



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 02:08 PM GMT

PDB ID : 4AJ5
Title : Crystal structure of the Ska core complex
Authors : Jeyaprakash, A.A.; Santamaria, A.; Jayachandran, U.; Chan, Y.W.; Benda, C.; Nigg, E.A.; Conti, E.
Deposited on : 2012-02-15
Resolution : 3.32 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

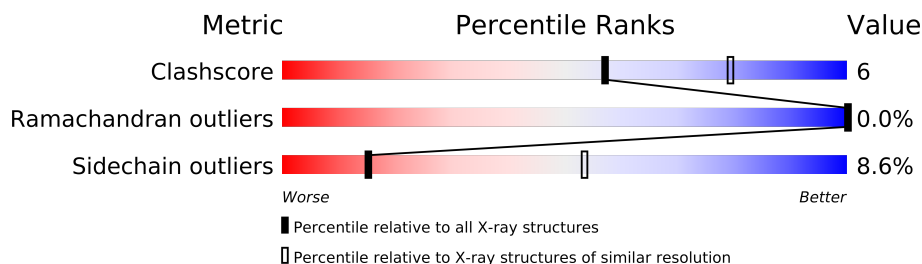
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : **FAILED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.32 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))
Clashscore	79885	1016 (3.42-3.22)
Ramachandran outliers	78287	1699 (3.44-3.20)
Sidechain outliers	78261	1697 (3.44-3.20)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	1	101	
1	2	101	
1	3	101	
1	4	101	
1	U	101	
1	V	101	
1	W	101	
1	X	101	
1	Y	101	
1	Z	101	
2	A	91	
2	B	91	
2	C	91	
2	D	91	
2	E	91	
2	F	91	
2	G	91	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	91	
2	I	91	
2	J	91	
3	K	123	
3	L	123	
3	M	123	
3	N	123	
3	O	123	
3	P	123	
3	Q	123	
3	R	123	
3	S	123	
3	T	123	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21691 atoms, of which 0 are hydrogen and 0 are deuterium.

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 SPINDLE AND KINETOCHORE-ASSOCIATEDPROTEIN 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	99	Total	C	N	O	S	0	0	0
			740	458	128	151	3			
1	2	100	Total	C	N	O	S	0	0	0
			787	491	135	156	5			
1	3	98	Total	C	N	O	S	0	0	0
			738	459	126	149	4			
1	4	98	Total	C	N	O	S	0	0	0
			775	484	134	151	6			
1	U	100	Total	C	N	O	S	0	0	0
			773	484	131	152	6			
1	V	98	Total	C	N	O	S	0	0	0
			725	448	126	148	3			
1	W	98	Total	C	N	O	S	0	0	0
			727	449	128	146	4			
1	X	98	Total	C	N	O	S	0	0	0
			729	453	126	147	3			
1	Y	99	Total	C	N	O	S	0	0	0
			763	479	133	146	5			
1	Z	97	Total	C	N	O	S	0	0	0
			723	446	127	146	4			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	58	ILE	VAL	ENGINEERED MUTATION	UNP Q8IX90
2	58	ILE	VAL	ENGINEERED MUTATION	UNP Q8IX90
3	58	ILE	VAL	ENGINEERED MUTATION	UNP Q8IX90
4	58	ILE	VAL	ENGINEERED MUTATION	UNP Q8IX90
U	58	ILE	VAL	ENGINEERED MUTATION	UNP Q8IX90
V	58	ILE	VAL	ENGINEERED MUTATION	UNP Q8IX90
W	58	ILE	VAL	ENGINEERED MUTATION	UNP Q8IX90
X	58	ILE	VAL	ENGINEERED MUTATION	UNP Q8IX90

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
Y	58	ILE	VAL	ENGINEERED MUTATION	UNP Q8IX90
Z	58	ILE	VAL	ENGINEERED MUTATION	UNP Q8IX90

- Molecule 2 is a protein called SPINDLE AND KINETOCHORE-ASSOCIATEDPROTEIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	79	Total	C	N	O	S	0	0	0
			588	363	99	123	3			
2	B	87	Total	C	N	O	S	0	0	0
			656	406	109	138	3			
2	C	79	Total	C	N	O	S	0	0	0
			595	369	100	123	3			
2	D	86	Total	C	N	O	S	0	0	0
			646	399	108	136	3			
2	E	86	Total	C	N	O	S	0	0	0
			630	387	108	132	3			
2	F	82	Total	C	N	O	S	0	0	0
			585	362	102	118	3			
2	G	86	Total	C	N	O	S	0	0	0
			637	392	108	134	3			
2	H	83	Total	C	N	O	S	0	0	0
			633	391	104	135	3			
2	I	86	Total	C	N	O	S	0	0	0
			645	398	109	135	3			
2	J	86	Total	C	N	O	S	0	0	0
			639	396	105	135	3			

