



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 12, 2024 – 11:04 AM EST

PDB ID : 3NFG
Title : Crystal structure of Dimerization module of RNA polymerase I subcomplex A49/A34.5
Authors : Geiger, S.R.
Deposited on : 2010-06-10
Resolution : 2.51 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

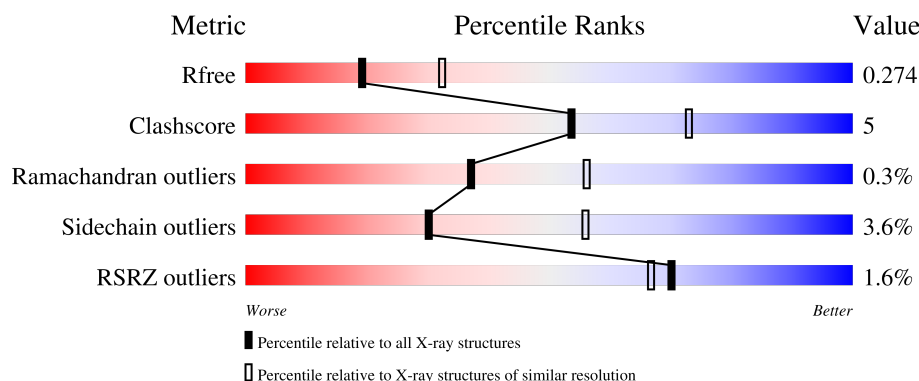
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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}	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (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 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	102	<div> <div>2%</div> <div>78% 14% 8%</div> </div>
1	C	102	<div> <div>75% 18% 7%</div> </div>
1	E	102	<div> <div>78% 16% 6%</div> </div>
1	G	102	<div> <div>2%</div> <div>77% 16% 7%</div> </div>
1	I	102	<div> <div>2%</div> <div>77% 15% 8%</div> </div>

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Mol	Chain	Length	Quality of chain
1	K	102	<div> <div>%</div> <div> </div> <div>81%12%7%</div> </div>
1	M	102	<div> <div> </div> <div>83%9%8%</div> </div>
1	O	102	<div> <div> </div> <div>75%16%8%</div> </div>
2	B	123	<div> <div>%</div> <div> </div> <div>82%15%..</div> </div>
2	D	123	<div> <div> </div> <div>76%21%..</div> </div>
2	F	123	<div> <div>%</div> <div> </div> <div>85%12%. </div> </div>
2	H	123	<div> <div>7%</div> <div> </div> <div>85%12%..</div> </div>
2	J	123	<div> <div>5%</div> <div> </div> <div>80%17%..</div> </div>
2	L	123	<div> <div>%</div> <div> </div> <div>79%15%. .</div> </div>
2	N	123	<div> <div>%</div> <div> </div> <div>82%15%. </div> </div>
2	P	123	<div> <div>2%</div> <div> </div> <div>83%14%. </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13795 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 DNA-directed RNA polymerase I subunit RPA49.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	94	Total	C	N	O	Se	0	1	0
			770	487	131	151	1			
1	C	95	Total	C	N	O	Se	0	0	0
			775	492	129	153	1			
1	E	96	Total	C	N	O	Se	0	0	0
			786	498	133	154	1			
1	G	95	Total	C	N	O	Se	0	0	0
			768	486	129	152	1			
1	I	94	Total	C	N	O	Se	0	0	0
			763	483	128	151	1			
1	K	95	Total	C	N	O	Se	0	0	0
			774	489	132	152	1			
1	M	94	Total	C	N	O	Se	0	0	0
			769	486	131	151	1			
1	O	94	Total	C	N	O	Se	0	0	0
			763	483	128	151	1			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q6FNZ9
A	-1	SER	-	expression tag	UNP Q6FNZ9
A	0	HIS	-	expression tag	UNP Q6FNZ9
A	72	MSE	VAL	engineered mutation	UNP Q6FNZ9
C	-2	GLY	-	expression tag	UNP Q6FNZ9
C	-1	SER	-	expression tag	UNP Q6FNZ9
C	0	HIS	-	expression tag	UNP Q6FNZ9
C	72	MSE	VAL	engineered mutation	UNP Q6FNZ9
E	-2	GLY	-	expression tag	UNP Q6FNZ9
E	-1	SER	-	expression tag	UNP Q6FNZ9
E	0	HIS	-	expression tag	UNP Q6FNZ9
E	72	MSE	VAL	engineered mutation	UNP Q6FNZ9
G	-2	GLY	-	expression tag	UNP Q6FNZ9

