



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 04:29 pm BST

PDB ID : 2Z3F  
Title : Crystal structure of spCia1/Asf1 complexed with Cac2 peptide  
Authors : Malay, A.D.; Padmanabhan, B.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2007-06-04  
Resolution : 2.70 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

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

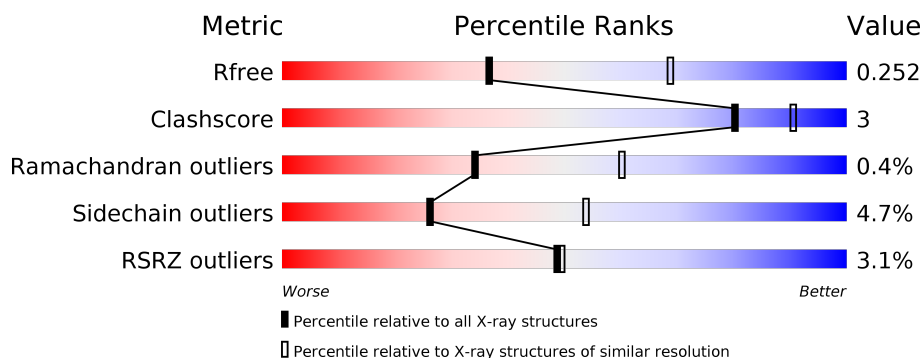
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 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	161	<div> <div>88%</div> <div>10%</div> <div>..</div> </div>
1	B	161	<div> <div>4%</div> <div>86%</div> <div>12%</div> <div>..</div> </div>
1	C	161	<div> <div>7%</div> <div>84%</div> <div>14%</div> <div>..</div> </div>
1	D	161	<div> <div>3%</div> <div>84%</div> <div>14%</div> <div>..</div> </div>
1	E	161	<div> <div>2%</div> <div>85%</div> <div>13%</div> <div>..</div> </div>
1	F	161	<div> <div>3%</div> <div>88%</div> <div>11%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	161	 3% 90% 9% ..
1	H	161	 2% 89% 9% ..
2	I	20	 50% 50%
2	J	20	 30% 20% 50%
2	K	20	 5% 25% 10% 65%
2	L	20	 40% 5% 55%
2	M	20	 45% 5% 50%
2	N	20	 35% 15% 50%
2	O	20	 50% 50%
2	P	20	 40% 10% 50%
2	Q	20	 25% 75%
2	R	20	 5% 25% 75%
2	T	20	 5% 25% 75%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11308 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 Histone chaperone cia1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	160	Total	C	N	O	S	0	0	0
			1284	829	202	249	4			
1	B	160	Total	C	N	O	S	0	0	0
			1284	829	202	249	4			
1	C	160	Total	C	N	O	S	0	0	0
			1284	829	202	249	4			
1	D	160	Total	C	N	O	S	0	0	0
			1284	829	202	249	4			
1	E	160	Total	C	N	O	S	0	0	0
			1284	829	202	249	4			
1	F	159	Total	C	N	O	S	0	0	0
			1278	826	201	247	4			
1	G	160	Total	C	N	O	S	0	0	0
			1284	829	202	249	4			
1	H	160	Total	C	N	O	S	0	0	0
			1284	829	202	249	4			

- Molecule 2 is a protein called SPAC26H5.03 protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	10	Total	C	N	O	0	0	0
			81	54	14	13			
2	J	10	Total	C	N	O	0	0	0
			81	54	14	13			
2	K	7	Total	C	N	O	0	0	0
			52	34	10	8			
2	L	9	Total	C	N	O	0	0	0
			72	48	12	12			
2	M	10	Total	C	N	O	0	0	0
			81	54	14	13			
2	N	10	Total	C	N	O	0	0	0
			81	54	14	13			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	O	10	Total	C	N	O	0	0	0
			81	54	14	13			
2	P	10	Total	C	N	O	0	0	0
			81	54	14	13			
2	Q	5	Total	C	N	O	0	0	0
			40	28	5	7			
2	R	5	Total	C	N	O	0	0	0
			40	28	5	7			
2	T	5	Total	C	N	O	0	0	0
			40	28	5	7			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	45	Total	O	0	0
			45	45		
3	B	27	Total	O	0	0
			27	27		
3	J	1	Total	O	0	0
			1	1		
3	C	37	Total	O	0	0
			37	37		
3	D	43	Total	O	0	0
			43	43		
3	L	3	Total	O	0	0
			3	3		
3	E	32	Total	O	0	0
			32	32		
3	M	1	Total	O	0	0
			1	1		
3	F	39	Total	O	0	0
			39	39		
3	N	2	Total	O	0	0
			2	2		
3	G	35	Total	O	0	0
			35	35		
3	O	1	Total	O	0	0
			1	1		
3	H	44	Total	O	0	0
			44	44		
3	P	1	Total	O	0	0
			1	1		

