



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:05 AM GMT

PDB ID : 2VTX
Title : ACTIVATION OF NUCLEOPLASMIN, AN OLIGOMERIC HISTONE CHAPERONE, CHALLENGES ITS STABILITY
Authors : Taneva, S.G.; Munoz, I.G.; Franco, G.; Falces, J.; Arregi, I.; Muga, A.; Montoya, G.; Urbaneja, M.A.; Banuelos, S.
Deposited on : 2008-05-16
Resolution : 2.50 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

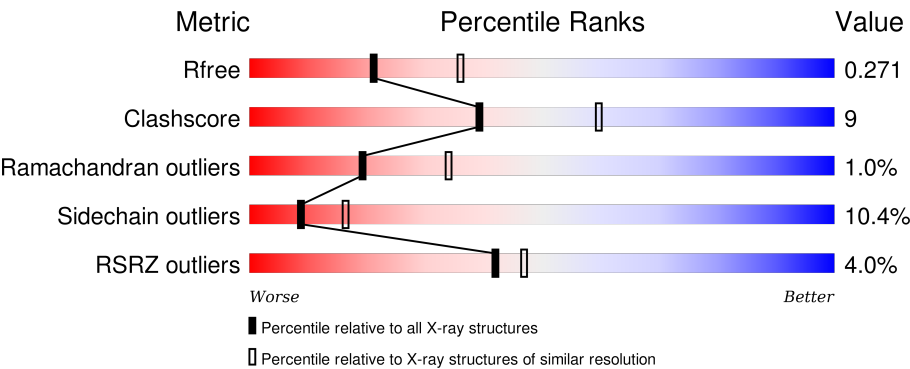
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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. 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	120	
1	B	120	
1	C	120	
1	D	120	
1	E	120	

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Mol	Chain	Length	Quality of chain
1	G	120	<div><div><div></div><div></div><div></div><div></div></div><div><div>2%</div><div>61%</div><div>15%</div><div>• •</div><div>22%</div></div></div>
1	H	120	<div><div><div></div><div></div><div></div><div></div></div><div><div>3%</div><div>58%</div><div>16%</div><div>5%</div><div>21%</div></div></div>
1	I	120	<div><div><div></div><div></div><div></div><div></div></div><div><div>2%</div><div>50%</div><div>24%</div><div>6%</div><div>20%</div></div></div>
1	K	120	<div><div><div></div><div></div><div></div><div></div></div><div><div>3%</div><div>53%</div><div>23%</div><div>•</div><div>23%</div></div></div>
2	J	120	<div><div><div></div><div></div><div></div><div></div></div><div><div>3%</div><div>52%</div><div>24%</div><div>•</div><div>23%</div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7259 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 NPM-A PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	92	Total	C	N	O	S	0	0	0
			713	460	117	131	5			
1	B	96	Total	C	N	O	S	0	0	0
			734	471	122	136	5			
1	C	89	Total	C	N	O	S	0	0	0
			684	442	112	126	4			
1	D	89	Total	C	N	O	S	0	0	0
			676	437	111	124	4			
1	E	91	Total	C	N	O	S	0	0	0
			696	451	115	126	4			
1	G	94	Total	C	N	O	S	0	0	0
			725	467	120	134	4			
1	H	95	Total	C	N	O	S	0	0	0
			720	461	118	137	4			
1	I	96	Total	C	N	O	S	0	0	0
			725	466	121	134	4			
1	K	93	Total	C	N	O	S	0	0	0
			706	455	116	130	5			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	ASP	SER	ENGINEERED MUTATION	UNP Q6GQG6
A	4	ASP	THR	ENGINEERED MUTATION	UNP Q6GQG6
A	6	ASP	SER	ENGINEERED MUTATION	UNP Q6GQG6
A	8	ASP	THR	ENGINEERED MUTATION	UNP Q6GQG6
A	9	ASP	SER	ENGINEERED MUTATION	UNP Q6GQG6
A	16	ASP	SER	ENGINEERED MUTATION	UNP Q6GQG6
A	67	ASP	THR	ENGINEERED MUTATION	UNP Q6GQG6
A	97	ASP	THR	ENGINEERED MUTATION	UNP Q6GQG6
B	3	ASP	SER	ENGINEERED MUTATION	UNP Q6GQG6
B	4	ASP	THR	ENGINEERED MUTATION	UNP Q6GQG6
B	6	ASP	SER	ENGINEERED MUTATION	UNP Q6GQG6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	8	ASP	THR	ENGINEERED MUTATION	UNP Q6GQG6
B	9	ASP	SER	ENGINEERED MUTATION	UNP Q6GQG6
B	16	ASP	SER	ENGINEERED MUTATION	UNP Q6GQG6
B	67	ASP	THR	ENGINEERED MUTATION	UNP Q6GQG6
B	97	ASP	THR	ENGINEERED MUTATION	UNP Q6GQG6
C	3	ASP	SER	ENGINEERED MUTATION	UNP Q6GQG6
C	4	ASP	THR	ENGINEERED MUTATION	UNP Q6GQG6
C	6	ASP	SER	ENGINEERED MUTATION	UNP Q6GQG6
C	8	ASP	THR	ENGINEERED MUTATION	UNP Q6GQG6
C	9	ASP	SER	ENGINEERED MUTATION	UNP Q6GQG6
C	16	ASP	SER	ENGINEERED MUTATION	UNP Q6GQG6
C	67	ASP	THR	ENGINEERED MUTATION	UNP Q6GQG6
C	97	ASP	THR	ENGINEERED MUTATION	UNP Q6GQG6
D	3	ASP	SER	ENGINEERED MUTATION	UNP Q6GQG6
D	4	ASP	THR	ENGINEERED MUTATION	UNP Q6GQG6
D	6	ASP	SER	ENGINEERED MUTATION	UNP Q6GQG6
D	8	ASP	THR	ENGINEERED MUTATION	UNP Q6GQG6
D	9	ASP	SER	ENGINEERED MUTATION	UNP Q6GQG6
D	16	ASP	SER	ENGINEERED MUTATION	UNP Q6GQG6
D	67	ASP	THR	ENGINEERED MUTATION	UNP Q6GQG6
D	97	ASP	THR	ENGINEERED MUTATION	UNP Q6GQG6
E	3	ASP	SER	ENGINEERED MUTATION	UNP Q6GQG6
E	4	ASP	THR	ENGINEERED MUTATION	UNP Q6GQG6
E	6	ASP	SER	ENGINEERED MUTATION	UNP Q6GQG6
E	8	ASP	THR	ENGINEERED MUTATION	UNP Q6GQG6
E	9	ASP	SER	ENGINEERED MUTATION	UNP Q6GQG6
E	16	ASP	SER	ENGINEERED MUTATION	UNP Q6GQG6
E	67	ASP	THR	ENGINEERED MUTATION	UNP Q6GQG6
E	97	ASP	THR	ENGINEERED MUTATION	UNP Q6GQG6
G	3	ASP	SER	ENGINEERED MUTATION	UNP Q6GQG6
G	4	ASP	THR	ENGINEERED MUTATION	UNP Q6GQG6
G	6	ASP	SER	ENGINEERED MUTATION	UNP Q6GQG6
G	8	ASP	THR	ENGINEERED MUTATION	UNP Q6GQG6
G	9	ASP	SER	ENGINEERED MUTATION	UNP Q6GQG6
G	16	ASP	SER	ENGINEERED MUTATION	UNP Q6GQG6
G	67	ASP	THR	ENGINEERED MUTATION	UNP Q6GQG6
G	97	ASP	THR	ENGINEERED MUTATION	UNP Q6GQG6
H	3	ASP	SER	ENGINEERED MUTATION	UNP Q6GQG6
H	4	ASP	THR	ENGINEERED MUTATION	UNP Q6GQG6
H	6	ASP	SER	ENGINEERED MUTATION	UNP Q6GQG6
H	8	ASP	THR	ENGINEERED MUTATION	UNP Q6GQG6
H	9	ASP	SER	ENGINEERED MUTATION	UNP Q6GQG6

