



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:54 PM UTC

PDB ID : 1U5G / pdb_00001u5g
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

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

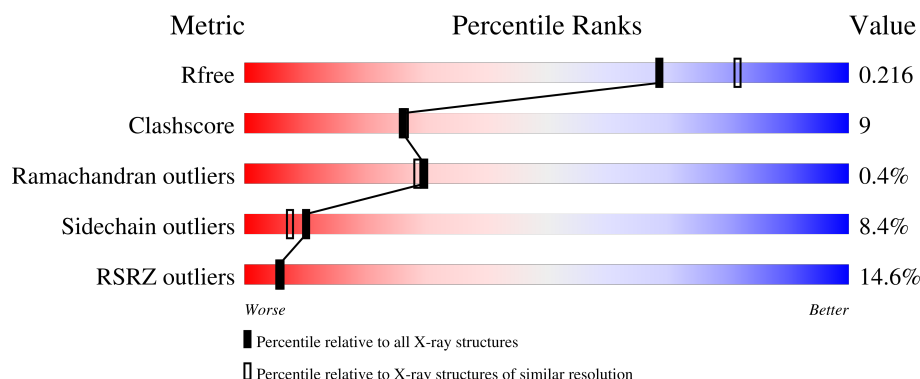
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 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	122	18% 61% 28% 5% 6%
1	B	122	2% 62% 25% 8% ...
1	C	122	2% 65% 29% ...
1	D	122	34% 57% 30% 6% 6%

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 mutation	UNP Q8BK74
A	102	SER	ASP	engineered mutation	UNP Q8BK74
B	101	GLY	SER	engineered mutation	UNP Q8BK74
B	102	SER	ASP	engineered mutation	UNP Q8BK74
C	101	GLY	SER	engineered mutation	UNP Q8BK74
C	102	SER	ASP	engineered mutation	UNP Q8BK74
D	101	GLY	SER	engineered mutation	UNP Q8BK74
D	102	SER	ASP	engineered mutation	UNP Q8BK74

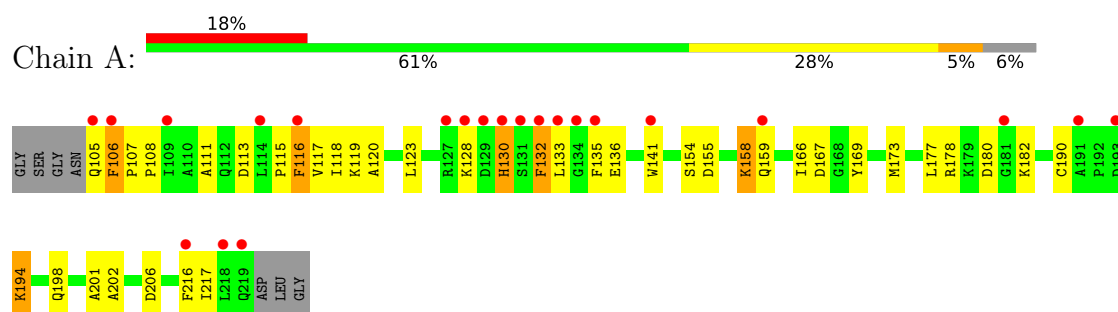
- Molecule 2 is water.

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		

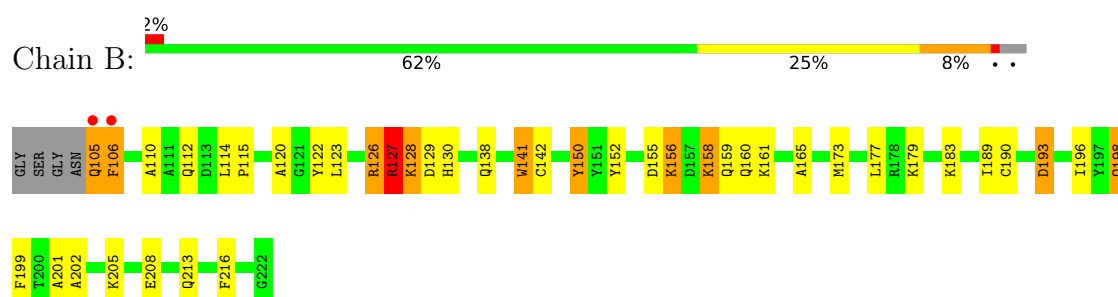
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