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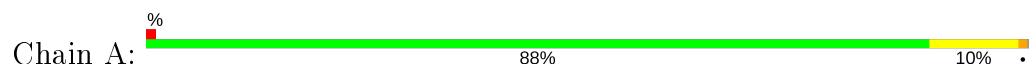
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	R	1	Total	O	0	0
			1	1		

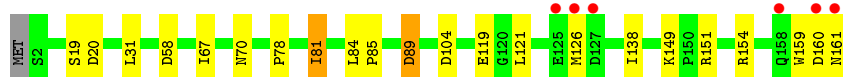
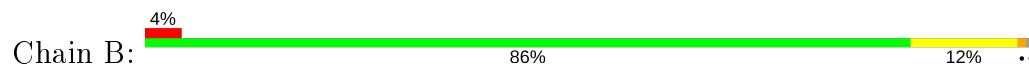
### 3 Residue-property plots [i](#)

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

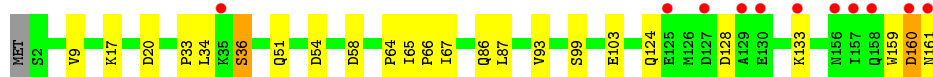
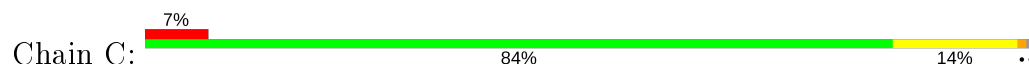
- Molecule 1: Histone chaperone cial



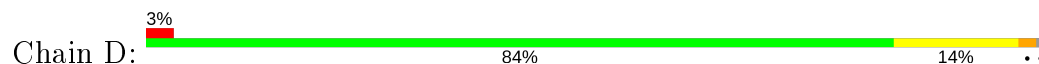
- Molecule 1: Histone chaperone cial



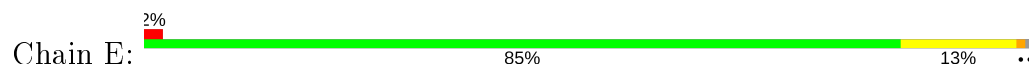
- Molecule 1: Histone chaperone cial



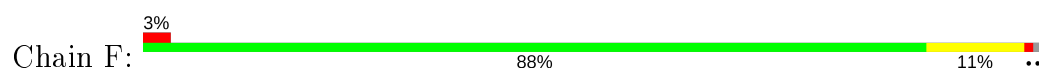
- Molecule 1: Histone chaperone cial



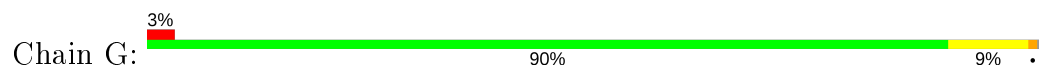
- Molecule 1: Histone chaperone cial



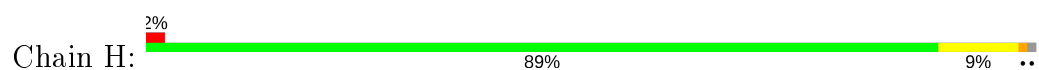
- Molecule 1: Histone chaperone cial



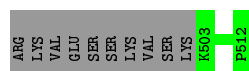
- Molecule 1: Histone chaperone cia1



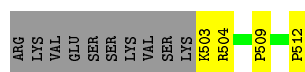
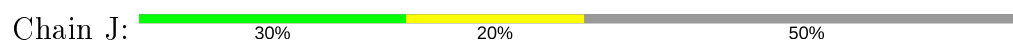
- Molecule 1: Histone chaperone cia1



