



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:13 PM UTC

PDB ID : 1U5E / pdb_00001u5e
Title : Crystal Structure of a N-terminal Fragment of SKAP-Hom Containing Both the Helical Dimerization Domain and the PH Domain
Authors : Tang, Y.; Swanson, K.D.; Neel, B.G.; Eck, M.J.
Deposited on : 2004-07-27
Resolution : 2.60 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
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

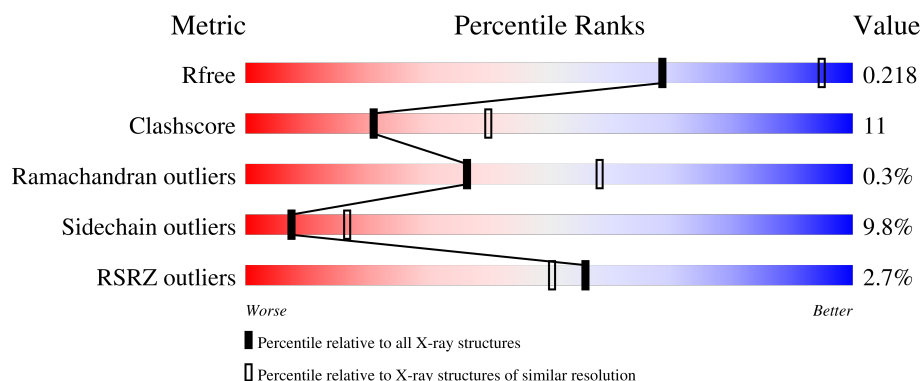
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	211	2% 26% 38% 13% • 19%
1	B	211	2% 32% 36% 11% • 20%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2807 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 Src-associated adaptor protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	170	Total	C	N	O	S	0	0	0
			1397	897	236	259	5			
1	B	168	Total	C	N	O	S	0	0	0
			1387	892	234	256	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	GLY	PRO	engineered mutation	UNP Q9Z2K4
A	13	SER	LEU	engineered mutation	UNP Q9Z2K4
B	12	GLY	PRO	engineered mutation	UNP Q9Z2K4
B	13	SER	LEU	engineered mutation	UNP Q9Z2K4

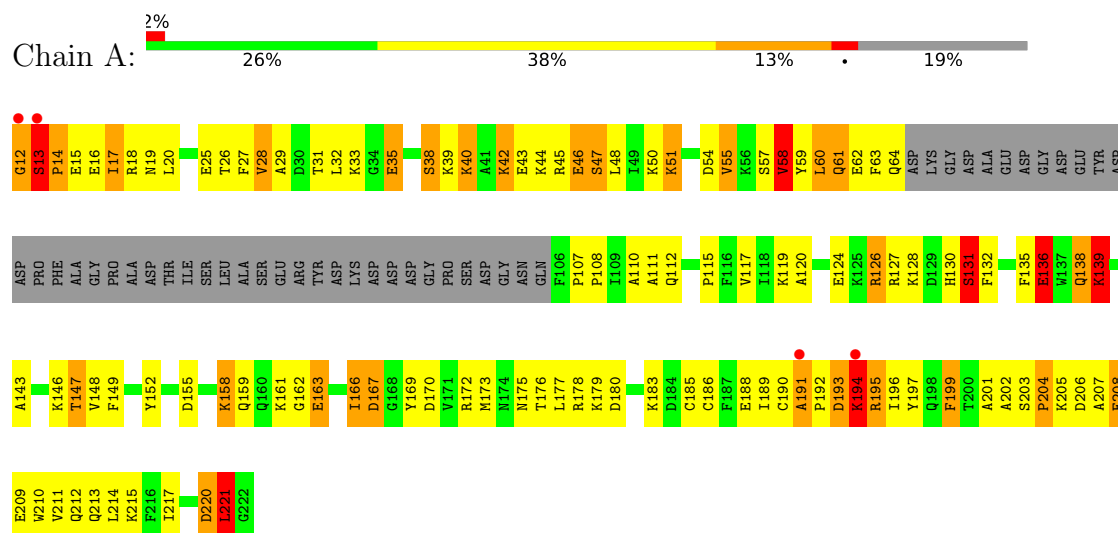
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	11	Total	O	0	0
			11	11		
2	B	12	Total	O	0	0
			12	12		