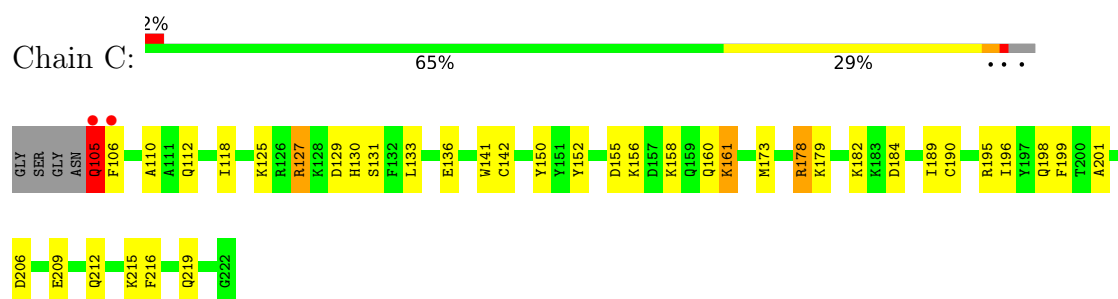
- Molecule 1: Src-associated adaptor protein



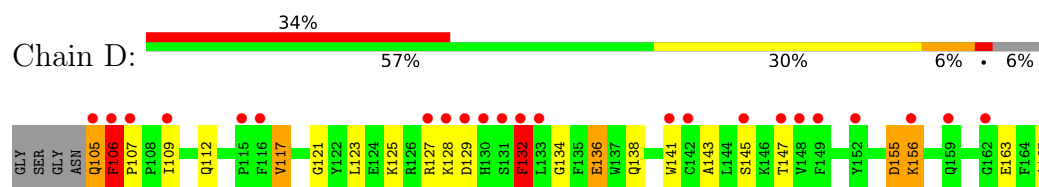
- Molecule 1: Src-associated adaptor protein

