W O R L D W I D E

wwPDB

PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

May 22, 2020 – 02:04 am BST

PDB ID	:	4Z88
Title	:	SH3-II of Drosophila Rim-binding protein with Aplip1 peptide
Authors	:	Driller, J.H.; Holton, N.; Siebert, M.; Boehme, M.A.; Wahl, M.C.; Sigrist, S.J.; Loll, B.
Deposited on	:	2015-04-08
Resolution	:	2.09 Å(reported)

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

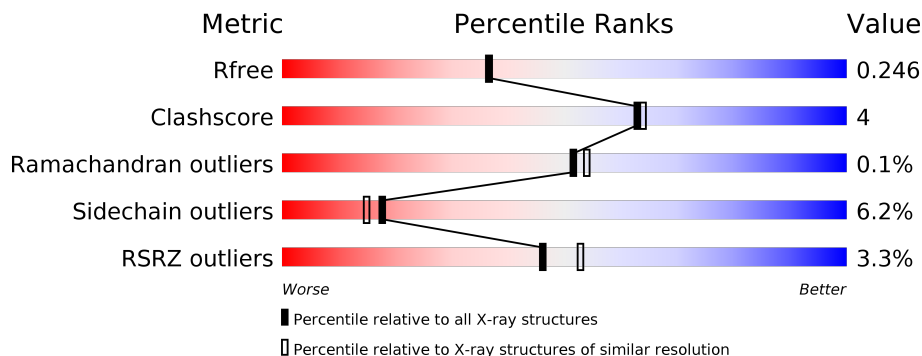|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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		0.246
Clashscore		4
Ramachandran outliers		0.1%
Sidechain outliers		6.2%
RSRZ outliers		3.3%

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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 <=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	73	10% / 73% / 15% · 11%
1	B	73	77% / 8% 5% 10%
1	C	73	82% / 7% 11%
1	D	73	89% / 7% ·
1	E	73	7% / 75% / 11% 14%
1	F	73	5% / 81% / 11% 8%

