



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:51 PM UTC

PDB ID : 4Z89 / pdb_00004z89
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

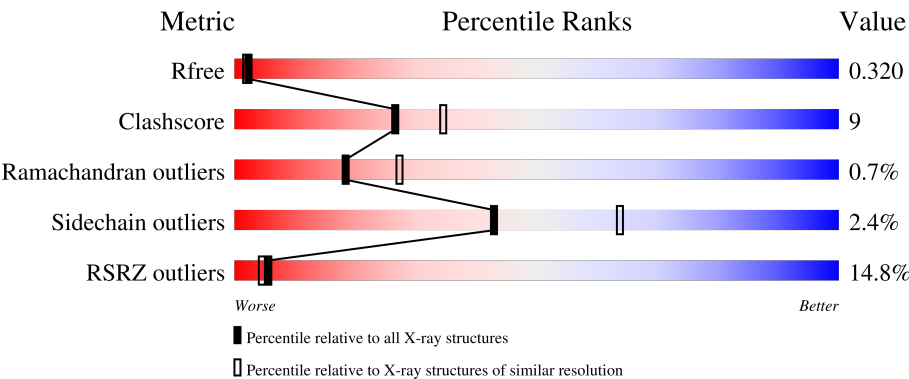
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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}	180053	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	73	63% 25% 11%
1	B	73	68% 21% 11%
1	C	73	71% 19% 10%
1	D	73	70% 19% 11%
1	E	73	68% 21% 10%

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Mol	Chain	Length	Quality of chain
1	F	73	
1	G	73	
1	H	73	
1	I	73	
1	J	73	
2	a	17	
2	b	17	
2	c	17	
2	d	17	
2	e	17	
2	f	17	
2	g	17	
2	h	17	
2	i	17	
2	j	17	

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

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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
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			

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

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 (CCD ID: CA) (formula: Ca).

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

- Molecule 4 is water.

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

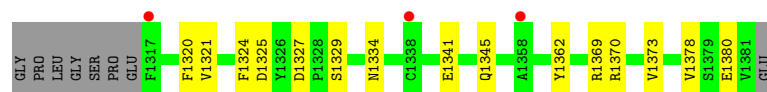
3 Residue-property plots [i](#)

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



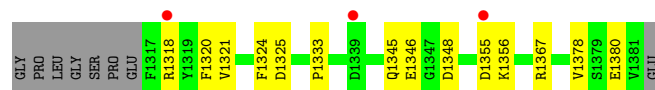
- Molecule 1: RIM-binding protein, isoform F



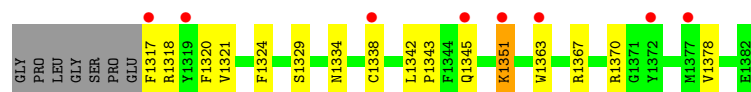
- Molecule 1: RIM-binding protein, isoform F



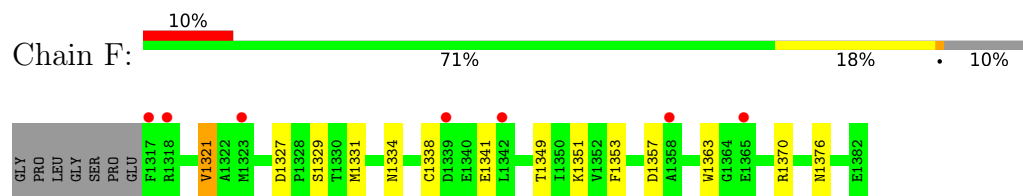
- Molecule 1: RIM-binding protein, isoform F



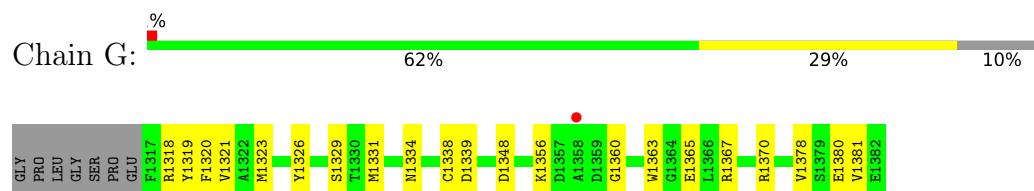
- Molecule 1: RIM-binding protein, isoform F