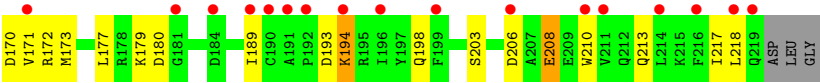


- Molecule 1: Src-associated adaptor protein



- 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, α , β , γ	59.61Å 65.69Å 143.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.10 25.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.4 (25.00-2.10) 99.4 (25.00-2.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.213 , 0.271 (Not available) , 0.216	Depositor DCC
R_{free} test set	1702 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	24.9	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4091	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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	1.72	10/985 (1.0%)	1.42	7/1323 (0.5%)
1	B	2.06	26/1006 (2.6%)	1.56	11/1350 (0.8%)
1	C	2.09	26/1006 (2.6%)	1.52	5/1350 (0.4%)
1	D	1.54	6/985 (0.6%)	1.37	13/1323 (1.0%)
All	All	1.87	68/3982 (1.7%)	1.47	36/5346 (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 (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	127	ARG	CD-NE	-9.60	1.32	1.46
1	C	131	SER	C-O	-9.57	1.12	1.23
1	B	127	ARG	CD-NE	-9.11	1.33	1.46
1	A	135	PHE	CA-C	9.02	1.63	1.52
1	B	115	PRO	N-CD	8.96	1.60	1.47
1	C	133	LEU	C-O	-8.61	1.12	1.24
1	D	107	PRO	CA-C	8.35	1.59	1.52
1	C	106	PHE	C-N	-8.21	1.23	1.33
1	B	128	LYS	C-O	-7.87	1.14	1.23
1	B	201	ALA	CA-CB	7.64	1.64	1.53
1	D	208	GLU	CA-C	7.53	1.62	1.52
1	A	107	PRO	CA-C	7.51	1.59	1.52
1	B	205	LYS	C-O	-7.33	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	202	ALA	N-CA	7.33	1.55	1.46
1	A	111	ALA	CA-CB	7.23	1.64	1.53
1	A	106	PHE	CA-C	7.12	1.61	1.52
1	B	138	GLN	C-O	7.12	1.32	1.24
1	B	150	TYR	C-O	7.02	1.32	1.23
1	C	201	ALA	CA-CB	6.88	1.63	1.53
1	A	117	VAL	N-CA	6.79	1.53	1.46
1	C	127	ARG	C-O	-6.78	1.14	1.23
1	B	126	ARG	CD-NE	-6.64	1.36	1.46
1	C	110	ALA	N-CA	-6.61	1.37	1.45
1	C	189	ILE	CA-C	6.42	1.60	1.52
1	C	178	ARG	C-O	-6.37	1.15	1.23
1	B	179	LYS	C-O	-6.30	1.15	1.24
1	C	199	PHE	CA-C	-6.27	1.45	1.52
1	D	155	ASP	CA-C	6.22	1.61	1.52
1	D	180	ASP	CA-C	6.19	1.60	1.53
1	A	123	LEU	C-O	-6.14	1.16	1.23
1	B	173	MET	SD-CE	6.11	1.94	1.79
1	A	106	PHE	N-CA	6.01	1.52	1.46
1	C	136	GLU	C-O	-5.97	1.16	1.24
1	C	189	ILE	C-O	5.96	1.30	1.24
1	C	173	MET	SD-CE	5.91	1.94	1.79
1	C	105	GLN	CA-C	-5.89	1.40	1.52
1	C	150	TYR	CA-C	-5.87	1.45	1.52
1	C	195	ARG	CG-CD	-5.81	1.35	1.52
1	B	161	LYS	CA-C	-5.79	1.44	1.52
1	B	196	ILE	CA-C	5.75	1.59	1.52
1	A	202	ALA	C-O	-5.68	1.16	1.24
1	C	215	LYS	N-CA	-5.52	1.39	1.46
1	D	109	ILE	CA-C	5.52	1.59	1.52
1	B	213	GLN	C-O	5.46	1.30	1.24
1	A	115	PRO	C-O	5.42	1.29	1.23
1	C	142	CYS	C-O	-5.41	1.17	1.24
1	B	141	TRP	N-CA	5.39	1.52	1.46
1	C	179	LYS	C-O	-5.35	1.17	1.24
1	C	206	ASP	N-CA	5.35	1.52	1.46
1	C	209	GLU	CA-C	5.33	1.59	1.52
1	B	189	ILE	CA-CB	-5.32	1.47	1.54
1	B	110	ALA	C-O	-5.31	1.17	1.23
1	A	173	MET	SD-CE	5.30	1.92	1.79
1	B	208	GLU	CA-C	-5.30	1.45	1.52
1	B	189	ILE	C-O	5.28	1.29	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	142	CYS	N-CA	5.24	1.52	1.46
1	C	201	ALA	CA-C	5.22	1.60	1.53
1	B	199	PHE	CD2-CE2	-5.21	1.23	1.38
1	B	159	GLN	CA-C	5.19	1.59	1.52
1	C	198	GLN	N-CA	-5.19	1.39	1.46
1	B	198	GLN	C-O	5.14	1.30	1.23
1	B	123	LEU	CA-C	5.11	1.58	1.52
1	B	216	PHE	CE1-CZ	-5.06	1.23	1.38
1	C	178	ARG	CB-CG	-5.06	1.37	1.52
1	D	106	PHE	CA-C	5.05	1.59	1.52
1	B	193	ASP	CA-CB	5.04	1.59	1.53
1	C	161	LYS	CD-CE	5.03	1.67	1.52
1	C	212	GLN	CG-CD	5.01	1.64	1.52

