Full wwPDB X-ray Structure Validation 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)

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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

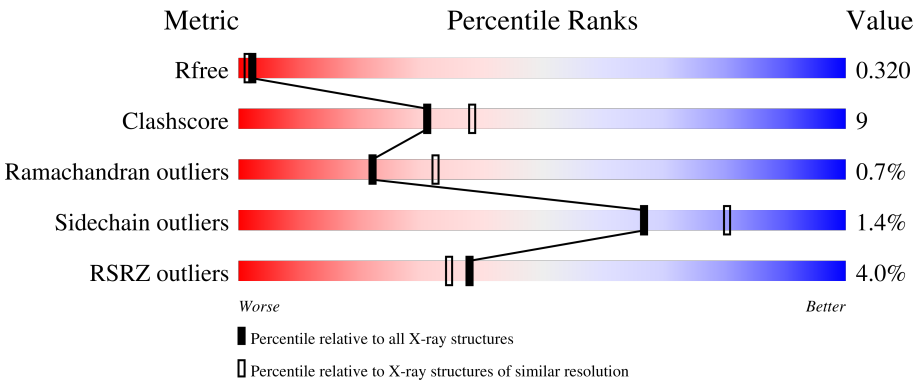
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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	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%

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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 (i)

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
			Total	C	N	O	S			
1	A	65	528	336	85	103	4	0	0	0
1	B	65	528	336	85	103	4	0	0	0
1	C	66	549	351	87	107	4	0	1	0
1	D	65	528	336	85	103	4	0	0	0
1	E	66	538	341	86	107	4	0	0	0
1	F	66	538	341	86	107	4	0	0	0
1	G	66	538	341	86	107	4	0	0	0
1	H	64	517	327	84	102	4	0	0	0
1	I	65	527	333	85	105	4	0	1	0
1	J	66	538	341	86	107	4	0	0	0

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

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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

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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
			Total	C	N	O			
2	a	12	90	56	19	15	0	0	0
			Total	C	N	O			
2	b	10	77	48	17	12	0	0	0
			Total	C	N	O			
2	c	12	90	56	19	15	0	0	0
			Total	C	N	O			
2	d	12	90	56	19	15	0	0	0
			Total	C	N	O			
2	e	11	79	50	16	13	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	f	10	73	47	15	11	0	0	0
2	g	8	62	39	14	9	0	0	0
2	h	8	62	39	14	9	0	0	0
2	i	8	62	39	14	9	0	0	0
2	j	12	90	56	19	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
			Total	Ca		
3	B	1	1	1	0	0

- Molecule 4 is water.

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

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: RIM-binding protein, isoform F

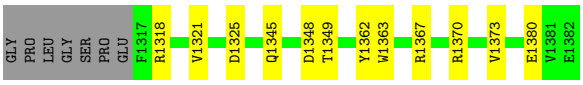
Chain A:

• Molecule 1: RIM-binding protein, isoform F

Chain B:

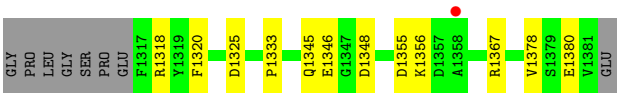
• Molecule 1: RIM-binding protein, isoform F

Chain C:



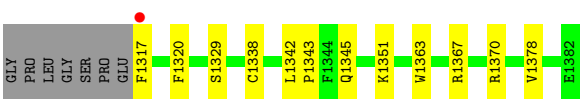
• Molecule 1: RIM-binding protein, isoform F

Chain D:



• Molecule 1: RIM-binding protein, isoform F

Chain E:



• Molecule 1: RIM-binding protein, isoform F

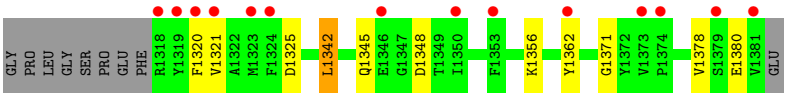
Chain F:

• Molecule 1: RIM-binding protein, isoform F

Chain G:

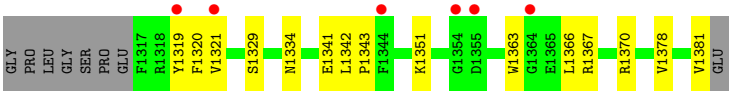
• Molecule 1: RIM-binding protein, isoform F

Chain H:



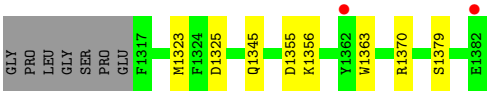
• Molecule 1: RIM-binding protein, isoform F

Chain I:



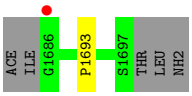
• Molecule 1: RIM-binding protein, isoform F

Chain J:



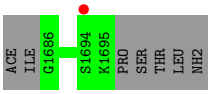
• Molecule 2: Voltage-dependent calcium channel type A subunit alpha-1

