



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:09 PM GMT

PDB ID : 1NOZ
Title : T4 DNA POLYMERASE FRAGMENT (RESIDUES 1-388) AT 110K
Authors : Wang, J.; Yu, P.; Lin, T.C.; Konigsberg, W.H.; Steitz, T.A.
Deposited on : 1996-02-16
Resolution : 2.20 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

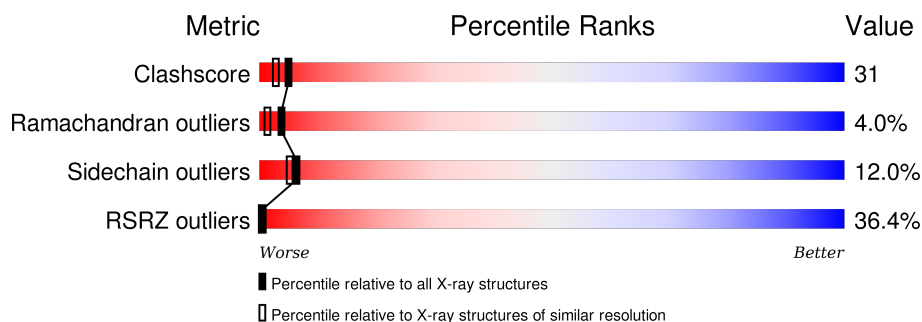
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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))
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	388	
1	B	388	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5725 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 POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	346	Total	C	N	O	S	0	0	0
			2840	1822	466	533	19			
1	B	346	Total	C	N	O	S	0	0	0
			2840	1822	466	533	19			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ASP	LYS	CONFLICT	UNP P04415
A	250	LEU	ILE	CONFLICT	UNP P04415
B	2	ASP	LYS	CONFLICT	UNP P04415
B	250	LEU	ILE	CONFLICT	UNP P04415

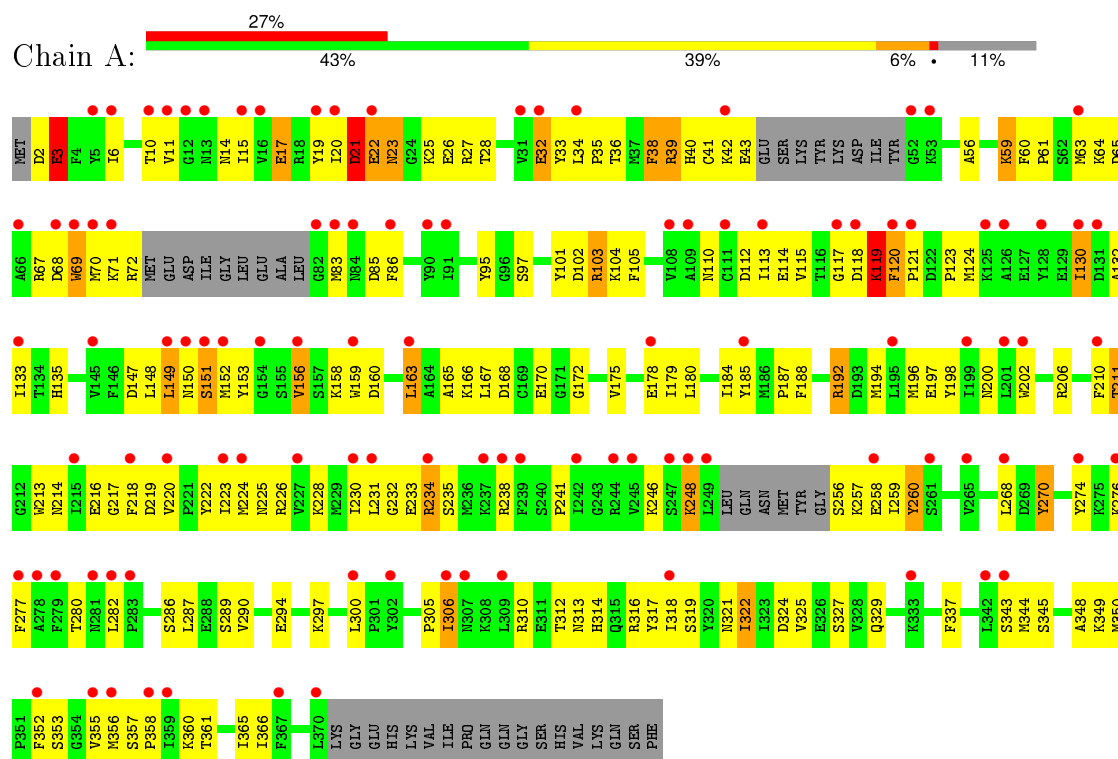
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	34	Total	O	0	0
			34	34		
2	B	11	Total	O	0	0
			11	11		

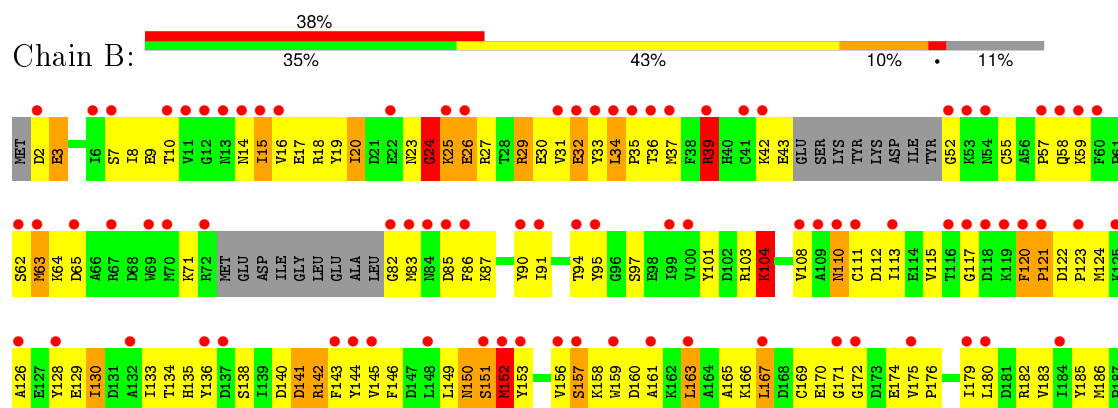
3 Residue-property plots

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: DNA POLYMERASE



• Molecule 1: DNA POLYMERASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	113.62Å 109.31Å 68.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.20 58.09 – 2.72	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-2.20) 82.2 (58.09-2.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 2.73Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.222 , (Not available) (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å ²)	44.9	Xtriage
Anisotropy	0.487	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 92.8	EDS
Estimated twinning fraction	0.017 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 20521 reflections	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	5725	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 9.11% 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 [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	0.65	0/2904	0.85	2/3911 (0.1%)
1	B	0.59	0/2904	0.89	3/3911 (0.1%)
All	All	0.62	0/5808	0.87	5/7822 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	24	GLY	N-CA-C	6.41	129.13	113.10
1	A	32	GLU	N-CA-C	-6.15	94.39	111.00
1	B	280	THR	N-CA-C	6.13	127.56	111.00
1	B	29	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	A	38	PHE	N-CA-C	5.73	126.46	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2840	0	2783	151	0
1	B	2840	0	2783	210	0
2	A	34	0	0	2	0
2	B	11	0	0	1	0
All	All	5725	0	5566	350	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 31.