- Molecule 3 is a protein called SPINDLE AND KINETOCHORE-ASSOCIATEDPROTEIN 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	108	Total	C	N	O	S	0	0	0
			813	511	132	166	4			
3	L	106	Total	C	N	O	S	0	0	0
			779	491	130	155	3			
3	M	109	Total	C	N	O	S	0	0	0
			800	505	133	158	4			
3	N	104	Total	C	N	O	S	0	0	0
			770	485	129	152	4			
3	O	109	Total	C	N	O	S	0	0	0
			840	528	140	168	4			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	105	Total	C	N	O	S	0	0	0
			776	491	125	155	5			
3	Q	102	Total	C	N	O	S	0	0	0
			729	457	123	145	4			
3	R	108	Total	C	N	O	S	0	0	0
			826	520	138	163	5			
3	S	107	Total	C	N	O	S	0	0	0
			785	495	129	157	4			
3	T	110	Total	C	N	O	S	0	0	0
			839	534	137	163	5			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-1	GLY	-	EXPRESSION TAG	UNP Q8WVK7
K	0	HIS	-	EXPRESSION TAG	UNP Q8WVK7
L	-1	GLY	-	EXPRESSION TAG	UNP Q8WVK7
L	0	HIS	-	EXPRESSION TAG	UNP Q8WVK7
M	-1	GLY	-	EXPRESSION TAG	UNP Q8WVK7
M	0	HIS	-	EXPRESSION TAG	UNP Q8WVK7
N	-1	GLY	-	EXPRESSION TAG	UNP Q8WVK7
N	0	HIS	-	EXPRESSION TAG	UNP Q8WVK7
O	-1	GLY	-	EXPRESSION TAG	UNP Q8WVK7
O	0	HIS	-	EXPRESSION TAG	UNP Q8WVK7
P	-1	GLY	-	EXPRESSION TAG	UNP Q8WVK7
P	0	HIS	-	EXPRESSION TAG	UNP Q8WVK7
Q	-1	GLY	-	EXPRESSION TAG	UNP Q8WVK7
Q	0	HIS	-	EXPRESSION TAG	UNP Q8WVK7
R	-1	GLY	-	EXPRESSION TAG	UNP Q8WVK7
R	0	HIS	-	EXPRESSION TAG	UNP Q8WVK7
S	-1	GLY	-	EXPRESSION TAG	UNP Q8WVK7
S	0	HIS	-	EXPRESSION TAG	UNP Q8WVK7
T	-1	GLY	-	EXPRESSION TAG	UNP Q8WVK7
T	0	HIS	-	EXPRESSION TAG	UNP Q8WVK7

3 Residue-property plots

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.

Note EDS failed to run properly.

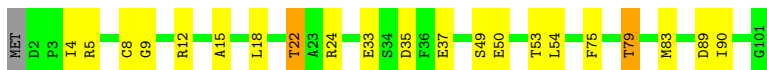
- Molecule 1: SPINDLE AND KINETOCHORE-ASSOCIATEDPROTEIN 3

Chain 1: 



- Molecule 1: SPINDLE AND KINETOCHORE-ASSOCIATEDPROTEIN 3

Chain 2: 



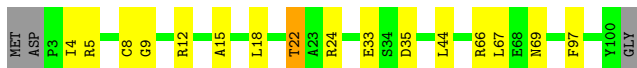
- Molecule 1: SPINDLE AND KINETOCHORE-ASSOCIATEDPROTEIN 3

Chain 3: 



- Molecule 1: SPINDLE AND KINETOCHORE-ASSOCIATEDPROTEIN 3

Chain 4: 



- Molecule 1: SPINDLE AND KINETOCHORE-ASSOCIATEDPROTEIN 3

Chain U: 



- Molecule 1: SPINDLE AND KINETOCHORE-ASSOCIATEDPROTEIN 3

Chain V: 



- Molecule 1: SPINDLE AND KINETOCHORE-ASSOCIATEDPROTEIN 3

Chain W:



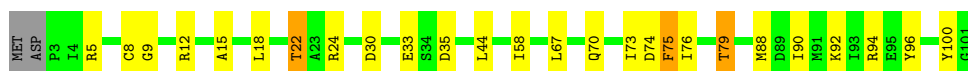
- Molecule 1: SPINDLE AND KINETOCHORE-ASSOCIATEDPROTEIN 3

Chain X:



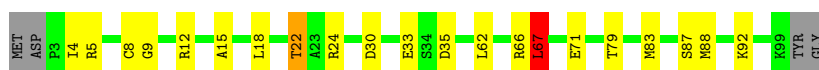
- Molecule 1: SPINDLE AND KINETOCHORE-ASSOCIATEDPROTEIN 3

Chain Y:



- Molecule 1: SPINDLE AND KINETOCHORE-ASSOCIATEDPROTEIN 3

Chain Z:



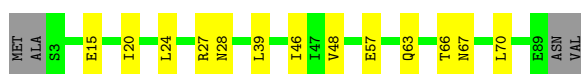
- Molecule 2: SPINDLE AND KINETOCHORE-ASSOCIATEDPROTEIN 1

Chain A:



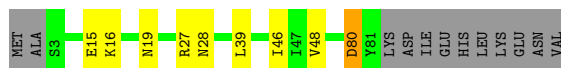
- Molecule 2: SPINDLE AND KINETOCHORE-ASSOCIATEDPROTEIN 1

Chain B:



- Molecule 2: SPINDLE AND KINETOCHORE-ASSOCIATEDPROTEIN 1

Chain C:



- Molecule 2: SPINDLE AND KINETOCHORE-ASSOCIATEDPROTEIN 1

Chain D:



- Molecule 2: SPINDLE AND KINETOCHORE-ASSOCIATEDPROTEIN 1

Chain E: 



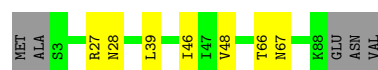
- Molecule 2: SPINDLE AND KINETOCHORE-ASSOCIATEDPROTEIN 1

Chain F: 



- Molecule 2: SPINDLE AND KINETOCHORE-ASSOCIATEDPROTEIN 1

Chain G: 



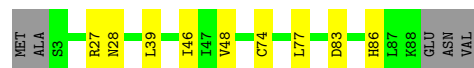
- Molecule 2: SPINDLE AND KINETOCHORE-ASSOCIATEDPROTEIN 1

Chain H: 



- Molecule 2: SPINDLE AND KINETOCHORE-ASSOCIATEDPROTEIN 1

Chain I: 



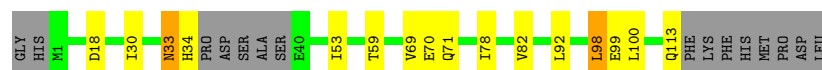
- Molecule 2: SPINDLE AND KINETOCHORE-ASSOCIATEDPROTEIN 1

Chain J: 



- Molecule 3: SPINDLE AND KINETOCHORE-ASSOCIATEDPROTEIN 2

Chain K: 



- Molecule 3: SPINDLE AND KINETOCHORE-ASSOCIATEDPROTEIN 2

Chain L: 



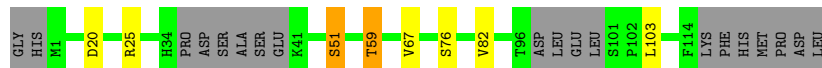
- Molecule 3: SPINDLE AND KINETOCHORE-ASSOCIATEDPROTEIN 2

Chain M: 



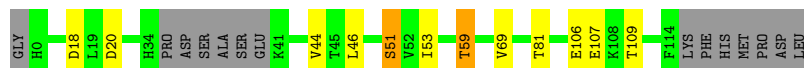
- Molecule 3: SPINDLE AND KINETOCHORE-ASSOCIATEDPROTEIN 2

Chain N:



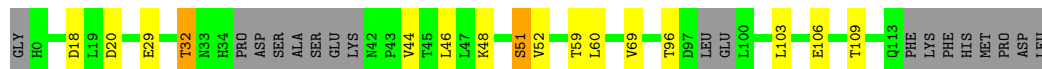
- Molecule 3: SPINDLE AND KINETOCHORE-ASSOCIATEDPROTEIN 2

Chain O:



- Molecule 3: SPINDLE AND KINETOCHORE-ASSOCIATEDPROTEIN 2

Chain P:



- Molecule 3: SPINDLE AND KINETOCHORE-ASSOCIATEDPROTEIN 2

Chain Q:



- Molecule 3: SPINDLE AND KINETOCHORE-ASSOCIATEDPROTEIN 2

Chain R:



- Molecule 3: SPINDLE AND KINETOCHORE-ASSOCIATEDPROTEIN 2

Chain S:



- Molecule 3: SPINDLE AND KINETOCHORE-ASSOCIATEDPROTEIN 2

Chain T:



4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	174.40Å 193.12Å 198.27Å 90.00° 95.21° 90.00°	Depositor
Resolution (Å)	69.03 – 3.32	Depositor
% Data completeness (in resolution range)	94.2 (69.03-3.32)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 3.33Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.234 , 0.280	Depositor
Wilson B-factor (Å ²)	104.4	Xtriage
Anisotropy	0.261	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	4 of 90969 reflections (0.004%)	Xtriage
Total number of atoms	21691	wwPDB-VP
Average B, all atoms (Å ²)	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	1	0.39	0/747	0.64	0/1012
1	2	0.46	0/796	0.70	0/1071
1	3	0.38	0/745	0.65	0/1008
1	4	0.42	0/783	0.65	0/1050
1	U	0.41	0/782	0.69	0/1055
1	V	0.40	0/733	0.64	0/993
1	W	0.41	0/734	0.68	1/991 (0.1%)
1	X	0.42	0/738	0.64	0/1000
1	Y	0.48	0/772	0.75	1/1039 (0.1%)
1	Z	0.42	0/729	0.71	1/984 (0.1%)
2	A	0.37	0/590	0.52	0/800
2	B	0.37	0/659	0.53	0/894
2	C	0.38	0/598	0.51	0/811
2	D	0.45	0/649	0.54	0/879
2	E	0.38	0/632	0.53	0/858
2	F	0.40	0/587	0.53	0/799
2	G	0.40	0/639	0.51	0/867
2	H	0.47	0/636	0.61	0/862
2	I	0.40	0/648	0.47	0/879
2	J	0.39	0/642	0.50	0/873
3	K	0.40	0/822	0.63	1/1117 (0.1%)
3	L	0.42	0/788	0.58	0/1074
3	M	0.40	0/809	0.59	0/1101
3	N	0.40	0/778	0.57	1/1056 (0.1%)
3	O	0.50	0/850	0.70	0/1152
3	P	0.42	0/785	0.61	0/1070
3	Q	0.43	0/736	0.58	0/1001
3	R	0.46	0/836	0.69	0/1134
3	S	0.42	0/794	0.63	0/1081
3	T	0.42	0/851	0.67	2/1155 (0.2%)
All	All	0.42	0/21888	0.62	7/29666 (0.0%)