- Molecule 2: SPAC26H5.03 protein



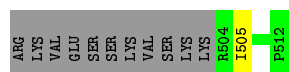
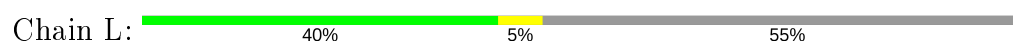
- Molecule 2: SPAC26H5.03 protein



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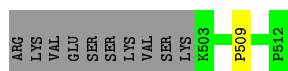
- Molecule 2: SPAC26H5.03 protein




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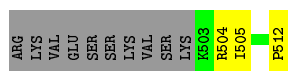


Chain M:  45% 5% 50%



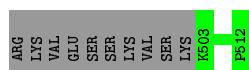
- Molecule 2: SPAC26H5.03 protein

Chain N:  35% 15% 50%



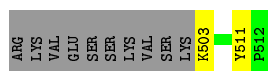
- Molecule 2: SPAC26H5.03 protein

Chain O:  50% 50%



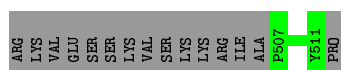
- Molecule 2: SPAC26H5.03 protein

Chain P:  40% 10% 50%



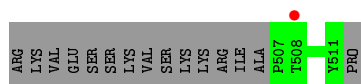
- Molecule 2: SPAC26H5.03 protein

Chain Q:  25% 75%



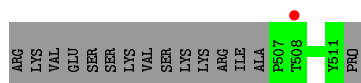
- Molecule 2: SPAC26H5.03 protein

Chain R:  5% 25% 75%



- Molecule 2: SPAC26H5.03 protein

Chain T:  5% 25% 75%



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	151.51Å 151.51Å 144.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.60 – 2.70 31.64 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (31.60-2.70) 99.9 (31.64-2.60)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.72 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.208 , 0.263 0.197 , 0.252	Depositor DCC
$R_{free}$ test set	2540 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.4	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 42.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h 0.000 for -l,-k,-h 0.000 for -h,-l,-k 0.000 for -h,l,k 0.021 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11308	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	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 23.39 % 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 4.7025e-03. 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, 0.333 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	1.11	2/1311 (0.2%)	1.02	7/1785 (0.4%)
1	B	0.96	0/1311	0.95	4/1785 (0.2%)
1	C	1.00	0/1311	0.94	3/1785 (0.2%)
1	D	0.96	0/1311	0.94	4/1785 (0.2%)
1	E	0.98	0/1311	0.97	7/1785 (0.4%)
1	F	1.06	1/1305 (0.1%)	0.98	5/1777 (0.3%)
1	G	1.02	3/1311 (0.2%)	0.94	4/1785 (0.2%)
1	H	0.95	0/1311	0.92	4/1785 (0.2%)
2	I	1.22	0/84	0.90	0/114
2	J	0.90	0/84	1.01	0/114
2	K	1.05	0/53	0.99	0/73
2	L	1.05	0/75	0.86	0/103
2	M	1.02	0/84	0.89	0/114
2	N	0.94	0/84	0.90	0/114
2	O	0.85	0/84	0.91	0/114
2	P	1.07	0/84	1.10	0/114
2	Q	1.26	0/42	1.12	0/58
2	R	1.54	0/42	0.99	0/58
2	T	1.43	0/42	1.05	0/58
All	All	1.01	6/11240 (0.1%)	0.96	38/15306 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	130	GLU	CG-CD	5.56	1.60	1.51
1	A	148	GLU	CD-OE2	5.41	1.31	1.25
1	G	130	GLU	CD-OE2	5.25	1.31	1.25
1	G	130	GLU	CD-OE1	5.18	1.31	1.25
1	F	115	ASN	CG-OD1	5.17	1.35	1.24
1	A	24	PHE	CE1-CZ	-5.00	1.27	1.37