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: Src-associated adaptor protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	106.20Å 56.74Å 89.11Å 90.00° 95.82° 90.00°	Depositor
Resolution (Å)	35.00 – 2.60 35.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.7 (35.00-2.60) 98.7 (35.00-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.179 , 0.216 0.185 , 0.218	Depositor DCC
R_{free} test set	819 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	50.6	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 50.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2807	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.96% 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	3.08	141/1426 (9.9%)	1.94	41/1909 (2.1%)
1	B	2.67	99/1416 (7.0%)	1.91	32/1895 (1.7%)
All	All	2.88	240/2842 (8.4%)	1.92	73/3804 (1.9%)

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	3

All (240) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	194	LYS	CA-C	14.02	1.71	1.52
1	A	13	SER	N-CA	13.75	1.60	1.46
1	A	13	SER	CA-C	13.48	1.69	1.52
1	A	163	GLU	C-O	-12.04	1.09	1.23
1	B	109	ILE	CG1-CD1	11.93	1.98	1.51
1	A	29	ALA	CA-CB	-11.64	1.34	1.53
1	A	201	ALA	C-O	-10.70	1.09	1.23
1	A	173	MET	SD-CE	-10.49	1.53	1.79
1	B	14	PRO	N-CA	10.41	1.62	1.47
1	B	217	ILE	CA-CB	10.40	1.67	1.54
1	A	211	VAL	C-O	-10.24	1.11	1.24
1	A	195	ARG	C-O	-9.74	1.12	1.24
1	A	120	ALA	CA-CB	-9.52	1.37	1.53
1	A	136	GLU	CG-CD	9.30	1.75	1.52
1	B	217	ILE	C-O	-9.27	1.13	1.24
1	A	115	PRO	CA-C	9.17	1.63	1.52
1	B	112	GLN	C-O	-9.11	1.11	1.24
1	A	107	PRO	C-O	-9.08	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	17	ILE	N-CA	-9.05	1.35	1.46
1	B	154	SER	N-CA	9.04	1.57	1.45
1	A	120	ALA	C-O	-8.98	1.12	1.23
1	B	120	ALA	C-O	-8.91	1.13	1.23
1	B	201	ALA	C-O	-8.90	1.12	1.23
1	A	209	GLU	CA-C	8.88	1.64	1.52
1	B	107	PRO	C-O	-8.84	1.17	1.25
1	B	57	SER	C-N	-8.82	1.24	1.34
1	A	139	LYS	CD-CE	8.69	1.78	1.52
1	A	190	CYS	CA-C	8.59	1.63	1.52
1	A	166	ILE	C-O	-8.50	1.12	1.24
1	A	205	LYS	C-O	-8.45	1.13	1.24
1	A	107	PRO	CA-C	8.40	1.57	1.52
1	B	139	LYS	CD-CE	8.38	1.77	1.52
1	B	33	LYS	C-O	8.32	1.33	1.23
1	A	119	LYS	N-CA	-8.30	1.36	1.46
1	B	26	THR	C-O	-8.24	1.14	1.24
1	A	126	ARG	NE-CZ	8.17	1.42	1.33
1	B	219	GLN	CA-C	-8.13	1.41	1.52
1	A	188	GLU	CA-C	8.10	1.62	1.52
