



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 4, 2026 – 08:19 PM UTC

PDB ID : 6AXG / pdb_00006axg
Title : Structure of RasGRP4 in complex with HRas
Authors : Kondo, Y.; Iwig, J.S.; Kuriyan, J.
Deposited on : 2017-09-06
Resolution : 3.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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
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

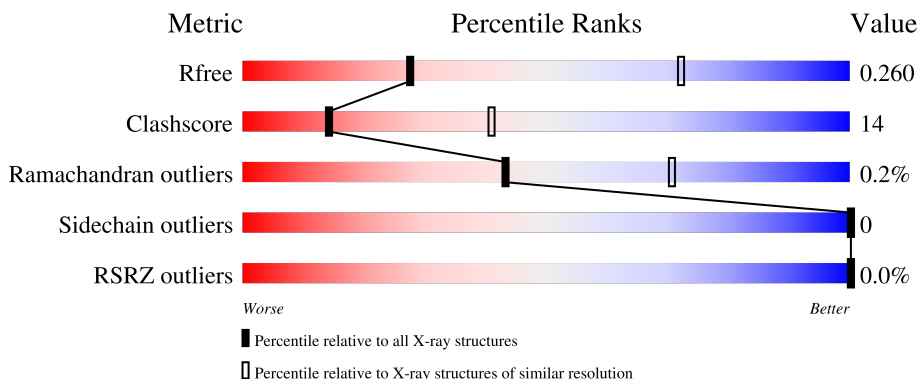
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	418	
1	C	418	
1	E	418	
1	G	418	
1	I	418	

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Mol	Chain	Length	Quality of chain
1	K	418	52% 28% 19%
2	B	170	61% 31% 8%
2	D	170	61% 32% 7%
2	F	170	% 62% 31% 7%
2	H	170	56% 36% • 8%
2	J	170	64% 29% 8%
2	L	170	59% 32% • 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 23168 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 RAS guanyl-releasing protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	0	0
			2659	1678	484	484	13			
1	C	336	Total	C	N	O	S	0	0	0
			2655	1679	484	478	14			
1	E	330	Total	C	N	O	S	0	0	0
			2600	1647	473	467	13			
1	G	320	Total	C	N	O	S	0	0	0
			2552	1621	463	455	13			
1	I	334	Total	C	N	O	S	0	0	0
			2624	1662	477	473	12			
1	K	337	Total	C	N	O	S	0	0	0
			2663	1686	485	478	14			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	43	SER	-	expression tag	UNP Q8TDF6
A	44	ASN	-	expression tag	UNP Q8TDF6
A	45	ALA	-	expression tag	UNP Q8TDF6
C	43	SER	-	expression tag	UNP Q8TDF6
C	44	ASN	-	expression tag	UNP Q8TDF6
C	45	ALA	-	expression tag	UNP Q8TDF6
E	43	SER	-	expression tag	UNP Q8TDF6
E	44	ASN	-	expression tag	UNP Q8TDF6
E	45	ALA	-	expression tag	UNP Q8TDF6
G	43	SER	-	expression tag	UNP Q8TDF6
G	44	ASN	-	expression tag	UNP Q8TDF6
G	45	ALA	-	expression tag	UNP Q8TDF6
I	43	SER	-	expression tag	UNP Q8TDF6
I	44	ASN	-	expression tag	UNP Q8TDF6
I	45	ALA	-	expression tag	UNP Q8TDF6
K	43	SER	-	expression tag	UNP Q8TDF6
K	44	ASN	-	expression tag	UNP Q8TDF6

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Chain	Residue	Modelled	Actual	Comment	Reference
K	45	ALA	-	expression tag	UNP Q8TDF6