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	54	ASP	CB-CG-OD1	7.88	125.39	118.30
1	E	58	ASP	CB-CG-OD2	7.54	125.09	118.30
1	A	77	ASP	CB-CG-OD2	7.18	124.76	118.30
1	A	54	ASP	CB-CG-OD1	7.15	124.74	118.30
1	B	20	ASP	CB-CG-OD2	6.91	124.52	118.30
1	A	37	ASP	CB-CG-OD2	6.89	124.50	118.30
1	G	160	ASP	CB-CG-OD2	6.75	124.38	118.30
1	D	20	ASP	CB-CG-OD1	6.55	124.19	118.30
1	F	77	ASP	CB-CG-OD2	6.33	124.00	118.30
1	G	128	ASP	CB-CG-OD2	6.30	123.97	118.30
1	A	104	ASP	CB-CG-OD2	6.25	123.93	118.30
1	G	37	ASP	CB-CG-OD2	6.20	123.88	118.30
1	H	104	ASP	CB-CG-OD2	6.12	123.80	118.30
1	F	104	ASP	CB-CG-OD2	6.09	123.78	118.30
1	B	89	ASP	CB-CG-OD2	6.09	123.78	118.30
1	A	58	ASP	CB-CG-OD2	6.06	123.75	118.30
1	D	58	ASP	CB-CG-OD2	5.81	123.53	118.30
1	H	128	ASP	CB-CG-OD2	5.80	123.52	118.30
1	C	20	ASP	CB-CG-OD1	5.70	123.43	118.30
1	E	104	ASP	CB-CG-OD2	5.70	123.43	118.30
1	A	128	ASP	CB-CG-OD2	5.67	123.40	118.30
1	A	20	ASP	CB-CG-OD2	5.63	123.37	118.30
1	E	160	ASP	CB-CG-OD2	5.61	123.35	118.30
1	H	82	ASP	CB-CG-OD2	5.60	123.34	118.30
1	B	160	ASP	CB-CG-OD2	5.48	123.23	118.30
1	E	54	ASP	CB-CG-OD1	5.43	123.19	118.30
1	E	37	ASP	CB-CG-OD2	5.35	123.11	118.30
1	F	37	ASP	CB-CG-OD2	5.32	123.09	118.30
1	E	82	ASP	CB-CG-OD2	5.31	123.08	118.30
1	E	137	ASP	CB-CG-OD2	5.30	123.07	118.30
1	D	127	ASP	CB-CG-OD1	5.24	123.02	118.30
1	C	160	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	104	ASP	CB-CG-OD2	5.16	122.94	118.30
1	G	104	ASP	CB-CG-OD2	5.11	122.90	118.30
1	F	128	ASP	CB-CG-OD2	5.07	122.87	118.30
1	F	81	ILE	CG1-CB-CG2	-5.05	100.28	111.40
1	H	58	ASP	CB-CG-OD2	5.05	122.84	118.30
1	D	160	ASP	CB-CG-OD2	5.04	122.83	118.30

There are no chirality outliers.

There are no planarity outliers.

## 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	1284	0	1281	5	0
1	B	1284	0	1281	9	0
1	C	1284	0	1281	12	0
1	D	1284	0	1281	14	0
1	E	1284	0	1281	11	0
1	F	1278	0	1276	9	0
1	G	1284	0	1281	4	0
1	H	1284	0	1281	5	0
2	I	81	0	87	0	0
2	J	81	0	87	1	0
2	K	52	0	58	1	0
2	L	72	0	74	0	0
2	M	81	0	87	1	0
2	N	81	0	87	2	0
2	O	81	0	87	0	0
2	P	81	0	87	0	0
2	Q	40	0	39	0	0
2	R	40	0	39	0	0
2	T	40	0	39	0	0
3	A	45	0	0	1	0
3	B	27	0	0	2	0
3	C	37	0	0	2	0
3	D	43	0	0	1	0
3	E	32	0	0	1	0
3	F	39	0	0	3	0
3	G	35	0	0	0	0
3	H	44	0	0	0	0
3	J	1	0	0	0	0
3	L	3	0	0	0	0
3	M	1	0	0	0	0
3	N	2	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
3	R	1	0	0	0	0
All	All	11308	0	11014	60	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 3.