All (350) 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:B:169:CYS:SG	1:B:170:GLU:HG3	2.05	0.97
1:A:114:GLU:HB2	1:A:132:ALA:HB3	1.53	0.88
1:B:179:ILE:HG22	1:B:322:ILE:HD11	1.62	0.82
1:A:67:ARG:O	1:A:71:LYS:HG2	1.81	0.81
1:B:10:THR:HG23	1:B:14:ASN:O	1.81	0.79
1:B:19:TYR:CE1	1:B:29:ARG:HG3	2.17	0.79
1:A:160:ASP:OD2	1:A:163:LEU:HB2	1.82	0.79
1:B:17:GLU:OE1	1:B:29:ARG:HD2	1.84	0.78
1:B:149:LEU:O	1:B:150:ASN:HB2	1.85	0.77
1:A:130:ILE:HD11	1:A:133:ILE:HG12	1.69	0.75
1:B:57:PRO:HG2	1:B:370:LEU:CD2	2.17	0.75
1:A:102:ASP:HB3	1:A:105:PHE:HD2	1.52	0.74
1:B:159:TRP:HD1	1:B:315:GLN:HA	1.52	0.74
1:B:113:ILE:HD11	1:B:218:PHE:CE2	2.23	0.74
1:A:130:ILE:HD11	1:A:133:ILE:CG1	2.19	0.73
1:A:158:LYS:HE2	1:A:185:TYR:CE2	2.23	0.73
1:B:143:PHE:HE1	1:B:182:ARG:HE	1.37	0.73
1:B:20:ILE:HG23	1:B:24:GLY:HA2	1.72	0.72
1:B:25:LYS:HA	1:B:25:LYS:HE2	1.72	0.72
1:A:230:ILE:HG22	1:A:231:LEU:HD22	1.72	0.71
1:B:156:VAL:HG11	1:B:314:HIS:CD2	2.25	0.70
1:B:110:ASN:HB2	1:B:211:THR:HG23	1.74	0.70
1:A:2:ASP:O	1:A:3:GLU:HB2	1.91	0.70
1:A:36:THR:HG22	1:A:59:LYS:HG3	1.74	0.69
1:B:90:TYR:CZ	1:B:94:THR:HG21	2.28	0.69
1:B:163:LEU:HD11	1:B:171:GLY:O	1.94	0.68
1:B:249:LEU:HB3	1:B:258:GLU:HB3	1.75	0.68
1:B:39:ARG:HH12	1:B:42:LYS:NZ	1.92	0.68
1:B:241:PRO:HD2	1:B:263:ASP:O	1.94	0.68
1:A:158:LYS:HE2	1:A:185:TYR:HE2	1.56	0.67
1:A:228:LYS:O	1:A:232:GLY:HA2	1.95	0.67
1:B:141:ASP:O	1:B:182:ARG:HG2	1.95	0.66
1:B:156:VAL:HG22	1:B:157:SER:H	1.61	0.66
1:A:56:ALA:HB2	1:B:340:LEU:HD22	1.78	0.66
1:B:280:THR:HG1	1:B:285:PHE:HZ	1.43	0.65
1:A:179:ILE:HG22	1:A:322:ILE:HD11	1.77	0.65
1:B:179:ILE:CG2	1:B:322:ILE:HD11	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:TRP:HZ2	1:A:290:VAL:HG21	1.63	0.64
1:A:248:LYS:O	1:A:258:GLU:HA	1.97	0.64
1:A:196:MET:HG3	1:A:231:LEU:HD11	1.78	0.64
1:A:23:ASN:ND2	1:A:25:LYS:HG3	2.13	0.63
1:B:151:SER:O	1:B:153:TYR:N	2.31	0.63
1:A:348:ALA:HB3	1:A:350:MET:HG2	1.81	0.63
1:A:11:VAL:O	1:A:14:ASN:HB2	1.98	0.63
1:B:166:LYS:O	1:B:172:GLY:HA3	1.99	0.62
1:A:149:LEU:HA	1:A:156:VAL:HG12	1.82	0.61
1:A:310:ARG:HD2	2:A:392:HOH:O	1.98	0.61
1:B:299:LYS:HE2	1:B:323:ILE:CG2	2.29	0.61
1:B:248:LYS:O	1:B:258:GLU:HA	1.99	0.61
1:A:211:THR:HG21	1:A:270:TYR:HD2	1.64	0.61
1:B:282:LEU:HB2	1:B:285:PHE:CE1	2.36	0.61
1:B:83:MET:SD	1:B:86:PHE:HB2	2.39	0.61
1:B:121:PRO:O	1:B:218:PHE:HE1	1.84	0.61
1:B:122:ASP:OD2	1:B:124:MET:HB2	2.01	0.61
1:B:179:ILE:HG22	1:B:322:ILE:CD1	2.30	0.60
1:B:19:TYR:HE1	1:B:29:ARG:HG3	1.63	0.60
1:A:110:ASN:ND2	1:A:329:GLN:HE21	1.98	0.60
1:B:103:ARG:HH11	1:B:103:ARG:HG3	1.64	0.60
1:B:33:TYR:CD2	1:B:86:PHE:CE1	2.90	0.59
1:A:61:PRO:HD2	1:A:65:ASP:OD2	2.03	0.59
1:A:121:PRO:O	1:A:218:PHE:HE1	1.85	0.59
1:B:8:ILE:HD13	1:B:17:GLU:HG3	1.85	0.59
1:A:213:TRP:CZ2	1:A:290:VAL:HG21	2.38	0.59
1:A:246:LYS:O	1:A:260:TYR:HA	2.03	0.59
1:A:124:MET:SD	1:A:256:SER:O	2.61	0.59
1:B:130:ILE:HD11	1:B:133:ILE:HG13	1.85	0.59
1:A:39:ARG:HB3	1:A:42:LYS:HG2	1.85	0.59
1:B:344:MET:HE2	1:B:355:VAL:HB	1.84	0.58
1:A:306:ILE:HD12	1:A:306:ILE:H	1.68	0.58
1:B:124:MET:SD	1:B:258:GLU:HG2	2.42	0.58
1:B:33:TYR:HD2	1:B:86:PHE:CE1	2.21	0.58
