WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2023 – 04:08 PM JST

PDB ID	:	6JKY
Title	:	Crystal structure of MvcA-UBE2N-Ub complex from Legionella pneumophila
Authors	:	Ouyang, S.Y.; Guan, H.
Deposited on	:	2019-03-03
Resolution	:	2.45 Å(reported)

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

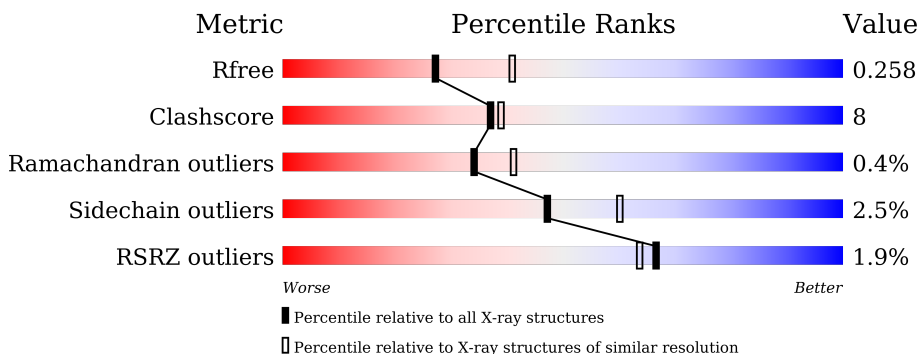|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.45 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	Percentile Ranks	Value
Rfree		0.258
Clashscore		8
Ramachandran outliers		0.4%
Sidechain outliers		2.5%
RSRZ outliers		1.9%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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% 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	385	82% 18%
1	D	385	% 79% 19% ••
2	B	152	6% 79% 16% • •
2	E	152	6% 66% 30% • •
3	C	79	% 84% 13% •
3	F	79	84% 10% • 5%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 9776 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 MvcA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	384	Total 3091	C 1967	N 514	O 596	S 14	0	0	0
1	D	381	Total 3069	C 1954	N 511	O 590	S 14	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	ALA	-	expression tag	UNP Q5ZTL3
A	12	SER	-	expression tag	UNP Q5ZTL3
A	83	ALA	CYS	engineered mutation	UNP Q5ZTL3
D	11	ALA	-	expression tag	UNP Q5ZTL3
D	12	SER	-	expression tag	UNP Q5ZTL3
D	83	ALA	CYS	engineered mutation	UNP Q5ZTL3

- Molecule 2 is a protein called Ubiquitin-conjugating enzyme E2 N.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	149	Total 1179	C 757	N 203	O 215	S 4	0	0	0
2	E	148	Total 1174	C 754	N 202	O 214	S 4	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	94	ALA	LYS	engineered mutation	UNP P61088
E	94	ALA	LYS	engineered mutation	UNP P61088

- Molecule 3 is a protein called Ub.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	76	Total 602	C 379	N 104	O 118	S 1	0	0	0
3	F	75	Total 598	C 377	N 103	O 117	S 1	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	CYS	-	expression tag	UNP A0A3P7ZMV6
C	-1	GLY	-	expression tag	UNP A0A3P7ZMV6
C	0	SER	-	expression tag	UNP A0A3P7ZMV6
F	-2	CYS	-	expression tag	UNP A0A3P7ZMV6
F	-1	GLY	-	expression tag	UNP A0A3P7ZMV6
F	0	SER	-	expression tag	UNP A0A3P7ZMV6

- Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	39	Total 39	O 39	0	0
4	B	5	Total 5	O 5	0	0
4	C	5	Total 5	O 5	0	0
4	D	10	Total 10	O 10	0	0
4	E	3	Total 3	O 3	0	0
4	F	1	Total 1	O 1	0	0