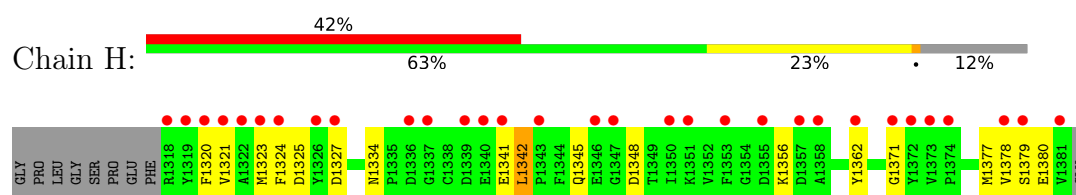
- Molecule 1: RIM-binding protein, isoform F



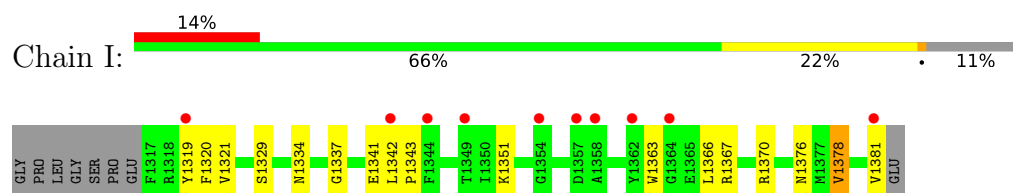
- Molecule 1: RIM-binding protein, isoform F



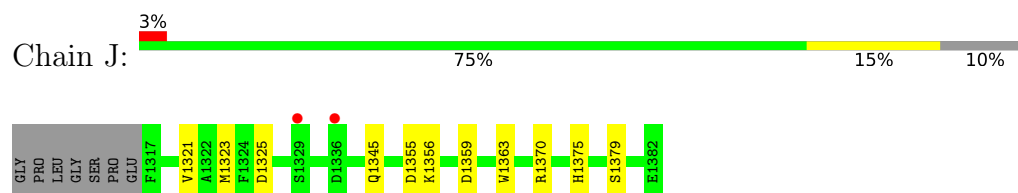
- Molecule 1: RIM-binding protein, isoform F



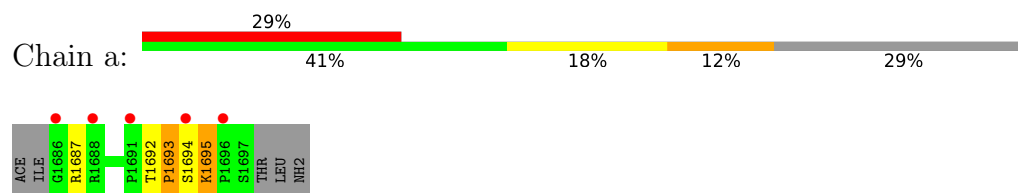
- Molecule 1: RIM-binding protein, isoform F



- Molecule 1: RIM-binding protein, isoform F

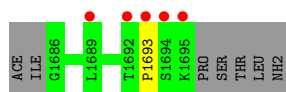


- Molecule 2: Voltage-dependent calcium channel type A subunit alpha-1

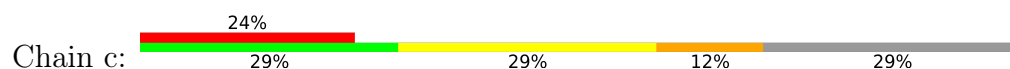


- Molecule 2: Voltage-dependent calcium channel type A subunit alpha-1

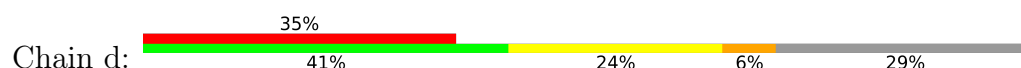




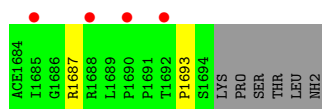
- Molecule 2: Voltage-dependent calcium channel type A subunit alpha-1



