



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:05 AM UTC

PDB ID : 2Z3F / pdb_00002z3f
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

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

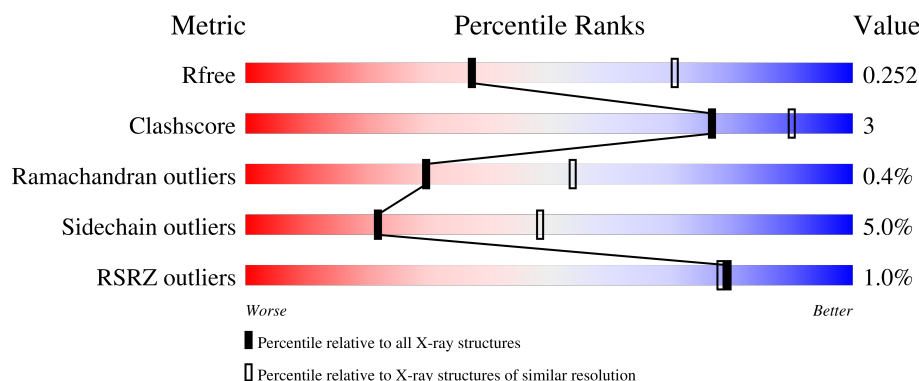
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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.



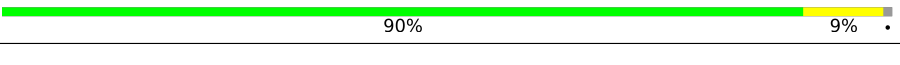
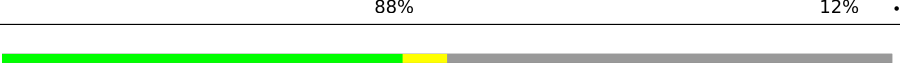
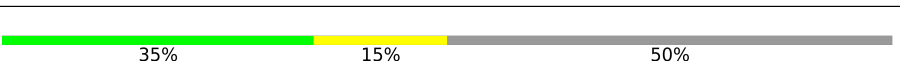
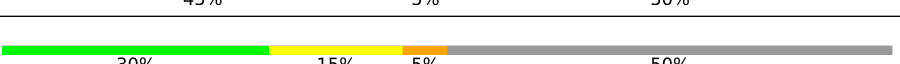
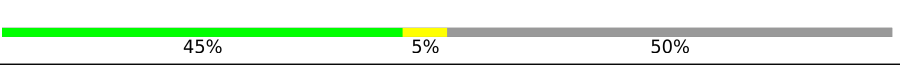
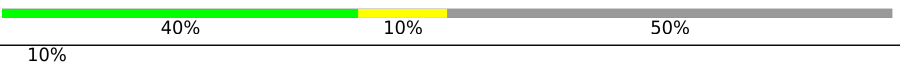
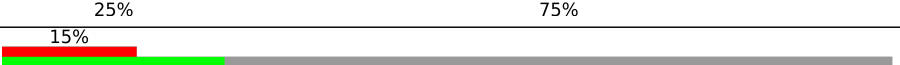
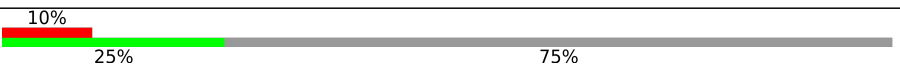
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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 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	161	
1	B	161	
1	C	161	
1	D	161	
1	E	161	

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Mol	Chain	Length	Quality of chain
1	F	161	 88% 9% ..
1	G	161	 90% 9% .
1	H	161	 88% 12% .
2	I	20	 45% 5% 50%
2	J	20	 35% 15% 50%
2	K	20	 5% 25% 10% 65%
2	L	20	 5% 35% 10% 55%
2	M	20	 45% 5% 50%
2	N	20	 30% 15% 5% 50%
2	O	20	 45% 5% 50%
2	P	20	 40% 10% 50%
2	Q	20	 10% 25% 75%
2	R	20	 15% 25% 75%
2	T	20	 10% 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 cial.