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Mol	Chain	Length	Quality of chain
1	G	73	11% / 78% / 12% · 8%
1	H	73	85% / 10% · ·
1	I	73	% / 84% / 7% 10%
1	J	73	77% / 15% · 7%
1	K	73	4% / 79% / 10% · 10%
1	L	73	% / 88% / 5% 7%
2	M	17	47% / 24% / 29%
2	N	17	29% / 71%
2	O	17	65% / 35%
2	P	17	24% / 18% / 6% / 53%
2	Q	17	76% / 6% 18%
2	R	17	29% / 6% 6% / 59%
2	S	17	65% / 18% / 18%
2	T	17	18% / 12% / 71%
2	U	17	6% / 65% / 12% / 24%
2	V	17	35% / 6% / 59%
2	W	17	65% / 12% / 24%
2	X	17	41% / 59%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7564 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 RIM-binding protein, isoform F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	65	Total	C	N	O	S	0	1	0
			532	335	85	108	4			
1	B	66	Total	C	N	O	S	0	0	0
			538	341	86	107	4			
1	C	65	Total	C	N	O	S	0	0	0
			528	336	85	103	4			
1	D	70	Total	C	N	O	S	0	0	0
			564	356	90	114	4			
1	E	63	Total	C	N	O	S	0	0	0
			506	321	80	101	4			
1	F	67	Total	C	N	O	S	0	0	0
			543	344	87	108	4			
1	G	67	Total	C	N	O	S	0	0	0
			537	340	87	106	4			
1	H	70	Total	C	N	O	S	0	0	0
			564	356	90	114	4			
1	I	66	Total	C	N	O	S	0	0	0
			538	341	86	107	4			
1	J	68	Total	C	N	O	S	0	0	0
			550	349	88	109	4			
1	K	66	Total	C	N	O	S	0	0	0
			537	341	86	106	4			
1	L	68	Total	C	N	O	S	0	0	0
			550	349	88	109	4			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1310	GLY	-	expression tag	UNP A0A0B4JDC9
A	1311	PRO	-	expression tag	UNP A0A0B4JDC9
A	1312	LEU	-	expression tag	UNP A0A0B4JDC9
A	1313	GLY	-	expression tag	UNP A0A0B4JDC9
A	1314	SER	-	expression tag	UNP A0A0B4JDC9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1315	PRO	-	expression tag	UNP A0A0B4JDC9
A	1316	GLU	-	expression tag	UNP A0A0B4JDC9
A	1317	PHE	-	expression tag	UNP A0A0B4JDC9
B	1310	GLY	-	expression tag	UNP A0A0B4JDC9
B	1311	PRO	-	expression tag	UNP A0A0B4JDC9
B	1312	LEU	-	expression tag	UNP A0A0B4JDC9
B	1313	GLY	-	expression tag	UNP A0A0B4JDC9
B	1314	SER	-	expression tag	UNP A0A0B4JDC9
B	1315	PRO	-	expression tag	UNP A0A0B4JDC9
B	1316	GLU	-	expression tag	UNP A0A0B4JDC9
B	1317	PHE	-	expression tag	UNP A0A0B4JDC9
C	1310	GLY	-	expression tag	UNP A0A0B4JDC9
C	1311	PRO	-	expression tag	UNP A0A0B4JDC9
C	1312	LEU	-	expression tag	UNP A0A0B4JDC9
C	1313	GLY	-	expression tag	UNP A0A0B4JDC9
C	1314	SER	-	expression tag	UNP A0A0B4JDC9
C	1315	PRO	-	expression tag	UNP A0A0B4JDC9
C	1316	GLU	-	expression tag	UNP A0A0B4JDC9
C	1317	PHE	-	expression tag	UNP A0A0B4JDC9
D	1310	GLY	-	expression tag	UNP A0A0B4JDC9
D	1311	PRO	-	expression tag	UNP A0A0B4JDC9
D	1312	LEU	-	expression tag	UNP A0A0B4JDC9
D	1313	GLY	-	expression tag	UNP A0A0B4JDC9
D	1314	SER	-	expression tag	UNP A0A0B4JDC9
D	1315	PRO	-	expression tag	UNP A0A0B4JDC9
D	1316	GLU	-	expression tag	UNP A0A0B4JDC9
D	1317	PHE	-	expression tag	UNP A0A0B4JDC9
E	1310	GLY	-	expression tag	UNP A0A0B4JDC9
E	1311	PRO	-	expression tag	UNP A0A0B4JDC9
E	1312	LEU	-	expression tag	UNP A0A0B4JDC9
E	1313	GLY	-	expression tag	UNP A0A0B4JDC9
E	1314	SER	-	expression tag	UNP A0A0B4JDC9
E	1315	PRO	-	expression tag	UNP A0A0B4JDC9
E	1316	GLU	-	expression tag	UNP A0A0B4JDC9
E	1317	PHE	-	expression tag	UNP A0A0B4JDC9
F	1310	GLY	-	expression tag	UNP A0A0B4JDC9
F	1311	PRO	-	expression tag	UNP A0A0B4JDC9
F	1312	LEU	-	expression tag	UNP A0A0B4JDC9
F	1313	GLY	-	expression tag	UNP A0A0B4JDC9
F	1314	SER	-	expression tag	UNP A0A0B4JDC9
F	1315	PRO	-	expression tag	UNP A0A0B4JDC9
F	1316	GLU	-	expression tag	UNP A0A0B4JDC9

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1317	PHE	-	expression tag	UNP A0A0B4JDC9
G	1310	GLY	-	expression tag	UNP A0A0B4JDC9
G	1311	PRO	-	expression tag	UNP A0A0B4JDC9
G	1312	LEU	-	expression tag	UNP A0A0B4JDC9
G	1313	GLY	-	expression tag	UNP A0A0B4JDC9
G	1314	SER	-	expression tag	UNP A0A0B4JDC9
G	1315	PRO	-	expression tag	UNP A0A0B4JDC9
G	1316	GLU	-	expression tag	UNP A0A0B4JDC9
G	1317	PHE	-	expression tag	UNP A0A0B4JDC9
H	1310	GLY	-	expression tag	UNP A0A0B4JDC9
H	1311	PRO	-	expression tag	UNP A0A0B4JDC9
H	1312	LEU	-	expression tag	UNP A0A0B4JDC9
H	1313	GLY	-	expression tag	UNP A0A0B4JDC9
H	1314	SER	-	expression tag	UNP A0A0B4JDC9
H	1315	PRO	-	expression tag	UNP A0A0B4JDC9
H	1316	GLU	-	expression tag	UNP A0A0B4JDC9
H	1317	PHE	-	expression tag	UNP A0A0B4JDC9
I	1310	GLY	-	expression tag	UNP A0A0B4JDC9
I	1311	PRO	-	expression tag	UNP A0A0B4JDC9
I	1312	LEU	-	expression tag	UNP A0A0B4JDC9
I	1313	GLY	-	expression tag	UNP A0A0B4JDC9
I	1314	SER	-	expression tag	UNP A0A0B4JDC9
I	1315	PRO	-	expression tag	UNP A0A0B4JDC9
I	1316	GLU	-	expression tag	UNP A0A0B4JDC9
I	1317	PHE	-	expression tag	UNP A0A0B4JDC9
J	1310	GLY	-	expression tag	UNP A0A0B4JDC9
J	1311	PRO	-	expression tag	UNP A0A0B4JDC9
J	1312	LEU	-	expression tag	UNP A0A0B4JDC9
J	1313	GLY	-	expression tag	UNP A0A0B4JDC9
J	1314	SER	-	expression tag	UNP A0A0B4JDC9
J	1315	PRO	-	expression tag	UNP A0A0B4JDC9
J	1316	GLU	-	expression tag	UNP A0A0B4JDC9
J	1317	PHE	-	expression tag	UNP A0A0B4JDC9
K	1310	GLY	-	expression tag	UNP A0A0B4JDC9
K	1311	PRO	-	expression tag	UNP A0A0B4JDC9
K	1312	LEU	-	expression tag	UNP A0A0B4JDC9
K	1313	GLY	-	expression tag	UNP A0A0B4JDC9
K	1314	SER	-	expression tag	UNP A0A0B4JDC9
K	1315	PRO	-	expression tag	UNP A0A0B4JDC9
K	1316	GLU	-	expression tag	UNP A0A0B4JDC9
K	1317	PHE	-	expression tag	UNP A0A0B4JDC9
L	1310	GLY	-	expression tag	UNP A0A0B4JDC9