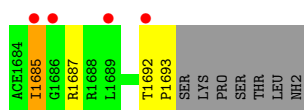
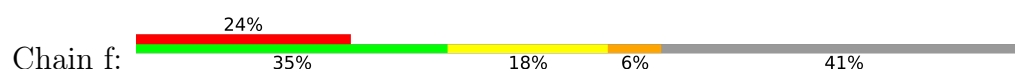
- Molecule 2: Voltage-dependent calcium channel type A subunit alpha-1



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



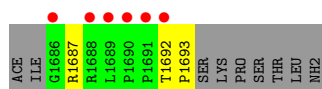
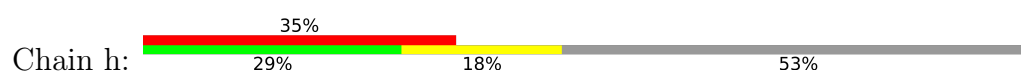
- Molecule 2: Voltage-dependent calcium channel type A subunit alpha-1



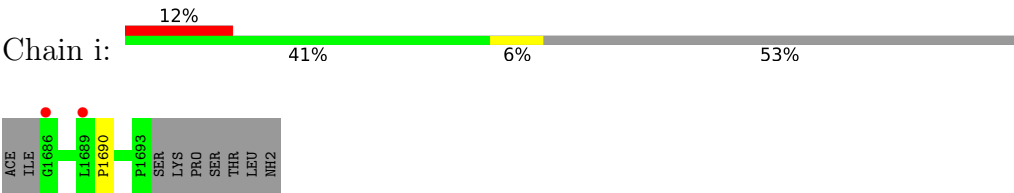
- Molecule 2: Voltage-dependent calcium channel type A subunit alpha-1



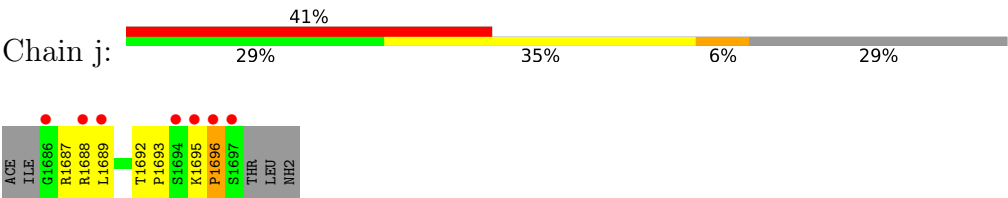
- Molecule 2: Voltage-dependent calcium channel type A subunit alpha-1



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



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



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	3.16 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.255 , 0.312 0.258 , 0.320	Depositor DCC
R_{free} test set	1262 reflections (4.77%)	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)	0.36 , 62.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.37	0/545	0.87	0/737
1	B	0.35	0/545	0.84	0/737
1	C	0.35	0/571	0.83	0/772
1	D	0.39	0/545	0.92	0/737
1	E	0.41	0/555	1.02	3/749 (0.4%)
1	F	0.40	0/555	0.91	2/749 (0.3%)
1	G	0.37	0/555	0.91	2/749 (0.3%)
1	H	0.36	0/533	1.04	5/721 (0.7%)
1	I	0.36	0/546	0.94	1/739 (0.1%)
1	J	0.35	0/555	0.87	0/749
2	a	0.43	0/93	1.29	2/126 (1.6%)
2	b	0.30	0/79	0.93	0/106
2	c	0.44	0/93	1.39	2/126 (1.6%)
2	d	0.43	0/93	1.06	0/126
2	e	0.43	0/79	0.99	0/108
2	f	0.40	0/73	0.88	0/100
2	g	0.37	0/64	0.79	0/87
2	h	0.50	0/64	1.29	0/87
2	i	0.35	0/64	0.65	0/87
2	j	0.52	0/93	1.27	0/126
All	All	0.38	0/6300	0.94	17/8518 (0.2%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	1334	ASN	CA-C-N	7.22	126.92	119.56
1	G	1334	ASN	C-N-CA	7.22	126.92	119.56
1	E	1334	ASN	CA-C-N	6.88	126.57	119.56
1	E	1334	ASN	C-N-CA	6.88	126.57	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	1327	ASP	CA-C-N	5.77	126.17	119.47
1	F	1327	ASP	C-N-CA	5.77	126.17	119.47
1	E	1318	ARG	N-CA-C	5.56	118.28	109.50
1	H	1377	MET	N-CA-C	-5.47	106.51	114.12
1	H	1334	ASN	CA-C-N	5.45	125.06	119.56
1	H	1334	ASN	C-N-CA	5.45	125.06	119.56
2	c	1692	THR	CA-C-N	5.35	126.53	119.84
2	c	1692	THR	C-N-CA	5.35	126.53	119.84
1	I	1337	GLY	N-CA-C	5.22	120.07	113.24
2	a	1695	LYS	CA-C-N	5.06	126.16	119.84
2	a	1695	LYS	C-N-CA	5.06	126.16	119.84
1	H	1327	ASP	CA-C-N	5.04	125.31	119.47
1	H	1327	ASP	C-N-CA	5.04	125.31	119.47