- Molecule 2 is a protein called GTPase HRas.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	156	Total	C	N	O	S	0	0	0
			1230	766	214	244	6			
2	D	158	Total	C	N	O	S	0	0	0
			1232	769	207	249	7			
2	F	158	Total	C	N	O	S	0	0	0
			1251	780	215	250	6			
2	H	157	Total	C	N	O	S	0	0	0
			1242	774	213	249	6			
2	J	157	Total	C	N	O	S	0	0	0
			1240	771	216	246	7			
2	L	155	Total	C	N	O	S	0	0	0
			1220	761	212	240	7			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P01112
B	-2	ALA	-	expression tag	UNP P01112
B	-1	MET	-	expression tag	UNP P01112
B	0	ALA	-	expression tag	UNP P01112
D	-3	GLY	-	expression tag	UNP P01112
D	-2	ALA	-	expression tag	UNP P01112
D	-1	MET	-	expression tag	UNP P01112
D	0	ALA	-	expression tag	UNP P01112
F	-3	GLY	-	expression tag	UNP P01112
F	-2	ALA	-	expression tag	UNP P01112
F	-1	MET	-	expression tag	UNP P01112
F	0	ALA	-	expression tag	UNP P01112
H	-3	GLY	-	expression tag	UNP P01112
H	-2	ALA	-	expression tag	UNP P01112
H	-1	MET	-	expression tag	UNP P01112
H	0	ALA	-	expression tag	UNP P01112
J	-3	GLY	-	expression tag	UNP P01112
J	-2	ALA	-	expression tag	UNP P01112
J	-1	MET	-	expression tag	UNP P01112
J	0	ALA	-	expression tag	UNP P01112
L	-3	GLY	-	expression tag	UNP P01112

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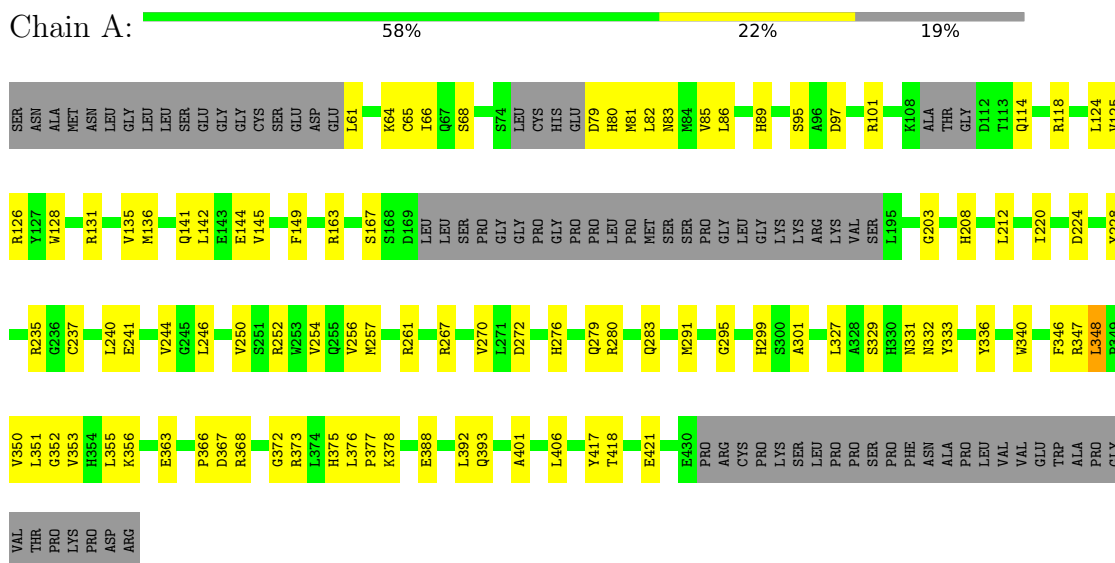
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Chain	Residue	Modelled	Actual	Comment	Reference
L	-2	ALA	-	expression tag	UNP P01112
L	-1	MET	-	expression tag	UNP P01112
L	0	ALA	-	expression tag	UNP P01112