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	127	ARG	NE-CZ-NH1	10.03	131.53	121.50
1	B	112	GLN	OE1-CD-NE2	-9.81	112.79	122.60
1	A	135	PHE	N-CA-C	9.62	125.20	108.75
1	B	114	LEU	CA-C-N	9.21	129.33	120.31
1	B	114	LEU	C-N-CA	9.21	129.33	120.31
1	B	127	ARG	NE-CZ-NH2	-8.89	111.20	119.20
1	A	116	PHE	CA-C-N	-8.28	110.22	121.80
1	A	116	PHE	C-N-CA	-8.28	110.22	121.80
1	A	106	PHE	N-CA-C	8.01	124.53	113.16
1	C	127	ARG	NE-CZ-NH2	-7.92	112.07	119.20
1	C	106	PHE	CA-C-N	-7.69	112.46	120.38
1	C	106	PHE	C-N-CA	-7.69	112.46	120.38
1	A	216	PHE	N-CA-C	-7.29	103.64	112.54
1	D	107	PRO	N-CA-C	7.14	119.41	110.70
1	D	134	GLY	N-CA-C	-6.94	102.46	112.17
1	A	130	HIS	N-CA-C	6.82	122.26	113.88
1	D	117	VAL	N-CA-CB	-6.74	104.25	111.46
1	B	156	LYS	N-CA-C	6.73	121.20	112.92
1	B	112	GLN	CG-CD-NE2	6.68	126.42	116.40
1	C	127	ARG	NE-CZ-NH1	6.12	127.62	121.50
1	D	180	ASP	N-CA-C	5.89	117.68	109.31
1	A	113	ASP	N-CA-C	5.80	120.22	113.20
1	B	106	PHE	CB-CA-C	5.65	121.30	110.17
1	B	156	LYS	N-CA-CB	-5.47	102.57	110.56
1	B	122	TYR	N-CA-C	-5.29	100.67	109.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	123	LEU	CA-C-N	-5.23	115.50	122.72
1	D	123	LEU	C-N-CA	-5.23	115.50	122.72
1	D	136	GLU	CA-CB-CG	-5.23	103.64	114.10
1	B	126	ARG	CB-CG-CD	5.20	123.26	111.30
1	D	203	SER	N-CA-CB	-5.16	105.98	111.29
1	D	210	TRP	CA-C-N	5.14	127.14	120.56
1	D	210	TRP	C-N-CA	5.14	127.14	120.56
1	C	118	ILE	N-CA-C	5.04	115.81	110.72
1	D	121	GLY	N-CA-C	-5.03	104.88	111.37
1	D	143	ALA	CA-C-N	-5.01	115.72	123.14
1	D	143	ALA	C-N-CA	-5.01	115.72	123.14

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	16	0
1	B	980	0	956	17	0
1	C	980	0	956	17	0
1	D	959	0	938	23	0
2	A	23	0	0	3	0
2	B	82	0	0	4	0
2	C	88	0	0	4	0
2	D	20	0	0	1	0
All	All	4091	0	3788	72	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 (72) 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:N	1:C:105:GLN:NE2	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:HE21	1:C:105:GLN:HA	1.48	0.77
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:C:105:GLN:NE2	1:C:105:GLN:CA	2.13	0.61
1:D:168:GLY:HA3	1:D:194:LYS:NZ	2.15	0.61
1:D:168:GLY:HA3	1:D:194:LYS:HZ3	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
1:A:132:PHE:CE2	1:A:136:GLU:HG3	2.37	0.59
1:A:119:LYS:NZ	2:A:234:HOH:O	2.31	0.58
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:D:127:ARG:HG3	1:D:138:GLN:CD	2.29	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: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:B:158:LYS:N	1:B:158:LYS:HD3	2.26	0.50
1:D:169:TYR:CD2	1:D:189:ILE:HG22	2.46	0.50
1:A:130:HIS:HA	1:A:132:PHE:CE2	2.47	0.50
1:C:182:LYS:NZ	2:C:284:HOH:O	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:OD2	1:B:193:ASP:N	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:B:183:LYS:NZ	2:B:233:HOH:O	2.38	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:D:105:GLN:NE2	1:D:165:ALA:H	2.16	0.44
1:B:105:GLN:N	1:B:150:TYR:HH	2.15	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:105:GLN:NE2	1:B:165:ALA:HB2	2.34	0.43
1:B:158:LYS:N	1:B:158:LYS:CD	2.81	0.43
1:D:171:VAL:O	1:D:171:VAL:HG13	2.18	0.42
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:A:166:ILE:O	1:A:169:TYR:HB2	2.21	0.41
1:B:141:TRP:CE2	1:B:155:ASP:HB3	2.56	0.41
1:D:167:ASP:O	1:D:194:LYS:NZ	2.52	0.41
1:A:141:TRP:CD1	1:A:155:ASP:HB3	2.56	0.41
1:B:120:ALA:HB1	1:B:141:TRP:CZ2	2.56	0.41

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	113/122 (93%)	104 (92%)	8 (7%)	1 (1%)	14	10
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%)	14	10
All	All	458/488 (94%)	429 (94%)	27 (6%)	2 (0%)	30	28