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Chain	Residue	Modelled	Actual	Comment	Reference
L	1311	PRO	-	expression tag	UNP A0A0B4JDC9
L	1312	LEU	-	expression tag	UNP A0A0B4JDC9
L	1313	GLY	-	expression tag	UNP A0A0B4JDC9
L	1314	SER	-	expression tag	UNP A0A0B4JDC9
L	1315	PRO	-	expression tag	UNP A0A0B4JDC9
L	1316	GLU	-	expression tag	UNP A0A0B4JDC9
L	1317	PHE	-	expression tag	UNP A0A0B4JDC9

• Molecule 2 is a protein called JNK-interacting protein 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	M	12	Total	C	N	O	0	0	1
			95	61	20	14			
2	N	5	Total	C	N	O	0	0	0
			39	27	5	7			
2	O	11	Total	C	N	O	0	0	1
			84	55	16	13			
2	P	8	Total	C	N	O	0	0	0
			70	45	15	10			
2	Q	14	Total	C	N	O	0	0	1
			117	73	28	16			
2	R	7	Total	C	N	O	0	0	0
			59	39	11	9			
2	S	14	Total	C	N	O	0	0	1
			117	73	28	16			
2	T	5	Total	C	N	O	0	0	0
			46	29	12	5			
2	U	13	Total	C	N	O	0	0	1
			106	67	24	15			
2	V	7	Total	C	N	O	0	0	0
			63	40	14	9			
2	W	13	Total	C	N	O	0	0	1
			106	67	24	15			
2	X	7	Total	C	N	O	0	0	0
			63	40	14	9			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	148	ACE	-	acetylation	UNP Q9W0K0
M	164	NH2	-	amidation	UNP Q9W0K0
N	148	ACE	-	acetylation	UNP Q9W0K0