Chain a:



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

Chain b:

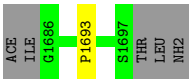


• Molecule 2: Voltage-dependent calcium channel type A subunit alpha-1

Chain c:

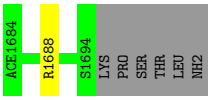
• Molecule 2: Voltage-dependent calcium channel type A subunit alpha-1

Chain d:



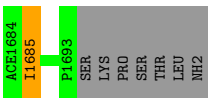
• Molecule 2: Voltage-dependent calcium channel type A subunit alpha-1

Chain e:



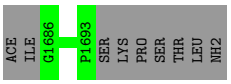
• Molecule 2: Voltage-dependent calcium channel type A subunit alpha-1

Chain f:



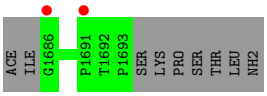
• Molecule 2: Voltage-dependent calcium channel type A subunit alpha-1

Chain g:



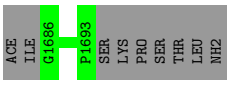
• Molecule 2: Voltage-dependent calcium channel type A subunit alpha-1

Chain h:



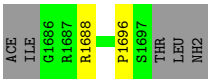
• Molecule 2: Voltage-dependent calcium channel type A subunit alpha-1

Chain i: 47% 53%



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

Chain j: 59% 12% 29%



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 43.87 – 2.64	Depositor EDS
% Data completeness (in resolution range)	97.2 (43.87-2.64) 97.2 (43.87-2.64)	Depositor 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 0.257 , 0.320	Depositor 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 (i)

5.1 Standard geometry (i)

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

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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.