1:B:2:ASP:O	1:B:3:GLU:HB3	2.03	0.58
1:A:228:LYS:HG3	1:A:233:GLU:HG3	1.85	0.58
1:B:203:GLU:OE2	1:B:238:ARG:HD2	2.04	0.58
1:A:318:ILE:O	1:A:322:ILE:HG23	2.04	0.58
1:B:306:ILE:HG22	1:B:307:ASN:N	2.19	0.58
1:A:83:MET:O	1:A:86:PHE:HB3	2.04	0.58
1:B:37:MET:SD	1:B:370:LEU:HB3	2.44	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:SER:OG	1:A:352:PHE:HA	2.03	0.57
1:B:135:HIS:HD2	1:B:198:TYR:OH	1.88	0.57
1:B:156:VAL:HB	1:B:310:ARG:NH2	2.20	0.57
1:B:15:ILE:HG21	1:B:90:TYR:CD2	2.40	0.57
1:B:83:MET:C	1:B:85:ASP:H	2.07	0.57
1:A:344:MET:SD	1:B:366:ILE:HG12	2.45	0.57
1:B:143:PHE:HE1	1:B:182:ARG:NE	2.02	0.56
1:B:113:ILE:HD11	1:B:218:PHE:HE2	1.68	0.56
1:B:302:TYR:HE1	1:B:309:LEU:HD22	1.71	0.56
1:B:19:TYR:O	1:B:26:GLU:HA	2.06	0.56
1:A:38:PHE:HD2	1:A:69:TRP:CZ3	2.24	0.56
1:B:309:LEU:HD11	1:B:313:ASN:HB3	1.87	0.56
1:A:286:SER:O	1:A:290:VAL:HG23	2.06	0.56
1:A:33:TYR:HD2	1:A:86:PHE:CE1	2.24	0.56
1:B:235:SER:O	1:B:238:ARG:HB2	2.06	0.56
1:A:214:ASN:HD21	1:A:217:GLY:HA3	1.69	0.56
1:A:358:PRO:HA	1:B:362:TRP:HB2	1.86	0.56
1:A:149:LEU:HD11	1:A:187:PRO:HB2	1.87	0.56
1:B:16:VAL:HG12	1:B:30:GLU:HG3	1.86	0.56
1:B:326:GLU:HB3	2:B:394:HOH:O	2.06	0.56
1:B:37:MET:HG2	1:B:59:LYS:HA	1.88	0.56
1:B:308:LYS:HG3	1:B:311:GLU:HG3	1.87	0.56
1:A:6:ILE:HD13	1:A:20:ILE:HG12	1.87	0.55
1:B:310:ARG:O	1:B:314:HIS:HB2	2.06	0.55
1:A:43:GLU:HG2	1:A:69:TRP:CZ3	2.41	0.55
1:B:152:MET:SD	1:B:153:TYR:CD1	3.00	0.55
1:A:158:LYS:NZ	1:A:158:LYS:HB3	2.22	0.55
1:B:163:LEU:HD22	1:B:163:LEU:O	2.06	0.55
1:A:235:SER:HA	1:A:238:ARG:HG3	1.89	0.55
1:A:366:ILE:HG12	1:B:344:MET:SD	2.47	0.55
1:A:357:SER:OG	1:A:360:LYS:HB2	2.07	0.54
1:B:110:ASN:HA	1:B:211:THR:O	2.08	0.54
1:B:299:LYS:HE2	1:B:323:ILE:HG21	1.89	0.54
1:A:38:PHE:HB2	1:A:69:TRP:CH2	2.42	0.54
1:A:274:TYR:CE2	1:A:280:THR:HG21	2.42	0.54
1:B:226:ARG:NH2	1:B:229:MET:SD	2.80	0.54
1:B:57:PRO:HG2	1:B:370:LEU:HD23	1.90	0.54
1:B:270:TYR:HA	1:B:273:LEU:HG	1.90	0.54
1:A:63:MET:HG2	1:A:67:ARG:HH21	1.72	0.54
1:A:259:ILE:O	1:A:260:TYR:HB2	2.07	0.53
1:A:102:ASP:HB3	1:A:105:PHE:CD2	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:ARG:HG3	1:A:317:TYR:CD2	2.43	0.53
1:B:36:THR:O	1:B:59:LYS:HG3	2.09	0.53
1:B:64:LYS:HG3	1:B:65:ASP:N	2.23	0.53
1:B:145:VAL:CG2	1:B:183:VAL:HG13	2.39	0.53
1:B:308:LYS:CG	1:B:311:GLU:HB2	2.38	0.53
1:A:344:MET:HB3	1:A:355:VAL:HG22	1.91	0.53
1:B:233:GLU:O	1:B:234:ARG:HB3	2.09	0.52
1:A:34:LEU:CD2	1:A:70:MET:HG3	2.38	0.52
1:A:188:PHE:CD1	1:A:194:MET:HG3	2.43	0.52
1:B:302:TYR:OH	1:B:309:LEU:HD13	2.10	0.52
1:B:85:ASP:CG	1:B:367:PHE:HZ	2.12	0.52
1:B:357:SER:HB3	1:B:360:LYS:HB2	1.89	0.52
1:A:211:THR:HG23	1:A:268:LEU:O	2.10	0.52
1:B:213:TRP:NE1	1:B:271:LEU:HD13	2.25	0.52
1:A:135:HIS:HD2	1:A:198:TYR:OH	1.93	0.52
1:A:36:THR:O	1:A:59:LYS:HG3	2.10	0.52
1:A:166:LYS:O	1:A:172:GLY:HA3	2.10	0.52
1:B:201:LEU:O	1:B:205:LYS:HG3	2.10	0.52
1:B:117:GLY:HA2	1:B:153:TYR:OH	2.10	0.51
1:A:69:TRP:HA	1:A:72:ARG:CZ	2.40	0.51
1:B:8:ILE:CD1	1:B:17:GLU:HG3	2.41	0.51
1:A:156:VAL:HG11	1:A:314:HIS:CD2	2.45	0.51
1:A:117:GLY:HA2	1:A:153:TYR:CZ	2.44	0.51
1:B:103:ARG:HH12	1:B:108:VAL:HG21	1.76	0.51