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
3	K	0	1
3	R	0	1
All	All	0	2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Z	67	LEU	CA-CB-CG	5.96	129.02	115.30
3	T	98	LEU	CA-CB-CG	5.89	128.86	115.30
3	K	98	LEU	CA-CB-CG	5.69	128.39	115.30
3	T	103	LEU	CA-CB-CG	5.37	127.64	115.30
1	W	67	LEU	CA-CB-CG	5.07	126.96	115.30
3	N	103	LEU	CA-CB-CG	5.03	126.87	115.30
1	Y	75	PHE	N-CA-C	-5.02	97.45	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	K	99	GLU	Peptide
3	R	99	GLU	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	740	0	0	5	0
1	2	787	0	0	10	0
1	3	738	0	0	7	0
1	4	775	0	0	6	0
1	U	773	0	0	8	0
1	V	725	0	0	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	W	727	0	0	6	0
1	X	729	0	0	8	0
1	Y	763	0	0	12	1
1	Z	723	0	0	10	0
2	A	588	0	0	5	0
2	B	656	0	0	3	0
2	C	595	0	0	3	0
2	D	646	0	0	4	0
2	E	630	0	0	3	0
2	F	585	0	0	5	0
2	G	637	0	0	2	0
2	H	633	0	0	5	1
2	I	645	0	0	1	0
2	J	639	0	0	4	0
3	K	813	0	0	4	0
3	L	779	0	0	4	0
3	M	800	0	0	5	0
3	N	770	0	0	4	0
3	O	840	0	0	5	0
3	P	776	0	0	7	0
3	Q	729	0	0	4	0
3	R	826	0	1	7	0
3	S	785	0	0	3	0
3	T	839	0	0	4	0
All	All	21691	0	1	139	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (139) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:Y:18:LEU:O	1:Y:22:THR:OG1	1.98	0.82
3:M:18:ASP:OD1	3:P:51:SER:OG	2.00	0.79
1:X:18:LEU:O	1:X:22:THR:OG1	2.03	0.76
1:V:18:LEU:O	1:V:22:THR:OG1	2.05	0.75
1:1:18:LEU:O	1:1:22:THR:OG1	2.05	0.75
1:4:18:LEU:O	1:4:22:THR:OG1	2.06	0.73
1:U:18:LEU:O	1:U:22:THR:OG1	2.06	0.73
3:Q:18:ASP:OD1	3:R:51:SER:OG	2.07	0.72
3:O:59:THR:OG1	1:Z:30:ASP:OD1	2.07	0.72
1:3:18:LEU:O	1:3:22:THR:OG1	2.07	0.71
1:Z:18:LEU:O	1:Z:22:THR:OG1	2.09	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:67:ASN:ND2	3:K:70:GLU:OE1	2.24	0.70
3:O:51:SER:OG	3:P:18:ASP:OD1	2.09	0.70
1:V:82:LEU:O	1:V:86:ASN:ND2	2.26	0.69
1:Z:83:MET:O	1:Z:87:SER:N	2.26	0.68
1:U:99:LYS:NZ	1:U:100:TYR:O	2.28	0.67
2:F:16:LYS:NZ	3:P:20:ASP:OD1	2.27	0.67
1:2:18:LEU:O	1:2:22:THR:OG1	2.12	0.67
2:G:67:ASN:ND2	3:Q:70:GLU:OE1	2.28	0.67
1:2:50:GLU:O	1:2:54:LEU:N	2.30	0.65
1:W:67:LEU:O	1:W:71:GLU:N	2.31	0.64
1:2:50:GLU:O	1:2:53:THR:N	2.30	0.63
1:W:18:LEU:O	1:W:22:THR:OG1	2.16	0.63
1:U:75:PHE:O	1:U:79:THR:N	2.31	0.63
1:4:15:ALA:O	1:4:18:LEU:N	2.32	0.62
3:N:51:SER:OG	3:O:18:ASP:OD1	2.18	0.61
2:E:27:ARG:NH2	2:E:28:ASN:OD1	2.33	0.61
1:Y:15:ALA:O	1:Y:18:LEU:N	2.34	0.61
3:R:70:GLU:O	3:R:74:SER:N	2.34	0.61
3:M:42:ASN:OD1	3:M:42:ASN:N	2.34	0.61
1:1:15:ALA:O	1:1:18:LEU:N	2.34	0.60
2:D:66:THR:O	2:D:70:LEU:N	2.34	0.60
1:X:15:ALA:O	1:X:18:LEU:N	2.35	0.60
3:P:29:GLU:O	3:P:32:THR:OG1	2.19	0.60
3:P:106:GLU:O	3:P:109:THR:OG1	2.18	0.60
1:3:15:ALA:O	1:3:18:LEU:N	2.34	0.59
1:Y:67:LEU:O	1:Y:70:GLN:N	2.35	0.59
3:L:18:ASP:OD1	3:S:51:SER:OG	2.21	0.59
2:F:27:ARG:NH2	2:F:28:ASN:OD1	2.36	0.58
1:W:8:CYS:O	1:W:12:ARG:N	2.36	0.58
3:S:105:LYS:O	3:S:109:THR:OG1	2.21	0.58
1:X:8:CYS:O	1:X:12:ARG:N	2.37	0.57
1:Z:15:ALA:O	1:Z:18:LEU:N	2.38	0.57
1:Z:88:MET:O	1:Z:92:LYS:N	2.38	0.56
1:Y:75:PHE:O	1:Y:79:THR:N	2.38	0.56
1:3:8:CYS:O	1:3:12:ARG:N	2.38	0.56
2:I:27:ARG:NH2	2:I:28:ASN:OD1	2.38	0.56
1:Z:8:CYS:O	1:Z:12:ARG:N	2.39	0.56
1:Y:8:CYS:O	1:Y:12:ARG:N	2.39	0.56
1:V:8:CYS:O	1:V:12:ARG:N	2.39	0.56
1:1:8:CYS:O	1:1:12:ARG:N	2.39	0.56
2:D:27:ARG:NH2	2:D:28:ASN:OD1	2.39	0.55
2:H:67:ASN:ND2	3:R:70:GLU:OE1	2.39	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:W:15:ALA:O	1:W:18:LEU:N	2.39	0.55
1:V:5:ARG:O	1:V:9:GLY:N	2.40	0.55
1:2:15:ALA:O	1:2:18:LEU:N	2.40	0.54
2:A:27:ARG:NH2	2:A:28:ASN:OD1	2.40	0.54
2:C:27:ARG:NH2	2:C:28:ASN:OD1	2.40	0.54
1:Z:5:ARG:O	1:Z:9:GLY:N	2.41	0.54
1:2:8:CYS:O	1:2:12:ARG:N	2.40	0.54
3:R:96:THR:OG1	3:R:96:THR:O	2.26	0.54
1:4:5:ARG:O	1:4:9:GLY:N	2.41	0.54
1:Y:5:ARG:O	1:Y:9:GLY:N	2.41	0.54
1:U:15:ALA:O	1:U:18:LEU:N	2.41	0.53
2:A:54:ASN:OD1	3:L:56:ARG:NH1	2.42	0.53
1:U:8:CYS:O	1:U:12:ARG:N	2.42	0.53
1:1:5:ARG:O	1:1:9:GLY:N	2.42	0.53
2:B:27:ARG:NH2	2:B:28:ASN:OD1	2.42	0.53
2:J:27:ARG:NH2	2:J:28:ASN:OD1	2.42	0.53
1:V:49:SER:O	1:V:53:THR:OG1	2.27	0.52
1:4:8:CYS:O	1:4:12:ARG:N	2.43	0.52
1:U:5:ARG:O	1:U:9:GLY:N	2.43	0.51
1:3:5:ARG:O	1:3:9:GLY:N	2.44	0.51
2:G:27:ARG:NH2	2:G:28:ASN:OD1	2.44	0.51
1:2:49:SER:O	1:2:53:THR:N	2.44	0.51
1:2:5:ARG:O	1:2:9:GLY:N	2.44	0.51
1:W:5:ARG:O	1:W:9:GLY:N	2.44	0.51
1:V:33:GLU:O	1:V:35:ASP:N	2.44	0.51
1:Y:96:TYR:O	1:Y:100:TYR:N	2.44	0.50
1:Y:33:GLU:O	1:Y:35:ASP:N	2.44	0.50
1:2:33:GLU:O	1:2:35:ASP:N	2.44	0.50
1:W:33:GLU:O	1:W:35:ASP:N	2.44	0.50
1:U:33:GLU:O	1:U:35:ASP:N	2.44	0.50
1:X:5:ARG:O	1:X:9:GLY:N	2.44	0.50
3:N:59:THR:OG1	1:Y:30:ASP:OD1	2.28	0.49
2:H:27:ARG:NH2	2:H:28:ASN:OD1	2.45	0.49
1:X:33:GLU:O	1:X:35:ASP:N	2.45	0.49
2:H:74:CYS:SG	3:R:77:ARG:NH2	2.86	0.48
2:D:81:TYR:O	2:D:85:GLU:N	2.46	0.48
1:X:70:GLN:O	1:X:74:ASP:N	2.46	0.48
1:2:79:THR:O	1:2:83:MET:N	2.47	0.48
1:Y:70:GLN:O	1:Y:73:ILE:N	2.46	0.48
1:3:33:GLU:O	1:3:35:ASP:N	2.47	0.48
1:Z:33:GLU:O	1:Z:35:ASP:N	2.47	0.48
1:1:33:GLU:O	1:1:35:ASP:N	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:M:28:TYR:O	3:M:32:THR:OG1	2.30	0.47
1:V:15:ALA:O	1:V:18:LEU:N	2.47	0.47
3:K:33:ASN:OD1	3:K:33:ASN:N	2.48	0.47
3:O:106:GLU:O	3:O:109:THR:OG1	2.32	0.47
1:4:33:GLU:O	1:4:35:ASP:N	2.48	0.47
1:2:75:PHE:O	1:2:79:THR:OG1	2.34	0.46
1:X:90:ILE:O	1:X:94:ARG:N	2.48	0.46
2:A:67:ASN:ND2	3:L:70:GLU:OE1	2.49	0.46
2:F:64:GLU:O	2:F:68:ASN:N	2.49	0.46
2:D:16:LYS:NZ	3:O:20:ASP:OD1	2.49	0.46
2:F:62:TYR:O	2:F:66:THR:N	2.50	0.45
2:H:73:LEU:O	2:H:77:LEU:N	2.50	0.45
3:Q:51:SER:OG	3:T:18:ASP:OD1	2.35	0.45
2:J:64:GLU:OE1	3:T:63:ARG:NH2	2.49	0.44
1:Z:62:LEU:O	1:Z:66:ARG:N	2.50	0.44
1:Y:90:ILE:O	1:Y:94:ARG:N	2.51	0.44
2:C:16:LYS:NZ	3:N:20:ASP:OD1	2.50	0.44
3:M:59:THR:OG1	1:U:30:ASP:OD1	2.35	0.44
1:4:66:ARG:O	1:4:69:ASN:N	2.51	0.43
3:T:61:TYR:CD1	3:T:61:TYR:C	2.91	0.43
2:C:80:ASP:OD1	2:C:80:ASP:N	2.50	0.43
3:Q:28:TYR:O	3:Q:32:THR:OG1	2.37	0.43
1:Y:88:MET:O	1:Y:92:LYS:N	2.52	0.42
3:T:115:LYS:O	3:T:116:PHE:CG	2.73	0.42
2:A:20:ILE:CG1	3:L:23:GLN:NE2	2.82	0.42
3:R:71:GLN:O	3:R:75:LYS:N	2.52	0.42
3:P:59:THR:OG1	3:P:60:LEU:N	2.52	0.42
2:J:62:TYR:O	2:J:66:THR:N	2.53	0.42
2:B:20:ILE:O	2:B:24:LEU:N	2.53	0.42
3:K:18:ASP:OD1	3:M:51:SER:OG	2.38	0.42
2:A:20:ILE:O	2:A:24:LEU:N	2.53	0.42
2:F:60:ILE:O	2:F:64:GLU:N	2.53	0.42
3:K:59:THR:OG1	3:N:25:ARG:NH1	2.53	0.41
3:R:89:ILE:O	3:R:93:GLN:N	2.52	0.41
2:H:20:ILE:O	2:H:24:LEU:N	2.53	0.41
2:E:20:ILE:O	2:E:24:LEU:N	2.53	0.41
1:3:52:GLN:O	1:3:56:ASP:N	2.53	0.41
3:S:71:GLN:O	3:S:75:LYS:N	2.54	0.40
2:J:20:ILE:O	2:J:24:LEU:N	2.54	0.40
3:P:48:LYS:O	3:P:52:VAL:N	2.54	0.40
2:B:63:GLN:O	2:B:67:ASN:N	2.54	0.40
1:3:61:LEU:O	1:3:65:ALA:N	2.54	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:67:LEU:O	1:X:71:GLU:N	2.53	0.40
1:Z:67:LEU:O	1:Z:71:GLU:N	2.53	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:61:GLN:OE1	1:Y:70:GLN:NE2[3_445]	2.04	0.16