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	17	0
1	B	528	0	470	11	0
1	C	549	0	486	11	0
1	D	528	0	470	12	0
1	E	538	0	476	10	0
1	F	538	0	476	11	0
1	G	538	0	477	14	0
1	H	517	0	462	8	0
1	I	527	0	468	10	0
1	J	538	0	477	6	0
2	a	90	0	97	4	0
2	b	77	0	85	1	0
2	c	90	0	97	4	0
2	d	90	0	97	3	0
2	e	79	0	87	2	0
2	f	73	0	82	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	g	62	0	67	0	0
2	h	62	0	67	3	0
2	i	62	0	67	1	0
2	j	90	0	97	4	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	1	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	1	0
4	f	3	0	0	0	0
4	g	1	0	0	0	0
4	j	3	0	0	0	0
All	All	6239	0	5575	109	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 (109) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:1376:ASN:HB2	2:f:1692:THR:HG22	1.79	0.65
1:G:1321:VAL:HG13	1:G:1323:MET:HE3	1.79	0.64
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:D:1318:ARG:HH11	1:D:1380:GLU:CD	2.14	0.55
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:D:1324:PHE:CE1	2:d:1696:PRO:HA	2.42	0.54
1:F:1351:LYS:HE3	1:F:1353:PHE:CZ	2.43	0.54
1:J:1375:HIS:CD2	2:j:1689:LEU:HD21	2.43	0.54
1:H:1323:MET:HE2	1:H:1379:SER:HB3	1.90	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
2:d:1694:SER:OG	2:d:1695:LYS:N	2.43	0.51
1:H:1342:LEU:HD13	1:H:1371:GLY:HA3	1.93	0.51
1:D:1345:GLN:OE1	1:E:1345:GLN:NE2	2.43	0.51
2:a:1694:SER:OG	2:a:1695:LYS:N	2.44	0.51
1:A:1374:PRO:HG2	1:A:1377:MET:HG3	1.92	0.51
1:H:1341:GLU:OE2	2:h:1687:ARG:NH2	2.44	0.51
1:D:1318:ARG:HD2	1:D:1380:GLU:HG3	1.93	0.50
1:I:1376:ASN:ND2	2:i:1690:PRO:O	2.44	0.49
1:A:1341:GLU:HG3	2:a:1687:ARG:HH21	1.76	0.49
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:C:1340:GLU:HB3	2:c:1687:ARG:HH21	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:d:1692:THR:HA	2:d:1693:PRO:HD3	1.76	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
2:j:1692:THR:HA	2:j:1693:PRO:HD3	1.71	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:H:1324:PHE:CD2	2:h:1693:PRO:HG2	2.51	0.45
2:j:1695:LYS:HA	2:j:1696:PRO:HD3	1.53	0.45
2:c:1692:THR:HA	2:c:1693:PRO:HD3	1.65	0.45
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
2:e:1687:ARG:NE	4:e:1802:HOH:O	2.45	0.45
2:c:1695:LYS:HG3	2:c:1696:PRO:HD2	1.99	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:F:1334:ASN:ND2	2:f:1687:ARG:HG2	2.32	0.44
2:h:1692:THR:HA	2:h:1693:PRO:HD3	1.83	0.44
1:A:1340:GLU:HB2	2:a:1687:ARG:HH22	1.82	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:E:1324:PHE:CE2	2:e:1693:PRO:HD2	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:I:1320:PHE:HB3	1:I:1378:VAL:HG13	2.02	0.42
2:f:1692:THR:HA	2:f:1693:PRO:HD3	1.86	0.41
1:C:1370:ARG:NH2	4:a:1801:HOH:O	2.33	0.41
1:G:1326:TYR:HD1	1:G:1331:MET:HE2	1.84	0.41
2:a:1692:THR:HA	2:a:1693:PRO:HD3	1.82	0.41
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:J:1359:ASP:HB3	2:j:1687:ARG:O	2.20	0.40
1:B:1324:PHE:CD2	2:b:1693:PRO:HG2	2.56	0.40
1:C:1375:HIS:CE1	2:c:1689:LEU:HD21	2.56	0.40
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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%)	18	27

