WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Jan 4, 2024 – 07:34 am GMT

PDB ID	:	4Z89
Title	:	SH3-II of Drosophila Rim-binding protein bound to a Cacophony derived 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	:	2.64 Å(reported)

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

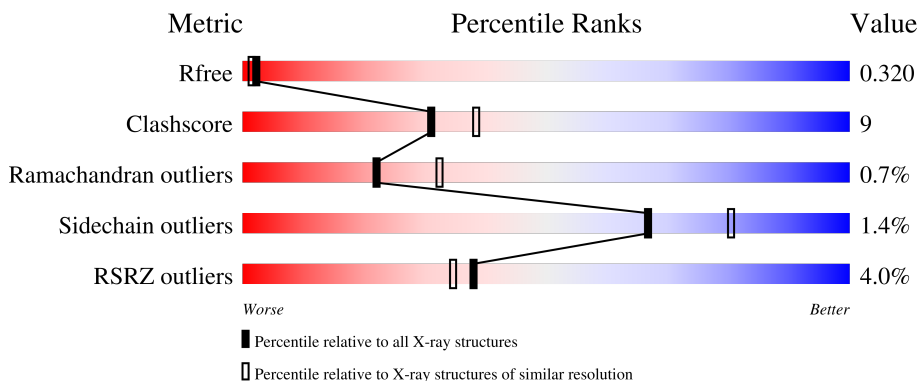|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.64 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		0.320
Clashscore		9
Ramachandran outliers		0.7%
Sidechain outliers		1.4%
RSRZ outliers		4.0%

Worse   *Better*

▮ Percentile relative to all X-ray structures

❚ Percentile relative to X-ray structures of similar resolution
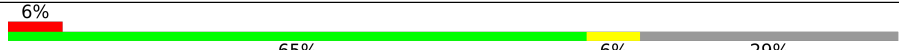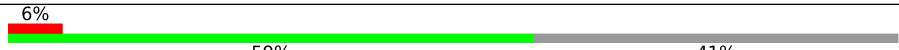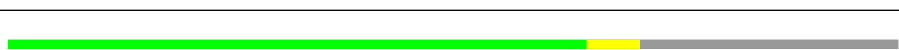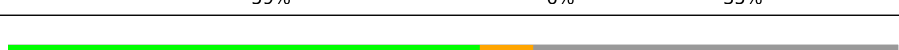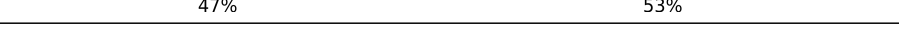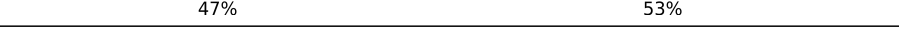
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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	73	66% 22% • 11%
1	B	73	71% 18% 11%
1	C	73	74% 16% 10%
1	D	73	.% 73% 16% 11%
1	E	73	.% 74% 16% 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	73	73% · 18% · 10%
1	G	73	3% · 68% · 22% · 10%
1	H	73	19% · 73% · 14% · 12%
1	I	73	8% · 68% · 21% · 11%
1	J	73	3% · 79% · 11% · 10%
2	a	17	6% · 65% · 6% · 29%
2	b	17	6% · 59% · 41%
2	c	17	59% · 12% · 29%
2	d	17	65% · 6% · 29%
2	e	17	59% · 6% · 35%
2	f	17	53% · 6% · 41%
2	g	17	47% · 53%
2	h	17	12% · 47% · 53%
2	i	17	47% · 53%
2	j	17	59% · 12% · 29%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 6239 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	0	0
			528	336	85	103	4			
1	B	65	Total	C	N	O	S	0	0	0
			528	336	85	103	4			
1	C	66	Total	C	N	O	S	0	1	0
			549	351	87	107	4			
1	D	65	Total	C	N	O	S	0	0	0
			528	336	85	103	4			
1	E	66	Total	C	N	O	S	0	0	0
			538	341	86	107	4			
1	F	66	Total	C	N	O	S	0	0	0
			538	341	86	107	4			
1	G	66	Total	C	N	O	S	0	0	0
			538	341	86	107	4			
1	H	64	Total	C	N	O	S	0	0	0
			517	327	84	102	4			
1	I	65	Total	C	N	O	S	0	1	0
			527	333	85	105	4			
1	J	66	Total	C	N	O	S	0	0	0
			538	341	86	107	4			

There are 80 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
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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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
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

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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

