



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:53 AM GMT

PDB ID : 3NFF
Title : Crystal structure of extended Dimerization module of RNA polymerase I sub-complex A49/A34.5
Authors : Geiger, S.R.; Lorenzen, K.; Schrieck, A.; Hanecker, P.; Kostrewa, D.; Heck, A.J.R.; Cramer, P.
Deposited on : 2010-06-10
Resolution : 3.24 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

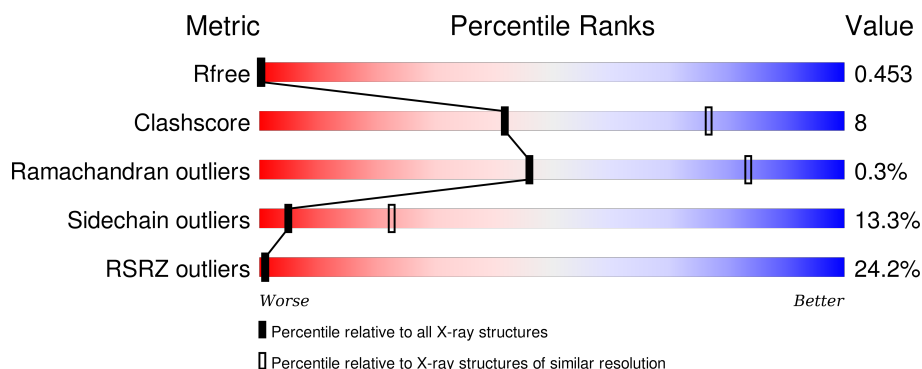
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.24 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	1092 (3.28-3.20)
Clashscore	102246	1227 (3.28-3.20)
Ramachandran outliers	100387	1204 (3.28-3.20)
Sidechain outliers	100360	1203 (3.28-3.20)
RSRZ outliers	91569	1097 (3.28-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	122	<div> <div>22%</div> <div>57%</div> <div>22%</div> <div>19%</div> </div>
1	C	122	<div> <div>19%</div> <div>66%</div> <div>9%</div> <div>24%</div> </div>
1	E	122	<div> <div>13%</div> <div>57%</div> <div>18%</div> <div>24%</div> </div>
1	G	122	<div> <div>33%</div> <div>62%</div> <div>13%</div> <div>24%</div> </div>
2	B	121	<div> <div>16%</div> <div>57%</div> <div>28%</div> <div>5%</div> <div>9%</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	121	<div><div></div><div>17%</div><div>59%</div><div>28%</div><div>•</div><div>9%</div></div>
2	F	121	<div><div></div><div>36%</div><div>68%</div><div>21%</div><div>•</div><div>9%</div></div>
2	H	121	<div><div></div><div>7%</div><div>45%</div><div>37%</div><div>8%</div><div>•</div><div>8%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6539 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 RNA polymerase I subunit A49.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	99	Total	C	N	O	S	0	1	0
			805	511	135	158	1			
1	C	93	Total	C	N	O	S	0	1	0
			759	481	127	150	1			
1	E	93	Total	C	N	O	S	0	1	0
			759	481	127	150	1			
1	G	93	Total	C	N	O	S	0	1	0
			759	481	127	150	1			

There are 16 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	MET	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	MET	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	MET	VAL	ENGINEERED MUTATION	UNP Q6FNZ9
G	-2	GLY	-	EXPRESSION TAG	UNP Q6FNZ9
G	-1	SER	-	EXPRESSION TAG	UNP Q6FNZ9
G	0	HIS	-	EXPRESSION TAG	UNP Q6FNZ9
G	72	MET	VAL	ENGINEERED MUTATION	UNP Q6FNZ9

- Molecule 2 is a protein called RNA polymerase I subunit A34.5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	110	Total 863	C 546	N 140	O 175	S 2	0	0	0
2	D	110	Total 863	C 546	N 140	O 175	S 2	0	0	0
2	F	110	Total 863	C 546	N 140	O 175	S 2	0	0	0
2	H	111	Total 868	C 549	N 141	O 176	S 2	0	0	0