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-1	SER	-	expression tag	UNP Q6FNZ9
G	0	HIS	-	expression tag	UNP Q6FNZ9
G	72	MSE	VAL	engineered mutation	UNP Q6FNZ9
I	-2	GLY	-	expression tag	UNP Q6FNZ9
I	-1	SER	-	expression tag	UNP Q6FNZ9
I	0	HIS	-	expression tag	UNP Q6FNZ9
I	72	MSE	VAL	engineered mutation	UNP Q6FNZ9
K	-2	GLY	-	expression tag	UNP Q6FNZ9
K	-1	SER	-	expression tag	UNP Q6FNZ9
K	0	HIS	-	expression tag	UNP Q6FNZ9
K	72	MSE	VAL	engineered mutation	UNP Q6FNZ9
M	-2	GLY	-	expression tag	UNP Q6FNZ9
M	-1	SER	-	expression tag	UNP Q6FNZ9
M	0	HIS	-	expression tag	UNP Q6FNZ9
M	72	MSE	VAL	engineered mutation	UNP Q6FNZ9
O	-2	GLY	-	expression tag	UNP Q6FNZ9
O	-1	SER	-	expression tag	UNP Q6FNZ9
O	0	HIS	-	expression tag	UNP Q6FNZ9
O	72	MSE	VAL	engineered mutation	UNP Q6FNZ9

- Molecule 2 is a protein called DNA-directed RNA polymerase I subunit RPA34.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	120	Total	C	N	O	S	Se	0	0	0
			942	593	156	191	1	1			
2	D	120	Total	C	N	O	S	Se	0	0	0
			942	593	156	191	1	1			
2	F	120	Total	C	N	O	S	Se	0	0	0
			938	591	156	189	1	1			
2	H	120	Total	C	N	O	S	Se	0	0	0
			935	589	155	189	1	1			
2	J	120	Total	C	N	O	S	Se	0	0	0
			939	590	156	191	1	1			
2	L	120	Total	C	N	O	S	Se	0	0	0
			942	593	156	191	1	1			
2	N	120	Total	C	N	O	S	Se	0	0	0
			942	593	156	191	1	1			
2	P	119	Total	C	N	O	S	Se	0	0	0
			938	591	155	190	1	1			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	21	MSE	-	expression tag	UNP Q6FQI3
B	22	GLY	-	expression tag	UNP Q6FQI3
B	23	MET	-	expression tag	UNP Q6FQI3
B	24	GLY	-	expression tag	UNP Q6FQI3
B	55	MSE	LEU	engineered mutation	UNP Q6FQI3
D	21	MSE	-	expression tag	UNP Q6FQI3
D	22	GLY	-	expression tag	UNP Q6FQI3
D	23	MET	-	expression tag	UNP Q6FQI3
D	24	GLY	-	expression tag	UNP Q6FQI3
D	55	MSE	LEU	engineered mutation	UNP Q6FQI3
F	21	MSE	-	expression tag	UNP Q6FQI3
F	22	GLY	-	expression tag	UNP Q6FQI3
F	23	MET	-	expression tag	UNP Q6FQI3
F	24	GLY	-	expression tag	UNP Q6FQI3
F	55	MSE	LEU	engineered mutation	UNP Q6FQI3
H	21	MSE	-	expression tag	UNP Q6FQI3
H	22	GLY	-	expression tag	UNP Q6FQI3
H	23	MET	-	expression tag	UNP Q6FQI3
H	24	GLY	-	expression tag	UNP Q6FQI3
H	55	MSE	LEU	engineered mutation	UNP Q6FQI3
J	21	MSE	-	expression tag	UNP Q6FQI3
J	22	GLY	-	expression tag	UNP Q6FQI3
J	23	MET	-	expression tag	UNP Q6FQI3
J	24	GLY	-	expression tag	UNP Q6FQI3
J	55	MSE	LEU	engineered mutation	UNP Q6FQI3
L	21	MSE	-	expression tag	UNP Q6FQI3
L	22	GLY	-	expression tag	UNP Q6FQI3
L	23	MET	-	expression tag	UNP Q6FQI3
L	24	GLY	-	expression tag	UNP Q6FQI3
L	55	MSE	LEU	engineered mutation	UNP Q6FQI3
N	21	MSE	-	expression tag	UNP Q6FQI3
N	22	GLY	-	expression tag	UNP Q6FQI3
N	23	MET	-	expression tag	UNP Q6FQI3
N	24	GLY	-	expression tag	UNP Q6FQI3
N	55	MSE	LEU	engineered mutation	UNP Q6FQI3
P	21	MSE	-	expression tag	UNP Q6FQI3
P	22	GLY	-	expression tag	UNP Q6FQI3
P	23	MET	-	expression tag	UNP Q6FQI3
P	24	GLY	-	expression tag	UNP Q6FQI3
P	55	MSE	LEU	engineered mutation	UNP Q6FQI3

