



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:33 PM GMT

PDB ID : 1U5G  
Title : Crystal Structure of the PH Domain of SKAP-Hom  
Authors : Tang, Y.; Swanson, K.; Neel, B.G.; Eck, M.J.  
Deposited on : 2004-07-27  
Resolution : 2.10 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

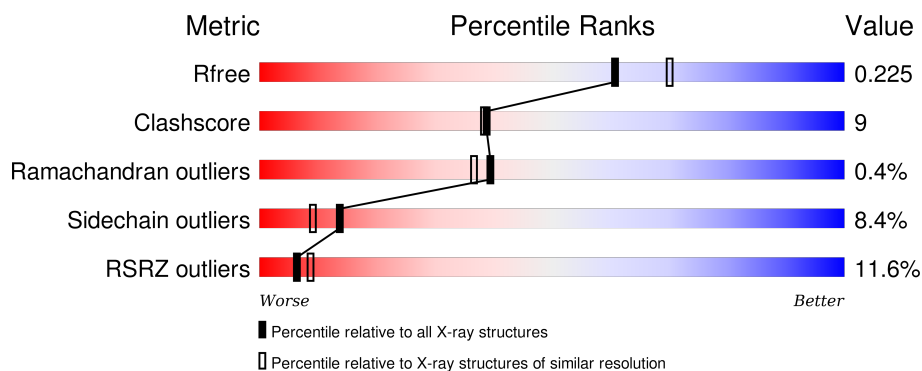
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	122	<div> <div>16%</div> <div>67%</div> <div>20%</div> <div>7%</div> <div>6%</div> </div>
1	B	122	<div> <div>2%</div> <div>64%</div> <div>26%</div> <div>5%</div> <div>• •</div> </div>
1	C	122	<div> <div>2%</div> <div>63%</div> <div>29%</div> <div>• • •</div> </div>
1	D	122	<div> <div>24%</div> <div>64%</div> <div>24%</div> <div>6%</div> <div>• 6%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4091 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	115	Total	C	N	O	S	0	0	0
			959	620	163	171	5			
1	B	118	Total	C	N	O	S	0	0	0
			980	632	166	177	5			
1	C	118	Total	C	N	O	S	0	0	0
			980	632	166	177	5			
1	D	115	Total	C	N	O	S	0	0	0
			959	620	163	171	5			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	101	GLY	SER	ENGINEERED	UNP Q8BK74
A	102	SER	ASP	ENGINEERED	UNP Q8BK74
B	101	GLY	SER	ENGINEERED	UNP Q8BK74
B	102	SER	ASP	ENGINEERED	UNP Q8BK74
C	101	GLY	SER	ENGINEERED	UNP Q8BK74
C	102	SER	ASP	ENGINEERED	UNP Q8BK74
D	101	GLY	SER	ENGINEERED	UNP Q8BK74
D	102	SER	ASP	ENGINEERED	UNP Q8BK74

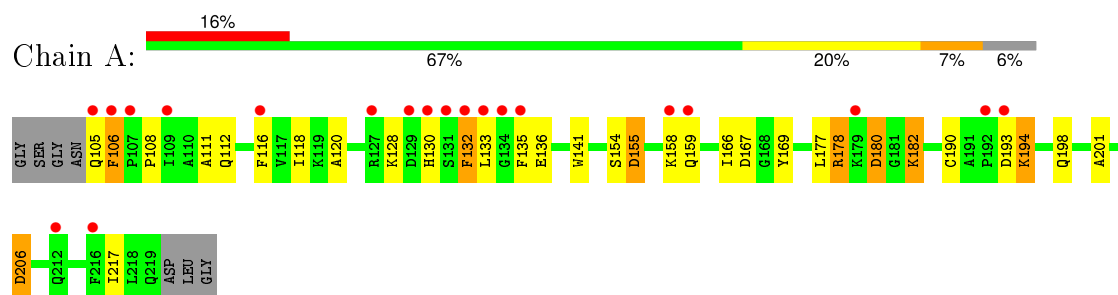
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	23	Total	O	0	0
			23	23		
2	B	82	Total	O	0	0
			82	82		
2	C	88	Total	O	0	0
			88	88		
2	D	20	Total	O	0	0
			20	20		

