Full wwPDB X-ray Structure Validation Report (i)

Aug 15, 2023 – 10:12 PM EDT

PDB ID	:	1U5E
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 (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 (1)) were used in the production of this report:

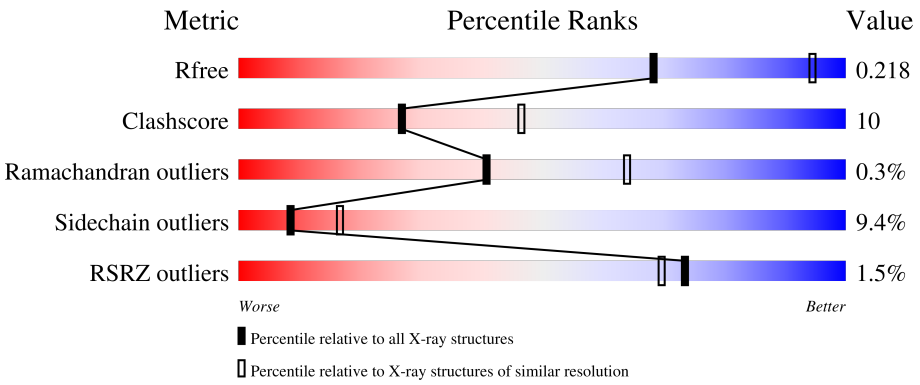
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.60 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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 <=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	40% 28% 10% • 19%
1	B	211	2% 43% 29% 5% • 20%

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	170	1397	897	236	259	5	0	0	0
1	B	168	1387	892	234	256	5	0	0	0

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.

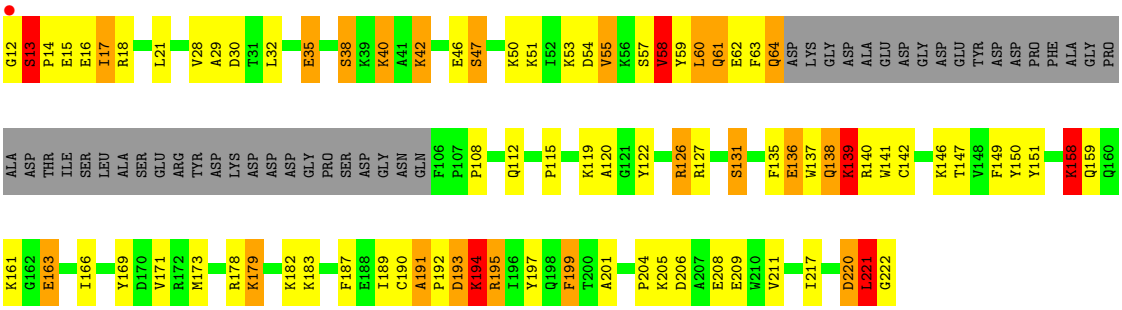
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	11	11	11	0	0
2	B	12	12	12	0	0

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.

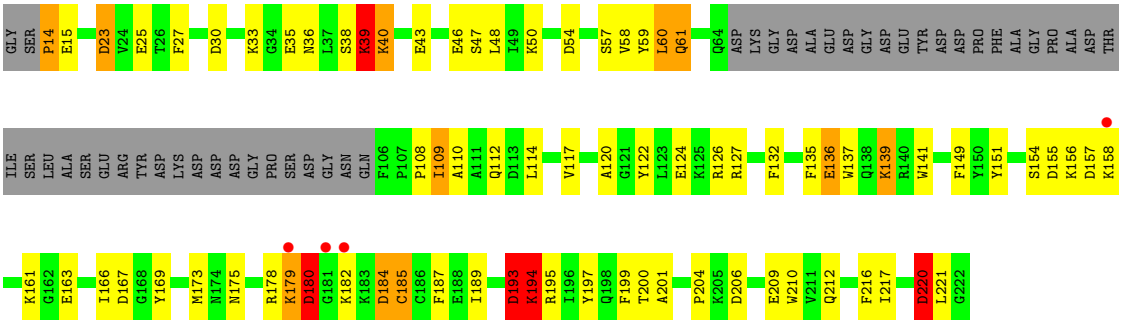
- Molecule 1: Src-associated adaptor protein

Chain A:



- Molecule 1: Src-associated adaptor protein

Chain B:



4 Data and refinement statistics (i)

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 32.38 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.7 (35.00-2.60) 98.7 (32.38-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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)	0.40 , 53.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

[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)

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	2.61	86/1426 (6.0%)	1.72	24/1909 (1.3%)
1	B	2.23	53/1416 (3.7%)	1.71	29/1895 (1.5%)
All	All	2.43	139/2842 (4.9%)	1.72	53/3804 (1.4%)

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 (139) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	136	GLU	CG-CD	15.56	1.75	1.51
1	A	16	GLU	CD-OE2	12.29	1.39	1.25
1	B	58	VAL	CB-CG1	-11.86	1.27	1.52
1	A	139	LYS	CD-CE	10.90	1.78	1.51
1	A	47	SER	CB-OG	-10.83	1.28	1.42
1	A	136	GLU	CD-OE2	10.59	1.37	1.25
1	B	139	LYS	CD-CE	10.54	1.77	1.51
1	B	149	PHE	CD1-CE1	9.41	1.58	1.39
1	A	150	TYR	CD2-CE2	9.24	1.53	1.39
1	B	14	PRO	N-CA	9.07	1.62	1.47
1	A	195	ARG	CG-CD	-8.93	1.29	1.51
1	A	62	GLU	CD-OE1	8.92	1.35	1.25
1	A	135	PHE	CE1-CZ	-8.90	1.20	1.37
1	B	210	TRP	CB-CG	-8.84	1.34	1.50
1	A	136	GLU	CB-CG	8.57	1.68	1.52
1	A	29	ALA	CA-CB	-8.56	1.34	1.52
1	A	61	GLN	CG-CD	8.53	1.70	1.51
1	A	194	LYS	CD-CE	8.11	1.71	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	138	GLN	CG-CD	7.88	1.69	1.51
1	A	150	TYR	CE2-CZ	7.86	1.48	1.38
1	A	57	SER	CB-OG	-7.81	1.32	1.42
1	B	212	GLN	CG-CD	7.74	1.68	1.51
1	A	42	LYS	CD-CE	7.66	1.70	1.51
1	B	127	ARG	CZ-NH1	-7.51	1.23	1.33
1	A	120	ALA	CA-CB	-7.32	1.37	1.52
1	A	139	LYS	CE-NZ	7.29	1.67	1.49
1	A	13	SER	N-CA	7.22	1.60	1.46
1	A	163	GLU	C-O	-7.19	1.09	1.23
1	A	135	PHE	CG-CD2	-7.18	1.27	1.38
1	A	194	LYS	CA-C	7.16	1.71	1.52
1	A	201	ALA	C-O	-7.15	1.09	1.23
1	A	150	TYR	CE1-CZ	7.14	1.47	1.38
1	A	18	ARG	CZ-NH1	-7.00	1.24	1.33
1	B	109	ILE	CG1-CD1	6.93	1.98	1.50
1	A	126	ARG	NE-CZ	6.91	1.42	1.33
1	A	193	ASP	CB-CG	6.76	1.66	1.51
1	B	139	LYS	CB-CG	6.76	1.70	1.52
1	B	30	ASP	CB-CG	6.73	1.65	1.51
1	A	171	VAL	CB-CG1	-6.68	1.38	1.52
1	B	117	VAL	CB-CG1	-6.68	1.38	1.52
1	B	136	GLU	CD-OE2	6.67	1.32	1.25
1	B	156	LYS	CB-CG	6.67	1.70	1.52
1	A	63	PHE	CD1-CE1	-6.61	1.26	1.39
1	A	16	GLU	CB-CG	-6.60	1.39	1.52
1	A	35	GLU	CD-OE1	6.59	1.32	1.25
1	B	122	TYR	CD2-CE2	6.54	1.49	1.39
1	A	13	SER	CB-OG	6.53	1.50	1.42
1	B	25	GLU	CD-OE1	6.50	1.32	1.25
1	A	194	LYS	CG-CD	6.48	1.74	1.52
1	A	58	VAL	CB-CG2	-6.45	1.39	1.52
1	A	146	LYS	CD-CE	6.45	1.67	1.51
1	B	47	SER	CB-OG	-6.39	1.33	1.42
1	A	197	TYR	CE1-CZ	-6.35	1.30	1.38
1	A	35	GLU	CD-OE2	-6.31	1.18	1.25
1	B	39	LYS	CD-CE	6.30	1.67	1.51
1	B	139	LYS	CG-CD	6.28	1.73	1.52
1	A	13	SER	CA-C	6.26	1.69	1.52
1	A	161	LYS	CE-NZ	6.23	1.64	1.49