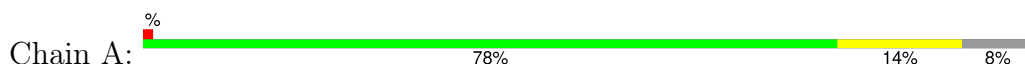
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	7	Total O 7 7	0	0
3	B	14	Total O 14 14	0	0
3	C	6	Total O 6 6	0	0
3	D	8	Total O 8 8	0	0
3	E	4	Total O 4 4	0	0
3	F	17	Total O 17 17	0	0
3	G	4	Total O 4 4	0	0
3	H	6	Total O 6 6	0	0
3	I	6	Total O 6 6	0	0
3	J	2	Total O 2 2	0	0
3	K	15	Total O 15 15	0	0
3	L	2	Total O 2 2	0	0
3	M	8	Total O 8 8	0	0
3	N	5	Total O 5 5	0	0
3	O	3	Total O 3 3	0	0
3	P	2	Total O 2 2	0	0

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: DNA-directed RNA polymerase I subunit RPA49



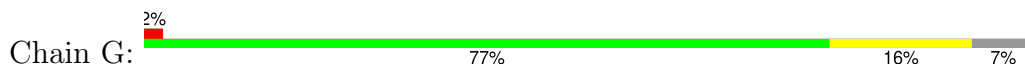
- Molecule 1: DNA-directed RNA polymerase I subunit RPA49



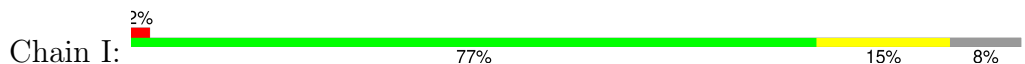
- Molecule 1: DNA-directed RNA polymerase I subunit RPA49



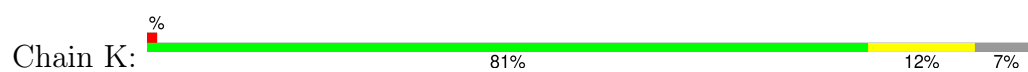
- Molecule 1: DNA-directed RNA polymerase I subunit RPA49



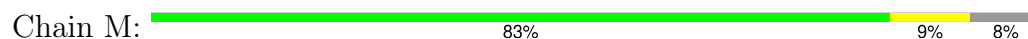
- Molecule 1: DNA-directed RNA polymerase I subunit RPA49



- Molecule 1: DNA-directed RNA polymerase I subunit RPA49



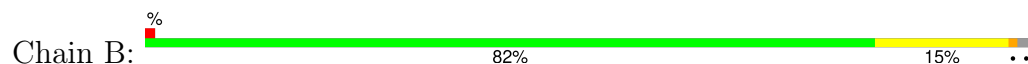
- Molecule 1: DNA-directed RNA polymerase I subunit RPA49



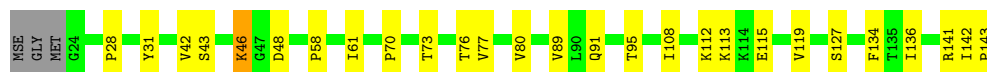
- Molecule 1: DNA-directed RNA polymerase I subunit RPA49



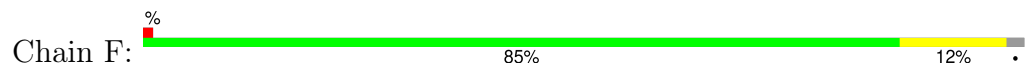
- Molecule 2: DNA-directed RNA polymerase I subunit RPA34



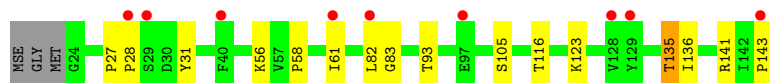
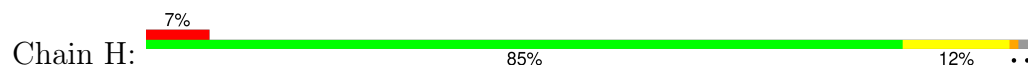
- Molecule 2: DNA-directed RNA polymerase I subunit RPA34



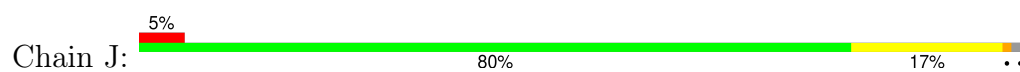
- Molecule 2: DNA-directed RNA polymerase I subunit RPA34