3 Residue-property plots ⓘ

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.
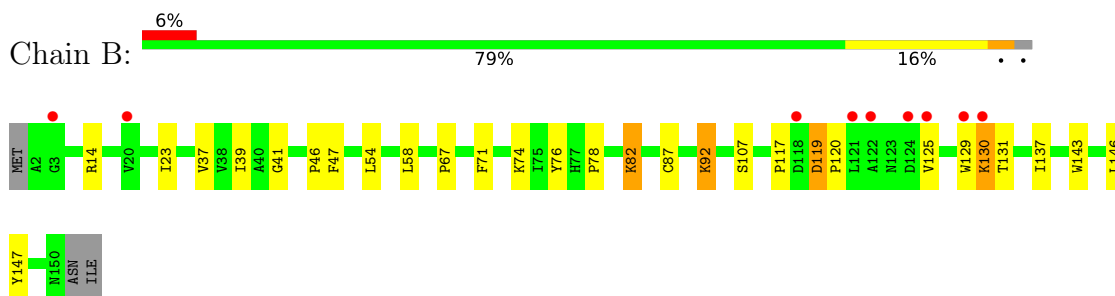
- Molecule 1: MvcA
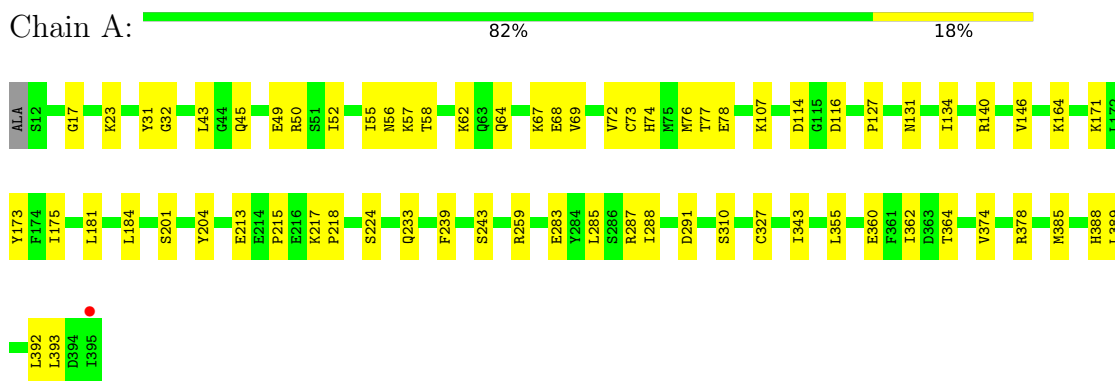
- Molecule 1: MvcA
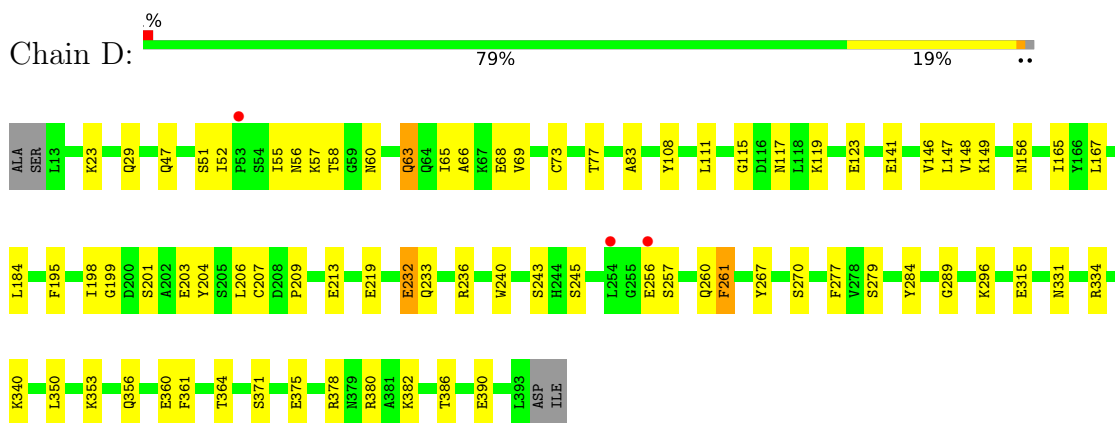
- Molecule 2: Ubiquitin-conjugating enzyme E2 N