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%)	14	11
1	B	102/104 (98%)	95 (93%)	7 (7%)	14	12
1	C	102/104 (98%)	98 (96%)	4 (4%)	28	31
1	D	100/104 (96%)	84 (84%)	16 (16%)	2	1
All	All	404/416 (97%)	370 (92%)	34 (8%)	10	7

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

Mol	Chain	Res	Type
1	A	128	LYS
1	A	132	PHE
1	A	133	LEU
1	A	154	SER
1	A	158	LYS
1	A	182	LYS

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Mol	Chain	Res	Type
1	A	194	LYS
1	B	105	GLN
1	B	106	PHE
1	B	126	ARG
1	B	127	ARG
1	B	128	LYS
1	B	156	LYS
1	B	158	LYS
1	C	105	GLN
1	C	158	LYS
1	C	161	LYS
1	C	178	ARG
1	D	105	GLN
1	D	106	PHE
1	D	112	GLN
1	D	117	VAL
1	D	125	LYS
1	D	128	LYS
1	D	129	ASP
1	D	132	PHE
1	D	145	SER
1	D	156	LYS
1	D	163	GLU
1	D	170	ASP
1	D	179	LYS
1	D	193	ASP
1	D	194	LYS
1	D	208	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	219	GLN
1	B	105	GLN
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 [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

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	115/122 (94%)	1.33	22 (19%) 3 3	34, 54, 84, 101	0
1	B	118/122 (96%)	0.23	2 (1%) 69 71	25, 34, 52, 68	0
1	C	118/122 (96%)	-0.00	2 (1%) 69 71	24, 31, 47, 60	0
1	D	115/122 (94%)	1.72	42 (36%) 1 1	39, 59, 87, 100	0
All	All	466/488 (95%)	0.81	68 (14%) 6 6	24, 44, 80, 101	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	133	LEU	9.7
1	A	135	PHE	6.5
1	B	105	GLN	5.7
1	C	106	PHE	5.5
1	A	132	PHE	5.0
1	D	133	LEU	4.7
1	D	132	PHE	4.7
1	A	105	GLN	4.4
1	A	106	PHE	4.3
1	D	106	PHE	4.2
1	A	116	PHE	4.0
1	D	168	GLY	4.0
1	D	191	ALA	3.9
1	C	105	GLN	3.8
1	A	216	PHE	3.7
1	B	106	PHE	3.6
1	A	159	GLN	3.5
1	A	131	SER	3.4
1	A	218	LEU	3.4
1	D	216	PHE	3.4
1	D	169	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	134	GLY	3.3
1	A	109	ILE	3.3
1	D	199	PHE	3.2
1	D	171	VAL	3.1
1	D	130	HIS	3.1
1	D	142	CYS	3.1
1	A	130	HIS	3.0
1	D	196	ILE	3.0
1	D	128	LYS	2.9
1	D	127	ARG	2.7
1	A	141	TRP	2.7
1	D	149	PHE	2.7
1	D	109	ILE	2.7
1	D	107	PRO	2.6
1	D	218	LEU	2.6
1	A	127	ARG	2.6
1	D	219	GLN	2.5
1	D	211	VAL	2.5
1	A	193	ASP	2.5
1	D	129	ASP	2.5
1	D	131	SER	2.5
1	D	159	GLN	2.5
1	D	116	PHE	2.5
1	D	152	TYR	2.4
1	D	145	SER	2.4
1	A	181	GLY	2.4
1	D	214	LEU	2.4
1	D	141	TRP	2.4
1	A	219	GLN	2.3
1	D	148	VAL	2.3
1	D	190	CYS	2.3
1	D	162	GLY	2.3
1	D	181	GLY	2.3
1	D	210	TRP	2.3
1	D	192	PRO	2.2
1	D	189	ILE	2.2
1	A	191	ALA	2.2
1	D	105	GLN	2.2
1	A	129	ASP	2.2
1	D	206	ASP	2.2
1	A	128	LYS	2.2
1	D	147	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	114	LEU	2.1
1	D	184	ASP	2.1
1	D	156	LYS	2.1
1	D	115	PRO	2.0
1	D	194	LYS	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.