1	A	128	LYS	CA-C	-8.07	1.42	1.52
1	B	24	VAL	C-O	-8.04	1.15	1.24
1	A	28	VAL	CA-C	-7.98	1.43	1.52
1	A	15	GLU	CA-C	-7.96	1.42	1.52
1	B	57	SER	C-O	-7.92	1.13	1.24
1	B	42	LYS	C-O	-7.92	1.14	1.24
1	B	137	TRP	C-O	-7.84	1.14	1.23
1	A	210	TRP	N-CA	-7.83	1.37	1.46
1	A	143	ALA	CA-C	-7.82	1.43	1.52
1	A	48	LEU	N-CA	-7.75	1.36	1.46
1	B	47	SER	CA-C	7.62	1.62	1.52
1	A	195	ARG	CG-CD	-7.61	1.29	1.52
1	B	40	LYS	CA-C	7.58	1.62	1.52
1	A	192	PRO	N-CA	7.55	1.56	1.47
1	A	191	ALA	CA-C	7.54	1.62	1.52
1	B	178	ARG	C-O	7.52	1.32	1.24
1	A	54	ASP	C-O	-7.50	1.14	1.24
1	A	63	PHE	C-O	-7.48	1.13	1.23
1	B	58	VAL	CB-CG1	-7.46	1.27	1.52
1	A	61	GLN	CG-CD	7.45	1.70	1.52
1	A	45	ARG	N-CA	-7.39	1.37	1.46
1	A	194	LYS	CG-CD	7.34	1.74	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	196	ILE	C-O	-7.34	1.16	1.24
1	A	16	GLU	CD-OE2	7.27	1.39	1.25
1	A	29	ALA	CA-C	7.25	1.62	1.52
1	B	184	ASP	CA-C	7.22	1.62	1.52
1	B	154	SER	C-O	7.21	1.33	1.23
1	B	145	SER	C-O	-7.19	1.15	1.23
1	A	175	ASN	C-O	-7.15	1.14	1.24
1	A	212	GLN	C-O	-7.12	1.16	1.24
1	B	139	LYS	CG-CD	7.11	1.73	1.52
1	B	49	ILE	C-O	-7.10	1.16	1.24
1	A	158	LYS	C-O	-7.09	1.14	1.23
1	A	127	ARG	CA-C	7.05	1.61	1.52
1	B	48	LEU	CB-CG	-7.04	1.39	1.53
1	A	47	SER	CB-OG	-6.99	1.28	1.42
1	A	40	LYS	N-CA	-6.95	1.38	1.46
1	A	146	LYS	C-O	-6.95	1.15	1.24
1	B	43	GLU	CA-C	-6.94	1.43	1.52
1	A	204	PRO	CA-CB	6.91	1.63	1.53
1	A	57	SER	CA-C	-6.91	1.43	1.52
1	A	221	LEU	CA-C	6.89	1.61	1.52
1	A	207	ALA	CA-CB	-6.88	1.42	1.53
1	B	188	GLU	N-CA	-6.87	1.37	1.45
1	A	138	GLN	CG-CD	6.85	1.69	1.52
1	A	59	TYR	N-CA	-6.83	1.36	1.46
1	A	42	LYS	C-O	-6.79	1.16	1.24
1	B	127	ARG	CZ-NH1	-6.76	1.23	1.32
1	B	212	GLN	CG-CD	6.72	1.68	1.52
1	A	117	VAL	C-O	-6.68	1.14	1.23
1	A	191	ALA	CA-CB	6.67	1.64	1.53
1	B	155	ASP	C-O	-6.67	1.15	1.24
1	A	212	GLN	CA-C	6.65	1.61	1.52
1	A	149	PHE	N-CA	-6.61	1.38	1.46
1	A	202	ALA	CA-C	6.59	1.61	1.52
1	A	208	GLU	C-O	-6.50	1.16	1.24
1	A	201	ALA	N-CA	-6.49	1.37	1.45
1	B	148	VAL	CA-C	-6.47	1.44	1.52
1	B	149	PHE	CD1-CE1	6.47	1.58	1.38
1	A	13	SER	CA-CB	6.43	1.61	1.53
1	B	62	GLU	CA-C	6.42	1.61	1.52
1	B	169	TYR	C-O	-6.40	1.15	1.23
1	A	17	ILE	CG1-CD1	6.40	1.76	1.51
1	B	55	VAL	N-CA	-6.38	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	180	ASP	CA-C	-6.38	1.44	1.52
1	A	176	THR	C-O	-6.38	1.15	1.24
1	A	31	THR	CA-CB	-6.37	1.43	1.53