1:A:206:ARG:NH2	1:A:238:ARG:O	2.44	0.51
1:A:113:ILE:HG22	1:A:133:ILE:HG12	1.91	0.51
1:B:64:LYS:HG3	1:B:65:ASP:H	1.75	0.51
1:B:113:ILE:HD12	1:B:115:VAL:HG23	1.93	0.51
1:A:179:ILE:HG22	1:A:322:ILE:CD1	2.40	0.51
1:B:200:ASN:O	1:B:204:GLN:HG3	2.11	0.51
1:A:233:GLU:O	1:A:234:ARG:CB	2.58	0.51
1:B:121:PRO:HB3	1:B:128:TYR:CD2	2.46	0.51
1:A:159:TRP:HB3	1:A:185:TYR:CE1	2.46	0.51
1:A:33:TYR:CD2	1:A:86:PHE:CE1	2.99	0.50
1:B:308:LYS:O	1:B:308:LYS:HG2	2.11	0.50
1:B:308:LYS:HG2	1:B:311:GLU:HB2	1.93	0.50
1:B:71:LYS:HG2	1:B:71:LYS:O	2.11	0.50
1:A:123:PRO:HG3	1:A:218:PHE:CD1	2.46	0.50
1:A:216:GLU:HA	2:A:420:HOH:O	2.10	0.50
1:A:38:PHE:HB3	1:A:60:PHE:CZ	2.47	0.50
1:A:358:PRO:HG3	1:B:362:TRP:CE3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:VAL:HG12	1:B:260:TYR:CE2	2.46	0.50
1:B:103:ARG:NH1	1:B:103:ARG:HG3	2.27	0.50
1:B:190:ASN:OD1	1:B:193:ASP:HB2	2.12	0.50
1:A:118:ASP:O	1:A:120:PHE:N	2.45	0.49
1:B:292:GLN:NE2	1:B:298:GLY:HA2	2.27	0.49
1:B:136:TYR:CE2	1:B:138:SER:HA	2.47	0.49
1:B:19:TYR:CZ	1:B:27:ARG:HB2	2.46	0.49
1:A:115:VAL:HG22	1:A:130:ILE:HA	1.93	0.49
1:B:57:PRO:HG2	1:B:370:LEU:HD21	1.95	0.49
1:B:146:PHE:HB3	1:B:194:MET:CG	2.43	0.49
1:A:36:THR:O	1:A:59:LYS:HA	2.13	0.49
1:B:299:LYS:HE2	1:B:323:ILE:HG22	1.93	0.49
1:B:245:VAL:HG12	1:B:260:TYR:CD2	2.47	0.49
1:B:183:VAL:HG21	1:B:322:ILE:HD13	1.93	0.49
1:A:34:LEU:HD23	1:A:70:MET:HG3	1.94	0.49
1:A:121:PRO:HB2	1:A:218:PHE:CE1	2.47	0.49
1:B:236:MET:O	1:B:239:PHE:HB2	2.13	0.49
1:B:215:ILE:HA	1:B:219:ASP:HB2	1.95	0.48
1:A:219:ASP:O	1:A:223:ILE:HG13	2.13	0.48
1:B:134:THR:HA	1:B:144:TYR:O	2.13	0.48
1:B:226:ARG:HE	1:B:226:ARG:HA	1.78	0.48
1:A:321:ASN:O	1:A:325:VAL:HG23	2.13	0.48
1:B:152:MET:SD	1:B:153:TYR:N	2.87	0.48
1:A:23:ASN:HD21	1:A:25:LYS:HG3	1.76	0.48
1:B:140:ASP:O	1:B:142:ARG:N	2.46	0.48
1:B:153:TYR:HD1	1:B:153:TYR:H	1.62	0.48
1:A:17:GLU:O	1:A:28:THR:HA	2.14	0.47
1:B:10:THR:O	1:B:244:ARG:NH2	2.47	0.47
1:B:175:VAL:HG22	1:B:323:ILE:HD11	1.96	0.47
1:A:167:LEU:O	1:A:170:GLU:HG2	2.13	0.47
1:A:147:ASP:O	1:A:187:PRO:HA	2.14	0.47
1:B:165:ALA:HB2	1:B:180:LEU:CD1	2.44	0.47
1:A:38:PHE:CD2	1:A:69:TRP:CZ3	3.03	0.47
1:A:192:ARG:HB2	1:A:192:ARG:NH1	2.30	0.47
1:A:163:LEU:HA	1:A:163:LEU:HD23	1.71	0.47
1:A:102:ASP:OD2	1:A:104:LYS:HE2	2.15	0.47
1:B:34:LEU:HA	1:B:35:PRO:HD3	1.75	0.47
1:A:119:LYS:O	1:A:120:PHE:CB	2.63	0.47
1:B:129:GLU:HA	1:B:191:GLU:OE2	2.15	0.47
1:B:156:VAL:HG22	1:B:157:SER:N	2.29	0.47
1:B:292:GLN:O	1:B:296:LYS:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:VAL:HG23	1:B:183:VAL:HG13	1.96	0.46
1:B:121:PRO:HB3	1:B:128:TYR:HD2	1.81	0.46
1:B:206:ARG:NH2	1:B:238:ARG:O	2.47	0.46
1:A:276:LYS:NZ	1:A:356:MET:SD	2.80	0.46
1:B:176:PRO:HD2	1:B:179:ILE:HD12	1.97	0.46
1:A:35:PRO:HD3	1:A:86:PHE:CE1	2.51	0.46
1:B:213:TRP:CZ2	1:B:290:VAL:HG21	2.50	0.46
1:A:119:LYS:O	1:A:120:PHE:HB2	2.15	0.46
1:A:175:VAL:CG2	1:A:319:SER:HB3	2.45	0.46
1:B:159:TRP:CH2	1:B:161:ALA:HA	2.51	0.46
1:A:10:THR:HA	1:A:14:ASN:O	2.16	0.46
1:B:34:LEU:HD11	1:B:63:MET:HG2	1.98	0.46
1:A:10:THR:CG2	1:A:15:ILE:HD13	2.44	0.46
1:B:309:LEU:CD1	1:B:313:ASN:HB3	2.45	0.46