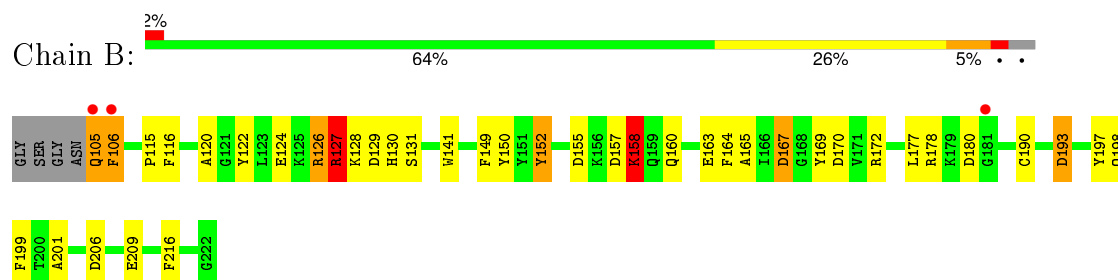
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

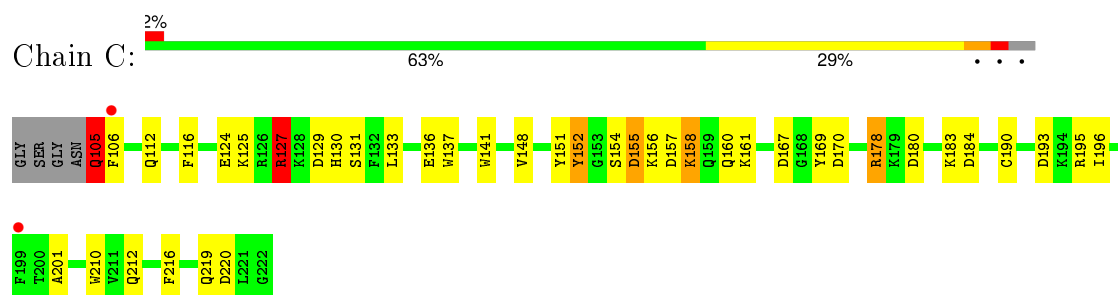
- Molecule 1: Src-associated adaptor protein



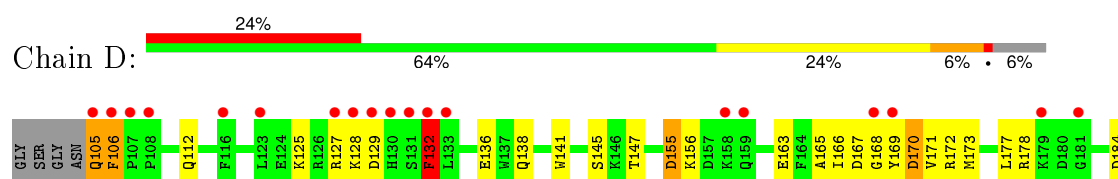
- Molecule 1: Src-associated adaptor protein

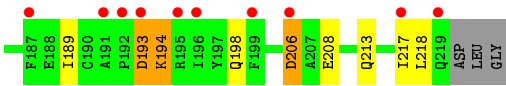


- Molecule 1: Src-associated adaptor protein



- Molecule 1: Src-associated adaptor protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.61Å 65.69Å 143.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.10 24.67 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.4 (25.00-2.10) 99.5 (24.67-2.10)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.77 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, $R_{free}$	0.213 , 0.271 0.220 , 0.225	Depositor DCC
$R_{free}$ test set	1702 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.9	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 58.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 33567 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4091	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	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 32.44 % 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 9.3921e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	1.41	2/985 (0.2%)	1.20	7/1323 (0.5%)
1	B	1.77	17/1006 (1.7%)	1.60	14/1350 (1.0%)
1	C	1.81	24/1006 (2.4%)	1.48	12/1350 (0.9%)
1	D	1.24	0/985	1.18	7/1323 (0.5%)
All	All	1.58	43/3982 (1.1%)	1.38	40/5346 (0.7%)