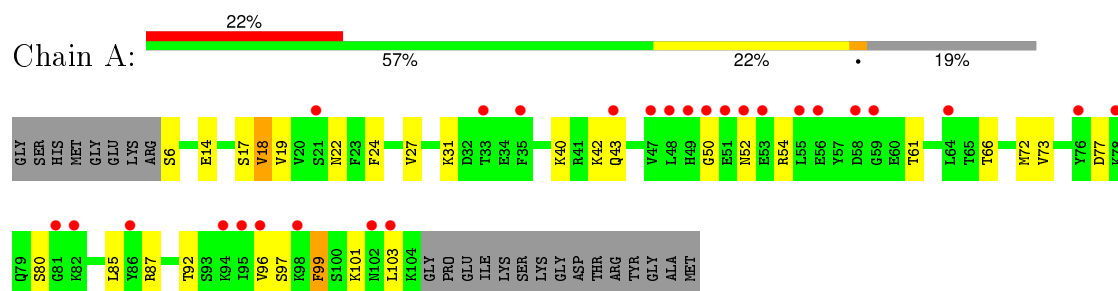
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	23	MET	-	EXPRESSION TAG	UNP Q6FQI3
B	24	GLY	-	EXPRESSION TAG	UNP Q6FQI3
B	55	MET	LEU	ENGINEERED MUTATION	UNP Q6FQI3
D	23	MET	-	EXPRESSION TAG	UNP Q6FQI3
D	24	GLY	-	EXPRESSION TAG	UNP Q6FQI3
D	55	MET	LEU	ENGINEERED MUTATION	UNP Q6FQI3
F	23	MET	-	EXPRESSION TAG	UNP Q6FQI3
F	24	GLY	-	EXPRESSION TAG	UNP Q6FQI3
F	55	MET	LEU	ENGINEERED MUTATION	UNP Q6FQI3
H	23	MET	-	EXPRESSION TAG	UNP Q6FQI3
H	24	GLY	-	EXPRESSION TAG	UNP Q6FQI3
H	55	MET	LEU	ENGINEERED MUTATION	UNP Q6FQI3

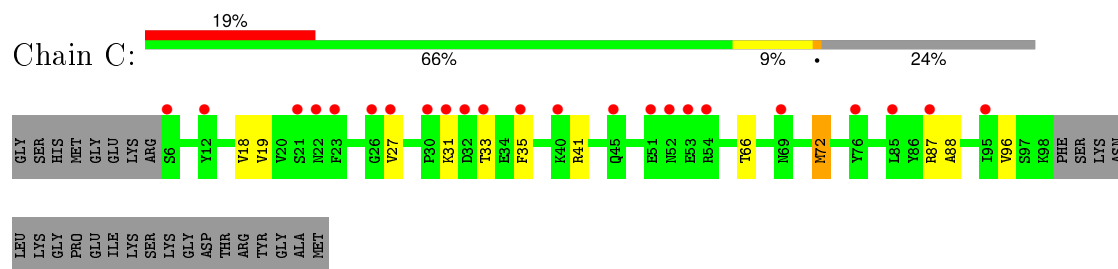
3 Residue-property plots [i](#)

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

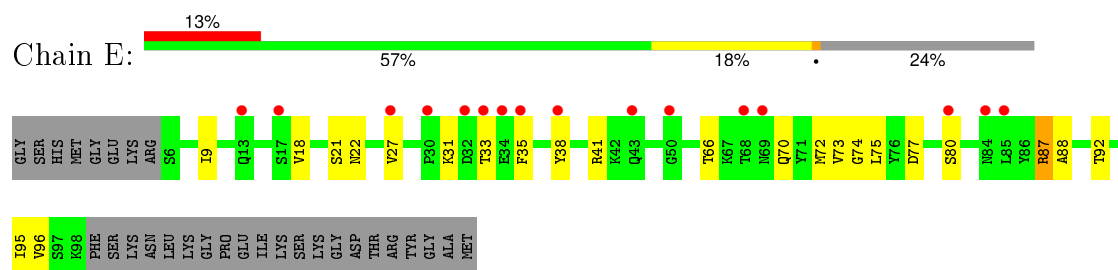
- Molecule 1: RNA polymerase I subunit A49



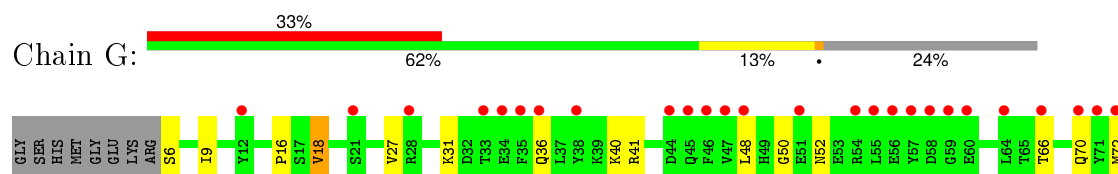
- Molecule 1: RNA polymerase I subunit A49