All (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
1:E:1317:PHE:HZ	1:E:1351:LYS:HD2	1.56	0.70
1:G:1348:ASP:OD2	1:G:1367:ARG:NH2	2.23	0.69
1:D:1355:ASP:OD1	1:D:1356:LYS:N	2.24	0.68
1:A:1334:ASN:ND2	1:A:1341:GLU:OE2	2.27	0.68
1:I:1334:ASN:ND2	1:I:1341:GLU:OE2	2.24	0.67
1:A:1369:ARG:NH1	1:B:1327:ASP:OD2	2.28	0.66
1:D:1348:ASP:OD2	1:D:1367:ARG:NH2	2.28	0.66
1:G:1365:GLU:OE2	4:G:1401:HOH:O	2.11	0.66
1:I:1329:SER:O	4:I:1401:HOH:O	2.12	0.66
1:G:1339:ASP:OD2	4:G:1402:HOH:O	2.14	0.65
1:A:1348:ASP:OD2	1:A:1367:ARG:NH2	2.32	0.63
1:A:1331:MET:O	1:C:1370:ARG:NH1	2.32	0.63
1:C:1363[B]:TRP:CH2	1:C:1370:ARG:HD3	2.33	0.63
1:A:1379:SER:HB3	1:G:1319:TYR:HE2	1.65	0.62
1:D:1345:GLN:OE1	1:E:1367:ARG:NH2	2.33	0.61
1:F:1357:ASP:OD2	4:F:1401:HOH:O	2.17	0.59
1:A:1327:ASP:OD2	1:B:1369:ARG:NH1	2.36	0.58
1:A:1379:SER:HB3	1:G:1319:TYR:CE2	2.40	0.56
1:E:1329:SER:HB3	1:E:1338:CYS:SG	2.46	0.56
1:J:1363:TRP:CH2	1:J:1370:ARG:HD3	2.41	0.55
1:F:1363:TRP:CH2	1:F:1370:ARG:HD3	2.42	0.55
1:F:1351:LYS:HE3	1:F:1353:PHE:CZ	2.43	0.54
1:B:1334:ASN:ND2	1:B:1341:GLU:OE2	2.42	0.53
1:G:1318:ARG:HD2	1:G:1380:GLU:OE2	2.10	0.52
1:J:1355:ASP:OD1	1:J:1356:LYS:N	2.37	0.52
1:H:1342:LEU:HD13	1:H:1371:GLY:HA3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1318:ARG:HH11	1:D:1380:GLU:CD	2.14	0.51
1:D:1345:GLN:OE1	1:E:1345:GLN:NE2	2.43	0.51
1:A:1374:PRO:HG2	1:A:1377:MET:HG3	1.92	0.51
1:D:1318:ARG:HD2	1:D:1380:GLU:HG3	1.93	0.50
1:D:1320:PHE:HB3	1:D:1378:VAL:HB	1.94	0.49
1:D:1318:ARG:NH1	1:D:1380:GLU:OE2	2.46	0.49
1:D:1345:GLN:NE2	1:E:1345:GLN:HG3	2.27	0.48
1:A:1333:PRO:HB3	1:C:1363[B]:TRP:CE3	2.47	0.48
1:G:1363:TRP:CH2	1:G:1370:ARG:HD3	2.49	0.48
1:G:1320:PHE:HB3	1:G:1378:VAL:HG22	1.96	0.47
1:G:1329:SER:HB3	1:G:1338:CYS:SG	2.55	0.47
1:I:1319:TYR:O	1:I:1381:VAL:HG22	2.13	0.47
1:I:1363:TRP:CH2	1:I:1370:ARG:HD3	2.49	0.46
1:E:1363:TRP:CH2	1:E:1370:ARG:HD2	2.51	0.46
1:J:1325:ASP:HA	1:J:1345:GLN:HA	1.97	0.46
1:B:1320:PHE:CE1	1:B:1380:GLU:HB3	2.51	0.46
1:D:1333:PRO:HB3	1:I:1363:TRP:CE3	2.50	0.46
1:F:1351:LYS:HE3	1:F:1353:PHE:HZ	1.80	0.46
1:A:1320:PHE:HB3	1:A:1378:VAL:HB	1.98	0.46
1:G:1320:PHE:HD2	1:G:1378:VAL:HG13	1.81	0.46
1:E:1342:LEU:HA	1:E:1343:PRO:HD3	1.75	0.46
1:B:1362:TYR:N	1:B:1373:VAL:O	2.43	0.45
1:F:1329:SER:HB3	1:F:1338:CYS:SG	2.56	0.45
1:I:1342:LEU:HA	1:I:1343:PRO:HD3	1.81	0.44
1:C:1321:VAL:HG12	1:C:1349:THR:HG22	1.98	0.44
1:B:1370:ARG:HD2	1:F:1331:MET:HA	1.99	0.44
1:C:1325:ASP:HA	1:C:1345:GLN:HA	1.99	0.43
1:F:1334:ASN:ND2	1:F:1341:GLU:OE2	2.38	0.43
1:H:1320:PHE:HE1	1:H:1380:GLU:HG2	1.83	0.43
1:G:1319:TYR:O	1:G:1381:VAL:HG22	2.18	0.43
1:F:1321:VAL:HG22	1:F:1349:THR:HG22	2.01	0.43
1:A:1342:LEU:HA	1:A:1343:PRO:HD3	1.80	0.43
1:B:1320:PHE:HB3	1:B:1378:VAL:HB	2.00	0.43
1:D:1325:ASP:OD1	1:D:1346:GLU:HG3	2.18	0.43
1:H:1325:ASP:O	4:H:1401:HOH:O	2.21	0.43
1:H:1345:GLN:HB3	1:H:1348:ASP:OD1	2.20	0.42
1:I:1366:LEU:HD11	1:I:1367:ARG:NH1	2.34	0.42
1:A:1369:ARG:NH1	1:B:1329:SER:OG	2.52	0.42
1:B:1325:ASP:HA	1:B:1345:GLN:HA	2.01	0.42
1:A:1365:GLU:HB2	1:A:1370:ARG:HG2	2.02	0.42
1:H:1356:LYS:HB2	1:H:1362:TYR:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1320:PHE:HB3	1:I:1378:VAL:HG13	2.02	0.42
1:A:1342:LEU:HA	1:A:1342:LEU:HD12	1.87	0.41
1:C:1362:TYR:O	1:C:1373:VAL:N	2.49	0.41
1:C:1318:ARG:HD2	1:C:1380:GLU:OE2	2.19	0.41
1:A:1333:PRO:O	4:A:1401:HOH:O	2.21	0.41
1:B:1320:PHE:CZ	1:B:1380:GLU:HB3	2.56	0.41
1:E:1320:PHE:HB3	1:E:1378:VAL:HB	2.03	0.41
1:F:1376:ASN:OD1	1:F:1376:ASN:N	2.54	0.40

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 (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	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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 (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	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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1342	LEU
1	H	1321	VAL
1	H	1342	LEU
1	H	1378	VAL
1	I	1321	VAL
2	c	1695	LYS
2	e	1688	ARG
2	f	1685	ILE
2	j	1688	ARG

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 (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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 (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%)	-0.01	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

All (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
1	H	1323	MET	3.3
1	I	1355	ASP	3.2
1	E	1317	PHE	3.1
1	H	1321	VAL	3.1
1	H	1318	ARG	3.1
1	H	1324	PHE	3.0
2	h	1691	PRO	2.9
2	b	1694	SER	2.8
1	H	1320	PHE	2.8
1	H	1346	GLU	2.7
1	I	1364	GLY	2.7
1	I	1354	GLY	2.5
1	H	1319	TYR	2.5
2	a	1686	GLY	2.5
1	I	1344	PHE	2.4
1	J	1362	TYR	2.3
1	H	1379	SER	2.3
1	G	1321	VAL	2.3
1	H	1381	VAL	2.3
1	I	1321	VAL	2.3
1	G	1382	GLU	2.2
2	h	1686	GLY	2.2
1	I	1319	TYR	2.1
1	J	1382	GLU	2.0
1	D	1358	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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 (i)

There are no such residues in this entry.