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	D	0	1
All	All	0	3

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	115	PRO	N-CD	8.89	1.60	1.47
1	B	199	PHE	CD2-CE2	-8.11	1.23	1.39
1	C	127	ARG	CD-NE	-8.03	1.32	1.46
1	C	152	TYR	CG-CD1	7.99	1.49	1.39
1	B	127	ARG	CD-NE	-7.62	1.33	1.46
1	B	216	PHE	CE1-CZ	-7.31	1.23	1.37
1	C	137	TRP	CE3-CZ3	-6.93	1.26	1.38
1	C	195	ARG	CG-CD	-6.77	1.35	1.51
1	B	169	TYR	CG-CD1	-6.73	1.30	1.39
1	C	151	TYR	CE2-CZ	6.69	1.47	1.38
1	C	161	LYS	CD-CE	6.51	1.67	1.51
1	B	164	PHE	CE1-CZ	-6.35	1.25	1.37
1	B	169	TYR	CD2-CE2	-5.99	1.30	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	169	TYR	CE1-CZ	5.94	1.46	1.38
1	C	131	SER	C-O	-5.89	1.12	1.23
1	C	152	TYR	CE1-CZ	5.88	1.46	1.38
1	C	212	GLN	CG-CD	5.88	1.64	1.51
1	B	124	GLU	CD-OE1	-5.88	1.19	1.25
1	A	111	ALA	CA-CB	5.83	1.64	1.52
1	B	149	PHE	CE1-CZ	-5.81	1.26	1.37
1	B	201	ALA	CA-CB	5.76	1.64	1.52
1	C	178	ARG	CB-CG	-5.66	1.37	1.52
1	C	148	VAL	CB-CG1	-5.66	1.41	1.52
1	C	133	LEU	C-O	-5.62	1.12	1.23
1	B	126	ARG	CD-NE	-5.58	1.36	1.46
1	C	106	PHE	C-N	-5.56	1.23	1.34
1	B	209	GLU	CD-OE1	-5.51	1.19	1.25
1	C	210	TRP	CB-CG	-5.49	1.40	1.50
1	A	182	LYS	CD-CE	5.48	1.65	1.51
1	C	158	LYS	CD-CE	5.39	1.64	1.51
1	B	197	TYR	CD1-CE1	-5.38	1.31	1.39
1	C	154	SER	CA-CB	5.34	1.60	1.52
1	C	136	GLU	CD-OE2	-5.33	1.19	1.25
1	C	183	LYS	CD-CE	5.23	1.64	1.51
1	C	201	ALA	CA-CB	5.22	1.63	1.52
1	C	124	GLU	CD-OE1	-5.19	1.20	1.25
1	C	151	TYR	CD1-CE1	5.16	1.47	1.39
1	B	131	SER	CA-CB	5.14	1.60	1.52
1	C	178	ARG	CG-CD	-5.12	1.39	1.51
1	B	152	TYR	CE2-CZ	5.11	1.45	1.38
1	C	151	TYR	CD2-CE2	-5.09	1.31	1.39
1	B	152	TYR	CD2-CE2	5.06	1.47	1.39
1	B	122	TYR	CE2-CZ	5.01	1.45	1.38