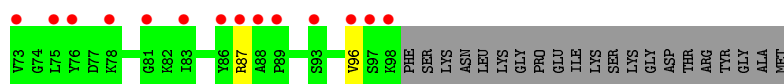


- Molecule 1: RNA polymerase I subunit A49

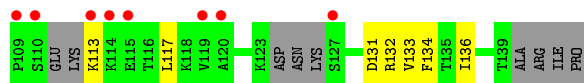


- Molecule 1: RNA polymerase I subunit A49

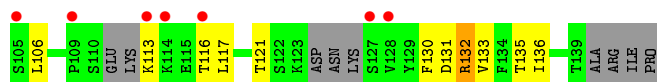




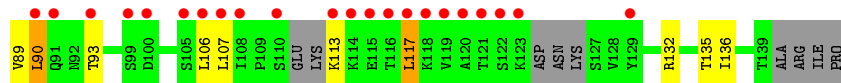
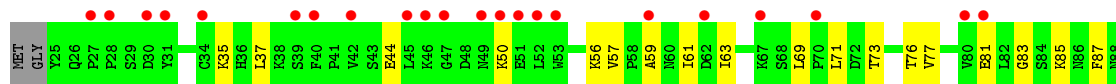
• Molecule 2: RNA polymerase I subunit A34.5



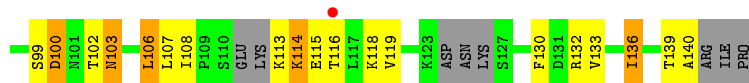
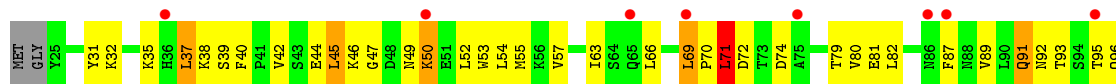
• Molecule 2: RNA polymerase I subunit A34.5



• Molecule 2: RNA polymerase I subunit A34.5



• Molecule 2: RNA polymerase I subunit A34.5



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	108.93Å 221.77Å 129.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.10 – 3.24 77.97 – 3.24	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.10-3.24) 95.7 (77.97-3.24)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	0.21	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 3.26Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, R_{free}	0.287 , 0.361 0.358 , 0.453	Depositor DCC
R_{free} test set	1233 reflections (5.09%)	DCC
Wilson B-factor (Å ²)	103.8	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 198.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Outliers	0 of 24236 reflections	Xtriage
F_o, F_c correlation	0.72	EDS
Total number of atoms	6539	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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	0.50	0/825	1.00	6/1110 (0.5%)
1	C	0.47	0/778	0.75	1/1048 (0.1%)
1	E	0.47	0/778	0.68	0/1048
1	G	0.41	0/778	0.73	0/1048
2	B	0.56	0/876	0.88	2/1184 (0.2%)
2	D	0.55	0/876	0.83	1/1184 (0.1%)
2	F	0.49	0/876	0.78	1/1184 (0.1%)
2	H	0.59	0/881	1.04	6/1191 (0.5%)
All	All	0.51	0/6668	0.85	17/8997 (0.2%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	99	PHE	CB-CA-C	-11.41	87.57	110.40
1	A	42	LYS	CB-CA-C	-11.27	87.87	110.40
1	A	97	SER	CB-CA-C	9.53	128.21	110.10
2	H	46	LYS	CB-CA-C	-8.47	93.46	110.40
1	A	42	LYS	N-CA-C	-8.18	88.91	111.00
2	H	96	GLN	N-CA-CB	-7.54	97.02	110.60
2	F	56	LYS	N-CA-C	-7.16	91.68	111.00
2	H	114	LYS	N-CA-C	6.89	129.60	111.00
2	H	71	LEU	CB-CA-C	-6.50	97.84	110.20
1	A	97	SER	N-CA-C	-6.44	93.62	111.00
1	C	72	MET	N-CA-C	6.42	128.32	111.00
1	A	43	GLN	N-CA-CB	-6.01	99.79	110.60
2	B	91	GLN	N-CA-C	-5.66	95.71	111.00
2	H	115	GLU	N-CA-CB	-5.32	101.02	110.60
2	D	121	THR	CB-CA-C	-5.08	97.88	111.60
2	H	139	THR	N-CA-C	5.05	124.63	111.00
2	B	96	GLN	N-CA-CB	-5.02	101.57	110.60

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	805	0	799	17	0
1	C	759	0	754	11	0
1	E	759	0	754	16	0
1	G	759	0	754	16	0
2	B	863	0	871	22	0
2	D	863	0	871	26	0
2	F	863	0	871	16	0
2	H	868	0	876	32	0
All	All	6539	0	6550	110	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 8.