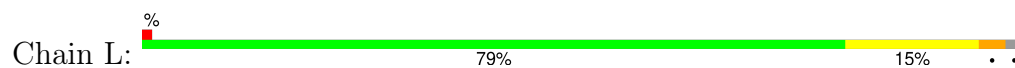
- Molecule 2: DNA-directed RNA polymerase I subunit RPA34



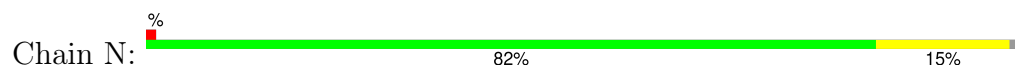
- Molecule 2: DNA-directed RNA polymerase I subunit RPA34



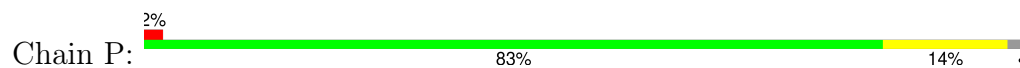
- Molecule 2: DNA-directed RNA polymerase I subunit RPA34



- Molecule 2: DNA-directed RNA polymerase I subunit RPA34



- Molecule 2: DNA-directed RNA polymerase I subunit RPA34



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.43Å 132.92Å 118.29Å 90.00° 102.84° 90.00°	Depositor
Resolution (Å)	49.68 – 2.51 49.68 – 2.51	Depositor EDS
% Data completeness (in resolution range)	(Not available) (49.68-2.51) 96.9 (49.68-2.51)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.51Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, R_{free}	0.194 , 0.243 0.221 , 0.274	Depositor DCC
R_{free} test set	3521 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	56.0	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 88.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13795	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.30% 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, 0.333 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	0.48	0/788	0.81	2/1059 (0.2%)
1	C	0.46	0/788	0.71	0/1058
1	E	0.49	0/799	0.75	0/1072
1	G	0.51	0/780	0.73	0/1049
1	I	0.47	0/775	0.72	0/1042
1	K	0.50	0/786	0.78	0/1056
1	M	0.54	0/781	0.75	0/1049
1	O	0.51	0/775	0.77	0/1042
2	B	0.54	0/957	0.78	0/1292
2	D	0.53	0/957	0.76	0/1292
2	F	0.54	0/953	0.74	0/1287
2	H	0.45	0/950	0.77	1/1284 (0.1%)
2	J	0.47	0/954	0.75	0/1288
2	L	0.56	0/957	0.83	1/1292 (0.1%)
2	N	0.54	0/957	0.79	0/1292
2	P	0.48	0/953	0.82	2/1287 (0.2%)
All	All	0.51	0/13910	0.77	6/18741 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	48	ASP	CB-CA-C	8.22	126.85	110.40
2	P	49	ASN	N-CA-CB	-7.50	97.10	110.60
2	H	83	GLY	N-CA-C	-6.92	95.80	113.10
1	A	65[A]	THR	N-CA-CB	6.20	122.08	110.30
1	A	65[B]	THR	N-CA-CB	6.20	122.08	110.30
2	L	47	GLY	N-CA-C	-5.22	100.04	113.10

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	770	0	767	8	0
1	C	775	0	763	11	0
1	E	786	0	776	10	0
1	G	768	0	756	10	0
1	I	763	0	754	10	0
1	K	774	0	767	6	0
1	M	769	0	765	5	0
1	O	763	0	754	13	0
2	B	942	0	954	13	0
2	D	942	0	954	18	0
2	F	938	0	950	10	0
2	H	935	0	941	14	0
2	J	939	0	945	12	0
2	L	942	0	954	12	0
2	N	942	0	954	11	0
2	P	938	0	951	8	0
3	A	7	0	0	0	0
3	B	14	0	0	0	0
3	C	6	0	0	0	0
3	D	8	0	0	1	0
3	E	4	0	0	0	0
3	F	17	0	0	0	0
3	G	4	0	0	0	0
3	H	6	0	0	0	0
3	I	6	0	0	0	0
3	J	2	0	0	0	0
3	K	15	0	0	0	0
3	L	2	0	0	0	0
3	M	8	0	0	0	0
3	N	5	0	0	0	0
3	O	3	0	0	0	0
3	P	2	0	0	0	0
All	All	13795	0	13705	132	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 5.