All (60) 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:F:81:ILE:HG23	3:F:274:HOH:O	1.90	0.71
1:D:51:GLN:HE21	1:E:33:PRO:HD2	1.58	0.68
1:D:33:PRO:N	1:D:67:ILE:HD11	2.12	0.64
1:D:51:GLN:NE2	1:E:33:PRO:HD2	2.14	0.61
1:F:81:ILE:CG2	3:F:274:HOH:O	2.47	0.61
1:C:36:SER:OG	1:C:103:GLU:OE2	2.18	0.60
1:C:64:PRO:O	1:C:66:PRO:HD3	2.01	0.60
1:C:33:PRO:N	1:C:67:ILE:HD11	2.17	0.60
1:E:36:SER:HB3	3:E:552:HOH:O	2.01	0.59
1:B:89:ASP:OD2	3:B:173:HOH:O	2.17	0.58
1:B:81:ILE:HD13	1:B:84:LEU:CD1	2.34	0.58
1:C:124:GLN:OE1	3:C:178:HOH:O	2.17	0.58
2:N:504:ARG:O	2:N:505:ILE:HG23	2.06	0.56
1:C:65:ILE:HG22	1:C:66:PRO:O	2.07	0.55
1:C:87:LEU:HB3	3:C:196:HOH:O	2.07	0.54
1:E:81:ILE:HD13	1:E:84:LEU:CD1	2.37	0.54
1:B:70:ASN:OD1	2:J:509:PRO:HA	2.09	0.53
1:D:51:GLN:HE21	1:E:33:PRO:CD	2.22	0.53
1:B:85:PRO:HG2	3:B:173:HOH:O	2.08	0.52
1:D:36:SER:OG	1:D:103:GLU:OE2	2.23	0.52
1:C:93:VAL:HB	2:N:512:PRO:HB3	1.92	0.51
1:D:64:PRO:O	1:D:66:PRO:HD3	2.12	0.49
1:D:33:PRO:CD	1:D:67:ILE:HD11	2.43	0.49
1:E:70:ASN:OD1	2:M:509:PRO:HA	2.12	0.49
1:F:31:LEU:HA	1:F:67:ILE:HG23	1.96	0.47
1:C:34:LEU:HA	1:C:160:ASP:OD2	2.14	0.47
1:E:140:LYS:NZ	1:G:140:LYS:NZ	2.63	0.47
1:A:119:GLU:OE2	1:C:17:LYS:HD2	2.14	0.47
2:K:504:ARG:HG3	2:K:505:ILE:N	2.29	0.47
1:B:31:LEU:O	1:B:67:ILE:HG12	2.15	0.46
1:E:81:ILE:HD13	1:E:84:LEU:HD12	1.97	0.46
1:E:140:LYS:NZ	1:G:140:LYS:HZ2	2.14	0.46
1:B:81:ILE:HD13	1:B:84:LEU:HD12	1.97	0.45
1:A:87:LEU:HG	1:A:136:VAL:HB	1.99	0.44
1:E:81:ILE:HA	1:E:84:LEU:HD12	2.00	0.44
1:F:81:ILE:HD13	1:F:81:ILE:HG21	1.70	0.44
1:D:133:LYS:HG2	1:H:50:SER:HA	1.99	0.44
1:G:96:ILE:HG13	1:G:112:TYR:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:115:ASN:O	1:H:143:ARG:HA	2.18	0.43
1:B:121:LEU:HD11	1:B:126:MET:SD	2.58	0.43
1:A:81:ILE:HG21	1:A:81:ILE:HD13	1.79	0.43
1:D:19:SER:O	1:D:78:PRO:HG3	2.18	0.43
1:D:122:ASN:ND2	3:D:203:HOH:O	2.40	0.43
1:F:19:SER:O	1:F:78:PRO:HG3	2.19	0.42
1:A:64:PRO:HB3	1:D:129:ALA:HB2	2.01	0.42
1:C:33:PRO:CA	1:C:67:ILE:HD11	2.50	0.42
1:C:33:PRO:CD	1:C:67:ILE:HD11	2.49	0.42
1:B:119:GLU:OE2	1:D:17:LYS:HD2	2.20	0.41
1:E:19:SER:O	1:E:78:PRO:HG3	2.21	0.41
1:G:4:VAL:HA	1:G:29:GLU:O	2.21	0.41
1:H:29:GLU:HA	1:H:68:GLY:O	2.21	0.41
1:D:65:ILE:HG22	1:D:66:PRO:O	2.21	0.41
1:F:15:PRO:HD3	1:H:144:SER:HB2	2.02	0.41
1:H:19:SER:O	1:H:78:PRO:HG3	2.20	0.41
1:F:87:LEU:HG	1:F:136:VAL:HB	2.01	0.41
1:B:19:SER:O	1:B:78:PRO:HG3	2.21	0.41
1:F:154:ARG:HG2	3:F:475:HOH:O	2.20	0.41
1:A:96:ILE:HG23	3:A:172:HOH:O	2.20	0.40
1:D:33:PRO:CA	1:D:67:ILE:HD11	2.51	0.40
1:C:51:GLN:HE21	1:F:33:PRO:HD2	1.86	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	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
1	B	158/161 (98%)	156 (99%)	1 (1%)	1 (1%)	25	50
1	C	158/161 (98%)	150 (95%)	7 (4%)	1 (1%)	25	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	158/161 (98%)	152 (96%)	5 (3%)	1 (1%)	25	50
1	E	158/161 (98%)	156 (99%)	1 (1%)	1 (1%)	25	50
1	F	157/161 (98%)	153 (98%)	4 (2%)	0	100	100
1	G	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
1	H	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
2	I	8/20 (40%)	7 (88%)	1 (12%)	0	100	100
2	J	8/20 (40%)	6 (75%)	2 (25%)	0	100	100
2	K	5/20 (25%)	5 (100%)	0	0	100	100
2	L	7/20 (35%)	6 (86%)	1 (14%)	0	100	100
2	M	8/20 (40%)	8 (100%)	0	0	100	100
2	N	8/20 (40%)	7 (88%)	1 (12%)	0	100	100
2	O	8/20 (40%)	7 (88%)	1 (12%)	0	100	100
2	P	8/20 (40%)	7 (88%)	0	1 (12%)	0	0
2	Q	3/20 (15%)	3 (100%)	0	0	100	100
2	R	3/20 (15%)	2 (67%)	1 (33%)	0	100	100
2	T	3/20 (15%)	2 (67%)	1 (33%)	0	100	100
All	All	1332/1508 (88%)	1292 (97%)	35 (3%)	5 (0%)	34	60