All (110) 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:D:63:ILE:HG13	1:C:72:MET:CE	1.63	1.28
2:B:95:THR:O	2:B:99:SER:HB2	1.58	1.01
2:D:63:ILE:HG13	1:C:72:MET:HE1	1.01	1.00
2:F:57:VAL:HG21	1:G:72:MET:CE	1.92	0.98
2:D:63:ILE:CG1	1:C:72:MET:HE1	1.95	0.97
2:H:42:VAL:HG13	2:H:45:LEU:HD12	1.46	0.94
1:A:73:VAL:HG11	2:B:106:LEU:HD11	1.54	0.89
2:D:93:THR:HG21	2:D:132:ARG:HA	1.59	0.83
2:F:57:VAL:CG2	1:G:72:MET:CE	2.57	0.82
2:H:93:THR:HG21	2:H:132:ARG:HA	1.60	0.81
2:B:95:THR:O	2:B:99:SER:CB	2.30	0.78
2:D:57:VAL:HG22	2:D:136:ILE:HD13	1.65	0.78
2:D:63:ILE:HG13	1:C:72:MET:HE3	1.65	0.76
2:H:91:GLN:O	2:H:95:THR:HG23	1.87	0.75
2:H:37:LEU:HB2	2:H:114:LYS:O	1.90	0.71
2:F:57:VAL:HG21	1:G:72:MET:HE1	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:63:ILE:CG1	1:C:72:MET:CE	2.58	0.66
2:B:92:ASN:HD21	2:B:133:VAL:HB	1.61	0.66
2:B:54:LEU:HB3	2:B:133:VAL:HG13	1.79	0.65
1:A:19:VAL:HB	2:H:107:LEU:HD12	1.80	0.64
2:D:92:ASN:HB3	2:D:98:GLY:HA3	1.82	0.62
2:F:57:VAL:HG21	1:G:72:MET:HE3	1.76	0.61
1:A:52:ASN:HB3	1:E:33:THR:HA	1.82	0.61
2:D:57:VAL:CG2	2:D:136:ILE:HD13	2.31	0.60
2:F:57:VAL:CG2	1:G:72:MET:HE2	2.31	0.60
1:A:72:MET:HG2	1:A:85:LEU:HD22	1.83	0.60
1:A:40:LYS:HB2	2:H:31:TYR:CE1	2.37	0.59
2:B:101:ASN:HB3	2:B:104:LEU:HD12	1.85	0.57
2:B:92:ASN:ND2	2:B:133:VAL:HB	2.19	0.57
2:B:55:MET:HB3	2:B:57:VAL:HG23	1.85	0.57
2:H:42:VAL:HG21	2:H:108:ILE:HD13	1.87	0.57
2:B:66:LEU:HD21	2:B:82:LEU:HB3	1.85	0.57
1:C:88:ALA:HB2	1:G:18:VAL:HG13	1.88	0.56
1:C:35:PHE:HA	1:G:50:GLY:HA2	1.87	0.56
2:F:135:THR:HG21	2:H:140:ALA:O	2.05	0.56
1:C:33:THR:HA	1:G:52:ASN:HB3	1.86	0.56
2:D:116:THR:HG22	1:G:36:GLN:HG3	1.89	0.55
2:H:113:LYS:HD2	2:H:116:THR:HG21	1.88	0.55
2:B:80:VAL:O	2:B:87:PHE:HB2	2.07	0.54
2:B:91:GLN:HG2	2:B:134:PHE:CE1	2.43	0.54
2:B:91:GLN:HG2	2:B:134:PHE:HE1	1.71	0.54
1:A:24:PHE:O	2:H:103:ASN:HA	2.08	0.54
1:E:73:VAL:HG11	2:H:106:LEU:HD11	1.90	0.53
1:A:22:ASN:HD22	1:E:92:THR:HG22	1.74	0.52
2:D:31:TYR:CE1	1:G:40:LYS:HB2	2.45	0.52
1:A:73:VAL:HG11	2:B:106:LEU:CD1	2.33	0.51
2:D:70:PRO:HG3	1:G:6:SER:HB2	1.93	0.51
2:F:61:ILE:HD11	2:F:87:PHE:CE1	2.45	0.51
1:A:72:MET:HE1	2:B:63:ILE:HG13	1.92	0.50
2:D:136:ILE:H	2:D:136:ILE:HD12	1.76	0.50
2:D:55:MET:HB2	1:C:72:MET:HB2	1.94	0.50
1:E:73:VAL:HG11	2:H:106:LEU:CD1	2.41	0.49
2:H:106:LEU:O	2:H:119:VAL:HA	2.12	0.49
2:D:53:TRP:HZ3	2:D:71:LEU:HD13	1.77	0.49
2:B:55:MET:HG2	2:B:134:PHE:HB2	1.94	0.49
2:D:37:LEU:HD23	1:G:16:PRO:O	2.12	0.49
1:A:17:SER:HB3	2:H:38:LYS:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:PHE:HB3	1:A:103:LEU:HD13	1.94	0.49
2:H:91:GLN:O	2:H:95:THR:CG2	2.59	0.48
2:B:103:ASN:O	1:E:21:SER:O	2.31	0.48