- Molecule 2: Ubiquitin-conjugating enzyme E2 N

Chain E:

6%

66%   30%

MET ALA G3 L4 P5 R6 R7 I23 D28 E29 S30 N31 F35 H36 V37 V38 I39 A40 G41 P42 S45 P46 F47 T51 F52 K53 L54 E55 L56 F57 L58 M64 V69 R70 F71 M72 I75 P78 N79 V80 D81 R85 I86 C87 L88 D89 I90 L91 K92

L99 Q100 I101 L105 Q109 L112 N116 P117 D118 D119 E127 Q128 W129 E133 A134 Q135 E138 R141 L146 Y147 N150 ASN ILE

• Molecule 3: Ub

Chain C:

%

84%   13%

CYS G-1 S0 M1 K6 K11 E18 D39 R54 Y59 K63 L69 R74 GLY GLY

• Molecule 3: Ub

Chain F:

84%   10%   5%

CYS GLY S0 T22 V26 E51 T55 L56 S57 D58 Y59 N60 I61 R72 L73 R74 GLY GLY

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	104.33Å 107.61Å 263.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.14 – 2.45 65.14 – 2.45	Depositor EDS
% Data completeness (in resolution range)	96.4 (65.14-2.45) 96.4 (65.14-2.45)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.209 , 0.258 0.208 , 0.258	Depositor DCC
R_{free} test set	2639 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	58.5	Xtriage
Anisotropy	0.627	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 46.5	EDS
L-test for twinning[2]	$< |L| > = 0.46, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.067 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9776	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 3.28% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.26	0/3157	0.43	0/4258
1	D	0.26	0/3135	0.46	0/4228
2	B	0.33	0/1209	0.51	1/1648 (0.1%)
2	E	0.33	0/1204	0.61	1/1641 (0.1%)
3	C	0.32	0/608	0.48	0/817
3	F	0.41	0/604	0.52	0/812
All	All	0.29	0/9917	0.49	2/13404 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	92	LYS	CD-CE-NZ	6.95	127.69	111.70
2	E	92	LYS	CB-CG-CD	5.41	125.66	111.60

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	3091	0	3053	38	0
1	D	3069	0	3033	51	0
2	B	1179	0	1185	20	0
2	E	1174	0	1180	37	0
3	C	602	0	629	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	598	0	626	4	0
4	A	39	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	10	0	0	1	0
4	E	3	0	0	0	0
4	F	1	0	0	0	0
All	All	9776	0	9706	152	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 8.