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	1	97/101 (96%)	89 (92%)	8 (8%)	0	100	100
1	2	98/101 (97%)	88 (90%)	10 (10%)	0	100	100
1	3	96/101 (95%)	86 (90%)	10 (10%)	0	100	100
1	4	96/101 (95%)	85 (88%)	11 (12%)	0	100	100
1	U	98/101 (97%)	87 (89%)	11 (11%)	0	100	100
1	V	96/101 (95%)	85 (88%)	11 (12%)	0	100	100
1	W	96/101 (95%)	89 (93%)	7 (7%)	0	100	100
1	X	96/101 (95%)	87 (91%)	9 (9%)	0	100	100
1	Y	97/101 (96%)	85 (88%)	12 (12%)	0	100	100
1	Z	95/101 (94%)	86 (90%)	9 (10%)	0	100	100
2	A	77/91 (85%)	76 (99%)	1 (1%)	0	100	100
2	B	85/91 (93%)	83 (98%)	2 (2%)	0	100	100
2	C	77/91 (85%)	75 (97%)	2 (3%)	0	100	100
2	D	84/91 (92%)	82 (98%)	2 (2%)	0	100	100
2	E	84/91 (92%)	83 (99%)	1 (1%)	0	100	100
2	F	80/91 (88%)	78 (98%)	2 (2%)	0	100	100
2	G	84/91 (92%)	83 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	81/91 (89%)	77 (95%)	4 (5%)	0	100	100
2	I	84/91 (92%)	83 (99%)	1 (1%)	0	100	100
2	J	84/91 (92%)	82 (98%)	2 (2%)	0	100	100
3	K	104/123 (85%)	95 (91%)	8 (8%)	1 (1%)	22	74
3	L	102/123 (83%)	96 (94%)	6 (6%)	0	100	100
3	M	103/123 (84%)	96 (93%)	7 (7%)	0	100	100
3	N	98/123 (80%)	96 (98%)	2 (2%)	0	100	100
3	O	105/123 (85%)	90 (86%)	15 (14%)	0	100	100
3	P	99/123 (80%)	93 (94%)	6 (6%)	0	100	100
3	Q	96/123 (78%)	93 (97%)	3 (3%)	0	100	100
3	R	104/123 (85%)	94 (90%)	10 (10%)	0	100	100
3	S	103/123 (84%)	96 (93%)	7 (7%)	0	100	100
3	T	106/123 (86%)	96 (91%)	10 (9%)	0	100	100
All	All	2805/3150 (89%)	2614 (93%)	190 (7%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	K	30	ILE