1:A:297:LYS:HE2	1:A:297:LYS:HA	1.98	0.46
1:A:228:LYS:O	1:A:232:GLY:CA	2.62	0.46
1:B:126:ALA:O	1:B:226:ARG:NH2	2.48	0.46
1:B:175:VAL:HG22	1:B:323:ILE:CD1	2.45	0.46
1:A:20:ILE:HG13	1:A:105:PHE:HB3	1.98	0.45
1:B:113:ILE:HG22	1:B:133:ILE:HG12	1.98	0.45
1:B:313:ASN:C	1:B:314:HIS:O	2.52	0.45
1:B:82:GLY:O	1:B:85:ASP:HB2	2.17	0.45
1:A:123:PRO:HA	1:A:222:TYR:CD2	2.52	0.45
1:B:144:TYR:HB3	1:B:186:MET:HE1	1.98	0.45
1:A:361:THR:O	1:A:365:ILE:HG12	2.15	0.45
1:B:207:PRO:O	1:B:265:VAL:HG13	2.17	0.45
1:A:213:TRP:CH2	1:A:290:VAL:HG11	2.51	0.45
1:B:300:LEU:HD12	1:B:301:PRO:HD2	1.99	0.45
1:A:206:ARG:HD3	1:A:241:PRO:HD3	1.98	0.45
1:B:101:TYR:CD1	1:B:101:TYR:N	2.84	0.45
1:B:62:SER:O	1:B:64:LYS:N	2.49	0.45
1:A:32:GLU:H	1:A:32:GLU:CD	2.19	0.45
1:B:120:PHE:O	1:B:122:ASP:N	2.49	0.45
1:B:314:HIS:O	1:B:316:ARG:N	2.50	0.45
1:B:233:GLU:O	1:B:234:ARG:CB	2.64	0.45
1:A:119:LYS:HA	1:A:119:LYS:HD2	1.76	0.45
1:B:112:ASP:HB2	1:B:325:VAL:CG2	2.47	0.45
1:B:134:THR:N	1:B:321:ASN:HD21	2.13	0.45
1:B:123:PRO:HG3	1:B:218:PHE:CD1	2.52	0.45
1:B:31:VAL:HG12	1:B:32:GLU:O	2.17	0.45
1:A:10:THR:HG22	1:A:15:ILE:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:GLU:HG3	1:B:3:GLU:O	2.15	0.44
1:B:149:LEU:O	1:B:150:ASN:CB	2.61	0.44
1:B:305:PRO:O	1:B:306:ILE:HG12	2.17	0.44
1:A:358:PRO:HA	1:B:362:TRP:CG	2.51	0.44
1:A:192:ARG:HB2	1:A:192:ARG:HH11	1.82	0.44
1:B:42:LYS:HG2	1:B:85:ASP:OD1	2.17	0.44
1:B:146:PHE:CD1	1:B:146:PHE:N	2.86	0.44
1:B:167:LEU:HB2	1:B:169:CYS:SG	2.58	0.44
1:A:36:THR:HG22	1:A:36:THR:O	2.18	0.44
1:B:87:LYS:O	1:B:91:ILE:HG13	2.18	0.44
1:B:167:LEU:CB	1:B:169:CYS:SG	3.06	0.44
1:B:327:SER:O	1:B:330:ALA:HB3	2.18	0.44
1:A:156:VAL:HG21	1:A:314:HIS:HB2	2.00	0.44
1:B:356:MET:HE3	1:B:356:MET:HB3	1.88	0.44
1:B:90:TYR:CE2	1:B:94:THR:HG21	2.53	0.43
1:B:91:ILE:O	1:B:95:TYR:HB2	2.18	0.43
1:A:225:ASN:ND2	1:A:260:TYR:OH	2.51	0.43
1:A:274:TYR:HE2	1:A:280:THR:HG21	1.83	0.43
1:A:165:ALA:HB2	1:A:180:LEU:CD1	2.47	0.43
1:B:143:PHE:HZ	1:B:182:ARG:HH21	1.65	0.43
1:B:163:LEU:HD22	1:B:172:GLY:CA	2.48	0.43
1:B:62:SER:HB3	1:B:64:LYS:HG2	2.00	0.43
1:B:280:THR:OG1	1:B:285:PHE:HZ	1.98	0.43
1:A:95:TYR:O	1:A:349:LYS:NZ	2.47	0.43
1:B:7:SER:HB3	1:B:18:ARG:HB2	1.99	0.43
1:B:120:PHE:N	1:B:121:PRO:CD	2.82	0.43
1:A:149:LEU:HB3	1:A:156:VAL:HG12	2.01	0.43
1:B:342:LEU:O	1:B:346:TYR:CD2	2.71	0.43
1:B:262:ILE:HD13	1:B:267:ILE:HD11	2.01	0.43
1:B:200:ASN:ND2	1:B:204:GLN:OE1	2.51	0.43
1:A:149:LEU:CD2	1:A:158:LYS:HA	2.49	0.43
1:A:184:ILE:O	1:A:184:ILE:HG22	2.17	0.43
1:B:249:LEU:N	1:B:249:LEU:HD23	2.34	0.43
1:B:140:ASP:O	1:B:142:ARG:CD	2.66	0.43
1:B:228:LYS:O	1:B:232:GLY:N	2.51	0.43
1:B:159:TRP:CD1	1:B:318:ILE:HB	2.54	0.42
1:B:169:CYS:SG	1:B:170:GLU:N	2.92	0.42
1:B:144:TYR:HD2	1:B:186:MET:HE2	1.84	0.42
1:A:19:TYR:O	1:A:26:GLU:HA	2.18	0.42
1:B:329:GLN:O	1:B:333:LYS:HG3	2.20	0.42
1:B:274:TYR:O	1:B:278:ALA:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:GLY:O	1:B:235:SER:HB2	2.20	0.42
1:A:202:TRP:HZ2	1:A:210:PHE:CZ	2.37	0.42
1:A:22:GLU:H	1:A:22:GLU:HG3	1.54	0.42
1:A:197:GLU:O	1:A:200:ASN:HB2	2.20	0.42
1:B:305:PRO:HG2	1:B:306:ILE:H	1.84	0.42