1	B	187	PHE	CG-CD2	-6.21	1.29	1.38
1	B	137	TRP	CG-CD1	-6.12	1.28	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	61	GLN	CG-CD	6.08	1.65	1.51
1	B	112	GLN	C-O	-6.08	1.11	1.23
1	B	59	TYR	CE2-CZ	6.06	1.46	1.38
1	A	211	VAL	C-O	-6.00	1.11	1.23
1	A	112	GLN	CG-CD	5.97	1.64	1.51
1	A	59	TYR	CB-CG	-5.93	1.42	1.51
1	A	42	LYS	CE-NZ	5.90	1.63	1.49
1	A	199	PHE	CD2-CE2	-5.88	1.27	1.39
1	B	201	ALA	C-O	-5.88	1.12	1.23
1	B	161	LYS	CD-CE	5.86	1.65	1.51
1	A	195	ARG	C-O	-5.86	1.12	1.23
1	B	139	LYS	CE-NZ	5.81	1.63	1.49
1	A	122	TYR	CG-CD1	-5.81	1.31	1.39
1	A	53	LYS	CD-CE	5.79	1.65	1.51
1	B	154	SER	N-CA	5.79	1.57	1.46
1	A	127	ARG	CZ-NH1	-5.76	1.25	1.33
1	A	192	PRO	N-CA	5.73	1.56	1.47
1	B	194	LYS	CD-CE	5.71	1.65	1.51
1	A	197	TYR	CD1-CE1	5.68	1.47	1.39
1	B	195	ARG	CB-CG	-5.64	1.37	1.52
1	B	217	ILE	CA-CB	5.64	1.67	1.54
1	B	122	TYR	CD1-CE1	5.62	1.47	1.39
1	A	13	SER	CA-CB	5.62	1.61	1.52
1	A	16	GLU	CD-OE1	5.60	1.31	1.25
1	B	14	PRO	CB-CG	5.60	1.77	1.50
1	B	216	PHE	CB-CG	5.59	1.60	1.51
1	A	199	PHE	CE1-CZ	-5.57	1.26	1.37
1	B	178	ARG	CZ-NH1	-5.57	1.25	1.33
1	B	33	LYS	C-O	5.55	1.33	1.23
1	B	155	ASP	CB-CG	-5.54	1.40	1.51
1	A	209	GLU	CD-OE1	5.54	1.31	1.25
1	A	64	GLN	CB-CG	-5.53	1.37	1.52
1	A	126	ARG	CB-CG	5.53	1.67	1.52
1	A	120	ALA	C-O	-5.51	1.12	1.23
1	B	57	SER	CA-CB	-5.49	1.44	1.52
1	B	46	GLU	CD-OE1	5.49	1.31	1.25
1	A	191	ALA	CA-CB	5.48	1.64	1.52
1	A	119	LYS	CE-NZ	-5.47	1.35	1.49
1	A	182	LYS	CD-CE	5.47	1.65	1.51
1	A	187	PHE	CE1-CZ	5.47	1.47	1.37
1	B	197	TYR	CE2-CZ	5.47	1.45	1.38
1	A	166	ILE	C-O	-5.46	1.12	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	135	PHE	CG-CD1	-5.46	1.30	1.38
1	A	17	ILE	N-CA	-5.46	1.35	1.46
1	A	141	TRP	CE3-CZ3	5.43	1.47	1.38
1	A	142	CYS	CB-SG	-5.43	1.73	1.81
1	A	40	LYS	CE-NZ	5.43	1.62	1.49
1	B	209	GLU	CD-OE2	5.43	1.31	1.25
1	B	15	GLU	CD-OE2	5.42	1.31	1.25
1	B	50	LYS	CD-CE	5.39	1.64	1.51
1	B	217	ILE	C-O	-5.39	1.13	1.23
1	B	120	ALA	C-O	-5.38	1.13	1.23
1	A	194	LYS	CB-CG	5.33	1.67	1.52
1	B	132	PHE	CG-CD1	-5.33	1.30	1.38
1	B	141	TRP	CB-CG	5.33	1.59	1.50
1	B	59	TYR	CB-CG	-5.33	1.43	1.51
1	A	62	GLU	CD-OE2	5.32	1.31	1.25
1	A	115	PRO	CA-C	5.29	1.63	1.52
1	B	184	ASP	CB-CG	5.29	1.62	1.51
1	A	197	TYR	CG-CD1	-5.28	1.32	1.39
1	A	50	LYS	CE-NZ	5.25	1.62	1.49
1	A	151	TYR	CB-CG	-5.20	1.43	1.51
1	A	190	CYS	CB-SG	5.16	1.91	1.82
1	A	54	ASP	CB-CG	5.15	1.62	1.51
1	B	151	TYR	CD1-CE1	5.15	1.47	1.39
1	A	63	PHE	C-O	-5.12	1.13	1.23
1	B	154	SER	C-O	5.12	1.33	1.23
1	A	137	TRP	CZ3-CH2	5.11	1.48	1.40
1	A	194	LYS	CE-NZ	5.08	1.61	1.49
1	A	135	PHE	CE2-CZ	-5.08	1.27	1.37
1	A	119	LYS	N-CA	-5.08	1.36	1.46
1	A	149	PHE	CE1-CZ	-5.07	1.27	1.37
1	A	179	LYS	CB-CG	5.07	1.66	1.52
1	A	50	LYS	CD-CE	5.05	1.63	1.51
1	A	205	LYS	C-O	-5.05	1.13	1.23
1	B	57	SER	C-O	-5.03	1.13	1.23
1	A	220	ASP	CB-CG	5.03	1.62	1.51
1	A	40	LYS	CD-CE	5.01	1.63	1.51
1	B	27	PHE	CE1-CZ	-5.00	1.27	1.37