1	A	194	LYS	CD-CE	6.36	1.71	1.52
1	B	178	ARG	CA-C	6.34	1.60	1.52
1	A	48	LEU	C-O	-6.34	1.16	1.24
1	A	214	LEU	C-O	-6.33	1.16	1.24
1	A	119	LYS	CA-C	-6.29	1.44	1.52
1	A	136	GLU	CD-OE2	6.29	1.37	1.25
1	A	18	ARG	CZ-NH1	-6.28	1.24	1.32
1	A	124	GLU	N-CA	6.27	1.53	1.45
1	B	116	PHE	C-N	-6.25	1.27	1.33
1	A	136	GLU	CA-C	6.20	1.61	1.52
1	A	215	LYS	C-O	-6.18	1.16	1.24
1	B	136	GLU	CA-CB	6.17	1.63	1.53
1	A	148	VAL	CA-CB	6.14	1.62	1.54
1	B	209	GLU	C-O	-6.13	1.17	1.24
1	B	20	LEU	CA-C	-6.11	1.45	1.52
1	B	139	LYS	CB-CG	6.11	1.70	1.52
1	A	135	PHE	CE1-CZ	-6.07	1.20	1.38
1	B	158	LYS	CA-CB	6.07	1.64	1.53
1	A	26	THR	C-O	-6.07	1.17	1.24
1	B	133	LEU	N-CA	-6.06	1.38	1.46
1	B	156	LYS	CB-CG	6.03	1.70	1.52
1	B	120	ALA	CA-C	-6.01	1.45	1.52
1	A	42	LYS	CD-CE	5.98	1.70	1.52
1	B	42	LYS	CA-C	-5.98	1.44	1.52
1	B	109	ILE	CA-CB	5.98	1.63	1.54
1	A	17	ILE	CA-C	-5.97	1.45	1.52
1	A	139	LYS	CE-NZ	5.97	1.67	1.49
1	B	113	ASP	CA-CB	5.97	1.62	1.53
1	A	202	ALA	C-O	-5.97	1.16	1.24
1	A	58	VAL	C-O	-5.96	1.16	1.24
1	A	188	GLU	N-CA	-5.95	1.38	1.45
1	A	220	ASP	N-CA	-5.94	1.38	1.46
1	B	164	PHE	CA-C	5.90	1.59	1.52
1	B	155	ASP	N-CA	5.87	1.53	1.46
1	A	132	PHE	N-CA	-5.85	1.38	1.46
1	A	25	GLU	C-O	-5.85	1.17	1.24
1	B	107	PRO	CA-C	5.83	1.55	1.51
1	A	152	TYR	CA-C	5.77	1.59	1.52
1	A	172	ARG	C-O	-5.76	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	51	LYS	C-O	-5.73	1.17	1.24
1	B	172	ARG	CA-CB	-5.73	1.44	1.53
1	A	54	ASP	CA-C	-5.73	1.44	1.52
1	A	158	LYS	C-N	-5.72	1.26	1.33
1	A	20	LEU	C-O	-5.70	1.17	1.24
1	B	173	MET	C-O	-5.69	1.16	1.23
1	A	208	GLU	C-N	-5.67	1.26	1.33
1	A	193	ASP	C-O	5.67	1.31	1.24
1	A	33	LYS	CG-CD	5.66	1.69	1.52
1	B	53	LYS	C-O	-5.66	1.17	1.24
1	B	14	PRO	CB-CG	5.66	1.77	1.49
1	A	33	LYS	C-O	5.66	1.30	1.23
1	B	48	LEU	C-O	-5.65	1.17	1.24
1	B	36	ASN	CG-OD1	5.64	1.34	1.23
1	A	12	GLY	C-N	5.64	1.41	1.33
1	A	135	PHE	C-O	-5.63	1.17	1.23
1	A	186	CYS	N-CA	-5.63	1.39	1.46
1	B	195	ARG	C-O	-5.60	1.17	1.23
1	A	214	LEU	CA-C	-5.59	1.45	1.52
1	B	50	LYS	CG-CD	5.58	1.69	1.52
1	A	62	GLU	CA-C	-5.57	1.45	1.52
1	A	193	ASP	CB-CG	5.56	1.66	1.52
1	A	27	PHE	CA-C	-5.55	1.45	1.52
1	B	30	ASP	CB-CG	5.54	1.65	1.52
1	B	196	ILE	CB-CG1	-5.53	1.42	1.53
1	B	217	ILE	CA-C	-5.53	1.45	1.52
1	A	136	GLU	CA-CB	5.51	1.62	1.53
1	B	32	LEU	N-CA	-5.51	1.38	1.46
1	B	36	ASN	N-CA	-5.50	1.39	1.46
1	A	203	SER	N-CA	-5.49	1.40	1.46
