



Full wwPDB X-ray Structure Validation Report i

May 26, 2020 – 11:32 pm BST

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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the i symbol.

The following versions of software and data (see references ①) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

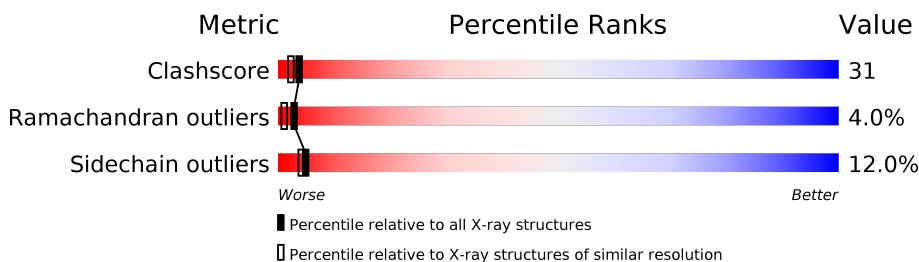
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

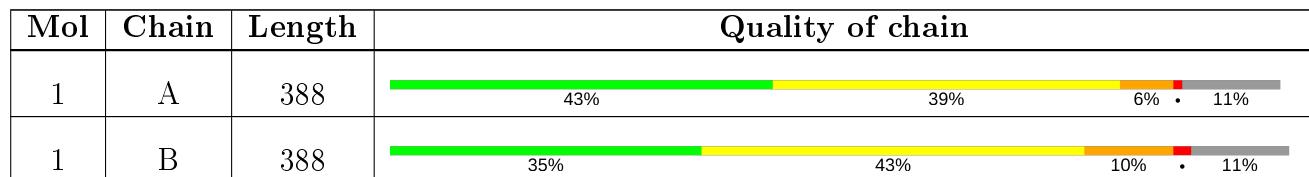
The reported resolution of this entry is 2.20 Å.

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	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (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 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 <=5%



2 Entry composition (i)

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			

Mol	Chain	Residues	Total	C	N	O	S	ZeroOcc	AltConf	Trace
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.

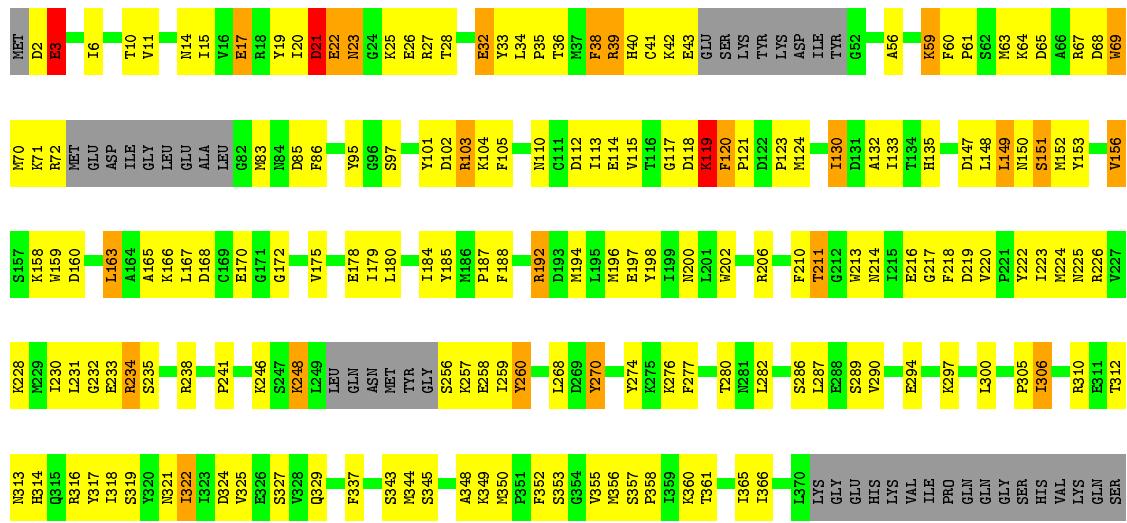
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	34	Total O 34 34	0	0
2	B	11	Total O 11 11	0	0

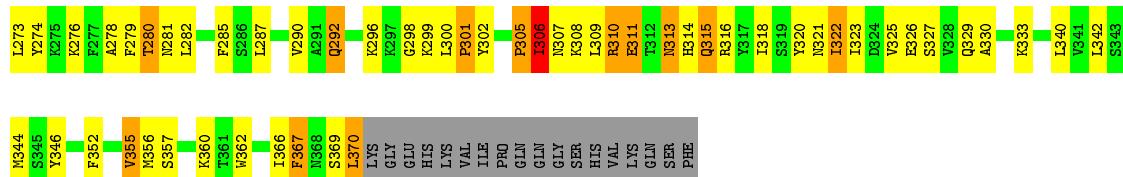
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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

Chain A: 





4 Data and refinement statistics i

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
$\langle I/\sigma(I) \rangle^1$	0.67 (at 2.73Å)	Xtriage
Refinement program	X-PLOR	Depositor
R , R_{free}	0.222 , (Not available) 0.314 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	46.8	Xtriage
Anisotropy	0.478	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 92.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for k,h,-l	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 9.09% 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 [\(i\)](#)