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	30	ASP	CB-CG-OD2	14.13	131.01	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	193	ASP	CB-CG-OD2	12.63	129.67	118.30
1	A	178	ARG	NE-CZ-NH2	-11.58	114.51	120.30
1	A	178	ARG	NE-CZ-NH1	11.35	125.97	120.30
1	A	30	ASP	CB-CG-OD1	11.12	128.31	118.30
1	B	206	ASP	CB-CG-OD2	11.05	128.25	118.30
1	A	127	ARG	NE-CZ-NH2	10.71	125.66	120.30
1	A	195	ARG	NE-CZ-NH1	10.39	125.50	120.30
1	B	155	ASP	CB-CG-OD2	9.47	126.82	118.30
1	A	206	ASP	CB-CG-OD2	9.43	126.79	118.30
1	B	136	GLU	OE1-CD-OE2	8.43	133.42	123.30
1	A	136	GLU	OE1-CD-OE2	-8.30	113.34	123.30
1	A	206	ASP	CB-CG-OD1	-8.04	111.06	118.30
1	A	146	LYS	CD-CE-NZ	7.28	128.43	111.70
1	B	193	ASP	OD1-CG-OD2	-7.18	109.66	123.30
1	A	222	GLY	CA-C-O	-7.11	107.80	120.60
1	B	184	ASP	CB-CG-OD1	7.05	124.64	118.30
1	B	60	LEU	CB-CG-CD1	7.04	122.97	111.00
1	B	126	ARG	NE-CZ-NH1	-7.03	116.78	120.30
1	A	42	LYS	CD-CE-NZ	6.92	127.62	111.70
1	B	109	ILE	CG1-CB-CG2	-6.85	96.32	111.40
1	B	23	ASP	CB-CG-OD1	6.84	124.46	118.30
1	B	167	ASP	CB-CG-OD2	6.65	124.28	118.30
1	A	126	ARG	NE-CZ-NH1	-6.65	116.98	120.30
1	A	158	LYS	CD-CE-NZ	-6.62	96.47	111.70
1	B	30	ASP	OD1-CG-OD2	-6.55	110.84	123.30
1	B	206	ASP	CB-CG-OD1	-6.55	112.41	118.30
1	B	157	ASP	CB-CG-OD2	6.53	124.17	118.30
1	B	161	LYS	CD-CE-NZ	6.27	126.12	111.70
1	B	155	ASP	CB-CG-OD1	-6.25	112.67	118.30
1	B	173	MET	CG-SD-CE	6.09	109.95	100.20
1	A	193	ASP	CB-CG-OD2	6.01	123.71	118.30
1	B	114	LEU	CB-CG-CD1	-5.91	100.95	111.00
1	A	16	GLU	OE1-CD-OE2	5.89	130.37	123.30
1	A	194	LYS	CD-CE-NZ	5.87	125.20	111.70
1	B	59	TYR	CB-CG-CD1	-5.84	117.50	121.00
1	B	139	LYS	N-CA-CB	5.68	120.82	110.60
1	B	178	ARG	NE-CZ-NH2	5.68	123.14	120.30
1	B	180	ASP	CB-CG-OD2	5.54	123.29	118.30
1	A	221	LEU	CB-CG-CD2	5.45	120.26	111.00
1	B	185	CYS	N-CA-C	5.45	125.71	111.00
1	B	23	ASP	OD1-CG-OD2	-5.44	112.96	123.30
1	B	220	ASP	CA-C-N	-5.38	105.36	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	140	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	B	39	LYS	CB-CG-CD	5.37	125.57	111.60
1	A	21	LEU	CB-CG-CD2	-5.37	101.88	111.00
1	B	126	ARG	N-CA-CB	-5.32	101.03	110.60
1	A	54	ASP	CB-CG-OD2	5.28	123.06	118.30
1	A	173	MET	CG-SD-CE	5.27	108.63	100.20
1	A	60	LEU	CA-CB-CG	5.26	127.39	115.30
1	A	139	LYS	CB-CG-CD	5.15	125.00	111.60
1	B	179	LYS	CD-CE-NZ	-5.13	99.90	111.70
1	A	15	GLU	OE1-CD-OE2	5.06	129.38	123.30