1	A	110	ALA	CA-CB	5.45	1.62	1.53
1	B	120	ALA	N-CA	-5.44	1.39	1.46
1	A	195	ARG	CA-CB	-5.44	1.45	1.53
1	A	47	SER	N-CA	-5.44	1.40	1.46
1	B	108	PRO	C-O	-5.40	1.17	1.23
1	B	127	ARG	CD-NE	-5.39	1.38	1.46
1	A	19	ASN	N-CA	5.36	1.52	1.46
1	B	164	PHE	C-O	-5.34	1.17	1.23
1	B	121	GLY	C-O	-5.34	1.16	1.23
1	A	192	PRO	CA-C	5.33	1.59	1.52
1	B	154	SER	CA-C	5.33	1.59	1.52
1	A	136	GLU	CB-CG	5.33	1.68	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	62	GLU	CD-OE1	5.32	1.35	1.25
1	B	176	THR	C-O	-5.32	1.17	1.24
1	A	31	THR	N-CA	-5.30	1.39	1.46
1	B	32	LEU	CG-CD2	-5.29	1.35	1.52
1	A	206	ASP	CG-OD2	5.29	1.35	1.25
1	A	19	ASN	CA-CB	-5.28	1.45	1.53
1	B	184	ASP	C-O	5.27	1.30	1.24
1	A	206	ASP	C-O	-5.27	1.18	1.24
1	B	33	LYS	N-CA	5.26	1.52	1.46
1	A	128	LYS	C-O	-5.25	1.18	1.24
1	B	122	TYR	CA-CB	5.24	1.61	1.53
1	B	203	SER	N-CA	5.23	1.51	1.46
1	B	61	GLN	CG-CD	5.20	1.65	1.52
1	A	199	PHE	C-O	5.20	1.30	1.23
1	B	25	GLU	CA-C	5.20	1.59	1.52
1	B	197	TYR	CA-CB	5.20	1.60	1.53
1	A	131	SER	CA-C	5.19	1.59	1.52
1	A	35	GLU	C-O	-5.19	1.16	1.23
1	B	30	ASP	N-CA	5.18	1.52	1.46
1	A	135	PHE	CG-CD2	-5.18	1.27	1.38
1	B	24	VAL	CA-C	5.17	1.58	1.52
1	A	197	TYR	C-O	-5.15	1.17	1.24
1	A	39	LYS	CA-C	5.15	1.59	1.52
1	A	172	ARG	CA-C	-5.15	1.46	1.52
1	A	170	ASP	N-CA	-5.14	1.39	1.45
1	A	155	ASP	C-O	5.14	1.31	1.24
1	A	127	ARG	CZ-NH1	-5.14	1.25	1.32
1	B	210	TRP	CB-CG	-5.13	1.34	1.50
1	A	130	HIS	C-N	-5.13	1.27	1.33
1	A	163	GLU	C-N	-5.12	1.27	1.33
1	A	39	LYS	CG-CD	5.11	1.67	1.52
1	B	202	ALA	C-O	-5.10	1.17	1.24
1	A	112	GLN	CG-CD	5.09	1.64	1.52
1	A	161	LYS	CE-NZ	5.09	1.64	1.49
1	B	216	PHE	C-O	-5.09	1.18	1.24
1	A	111	ALA	C-O	-5.09	1.18	1.24
1	A	191	ALA	N-CA	5.08	1.53	1.46
1	B	173	MET	SD-CE	-5.08	1.66	1.79
1	A	110	ALA	C-O	-5.07	1.17	1.23
1	B	179	LYS	CA-C	5.07	1.59	1.53
1	B	172	ARG	NE-CZ	5.06	1.38	1.33
1	B	45	ARG	CA-CB	-5.05	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	178	ARG	CZ-NH2	-5.05	1.26	1.33
1	B	195	ARG	CB-CG	-5.04	1.37	1.52
1	B	125	LYS	CA-C	-5.04	1.46	1.52
1	B	207	ALA	N-CA	-5.04	1.40	1.46
1	A	172	ARG	N-CA	5.04	1.52	1.46
1	A	148	VAL	C-O	5.04	1.29	1.24
1	B	170	ASP	C-O	-5.04	1.17	1.23
1	A	57	SER	CB-OG	-5.03	1.32	1.42
1	B	63	PHE	C-O	-5.02	1.17	1.23
1	A	126	ARG	CB-CG	5.01	1.67	1.52
1	A	170	ASP	CG-OD1	5.01	1.34	1.25
1	B	21	LEU	C-O	-5.00	1.17	1.24