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	127	ARG	NE-CZ-NH1	22.46	131.53	120.30
1	B	127	ARG	NE-CZ-NH2	-18.21	111.20	120.30
1	C	127	ARG	NE-CZ-NH2	-16.46	112.07	120.30
1	C	127	ARG	NE-CZ-NH1	14.64	127.62	120.30
1	B	167	ASP	CB-CG-OD2	10.71	127.94	118.30
1	A	180	ASP	CB-CG-OD2	8.93	126.33	118.30
1	B	157	ASP	CB-CG-OD2	8.76	126.18	118.30
1	C	193	ASP	CB-CG-OD2	8.73	126.16	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	178	ARG	NE-CZ-NH1	8.70	124.65	120.30
1	A	178	ARG	NE-CZ-NH2	-7.81	116.39	120.30
1	B	170	ASP	CB-CG-OD2	6.95	124.56	118.30
1	D	178	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	D	206	ASP	CB-CG-OD2	6.77	124.39	118.30
1	A	193	ASP	CB-CG-OD2	6.66	124.29	118.30
1	B	126	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	B	126	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	D	155	ASP	CB-CG-OD2	6.47	124.12	118.30
1	C	178	ARG	NE-CZ-NH1	6.39	123.49	120.30
1	B	158	LYS	CD-CE-NZ	6.23	126.03	111.70
1	C	170	ASP	CB-CG-OD2	6.21	123.89	118.30
1	D	193	ASP	CB-CG-OD2	6.16	123.84	118.30
1	D	170	ASP	CB-CG-OD2	5.93	123.64	118.30
1	A	155	ASP	CB-CG-OD2	5.88	123.59	118.30
1	B	193	ASP	CB-CG-OD1	5.87	123.58	118.30
1	B	172	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	B	206	ASP	CB-CG-OD1	5.78	123.50	118.30
1	C	167	ASP	CB-CG-OD1	5.68	123.41	118.30
1	C	180	ASP	CB-CG-OD2	5.66	123.39	118.30
1	D	184	ASP	CB-CG-OD2	5.66	123.39	118.30
1	C	157	ASP	CB-CG-OD2	5.65	123.39	118.30
1	D	178	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	C	220	ASP	CB-CG-OD1	5.55	123.30	118.30
1	B	106	PHE	CB-CA-C	5.45	121.30	110.40
1	C	124	GLU	OE1-CD-OE2	-5.42	116.80	123.30
1	C	155	ASP	CB-CG-OD2	5.41	123.17	118.30
1	A	206	ASP	CB-CG-OD2	5.37	123.13	118.30
1	B	180	ASP	CB-CG-OD2	5.34	123.11	118.30
1	C	183	LYS	CD-CE-NZ	-5.34	99.42	111.70
1	A	135	PHE	N-CA-C	5.26	125.20	111.00
1	A	106	PHE	N-CA-C	5.01	124.53	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	GLN	Peptide
1	C	105	GLN	Mainchain
1	D	132	PHE	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	959	0	938	15	0
1	B	980	0	956	16	0
1	C	980	0	956	16	0
1	D	959	0	938	23	0
2	A	23	0	0	2	0
2	B	82	0	0	3	0
2	C	88	0	0	3	0
2	D	20	0	0	1	0
All	All	4091	0	3788	69	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 9.