All (152) 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)
2:E:56:LEU:HG	2:E:69:VAL:HG12	1.57	0.87
1:A:78:GLU:OE1	1:A:378:ARG:NH2	2.12	0.83
1:A:52:ILE:HD11	1:A:393:LEU:HD21	1.69	0.75
1:D:69:VAL:HG11	1:D:386:THR:HG22	1.67	0.74
1:A:134:ILE:HG12	1:A:343:ILE:CD1	2.19	0.72
2:B:46:PRO:HG3	2:B:137:ILE:HG23	1.71	0.72
1:D:47:GLN:NE2	1:D:51:SER:OG	2.23	0.71
2:E:146:LEU:HD12	2:E:147:TYR:CE2	2.24	0.71
2:E:79:ASN:ND2	2:E:119:ASP:OD2	2.23	0.71
2:E:146:LEU:HD12	2:E:147:TYR:CZ	2.27	0.70
2:E:58:LEU:HD21	2:E:101:ILE:HD11	1.75	0.69
1:D:199:GLY:O	1:D:204:TYR:OH	2.13	0.67
2:B:82:LYS:HD3	2:B:82:LYS:H	1.59	0.67
1:D:184:LEU:O	1:D:233:GLN:NE2	2.27	0.67
2:E:135:GLN:N	2:E:135:GLN:OE1	2.28	0.66
1:D:233:GLN:OE1	1:D:236:ARG:NH1	2.29	0.65
1:D:371:SER:O	1:D:375:GLU:HG2	1.96	0.65
1:D:65:ILE:O	1:D:69:VAL:HG13	1.97	0.65
1:A:217:LYS:HG2	1:A:218:PRO:HD2	1.78	0.64
2:E:55:GLU:OE2	2:E:70:ARG:NE	2.29	0.64
2:E:23:ILE:HG23	2:E:39:ILE:HG13	1.80	0.64
1:A:55:ILE:HD13	1:A:64:GLN:HB3	1.79	0.62
2:E:86:ILE:HG22	2:E:87:CYS:H	1.64	0.62
2:B:130:LYS:O	2:B:130:LYS:HD3	2.00	0.62
2:E:29:GLU:OE1	2:E:29:GLU:N	2.31	0.61
1:D:52:ILE:O	1:D:55:ILE:HG13	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ILE:HG12	1:A:343:ILE:HD13	1.81	0.61
2:B:119:ASP:HB3	2:B:120:PRO:HD2	1.81	0.61
2:B:119:ASP:HB3	2:B:120:PRO:CD	2.30	0.61
1:D:111:LEU:HD11	1:D:115:GLY:HA2	1.82	0.60
1:D:261:PHE:HE2	1:D:289:GLY:C	2.05	0.60
1:A:134:ILE:HG12	1:A:343:ILE:HD11	1.83	0.60
1:A:50:ARG:NH2	3:C:69:LEU:O	2.34	0.59
2:B:74:LYS:HE3	2:B:143:TRP:CZ3	2.37	0.59
1:D:256:GLU:O	1:D:256:GLU:HG2	2.03	0.59
2:E:56:LEU:HG	2:E:69:VAL:CG1	2.30	0.59
1:D:141:GLU:HG3	1:D:240:TRP:CZ3	2.38	0.58
1:D:66:ALA:HA	1:D:69:VAL:HG22	1.85	0.58
1:A:57:LYS:HE2	1:A:393:LEU:HD22	1.85	0.58
1:A:127:PRO:HB3	1:A:259:ARG:HD3	1.85	0.58
2:E:138:GLU:OE1	2:E:141:ARG:NH2	2.36	0.58
2:B:117:PRO:HB3	2:B:129:TRP:HB3	1.85	0.57
1:D:198:ILE:HG12	1:D:219:GLU:HG3	1.87	0.56
2:E:54:LEU:HD21	2:E:71:PHE:CZ	2.40	0.56
1:D:60:ASN:OD1	1:D:63:GLN:NE2	2.37	0.56
1:D:83:ALA:HB1	1:D:245:SER:O	2.04	0.56
2:E:42:PRO:O	2:E:45:SER:HB3	2.06	0.56
1:A:140:ARG:HG3	1:A:243:SER:HB2	1.87	0.55
1:D:296:LYS:NZ	1:D:315:GLU:OE2	2.36	0.55
2:B:54:LEU:HD13	2:B:71:PHE:HA	1.88	0.54
1:D:361:PHE:O	1:D:364:THR:HG22	2.07	0.54
1:D:260:GLN:O	1:D:261:PHE:CD2	2.61	0.54