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%)	54 (96%)	2 (4%)	31	50
1	B	56/62 (90%)	55 (98%)	1 (2%)	51	71
1	C	58/62 (94%)	58 (100%)	0	100	100
1	D	56/62 (90%)	55 (98%)	1 (2%)	51	71
1	E	57/62 (92%)	55 (96%)	2 (4%)	32	51
1	F	57/62 (92%)	56 (98%)	1 (2%)	51	71
1	G	57/62 (92%)	57 (100%)	0	100	100
1	H	55/62 (89%)	52 (94%)	3 (6%)	19	32
1	I	56/62 (90%)	54 (96%)	2 (4%)	31	50
1	J	57/62 (92%)	56 (98%)	1 (2%)	51	71
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%)	9 (100%)	0	100	100
2	f	8/14 (57%)	7 (88%)	1 (12%)	4	6
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%)	640 (98%)	16 (2%)	43	64

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1321	VAL
1	A	1342	LEU
1	B	1321	VAL
1	D	1321	VAL
1	E	1321	VAL
1	E	1351	LYS
1	F	1321	VAL
1	H	1321	VAL
1	H	1342	LEU
1	H	1378	VAL
1	I	1321	VAL

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	1375	HIS
1	F	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 oligosaccharides 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(Å ²)	Q<0.9
1	A	65/73 (89%)	0.55	1 (1%) 72 69	31, 42, 54, 71	0
1	B	65/73 (89%)	0.64	3 (4%) 37 31	32, 40, 53, 64	0
1	C	66/73 (90%)	0.63	3 (4%) 38 32	20, 42, 57, 72	1 (1%)
1	D	65/73 (89%)	0.86	3 (4%) 37 31	35, 45, 70, 76	0
1	E	66/73 (90%)	1.00	8 (12%) 8 7	34, 48, 69, 99	0
1	F	66/73 (90%)	0.98	7 (10%) 11 9	29, 46, 72, 89	0
1	G	66/73 (90%)	0.73	1 (1%) 72 69	36, 47, 61, 63	0
1	H	64/73 (87%)	2.07	31 (48%) 0 0	46, 75, 107, 138	0
1	I	65/73 (89%)	1.28	10 (15%) 5 4	35, 58, 77, 86	1 (1%)
1	J	66/73 (90%)	0.69	2 (3%) 52 47	35, 47, 66, 83	0
2	a	12/17 (70%)	1.78	5 (41%) 0 0	43, 56, 84, 85	0
2	b	10/17 (58%)	1.74	5 (50%) 0 0	41, 51, 94, 130	0
2	c	12/17 (70%)	1.69	4 (33%) 1 0	41, 48, 84, 85	0
2	d	12/17 (70%)	1.95	6 (50%) 0 0	40, 60, 79, 115	0
2	e	10/17 (58%)	1.64	4 (40%) 1 0	50, 65, 73, 74	0
2	f	9/17 (52%)	1.69	4 (44%) 0 0	48, 55, 75, 79	0
2	g	8/17 (47%)	0.98	0 100 100	44, 48, 58, 70	0
2	h	8/17 (47%)	3.09	6 (75%) 0 0	76, 87, 106, 107	0
2	i	8/17 (47%)	1.62	2 (25%) 2 1	52, 58, 67, 82	0
2	j	12/17 (70%)	1.99	7 (58%) 0 0	53, 61, 77, 91	0
All	All	755/900 (83%)	1.06	112 (14%) 5 4	20, 48, 84, 138	2 (0%)