- Molecule 2 is a protein called Voltage-dependent calcium channel type A subunit alpha-1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	a	12	Total	C	N	O	0	0	0
			90	56	19	15			
2	b	10	Total	C	N	O	0	0	0
			77	48	17	12			
2	c	12	Total	C	N	O	0	0	0
			90	56	19	15			
2	d	12	Total	C	N	O	0	0	0
			90	56	19	15			
2	e	11	Total	C	N	O	0	0	0
			79	50	16	13			

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	f	10	Total 73	C 47	N 15	O 11	0	0	0
2	g	8	Total 62	C 39	N 14	O 9	0	0	0
2	h	8	Total 62	C 39	N 14	O 9	0	0	0
2	i	8	Total 62	C 39	N 14	O 9	0	0	0
2	j	12	Total 90	C 56	N 19	O 15	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	1684	ACE	-	acetylation	UNP P91645
a	1700	NH2	-	amidation	UNP P91645
b	1684	ACE	-	acetylation	UNP P91645
b	1700	NH2	-	amidation	UNP P91645
c	1684	ACE	-	acetylation	UNP P91645
c	1700	NH2	-	amidation	UNP P91645
d	1684	ACE	-	acetylation	UNP P91645
d	1700	NH2	-	amidation	UNP P91645
e	1684	ACE	-	acetylation	UNP P91645
e	1700	NH2	-	amidation	UNP P91645
f	1684	ACE	-	acetylation	UNP P91645
f	1700	NH2	-	amidation	UNP P91645
g	1684	ACE	-	acetylation	UNP P91645
g	1700	NH2	-	amidation	UNP P91645
h	1684	ACE	-	acetylation	UNP P91645
h	1700	NH2	-	amidation	UNP P91645
i	1684	ACE	-	acetylation	UNP P91645
i	1700	NH2	-	amidation	UNP P91645
j	1684	ACE	-	acetylation	UNP P91645
j	1700	NH2	-	amidation	UNP P91645

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Ca 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	16	Total 16	O 16	0	0
4	B	19	Total 19	O 19	0	0
4	C	9	Total 9	O 9	0	0
4	D	10	Total 10	O 10	0	0
4	E	14	Total 14	O 14	0	0
4	F	16	Total 16	O 16	0	0
4	G	10	Total 10	O 10	0	0
4	H	3	Total 3	O 3	0	0
4	I	6	Total 6	O 6	0	0
4	J	14	Total 14	O 14	0	0
4	a	3	Total 3	O 3	0	0
4	b	1	Total 1	O 1	0	0
4	c	1	Total 1	O 1	0	0
4	d	1	Total 1	O 1	0	0
4	e	4	Total 4	O 4	0	0
4	f	3	Total 3	O 3	0	0
4	g	1	Total 1	O 1	0	0
4	j	3	Total 3	O 3	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: RIM-binding protein, isoform F

Chain A:

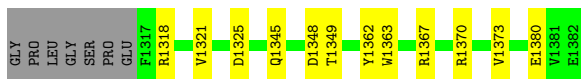
- Molecule 1: RIM-binding protein, isoform F

Chain B:

- Molecule 1: RIM-binding protein, isoform F

Chain C:
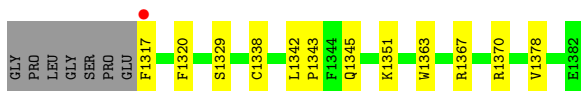

- Molecule 1: RIM-binding protein, isoform F

Chain D:

- Molecule 1: RIM-binding protein, isoform F

Chain E:

- Molecule 1: RIM-binding protein, isoform F

Chain F:

73% 18% 10%

GLY PRO LEU GLY SER PRO GLU F1317 V1321 S1329 T1330 M1331 N1334 C1338 E1341 T1349 I1350 K1351 V1352 F1353 D1357 W1363 R1370 N1376 E1382

• Molecule 1: RIM-binding protein, isoform F

Chain G:

3% 68% 22% 10%

GLY PRO LEU GLY SER PRO GLU F1317 R1318 Y1319 F1320 V1321 S1329 C1338 D1339 D1348 K1356 G1360 W1363 G1364 E1365 L1366 R1367 R1370 V1378 S1379 E1380 V1381 E1382

• Molecule 1: RIM-binding protein, isoform F

Chain H:

19% 73% 14% • 12%

GLY PRO LEU GLY SER PRO GLU PHE R1318 Y1319 F1320 V1321 A1322 M1323 F1324 D1325 L1342 Q1345 E1346 G1347 D1348 T1349 I1350 F1353 K1356 Y1362 G1371 Y1373 V1373 F1374 V1378 S1379 E1380 V1381 GLU
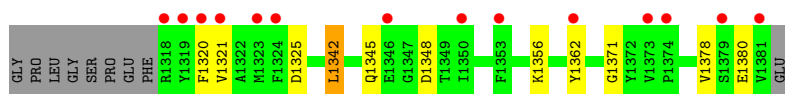
• Molecule 1: RIM-binding protein, isoform F

Chain I:

8% 68% 21% 11%

GLY PRO LEU GLY SER PRO GLU F1317 R1318 Y1319 F1320 V1321 S1329 N1334 E1341 L1342 P1343 F1344 K1351 G1354 D1355 W1363 G1364 E1365 L1366 R1367 R1370 V1378 V1381 GLU

• Molecule 1: RIM-binding protein, isoform F

Chain J:

3% 79% 11% 10%

GLY PRO LEU GLY SER PRO GLU F1317 M1323 F1324 D1325 Q1345 D1355 K1356 Y1362 W1363 R1370 S1379 E1382
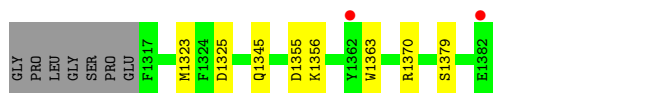
• Molecule 2: Voltage-dependent calcium channel type A subunit alpha-1

Chain a:

6% 65% 6% 29%

ACE ILE G1686 P1693 S1697 THR LEU NH2
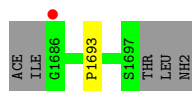
• Molecule 2: Voltage-dependent calcium channel type A subunit alpha-1

Chain b:

6% 59% 41%
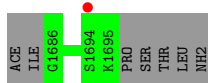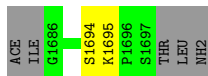
ACE ILE G1686 S1694 K1695 PRO SER THR LEU NH2

- Molecule 2: Voltage-dependent calcium channel type A subunit alpha-1

Chain c: 59%   12%   29%

ACE ILE G1686 S1694 K1695 P1696 S1697 THR LEU NH2

- Molecule 2: Voltage-dependent calcium channel type A subunit alpha-1

Chain d: 65%   6%   29%

ACE ILE G1686 P1693 S1697 THR LEU NH2

- Molecule 2: Voltage-dependent calcium channel type A subunit alpha-1

Chain e: 59%   6%   35%

ACE1684 R1688 S1694 LYS PRO SER THR LEU NH2

- Molecule 2: Voltage-dependent calcium channel type A subunit alpha-1

Chain f: 53%   6%   41%

ACE1684 I1685 P1693 SER LYS PRO SER THR LEU NH2

- Molecule 2: Voltage-dependent calcium channel type A subunit alpha-1

Chain g: 47%   53%

ACE ILE G1686 P1693 SER LYS PRO SER THR LEU NH2

- Molecule 2: Voltage-dependent calcium channel type A subunit alpha-1

12%

Chain h: 47%   53%

ACE ILE G1686 P1691 T1692 P1693 SER LYS PRO SER THR LEU NH2

- Molecule 2: Voltage-dependent calcium channel type A subunit alpha-1

Chain i:

47%　　　　　　53%

ACE ILE G1686 P1693 SER LYS PRO SER THR LEU NH2
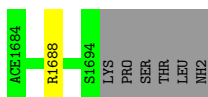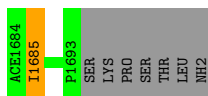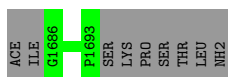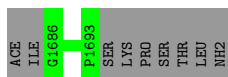
• Molecule 2: Voltage-dependent calcium channel type A subunit alpha-1

Chain j:

59%　　　　12%　　　29%

ACE ILE G1686 R1687 R1688 P1696 S1697 THR LEU NH2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	58.30Å 122.22Å 68.54Å 90.00° 113.17° 90.00°	Depositor
Resolution (Å)	43.87 – 2.64	Depositor
	43.87 – 2.64	EDS
% Data completeness (in resolution range)	97.2 (43.87-2.64)	Depositor
	97.2 (43.87-2.64)	EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.16 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.255 , 0.312	Depositor
	0.257 , 0.320	DCC
R_{free} test set	1262 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	35.9	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 56.9	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	6239	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.63 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.1635e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