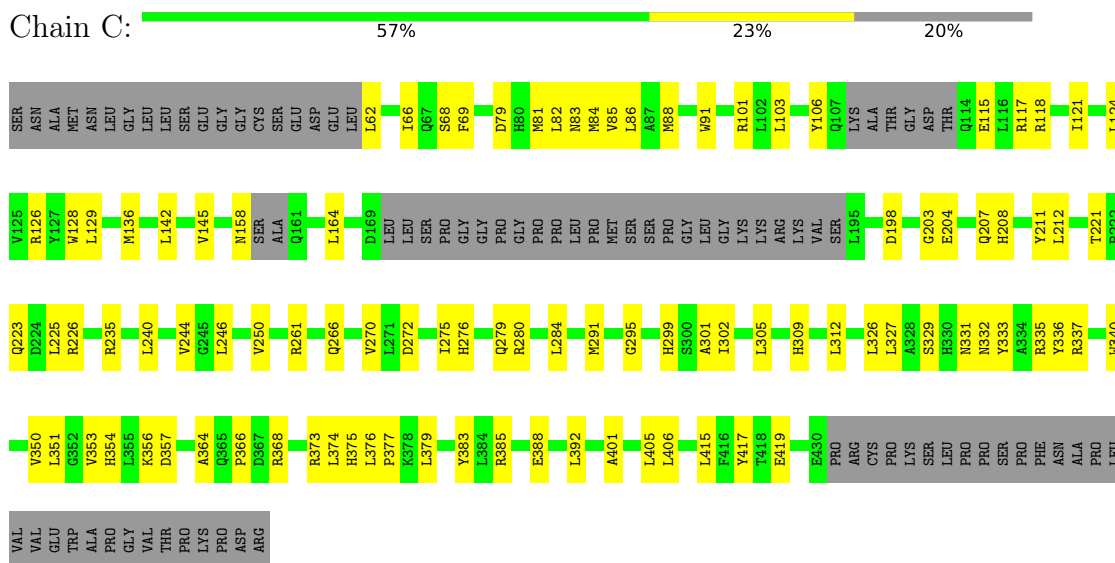
3 Residue-property plots

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: RAS guanyl-releasing protein 4



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Chain E:  58% 21% 21%

SER	ASN	ALA	MET	ASN	LEU	GLY	LEU	LEU	LEU	SER	GLU	GLY	CYS	SER	GLU	ASP	GLU	LEU	L62	C65	I66	O67	S68	F69	ASP	SER	ALA	GLY	SER	LEU	CYS	HIS	E78	M84	M88	H89	S90	W91	L98	Q107	LYS	ALA	THR	GLY	ASP	THR	Q114	E115	L116	R117	I121	V125		
W128	R131	H132	M136	Q141	L142	E143	E144	V145	F149	V153	M158	D169	LEU	SER	PRO	GLY	GLY	PRO	GLY	LEU	PRO	PRO	LEU	PRO	MET	SER	SER	PRO	GLY	LEU	LYS	ARG	LYS	VAL	L195	Q203	Q207	Y211	T221	Q223	D224	V234												
R235	G236	C237	E241	V244	Q254	Q255	L259	Q266	R267	V270	L271	D272	K273	F274	I275	H276	V277	R280	N286	F287	N288	N291	G295	D307	L327	A328	S329	N332	Y333	W340	L348	P349	V350	L351	K356	E363	A364	S365	P366	D367	R368													
D371	G372	R373	L374	H375	L376	P377	R378	L379	N380	N381	L382	Y383	L392	Q395	A401	L406	L415	F416	Y417	F418	E419	L422	A428	R429	E430	PRO	ARG	CYS	PRO	LYS	SER	LEU	PRO	SER	PRO	PHE	ASN	ALA	PRO	LEU	VAL	VAL	TRP	ALA	PRO	GLY	VAL	THR	PRO					
LYS	PRO	ASP	ARG																																																			

- Molecule 1: RAS guanyl-releasing protein 4

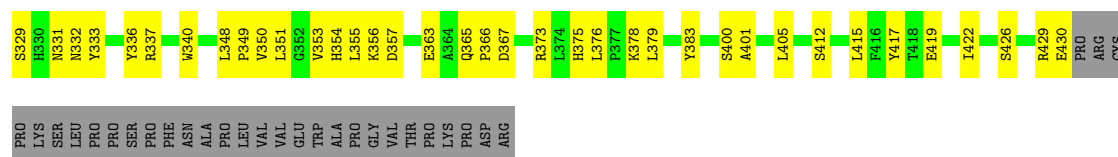
Chain G:  48% 28% 23%

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- Molecule 1: RAS guanyl-releasing protein 4