All (132) 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)
2:H:28:PRO:HB2	2:H:31:TYR:HD2	1.40	0.87
2:H:28:PRO:HG2	2:H:31:TYR:CD2	2.14	0.83
2:H:28:PRO:HB2	2:H:31:TYR:CD2	2.17	0.80
2:N:141:ARG:O	2:N:143:PRO:HD3	1.85	0.76
2:L:28:PRO:HB2	2:L:31:TYR:CD2	2.24	0.72
1:E:36:GLN:HE21	2:F:116:THR:HG22	1.54	0.72
2:H:28:PRO:CB	2:H:31:TYR:CD2	2.74	0.71
1:C:95:ILE:HD12	1:I:24:PHE:HE2	1.57	0.68
2:D:42:VAL:HG22	2:D:108:ILE:HD12	1.74	0.68
2:N:28:PRO:HB2	2:N:31:TYR:CD2	2.29	0.67
2:J:66:LEU:HD21	2:J:82:LEU:HD22	1.77	0.67
2:B:58:PRO:HD2	2:B:61:ILE:HD12	1.77	0.67
2:B:138:GLU:OE1	2:B:141:ARG:NH2	2.28	0.67
2:J:56:LYS:HB3	2:J:135:THR:HG23	1.78	0.66
2:H:28:PRO:CG	2:H:31:TYR:CD2	2.80	0.64
2:D:28:PRO:HB2	2:D:31:TYR:CD2	2.33	0.64
2:L:28:PRO:HB2	2:L:31:TYR:HD2	1.60	0.63
2:L:71:LEU:HD12	2:L:80:VAL:HG11	1.82	0.62
2:P:45:LEU:HD21	2:P:52:LEU:HD13	1.82	0.62
2:N:28:PRO:HB2	2:N:31:TYR:HD2	1.65	0.60
1:I:52:ASN:HB3	1:I:55:LEU:H	1.67	0.59
2:B:28:PRO:HB2	2:B:31:TYR:CD2	2.38	0.59
1:I:13:GLN:HE21	1:I:15:ASP:H	1.51	0.59
2:N:58:PRO:HD2	2:N:61:ILE:HD12	1.84	0.59
2:D:141:ARG:O	2:D:143:PRO:HD3	2.02	0.59
2:N:71:LEU:HD23	2:N:80:VAL:HG21	1.84	0.59
2:N:42:VAL:O	2:N:45:LEU:HB2	2.02	0.59
2:D:142:ILE:HG13	2:F:133:VAL:HG11	1.85	0.59
2:F:71:LEU:HD23	2:F:80:VAL:HG21	1.84	0.58
1:G:13:GLN:HE21	1:G:15:ASP:H	1.51	0.58
2:L:58:PRO:HD2	2:L:61:ILE:HD12	1.86	0.58
1:C:13:GLN:HE21	1:C:15:ASP:H	1.52	0.58
1:K:78:LYS:HE3	2:N:51:GLU:HG3	1.85	0.58
2:D:112:LYS:O	2:D:113:LYS:HG3	2.02	0.58
2:D:113:LYS:HD3	2:D:115:GLU:OE2	2.03	0.57
2:L:44:GLU:HB3	2:L:50:LYS:HD2	1.85	0.57
2:H:58:PRO:HD2	2:H:61:ILE:HD12	1.85	0.57
1:O:36:GLN:HE21	2:P:116:THR:HG22	1.70	0.57
1:C:29:VAL:HB	2:D:119:VAL:HG21	1.86	0.56
2:L:91:GLN:HE22	2:L:132:ARG:HH11	1.53	0.56
2:P:58:PRO:HD2	2:P:61:ILE:HD12	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:58:PRO:HD2	2:F:61:ILE:HD12	1.86	0.56
1:E:13:GLN:HE21	1:E:15:ASP:H	1.54	0.56
1:K:13:GLN:HE21	1:K:15:ASP:H	1.54	0.56
2:D:43:SER:O	2:D:46:LYS:HG2	2.06	0.55
2:P:28:PRO:HB2	2:P:31:TYR:CD2	2.43	0.55
1:A:9:ILE:HD11	2:B:69:LEU:HG	1.88	0.54
1:O:13:GLN:HE21	1:O:15:ASP:H	1.53	0.53
1:M:43:GLN:HE22	1:M:70:GLN:HB3	1.73	0.53
2:L:46:LYS:HE3	2:L:123:LYS:HE3	1.91	0.53
1:C:18:VAL:HG12	2:D:108:ILE:HG22	1.91	0.53
1:G:23:PHE:HB2	1:G:27:VAL:HG11	1.91	0.53
2:D:28:PRO:HB2	2:D:31:TYR:HD2	1.74	0.53
2:D:58:PRO:HD2	2:D:61:ILE:HD12	1.91	0.52
2:J:46:LYS:HE2	2:J:122:SER:HA	1.91	0.52
1:A:22:ASN:HD22	1:O:92:THR:HG22	1.74	0.52
2:B:28:PRO:HB2	2:B:31:TYR:HD2	1.75	0.51
2:F:61:ILE:HD13	2:F:82:LEU:HD11	1.92	0.51
1:A:38:TYR:HB2	1:O:47:VAL:HG23	1.92	0.51
2:H:28:PRO:CB	2:H:31:TYR:HD2	2.13	0.51
1:E:52:ASN:HD21	1:G:30:PRO:HG2	1.76	0.50
1:K:31:LYS:NZ	2:L:125:ASN:OD1	2.45	0.50
1:K:29:VAL:HB	2:L:119:VAL:HG21	1.93	0.50
2:F:51:GLU:OE2	1:G:78:LYS:HE2	2.12	0.50
2:D:80:VAL:HG23	2:D:89:VAL:HG21	1.92	0.49
2:D:58:PRO:HD3	2:D:136:ILE:O	2.12	0.49
2:F:42:VAL:O	2:F:45:LEU:HB2	2.12	0.49
1:I:56:GLU:HG3	1:I:98:LYS:HD3	1.93	0.49
2:J:46:LYS:HD3	2:J:123:LYS:HG3	1.92	0.49
2:B:57:VAL:CG2	1:O:70:GLN:HG3	2.42	0.49
2:J:58:PRO:HD2	2:J:61:ILE:HD12	1.93	0.49
2:B:111:GLU:HB3	2:D:95:THR:HG21	1.94	0.49
2:P:82:LEU:HD12	2:P:87:PHE:CD2	2.48	0.49
2:B:27:PRO:O	2:B:28:PRO:O	2.30	0.49
1:E:30:PRO:HG2	1:G:52:ASN:HD21	1.77	0.49
2:L:141:ARG:O	2:L:143:PRO:HD3	2.13	0.49