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Chain	Residue	Modelled	Actual	Comment	Reference
H	16	ASP	SER	ENGINEERED MUTATION	UNP Q6GQG6
H	67	ASP	THR	ENGINEERED MUTATION	UNP Q6GQG6
H	97	ASP	THR	ENGINEERED MUTATION	UNP Q6GQG6
I	3	ASP	SER	ENGINEERED MUTATION	UNP Q6GQG6
I	4	ASP	THR	ENGINEERED MUTATION	UNP Q6GQG6
I	6	ASP	SER	ENGINEERED MUTATION	UNP Q6GQG6
I	8	ASP	THR	ENGINEERED MUTATION	UNP Q6GQG6
I	9	ASP	SER	ENGINEERED MUTATION	UNP Q6GQG6
I	16	ASP	SER	ENGINEERED MUTATION	UNP Q6GQG6
I	67	ASP	THR	ENGINEERED MUTATION	UNP Q6GQG6
I	97	ASP	THR	ENGINEERED MUTATION	UNP Q6GQG6
K	3	ASP	SER	ENGINEERED MUTATION	UNP Q6GQG6
K	4	ASP	THR	ENGINEERED MUTATION	UNP Q6GQG6
K	6	ASP	SER	ENGINEERED MUTATION	UNP Q6GQG6
K	8	ASP	THR	ENGINEERED MUTATION	UNP Q6GQG6
K	9	ASP	SER	ENGINEERED MUTATION	UNP Q6GQG6
K	16	ASP	SER	ENGINEERED MUTATION	UNP Q6GQG6
K	67	ASP	THR	ENGINEERED MUTATION	UNP Q6GQG6
K	97	ASP	THR	ENGINEERED MUTATION	UNP Q6GQG6

- Molecule 2 is a protein called NPM-A PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	93	Total	C	N	O	S	0	0	0
			707	456	117	130	4			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	3	ASP	SER	ENGINEERED MUTATION	UNP Q6GQG6
J	4	ASP	THR	ENGINEERED MUTATION	UNP Q6GQG6
J	6	ASP	SER	ENGINEERED MUTATION	UNP Q6GQG6
J	8	ASP	THR	ENGINEERED MUTATION	UNP Q6GQG6
J	9	ASP	SER	ENGINEERED MUTATION	UNP Q6GQG6
J	16	ASP	SER	ENGINEERED MUTATION	UNP Q6GQG6
J	67	ASP	THR	ENGINEERED MUTATION	UNP Q6GQG6
J	75	VAL	SER	CONFLICT	UNP Q6GQG6
J	97	ASP	THR	ENGINEERED MUTATION	UNP Q6GQG6