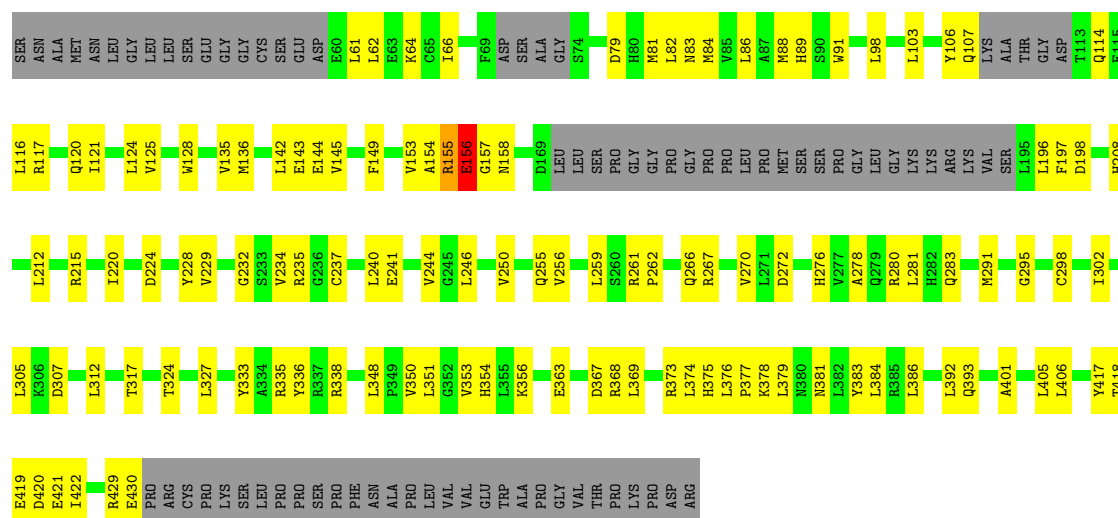
Chain I:  55% 25% 20%

SER	ASN	ALA	MET	ASN	LEU	GLY	LEU	SER	GLU	ASP	GLU	L61	L62	E63	I66	F69	ASP	SER	ALA	GLY	SER	LEU	CYS	H77	E78	D79	H80	M81	M84	V85	M88	W91	V92	L93	P94	L103	Y106	Q107	LYS	ALA	THR	GLY	ASP	THR	Q114
L119	Q120	I121	C122	H123	L124	V125	R126	W128	M136	L142	E143	E144	F149	V153	Q161	D169	LEU	SER	PRO	GLY	GLY	PRO	GLY	PRO	PRO	LEU	PRO	MET	SER	SER	PRO	GLY	LEU	GLY	LYS	LYS	ARG	LYS	V193	L196	F197	L200	G203	H208	Y211
T221	P222	Q223	S227	Y228	G232	C237	V244	G245	L246	V250	S251	R252	Q255	V256	L259	R261	P262	Q266	R267	V270	K273	V277	R280	Q283	N286	F287	N288	T289	L290	M291	G295	R304	L305	H309	L312	T317	L327	A328							



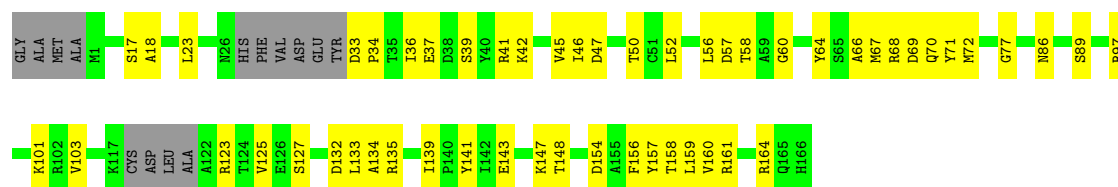
• Molecule 1: RAS guanyl-releasing protein 4