1:A:220:VAL:O	1:A:224:MET:HG2	2.20	0.42
1:A:147:ASP:OD2	1:A:314:HIS:CE1	2.72	0.42
1:A:358:PRO:HA	1:B:362:TRP:CB	2.49	0.42
1:B:292:GLN:O	1:B:296:LYS:N	2.52	0.42
1:A:343:SER:HB2	1:B:369:SER:HB2	2.01	0.42
1:A:41:CYS:HB3	1:B:279:PHE:CG	2.54	0.42
1:A:10:THR:HG21	1:A:86:PHE:CD2	2.55	0.42
1:A:270:TYR:OH	1:A:337:PHE:HB2	2.19	0.42
1:B:196:MET:CE	1:B:238:ARG:NH2	2.82	0.42
1:B:9:GLU:CG	1:B:10:THR:H	2.32	0.42
1:B:117:GLY:HA3	1:B:128:TYR:CD2	2.54	0.42
1:B:134:THR:OG1	1:B:321:ASN:ND2	2.50	0.42
1:B:115:VAL:HG22	1:B:130:ILE:HA	2.02	0.42
1:A:166:LYS:HB3	1:A:170:GLU:HG3	2.01	0.42
1:A:112:ASP:CB	1:A:325:VAL:HG22	2.50	0.41
1:B:104:LYS:N	1:B:104:LYS:HD2	2.34	0.41
1:B:103:ARG:CG	1:B:103:ARG:NH1	2.82	0.41
1:B:273:LEU:HD23	1:B:273:LEU:N	2.35	0.41
1:A:101:TYR:N	1:A:101:TYR:CD1	2.88	0.41
1:B:130:ILE:CD1	1:B:133:ILE:HG13	2.49	0.41
1:A:42:LYS:HG3	1:A:85:ASP:OD2	2.21	0.41
1:A:38:PHE:HB2	1:A:69:TRP:CZ2	2.55	0.41
1:A:168:ASP:HB2	1:A:300:LEU:HD13	2.03	0.41
1:B:299:LYS:HG3	1:B:300:LEU:N	2.34	0.41
1:B:227:VAL:O	1:B:232:GLY:N	2.53	0.41
1:B:144:TYR:HD2	1:B:186:MET:CE	2.33	0.41
1:A:112:ASP:HB2	1:A:325:VAL:HG22	2.02	0.41
1:A:3:GLU:OE1	1:A:3:GLU:HA	2.21	0.41
1:B:85:ASP:CG	1:B:367:PHE:CZ	2.94	0.41
1:B:202:TRP:CD1	1:B:239:PHE:HE1	2.38	0.41
1:B:203:GLU:CD	1:B:238:ARG:HH11	2.24	0.41
1:A:166:LYS:C	1:A:172:GLY:HA3	2.41	0.41
1:A:21:ASP:OD2	1:A:22:GLU:N	2.54	0.41
1:B:2:ASP:O	1:B:3:GLU:CB	2.66	0.41
1:A:135:HIS:CD2	1:A:198:TYR:OH	2.71	0.41
1:B:188:PHE:CD1	1:B:194:MET:HG3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:VAL:HA	1:B:29:ARG:O	2.21	0.41
1:B:309:LEU:HA	1:B:309:LEU:HD12	1.96	0.41
1:B:320:TYR:O	1:B:323:ILE:HB	2.21	0.41
1:A:61:PRO:HD2	1:A:65:ASP:CG	2.42	0.41
1:B:198:TYR:HE2	1:B:223:ILE:HD13	1.85	0.41
1:A:324:ASP:O	1:A:327:SER:HB2	2.20	0.41
1:A:277:PHE:O	1:B:55:CYS:HA	2.21	0.41
1:A:113:ILE:HG21	1:A:223:ILE:HD11	2.02	0.41
1:A:43:GLU:OE2	1:A:72:ARG:NH1	2.54	0.41
1:B:308:LYS:O	1:B:308:LYS:CG	2.68	0.41
1:A:148:LEU:HB2	1:A:194:MET:SD	2.61	0.41
1:B:159:TRP:HB3	1:B:185:TYR:CE1	2.56	0.40
1:B:234:ARG:HA	1:B:237:LYS:HB2	2.02	0.40
1:A:196:MET:O	1:A:200:ASN:ND2	2.52	0.40
1:A:357:SER:HA	1:A:358:PRO:HD3	1.98	0.40
1:A:103:ARG:HG3	1:A:103:ARG:O	2.20	0.40
1:B:145:VAL:HG21	1:B:183:VAL:HG13	2.03	0.40
1:B:35:PRO:HG3	1:B:86:PHE:HD1	1.85	0.40
1:B:167:LEU:HA	1:B:174:GLU:CG	2.52	0.40
1:B:18:ARG:NH1	1:B:26:GLU:OE2	2.54	0.40
1:B:39:ARG:HH12	1:B:42:LYS:HZ1	1.68	0.40
1:B:352:PHE:O	1:B:355:VAL:HG13	2.21	0.40
1:B:201:LEU:HD11	1:B:205:LYS:HD2	2.04	0.40
1:A:64:LYS:HD3	1:A:68:ASP:OD2	2.21	0.40
1:A:40:HIS:O	1:A:43:GLU:HG3	2.22	0.40
1:A:276:LYS:HG2	1:B:52:GLY:O	2.21	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	338/388 (87%)	299 (88%)	27 (8%)	12 (4%)	4	2
1	B	338/388 (87%)	294 (87%)	29 (9%)	15 (4%)	3	1
All	All	676/776 (87%)	593 (88%)	56 (8%)	27 (4%)	4	1

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	120	PHE
1	A	150	ASN
1	A	257	LYS
1	B	3	GLU
1	B	141	ASP
1	B	152	MET
1	B	167	LEU
1	B	305	PRO
1	B	306	ILE
1	A	3	GLU
1	A	119	LYS
1	A	234	ARG
1	B	24	GLY
1	B	234	ARG
1	B	281	ASN
1	A	21	ASP
1	A	151	SER
1	A	152	MET
1	B	63	MET