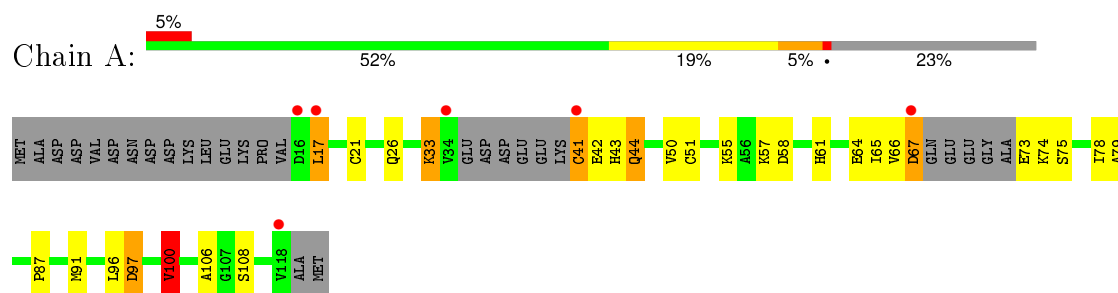
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	32	Total 32	O 32	0	0
3	B	29	Total 29	O 29	0	0
3	C	21	Total 21	O 21	0	0
3	D	16	Total 16	O 16	0	0
3	E	15	Total 15	O 15	0	0
3	G	16	Total 16	O 16	0	0
3	H	16	Total 16	O 16	0	0
3	I	11	Total 11	O 11	0	0
3	J	7	Total 7	O 7	0	0
3	K	10	Total 10	O 10	0	0

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.