2:H:141:ARG:O	2:H:143:PRO:HD3	2.13	0.49
1:C:56:GLU:HB2	1:C:96:VAL:HG13	1.95	0.49
1:A:38:TYR:HB2	1:O:47:VAL:CG2	2.43	0.48
2:F:58:PRO:HD3	2:F:136:ILE:O	2.14	0.47
2:H:28:PRO:HG2	2:H:31:TYR:CG	2.48	0.47
2:L:41:PRO:HG2	1:M:75:LEU:CD1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:LYS:HD3	1:C:42:LYS:HE3	1.97	0.47
3:D:9:HOH:O	1:I:41:ARG:HD3	2.15	0.47
2:P:28:PRO:HB2	2:P:31:TYR:HD2	1.79	0.47
1:A:51:GLU:HG3	1:A:56:GLU:HG2	1.95	0.47
1:G:36:GLN:HE21	2:H:116:THR:HG22	1.79	0.47
2:B:27:PRO:O	2:B:28:PRO:C	2.53	0.47
1:I:9:ILE:HD11	2:J:69:LEU:HG	1.96	0.46
2:J:28:PRO:HB2	2:J:31:TYR:CD2	2.51	0.46
2:B:41:PRO:HD3	1:O:86:TYR:OH	2.16	0.46
2:F:45:LEU:HD21	2:F:52:LEU:HD22	1.98	0.46
1:I:36:GLN:HE21	2:J:116:THR:HG22	1.80	0.46
1:C:71:TYR:HA	2:J:55:MSE:O	2.16	0.45
1:C:79:GLN:HB2	2:J:49:ASN:HD21	1.80	0.45
1:O:52:ASN:HB3	1:O:55:LEU:H	1.81	0.45
2:D:70:PRO:HD2	2:D:80:VAL:HG13	1.99	0.45
2:J:57:VAL:HG11	2:J:63:ILE:HD11	1.98	0.45
2:B:32:LYS:NZ	1:O:14:GLU:OE1	2.50	0.45
2:P:58:PRO:HD3	2:P:136:ILE:O	2.17	0.44
2:D:80:VAL:CG2	2:D:89:VAL:HG21	2.47	0.44
1:E:24:PHE:HE2	1:G:95:ILE:HD12	1.82	0.44
1:A:20:VAL:HB	1:O:90:VAL:HG22	2.00	0.44
2:B:54:LEU:O	2:B:133:VAL:HA	2.17	0.44
2:B:35:LYS:HG2	2:B:115:GLU:HG3	2.00	0.43
1:M:29:VAL:HB	2:N:119:VAL:HG21	1.99	0.43
1:C:95:ILE:HD12	1:I:24:PHE:CE2	2.45	0.43
2:H:61:ILE:HD13	2:H:82:LEU:HD11	2.00	0.43
2:D:76:THR:HG22	2:D:77:VAL:HG23	1.99	0.43
1:C:52:ASN:HB2	1:C:55:LEU:H	1.82	0.43
1:O:29:VAL:HB	2:P:119:VAL:HG21	2.00	0.43
1:E:29:VAL:HB	2:F:119:VAL:HG21	2.00	0.43
2:H:56:LYS:HB3	2:H:135:THR:HG23	2.01	0.42
1:A:92:THR:HG22	1:O:22:ASN:HD22	1.85	0.42
1:E:70:GLN:NE2	1:E:87:ARG:HH21	2.18	0.42
1:K:24:PHE:HE2	1:M:95:ILE:HD12	1.85	0.42
1:C:7:ILE:HD12	1:I:76:TYR:CE1	2.54	0.42
2:L:79:THR:HB	2:L:86:ASN:ND2	2.34	0.42
2:H:58:PRO:HD3	2:H:136:ILE:O	2.19	0.42
2:N:66:LEU:HD21	2:N:82:LEU:HD13	2.01	0.42
1:E:90:VAL:HG22	1:G:20:VAL:HB	2.01	0.41
1:O:75:LEU:HD12	1:O:75:LEU:HA	1.93	0.41
2:D:91:GLN:HG3	2:D:134:PHE:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:27:PRO:HB2	2:H:28:PRO:HD2	2.02	0.41
1:A:52:ASN:HD22	1:A:54:ARG:H	1.67	0.41
1:E:38:TYR:HB2	1:G:47:VAL:CG2	2.50	0.41
2:N:142:ILE:HD13	2:N:142:ILE:HA	1.93	0.41
1:E:52:ASN:HD22	1:E:55:LEU:HD12	1.86	0.40
1:I:18:VAL:HG12	2:J:108:ILE:HG22	2.02	0.40
2:N:115:GLU:HG3	2:N:116:THR:HG23	2.02	0.40
1:G:53:GLU:HG2	1:G:54:ARG:N	2.37	0.40
1:K:7:ILE:HD12	1:M:76:TYR:CE1	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	93/102 (91%)	90 (97%)	3 (3%)	0	100	100
1	C	93/102 (91%)	90 (97%)	3 (3%)	0	100	100
1	E	94/102 (92%)	92 (98%)	2 (2%)	0	100	100
1	G	93/102 (91%)	90 (97%)	3 (3%)	0	100	100
1	I	92/102 (90%)	89 (97%)	3 (3%)	0	100	100
1	K	93/102 (91%)	90 (97%)	3 (3%)	0	100	100
1	M	92/102 (90%)	89 (97%)	3 (3%)	0	100	100
1	O	92/102 (90%)	89 (97%)	3 (3%)	0	100	100
2	B	118/123 (96%)	111 (94%)	6 (5%)	1 (1%)	16	31
2	D	118/123 (96%)	113 (96%)	4 (3%)	1 (1%)	16	31
2	F	118/123 (96%)	109 (92%)	9 (8%)	0	100	100
2	H	118/123 (96%)	110 (93%)	7 (6%)	1 (1%)	16	31
2	J	118/123 (96%)	112 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	118/123 (96%)	108 (92%)	8 (7%)	2 (2%)	7	14
2	N	118/123 (96%)	115 (98%)	3 (2%)	0	100	100
2	P	117/123 (95%)	107 (92%)	10 (8%)	0	100	100
All	All	1685/1800 (94%)	1604 (95%)	76 (4%)	5 (0%)	37	56

