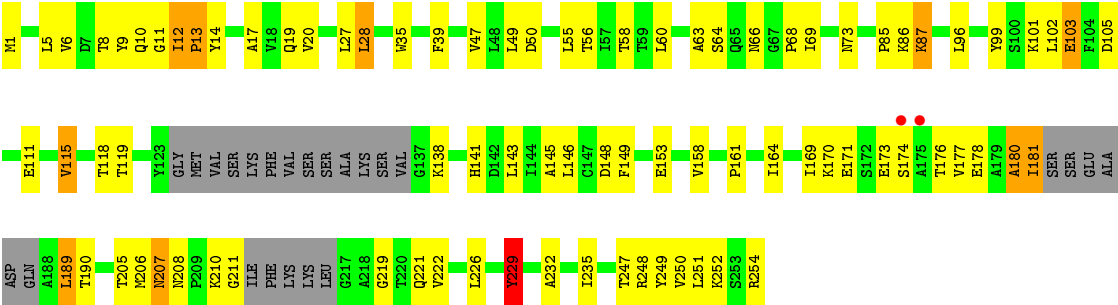


• Molecule 1: Matrix protein M





● Molecule 1: Matrix protein M



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	62.01Å 62.01Å 275.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	53.70 – 2.83 52.71 – 2.83	Depositor EDS
% Data completeness (in resolution range)	99.0 (53.70-2.83) 99.5 (52.71-2.83)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	0.20	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.81Å)	Xtriage
Refinement program	BUSTER-TNT, BUSTER 2.11.2	Depositor
R, R_{free}	0.185 , 0.229 0.189 , 0.215	Depositor DCC
R_{free} test set	1403 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	70.4	Xtriage
Anisotropy	0.595	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 66.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.468 for -h,-k,l 0.469 for h,-h-k,-l 0.468 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7114	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, CL

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	0.60	0/1719	0.87	0/2336
1	B	0.60	0/1760	0.88	1/2390 (0.0%)
1	C	0.57	0/1786	0.88	0/2427
1	D	0.59	0/1790	0.89	0/2432
All	All	0.59	0/7055	0.88	1/9585 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	248	ARG	NE-CZ-NH1	-5.27	117.66	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	12	ILE	Mainchain
1	B	12	ILE	Mainchain

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	1689	0	1750	53	0
1	B	1730	0	1799	83	3
1	C	1756	0	1820	61	0
1	D	1760	0	1823	68	3
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	D	1	0	0	1	0
4	A	42	0	0	2	0
4	B	37	0	0	4	0
4	C	49	0	0	5	0
4	D	46	0	0	2	0
All	All	7114	0	7192	242	3

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 17.