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	34	0
1	B	1387	0	1389	26	0
2	A	11	0	0	10	0
2	B	12	0	0	4	0
All	All	2807	0	2785	57	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 10.

All (57) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:LYS:CD	1:A:139:LYS:CE	1.78	1.62
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
1:B:14:PRO:CB	1:B:14:PRO:CG	1.77	1.54
1:A:136:GLU:CD	1:A:136:GLU:CG	1.75	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: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:64:GLN:C	2:A:231:HOH:O	2.35	0.66
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	0.58
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: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:B:185:CYS:HB3	1:B:204:PRO:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:LYS:HA	1:B:158:LYS:HD3	1.87	0.43
1:A:126:ARG:CZ	1:A:131:SER:OG	2.67	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:B:175:ASN:OD1	1:B:175:ASN:C	2.58	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:166:ILE:HG21	1:B:166:ILE:HD13	1.88	0.40

There are no symmetry-related clashes.

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	166/211 (79%)	155 (93%)	10 (6%)	1 (1%)	25 47
1	B	164/211 (78%)	155 (94%)	9 (6%)	0	100 100
All	All	330/422 (78%)	310 (94%)	19 (6%)	1 (0%)	41 64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	193	ASP

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	149/181 (82%)	134 (90%)	15 (10%)	7 14
1	B	148/181 (82%)	135 (91%)	13 (9%)	10 19
All	All	297/362 (82%)	269 (91%)	28 (9%)	8 17

All (28) 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	138	GLN
1	A	139	LYS
1	A	158	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	163	GLU
1	B	180	ASP
1	B	184	ASP
1	B	193	ASP
1	B	194	LYS
1	B	220	ASP

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Mol	Chain	Res	Type
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 monosaccharides 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%)	-0.23	1 (0%)	89	88	42, 57, 85, 100	0
1	B	168/211 (79%)	-0.15	4 (2%)	59	53	43, 60, 88, 105	0
All	All	338/422 (80%)	-0.19	5 (1%)	73	70	42, 58, 87, 105	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	182	LYS	2.8
1	B	179	LYS	2.7
1	B	181	GLY	2.7
1	A	12	GLY	2.3
1	B	158	LYS	2.3

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.