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Chain	Residue	Modelled	Actual	Comment	Reference
N	164	NH2	-	amidation	UNP Q9W0K0
O	148	ACE	-	acetylation	UNP Q9W0K0
O	164	NH2	-	amidation	UNP Q9W0K0
P	148	ACE	-	acetylation	UNP Q9W0K0
P	164	NH2	-	amidation	UNP Q9W0K0
Q	148	ACE	-	acetylation	UNP Q9W0K0
Q	164	NH2	-	amidation	UNP Q9W0K0
R	148	ACE	-	acetylation	UNP Q9W0K0
R	164	NH2	-	amidation	UNP Q9W0K0
S	148	ACE	-	acetylation	UNP Q9W0K0
S	164	NH2	-	amidation	UNP Q9W0K0
T	148	ACE	-	acetylation	UNP Q9W0K0
T	164	NH2	-	amidation	UNP Q9W0K0
U	148	ACE	-	acetylation	UNP Q9W0K0
U	164	NH2	-	amidation	UNP Q9W0K0
V	148	ACE	-	acetylation	UNP Q9W0K0
V	164	NH2	-	amidation	UNP Q9W0K0
W	148	ACE	-	acetylation	UNP Q9W0K0
W	164	NH2	-	amidation	UNP Q9W0K0
X	148	ACE	-	acetylation	UNP Q9W0K0
X	164	NH2	-	amidation	UNP Q9W0K0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).
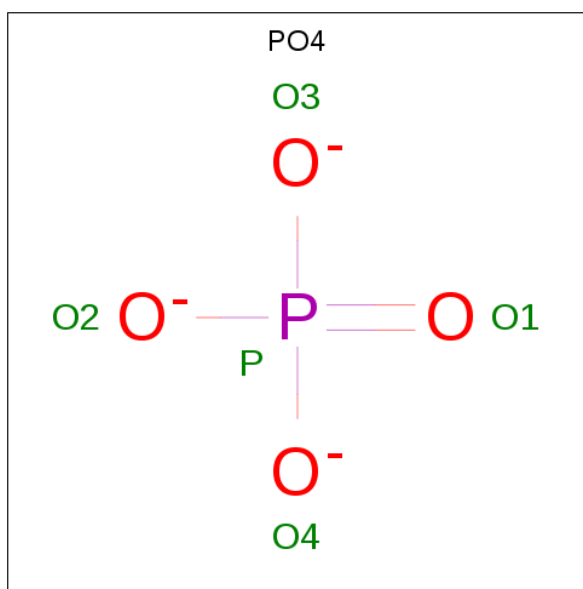
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total 5	O 4	P 1	0	0
3	C	1	Total 5	O 4	P 1	0	0
3	E	1	Total 5	O 4	P 1	0	0
3	F	1	Total 5	O 4	P 1	0	0
3	G	1	Total 5	O 4	P 1	0	0
3	H	1	Total 5	O 4	P 1	0	0
3	I	1	Total 5	O 4	P 1	0	0
3	J	1	Total 5	O 4	P 1	0	0
3	K	1	Total 5	O 4	P 1	0	0
3	L	1	Total 5	O 4	P 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total 5	O 5	0	0
4	B	5	Total 5	O 5	0	0
4	C	3	Total 3	O 3	0	0
4	D	3	Total 3	O 3	0	0
4	E	5	Total 5	O 5	0	0
4	F	6	Total 6	O 6	0	0
4	G	3	Total 3	O 3	0	0
4	H	2	Total 2	O 2	0	0
4	I	5	Total 5	O 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	J	4	Total 4	O 4	0	0
4	K	4	Total 4	O 4	0	0
4	L	1	Total 1	O 1	0	0
4	M	2	Total 2	O 2	0	0
4	O	1	Total 1	O 1	0	0
4	Q	5	Total 5	O 5	0	0
4	W	1	Total 1	O 1	0	0
4	X	2	Total 2	O 2	0	0

3 Residue-property plots (i)

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.
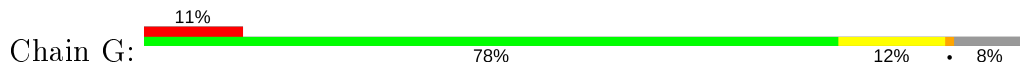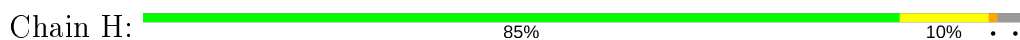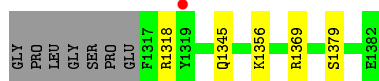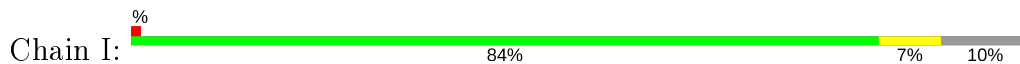
- Molecule 1: RIM-binding protein, isoform F
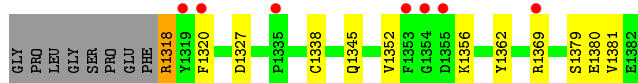
Chain A:

- Molecule 1: RIM-binding protein, isoform F

Chain B:

- Molecule 1: RIM-binding protein, isoform F

Chain C:
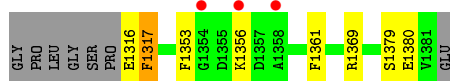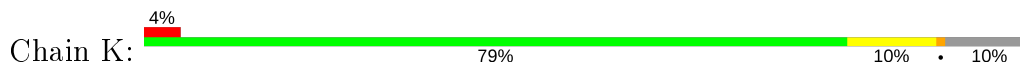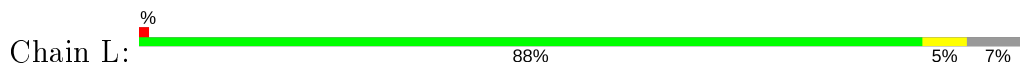
- Molecule 1: RIM-binding protein, isoform F

Chain D:

- Molecule 1: RIM-binding protein, isoform F

Chain E:

- Molecule 1: RIM-binding protein, isoform F

Chain F:

GLY PRO LEU GLY S1314 R1318 F1324 T1330 D1336 G1337 C1338 K1356 D1357 A1358 Y1362 R1369 S1379 E1380 VAL GLU

• Molecule 1: RIM-binding protein, isoform F

Chain G:

GLY PRO LEU GLY SER P1315 E1316 F1317 F1320 D1325 P1335 D1336 G1337 Q1345 F1353 K1356 D1357 A1358 D1359 G1360 F1361 Y1362 R1369 S1379 E1380 V1381 GLU

• Molecule 1: RIM-binding protein, isoform F

Chain H:

GLY PRO LEU G1313 S1314 R1318 P1333 K1356 D1359 R1369 S1379 E1380 V1381 E1382

• Molecule 1: RIM-binding protein, isoform F

Chain I:

GLY PRO LEU GLY SER PRO GLU F1317 R1318 Y1319 Q1345 K1356 R1369 S1379 E1382

• Molecule 1: RIM-binding protein, isoform F

Chain J:

GLY PRO LEU GLY S1314 F1317 R1318 Y1319 N1334 E1340 G1354 D1355 K1356 R1367 G1368 R1369 S1379 E1380 V1381 GLU

• Molecule 1: RIM-binding protein, isoform F

Chain K:

GLY PRO LEU GLY SER PRO E1316 F1317 F1353 G1354 D1355 K1356 D1357 A1358 F1361 R1369 S1379 E1380 V1381 GLU

• Molecule 1: RIM-binding protein, isoform F

Chain L:

GLY PRO LEU GLY S1314 K1356 D1357 A1358 R1369 S1379 E1380 V1381 GLU
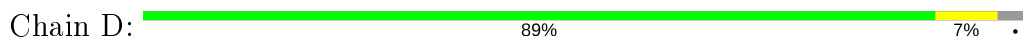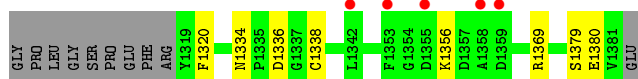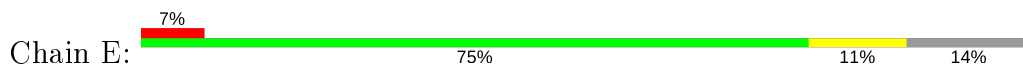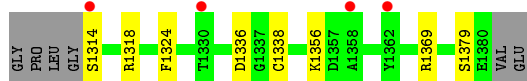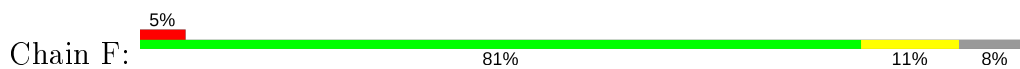
- Molecule 2: JNK-interacting protein 1

Chain M:

| 47% | 24% | 29% |

ACE THR ARG ARG **R153** K160 K163 ?164

- Molecule 2: JNK-interacting protein 1

Chain N:

| 29% | 71% |

ACE THR ARG ARG ARG LYS L155 P159 LYS ASN LYS LYS NH2

- Molecule 2: JNK-interacting protein 1

Chain O:

| 65% | 35% |

ACE THR ARG ARG ARG K154 ?164
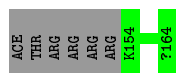
- Molecule 2: JNK-interacting protein 1

Chain P:

| 24% | 18% | 6% | 53% |

ACE THR ARG ARG R152 R153 I158 P159 LYS ASN LYS NH2
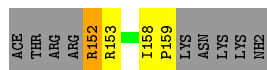
- Molecule 2: JNK-interacting protein 1

Chain Q:

| 76% | 6% | 18% |

ACE THR ARG R151 R152 R153 ?164
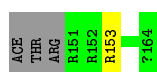
- Molecule 2: JNK-interacting protein 1

Chain R:

| 29% | 6% | 6% | 59% |

ACE THR ARG ARG R153 P159 LYS ASN LYS LYS NH2

- Molecule 2: JNK-interacting protein 1

Chain S:

| 65% | 18% | 18% |

ACE THR ARG R151 R152 R153 I158 P159 K160 ?164

- Molecule 2: JNK-interacting protein 1

Chain T:

18%   12%   71%

ACE THR ARG ARG R152 R153 K154 L155 P156 GLU ILE PRO LYS ASN LYS LYS NH2

• Molecule 2: JNK-interacting protein 1

6%

Chain U:

65%   12%   24%

ACE THR ARG ARG R152 R153 K162 K163 ?164

• Molecule 2: JNK-interacting protein 1

Chain V:

35%   6%   59%

ACE THR ARG ARG R152 R153 I158 PRO LYS ASN LYS LYS NH2

• Molecule 2: JNK-interacting protein 1

Chain W:

65%   12%   24%

ACE THR ARG ARG R152 R153 K160 ?164

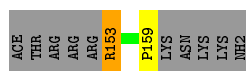• Molecule 2: JNK-interacting protein 1

Chain X:

41%   59%

ACE THR ARG ARG R152 I158 PRO LYS ASN LYS LYS NH2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	108.28Å 62.42Å 163.64Å 90.00° 90.27° 90.00°	Depositor
Resolution (Å)	45.25 – 2.09 45.25 – 2.09	Depositor EDS
% Data completeness (in resolution range)	98.5 (45.25-2.09) 98.9 (45.25-2.09)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.209 , 0.236 0.222 , 0.246	Depositor DCC
R_{free} test set	3042 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å^2)	35.1	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 36.9	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.178 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.187 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.099 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.115 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.078 for -h,-k,l	Xtriage
Reported twinning fraction	0.135 for H, K, L 0.126 for -1/2H-3/2K, -1/2H+1/2K, -L 0.146 for -1/2H+3/2K, 1/2H+1/2K, -L 0.193 for 1/2H-3/2K, -1/2H-1/2K, -L 0.182 for 1/2H+3/2K, 1/2H-1/2K, -L 0.218 for -h,-k,l	Depositor
Outliers	1 of 64777 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7564	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, NH2

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	0.36	0/551	0.62	0/744
1	B	0.50	0/555	0.98	4/749 (0.5%)
1	C	0.48	0/545	0.63	0/737
1	D	0.37	0/582	0.61	0/786
1	E	0.38	0/522	0.62	0/707
1	F	0.44	0/561	0.68	0/759
1	G	0.44	0/554	0.74	1/749 (0.1%)
1	H	0.48	0/582	0.90	4/786 (0.5%)
1	I	0.42	0/555	0.59	0/749
1	J	0.40	0/568	0.62	0/769
1	K	0.45	0/554	0.69	1/749 (0.1%)
1	L	0.40	0/568	0.58	0/769
2	M	0.47	0/95	0.83	0/124
2	N	0.36	0/40	0.43	0/55
2	O	0.42	0/84	0.57	0/110
2	P	0.40	0/71	0.85	0/94
2	Q	0.37	0/117	0.67	0/152
2	R	0.33	0/60	0.51	0/80
2	S	0.47	0/117	0.69	0/152
2	T	0.37	0/46	0.63	0/59
2	U	0.50	0/106	0.80	0/138
2	V	0.39	0/63	0.83	0/82
2	W	0.42	0/106	0.68	0/138
2	X	0.34	0/63	0.58	0/82
All	All	0.43	0/7665	0.70	10/10319 (0.1%)

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	J	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1369	ARG	NE-CZ-NH2	14.39	127.50	120.30
1	H	1369	ARG	NE-CZ-NH2	11.05	125.83	120.30
1	B	1369	ARG	NE-CZ-NH1	-10.06	115.27	120.30
1	H	1369	ARG	NE-CZ-NH1	-9.02	115.79	120.30
1	H	1369	ARG	CG-CD-NE	6.95	126.40	111.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1381	VAL	Peptide
1	J	1380	GLU	Peptide

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	532	0	471	8	0
1	B	538	0	476	12	0
1	C	528	0	470	1	0
1	D	564	0	497	2	0
1	E	506	0	448	5	0
1	F	543	0	479	4	0
1	G	537	0	477	6	0
1	H	564	0	497	4	0
1	I	538	0	476	2	0
1	J	550	0	488	10	0
1	K	537	0	476	7	0
1	L	550	0	488	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	M	95	0	112	1	0
2	N	39	0	41	0	0
2	O	84	0	99	0	0
2	P	70	0	80	8	0
2	Q	117	0	138	2	0
2	R	59	0	67	3	0
2	S	117	0	138	3	0
2	T	46	0	56	2	0
2	U	106	0	125	0	0
2	V	63	0	73	2	0
2	W	106	0	125	1	0
2	X	63	0	73	0	0
3	A	5	0	0	1	0
3	B	5	0	0	1	0
3	C	5	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	1	0
3	G	5	0	0	0	0
3	H	5	0	0	1	0
3	I	5	0	0	1	0
3	J	5	0	0	0	0
3	K	5	0	0	0	0
3	L	5	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	3	0	0	0	0
4	D	3	0	0	0	0
4	E	5	0	0	0	0
4	F	6	0	0	0	0
4	G	3	0	0	0	0
4	H	2	0	0	0	0
4	I	5	0	0	0	0
4	J	4	0	0	0	0
4	K	4	0	0	0	0
4	L	1	0	0	0	0
4	M	2	0	0	0	0
4	O	1	0	0	0	0
4	Q	5	0	0	0	0
4	W	1	0	0	0	0
4	X	2	0	0	0	0
All	All	7564	0	6870	62	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 4.