Chain K: 52% 28% 19%



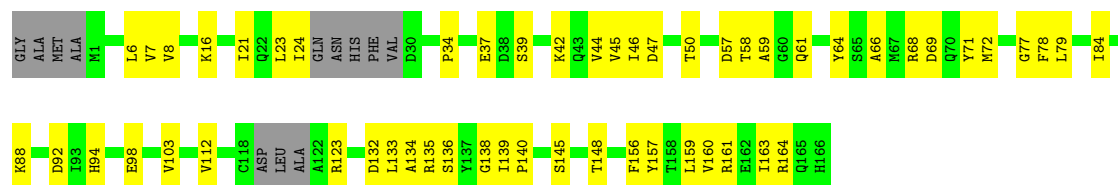
• Molecule 2: GTPase HRas

Chain B: 61% 31% 8%



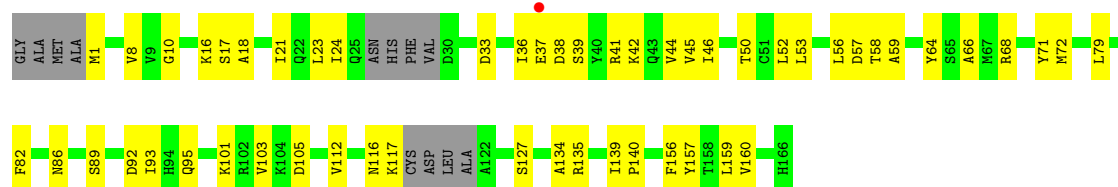
• Molecule 2: GTPase HRas

Chain D: 61% 32% 7%

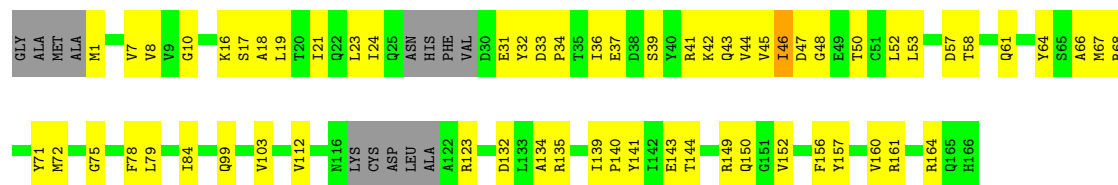


• Molecule 2: GTPase HRas

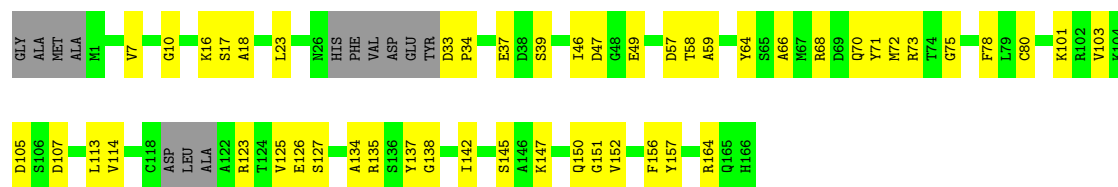
Chain F: 62% 31% 7%



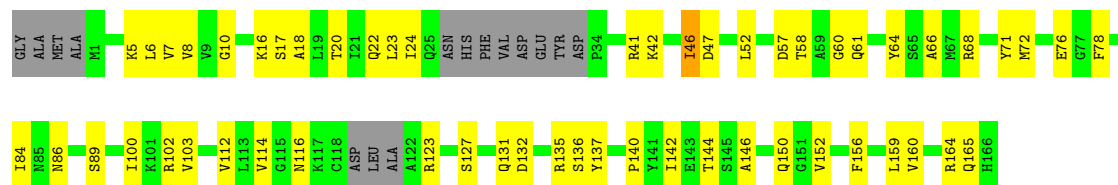
- Molecule 2: GTPase HRas



- Molecule 2: GTPase HRas



- Molecule 2: GTPase HRas



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 1 2	Depositor
Cell constants a, b, c, α , β , γ	114.11Å 114.11Å 680.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.21 – 3.30 49.21 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.7 (49.21-3.30) 96.3 (49.21-3.30)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 3.33Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.227 , 0.260 0.230 , 0.260	Depositor DCC
R_{free} test set	3814 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	72.0	Xtriage
Anisotropy	0.386	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 63.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.33$, $\langle L^2 \rangle = 0.16$	Xtriage
Estimated twinning fraction	0.347 for -h,-k,l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	23168	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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	0.18	0/2716	0.45	0/3687
1	C	0.17	0/2713	0.46	0/3682
1	E	0.17	0/2657	0.44	0/3608
1	G	0.18	0/2610	0.48	0/3545
1	I	0.17	0/2682	0.44	0/3645
1	K	0.17	0/2721	0.43	0/3694
2	B	0.18	0/1244	0.45	0/1675
2	D	0.18	0/1247	0.45	0/1683
2	F	0.16	0/1266	0.42	0/1705
2	H	0.17	0/1257	0.46	0/1694
2	J	0.18	0/1254	0.49	0/1688
2	L	0.18	0/1234	0.50	0/1660
All	All	0.18	0/23601	0.45	0/31966

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	K	0	2
2	H	0	1
2	L	0	2
All	All	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	348	LEU	Peptide
1	C	235	ARG	Peptide
2	H	46	ILE	Peptide
1	K	155	ARG	Peptide
1	K	156	GLU	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2659	0	2594	83	1
1	C	2655	0	2603	79	0
1	E	2600	0	2544	61	0
1	G	2552	0	2521	86	0
1	I	2624	0	2556	82	1
1	K	2663	0	2616	87	0
2	B	1230	0	1213	44	0
2	D	1232	0	1190	39	0
2	F	1251	0	1226	36	0
2	H	1242	0	1213	48	0
2	J	1240	0	1224	39	0
2	L	1220	0	1209	44	0
All	All	23168	0	22709	653	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 14.