1	A	260	TYR
1	B	121	PRO
1	A	39	ARG
1	A	305	PRO
1	B	39	ARG
1	B	150	ASN
1	B	104	LYS
1	B	301	PRO

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	312/350 (89%)	280 (90%)	32 (10%)	9	8
1	B	312/350 (89%)	269 (86%)	43 (14%)	4	3
All	All	624/700 (89%)	549 (88%)	75 (12%)	6	5

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	17	GLU
1	A	21	ASP
1	A	22	GLU
1	A	23	ASN
1	A	27	ARG
1	A	59	LYS
1	A	69	TRP
1	A	97	SER
1	A	103	ARG
1	A	119	LYS
1	A	130	ILE
1	A	149	LEU
1	A	151	SER
1	A	156	VAL
1	A	163	LEU
1	A	178	GLU
1	A	192	ARG
1	A	211	THR
1	A	226	ARG
1	A	248	LYS
1	A	270	TYR
1	A	282	LEU
1	A	287	LEU
1	A	289	SER
1	A	294	GLU
1	A	306	ILE
1	A	312	THR
1	A	313	ASN
1	A	316	ARG
1	A	322	ILE
1	A	353	SER
1	B	15	ILE
1	B	20	ILE

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Mol	Chain	Res	Type
1	B	23	ASN
1	B	25	LYS
1	B	26	GLU
1	B	32	GLU
1	B	34	LEU
1	B	39	ARG
1	B	43	GLU
1	B	58	GLN
1	B	97	SER
1	B	104	LYS
1	B	110	ASN
1	B	111	CYS
1	B	120	PHE
1	B	130	ILE
1	B	142	ARG
1	B	151	SER
1	B	152	MET
1	B	157	SER
1	B	158	LYS
1	B	160	ASP
1	B	163	LEU
1	B	191	GLU
1	B	200	ASN
1	B	205	LYS
1	B	206	ARG
1	B	226	ARG
1	B	230	ILE
1	B	234	ARG
1	B	259	ILE
1	B	276	LYS
1	B	287	LEU
1	B	292	GLN
1	B	306	ILE
1	B	310	ARG
1	B	311	GLU
1	B	313	ASN
1	B	315	GLN
1	B	322	ILE
1	B	355	VAL
1	B	367	PHE
1	B	370	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	58	GLN
1	A	110	ASN
1	A	135	HIS
1	A	190	ASN
1	A	214	ASN
1	A	225	ASN
1	A	313	ASN
1	A	321	ASN
1	B	14	ASN
1	B	135	HIS
1	B	200	ASN
1	B	204	GLN
1	B	292	GLN
1	B	313	ASN
1	B	321	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	346/388 (89%)	1.73	105 (30%) 1 0	20, 39, 61, 72	0
1	B	346/388 (89%)	2.14	147 (42%) 0 0	25, 54, 87, 101	0
All	All	692/776 (89%)	1.93	252 (36%) 0 0	20, 46, 78, 101	0

All (252) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	249	LEU	11.7
1	B	82	GLY	8.4
1	B	298	GLY	7.8
1	B	120	PHE	7.4
1	B	245	VAL	7.4
1	A	11	VAL	7.3
1	B	239	PHE	7.0
1	B	163	LEU	7.0
1	B	304	GLY	6.8
1	B	148	LEU	6.8
1	A	249	LEU	6.7
1	B	11	VAL	6.3
1	B	83	MET	5.9
1	B	119	LYS	5.8
1	B	201	LEU	5.8
1	A	86	PHE	5.7
1	B	281	ASN	5.6
1	B	118	ASP	5.6
1	A	150	ASN	5.5
1	A	12	GLY	5.4
1	B	230	ILE	5.4
1	A	126	ALA	5.4
1	B	15	ILE	5.3
1	B	285	PHE	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	121	PRO	5.1
1	B	305	PRO	5.1
1	B	72	ARG	5.1
1	A	152	MET	4.9
1	B	13	ASN	4.8
1	B	86	PHE	4.7
1	A	111	CYS	4.7
1	A	277	PHE	4.6
1	A	83	MET	4.6
1	B	152	MET	4.5
1	B	12	GLY	4.5
1	B	145	VAL	4.5
1	A	69	TRP	4.5
1	B	202	TRP	4.5
1	B	121	PRO	4.5
1	A	6	ILE	4.4
1	B	292	GLN	4.4
1	A	220	VAL	4.4
1	B	302	TYR	4.4
1	B	309	LEU	4.3
1	B	125	LYS	4.3
1	A	178	GLU	4.3
1	B	218	PHE	4.3
1	B	311	GLU	4.2
1	B	260	TYR	4.2
1	B	198	TYR	4.2
1	B	84	ASN	4.2
1	B	247	SER	4.1
1	A	52	GLY	4.1
1	B	370	LEU	4.1
1	A	248	LYS	4.1
1	A	218	PHE	4.1
1	B	6	ILE	4.0
1	A	279	PHE	4.0
1	B	16	VAL	3.8
1	A	120	PHE	3.8
1	B	52	GLY	3.8
1	B	90	TYR	3.8
1	A	118	ASP	3.8
1	A	227	VAL	3.8
1	B	179	ILE	3.7
1	B	205	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	248	LYS	3.7
1	B	229	MET	3.7
1	A	159	TRP	3.7
1	B	108	VAL	3.7
1	A	154	GLY	3.7
1	A	278	ALA	3.7
1	B	184	ILE	3.6
1	B	117	GLY	3.6