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	28	PRO
2	H	123	LYS
2	D	46	LYS
2	L	46	LYS
2	L	48	ASP

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	88/92 (96%)	84 (96%)	4 (4%)	23	46
1	C	87/92 (95%)	83 (95%)	4 (5%)	23	45
1	E	88/92 (96%)	84 (96%)	4 (4%)	23	46
1	G	86/92 (94%)	83 (96%)	3 (4%)	31	57
1	I	86/92 (94%)	83 (96%)	3 (4%)	31	57
1	K	87/92 (95%)	82 (94%)	5 (6%)	17	35
1	M	87/92 (95%)	84 (97%)	3 (3%)	32	58
1	O	86/92 (94%)	82 (95%)	4 (5%)	22	44
2	B	112/112 (100%)	109 (97%)	3 (3%)	40	67
2	D	112/112 (100%)	109 (97%)	3 (3%)	40	67
2	F	111/112 (99%)	109 (98%)	2 (2%)	54	78
2	H	110/112 (98%)	107 (97%)	3 (3%)	40	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	J	111/112 (99%)	106 (96%)	5 (4%)	23	46
2	L	112/112 (100%)	107 (96%)	5 (4%)	23	46
2	N	112/112 (100%)	110 (98%)	2 (2%)	54	78
2	P	112/112 (100%)	108 (96%)	4 (4%)	30	56
All	All	1587/1632 (97%)	1530 (96%)	57 (4%)	30	56