All (242) 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:B:229:TYR:HB2	1:D:229:TYR:CD2	1.29	1.57
1:B:226:LEU:O	1:B:229:TYR:CE2	1.76	1.38
1:B:229:TYR:CB	1:D:229:TYR:HD2	1.35	1.36
1:D:180:ALA:N	1:D:210:LYS:HD3	1.57	1.16
1:B:229:TYR:CB	1:D:229:TYR:CD2	2.17	1.15
1:D:180:ALA:H	1:D:210:LYS:HD3	0.98	1.12
1:B:226:LEU:O	1:B:229:TYR:CZ	2.04	1.11
1:B:138:LYS:HA	1:B:168:SER:OG	1.50	1.09
1:A:140:THR:O	1:A:167:VAL:O	1.79	1.01
1:B:229:TYR:HB3	4:B:432:HOH:O	1.61	0.98
1:C:181:ILE:HA	1:C:210:LYS:HG3	1.45	0.97
1:D:180:ALA:H	1:D:210:LYS:CD	1.78	0.96
1:D:176:THR:HG22	1:D:177:VAL:H	1.35	0.92
1:B:226:LEU:O	1:B:229:TYR:HE2	1.35	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:GLY:O	1:B:138:LYS:HD3	1.70	0.90
1:B:137:GLY:C	1:B:138:LYS:HD3	1.91	0.90
1:C:169:ILE:HB	1:C:172:SER:HB3	1.54	0.89
1:B:226:LEU:O	1:B:229:TYR:OH	1.92	0.86
1:D:180:ALA:CA	1:D:210:LYS:HD3	2.05	0.86
1:B:138:LYS:O	1:B:138:LYS:NZ	2.08	0.85
1:C:139:LYS:HD3	1:C:139:LYS:H	1.40	0.84
1:C:138:LYS:O	1:C:138:LYS:HG2	1.78	0.84
1:B:121:LYS:HZ1	1:B:123:TYR:HB3	1.43	0.83
1:B:229:TYR:HB2	1:D:229:TYR:CE2	2.09	0.83
1:B:138:LYS:HA	1:B:168:SER:CB	2.10	0.80
1:B:121:LYS:NZ	1:B:123:TYR:HB3	1.96	0.80
1:B:138:LYS:CA	1:B:168:SER:OG	2.29	0.80
1:B:138:LYS:O	1:B:139:LYS:HB2	1.82	0.79
1:A:205:THR:HG22	1:A:221:GLN:HG2	1.63	0.79
1:D:141:HIS:HE1	1:D:174:SER:HA	1.50	0.77
1:A:9:TYR:HE1	1:A:11:GLY:HA3	1.51	0.76
1:A:139:LYS:N	1:A:168:SER:OG	2.20	0.75
1:D:180:ALA:HA	1:D:210:LYS:HD3	1.69	0.74
1:B:137:GLY:O	1:B:138:LYS:HB3	1.87	0.74
1:D:207:ASN:HD22	1:D:208:ASN:H	1.36	0.73
1:B:229:TYR:OH	1:D:99:TYR:CE2	2.42	0.72
1:A:28:LEU:HD12	1:A:101:LYS:HG2	1.71	0.72
1:D:181:ILE:HA	1:D:211:GLY:HA3	1.71	0.72
1:B:138:LYS:O	1:B:139:LYS:CB	2.38	0.71
1:A:9:TYR:CE1	1:A:11:GLY:HA3	2.24	0.71
1:B:190:THR:OG1	1:B:247:THR:HG21	1.91	0.71
1:D:205:THR:HG22	1:D:221:GLN:HG2	1.72	0.71
1:A:138:LYS:C	1:A:139:LYS:HD3	2.11	0.71
1:D:189:LEU:O	1:D:207:ASN:ND2	2.17	0.71
1:C:205:THR:HG22	1:C:221:GLN:HG2	1.72	0.70
1:B:205:THR:HG22	1:B:221:GLN:HG2	1.71	0.70
1:C:209:PRO:HG3	1:C:218:ALA:N	2.07	0.70
1:C:139:LYS:HD3	1:C:139:LYS:N	2.04	0.69
1:B:206:MET:CE	1:B:209:PRO:HB3	2.23	0.69
1:C:190:THR:OG1	1:C:247:THR:HG21	1.94	0.68
1:D:145:ALA:HB2	1:D:164:ILE:HD11	1.75	0.68
1:A:145:ALA:HB2	1:A:164:ILE:HD11	1.75	0.67
1:C:170:LYS:O	1:C:171:GLU:HG2	1.95	0.67
1:D:141:HIS:CE1	1:D:174:SER:HA	2.31	0.66
1:A:190:THR:HG22	4:A:435:HOH:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:ALA:HB2	1:C:164:ILE:HD11	1.78	0.66
1:B:145:ALA:HB2	1:B:164:ILE:HD11	1.76	0.65
1:B:137:GLY:O	1:B:138:LYS:CB	2.44	0.65
1:B:229:TYR:CA	1:D:229:TYR:CD2	2.80	0.64
1:A:190:THR:OG1	1:A:247:THR:HG21	1.97	0.64