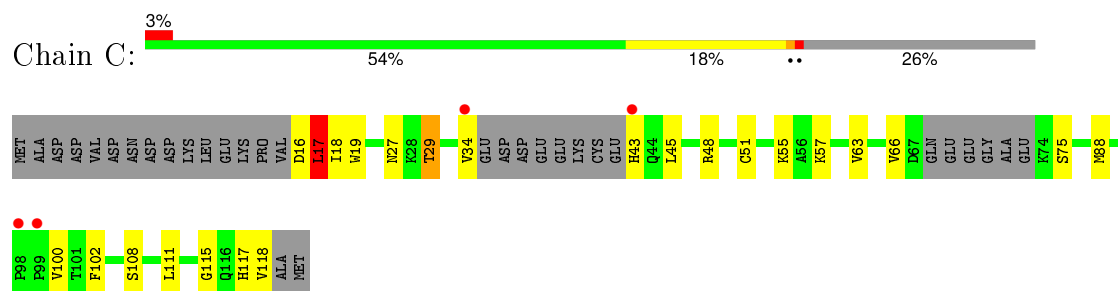
• Molecule 1: NPM-A PROTEIN



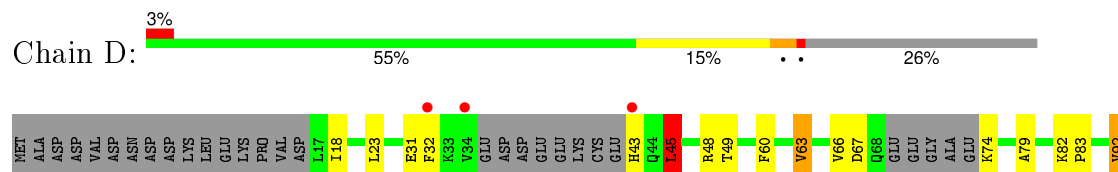
• Molecule 1: NPM-A PROTEIN



• Molecule 1: NPM-A PROTEIN

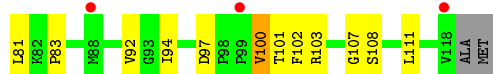


• Molecule 1: NPM-A PROTEIN





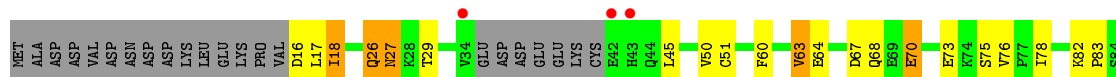
• Molecule 1: NPM-A PROTEIN



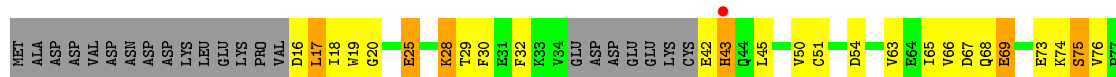
• Molecule 1: NPM-A PROTEIN



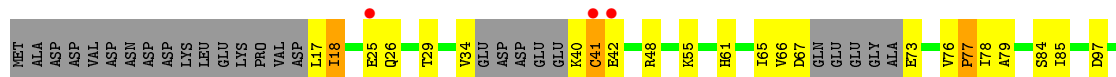
• Molecule 1: NPM-A PROTEIN



• Molecule 1: NPM-A PROTEIN

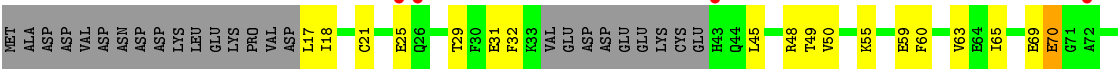


• Molecule 1: NPM-A PROTEIN





● Molecule 2: NPM-A PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.03Å 94.60Å 176.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.50 39.91 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.00-2.50) 100.0 (39.91-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.54 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.182 , 0.269 0.189 , 0.271	Depositor DCC
R_{free} test set	1984 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	40.3	Xtriage
Anisotropy	0.283	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 54.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 39553 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7259	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.84	13/726 (1.8%)	1.26	5/981 (0.5%)
1	B	1.78	12/747 (1.6%)	1.20	2/1010 (0.2%)
1	C	1.52	3/697 (0.4%)	1.18	1/945 (0.1%)
1	D	1.52	3/688 (0.4%)	1.22	1/931 (0.1%)
1	E	1.56	6/709 (0.8%)	1.23	6/960 (0.6%)
1	G	1.55	3/738 (0.4%)	1.13	0/998
1	H	1.50	5/733 (0.7%)	1.22	3/993 (0.3%)
1	I	1.52	8/739 (1.1%)	1.21	2/1002 (0.2%)
1	K	1.41	4/719 (0.6%)	1.15	1/975 (0.1%)
2	J	1.50	5/721 (0.7%)	1.16	2/979 (0.2%)
All	All	1.58	62/7217 (0.9%)	1.20	23/9774 (0.2%)

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	B	0	2
1	D	0	1
1	E	0	1
1	H	0	1
1	I	0	2
2	J	0	1
All	All	0	9

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	108	SER	CB-OG	12.47	1.58	1.42
1	G	51	CYS	CB-SG	-10.73	1.64	1.82
1	I	25	GLU	CG-CD	10.69	1.68	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	51	CYS	CB-SG	-10.02	1.65	1.82
2	J	108	SER	CB-OG	8.74	1.53	1.42
1	I	108	SER	CB-OG	8.73	1.53	1.42
1	I	63	VAL	CB-CG1	-8.59	1.34	1.52
1	A	73	GLU	CB-CG	8.55	1.68	1.52
1	G	42	GLU	CB-CG	8.48	1.68	1.52
1	B	51	CYS	CB-SG	-8.33	1.68	1.82
2	J	59	GLU	CD-OE2	8.33	1.34	1.25
1	C	51	CYS	CB-SG	-8.08	1.68	1.82
1	A	33	LYS	CE-NZ	7.99	1.69	1.49
1	B	103	ARG	CB-CG	7.83	1.73	1.52
1	B	25	GLU	CB-CG	-7.52	1.37	1.52
1	E	108	SER	CB-OG	7.40	1.51	1.42
1	E	51	CYS	CB-SG	-7.33	1.69	1.82
1	E	55	LYS	C-O	-7.25	1.09	1.23
1	H	16	ASP	CB-CG	7.14	1.66	1.51
1	A	87	PRO	N-CA	-7.09	1.35	1.47
1	K	108	SER	CB-OG	7.08	1.51	1.42
1	G	42	GLU	CG-CD	6.97	1.62	1.51
1	A	33	LYS	CD-CE	6.94	1.68	1.51
1	D	92	VAL	CB-CG2	6.70	1.67	1.52
1	H	50	VAL	CB-CG1	-6.65	1.38	1.52
2	J	25	GLU	CG-CD	6.59	1.61	1.51
1	K	73	GLU	CA-CB	6.58	1.68	1.53
1	A	57	LYS	CE-NZ	6.58	1.65	1.49
1	A	108	SER	CB-OG	6.53	1.50	1.42
1	I	67	ASP	CB-CG	6.43	1.65	1.51
1	K	25	GLU	CG-CD	6.30	1.61	1.51
1	E	100	VAL	CB-CG1	6.21	1.65	1.52
2	J	21	CYS	CB-SG	-6.18	1.71	1.82
2	J	55	LYS	CE-NZ	5.99	1.64	1.49
1	C	55	LYS	CE-NZ	5.93	1.63	1.49
1	I	51	CYS	CB-SG	-5.93	1.72	1.81
1	B	31	GLU	CB-CG	5.87	1.63	1.52
1	C	57	LYS	CD-CE	5.84	1.65	1.51
1	D	60	PHE	CE1-CZ	5.82	1.48	1.37
1	A	66	VAL	CB-CG1	5.79	1.65	1.52
1	A	44	GLN	CG-CD	5.79	1.64	1.51
1	I	25	GLU	CB-CG	5.74	1.63	1.52
1	A	51	CYS	CB-SG	-5.71	1.72	1.81
1	B	55	LYS	CD-CE	5.63	1.65	1.51
1	B	74	LYS	CD-CE	5.60	1.65	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	107	GLY	N-CA	-5.56	1.37	1.46
1	H	63	VAL	CB-CG1	-5.49	1.41	1.52
1	B	73	GLU	CG-CD	5.49	1.60	1.51
1	H	60	PHE	CE2-CZ	5.44	1.47	1.37
1	A	79	ALA	CA-CB	-5.35	1.41	1.52
1	B	75	SER	CB-OG	-5.35	1.35	1.42
1	D	108	SER	CB-OG	5.35	1.49	1.42
1	B	67	ASP	CB-CG	5.34	1.62	1.51
1	E	31	GLU	CG-CD	5.32	1.59	1.51
1	K	76	VAL	CB-CG2	5.29	1.64	1.52
1	A	33	LYS	CG-CD	5.29	1.70	1.52
1	A	55	LYS	CE-NZ	5.28	1.62	1.49
1	A	21	CYS	CB-SG	-5.24	1.73	1.81
1	B	60	PHE	CE2-CZ	-5.22	1.27	1.37
1	I	100	VAL	CB-CG2	5.01	1.63	1.52
1	B	68	GLN	N-CA	5.01	1.56	1.46
1	I	75	SER	CB-OG	-5.00	1.35	1.42