1:D:209:PRO:O	1:D:213:GLU:HG2	2.08	0.54
1:A:175:ILE:HG12	1:A:181:LEU:HG	1.90	0.54
1:A:283:GLU:OE2	1:A:287:ARG:NH2	2.41	0.54
1:D:108:TYR:HB3	1:D:340:LYS:HB3	1.90	0.54
1:A:184:LEU:O	1:A:233:GLN:NE2	2.35	0.54
2:E:38:VAL:HA	2:E:52:PHE:O	2.08	0.53
2:B:146:LEU:HB3	2:B:147:TYR:CD1	2.43	0.53
2:E:87:CYS:O	2:E:88:LEU:HG	2.07	0.53
3:C:1:MET:HB2	3:C:63:LYS:HB3	1.90	0.53
1:A:68:GLU:O	1:A:72:VAL:HG22	2.09	0.53
1:A:23:LYS:HB3	1:A:355:LEU:HD13	1.91	0.53
2:B:76:TYR:HB2	2:B:143:TRP:CE3	2.44	0.53
1:D:261:PHE:CE2	1:D:289:GLY:C	2.82	0.53
3:F:51:GLU:HG2	3:F:59:TYR:OH	2.09	0.52
2:E:37:VAL:O	2:E:53:LYS:HA	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:87:CYS:SG	2:E:88:LEU:N	2.83	0.51
1:D:60:ASN:HB3	1:D:63:GLN:HG2	1.92	0.51
1:A:56:ASN:OD1	1:A:58:THR:OG1	2.22	0.51
1:D:146:VAL:HG13	1:D:203:GLU:HB3	1.91	0.51
3:C:-1:GLY:N	3:C:18:GLU:OE1	2.38	0.51
2:B:37:VAL:HB	2:B:54:LEU:HB2	1.93	0.51
1:D:147:LEU:HB2	1:D:206:LEU:HD11	1.92	0.50
1:D:51:SER:HB3	1:D:68:GLU:OE1	2.12	0.50
2:E:146:LEU:CD1	2:E:147:TYR:CZ	2.95	0.50
1:D:77:THR:HB	1:D:378:ARG:HD3	1.93	0.50
2:E:47:PHE:CE1	2:E:75:ILE:HD11	2.47	0.50
1:A:45:GLN:O	1:A:49:GLU:HG3	2.12	0.50
1:D:284:TYR:OH	4:D:401:HOH:O	2.19	0.49
2:E:54:LEU:HD21	2:E:71:PHE:CE2	2.47	0.49
2:B:82:LYS:H	2:B:82:LYS:CD	2.24	0.49
2:E:81:ASP:OD1	2:E:85:ARG:HG3	2.13	0.49
1:D:356:GLN:O	1:D:360:GLU:HG3	2.13	0.49
1:D:382:LYS:O	1:D:386:THR:HG23	2.13	0.48
1:A:52:ILE:HD11	1:A:393:LEU:CD2	2.40	0.48
1:A:285:LEU:O	1:A:288:ILE:HG12	2.13	0.48
2:E:6:ARG:O	2:E:6:ARG:HG3	2.12	0.48
1:A:114:ASP:OD1	1:A:114:ASP:N	2.47	0.48
1:D:55:ILE:HD13	1:D:57:LYS:HG2	1.95	0.48
1:D:119:LYS:O	1:D:123:GLU:HG2	2.13	0.48
1:A:74:HIS:O	1:A:74:HIS:CG	2.67	0.47
2:E:70:ARG:HH22	2:E:72:MET:HE1	1.80	0.47
2:E:28:ASP:HB3	2:E:31:ASN:O	2.15	0.47
1:A:171:LYS:HG2	1:A:173:TYR:CZ	2.49	0.47
3:C:54:ARG:NH1	3:C:59:TYR:OH	2.48	0.47
2:B:41:GLY:HA3	2:B:47:PHE:O	2.14	0.47
2:B:78:PRO:HA	2:B:125:VAL:HG13	1.97	0.47
1:D:117:ASN:N	1:D:117:ASN:OD1	2.48	0.47
1:D:267:TYR:HB3	1:D:270:SER:HB3	1.96	0.47
2:E:23:ILE:HD11	2:E:109:GLN:CD	2.35	0.47
1:A:43:LEU:HG	1:A:76:MET:HG2	1.97	0.46
1:D:386:THR:O	1:D:390:GLU:HG3	2.16	0.46
1:D:331:ASN:OD1	2:E:90:ILE:HD12	2.16	0.46
1:D:261:PHE:HE2	1:D:289:GLY:CA	2.29	0.46
2:E:52:PHE:CE1	2:E:75:ILE:HD13	2.51	0.45
1:D:69:VAL:O	1:D:73:CYS:N	2.46	0.45