2:F:89:VAL:HG22	2:F:136:ILE:HG13	1.95	0.48
2:H:49:ASN:HB3	2:H:50:LYS:HZ2	1.79	0.48
2:H:40:PHE:HB3	2:H:108:ILE:HG22	1.96	0.47
2:D:75:ALA:O	2:D:91:GLN:NE2	2.47	0.47
2:H:39:SER:HB3	2:H:114:LYS:HE2	1.97	0.47
2:H:100:ASP:OD1	2:H:102:THR:HG23	2.14	0.47
2:F:73:THR:HB	2:F:132:ARG:HH11	1.80	0.47
2:H:52:LEU:HD23	2:H:130:PHE:HA	1.96	0.46
2:B:52:LEU:HB3	2:B:131:ASP:H	1.80	0.46
2:F:44:GLU:HB3	2:F:50:LYS:HG3	1.98	0.46
2:F:107:LEU:HB3	2:F:117:LEU:HD22	1.98	0.46
2:F:59:ALA:HA	1:G:70:GLN:HE21	1.81	0.45
2:H:69:LEU:HD22	2:H:71:LEU:HD11	1.98	0.45
2:D:55:MET:HB3	2:D:57:VAL:HG23	1.97	0.45
2:F:57:VAL:HG23	1:G:72:MET:HE2	1.98	0.45
1:A:50:GLY:HA2	1:E:35:PHE:HA	1.99	0.45
2:B:31:TYR:HD1	1:E:38:TYR:O	1.99	0.45
2:D:92:ASN:O	2:D:98:GLY:HA3	2.17	0.45
2:H:108:ILE:N	2:H:118:LYS:O	2.47	0.44
2:F:87:PHE:HB3	2:F:136:ILE:HG23	1.98	0.44
2:D:85:LYS:HD2	2:D:87:PHE:CZ	2.53	0.44
1:E:75:LEU:HD13	2:H:44:GLU:HG3	2.00	0.43
2:B:58:PRO:HD3	2:B:136:ILE:O	2.18	0.43
1:E:70:GLN:N	2:H:57:VAL:O	2.52	0.43
1:C:19:VAL:HG11	1:G:48:LEU:HD13	2.00	0.43
1:E:72:MET:HG2	1:E:87:ARG:HA	2.00	0.43
2:H:89:VAL:HA	2:H:136:ILE:HG23	2.01	0.43
2:D:69:LEU:HB2	1:G:9:ILE:HD11	1.99	0.43
2:F:77:VAL:HG22	2:F:90:LEU:HA	2.00	0.43
2:H:87:PHE:HB3	2:H:136:ILE:HG22	2.00	0.43
2:D:136:ILE:N	2:D:136:ILE:HD12	2.35	0.42
1:A:6:SER:HB2	2:H:70:PRO:HB3	2.01	0.42
2:B:42:VAL:HA	2:B:45:LEU:HD12	2.02	0.42
2:D:44:GLU:HB3	2:D:50:LYS:HG3	2.02	0.42
1:A:92:THR:HG22	1:E:22:ASN:HD22	1.84	0.41
2:B:73:THR:HA	2:B:91:GLN:HE21	1.85	0.41
2:H:45:LEU:HD21	2:H:52:LEU:HD13	2.03	0.41
2:D:92:ASN:HB2	2:D:133:VAL:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:66:LEU:HD21	2:H:82:LEU:HB3	2.03	0.41
2:D:63:ILE:CG1	1:C:72:MET:HE3	2.42	0.41
2:B:68:SER:HA	1:E:9:ILE:H	1.85	0.41
1:A:24:PHE:HE2	1:E:95:ILE:HD12	1.86	0.41
1:A:77:ASP:HB3	1:A:80:SER:OG	2.21	0.41
2:D:51:GLU:OE1	2:D:131:ASP:HB2	2.21	0.40
1:E:74:GLY:O	2:H:53:TRP:N	2.50	0.40
1:E:77:ASP:HB3	1:E:80:SER:OG	2.21	0.40
2:F:93:THR:HG21	2:F:132:ARG:HA	2.02	0.40
2:H:80:VAL:HG12	2:H:87:PHE:HB2	2.03	0.40
1:A:18:VAL:HG13	1:E:88:ALA:HB2	2.03	0.40
2:H:54:LEU:HB3	2:H:133:VAL:HG13	2.02	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	98/122 (80%)	87 (89%)	11 (11%)	0	100	100
1	C	92/122 (75%)	83 (90%)	9 (10%)	0	100	100
1	E	92/122 (75%)	86 (94%)	6 (6%)	0	100	100
1	G	92/122 (75%)	85 (92%)	7 (8%)	0	100	100
2	B	104/121 (86%)	89 (86%)	15 (14%)	0	100	100
2	D	104/121 (86%)	83 (80%)	21 (20%)	0	100	100
2	F	104/121 (86%)	89 (86%)	14 (14%)	1 (1%)	19	62
2	H	105/121 (87%)	86 (82%)	18 (17%)	1 (1%)	19	62
All	All	791/972 (81%)	688 (87%)	101 (13%)	2 (0%)	46	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	83	GLY
2	H	47	GLY