1:D:190:THR:OG1	1:D:247:THR:HG21	1.97	0.64
1:B:137:GLY:HA3	4:B:431:HOH:O	1.98	0.63
1:C:180:ALA:O	1:C:181:ILE:HG23	1.99	0.63
1:B:139:LYS:N	1:B:168:SER:OG	2.32	0.62
1:A:226:LEU:O	1:A:229:TYR:HE2	1.83	0.62
1:C:170:LYS:HE3	1:C:171:GLU:OE2	1.99	0.62
1:C:12:ILE:HG13	1:C:13:PRO:HD3	1.83	0.60
1:C:209:PRO:HD3	4:C:444:HOH:O	2.00	0.60
1:D:12:ILE:CG1	1:D:13:PRO:HD3	2.32	0.60
1:D:12:ILE:HG13	1:D:13:PRO:HD3	1.84	0.60
1:D:232:ALA:HA	1:D:235:ILE:HD12	1.83	0.60
1:B:12:ILE:CG1	1:B:13:PRO:HD3	2.31	0.60
1:A:12:ILE:CG1	1:A:13:PRO:HD3	2.31	0.60
1:D:8:THR:OG1	1:D:119:THR:O	2.19	0.60
1:A:12:ILE:HG13	1:A:13:PRO:HD3	1.83	0.59
1:B:206:MET:HE3	1:B:209:PRO:HB3	1.83	0.59
1:C:12:ILE:CG1	1:C:13:PRO:HD3	2.32	0.59
1:A:232:ALA:HA	1:A:235:ILE:HD12	1.84	0.59
1:A:140:THR:OG1	1:A:141:HIS:N	2.35	0.59
1:B:12:ILE:HG13	1:B:13:PRO:HD3	1.83	0.59
1:B:229:TYR:OH	1:D:99:TYR:HE2	1.83	0.59
1:A:17:ALA:HB3	1:A:118:THR:HB	1.85	0.59
1:C:232:ALA:HA	1:C:235:ILE:HD12	1.85	0.59
1:D:28:LEU:HD12	1:D:101:LYS:HG2	1.85	0.58
1:C:181:ILE:HA	1:C:210:LYS:CG	2.27	0.58
1:A:123:TYR:HD1	1:A:124:GLY:H	1.52	0.58
1:C:181:ILE:O	1:C:210:LYS:NZ	2.30	0.58
1:C:180:ALA:HB2	1:C:211:GLY:O	2.04	0.57
1:A:190:THR:HG21	1:A:249:TYR:OH	2.03	0.57
1:C:190:THR:HG21	1:C:249:TYR:OH	2.04	0.57
1:B:17:ALA:HB3	1:B:118:THR:HB	1.87	0.57
1:D:190:THR:HG21	1:D:249:TYR:OH	2.05	0.56
1:B:229:TYR:N	1:B:229:TYR:HD2	2.03	0.56
1:C:17:ALA:HB3	1:C:118:THR:HB	1.87	0.56
1:B:229:TYR:N	1:B:229:TYR:CD2	2.74	0.56
1:C:103:GLU:HB2	4:C:423:HOH:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:ILE:CA	1:C:210:LYS:HG3	2.27	0.56
1:D:17:ALA:HB3	1:D:118:THR:HB	1.87	0.56
1:D:14:TYR:CD1	1:D:119:THR:HG22	2.42	0.55
1:B:9:TYR:CE2	1:B:11:GLY:HA3	2.41	0.55
1:D:64:SER:HB3	1:D:69:ILE:HG12	1.88	0.55
1:C:209:PRO:HG3	1:C:218:ALA:CA	2.37	0.55
1:B:190:THR:HG21	1:B:249:TYR:OH	2.06	0.55
1:C:64:SER:HB3	1:C:69:ILE:HG12	1.89	0.55
1:D:180:ALA:HA	1:D:210:LYS:CD	2.35	0.55
1:D:180:ALA:HA	1:D:210:LYS:CG	2.36	0.55
1:A:70:LEU:HG	1:A:92:ALA:HB2	1.89	0.55
1:D:176:THR:CG2	1:D:177:VAL:H	2.14	0.54
1:B:64:SER:HB3	1:B:69:ILE:HG12	1.89	0.54
1:B:137:GLY:O	1:B:138:LYS:CD	2.50	0.54
1:B:230:VAL:HG23	1:B:234:SER:HB2	1.89	0.54
1:B:231:GLN:O	1:B:234:SER:N	2.41	0.54
1:B:40:GLN:HG2	1:B:127:SER:C	2.28	0.54
1:D:176:THR:HG22	1:D:177:VAL:N	2.16	0.53
1:B:209:PRO:HG2	1:B:217:GLY:HA2	1.90	0.53
1:D:141:HIS:CD2	1:D:169:ILE:HD12	2.44	0.53
1:A:60:LEU:HD23	1:A:71:LYS:HB2	1.91	0.53
1:B:121:LYS:NZ	1:B:123:TYR:CB	2.70	0.53
1:A:64:SER:HB3	1:A:69:ILE:HG12	1.90	0.53
1:C:12:ILE:HG13	1:C:13:PRO:CD	2.40	0.52
1:A:12:ILE:HG13	1:A:13:PRO:CD	2.40	0.52
1:B:231:GLN:CB	1:B:234:SER:OG	2.58	0.52