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	159	TRP
1	D	159	TRP
1	B	159	TRP
1	E	159	TRP
2	P	511	TYR

### 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	148/149 (99%)	143 (97%)	5 (3%)	37	66
1	B	148/149 (99%)	141 (95%)	7 (5%)	26	54
1	C	148/149 (99%)	140 (95%)	8 (5%)	22	47
1	D	148/149 (99%)	139 (94%)	9 (6%)	18	41
1	E	148/149 (99%)	139 (94%)	9 (6%)	18	41
1	F	147/149 (99%)	143 (97%)	4 (3%)	44	74
1	G	148/149 (99%)	142 (96%)	6 (4%)	30	59
1	H	148/149 (99%)	142 (96%)	6 (4%)	30	59
2	I	9/19 (47%)	9 (100%)	0	100	100
2	J	9/19 (47%)	6 (67%)	3 (33%)	0	0
2	K	6/19 (32%)	6 (100%)	0	100	100
2	L	8/19 (42%)	7 (88%)	1 (12%)	4	10
2	M	9/19 (47%)	9 (100%)	0	100	100
2	N	9/19 (47%)	9 (100%)	0	100	100
2	O	9/19 (47%)	9 (100%)	0	100	100
2	P	9/19 (47%)	8 (89%)	1 (11%)	6	14
2	Q	5/19 (26%)	5 (100%)	0	100	100
2	R	5/19 (26%)	5 (100%)	0	100	100
2	T	5/19 (26%)	5 (100%)	0	100	100
All	All	1266/1401 (90%)	1207 (95%)	59 (5%)	26	54

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	VAL
1	A	58	ASP
1	A	74	PHE
1	A	81	ILE
1	A	88	SER
1	B	58	ASP
1	B	81	ILE
1	B	138	ILE
1	B	149	LYS
1	B	151	ARG
1	B	154	ARG
1	B	161	ASN

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Mol	Chain	Res	Type
2	J	503	LYS
2	J	504	ARG
2	J	512	PRO
1	C	9	VAL
1	C	36	SER
1	C	58	ASP
1	C	86	GLN
1	C	99	SER
1	C	128	ASP
1	C	133	LYS
1	C	161	ASN
1	D	2	SER
1	D	9	VAL
1	D	36	SER
1	D	58	ASP
1	D	86	GLN
1	D	88	SER
1	D	99	SER
1	D	128	ASP
1	D	133	LYS
2	L	505	ILE
1	E	2	SER
1	E	9	VAL
1	E	58	ASP
1	E	81	ILE
1	E	138	ILE
1	E	149	LYS
1	E	151	ARG
1	E	154	ARG
1	E	158	GLN
1	F	9	VAL
1	F	58	ASP
1	F	74	PHE
1	F	81	ILE
1	G	58	ASP
1	G	104	ASP
1	G	127	ASP
1	G	135	LYS
1	G	148	GLU
1	G	161	ASN
1	H	10	ASN
1	H	58	ASP