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	1	74/92 (80%)	67 (90%)	7 (10%)	12	46
1	2	84/92 (91%)	77 (92%)	7 (8%)	16	56
1	3	76/92 (83%)	69 (91%)	7 (9%)	13	48
1	4	84/92 (91%)	78 (93%)	6 (7%)	21	64
1	U	81/92 (88%)	77 (95%)	4 (5%)	35	78
1	V	70/92 (76%)	67 (96%)	3 (4%)	40	82

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	W	71/92 (77%)	65 (92%)	6 (8%)	15	54
1	X	70/92 (76%)	65 (93%)	5 (7%)	21	64
1	Y	79/92 (86%)	72 (91%)	7 (9%)	14	51
1	Z	73/92 (79%)	68 (93%)	5 (7%)	22	67
2	A	66/87 (76%)	60 (91%)	6 (9%)	14	49
2	B	73/87 (84%)	66 (90%)	7 (10%)	12	45
2	C	67/87 (77%)	61 (91%)	6 (9%)	14	50
2	D	71/87 (82%)	68 (96%)	3 (4%)	40	82
2	E	68/87 (78%)	62 (91%)	6 (9%)	14	52
2	F	60/87 (69%)	55 (92%)	5 (8%)	16	56
2	G	70/87 (80%)	66 (94%)	4 (6%)	29	74
2	H	72/87 (83%)	64 (89%)	8 (11%)	9	37
2	I	72/87 (83%)	65 (90%)	7 (10%)	12	45
2	J	70/87 (80%)	64 (91%)	6 (9%)	15	53
3	K	81/114 (71%)	70 (86%)	11 (14%)	5	26
3	L	74/114 (65%)	67 (90%)	7 (10%)	12	46
3	M	76/114 (67%)	66 (87%)	10 (13%)	6	28
3	N	73/114 (64%)	68 (93%)	5 (7%)	22	67
3	O	86/114 (75%)	78 (91%)	8 (9%)	13	48
3	P	76/114 (67%)	69 (91%)	7 (9%)	13	48
3	Q	63/114 (55%)	58 (92%)	5 (8%)	18	59
3	R	84/114 (74%)	77 (92%)	7 (8%)	16	56
3	S	75/114 (66%)	67 (89%)	8 (11%)	10	39
3	T	84/114 (74%)	76 (90%)	8 (10%)	12	46
All	All	2223/2930 (76%)	2032 (91%)	191 (9%)	15	53