1	B	34	LEU	3.6
1	A	20	ILE	3.5
1	A	163	LEU	3.5
1	B	195	LEU	3.5
1	A	242	ILE	3.5
1	B	243	GLY	3.5
1	B	14	ASN	3.5
1	B	111	CYS	3.5
1	B	113	ILE	3.5
1	A	145	VAL	3.5
1	B	157	SER	3.5
1	B	194	MET	3.4
1	B	246	LYS	3.4
1	A	300	LEU	3.4
1	B	95	TYR	3.4
1	B	153	TYR	3.4
1	A	223	ILE	3.4
1	A	247	SER	3.4
1	A	230	ILE	3.3
1	B	37	MET	3.3
1	B	308	LYS	3.3
1	B	60	PHE	3.3
1	A	231	LEU	3.3
1	A	130	ILE	3.3
1	A	70	MET	3.3
1	B	196	MET	3.3
1	B	277	PHE	3.2
1	B	279	PHE	3.2
1	A	53	LYS	3.2
1	A	333	LYS	3.2
1	B	91	ILE	3.2
1	B	41	CYS	3.2
1	A	370	LEU	3.2
1	A	281	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	69	TRP	3.1
1	A	125	LYS	3.1
1	A	215	ILE	3.1
1	A	358	PRO	3.1
1	B	180	LEU	3.1
1	B	266	SER	3.1
1	B	42	LYS	3.1
1	B	137	ASP	3.1
1	B	94	THR	3.1
1	B	209	ILE	3.1
1	B	189	ASP	3.1
1	A	19	TYR	3.1
1	B	190	ASN	3.0
1	A	117	GLY	3.0
1	A	149	LEU	3.0
1	B	204	GLN	3.0
1	A	32	GLU	3.0
1	B	156	VAL	3.0
1	B	175	VAL	3.0
1	B	144	TYR	3.0
1	A	239	PHE	3.0
1	B	303	ASP	3.0
1	A	185	TYR	3.0
1	A	282	LEU	3.0
1	B	238	ARG	3.0
1	B	172	GLY	2.9
1	A	268	LEU	2.9
1	B	257	LYS	2.9
1	B	267	ILE	2.9
1	A	245	VAL	2.9
1	B	171	GLY	2.9
1	A	202	TRP	2.9
1	A	201	LEU	2.9
1	B	58	GLN	2.9
1	A	113	ILE	2.9
1	B	222	TYR	2.8
1	A	66	ALA	2.8
1	B	161	ALA	2.8
1	B	35	PRO	2.8
1	A	5	TYR	2.8
1	A	31	VAL	2.8
1	A	258	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	338	ILE	2.8
1	A	302	TYR	2.8
1	B	306	ILE	2.8
1	B	39	ARG	2.8
1	B	128	TYR	2.7
1	A	68	ASP	2.7
1	A	307	ASN	2.7
1	A	22	GLU	2.7
1	B	307	ASN	2.7
1	A	261	SER	2.7
1	A	234	ARG	2.7
1	A	210	PHE	2.6
1	B	280	THR	2.6
1	B	25	LYS	2.6
1	A	108	VAL	2.6
1	A	356	MET	2.6
1	B	109	ALA	2.6
1	A	10	THR	2.6
1	A	15	ILE	2.6
1	A	276	LYS	2.6
1	A	16	VAL	2.6
1	A	355	VAL	2.6
1	B	234	ARG	2.5
1	A	195	LEU	2.5
1	B	70	MET	2.5
1	B	31	VAL	2.5
1	B	262	ILE	2.5
1	A	306	ILE	2.5
1	B	65	ASP	2.5
1	B	368	ASN	2.5
1	B	315	GLN	2.5
1	A	82	GLY	2.4
1	A	109	ALA	2.4
1	B	116	THR	2.4
1	A	91	ILE	2.4
1	A	359	ILE	2.4
1	B	99	ILE	2.4
1	B	143	PHE	2.4
1	B	301	PRO	2.4
1	A	42	LYS	2.4
1	B	36	THR	2.4
1	B	273	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	242	ILE	2.4
1	B	352	PHE	2.4
1	B	32	GLU	2.4
1	A	352	PHE	2.4
1	B	10	THR	2.4
1	B	110	ASN	2.3
1	B	313	ASN	2.3
1	B	57	PRO	2.3
1	B	159	TRP	2.3
1	B	268	LEU	2.3
1	B	282	LEU	2.3
1	B	310	ARG	2.3
1	B	33	TYR	2.3
1	B	283	PRO	2.3
1	A	367	PHE	2.3
1	A	342	LEU	2.3
1	B	123	PRO	2.3
1	B	126	ALA	2.3
1	B	67	ARG	2.3
1	A	265	VAL	2.3
1	A	13	ASN	2.3
1	B	7	SER	2.2
1	B	62	SER	2.2
1	B	296	LYS	2.2
1	B	54	ASN	2.2
1	A	128	TYR	2.2
1	A	224	MET	2.2
1	B	85	ASP	2.2
1	A	343	SER	2.2
1	A	84	ASN	2.2
1	B	53	LYS	2.2
1	A	156	VAL	2.2
1	A	309	LEU	2.2
1	A	199	ILE	2.2
1	A	318	ILE	2.1
1	B	341	VAL	2.1
1	A	90	TYR	2.1
1	B	2	ASP	2.1
1	B	100	VAL	2.1
1	B	265	VAL	2.1
1	A	71	LYS	2.1
1	B	26	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	59	LYS	2.1
1	B	360	LYS	2.1
1	A	274	TYR	2.1
1	A	34	LEU	2.1
1	A	63	MET	2.1
1	B	63	MET	2.1
1	A	133	ILE	2.1
1	A	238	ARG	2.1
1	A	131	ASP	2.1
1	A	283	PRO	2.1
1	B	167	LEU	2.1
1	A	244	ARG	2.1
1	B	132	ALA	2.0
1	B	136	TYR	2.0
1	A	237	LYS	2.0
1	B	22	GLU	2.0
1	B	151	SER	2.0
1	A	151	SER	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.