All (69) 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:105:GLN:HE21	1:C:105:GLN:N	1.08	1.43
1:C:105:GLN:NE2	1:C:105:GLN:N	1.66	1.41
1:C:105:GLN:HE21	1:C:105:GLN:CA	1.37	1.34
1:D:206:ASP:HB3	2:D:237:HOH:O	1.53	1.06
1:A:106:PHE:HB2	2:A:243:HOH:O	1.62	0.98
1:C:184:ASP:HB2	2:C:290:HOH:O	1.65	0.95
1:C:127:ARG:HD3	1:C:129:ASP:OD1	1.68	0.92
1:A:118:ILE:HD13	1:A:217:ILE:HD11	1.53	0.90
1:B:190:CYS:SG	2:B:299:HOH:O	2.30	0.89
1:B:127:ARG:HD3	1:B:129:ASP:OD1	1.77	0.83
1:A:190:CYS:SG	2:A:236:HOH:O	2.40	0.80
1:C:105:GLN:HA	1:C:105:GLN:HE21	1.48	0.77
1:C:105:GLN:NE2	1:C:105:GLN:CA	2.13	0.71
1:D:127:ARG:NE	1:D:138:GLN:HE22	1.89	0.71
1:C:190:CYS:HA	1:C:196:ILE:HD12	1.76	0.66
1:D:168:GLY:HA3	1:D:194:LYS:NZ	2.15	0.61
1:D:168:GLY:HA3	1:D:194:LYS:HZ1	1.66	0.61
1:D:127:ARG:HD2	1:D:132:PHE:HB3	1.83	0.60
1:D:127:ARG:HE	1:D:138:GLN:HE22	1.49	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:PHE:CE2	1:A:136:GLU:HG3	2.37	0.59
1:B:130:HIS:HE1	2:B:291:HOH:O	1.86	0.58
1:D:147:THR:O	1:D:166:ILE:HG12	2.03	0.58
1:C:127:ARG:CD	1:C:129:ASP:OD1	2.47	0.57
1:B:177:LEU:HD13	1:B:198:GLN:HB3	1.86	0.57
1:B:127:ARG:HD2	1:B:129:ASP:O	2.05	0.56
1:C:127:ARG:HD2	1:C:129:ASP:O	2.07	0.55
1:B:141:TRP:CD2	1:B:155:ASP:HB3	2.42	0.55
1:C:141:TRP:CD2	1:C:155:ASP:HB3	2.43	0.54
1:D:177:LEU:HD22	1:D:198:GLN:NE2	2.23	0.54
1:D:127:ARG:HG3	1:D:138:GLN:CD	2.29	0.53
1:D:132:PHE:CE2	1:D:136:GLU:HA	2.45	0.52
1:B:158:LYS:HD2	2:B:294:HOH:O	2.09	0.52
1:C:125:LYS:HE2	2:C:285:HOH:O	2.10	0.52
1:C:216:PHE:HA	1:C:219:GLN:HE21	1.76	0.51
1:D:169:TYR:CD2	1:D:189:ILE:HG22	2.46	0.50
1:B:158:LYS:HD3	1:B:158:LYS:N	2.26	0.50
1:A:130:HIS:HA	1:A:132:PHE:CE2	2.47	0.50
1:D:213:GLN:HE21	1:D:217:ILE:CD1	2.25	0.50
1:B:127:ARG:CD	1:B:129:ASP:OD1	2.55	0.50
1:A:201:ALA:HB1	1:A:206:ASP:OD2	2.13	0.49
1:D:141:TRP:CD1	1:D:155:ASP:HB3	2.48	0.49
1:A:120:ALA:HB1	1:A:141:TRP:CZ2	2.48	0.48
1:B:193:ASP:N	1:B:193:ASP:OD2	2.46	0.48
1:D:105:GLN:HE21	1:D:165:ALA:H	1.62	0.48
1:C:130:HIS:HE1	2:C:303:HOH:O	1.97	0.47
1:D:127:ARG:CD	1:D:138:GLN:HE22	2.28	0.47
1:B:152:TYR:CD2	1:B:160:GLN:HA	2.50	0.46
1:A:158:LYS:HE3	1:D:156:LYS:HE2	1.98	0.45
1:D:166:ILE:O	1:D:218:LEU:HD21	2.15	0.45
1:A:167:ASP:O	1:A:194:LYS:NZ	2.49	0.45
1:B:105:GLN:N	1:B:150:TYR:HH	2.15	0.45
1:D:105:GLN:NE2	1:D:165:ALA:H	2.16	0.44
1:A:178:ARG:HB3	1:A:180:ASP:OD2	2.18	0.44
1:C:152:TYR:CD2	1:C:160:GLN:HA	2.53	0.44
1:D:169:TYR:O	1:D:218:LEU:HD13	2.19	0.43
1:A:108:PRO:HB3	1:A:159:GLN:HG3	2.00	0.43
1:C:112:GLN:NE2	1:C:156:LYS:HG2	2.33	0.43
1:B:158:LYS:CD	1:B:158:LYS:N	2.81	0.43
1:B:105:GLN:NE2	1:B:165:ALA:HB2	2.34	0.43
1:D:171:VAL:HG13	1:D:171:VAL:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:172:ARG:HG3	1:D:173:MET:O	2.19	0.42
1:A:118:ILE:CD1	1:A:217:ILE:HD11	2.36	0.42
1:A:177:LEU:HD13	1:A:198:GLN:HB3	2.01	0.41
1:D:127:ARG:HG3	1:D:138:GLN:OE1	2.21	0.41
1:D:167:ASP:O	1:D:194:LYS:NZ	2.52	0.41
1:B:141:TRP:CE2	1:B:155:ASP:HB3	2.56	0.41
1:A:166:ILE:O	1:A:169:TYR:HB2	2.21	0.41
1:B:120:ALA:HB1	1:B:141:TRP:CZ2	2.56	0.41
1:A:141:TRP:CD1	1:A:155:ASP:HB3	2.56	0.41