The worst 5 of 62 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:1380:GLU:O	1:B:1380:GLU:HG2	1.66	0.93
1:G:1361:PHE:CE1	2:S:153:ARG:HG2	2.11	0.85
1:J:1380:GLU:O	1:J:1381:VAL:HG23	1.79	0.81
1:J:1317:PHE:HE1	1:J:1319:TYR:CE1	2.00	0.79
2:P:158:ILE:HG22	2:P:159:PRO:CD	2.13	0.78

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	64/73 (88%)	64 (100%)	0	0	100	100
1	B	64/73 (88%)	62 (97%)	2 (3%)	0	100	100
1	C	63/73 (86%)	63 (100%)	0	0	100	100
1	D	68/73 (93%)	67 (98%)	1 (2%)	0	100	100
1	E	61/73 (84%)	61 (100%)	0	0	100	100
1	F	65/73 (89%)	64 (98%)	1 (2%)	0	100	100
1	G	65/73 (89%)	65 (100%)	0	0	100	100
1	H	68/73 (93%)	66 (97%)	1 (2%)	1 (2%)	10	5
1	I	64/73 (88%)	64 (100%)	0	0	100	100
1	J	66/73 (90%)	65 (98%)	1 (2%)	0	100	100
1	K	64/73 (88%)	63 (98%)	1 (2%)	0	100	100
1	L	66/73 (90%)	65 (98%)	1 (2%)	0	100	100
2	M	10/17 (59%)	9 (90%)	1 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	N	3/17 (18%)	3 (100%)	0	0	100	100
2	O	9/17 (53%)	8 (89%)	1 (11%)	0	100	100
2	P	6/17 (35%)	6 (100%)	0	0	100	100
2	Q	12/17 (71%)	12 (100%)	0	0	100	100
2	R	5/17 (29%)	5 (100%)	0	0	100	100
2	S	12/17 (71%)	12 (100%)	0	0	100	100
2	T	3/17 (18%)	3 (100%)	0	0	100	100
2	U	11/17 (65%)	11 (100%)	0	0	100	100
2	V	5/17 (29%)	5 (100%)	0	0	100	100
2	W	11/17 (65%)	11 (100%)	0	0	100	100
2	X	5/17 (29%)	5 (100%)	0	0	100	100
All	All	870/1080 (81%)	859 (99%)	10 (1%)	1 (0%)	51	54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	1314	SER

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	57/62 (92%)	53 (93%)	4 (7%)	15	12
1	B	57/62 (92%)	54 (95%)	3 (5%)	22	20
1	C	56/62 (90%)	52 (93%)	4 (7%)	14	11
1	D	60/62 (97%)	57 (95%)	3 (5%)	24	23
1	E	54/62 (87%)	51 (94%)	3 (6%)	21	18
1	F	58/62 (94%)	54 (93%)	4 (7%)	15	12
1	G	57/62 (92%)	53 (93%)	4 (7%)	15	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	60/62 (97%)	57 (95%)	3 (5%)	24	23
1	I	57/62 (92%)	54 (95%)	3 (5%)	22	20
1	J	59/62 (95%)	56 (95%)	3 (5%)	24	22
1	K	57/62 (92%)	53 (93%)	4 (7%)	15	12
1	L	59/62 (95%)	55 (93%)	4 (7%)	16	13
2	M	11/15 (73%)	9 (82%)	2 (18%)	1	1
2	N	5/15 (33%)	5 (100%)	0	100	100
2	O	10/15 (67%)	10 (100%)	0	100	100
2	P	8/15 (53%)	7 (88%)	1 (12%)	4	2
2	Q	13/15 (87%)	13 (100%)	0	100	100
2	R	7/15 (47%)	6 (86%)	1 (14%)	3	1
2	S	13/15 (87%)	12 (92%)	1 (8%)	13	9
2	T	5/15 (33%)	5 (100%)	0	100	100
2	U	12/15 (80%)	10 (83%)	2 (17%)	2	1
2	V	7/15 (47%)	7 (100%)	0	100	100
2	W	12/15 (80%)	11 (92%)	1 (8%)	11	7
2	X	7/15 (47%)	7 (100%)	0	100	100
All	All	801/924 (87%)	751 (94%)	50 (6%)	18	15

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	1356	LYS
1	H	1379	SER
2	S	160	LYS
1	G	1369	ARG
1	H	1356	LYS

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

Mol	Chain	Res	Type
1	C	1334	ASN
1	F	1375	HIS
1	I	1345	GLN
1	K	1345	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