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	185	CYS	N-CA-C	10.08	125.71	111.30
1	B	219	GLN	CA-C-N	-8.00	112.16	123.20
1	B	219	GLN	C-N-CA	-8.00	112.16	123.20
1	A	40	LYS	N-CA-C	-7.93	102.23	111.03
1	A	107	PRO	N-CA-C	7.72	118.84	110.58
1	B	139	LYS	N-CA-CB	7.27	120.82	109.69
1	B	54	ASP	CA-C-O	-7.26	112.86	120.55
1	A	46	GLU	N-CA-C	-7.20	102.83	111.69
1	B	158	LYS	CA-C-O	7.19	127.34	119.15
1	A	127	ARG	NE-CZ-NH2	7.17	125.66	119.20
1	A	14	PRO	N-CA-C	6.91	124.97	113.78
1	A	180	ASP	N-CA-C	6.68	120.21	109.79
1	A	199	PHE	N-CA-C	6.59	120.27	109.72
1	A	60	LEU	N-CA-C	6.58	119.05	111.02
1	B	108	PRO	CA-C-O	-6.56	113.86	121.34
1	B	35	GLU	N-CA-C	-6.55	99.51	109.85
1	A	172	ARG	N-CA-C	6.54	118.80	108.79
1	B	134	GLY	N-CA-C	6.37	124.26	115.27
1	A	211	VAL	N-CA-C	-6.35	104.31	110.72
1	B	39	LYS	CB-CG-CD	6.20	125.57	111.30
1	B	220	ASP	CA-C-N	6.20	133.39	121.54
1	B	220	ASP	C-N-CA	6.20	133.39	121.54
1	B	36	ASN	N-CA-C	6.15	119.17	109.39
1	A	213	GLN	N-CA-C	-6.08	104.56	111.07
1	A	47	SER	N-CA-C	6.01	118.36	111.02
1	A	147	THR	CA-C-N	-6.00	114.65	122.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	147	THR	C-N-CA	-6.00	114.65	122.99
1	A	47	SER	CA-CB-OG	-5.96	99.18	111.10
1	A	139	LYS	CB-CG-CD	5.96	125.00	111.30
1	B	203	SER	CB-CA-C	-5.92	103.54	110.76
1	B	43	GLU	N-CA-C	-5.87	104.47	111.69
1	A	16	GLU	N-CA-C	5.86	119.69	112.54
1	B	169	TYR	N-CA-C	-5.85	102.11	110.59
1	B	205	LYS	N-CA-C	-5.85	104.99	111.36
1	A	13	SER	CA-C-O	5.80	126.35	120.38
1	B	220	ASP	O-C-N	5.80	130.66	122.83
1	B	55	VAL	CB-CA-C	-5.79	102.88	112.26
1	A	42	LYS	N-CA-CB	5.74	118.65	110.16
1	A	13	SER	CA-C-N	5.69	125.16	119.24
1	A	13	SER	C-N-CA	5.69	125.16	119.24
1	A	177	LEU	N-CA-C	-5.64	106.06	113.17
1	B	126	ARG	N-CA-CB	-5.64	101.03	111.52
1	A	25	GLU	N-CA-C	5.59	118.10	111.33
1	B	39	LYS	CA-C-N	5.58	127.76	120.28
1	B	39	LYS	C-N-CA	5.58	127.76	120.28
1	A	163	GLU	O-C-N	-5.54	117.44	123.26
1	B	193	ASP	OD1-CG-OD2	-5.51	109.66	122.90
1	B	15	GLU	N-CA-C	5.51	117.28	111.28
1	B	183	LYS	N-CA-C	5.49	119.14	112.23
1	B	30	ASP	CB-CG-OD2	5.48	131.01	118.40
1	A	158	LYS	CA-C-O	5.44	125.72	119.35
1	A	43	GLU	N-CA-C	-5.36	105.10	111.69
1	A	50	LYS	CG-CD-CE	5.30	123.49	111.30
1	A	131	SER	CA-CB-OG	-5.29	100.51	111.10
1	A	13	SER	N-CA-C	5.27	120.04	108.66
1	B	220	ASP	N-CA-C	5.23	115.92	108.54
1	B	147	THR	CB-CA-C	-5.22	102.32	110.94
1	A	178	ARG	NE-CZ-NH2	-5.21	114.51	119.20
1	A	146	LYS	CD-CE-NZ	5.17	128.43	111.90
1	A	211	VAL	CA-C-O	-5.16	115.38	120.85
1	A	158	LYS	N-CA-C	-5.15	106.68	113.17
1	A	194	LYS	N-CA-C	5.14	121.74	110.80
1	A	212	GLN	CA-CB-CG	5.13	124.36	114.10
1	A	44	LYS	N-CA-C	5.13	117.77	111.82
1	A	162	GLY	N-CA-C	-5.12	101.04	113.18
1	B	113	ASP	N-CA-C	-5.07	107.25	112.93
1	B	197	TYR	CA-C-O	5.06	125.89	120.32
1	B	216	PHE	N-CA-C	5.06	116.48	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	LYS	O-C-N	-5.05	116.03	122.34
1	A	185	CYS	N-CA-C	5.05	118.58	112.93
1	A	167	ASP	CB-CA-C	-5.04	103.60	109.80
1	B	30	ASP	OD1-CG-OD2	-5.02	110.84	122.90