1:B:230:VAL:CG2	1:B:234:SER:HB2	2.40	0.52
1:D:12:ILE:HG13	1:D:13:PRO:CD	2.40	0.51
1:A:2:GLU:HB3	1:A:113:LYS:O	2.10	0.51
1:B:12:ILE:HG13	1:B:13:PRO:CD	2.40	0.51
1:D:148:ASP:OD2	1:D:248:ARG:HD3	2.10	0.51
1:B:148:ASP:OD2	1:B:248:ARG:HD3	2.11	0.51
1:C:207:ASN:HB3	4:C:441:HOH:O	2.11	0.51
1:B:189:LEU:HD23	4:B:430:HOH:O	2.10	0.50
1:B:19:GLN:HG3	1:B:35:TRP:HB3	1.92	0.50
1:A:148:ASP:OD2	1:A:248:ARG:HD3	2.11	0.50
1:A:121:LYS:H	1:A:221:GLN:NE2	2.10	0.50
1:D:103:GLU:HB2	4:D:437:HOH:O	2.12	0.50
1:C:229:TYR:C	1:C:229:TYR:CD1	2.85	0.50
1:D:9:TYR:CE1	1:D:11:GLY:HA3	2.47	0.50
1:B:229:TYR:HH	1:D:99:TYR:HE2	1.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:TYR:C	1:C:229:TYR:HD1	2.15	0.49
1:B:140:THR:OG1	1:B:141:HIS:HD2	1.95	0.49
1:D:206:MET:O	1:D:219:GLY:HA2	2.12	0.49
1:B:209:PRO:CG	1:B:217:GLY:HA2	2.43	0.49
1:B:229:TYR:OH	1:D:99:TYR:CZ	2.57	0.49
1:A:9:TYR:CD2	1:A:121:LYS:HA	2.49	0.48
1:B:63:ALA:HB2	1:D:161:PRO:HB2	1.95	0.48
1:B:229:TYR:HB2	1:D:229:TYR:HD2	0.54	0.48
1:B:161:PRO:HB2	1:D:63:ALA:HB2	1.95	0.48
1:A:121:LYS:H	1:A:221:GLN:HE22	1.59	0.48
1:A:141:HIS:CD2	1:A:169:ILE:HD12	2.49	0.48
1:B:137:GLY:CA	4:B:431:HOH:O	2.60	0.48
1:A:106:LYS:NZ	4:A:415:HOH:O	2.47	0.48
1:C:209:PRO:HG3	1:C:218:ALA:H	1.78	0.47
1:C:190:THR:HA	1:C:207:ASN:ND2	2.29	0.47
1:D:181:ILE:HD12	1:D:210:LYS:O	2.13	0.47
1:A:161:PRO:HB2	1:C:63:ALA:HB2	1.95	0.47
1:D:19:GLN:HG3	1:D:35:TRP:HB3	1.96	0.47
1:B:138:LYS:C	1:B:168:SER:OG	2.53	0.47
1:C:21:ASP:HB3	1:C:113:LYS:HE3	1.97	0.47
1:D:181:ILE:HA	1:D:211:GLY:CA	2.43	0.47
1:D:226:LEU:O	3:D:301:CL:CL	2.69	0.47
1:A:1:MET:SD	1:A:1:MET:O	2.73	0.47
1:A:252:LYS:HE3	1:C:105:ASP:OD2	2.14	0.47
1:A:238:ILE:HD13	1:C:96:LEU:HD22	1.96	0.47
1:C:8:THR:OG1	1:C:119:THR:O	2.30	0.47
1:A:20:VAL:HG12	1:A:115:VAL:HG13	1.97	0.47
1:B:229:TYR:OH	1:D:99:TYR:OH	2.09	0.46
1:C:121:LYS:H	1:C:221:GLN:NE2	2.13	0.46
1:C:148:ASP:OD2	1:C:248:ARG:HD3	2.16	0.46
1:C:229:TYR:O	1:C:230:VAL:HB	2.15	0.46
1:C:19:GLN:HG3	1:C:35:TRP:HB3	1.96	0.46
1:A:3:SER:OG	1:A:53:LYS:HE3	2.14	0.46
1:A:189:LEU:O	1:A:189:LEU:HD13	2.16	0.46
1:C:9:TYR:CE2	1:C:11:GLY:HA3	2.50	0.46
1:D:229:TYR:C	1:D:229:TYR:CD1	2.90	0.46
1:B:138:LYS:HA	1:B:168:SER:HG	1.70	0.45
1:B:87:LYS:HB2	1:B:87:LYS:HE2	1.79	0.45
1:D:176:THR:HG22	1:D:177:VAL:HG12	1.98	0.45
1:B:227:GLY:C	1:B:229:TYR:CD2	2.89	0.45
1:B:231:GLN:HB3	1:B:234:SER:OG	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:ASP:OD1	1:D:248:ARG:NH1	2.50	0.45
1:C:180:ALA:HB1	1:C:210:LYS:O	2.17	0.45
1:B:121:LYS:HZ2	1:B:123:TYR:CB	2.28	0.45
1:B:187:GLN:HB2	1:B:210:LYS:HD3	1.97	0.45
1:C:252:LYS:HD3	4:C:413:HOH:O	2.16	0.45
1:B:226:LEU:C	1:B:229:TYR:HE2	2.12	0.45