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	67	ASP	CB-CG-OD1	9.81	127.13	118.30
2	J	48	ARG	NE-CZ-NH2	-8.57	116.02	120.30
1	A	58	ASP	CB-CG-OD2	8.26	125.73	118.30
1	E	94	ILE	CG1-CB-CG2	-7.27	95.41	111.40
1	B	48	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	A	50	VAL	CG1-CB-CG2	-6.20	100.98	110.90
1	A	17	LEU	CA-CB-CG	6.17	129.48	115.30
1	K	48	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	E	23	LEU	CB-CG-CD1	-5.73	101.26	111.00
1	H	50	VAL	CG1-CB-CG2	-5.72	101.75	110.90
1	B	48	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	E	97	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	D	45	LEU	CA-CB-CG	5.32	127.54	115.30
1	A	33	LYS	CD-CE-NZ	5.30	123.90	111.70
1	H	111	LEU	CA-CB-CG	5.27	127.43	115.30
1	I	100	VAL	CG1-CB-CG2	5.25	119.30	110.90
1	E	55	LYS	CD-CE-NZ	-5.23	99.68	111.70
1	A	100	VAL	CB-CA-C	-5.19	101.54	111.40
1	E	23	LEU	CB-CG-CD2	5.10	119.68	111.00
1	C	88	MET	CG-SD-CE	5.07	108.30	100.20
1	H	16	ASP	CB-CG-OD2	5.05	122.85	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	103	ARG	NE-CZ-NH1	5.03	122.82	120.30
2	J	100	VAL	CB-CA-C	-5.03	101.84	111.40