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 81	C 54	N 14	O 13	0	0	0
2	P	10	Total 81	C 54	N 14	O 13	0	0	0
2	Q	5	Total 40	C 28	N 5	O 7	0	0	0
2	R	5	Total 40	C 28	N 5	O 7	0	0	0
2	T	5	Total 40	C 28	N 5	O 7	0	0	0

- Molecule 3 is water.

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

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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, 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.

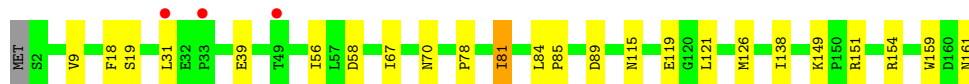
- Molecule 1: Histone chaperone cial

Chain A:  90% 9% ..



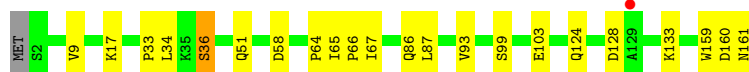
- Molecule 1: Histone chaperone cial

Chain B:  84% 14% ..



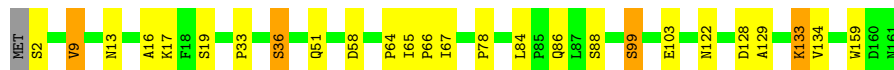
- Molecule 1: Histone chaperone cial

Chain C:  86% 13% ..



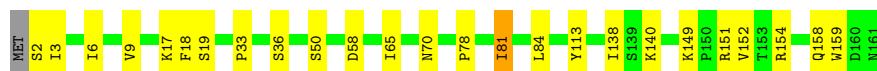
- Molecule 1: Histone chaperone cial

Chain D:  83% 14% ..

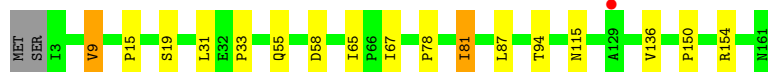
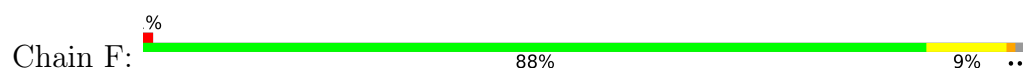


- Molecule 1: Histone chaperone cial

Chain E:  84% 15% ..



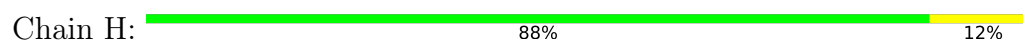
- Molecule 1: Histone chaperone cial



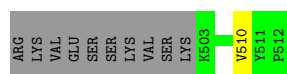
- Molecule 1: Histone chaperone cial



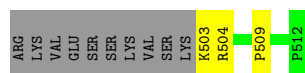
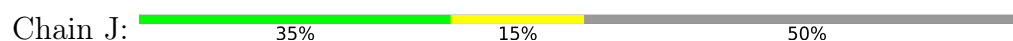
- Molecule 1: Histone chaperone cial



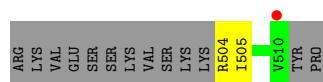
- Molecule 2: SPAC26H5.03 protein



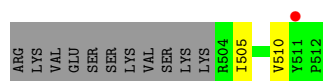
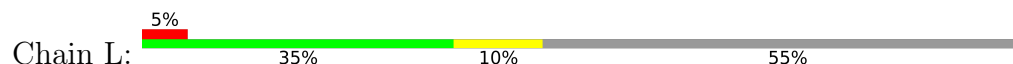
- Molecule 2: SPAC26H5.03 protein