11 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
3	PO4	F	1401	-	4,4,4	0.99	0	6,6,6	0.47	0
3	PO4	J	1401	-	4,4,4	0.95	0	6,6,6	0.53	0
3	PO4	G	1401	-	4,4,4	0.86	0	6,6,6	0.39	0
3	PO4	H	1401	-	4,4,4	0.92	0	6,6,6	0.72	0
3	PO4	L	1401	-	4,4,4	0.94	0	6,6,6	0.48	0
3	PO4	A	1401	-	4,4,4	1.03	0	6,6,6	0.47	0
3	PO4	E	1401	-	4,4,4	0.90	0	6,6,6	0.42	0
3	PO4	C	1401	-	4,4,4	0.85	0	6,6,6	0.49	0
3	PO4	I	1401	-	4,4,4	0.91	0	6,6,6	0.47	0
3	PO4	K	1401	-	4,4,4	0.86	0	6,6,6	0.43	0
3	PO4	B	1401	-	4,4,4	0.95	0	6,6,6	0.34	0

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.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1401	PO4	1	0
3	H	1401	PO4	1	0
3	A	1401	PO4	1	0
3	I	1401	PO4	1	0
3	B	1401	PO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	65/73 (89%)	0.61	7 (10%)	5	7	30, 44, 63, 68	0
1	B	66/73 (90%)	0.32	0	100	100	26, 36, 53, 61	0
1	C	65/73 (89%)	0.13	0	100	100	25, 35, 46, 50	0
1	D	70/73 (95%)	0.20	0	100	100	26, 34, 43, 46	0
1	E	63/73 (86%)	0.52	5 (7%)	12	16	32, 44, 60, 64	0
1	F	67/73 (91%)	0.70	4 (5%)	21	27	37, 49, 60, 72	0
1	G	67/73 (91%)	0.72	8 (11%)	4	5	27, 47, 64, 70	0
1	H	70/73 (95%)	0.26	0	100	100	30, 40, 51, 58	0
1	I	66/73 (90%)	0.16	1 (1%)	73	77	24, 34, 43, 48	0
1	J	68/73 (93%)	0.16	0	100	100	26, 36, 44, 52	0
1	K	66/73 (90%)	0.37	3 (4%)	33	38	26, 38, 57, 61	0
1	L	68/73 (93%)	0.58	1 (1%)	73	77	32, 40, 56, 67	0
2	M	11/17 (64%)	0.06	0	100	100	36, 39, 41, 42	0
2	N	5/17 (29%)	0.05	0	100	100	42, 43, 44, 45	0
2	O	10/17 (58%)	-0.05	0	100	100	37, 38, 40, 41	0
2	P	8/17 (47%)	0.18	0	100	100	37, 39, 48, 50	0
2	Q	13/17 (76%)	0.35	0	100	100	37, 43, 48, 48	0
2	R	7/17 (41%)	0.10	0	100	100	44, 47, 50, 54	0
2	S	13/17 (76%)	-0.00	0	100	100	40, 42, 45, 46	0
2	T	5/17 (29%)	0.17	0	100	100	46, 47, 52, 54	0
2	U	12/17 (70%)	0.56	1 (8%)	11	14	39, 45, 52, 63	0
2	V	7/17 (41%)	0.16	0	100	100	30, 31, 37, 40	0
2	W	12/17 (70%)	0.02	0	100	100	32, 40, 43, 48	0
2	X	7/17 (41%)	0.09	0	100	100	37, 46, 47, 51	0

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Mol	Chain	Analysed	$<$RSRZ$>$	#RSRZ$>$2		OWAB($Å^2$)	Q$<$0.9
All	All	911/1080 (84%)	0.36	30 (3%)	46 53	24, 40, 58, 72	0

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	U	152	ARG	4.5
1	F	1358	ALA	4.5
1	A	1319	TYR	4.4
1	G	1335	PRO	4.0
1	A	1353	PHE	3.7

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 (i)

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	PO4	E	1401	5/5	0.87	0.18	46,47,49,50	0
3	PO4	K	1401	5/5	0.94	0.13	39,40,42,42	0
3	PO4	J	1401	5/5	0.95	0.09	43,44,45,45	0
3	PO4	C	1401	5/5	0.96	0.14	36,37,38,39	0
3	PO4	I	1401	5/5	0.96	0.10	34,34,35,36	0
3	PO4	A	1401	5/5	0.96	0.18	40,40,42,42	0
3	PO4	H	1401	5/5	0.97	0.08	31,32,33,33	0
3	PO4	F	1401	5/5	0.97	0.09	35,36,36,38	0
3	PO4	G	1401	5/5	0.97	0.10	39,41,41,43	0
3	PO4	B	1401	5/5	0.98	0.07	36,36,37,38	0
3	PO4	L	1401	5/5	0.99	0.09	42,44,45,46	0

6.5 Other polymers (i)

There are no such residues in this entry.