1:D:87:LYS:HE2	1:D:87:LYS:HB2	1.85	0.45
1:A:112:VAL:HG11	1:A:115:VAL:HG22	1.99	0.45
1:D:181:ILE:CD1	1:D:181:ILE:H	2.30	0.45
1:B:21:ASP:HB3	1:B:113:LYS:HE3	1.98	0.44
1:A:63:ALA:HB2	1:C:161:PRO:HB2	1.99	0.44
1:A:96:LEU:HD22	1:C:238:ILE:HD13	2.00	0.44
1:C:151:ASP:O	1:C:155:ASN:N	2.50	0.44
1:B:141:HIS:CD2	1:B:169:ILE:HD12	2.53	0.44
1:B:206:MET:HE2	1:B:209:PRO:HB3	1.97	0.44
1:A:138:LYS:N	1:A:139:LYS:HE2	2.33	0.44
1:C:138:LYS:N	1:C:168:SER:HG	2.15	0.44
1:B:228:ALA:O	1:B:230:VAL:N	2.51	0.44
1:A:227:GLY:HA3	1:A:229:TYR:CE2	2.53	0.43
1:B:252:LYS:HE3	1:D:105:ASP:OD2	2.18	0.43
1:D:141:HIS:HE1	1:D:174:SER:CA	2.26	0.43
1:D:39:PHE:CD1	1:D:85:PRO:HD3	2.52	0.43
1:C:178:GLU:CD	1:C:179:ALA:O	2.56	0.43
1:C:148:ASP:OD1	1:C:248:ARG:NH1	2.52	0.43
1:A:39:PHE:CD1	1:A:85:PRO:HD3	2.53	0.43
1:B:232:ALA:HA	1:B:235:ILE:HD12	2.00	0.43
1:B:58:THR:HG22	1:B:73:ASN:HB2	1.99	0.43
1:A:226:LEU:O	1:A:229:TYR:CE2	2.67	0.43
1:C:121:LYS:H	1:C:221:GLN:HE22	1.64	0.43
1:A:140:THR:HG23	1:A:141:HIS:HD2	1.84	0.43
1:D:207:ASN:HD22	1:D:208:ASN:N	2.11	0.43
1:B:151:ASP:O	1:B:155:ASN:N	2.51	0.42
1:C:44:PRO:HA	1:C:45:PRO:HD3	1.94	0.42
1:C:58:THR:HG22	1:C:73:ASN:HB2	2.01	0.42
1:A:208:ASN:HD22	1:A:209:PRO:HD2	1.84	0.42
1:A:224:VAL:HG13	1:C:68:PRO:HD3	2.01	0.42
1:C:87:LYS:HE2	1:C:87:LYS:HB2	1.81	0.42
1:B:224:VAL:HG13	1:D:68:PRO:HD3	2.02	0.42
1:D:14:TYR:CE1	1:D:119:THR:HG22	2.55	0.42
1:D:180:ALA:HA	1:D:210:LYS:HG2	2.01	0.42
1:D:58:THR:HG22	1:D:73:ASN:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ASP:OD2	1:C:252:LYS:HE3	2.19	0.42
1:C:70:LEU:HG	1:C:92:ALA:HB2	2.01	0.41
1:A:58:THR:HG22	1:A:73:ASN:HB2	2.02	0.41
1:B:14:TYR:HA	1:B:122:PRO:HD3	2.02	0.41
1:A:148:ASP:OD1	1:A:248:ARG:NH1	2.53	0.41
1:B:238:ILE:HD12	1:D:96:LEU:HD22	2.02	0.41
1:B:13:PRO:O	1:B:13:PRO:HD2	2.21	0.41
1:D:149:PHE:HB2	1:D:158:VAL:HG13	2.03	0.41
1:C:209:PRO:CD	4:C:444:HOH:O	2.66	0.41
1:A:140:THR:O	1:A:141:HIS:O	2.38	0.41
1:C:164:ILE:HG22	1:C:165:LYS:HG2	2.03	0.41
1:C:139:LYS:N	1:C:168:SER:OG	2.54	0.41
1:D:247:THR:HG22	4:D:422:HOH:O	2.21	0.41
1:A:106:LYS:O	1:A:108:THR:HG23	2.21	0.41
1:A:229:TYR:O	1:A:230:VAL:HB	2.21	0.40
1:C:39:PHE:CD1	1:C:85:PRO:HD3	2.56	0.40
1:B:227:GLY:C	1:B:229:TYR:HD2	2.25	0.40
1:D:13:PRO:HD2	1:D:13:PRO:O	2.22	0.40
1:A:170:LYS:NZ	1:A:171:GLU:OE2	2.52	0.40
1:B:39:PHE:CD1	1:B:85:PRO:HD3	2.55	0.40
1:C:149:PHE:HB2	1:C:158:VAL:HG13	2.04	0.40
1:D:20:VAL:HG12	1:D:115:VAL:HG13	2.03	0.40
1:B:70:LEU:HG	1:B:92:ALA:HB2	2.03	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:VAL:N	1:D:170:LYS:NZ[1_655]	1.55	0.65
1:B:253:SER:OG	1:D:180:ALA:CB[1_655]	2.08	0.12
1:B:187:GLN:OE1	1:D:174:SER:O[1_655]	2.17	0.03