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	92/109 (84%)	82 (89%)	10 (11%)	8	33
1	C	87/109 (80%)	80 (92%)	7 (8%)	15	51
1	E	87/109 (80%)	80 (92%)	7 (8%)	15	51
1	G	87/109 (80%)	80 (92%)	7 (8%)	15	51
2	B	104/113 (92%)	84 (81%)	20 (19%)	2	9
2	D	104/113 (92%)	85 (82%)	19 (18%)	2	10
2	F	104/113 (92%)	92 (88%)	12 (12%)	7	30
2	H	104/113 (92%)	84 (81%)	20 (19%)	2	9
All	All	769/888 (87%)	667 (87%)	102 (13%)	5	22

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLU
1	A	18	VAL
1	A	27	VAL
1	A	31	LYS
1	A	54	ARG
1	A	61	THR
1	A	66	THR
1	A	87	ARG
1	A	96	VAL
1	A	101	LYS
2	B	30	ASP
2	B	37	LEU
2	B	63	ILE
2	B	69	LEU

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Mol	Chain	Res	Type
2	B	71	LEU
2	B	74	ASP
2	B	79	THR
2	B	80	VAL
2	B	81	GLU
2	B	88	ASN
2	B	91	GLN
2	B	92	ASN
2	B	94	SER
2	B	101	ASN
2	B	103	ASN
2	B	106	LEU
2	B	108	ILE
2	B	113	LYS
2	B	117	LEU
2	B	132	ARG
2	D	35	LYS
2	D	37	LEU
2	D	63	ILE
2	D	69	LEU
2	D	71	LEU
2	D	76	THR
2	D	79	THR
2	D	81	GLU
2	D	95	THR
2	D	99	SER
2	D	100	ASP
2	D	102	THR
2	D	103	ASN
2	D	106	LEU
2	D	113	LYS
2	D	117	LEU
2	D	130	PHE
2	D	132	ARG
2	D	135	THR
1	C	18	VAL
1	C	27	VAL
1	C	31	LYS
1	C	41	ARG
1	C	66	THR
1	C	87	ARG
1	C	96	VAL