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	41	CYS	Peptide
1	B	33	LYS	Peptide
1	B	40	LYS	Peptide
1	D	43	HIS	Peptide
1	E	33	LYS	Peptide
1	H	68	GLN	Peptide
1	I	16	ASP	Peptide
1	I	69	GLU	Peptide
2	J	69	GLU	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	713	0	724	12	0
1	B	734	0	732	16	0
1	C	684	0	687	9	0
1	D	676	0	677	12	0
1	E	696	0	702	10	0
1	G	725	0	732	13	0
1	H	720	0	710	13	0
1	I	725	0	718	18	0
1	K	706	0	703	17	0
2	J	707	0	705	18	0
3	A	32	0	0	0	0
3	B	29	0	0	2	0
3	C	21	0	0	0	0
3	D	16	0	0	0	0
3	E	15	0	0	0	0
3	G	16	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	16	0	0	1	0
3	I	11	0	0	0	0
3	J	7	0	0	0	0
3	K	10	0	0	0	0
All	All	7259	0	7090	126	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 (126) 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:A:33:LYS:NZ	1:A:33:LYS:CE	1.69	1.54
2:J:31:GLU:HA	2:J:101:THR:HG22	1.54	0.89
2:J:50:VAL:HG12	2:J:81:LEU:HD11	1.57	0.86
1:A:42:GLU:CD	1:A:43:HIS:H	1.85	0.80
1:B:34:VAL:HG13	1:B:38:GLU:N	1.98	0.79
1:H:18:ILE:O	1:H:18:ILE:HD12	1.86	0.76
2:J:31:GLU:CA	2:J:101:THR:HG22	2.17	0.74
2:J:50:VAL:CG1	2:J:81:LEU:HD11	2.19	0.72
2:J:88:MET:SD	1:K:79:ALA:HB1	2.31	0.70
1:B:34:VAL:CG1	1:B:34:VAL:O	2.39	0.70
1:D:32:PHE:CE2	1:D:98:PRO:HG3	2.27	0.69
1:G:25:GLU:OE1	1:G:25:GLU:HA	1.91	0.69
1:C:34:VAL:O	1:C:34:VAL:HG23	1.90	0.69
1:C:16:ASP:O	1:C:17:LEU:HB3	1.93	0.68
1:B:33:LYS:HD2	1:B:99:PRO:HB3	1.74	0.68
1:B:50:VAL:HG12	1:B:81:LEU:HD11	1.76	0.68
1:K:40:LYS:O	1:K:41:CYS:HB2	1.95	0.67
1:B:34:VAL:HG12	1:B:34:VAL:O	1.94	0.66
1:A:42:GLU:CD	1:A:43:HIS:N	2.48	0.66
1:D:111:LEU:HD23	1:D:111:LEU:C	2.17	0.65
1:B:66:VAL:O	3:B:2019:HOH:O	2.14	0.65
1:A:96:LEU:HD13	1:A:100:VAL:HG11	1.79	0.64
1:I:92:VAL:HG22	2:J:92:VAL:HG11	1.80	0.63
1:G:66:VAL:HG12	1:G:66:VAL:O	1.99	0.61
1:E:63:VAL:HG13	1:E:79:ALA:HB3	1.83	0.61
1:B:39:GLU:O	1:B:39:GLU:HG2	2.00	0.60
1:B:111:LEU:HD23	1:B:111:LEU:C	2.23	0.58
1:H:18:ILE:HD13	1:I:76:VAL:HG21	1.86	0.58
1:I:65:ILE:HD12	1:I:78:ILE:HG21	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:ARG:NH1	3:B:2025:HOH:O	2.38	0.55
1:A:42:GLU:OE1	1:A:43:HIS:N	2.39	0.55
1:E:65:ILE:HD11	1:E:102:PHE:CE2	2.41	0.55
1:K:18:ILE:CG2	1:K:18:ILE:O	2.55	0.55
1:H:18:ILE:C	1:H:18:ILE:CD1	2.76	0.54
1:I:50:VAL:HG12	1:I:81:LEU:HD11	1.90	0.54
1:G:84:SER:O	1:H:85:ILE:HD12	2.08	0.53
1:E:50:VAL:HG12	1:E:81:LEU:HD11	1.90	0.53
1:A:44:GLN:NE2	1:A:97:ASP:OD1	2.42	0.53
1:E:29:THR:HG23	1:E:101:THR:HG23	1.92	0.52
1:G:118:VAL:HG13	1:G:119:ALA:N	2.25	0.52
1:K:84:SER:C	1:K:85:ILE:HD13	2.29	0.51
1:H:27:ASN:N	1:H:27:ASN:HD22	2.08	0.51
1:D:92:VAL:HG22	1:E:92:VAL:HG11	1.91	0.51
2:J:50:VAL:HG12	2:J:81:LEU:CD1	2.37	0.51
1:B:66:VAL:HG22	1:B:75:SER:HB3	1.92	0.51
1:D:66:VAL:HA	1:D:74:LYS:O	2.11	0.51
1:A:64:GLU:OE2	1:A:75:SER:HB3	2.11	0.51
1:B:63:VAL:CG1	1:B:79:ALA:HB3	2.41	0.51
1:B:33:LYS:HE2	1:B:34:VAL:HG23	1.93	0.51
1:I:92:VAL:HG22	2:J:92:VAL:CG1	2.41	0.50
1:D:23:LEU:N	1:D:23:LEU:HD23	2.25	0.50
1:C:111:LEU:HD23	1:C:111:LEU:C	2.32	0.50
1:E:26:GLN:HB2	1:E:27:ASN:ND2	2.27	0.50
1:B:96:LEU:HD13	1:B:100:VAL:HG11	1.94	0.50
2:J:32:PHE:N	2:J:100:VAL:O	2.37	0.50
2:J:88:MET:SD	1:K:79:ALA:CB	3.00	0.50
1:G:85:ILE:HD12	1:K:84:SER:O	2.12	0.50
2:J:31:GLU:CB	2:J:101:THR:HG22	2.42	0.49
1:H:108:SER:HB2	3:H:2016:HOH:O	2.13	0.49
2:J:18:ILE:HD12	1:K:65:ILE:HD13	1.95	0.49
1:E:65:ILE:HD11	1:E:102:PHE:HE2	1.77	0.49