1:D:165:ILE:HD12	1:D:206:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:GLU:O	1:A:364:THR:HG23	2.17	0.45
1:A:69:VAL:O	1:A:73:CYS:N	2.50	0.45
1:A:388:HIS:CE1	1:A:392:LEU:HD11	2.52	0.44
1:A:201:SER:HB2	1:A:204:TYR:CZ	2.52	0.44
2:E:70:ARG:CZ	2:E:72:MET:SD	3.06	0.44
1:D:65:ILE:HD12	1:D:66:ALA:N	2.33	0.44
1:D:232:GLU:O	1:D:232:GLU:HG3	2.17	0.44
1:A:146:VAL:HG22	1:A:164:LYS:HG2	2.00	0.44
2:B:78:PRO:HD3	2:B:129:TRP:NE1	2.33	0.44
1:D:334:ARG:CZ	2:E:99:LEU:HD21	2.48	0.44
1:D:149:LYS:NZ	1:D:199:GLY:HA2	2.33	0.44
1:D:141:GLU:HG3	1:D:240:TRP:CH2	2.53	0.43
2:E:116:ASN:O	2:E:119:ASP:HB3	2.19	0.43
1:A:62:LYS:HA	1:A:62:LYS:HD2	1.95	0.43
2:B:23:ILE:HG23	2:B:39:ILE:HG13	2.01	0.43
2:E:70:ARG:NH1	2:E:72:MET:SD	2.92	0.43
2:E:71:PHE:HZ	2:E:112:LEU:HD11	1.83	0.43
1:D:350:LEU:HD12	1:D:353:LYS:HE2	2.00	0.43
2:B:58:LEU:HD23	2:B:67:PRO:HB3	2.01	0.43
3:F:22:THR:O	3:F:26:VAL:HG23	2.19	0.43
2:E:23:ILE:HD11	2:E:109:GLN:NE2	2.34	0.42
2:E:78:PRO:HD3	2:E:129:TRP:NE1	2.34	0.42
1:D:69:VAL:O	1:D:73:CYS:HB3	2.20	0.42
3:C:6:LYS:HA	3:C:11:LYS:O	2.20	0.42
1:A:374:VAL:HG12	1:A:378:ARG:HE	1.84	0.42
1:D:56:ASN:C	1:D:58:THR:H	2.23	0.42
2:B:39:ILE:HD12	2:B:54:LEU:HD23	2.01	0.42
1:D:29:GLN:HG3	1:D:277:PHE:HB3	2.02	0.42
3:F:56:LEU:O	3:F:61:ILE:HG12	2.20	0.42
1:D:148:VAL:HG22	1:D:203:GLU:HG2	2.02	0.41
1:A:74:HIS:HA	1:A:77:THR:HG22	2.03	0.41
1:A:389:LEU:O	1:A:393:LEU:HG	2.21	0.41
1:A:31:TYR:CD2	1:A:362:ILE:HD13	2.56	0.41
1:D:201:SER:HB2	1:D:204:TYR:CZ	2.56	0.41
1:A:69:VAL:HA	1:A:385:MET:HE3	2.01	0.41
1:A:213:GLU:C	1:A:215:PRO:HD3	2.42	0.41
2:B:78:PRO:HD3	2:B:129:TRP:CD1	2.56	0.41
2:B:92:LYS:HG2	3:C:39:ASP:HB3	2.03	0.41
3:F:55:THR:HG22	3:F:58:ASP:CG	2.41	0.41
1:A:17:GLY:HA3	1:A:131:ASN:OD1	2.21	0.40
1:D:167:LEU:HD21	1:D:195:PHE:HA	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:56:LEU:HD23	2:E:57:PHE:N	2.36	0.40
1:A:310:SER:HB3	1:A:327:CYS:HB3	2.04	0.40
2:E:58:LEU:CD2	2:E:101:ILE:HD11	2.49	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	382/385 (99%)	372 (97%)	9 (2%)	1 (0%)	41	49
1	D	379/385 (98%)	354 (93%)	25 (7%)	0	100	100
2	B	147/152 (97%)	140 (95%)	4 (3%)	3 (2%)	7	5
2	E	146/152 (96%)	136 (93%)	9 (6%)	1 (1%)	22	25
3	C	74/79 (94%)	73 (99%)	1 (1%)	0	100	100
3	F	73/79 (92%)	72 (99%)	1 (1%)	0	100	100
All	All	1201/1232 (98%)	1147 (96%)	49 (4%)	5 (0%)	34	41