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Mol	Chain	Res	Type
2	F	35	LYS
2	F	37	LEU
2	F	63	ILE
2	F	69	LEU
2	F	71	LEU
2	F	76	THR
2	F	81	GLU
2	F	85	LYS
2	F	90	LEU
2	F	106	LEU
2	F	113	LYS
2	F	117	LEU
1	E	18	VAL
1	E	27	VAL
1	E	31	LYS
1	E	41	ARG
1	E	66	THR
1	E	87	ARG
1	E	96	VAL
2	H	32	LYS
2	H	35	LYS
2	H	37	LEU
2	H	45	LEU
2	H	50	LYS
2	H	55	MET
2	H	63	ILE
2	H	69	LEU
2	H	71	LEU
2	H	72	ASP
2	H	74	ASP
2	H	79	THR
2	H	81	GLU
2	H	91	GLN
2	H	92	ASN
2	H	99	SER
2	H	100	ASP
2	H	103	ASN
2	H	106	LEU
2	H	136	ILE
1	G	18	VAL
1	G	27	VAL
1	G	31	LYS

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Mol	Chain	Res	Type
1	G	41	ARG
1	G	66	THR
1	G	87	ARG
1	G	96	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	84	ASN
2	B	91	GLN
2	B	92	ASN
2	D	88	ASN
2	D	91	GLN
2	D	92	ASN
2	D	101	ASN
1	C	43	GLN
1	E	43	GLN
1	E	84	ASN
2	H	91	GLN
1	G	43	GLN

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

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	99/122 (81%)	1.44	27 (27%) 1 1	57, 99, 151, 186	1 (1%)
1	C	93/122 (76%)	1.41	23 (24%) 1 1	61, 118, 174, 186	1 (1%)
1	E	93/122 (76%)	1.07	16 (17%) 2 2	39, 87, 146, 152	1 (1%)
1	G	93/122 (76%)	2.26	40 (43%) 0 0	87, 148, 194, 207	1 (1%)
2	B	110/121 (90%)	1.11	19 (17%) 2 1	42, 89, 150, 172	0
2	D	110/121 (90%)	1.22	20 (18%) 2 1	59, 106, 157, 178	0
2	F	110/121 (90%)	2.11	44 (40%) 0 0	61, 143, 225, 265	0
2	H	111/121 (91%)	0.78	9 (8%) 15 9	39, 89, 120, 134	0
All	All	819/972 (84%)	1.41	198 (24%) 1 1	39, 109, 177, 265	4 (0%)

All (198) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	59	GLY	14.3
1	G	47	VAL	10.8
2	F	116	THR	10.6
1	G	55	LEU	10.2
2	H	75	ALA	10.0
2	F	123	LYS	9.7
2	F	31	TYR	8.7
1	G	56	GLU	8.4
2	D	50	LYS	7.5
2	F	121	THR	7.3
2	B	113	LYS	6.9
2	F	52	LEU	6.6
1	G	66	THR	6.3
2	F	114	LYS	6.1
2	F	122	SER	6.0
2	D	127	SER	5.9

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Mol	Chain	Res	Type	RSRZ
1	A	48	LEU	5.9
2	H	69	LEU	5.7
1	A	78	LYS	5.6
2	F	115	GLU	5.6
1	A	81	GLY	5.6
2	B	110	SER	5.5
2	F	34	CYS	5.5
2	F	113	LYS	5.4
2	B	119	VAL	5.4
1	G	38	TYR	5.3
1	A	98	LYS	5.2
2	F	110	SER	5.1
1	E	80	SER	5.1
1	E	38	TYR	5.0
2	F	45	LEU	5.0
1	E	33	THR	4.9
2	F	27	PRO	4.9
1	C	52	ASN	4.9
2	F	49	ASN	4.9
2	F	105	SER	4.8
1	C	54	ARG	4.8
2	D	49	ASN	4.8
2	F	118	LYS	4.8
2	F	51	GLU	4.7
1	G	97	SER	4.7
2	B	45	LEU	4.7
2	F	47	GLY	4.7
2	F	50	LYS	4.6
2	B	31	TYR	4.5
1	G	54	ARG	4.5
1	A	56	GLU	4.5
1	G	58	ASP	4.5
2	F	117	LEU	4.4
1	G	71	TYR	4.4
1	C	6	SER	4.4
1	G	48	LEU	4.4
2	B	25	TYR	4.3
1	A	49	HIS	4.3
1	G	96	VAL	4.3
2	B	43	SER	4.3
1	G	93	SER	4.3
1	C	51	GLU	4.3