1	A	44	LYS	CA-CB-CG	-5.02	104.07	114.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	12	GLY	Peptide
1	A	13	SER	Peptide
1	A	221	LEU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1397	0	1396	35	0
1	B	1387	0	1389	29	0
2	A	11	0	0	10	0
2	B	12	0	0	5	0
All	All	2807	0	2785	61	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (61) 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:17:ILE:CD1	1:A:17:ILE:CG1	1.76	1.62
1:A:139:LYS:CD	1:A:139:LYS:CE	1.78	1.62
1:A:136:GLU:CD	1:A:136:GLU:CG	1.75	1.60
1:A:194:LYS:CD	1:A:194:LYS:CG	1.74	1.56
1:B:139:LYS:CD	1:B:139:LYS:CE	1.77	1.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:PRO:CB	1:B:14:PRO:CG	1.77	1.54
1:B:109:ILE:CD1	1:B:109:ILE:CG1	1.98	1.42
1:B:220:ASP:HB2	2:B:231:HOH:O	1.45	1.17
1:A:136:GLU:HG2	2:A:229:HOH:O	1.52	1.08
1:A:220:ASP:O	1:A:221:LEU:HD23	1.65	0.95
1:A:17:ILE:CD1	1:A:17:ILE:CB	2.64	0.76
1:A:147:THR:HG22	2:A:226:HOH:O	1.88	0.73
1:A:204:PRO:O	1:A:208:GLU:HG3	1.90	0.72
1:A:64:GLN:C	2:A:231:HOH:O	2.35	0.70
1:A:147:THR:CG2	2:A:226:HOH:O	2.39	0.70
1:B:39:LYS:O	1:B:43:GLU:HG3	1.94	0.67
1:A:147:THR:HB	2:A:225:HOH:O	1.98	0.62
1:A:189:ILE:HD12	1:A:199:PHE:CE1	2.35	0.62
1:A:38:SER:OG	1:B:35:GLU:OE2	2.21	0.59
1:B:61:GLN:HB2	2:B:226:HOH:O	2.02	0.59
1:A:42:LYS:O	1:A:46:GLU:HG2	2.03	0.58
1:B:39:LYS:HG2	1:B:40:LYS:N	2.19	0.57
1:B:128:LYS:NZ	2:B:233:HOH:O	2.37	0.56
1:B:180:ASP:HB3	1:B:182:LYS:H	1.70	0.56
1:B:193:ASP:O	1:B:194:LYS:HB2	2.06	0.54
1:A:55:VAL:O	1:A:58:VAL:HB	2.10	0.52
1:B:108:PRO:O	1:B:109:ILE:HD13	2.11	0.51
1:B:124:GLU:HB2	1:B:200:THR:HB	1.92	0.51
1:A:40:LYS:HD3	2:A:232:HOH:O	2.10	0.49
1:A:194:LYS:CD	1:A:194:LYS:CB	2.82	0.49
1:A:28:VAL:HA	1:A:32:LEU:HD12	1.95	0.48
1:B:136:GLU:HA	2:B:227:HOH:O	2.14	0.47
1:B:175:ASN:OD1	1:B:175:ASN:C	2.58	0.47
1:A:189:ILE:HD12	1:A:199:PHE:HE1	1.78	0.46
1:A:40:LYS:CD	2:A:232:HOH:O	2.64	0.45
1:A:61:GLN:HG3	2:A:230:HOH:O	2.17	0.45
1:A:51:LYS:NZ	1:B:23:ASP:OD2	2.43	0.45
1:B:169:TYR:HD2	1:B:189:ILE:HG22	1.82	0.45
1:A:17:ILE:CD1	1:A:17:ILE:CG2	2.96	0.44
1:B:109:ILE:HG23	1:B:109:ILE:HD12	1.99	0.44
1:B:179:LYS:HG2	1:B:179:LYS:O	2.16	0.44
1:A:139:LYS:CE	1:A:139:LYS:CG	2.85	0.44
1:B:124:GLU:O	1:B:199:PHE:HA	2.18	0.44
1:A:166:ILE:O	1:A:167:ASP:C	2.58	0.43
1:B:185:CYS:HB3	1:B:204:PRO:HA	2.00	0.43
1:B:158:LYS:HA	1:B:158:LYS:HD3	1.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:ARG:CZ	1:A:131:SER:OG	2.67	0.42
1:B:166:ILE:O	1:B:167:ASP:C	2.60	0.42
1:A:35:GLU:OE2	1:B:38:SER:OG	2.37	0.42
1:B:109:ILE:CD1	1:B:109:ILE:HG23	2.49	0.42
1:A:13:SER:HA	1:A:14:PRO:HD3	1.81	0.42
1:A:217:ILE:HD12	1:A:217:ILE:HG23	1.76	0.42
1:B:109:ILE:CD1	1:B:109:ILE:CB	2.87	0.42
1:B:110:ALA:HB1	2:B:232:HOH:O	2.19	0.42
1:A:169:TYR:CE2	1:A:191:ALA:HB2	2.54	0.42
1:A:108:PRO:HB3	1:A:159:GLN:HE21	1.85	0.41
1:A:40:LYS:CE	2:A:232:HOH:O	2.67	0.41
1:A:158:LYS:HD2	1:A:158:LYS:N	2.36	0.41
1:A:40:LYS:HE3	2:A:232:HOH:O	2.21	0.41
1:B:30:ASP:O	1:B:31:THR:C	2.62	0.41
1:B:166:ILE:HG21	1:B:166:ILE:HD13	1.88	0.40