1:H:18:ILE:C	1:H:18:ILE:HD12	2.31	0.49
1:I:18:ILE:HG23	1:I:18:ILE:O	2.13	0.48
1:A:91:MET:HA	1:A:91:MET:HE2	1.95	0.48
1:D:18:ILE:CG2	1:D:18:ILE:O	2.60	0.48
1:B:34:VAL:CG1	1:B:38:GLU:N	2.73	0.48
1:D:111:LEU:HD23	1:D:111:LEU:O	2.14	0.47
1:E:65:ILE:CD1	1:E:102:PHE:CE2	2.96	0.47
1:G:34:VAL:HG13	1:G:98:PRO:HG3	1.96	0.47
1:K:65:ILE:HD12	1:K:78:ILE:HG21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:68:GLN:O	1:I:69:GLU:CB	2.61	0.47
1:K:18:ILE:HG23	1:K:18:ILE:O	2.15	0.47
1:A:67:ASP:C	1:A:67:ASP:OD1	2.52	0.46
2:J:32:PHE:O	2:J:99:PRO:HA	2.15	0.46
1:I:32:PHE:CD2	1:I:45:LEU:HD22	2.50	0.46
1:B:38:GLU:O	1:B:39:GLU:HB3	2.16	0.46
1:G:98:PRO:CB	1:G:99:PRO:HA	2.46	0.46
1:A:65:ILE:HD12	1:A:78:ILE:HG21	1.98	0.46
1:I:91:MET:HE2	1:I:91:MET:HA	1.97	0.46
1:C:16:ASP:O	1:C:17:LEU:CB	2.63	0.45
1:C:34:VAL:O	1:C:34:VAL:CG2	2.60	0.45
2:J:65:ILE:HD12	2:J:78:ILE:HG21	1.97	0.45
1:I:25:GLU:O	1:I:28:LYS:HD2	2.16	0.45
1:I:19:TRP:CG	1:I:20:GLY:N	2.85	0.45
1:I:66:VAL:HA	1:I:74:LYS:O	2.16	0.44
1:K:18:ILE:HD13	1:K:115:GLY:O	2.17	0.44
1:E:52:LEU:HD13	1:E:83:PRO:HG3	1.98	0.44
1:K:40:LYS:O	1:K:41:CYS:CB	2.62	0.44
1:K:61:HIS:HA	1:K:106:ALA:O	2.18	0.44
1:H:64:GLU:OE2	1:H:75:SER:HB3	2.18	0.44
1:K:29:THR:HA	1:K:102:PHE:O	2.18	0.43
1:G:55:LYS:HD2	3:G:2005:HOH:O	2.18	0.43
1:K:104:LEU:CD1	1:K:111:LEU:HD13	2.49	0.43
1:D:45:LEU:O	1:D:95:GLU:HA	2.18	0.43
1:I:29:THR:HG23	1:I:101:THR:CG2	2.48	0.43
1:I:82:LYS:HA	1:I:83:PRO:HD3	1.92	0.43
2:J:112:TYR:CG	1:K:77:PRO:HG2	2.54	0.43
1:C:16:ASP:N	1:C:117:HIS:O	2.51	0.43
1:G:64:GLU:OE2	1:G:75:SER:HB3	2.19	0.42
1:I:17:LEU:HD22	1:I:18:ILE:N	2.34	0.42
1:H:26:GLN:C	1:H:27:ASN:HD22	2.23	0.42
1:G:66:VAL:HG22	1:G:75:SER:OG	2.19	0.42
1:A:91:MET:HA	1:A:91:MET:CE	2.49	0.42
1:K:65:ILE:HD11	1:K:78:ILE:HD13	2.01	0.42
1:C:19:TRP:CZ3	1:C:45:LEU:HD21	2.54	0.42
1:E:33:LYS:NZ	1:E:33:LYS:HB2	2.34	0.42
1:B:33:LYS:NZ	1:B:99:PRO:HD3	2.35	0.42
1:C:29:THR:HA	1:C:102:PHE:O	2.20	0.42
1:G:95:GLU:OE2	1:G:118:VAL:HG11	2.20	0.41
1:D:48:ARG:C	1:D:49:THR:HG23	2.40	0.41
1:D:63:VAL:CG1	1:D:79:ALA:HB3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:94:ILE:HD13	1:G:94:ILE:HG21	1.93	0.41
2:J:49:THR:H	2:J:114:SER:HG	1.69	0.41
1:H:63:VAL:HG13	1:H:63:VAL:O	2.20	0.41
1:C:48:ARG:HG2	1:C:115:GLY:HA2	2.03	0.41
1:H:27:ASN:ND2	1:H:27:ASN:N	2.68	0.41
2:J:49:THR:HG21	1:K:78:ILE:O	2.20	0.41
1:H:82:LYS:HA	1:H:83:PRO:HD3	1.94	0.41
1:G:34:VAL:HG21	1:G:42:GLU:HG2	2.03	0.40
1:I:54:ASP:HB2	2:J:60:PHE:HB2	2.03	0.40
1:D:18:ILE:HG23	1:D:18:ILE:O	2.17	0.40
1:A:61:HIS:HA	1:A:106:ALA:O	2.22	0.40
1:I:30:PHE:C	1:I:30:PHE:CD2	2.94	0.40
1:D:82:LYS:HA	1:D:83:PRO:HD3	1.97	0.40
1:H:76:VAL:O	1:H:78:ILE:HG23	2.21	0.40
1:I:42:GLU:O	1:I:43:HIS:HB2	2.22	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	86/120 (72%)	81 (94%)	5 (6%)	0	100	100
1	B	90/120 (75%)	87 (97%)	1 (1%)	2 (2%)	8	13
1	C	83/120 (69%)	79 (95%)	2 (2%)	2 (2%)	7	11
1	D	83/120 (69%)	79 (95%)	4 (5%)	0	100	100
1	E	85/120 (71%)	84 (99%)	1 (1%)	0	100	100
1	G	88/120 (73%)	86 (98%)	2 (2%)	0	100	100
1	H	91/120 (76%)	88 (97%)	2 (2%)	1 (1%)	17	31
1	I	92/120 (77%)	87 (95%)	4 (4%)	1 (1%)	17	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	87/120 (72%)	82 (94%)	4 (5%)	1 (1%)	17	31
2	J	89/120 (74%)	84 (94%)	3 (3%)	2 (2%)	8	13
All	All	874/1200 (73%)	837 (96%)	28 (3%)	9 (1%)	19	34