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Mol	Chain	Res	Type	RSRZ
1	G	98	LYS	4.2
1	G	33	THR	4.1
2	F	53	TRP	4.1
1	A	47	VAL	4.0
1	C	32	ASP	4.0
1	G	60	GLU	3.9
1	G	83	ILE	3.9
1	G	45	GLN	3.9
1	C	76	TYR	3.8
1	G	57	TYR	3.8
2	F	70	PRO	3.7
1	A	55	LEU	3.7
1	A	50	GLY	3.7
1	G	86	TYR	3.7
1	G	28	ARG	3.7
2	F	81	GLU	3.6
1	G	21	SER	3.6
2	D	45	LEU	3.6
1	G	73	VAL	3.5
1	C	69	ASN	3.5
2	D	46	LYS	3.5
1	C	27	VAL	3.5
1	A	64	LEU	3.5
2	F	28	PRO	3.4
2	D	116	THR	3.4
1	G	70	GLN	3.4
1	C	95	ILE	3.3
2	D	30	ASP	3.3
1	A	53	GLU	3.3
1	G	75	LEU	3.3
1	E	30	PRO	3.3
1	G	72	MET	3.3
1	E	34	GLU	3.3
2	F	80	VAL	3.2
1	E	32	ASP	3.2
2	B	37	LEU	3.1
2	F	106	LEU	3.1
2	F	93	THR	3.1
1	A	43	GLN	3.1
1	A	33	THR	3.1
1	E	17	SER	3.1
1	G	78	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	67	LYS	3.0
2	F	62	ASP	3.0
2	F	39	SER	3.0
1	C	21	SER	3.0
2	F	67	LYS	3.0
2	H	86	ASN	3.0
1	C	26	GLY	3.0
1	C	53	GLU	3.0
1	C	30	PRO	3.0
1	A	51	GLU	3.0
1	A	102	ASN	3.0
1	G	35	PHE	3.0
2	B	114	LYS	2.9
2	B	120	ALA	2.9
1	E	13	GLN	2.9
1	A	21	SER	2.9
1	A	86	TYR	2.9
2	D	75	ALA	2.8
2	D	128	VAL	2.8
2	F	107	LEU	2.8
2	D	113	LYS	2.7
2	F	40	PHE	2.7
2	D	102	THR	2.7
1	A	76	TYR	2.7
1	A	96	VAL	2.7
2	H	65	GLN	2.6
2	F	46	LYS	2.6
1	A	52	ASN	2.6
1	G	87	ARG	2.6
1	E	50	GLY	2.6
1	G	46	PHE	2.6
2	F	30	ASP	2.5
1	G	36	GLN	2.5
1	C	85	LEU	2.5
1	E	27	VAL	2.5
2	D	33	GLN	2.5
2	B	115	GLU	2.5
2	F	90	LEU	2.5
1	A	35	PHE	2.5
2	H	87	PHE	2.5
2	B	127	SER	2.5
2	D	79	THR	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	68	SER	2.4
2	F	108	ILE	2.4
1	C	22	ASN	2.4
1	G	88	ALA	2.4
2	B	93	THR	2.4
2	H	116	THR	2.4
1	C	12	TYR	2.4
1	C	31	LYS	2.4
2	B	38	LYS	2.4
1	G	44	ASP	2.4
1	A	82	LYS	2.4
2	F	91	GLN	2.4
1	C	33	THR	2.4
1	G	64	LEU	2.4
2	B	109	PRO	2.4
1	A	58	ASP	2.3
1	A	94	LYS	2.3
2	F	119	VAL	2.3
2	F	129	TYR	2.3
1	E	68	THR	2.3
1	A	95	ILE	2.3
1	G	34	GLU	2.3
2	D	105	SER	2.3
1	A	59	GLY	2.3
2	B	53	TRP	2.3
1	G	81	GLY	2.3
1	E	35	PHE	2.2
1	E	85	LEU	2.2
2	H	50	LYS	2.2
2	H	95	THR	2.2
1	C	23	PHE	2.2
1	C	40	LYS	2.2
2	F	99	SER	2.2
2	F	100	ASP	2.2
2	D	47	GLY	2.1
1	E	69	ASN	2.1
2	F	120	ALA	2.1
1	E	84	ASN	2.1
1	G	51	GLU	2.1
2	D	114	LYS	2.1
1	A	103	LEU	2.1
1	C	35	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	87	ARG	2.1
1	G	76	TYR	2.1
2	H	36	HIS	2.1
1	E	43	GLN	2.1
2	D	87	PHE	2.1
2	F	59	ALA	2.1
2	B	108	ILE	2.1
1	G	12	TYR	2.1
2	D	109	PRO	2.1
2	B	63	ILE	2.0
2	F	42	VAL	2.0
2	B	52	LEU	2.0
1	G	89	PRO	2.0
1	C	45	GLN	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.