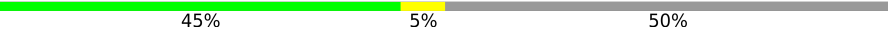
- Molecule 2: SPAC26H5.03 protein

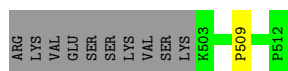


- Molecule 2: SPAC26H5.03 protein



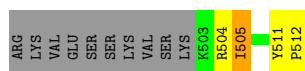
- Molecule 2: SPAC26H5.03 protein

Chain M:  45% 5% 50%

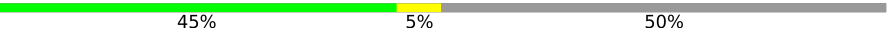


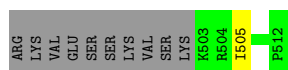
- Molecule 2: SPAC26H5.03 protein

Chain N:  30% 15% 5% 50%



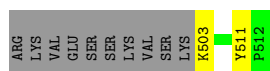
- Molecule 2: SPAC26H5.03 protein

Chain O:  45% 5% 50%



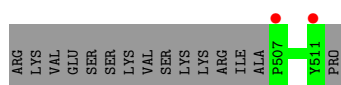
- Molecule 2: SPAC26H5.03 protein

Chain P:  40% 10% 50%



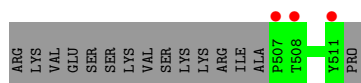
- Molecule 2: SPAC26H5.03 protein

Chain Q:  10% 25% 75%



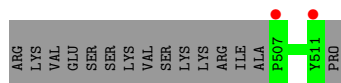
- Molecule 2: SPAC26H5.03 protein

Chain R:  15% 25% 75%



- Molecule 2: SPAC26H5.03 protein

Chain T:  10% 25% 75%



4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α , β , γ	151.51Å 151.51Å 144.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.60 – 2.70 31.60 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (31.60-2.70) 99.8 (31.60-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	45.4	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 33.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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 ²)	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.*

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 [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.40	5/1311 (0.4%)	1.12	3/1785 (0.2%)
1	B	1.24	1/1311 (0.1%)	1.11	1/1785 (0.1%)
1	C	1.26	0/1311	1.06	0/1785
1	D	1.22	4/1311 (0.3%)	1.06	1/1785 (0.1%)
1	E	1.23	3/1311 (0.2%)	1.10	2/1785 (0.1%)
1	F	1.32	5/1305 (0.4%)	1.10	2/1777 (0.1%)
1	G	1.19	1/1311 (0.1%)	1.08	2/1785 (0.1%)
1	H	1.21	1/1311 (0.1%)	1.09	2/1785 (0.1%)
2	I	1.23	0/84	1.33	1/114 (0.9%)
2	J	1.04	0/84	1.10	0/114
2	K	1.23	0/53	1.26	0/73
2	L	1.52	1/75 (1.3%)	1.20	0/103
2	M	1.19	0/84	1.23	0/114
2	N	1.04	0/84	1.24	1/114 (0.9%)
2	O	0.93	0/84	1.06	0/114
2	P	1.25	0/84	1.15	0/114
2	Q	1.58	0/42	1.36	0/58
2	R	1.37	0/42	1.06	0/58
2	T	1.49	0/42	1.22	0/58
All	All	1.26	21/11240 (0.2%)	1.10	15/15306 (0.1%)

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	69	ILE	CA-CB	-7.49	1.45	1.54
1	E	6	ILE	CA-CB	-6.37	1.46	1.54
1	F	115	ASN	CG-OD1	6.20	1.35	1.23
1	F	115	ASN	CA-C	-6.03	1.45	1.52
1	F	94	THR	CA-CB	-6.00	1.45	1.53
1	D	16	ALA	CA-CB	-5.97	1.43	1.53
1	A	114	VAL	C-O	-5.94	1.18	1.24
1	G	118	MET	SD-CE	5.68	1.93	1.79
1	F	9	VAL	C-O	-5.62	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	50	SER	CA-C	5.61	1.59	1.52
1	A	112	TYR	C-O	-5.58	1.17	1.23
1	D	84	LEU	C-O	-5.50	1.16	1.23
1	D	134	VAL	CA-CB	5.44	1.59	1.54
2	L	510	VAL	CA-C	5.38	1.59	1.52
1	F	55	GLN	C-O	-5.22	1.18	1.24
1	D	9	VAL	CA-CB	5.18	1.61	1.54
1	A	114	VAL	CA-C	-5.16	1.46	1.52
1	E	152	VAL	C-O	-5.12	1.17	1.24
1	B	115	ASN	CG-OD1	5.05	1.33	1.23
1	H	118	MET	SD-CE	5.04	1.92	1.79
1	E	113	TYR	C-O	-5.04	1.17	1.23