---

[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 ⓘ

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

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	0.33	0/545	0.55	0/737
1	B	0.30	0/545	0.50	0/737
1	C	0.32	0/571	0.54	0/772
1	D	0.33	0/545	0.62	0/737
1	E	0.34	0/555	0.57	0/749
1	F	0.35	0/555	0.57	0/749
1	G	0.32	0/555	0.51	0/749
1	H	0.30	0/533	0.56	0/721
1	I	0.28	0/546	0.56	0/739
1	J	0.30	0/555	0.55	0/749
2	a	0.27	0/93	0.80	0/126
2	b	0.22	0/79	0.75	0/106
2	c	0.30	0/93	0.74	0/126
2	d	0.28	0/93	0.71	0/126
2	e	0.28	0/79	0.62	0/108
2	f	0.30	0/73	0.84	0/100
2	g	0.22	0/64	0.58	0/87
2	h	0.32	0/64	0.84	0/87
2	i	0.26	0/64	0.49	0/87
2	j	0.28	0/93	0.69	0/126
All	All	0.31	0/6300	0.58	0/8518

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	528	0	470	15	0
1	B	528	0	470	10	0
1	C	549	0	486	8	0
1	D	528	0	470	11	0
1	E	538	0	476	9	0
1	F	538	0	476	9	0
1	G	538	0	477	12	0
1	H	517	0	462	5	0
1	I	527	0	468	9	0
1	J	538	0	477	4	0
2	a	90	0	97	0	0
2	b	77	0	85	0	0
2	c	90	0	97	0	0
2	d	90	0	97	0	0
2	e	79	0	87	0	0
2	f	73	0	82	0	0
2	g	62	0	67	0	0
2	h	62	0	67	0	0
2	i	62	0	67	0	0
2	j	90	0	97	0	0
3	B	1	0	0	0	0
4	A	16	0	0	1	0
4	B	19	0	0	0	0
4	C	9	0	0	0	0
4	D	10	0	0	0	0
4	E	14	0	0	0	0
4	F	16	0	0	1	0
4	G	10	0	0	2	1
4	H	3	0	0	1	0
4	I	6	0	0	1	1
4	J	14	0	0	0	0
4	a	3	0	0	0	0
4	b	1	0	0	0	0
4	c	1	0	0	0	0
4	d	1	0	0	0	0
4	e	4	0	0	0	0
4	f	3	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	g	1	0	0	0	0
4	j	3	0	0	0	0
All	All	6239	0	5575	80	1

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.

The worst 5 of 80 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1348:ASP:OD2	1:C:1367:ARG:NH2	2.16	0.78
1:I:1319:TYR:OH	1:I:1351:LYS:NZ	2.19	0.76
1:J:1323:MET:SD	1:J:1379:SER:OG	2.45	0.74
1:G:1356:LYS:HE2	1:G:1360:GLY:HA2	1.70	0.73
1:E:1317:PHE:CZ	1:E:1351:LYS:HD2	2.25	0.71

All (1) 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)
4:G:1403:HOH:O	4:I:1401:HOH:O[2_455]	2.18	0.02

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	63/73 (86%)	63 (100%)	0	0	100	100
1	B	63/73 (86%)	63 (100%)	0	0	100	100
1	C	65/73 (89%)	65 (100%)	0	0	100	100
1	D	63/73 (86%)	63 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	64/73 (88%)	64 (100%)	0	0	100	100
1	F	64/73 (88%)	64 (100%)	0	0	100	100
1	G	64/73 (88%)	64 (100%)	0	0	100	100
1	H	62/73 (85%)	62 (100%)	0	0	100	100
1	I	64/73 (88%)	62 (97%)	2 (3%)	0	100	100
1	J	64/73 (88%)	64 (100%)	0	0	100	100
2	a	10/17 (59%)	8 (80%)	1 (10%)	1 (10%)	0	0
2	b	8/17 (47%)	7 (88%)	1 (12%)	0	100	100
2	c	10/17 (59%)	8 (80%)	1 (10%)	1 (10%)	0	0
2	d	10/17 (59%)	7 (70%)	2 (20%)	1 (10%)	0	0
2	e	9/17 (53%)	9 (100%)	0	0	100	100
2	f	8/17 (47%)	6 (75%)	1 (12%)	1 (12%)	0	0
2	g	6/17 (35%)	6 (100%)	0	0	100	100
2	h	6/17 (35%)	6 (100%)	0	0	100	100
2	i	6/17 (35%)	6 (100%)	0	0	100	100
2	j	10/17 (59%)	7 (70%)	2 (20%)	1 (10%)	0	0
All	All	719/900 (80%)	704 (98%)	10 (1%)	5 (1%)	22	32