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Mol	Chain	Res	Type
1	H	104	ASP
1	H	127	ASP
1	H	135	LYS
1	H	161	ASN
2	P	503	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	ASN
1	A	156	ASN
1	B	105	ASN
1	B	156	ASN
1	C	10	ASN
1	C	51	GLN
1	C	105	ASN
1	C	124	GLN
1	D	51	GLN
1	D	105	ASN
1	F	105	ASN
1	F	156	ASN
1	G	105	ASN
1	H	105	ASN
1	H	156	ASN

### 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

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 ⓘ

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	160/161 (99%)	-0.33	1 (0%) 89 91	20, 32, 57, 68	0
1	B	160/161 (99%)	-0.17	6 (3%) 40 39	26, 40, 72, 78	0
1	C	160/161 (99%)	0.05	11 (6%) 16 15	19, 38, 74, 80	0
1	D	160/161 (99%)	-0.12	5 (3%) 49 49	20, 38, 74, 82	0
1	E	160/161 (99%)	-0.11	4 (2%) 57 59	26, 40, 72, 78	0
1	F	159/161 (98%)	-0.25	5 (3%) 49 49	20, 32, 58, 68	0
1	G	160/161 (99%)	-0.18	5 (3%) 49 49	24, 40, 64, 75	0
1	H	160/161 (99%)	-0.13	3 (1%) 66 69	23, 39, 64, 71	0
2	I	10/20 (50%)	-0.62	0 100 100	32, 36, 39, 42	0
2	J	10/20 (50%)	0.10	0 100 100	50, 54, 61, 63	0
2	K	7/20 (35%)	0.09	1 (14%) 2 1	53, 54, 61, 63	0
2	L	9/20 (45%)	-0.09	0 100 100	65, 68, 76, 80	0
2	M	10/20 (50%)	-0.64	0 100 100	37, 41, 44, 47	0
2	N	10/20 (50%)	-0.34	0 100 100	40, 47, 50, 50	0
2	O	10/20 (50%)	0.22	0 100 100	66, 67, 70, 74	0
2	P	10/20 (50%)	-0.18	0 100 100	45, 51, 55, 64	0
2	Q	5/20 (25%)	1.37	0 100 100	65, 69, 70, 71	0
2	R	5/20 (25%)	1.51	1 (20%) 1 0	67, 69, 70, 71	0
2	T	5/20 (25%)	1.72	1 (20%) 1 0	68, 70, 71, 72	0
All	All	1370/1508 (90%)	-0.14	43 (3%) 49 49	19, 38, 69, 82	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	161	ASN	4.6

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Mol	Chain	Res	Type	RSRZ
1	D	35	LYS	4.2
1	H	161	ASN	4.0
1	F	158	GLN	3.9
1	C	129	ALA	3.8
1	C	158	GLN	3.8
1	D	158	GLN	3.8
2	R	508	THR	3.7
1	G	160	ASP	3.7
1	H	158	GLN	3.5
1	F	129	ALA	3.3
1	C	35	LYS	3.3
1	E	161	ASN	3.2
1	C	125	GLU	3.2
1	C	160	ASP	3.1
1	B	161	ASN	3.1
1	E	125	GLU	3.1
1	G	161	ASN	3.1
1	G	158	GLN	3.0
2	K	510	VAL	3.0
1	F	127	ASP	3.0
2	T	508	THR	2.9
1	B	158	GLN	2.8
1	B	125	GLU	2.8
1	C	161	ASN	2.7
1	F	161	ASN	2.7
1	H	125	GLU	2.6
1	G	125	GLU	2.4
1	G	35	LYS	2.4
1	E	133	LYS	2.3
1	C	133	LYS	2.3
1	C	130	GLU	2.3
1	D	156	ASN	2.2
1	A	158	GLN	2.2
1	B	126	MET	2.2
1	B	127	ASP	2.2
1	C	156	ASN	2.1
1	C	157	ILE	2.1
1	E	35	LYS	2.1
1	C	127	ASP	2.1
1	B	160	ASP	2.1
1	F	133	LYS	2.1
1	D	125	GLU	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 carbohydrates 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.