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	510	VAL	N-CA-C	-6.98	106.25	111.90
1	E	65	ILE	N-CA-C	6.72	114.20	107.55
1	H	65	ILE	N-CA-C	6.01	113.03	107.56
1	F	65	ILE	N-CA-C	5.81	113.30	107.55
1	F	150	PRO	CA-C-O	-5.73	114.61	121.48
1	A	150	PRO	CA-C-O	-5.70	114.64	121.48
1	A	50	SER	N-CA-C	5.65	118.45	109.24
1	G	65	ILE	N-CA-C	5.64	112.69	107.56
1	A	36	SER	N-CA-C	5.46	118.16	110.14
1	G	3	ILE	N-CA-C	5.29	116.77	111.00
1	H	100	CYS	N-CA-C	5.17	117.32	108.90
2	N	505	ILE	N-CA-C	5.16	115.01	107.88
1	D	99	SER	N-CA-C	5.06	116.94	108.99
1	E	50	SER	N-CA-C	5.03	116.72	108.52
1	B	56	ILE	N-CA-C	-5.01	101.41	108.12

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	10	0
1	C	1284	0	1281	12	0
1	D	1284	0	1281	15	0
1	E	1284	0	1281	12	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	3	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	64	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 (64) 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: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:B:18:PHE:C	1:B:18:PHE:CD2	2.95	0.44
1:E:140:LYS:NZ	1:G:140:LYS:HZ2	2.16	0.44
1:G:96:ILE:HG13	1:G:112:TYR:HB2	2.00	0.44
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:HD13	1:A:81:ILE:HG21	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:17:LYS:O	1:E:18:PHE:C	2.61	0.42
1:F:19:SER:O	1:F:78:PRO:HG3	2.19	0.42
1:D:13:ASN:O	1:D:13:ASN:CG	2.63	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:B:19:SER:O	1:B:78:PRO:HG3	2.21	0.41
1:F:87:LEU:HG	1:F:136:VAL:HB	2.01	0.41
2:N:511:TYR:HA	2:N:512:PRO:C	2.45	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%)	21	44
1	C	158/161 (98%)	150 (95%)	7 (4%)	1 (1%)	21	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	158/161 (98%)	152 (96%)	5 (3%)	1 (1%)	21	44
1	E	158/161 (98%)	156 (99%)	1 (1%)	1 (1%)	21	44
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%)	30	54

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%)	144 (97%)	4 (3%)	39	69
1	B	148/149 (99%)	139 (94%)	9 (6%)	17	40
1	C	148/149 (99%)	140 (95%)	8 (5%)	20	45
1	D	148/149 (99%)	139 (94%)	9 (6%)	17	40
1	E	148/149 (99%)	138 (93%)	10 (7%)	14	35
1	F	147/149 (99%)	144 (98%)	3 (2%)	48	76
1	G	148/149 (99%)	141 (95%)	7 (5%)	23	51
1	H	148/149 (99%)	140 (95%)	8 (5%)	20	45
2	I	9/19 (47%)	9 (100%)	0	100	100
2	J	9/19 (47%)	7 (78%)	2 (22%)	1	3
2	K	6/19 (32%)	6 (100%)	0	100	100
2	L	8/19 (42%)	7 (88%)	1 (12%)	4	11
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%)	8 (89%)	1 (11%)	6	15
2	P	9/19 (47%)	8 (89%)	1 (11%)	6	15
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%)	1203 (95%)	63 (5%)	22	48