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	113/122 (93%)	104 (92%)	8 (7%)	1 (1%)	21	15
1	B	116/122 (95%)	113 (97%)	3 (3%)	0	100	100
1	C	116/122 (95%)	113 (97%)	3 (3%)	0	100	100
1	D	113/122 (93%)	99 (88%)	13 (12%)	1 (1%)	21	15
All	All	458/488 (94%)	429 (94%)	27 (6%)	2 (0%)	39	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	116	PHE
1	D	106	PHE

### 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	100/104 (96%)	93 (93%)	7 (7%)	19	15
1	B	102/104 (98%)	93 (91%)	9 (9%)	12	8
1	C	102/104 (98%)	97 (95%)	5 (5%)	31	28
1	D	100/104 (96%)	87 (87%)	13 (13%)	5	2
All	All	404/416 (97%)	370 (92%)	34 (8%)	14	9

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	A	128	LYS
1	A	132	PHE
1	A	133	LEU
1	A	154	SER
1	A	182	LYS
1	A	194	LYS
1	B	105	GLN
1	B	106	PHE
1	B	116	PHE
1	B	126	ARG
1	B	127	ARG
1	B	128	LYS
1	B	158	LYS
1	B	163	GLU
1	B	167	ASP
1	C	105	GLN
1	C	116	PHE
1	C	127	ARG
1	C	158	LYS
1	C	178	ARG
1	D	105	GLN
1	D	106	PHE
1	D	112	GLN

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Mol	Chain	Res	Type
1	D	125	LYS
1	D	128	LYS
1	D	129	ASP
1	D	132	PHE
1	D	145	SER
1	D	163	GLU
1	D	170	ASP
1	D	193	ASP
1	D	194	LYS
1	D	208	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	105	GLN
1	C	219	GLN
1	D	105	GLN
1	D	138	GLN
1	D	198	GLN
1	D	213	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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 ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	115/122 (94%)	1.13	20 (17%) 2 3	34, 54, 84, 101	0
1	B	118/122 (96%)	0.11	3 (2%) 61 67	25, 34, 52, 68	0
1	C	118/122 (96%)	0.04	2 (1%) 73 78	24, 31, 47, 60	0
1	D	115/122 (94%)	1.39	29 (25%) 1 1	39, 59, 87, 100	0
All	All	466/488 (95%)	0.66	54 (11%) 6 9	24, 44, 80, 101	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	133	LEU	15.1
1	A	130	HIS	8.5
1	A	135	PHE	7.7
1	D	192	PRO	7.2
1	D	133	LEU	6.9
1	D	130	HIS	6.4
1	A	134	GLY	6.4
1	D	132	PHE	6.3
1	A	106	PHE	6.2
1	A	192	PRO	5.7
1	A	132	PHE	5.7
1	A	193	ASP	5.5
1	D	131	SER	5.4
1	A	131	SER	5.2
1	D	106	PHE	5.0
1	D	129	ASP	4.9
1	D	168	GLY	4.6
1	A	105	GLN	4.6
1	C	106	PHE	4.5
1	D	193	ASP	4.5
1	D	128	LYS	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	116	PHE	4.4
1	D	191	ALA	4.2
1	D	159	GLN	3.9
1	A	116	PHE	3.9
1	B	105	GLN	3.6
1	A	129	ASP	3.6
1	D	181	GLY	3.4
1	A	216	PHE	3.4
1	B	106	PHE	3.2
1	D	107	PRO	3.1
1	D	196	ILE	3.1
1	D	108	PRO	2.9
1	A	127	ARG	2.9
1	A	107	PRO	2.9
1	B	181	GLY	2.8
1	D	199	PHE	2.5
1	A	158	LYS	2.5
1	D	169	TYR	2.4
1	D	217	ILE	2.4
1	A	212	GLN	2.3
1	D	123	LEU	2.3
1	D	158	LYS	2.3
1	D	179	LYS	2.3
1	D	105	GLN	2.2
1	A	109	ILE	2.2
1	D	206	ASP	2.1
1	C	199	PHE	2.1
1	A	159	GLN	2.1
1	D	219	GLN	2.1
1	D	127	ARG	2.1
1	A	179	LYS	2.1
1	D	195	ARG	2.1
1	D	187	PHE	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.