All (191) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	4	ILE
1	1	22	THR
1	1	53	THR
1	1	54	LEU
1	1	58	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	81	VAL
1	1	82	LEU
1	2	4	ILE
1	2	22	THR
1	2	24	ARG
1	2	37	GLU
1	2	79	THR
1	2	89	ASP
1	2	90	ILE
1	3	4	ILE
1	3	22	THR
1	3	44	LEU
1	3	53	THR
1	3	56	ASP
1	3	60	ILE
1	3	93	ILE
1	4	4	ILE
1	4	22	THR
1	4	24	ARG
1	4	44	LEU
1	4	67	LEU
1	4	97	PHE
2	A	19	ASN
2	A	39	LEU
2	A	46	ILE
2	A	48	VAL
2	A	63	GLN
2	A	73	LEU
2	B	15	GLU
2	B	39	LEU
2	B	46	ILE
2	B	48	VAL
2	B	57	GLU
2	B	66	THR
2	B	70	LEU
2	C	15	GLU
2	C	19	ASN
2	C	39	LEU
2	C	46	ILE
2	C	48	VAL
2	C	80	ASP
2	D	39	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	46	ILE
2	D	48	VAL
2	E	39	LEU
2	E	46	ILE
2	E	48	VAL
2	E	57	GLU
2	E	65	GLN
2	E	77	LEU
2	F	39	LEU
2	F	46	ILE
2	F	48	VAL
2	F	63	GLN
2	F	74	CYS
2	G	39	LEU
2	G	46	ILE
2	G	48	VAL
2	G	66	THR
2	H	39	LEU
2	H	46	ILE
2	H	48	VAL
2	H	57	GLU
2	H	61	GLN
2	H	65	GLN
2	H	66	THR
2	H	69	SER
2	I	39	LEU
2	I	46	ILE
2	I	48	VAL
2	I	74	CYS
2	I	77	LEU
2	I	83	ASP
2	I	86	HIS
2	J	39	LEU
2	J	46	ILE
2	J	48	VAL
2	J	57	GLU
2	J	63	GLN
2	J	83	ASP
3	K	33	ASN
3	K	34	HIS
3	K	53	ILE
3	K	69	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	K	71	GLN
3	K	78	ILE
3	K	82	VAL
3	K	92	LEU
3	K	98	LEU
3	K	100	LEU
3	K	113	GLN
3	L	55	SER
3	L	57	TYR
3	L	69	VAL
3	L	70	GLU
3	L	81	THR
3	L	85	THR
3	L	109	THR
3	M	0	HIS
3	M	46	LEU
3	M	51	SER
3	M	63	ARG
3	M	69	VAL
3	M	74	SER
3	M	82	VAL
3	M	100	LEU
3	M	103	LEU
3	M	113	GLN
3	N	51	SER
3	N	59	THR
3	N	67	VAL
3	N	76	SER
3	N	82	VAL
3	O	44	VAL
3	O	46	LEU
3	O	51	SER
3	O	53	ILE
3	O	59	THR
3	O	69	VAL
3	O	81	THR
3	O	107	GLU
3	P	32	THR
3	P	44	VAL
3	P	46	LEU
3	P	51	SER
3	P	69	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	P	96	THR
3	P	103	LEU
3	Q	51	SER
3	Q	53	ILE
3	Q	69	VAL
3	Q	81	THR
3	Q	89	ILE
3	R	47	LEU
3	R	51	SER
3	R	64	PHE
3	R	70	GLU
3	R	87	ASN
3	R	100	LEU
3	R	113	GLN
3	S	44	VAL
3	S	51	SER
3	S	53	ILE
3	S	74	SER
3	S	78	ILE
3	S	82	VAL
3	S	85	THR
3	S	112	GLU
3	T	44	VAL
3	T	55	SER
3	T	59	THR
3	T	79	CYS
3	T	98	LEU
3	T	100	LEU
3	T	108	LYS
3	T	109	THR
1	U	22	THR
1	U	24	ARG
1	U	79	THR
1	U	90	ILE
1	V	22	THR
1	V	24	ARG
1	V	67	LEU
1	W	22	THR
1	W	24	ARG
1	W	53	THR
1	W	58	ILE
1	W	69	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	W	99	LYS
1	X	4	ILE
1	X	22	THR
1	X	24	ARG
1	X	44	LEU
1	X	53	THR
1	Y	22	THR
1	Y	24	ARG
1	Y	44	LEU
1	Y	58	ILE
1	Y	74	ASP
1	Y	76	ILE
1	Y	79	THR
1	Z	4	ILE
1	Z	22	THR
1	Z	24	ARG
1	Z	67	LEU
1	Z	79	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.