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	211/254 (83%)	194 (92%)	12 (6%)	5 (2%)	6	12
1	B	217/254 (85%)	201 (93%)	10 (5%)	6 (3%)	5	10
1	C	221/254 (87%)	201 (91%)	16 (7%)	4 (2%)	8	19
1	D	222/254 (87%)	205 (92%)	13 (6%)	4 (2%)	8	19
All	All	871/1016 (86%)	801 (92%)	51 (6%)	19 (2%)	6	14

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	HIS
1	B	126	VAL
1	B	138	LYS
1	B	139	LYS
1	B	229	TYR
1	C	139	LYS
1	D	173	GLU
1	A	2	GLU
1	A	139	LYS
1	A	229	TYR
1	C	229	TYR
1	D	229	TYR
1	B	125	MET
1	D	180	ALA
1	C	174	SER
1	B	13	PRO
1	C	13	PRO
1	D	13	PRO
1	A	13	PRO

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	188/216 (87%)	155 (82%)	33 (18%)	2	2
1	B	193/216 (89%)	154 (80%)	39 (20%)	1	1
1	C	195/216 (90%)	155 (80%)	40 (20%)	1	1
1	D	195/216 (90%)	160 (82%)	35 (18%)	2	2
All	All	771/864 (89%)	624 (81%)	147 (19%)	1	1