There are no symmetry-related clashes.

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	166/211 (79%)	155 (93%)	10 (6%)	1 (1%)	21	42
1	B	164/211 (78%)	155 (94%)	9 (6%)	0	100	100
All	All	330/422 (78%)	310 (94%)	19 (6%)	1 (0%)	36	58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	193	ASP

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	149/181 (82%)	134 (90%)	15 (10%)	7	15
1	B	148/181 (82%)	134 (90%)	14 (10%)	8	18
All	All	297/362 (82%)	268 (90%)	29 (10%)	7	17

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	SER
1	A	38	SER
1	A	47	SER
1	A	55	VAL
1	A	58	VAL
1	A	60	LEU
1	A	131	SER
1	A	136	GLU
1	A	138	GLN
1	A	139	LYS
1	A	163	GLU
1	A	179	LYS
1	A	183	LYS
1	A	194	LYS
1	A	195	ARG
1	B	36	ASN
1	B	39	LYS
1	B	40	LYS
1	B	48	LEU
1	B	54	ASP
1	B	60	LEU
1	B	112	GLN
1	B	147	THR
1	B	156	LYS
1	B	180	ASP
1	B	184	ASP
1	B	208	GLU

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Mol	Chain	Res	Type
1	B	209	GLU
1	B	221	LEU

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

Mol	Chain	Res	Type
1	A	159	GLN
1	A	219	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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	170/211 (80%)	-0.09	4 (2%) 59 54	42, 57, 85, 100	0
1	B	168/211 (79%)	-0.08	5 (2%) 52 47	43, 60, 88, 105	0
All	All	338/422 (80%)	-0.09	9 (2%) 56 50	42, 58, 87, 105	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	14	PRO	5.4
1	A	194	LYS	3.5
1	A	12	GLY	3.4
1	B	222	GLY	3.2
1	B	179	LYS	3.1
1	A	13	SER	2.6
1	B	182	LYS	2.3
1	A	191	ALA	2.2
1	B	109	ILE	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.