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	j	1696	PRO
2	a	1693	PRO
2	c	1694	SER
2	d	1693	PRO
2	f	1685	ILE

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	56/62 (90%)	55 (98%)	1 (2%)	59	75
1	B	56/62 (90%)	56 (100%)	0	100	100
1	C	58/62 (94%)	58 (100%)	0	100	100
1	D	56/62 (90%)	56 (100%)	0	100	100
1	E	57/62 (92%)	57 (100%)	0	100	100
1	F	57/62 (92%)	57 (100%)	0	100	100
1	G	57/62 (92%)	57 (100%)	0	100	100
1	H	55/62 (89%)	52 (94%)	3 (6%)	21	33
1	I	56/62 (90%)	55 (98%)	1 (2%)	59	75
1	J	57/62 (92%)	57 (100%)	0	100	100
2	a	11/14 (79%)	11 (100%)	0	100	100
2	b	9/14 (64%)	9 (100%)	0	100	100
2	c	11/14 (79%)	10 (91%)	1 (9%)	9	13
2	d	11/14 (79%)	11 (100%)	0	100	100
2	e	9/14 (64%)	8 (89%)	1 (11%)	6	8
2	f	8/14 (57%)	7 (88%)	1 (12%)	4	5
2	g	7/14 (50%)	7 (100%)	0	100	100
2	h	7/14 (50%)	7 (100%)	0	100	100
2	i	7/14 (50%)	7 (100%)	0	100	100
2	j	11/14 (79%)	10 (91%)	1 (9%)	9	13
All	All	656/760 (86%)	647 (99%)	9 (1%)	67	80

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	f	1685	ILE
2	j	1688	ARG
1	H	1378	VAL
1	I	1321	VAL
2	c	1695	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	1375	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is 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 ⓘ

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	65/73 (89%)	-0.01	0	100	100	31, 42, 54, 71	0
1	B	65/73 (89%)	0.03	0	100	100	32, 40, 53, 64	0
1	C	66/73 (90%)	0.02	0	100	100	30, 42, 57, 72	0
1	D	65/73 (89%)	0.19	1 (1%)	73	71	35, 45, 70, 76	0
1	E	66/73 (90%)	0.21	1 (1%)	73	71	34, 48, 69, 99	0
1	F	66/73 (90%)	0.19	0	100	100	29, 46, 72, 89	0
1	G	66/73 (90%)	0.12	2 (3%)	50	46	36, 47, 61, 63	0
1	H	64/73 (87%)	1.31	14 (21%)	0	0	46, 75, 107, 138	0
1	I	65/73 (89%)	0.61	6 (9%)	9	7	39, 58, 77, 86	0
1	J	66/73 (90%)	0.16	2 (3%)	50	46	35, 47, 66, 83	0
2	a	12/17 (70%)	0.52	1 (8%)	11	9	43, 56, 84, 85	0
2	b	10/17 (58%)	0.47	1 (10%)	7	5	41, 51, 94, 130	0
2	c	12/17 (70%)	0.41	0	100	100	41, 48, 84, 85	0
2	d	12/17 (70%)	0.56	0	100	100	40, 60, 79, 115	0
2	e	10/17 (58%)	0.46	0	100	100	50, 65, 73, 74	0
2	f	9/17 (52%)	0.52	0	100	100	48, 55, 75, 79	0
2	g	8/17 (47%)	0.05	0	100	100	44, 48, 58, 70	0
2	h	8/17 (47%)	1.16	2 (25%)	0	0	76, 87, 106, 107	0
2	i	8/17 (47%)	0.39	0	100	100	52, 58, 67, 82	0
2	j	12/17 (70%)	0.53	0	100	100	53, 61, 77, 91	0
All	All	755/900 (83%)	0.31	30 (3%)	38	35	29, 48, 84, 138	0

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	1373	VAL	5.1
1	H	1362	TYR	4.7
1	H	1350	ILE	4.6
1	H	1353	PHE	3.7
1	H	1374	PRO	3.6

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 ⓘ

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	CA	B	1401	1/1	0.92	0.07	46,46,46,46	0

6.5　Other polymers ⓘ

There are no such residues in this entry.