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	5	LEU
1	A	6	VAL
1	A	10	GLN
1	A	12	ILE
1	A	27	LEU
1	A	28	LEU
1	A	47	VAL
1	A	49	LEU
1	A	50	ASP
1	A	55	LEU
1	A	56	THR
1	A	60	LEU
1	A	66	ASN
1	A	86	LYS
1	A	87	LYS
1	A	102	LEU
1	A	113	LYS
1	A	123	TYR
1	A	138	LYS
1	A	139	LYS
1	A	143	LEU
1	A	146	LEU
1	A	153	GLU
1	A	165	LYS
1	A	189	LEU
1	A	193	LYS
1	A	208	ASN
1	A	222	VAL
1	A	229	TYR
1	A	250	VAL
1	A	251	LEU
1	A	254	ARG

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Mol	Chain	Res	Type
1	B	1	MET
1	B	5	LEU
1	B	6	VAL
1	B	10	GLN
1	B	12	ILE
1	B	27	LEU
1	B	28	LEU
1	B	47	VAL
1	B	49	LEU
1	B	50	ASP
1	B	55	LEU
1	B	56	THR
1	B	60	LEU
1	B	66	ASN
1	B	87	LYS
1	B	96	LEU
1	B	102	LEU
1	B	123	TYR
1	B	125	MET
1	B	127	SER
1	B	138	LYS
1	B	139	LYS
1	B	146	LEU
1	B	153	GLU
1	B	165	LYS
1	B	170	LYS
1	B	189	LEU
1	B	193	LYS
1	B	201	ILE
1	B	206	MET
1	B	210	LYS
1	B	222	VAL
1	B	229	TYR
1	B	231	GLN
1	B	234	SER
1	B	236	SER
1	B	250	VAL
1	B	251	LEU
1	B	254	ARG
1	C	1	MET
1	C	5	LEU
1	C	6	VAL

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Mol	Chain	Res	Type
1	C	7	ASP
1	C	10	GLN
1	C	12	ILE
1	C	27	LEU
1	C	28	LEU
1	C	47	VAL
1	C	49	LEU
1	C	50	ASP
1	C	55	LEU
1	C	56	THR
1	C	60	LEU
1	C	66	ASN
1	C	86	LYS
1	C	87	LYS
1	C	93	THR
1	C	102	LEU
1	C	103	GLU
1	C	115	VAL
1	C	139	LYS
1	C	143	LEU
1	C	146	LEU
1	C	153	GLU
1	C	173	GLU
1	C	174	SER
1	C	176	THR
1	C	178	GLU
1	C	181	ILE
1	C	189	LEU
1	C	193	LYS
1	C	206	MET
1	C	208	ASN
1	C	210	LYS
1	C	222	VAL
1	C	229	TYR
1	C	250	VAL
1	C	251	LEU
1	C	254	ARG
1	D	1	MET
1	D	5	LEU
1	D	6	VAL
1	D	10	GLN
1	D	12	ILE

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Mol	Chain	Res	Type
1	D	27	LEU
1	D	28	LEU
1	D	47	VAL
1	D	49	LEU
1	D	50	ASP
1	D	55	LEU
1	D	56	THR
1	D	60	LEU
1	D	66	ASN
1	D	86	LYS
1	D	87	LYS
1	D	102	LEU
1	D	103	GLU
1	D	111	GLU
1	D	115	VAL
1	D	138	LYS
1	D	143	LEU
1	D	146	LEU
1	D	153	GLU
1	D	171	GLU
1	D	178	GLU
1	D	181	ILE
1	D	189	LEU
1	D	207	ASN
1	D	222	VAL
1	D	229	TYR
1	D	250	VAL
1	D	251	LEU
1	D	252	LYS
1	D	254	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	141	HIS
1	A	187	GLN
1	A	208	ASN
1	A	221	GLN
1	A	244	HIS
1	B	19	GLN
1	B	141	HIS

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Mol	Chain	Res	Type
1	C	19	GLN
1	C	141	HIS
1	C	208	ASN
1	C	221	GLN
1	D	19	GLN
1	D	141	HIS

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 ⓘ

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	219/254 (86%)	-0.23	0 100 100	58, 82, 124, 188	0
1	B	225/254 (88%)	-0.23	1 (0%) 92 91	55, 82, 131, 261	0
1	C	229/254 (90%)	-0.18	4 (1%) 70 66	59, 83, 131, 168	0
1	D	230/254 (90%)	-0.15	2 (0%) 84 83	57, 83, 132, 185	0
All	All	903/1016 (88%)	-0.20	7 (0%) 86 85	55, 83, 130, 261	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	175	ALA	7.2
1	C	175	ALA	5.9
1	B	126	VAL	3.3
1	C	172	SER	3.1
1	D	174	SER	2.9
1	C	174	SER	2.3
1	C	146	LEU	2.2

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 carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CL	D	301	1/1	0.97	0.18	115,115,115,115	0
2	CA	C	301	1/1	0.99	0.10	79,79,79,79	0
2	CA	A	301	1/1	0.99	0.14	70,70,70,70	0
2	CA	B	301	1/1	0.99	0.14	69,69,69,69	0
2	CA	D	302	1/1	1.00	0.11	74,74,74,74	0

6.5 Other polymers

There are no such residues in this entry.