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	39	GLU
1	C	17	LEU
1	I	43	HIS
1	K	41	CYS
1	B	41	CYS
1	C	27	ASN
1	H	70	GLU
2	J	104	LEU
2	J	70	GLU

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	80/105 (76%)	73 (91%)	7 (9%)	12	23
1	B	80/105 (76%)	73 (91%)	7 (9%)	12	23
1	C	76/105 (72%)	66 (87%)	10 (13%)	5	9
1	D	73/105 (70%)	65 (89%)	8 (11%)	8	14
1	E	76/105 (72%)	71 (93%)	5 (7%)	21	38
1	G	80/105 (76%)	72 (90%)	8 (10%)	9	18
1	H	77/105 (73%)	66 (86%)	11 (14%)	4	7
1	I	77/105 (73%)	71 (92%)	6 (8%)	16	29
1	K	77/105 (73%)	66 (86%)	11 (14%)	4	7
2	J	76/105 (72%)	69 (91%)	7 (9%)	11	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	772/1050 (74%)	692 (90%)	80 (10%)	9 16

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	26	GLN
1	A	41	CYS
1	A	67	ASP
1	A	74	LYS
1	A	97	ASP
1	A	100	VAL
1	B	26	GLN
1	B	33	LYS
1	B	39	GLU
1	B	41	CYS
1	B	68	GLN
1	B	73	GLU
1	B	97	ASP
1	C	17	LEU
1	C	18	ILE
1	C	29	THR
1	C	43	HIS
1	C	63	VAL
1	C	66	VAL
1	C	75	SER
1	C	100	VAL
1	C	108	SER
1	C	118	VAL
1	D	31	GLU
1	D	45	LEU
1	D	63	VAL
1	D	67	ASP
1	D	95	GLU
1	D	100	VAL
1	D	103	ARG
1	D	111	LEU
1	E	34	VAL
1	E	44	GLN
1	E	63	VAL
1	E	100	VAL
1	E	111	LEU

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Mol	Chain	Res	Type
1	G	16	ASP
1	G	17	LEU
1	G	42	GLU
1	G	55	LYS
1	G	68	GLN
1	G	97	ASP
1	G	100	VAL
1	G	118	VAL
1	H	17	LEU
1	H	18	ILE
1	H	26	GLN
1	H	27	ASN
1	H	29	THR
1	H	45	LEU
1	H	67	ASP
1	H	70	GLU
1	H	73	GLU
1	H	100	VAL
1	H	111	LEU
1	I	17	LEU
1	I	28	LYS
1	I	73	GLU
1	I	75	SER
1	I	95	GLU
1	I	100	VAL
2	J	17	LEU
2	J	29	THR
2	J	45	LEU
2	J	63	VAL
2	J	70	GLU
2	J	75	VAL
2	J	97	ASP
1	K	17	LEU
1	K	18	ILE
1	K	26	GLN
1	K	34	VAL
1	K	42	GLU
1	K	55	LYS
1	K	66	VAL
1	K	67	ASP
1	K	77	PRO
1	K	97	ASP

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Mol	Chain	Res	Type
1	K	100	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	44	GLN
1	B	26	GLN
1	D	27	ASN
1	E	117	HIS
1	G	26	GLN
1	H	27	ASN

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 carbohydrates 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	92/120 (76%)	0.10	6 (6%)	22 25	23, 34, 64, 73	0
1	B	96/120 (80%)	0.01	2 (2%)	67 71	24, 36, 71, 85	0
1	C	89/120 (74%)	0.16	4 (4%)	37 42	28, 45, 70, 81	0
1	D	89/120 (74%)	0.30	3 (3%)	49 54	29, 48, 72, 79	0
1	E	91/120 (75%)	0.27	7 (7%)	16 18	26, 44, 71, 83	0
1	G	94/120 (78%)	-0.10	2 (2%)	67 71	30, 47, 74, 80	0
1	H	95/120 (79%)	0.01	3 (3%)	51 56	30, 45, 73, 81	0
1	I	96/120 (80%)	-0.08	2 (2%)	67 71	31, 47, 74, 81	0
1	K	93/120 (77%)	0.12	4 (4%)	39 44	31, 51, 73, 88	0
2	J	93/120 (77%)	0.03	4 (4%)	39 44	31, 51, 73, 79	0
All	All	928/1200 (77%)	0.08	37 (3%)	42 47	23, 46, 73, 88	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	34	VAL	5.7
1	K	41	CYS	4.9
1	A	17	LEU	4.1
1	H	34	VAL	3.5
1	I	118	VAL	3.5
1	H	43	HIS	3.4
1	C	98	PRO	3.4
1	G	119	ALA	3.3
1	E	16	ASP	3.2
1	B	119	ALA	3.1
1	D	43	HIS	3.1
2	J	72	ALA	3.1
1	C	99	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	26	GLN	2.9
1	I	43	HIS	2.9
2	J	43	HIS	2.9
2	J	26	GLN	2.9
1	H	42	GLU	2.8
1	A	41	CYS	2.8
1	K	42	GLU	2.7
2	J	25	GLU	2.7
1	D	34	VAL	2.6
1	K	25	GLU	2.6
1	A	118	VAL	2.6
1	C	43	HIS	2.5
1	E	43	HIS	2.4
1	A	34	VAL	2.4
1	K	118	VAL	2.4
1	E	17	LEU	2.2
1	E	118	VAL	2.1
1	E	88	MET	2.1
1	B	42	GLU	2.1
1	E	42	GLU	2.1
1	A	16	ASP	2.1
1	E	99	PRO	2.1
1	A	67	ASP	2.0
1	D	32	PHE	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.