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	1357[A]	ASP	4.6
1	H	1373	VAL	4.6
1	E	1317	PHE	4.5
1	H	1362	TYR	4.5
2	a	1696	PRO	4.5
1	I	1358	ALA	4.2
2	c	1692	THR	4.2
1	F	1317	PHE	4.1
2	h	1692	THR	4.1
2	h	1690	PRO	4.0
1	H	1340	GLU	4.0
2	d	1694	SER	4.0
2	h	1691	PRO	4.0
2	h	1686	GLY	4.0
1	H	1358	ALA	3.9
2	a	1686	GLY	3.9
1	I	1342	LEU	3.9
1	H	1350	ILE	3.8
2	j	1694	SER	3.8
1	H	1374	PRO	3.7
1	H	1323	MET	3.6
1	H	1381	VAL	3.5
1	F	1339	ASP	3.4
2	b	1694	SER	3.4
1	H	1378	VAL	3.4
1	H	1379	SER	3.3
2	b	1692	THR	3.3
2	h	1689	LEU	3.2
1	H	1339	ASP	3.2
2	i	1689	LEU	3.1
1	E	1338	CYS	3.1
2	c	1694	SER	3.1
1	E	1351	LYS	3.0
1	H	1353	PHE	3.0
1	E	1319	TYR	3.0
1	H	1318	ARG	3.0
2	e	1688	ARG	3.0
1	H	1324	PHE	2.9
1	A	1317	PHE	2.9
1	B	1338	CYS	2.8
1	H	1346	GLU	2.8
1	D	1339	ASP	2.8
1	H	1336	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	1337	GLY	2.7
1	I	1344	PHE	2.7
2	e	1685	ILE	2.7
1	H	1372	TYR	2.7
2	f	1692	THR	2.7
2	d	1697	SER	2.7
1	H	1341	GLU	2.6
2	c	1697	SER	2.6
1	B	1317	PHE	2.6
2	d	1686	GLY	2.6
1	H	1357	ASP	2.6
1	H	1326	TYR	2.6
1	F	1358	ALA	2.6
2	e	1690	PRO	2.6
2	j	1696	PRO	2.6
1	E	1345	GLN	2.6
1	I	1319	TYR	2.6
1	I	1354	GLY	2.6
2	c	1696	PRO	2.6
2	d	1688	ARG	2.5
2	j	1697	SER	2.5
1	D	1318	ARG	2.5
2	a	1688	ARG	2.5
1	F	1323	MET	2.5
2	j	1689	LEU	2.5
1	I	1362	TYR	2.5
1	I	1364	GLY	2.5
1	H	1343	PRO	2.5
1	D	1355	ASP	2.3
2	d	1696	PRO	2.3
1	H	1355	ASP	2.3
1	E	1363	TRP	2.3
2	i	1686	GLY	2.3
1	H	1319	TYR	2.3
2	a	1691	PRO	2.3
2	b	1693	PRO	2.3
1	H	1321	VAL	2.3
1	H	1322	ALA	2.3
1	F	1365	GLU	2.3
2	d	1693	PRO	2.3
1	H	1371	GLY	2.3
2	f	1689	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	J	1329	SER	2.2
2	a	1694	SER	2.2
1	I	1381	VAL	2.2
1	I	1349	THR	2.2
1	J	1336	ASP	2.2
1	C	1320	PHE	2.2
1	B	1358	ALA	2.2
1	G	1358	ALA	2.2
1	F	1318	ARG	2.2
1	H	1320	PHE	2.2
1	E	1372	TYR	2.2
2	b	1695	LYS	2.2
1	H	1351	LYS	2.1
2	j	1695	LYS	2.1
2	h	1688	ARG	2.1
2	j	1686	GLY	2.1
1	H	1327	ASP	2.1
1	C	1317	PHE	2.1
2	e	1692	THR	2.1
1	C	1335	PRO	2.1
1	E	1377	MET	2.1
2	b	1689	LEU	2.1
1	H	1347	GLY	2.1
2	f	1685	ILE	2.1
2	j	1688	ARG	2.0
1	F	1342	LEU	2.0
2	f	1686	GLY	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	CA	B	1401	1/1	0.95	0.09	46,46,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.