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	119	ASP
2	B	87	CYS
2	B	131	THR
1	A	32	GLY
2	E	5	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	344/344 (100%)	338 (98%)	6 (2%)	60	73
1	D	341/344 (99%)	331 (97%)	10 (3%)	42	53
2	B	125/128 (98%)	121 (97%)	4 (3%)	39	50
2	E	125/128 (98%)	120 (96%)	5 (4%)	31	41
3	C	69/70 (99%)	69 (100%)	0	100	100
3	F	69/70 (99%)	67 (97%)	2 (3%)	42	53
All	All	1073/1084 (99%)	1046 (98%)	27 (2%)	47	60

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

Mol	Chain	Res	Type
1	A	67	LYS
1	A	107	LYS
1	A	116	ASP
1	A	224	SER
1	A	239	PHE
1	A	291	ASP
2	B	14	ARG
2	B	82	LYS
2	B	107	SER
2	B	130	LYS
1	D	23	LYS
1	D	63	GLN
1	D	156	ASN
1	D	207	CYS
1	D	232	GLU
1	D	243	SER
1	D	257	SER
1	D	261	PHE
1	D	279	SER
1	D	380	ARG
2	E	7	ARG
2	E	70	ARG

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Mol	Chain	Res	Type
2	E	87	CYS
2	E	118	ASP
2	E	127	GLU
3	F	22	THR
3	F	72	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	47	GLN
1	D	156	ASN
2	E	116	ASN
2	E	123	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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(Å²)	Q<0.9
1	A	384/385 (99%)	-0.18	1 (0%)	94	94	41, 62, 100, 153	0
1	D	381/385 (98%)	-0.06	3 (0%)	86	86	49, 73, 126, 164	0
2	B	149/152 (98%)	0.39	9 (6%)	21	18	52, 95, 143, 183	0
2	E	148/152 (97%)	0.42	9 (6%)	21	18	60, 100, 139, 179	0
3	C	76/79 (96%)	-0.23	1 (1%)	77	76	43, 66, 94, 138	0
3	F	75/79 (94%)	-0.03	0	100	100	51, 79, 109, 129	0
All	All	1213/1232 (98%)	0.01	23 (1%)	66	64	41, 76, 127, 183	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	121	LEU	6.8
2	B	122	ALA	6.1
1	D	254	LEU	4.6
2	B	124	ASP	4.4
2	B	125	VAL	3.8
2	E	56	LEU	3.5
2	E	118	ASP	3.2
2	B	3	GLY	3.1
3	C	-1	GLY	3.0
2	E	105	LEU	3.0
2	E	35	PHE	2.7
2	B	129	TRP	2.6
2	E	133	GLU	2.5
2	E	54	LEU	2.5
1	D	256	GLU	2.4
2	B	118	ASP	2.3
2	B	130	LYS	2.3
1	A	395	ILE	2.2
1	D	53	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	40	ALA	2.1
2	E	51	THR	2.1
2	E	64	MET	2.0
2	B	20	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.