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	VAL
1	A	58	ASP
1	A	81	ILE
1	A	88	SER
1	B	9	VAL
1	B	39	GLU
1	B	58	ASP
1	B	81	ILE
1	B	138	ILE
1	B	149	LYS
1	B	151	ARG
1	B	154	ARG

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Mol	Chain	Res	Type
1	B	161	ASN
2	J	503	LYS
2	J	504	ARG
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	3	ILE
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	81	ILE
1	G	9	VAL
1	G	58	ASP
1	G	104	ASP
1	G	127	ASP
1	G	135	LYS
1	G	148	GLU
1	G	161	ASN
2	O	505	ILE

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Mol	Chain	Res	Type
1	H	9	VAL
1	H	10	ASN
1	H	58	ASP
1	H	104	ASP
1	H	127	ASP
1	H	135	LYS
1	H	148	GLU
1	H	161	ASN
2	P	503	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	ASN
1	A	156	ASN
1	B	10	ASN
1	B	105	ASN
1	B	115	ASN
1	B	156	ASN
1	C	51	GLN
1	C	70	ASN
1	C	105	ASN
1	C	124	GLN
1	D	51	GLN
1	D	105	ASN
1	F	105	ASN
1	F	115	ASN
1	F	156	ASN
1	G	105	ASN
1	G	156	ASN
1	H	105	ASN
1	H	156	ASN
1	H	158	GLN

5.3.3 RNA ⓘ

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	160/161 (99%)	-0.40	0 100 100	20, 32, 57, 68	0
1	B	160/161 (99%)	-0.18	3 (1%) 66 63	26, 40, 72, 78	0
1	C	160/161 (99%)	-0.17	1 (0%) 85 85	19, 38, 74, 80	0
1	D	160/161 (99%)	-0.30	0 100 100	20, 38, 74, 82	0
1	E	160/161 (99%)	-0.22	0 100 100	26, 40, 72, 78	0
1	F	159/161 (98%)	-0.43	1 (0%) 85 85	20, 32, 58, 68	0
1	G	160/161 (99%)	-0.27	0 100 100	24, 40, 64, 75	0
1	H	160/161 (99%)	-0.29	0 100 100	23, 39, 64, 71	0
2	I	10/20 (50%)	-0.45	0 100 100	32, 36, 39, 42	0
2	J	10/20 (50%)	0.01	0 100 100	50, 54, 61, 63	0
2	K	7/20 (35%)	0.45	1 (14%) 6 5	53, 54, 61, 63	0
2	L	9/20 (45%)	0.75	1 (11%) 10 8	65, 68, 76, 80	0
2	M	10/20 (50%)	-0.39	0 100 100	37, 41, 44, 47	0
2	N	10/20 (50%)	-0.09	0 100 100	40, 47, 50, 50	0
2	O	10/20 (50%)	0.37	0 100 100	66, 67, 70, 74	0
2	P	10/20 (50%)	0.04	0 100 100	45, 51, 55, 64	0
2	Q	5/20 (25%)	1.39	2 (40%) 1 0	65, 69, 70, 71	0
2	R	5/20 (25%)	1.94	3 (60%) 0 0	67, 69, 70, 71	0
2	T	5/20 (25%)	1.72	2 (40%) 1 0	68, 70, 71, 72	0
All	All	1370/1508 (90%)	-0.24	14 (1%) 79 78	19, 38, 69, 82	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	129	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
2	T	507	PRO	2.7
2	Q	511	TYR	2.6
2	K	510	VAL	2.6
2	R	511	TYR	2.5
2	R	507	PRO	2.5
1	B	33	PRO	2.3
1	B	49	THR	2.3
2	R	508	THR	2.2
1	F	129	ALA	2.2
2	T	511	TYR	2.1
1	B	31	LEU	2.1
2	Q	507	PRO	2.1
2	L	511	TYR	2.1

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.