The worst 5 of 653 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:A:295:GLY:HA3	2:B:66:ALA:HB1	1.61	0.81
1:C:62:LEU:HB3	1:C:101:ARG:HH12	1.46	0.80
1:G:267:ARG:NH1	1:K:144:GLU:OE2	2.15	0.79
1:E:295:GLY:HA3	2:F:66:ALA:HB1	1.66	0.78
1:I:367:ASP:OD1	1:I:378:LYS:NZ	2.16	0.78

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ARG:NH1	1:I:144:GLU:OE2[1_565]	2.07	0.13

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	330/418 (79%)	319 (97%)	11 (3%)	0	100	100
1	C	328/418 (78%)	309 (94%)	19 (6%)	0	100	100
1	E	322/418 (77%)	308 (96%)	14 (4%)	0	100	100
1	G	312/418 (75%)	297 (95%)	14 (4%)	1 (0%)	36	65
1	I	326/418 (78%)	308 (94%)	18 (6%)	0	100	100
1	K	329/418 (79%)	304 (92%)	23 (7%)	2 (1%)	21	52
2	B	150/170 (88%)	145 (97%)	5 (3%)	0	100	100
2	D	152/170 (89%)	147 (97%)	5 (3%)	0	100	100
2	F	152/170 (89%)	145 (95%)	7 (5%)	0	100	100
2	H	151/170 (89%)	140 (93%)	11 (7%)	0	100	100
2	J	151/170 (89%)	141 (93%)	9 (6%)	1 (1%)	18	49
2	L	149/170 (88%)	140 (94%)	8 (5%)	1 (1%)	18	49
All	All	2852/3528 (81%)	2703 (95%)	144 (5%)	5 (0%)	43	71

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	J	151	GLY
1	G	349	PRO
1	K	156	GLU
1	K	157	GLY
2	L	137	TYR

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	283/362 (78%)	283 (100%)	0	100	100
1	C	284/362 (78%)	284 (100%)	0	100	100
1	E	276/362 (76%)	276 (100%)	0	100	100
1	G	276/362 (76%)	276 (100%)	0	100	100
1	I	278/362 (77%)	278 (100%)	0	100	100
1	K	285/362 (79%)	285 (100%)	0	100	100
2	B	133/145 (92%)	133 (100%)	0	100	100
2	D	132/145 (91%)	132 (100%)	0	100	100
2	F	135/145 (93%)	135 (100%)	0	100	100
2	H	134/145 (92%)	134 (100%)	0	100	100
2	J	135/145 (93%)	135 (100%)	0	100	100
2	L	132/145 (91%)	132 (100%)	0	100	100
All	All	2483/3042 (82%)	2483 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
2	J	166	HIS
1	K	387	GLN
2	L	61	GLN
2	L	43	GLN
2	D	94	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	338/418 (80%)	-0.65	0 100 100	40, 77, 124, 195	0
1	C	336/418 (80%)	-0.60	0 100 100	27, 84, 159, 225	0
1	E	330/418 (78%)	-0.46	0 100 100	46, 92, 147, 226	0
1	G	320/418 (76%)	-0.46	0 100 100	42, 94, 169, 216	0
1	I	334/418 (79%)	-0.52	0 100 100	40, 85, 147, 183	0
1	K	337/418 (80%)	-0.60	0 100 100	45, 81, 146, 212	0
2	B	156/170 (91%)	-0.62	0 100 100	32, 75, 115, 161	0
2	D	158/170 (92%)	-0.63	0 100 100	40, 76, 121, 174	0
2	F	158/170 (92%)	-0.40	1 (0%) 85 73	61, 89, 134, 181	0
2	H	157/170 (92%)	-0.39	0 100 100	48, 86, 142, 195	0
2	J	157/170 (92%)	-0.41	0 100 100	55, 86, 145, 227	0
2	L	155/170 (91%)	-0.42	0 100 100	57, 84, 124, 169	0
All	All	2936/3528 (83%)	-0.53	1 (0%) 100 100	27, 84, 145, 227	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	37	GLU	2.1

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.