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLU
1	A	47	VAL
1	A	66	THR
1	A	72	MSE
2	B	29	SER
2	B	78	SER
2	B	127	SER
1	C	14	GLU
1	C	72	MSE
1	C	75	LEU
1	C	92	THR
2	D	48	ASP
2	D	73	THR
2	D	127	SER
1	E	14	GLU
1	E	47	VAL
1	E	72	MSE
1	E	92	THR
2	F	97	GLU
2	F	127	SER
1	G	14	GLU
1	G	66	THR
1	G	72	MSE
2	H	93	THR
2	H	105	SER
2	H	135	THR
1	I	14	GLU
1	I	47	VAL
1	I	72	MSE
2	J	80	VAL
2	J	93	THR
2	J	105	SER

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Mol	Chain	Res	Type
2	J	127	SER
2	J	135	THR
1	K	14	GLU
1	K	32	ASP
1	K	43	GLN
1	K	66	THR
1	K	72	MSE
2	L	45	LEU
2	L	48	ASP
2	L	80	VAL
2	L	86	ASN
2	L	105	SER
1	M	14	GLU
1	M	72	MSE
1	M	87	ARG
2	N	93	THR
2	N	105	SER
1	O	14	GLU
1	O	66	THR
1	O	72	MSE
1	O	97	SER
2	P	84	SER
2	P	95	THR
2	P	96	GLN
2	P	105	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	C	13	GLN
1	C	36	GLN
1	C	84	ASN
2	D	92	ASN
1	E	13	GLN
1	E	36	GLN
1	E	52	ASN
1	E	70	GLN
2	F	92	ASN
1	G	13	GLN
1	G	36	GLN
1	G	84	ASN

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Mol	Chain	Res	Type
1	I	13	GLN
1	I	36	GLN
1	I	43	GLN
1	I	52	ASN
1	I	69	ASN
2	J	49	ASN
2	J	92	ASN
1	K	13	GLN
1	K	36	GLN
2	L	86	ASN
2	L	91	GLN
2	L	92	ASN
1	M	43	GLN
1	M	52	ASN
1	M	69	ASN
2	N	88	ASN
2	N	92	ASN
1	O	13	GLN
1	O	36	GLN

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 oligosaccharides 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, 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	93/102 (91%)	-0.10	1 (1%) 77 74	35, 74, 134, 155	1 (1%)
1	C	94/102 (92%)	0.06	0 100 100	48, 80, 122, 139	0
1	E	95/102 (93%)	-0.10	0 100 100	44, 72, 131, 168	0
1	G	94/102 (92%)	-0.05	2 (2%) 63 60	40, 75, 126, 139	0
1	I	93/102 (91%)	0.06	2 (2%) 62 59	43, 84, 121, 139	0
1	K	94/102 (92%)	-0.16	1 (1%) 77 74	41, 67, 126, 142	0
1	M	93/102 (91%)	-0.20	0 100 100	39, 67, 110, 135	0
1	O	93/102 (91%)	0.01	0 100 100	35, 75, 123, 142	0
2	B	119/123 (96%)	-0.13	1 (0%) 82 79	35, 64, 97, 130	0
2	D	119/123 (96%)	0.00	0 100 100	33, 77, 136, 156	0
2	F	119/123 (96%)	0.01	1 (0%) 82 79	39, 74, 112, 130	0
2	H	119/123 (96%)	0.66	9 (7%) 21 20	62, 111, 155, 164	0
2	J	119/123 (96%)	0.40	6 (5%) 35 32	60, 101, 152, 170	0
2	L	119/123 (96%)	-0.09	1 (0%) 82 79	38, 69, 124, 150	0
2	N	119/123 (96%)	0.16	1 (0%) 82 79	37, 82, 131, 142	0
2	P	118/123 (95%)	0.40	2 (1%) 69 65	46, 98, 151, 174	0
All	All	1700/1800 (94%)	0.07	27 (1%) 70 67	33, 81, 136, 174	1 (0%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	97	GLU	5.0
2	J	143	PRO	4.1
2	H	28	PRO	3.7
2	B	143	PRO	3.4
2	P	112	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	K	99	PHE	2.9
2	H	143	PRO	2.8
2	J	102	THR	2.7
2	F	143	PRO	2.7
2	H	82	LEU	2.7
2	J	82	LEU	2.6
2	H	128	VAL	2.6
1	I	27	VAL	2.6
2	N	112	LYS	2.5
2	H	40	PHE	2.4
2	J	100	ASP	2.4
2	H	129	TYR	2.3
2	H	61	ILE	2.3
2	H	29	SER	2.2
1	A	55	LEU	2.2
1	I	24	PHE	2.2
1	G	24	PHE	2.1
2	J	46	LYS	2.1
2	P	71	LEU	2.1
2	L	112	LYS	2.1
2	J	42	VAL	2.0
1	G	99	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 monosaccharides 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.