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($^{\circ}$)	Ideal($^{\circ}$)
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:A:348:ALA:HB3	1:A:350:MET:HG2	1.81	0.63
1:B:151:SER:O	1:B:153:TYR:N	2.31	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:A:211:THR:HG21	1:A:270:TYR:HD2	1.64	0.61
1:B:248:LYS:O	1:B:258:GLU:HA	1.99	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:121:PRO:O	1:A:218:PHE:HE1	1.85	0.59
1:A:61:PRO:HD2	1:A:65:ASP:OD2	2.03	0.59
1:B:8:ILE:HD13	1:B:17:GLU:HG3	1.85	0.59
1:A:124:MET:SD	1:A:256:SER:O	2.61	0.59
1:A:246:LYS:O	1:A:260:TYR:HA	2.03	0.59
1:A:213:TRP:CZ2	1:A:290:VAL:HG21	2.38	0.59
1:A:39:ARG:HB3	1:A:42:LYS:HG2	1.85	0.59
1:B:130:ILE:HD11	1:B:133:ILE:HG13	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:15:ILE:HG21	1:B:90:TYR:CD2	2.40	0.57
1:B:156:VAL:HB	1:B:310:ARG:NH2	2.20	0.57
1:A:344:MET:SD	1:B:366:ILE:HG12	2.45	0.57
1:B:83:MET:C	1:B:85:ASP:H	2.07	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:A:38:PHE:HD2	1:A:69:TRP:CZ3	2.24	0.56
1:B:19:TYR:O	1:B:26:GLU:HA	2.06	0.56
1:A:214:ASN:HD21	1:A:217:GLY:HA3	1.69	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:B:309:LEU:HD11	1:B:313:ASN:HB3	1.87	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:308:LYS:HG3	1:B:311:GLU:HG3	1.87	0.56
1:B:37:MET:HG2	1:B:59:LYS:HA	1.88	0.56
1:A:6:ILE:HD13	1:A:20:ILE:HG12	1.87	0.55
1:A:43:GLU:HG2	1:A:69:TRP:CZ3	2.41	0.55
1:B:310:ARG:O	1:B:314:HIS:HB2	2.06	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:A:38:PHE:HB2	1:A:69:TRP:CH2	2.42	0.54
1:B:299:LYS:HE2	1:B:323:ILE:HG21	1.89	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:270:TYR:HA	1:B:273:LEU:HG	1.90	0.54
1:B:57:PRO:HG2	1:B:370:LEU:HD23	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:A:34:LEU:CD2	1:A:70:MET:HG3	2.38	0.52
1:B:233:GLU:O	1:B:234:ARG:HB3	2.09	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:357:SER:HB3	1:B:360:LYS:HB2	1.89	0.52
1:B:85:ASP:CG	1:B:367:PHE:HZ	2.12	0.52
1:A:135:HIS:HD2	1:A:198:TYR:OH	1.93	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: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:A:69:TRP:HA	1:A:72:ARG:CZ	2.40	0.51
1:B:117:GLY:HA2	1:B:153:TYR:OH	2.10	0.51
1:A:117:GLY:HA2	1:A:153:TYR:CZ	2.44	0.51
1:A:156:VAL:HG11	1:A:314:HIS:CD2	2.45	0.51
1:B:8:ILE:CD1	1:B:17:GLU:HG3	2.41	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:A:179:ILE:HG22	1:A:322:ILE:CD1	2.40	0.51
1:B:113:ILE:HD12	1:B:115:VAL:HG23	1.93	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:A:159:TRP:HB3	1:A:185:TYR:CE1	2.46	0.51
1:B:121:PRO:HB3	1:B:128:TYR:CD2	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:216:GLU:HA	2:A:420:HOH:O	2.10	0.50
1:A:123:PRO:HG3	1:A:218:PHE:CD1	2.46	0.50
1:A:358:PRO:HG3	1:B:362:TRP:CE3	2.46	0.50
1:A:38:PHE:HB3	1:A:60:PHE:CZ	2.47	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:136:TYR:CE2	1:B:138:SER:HA	2.47	0.49
1:B:292:GLN:NE2	1:B:298:GLY:HA2	2.27	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:146:PHE:HB3	1:B:194:MET:CG	2.43	0.49
1:B:57:PRO:HG2	1:B:370:LEU:HD21	1.95	0.49
1:A:36:THR:O	1:A:59:LYS:HA	2.13	0.49
1:B:245:VAL:HG12	1:B:260:TYR:CD2	2.47	0.49
1:B:299:LYS:HE2	1:B:323:ILE:HG22	1.93	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:A:321:ASN:O	1:A:325:VAL:HG23	2.13	0.48
1:B:226:ARG:HE	1:B:226:ARG:HA	1.78	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:152:MET:SD	1:B:153:TYR:N	2.87	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:192:ARG:HB2	1:A:192:ARG:NH1	2.30	0.47
1:A:38:PHE:CD2	1:A:69:TRP:CZ3	3.03	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:A:119:LYS:O	1:A:120:PHE:CB	2.63	0.47
1:B:34:LEU:HA	1:B:35:PRO:HD3	1.75	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:A:276:LYS:NZ	1:A:356:MET:SD	2.80	0.46
1:B:121:PRO:HB3	1:B:128:TYR:HD2	1.81	0.46
1:B:145:VAL:HG23	1:B:183:VAL:HG13	1.96	0.46
1:B:206:ARG:NH2	1:B:238:ARG:O	2.47	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:A:35:PRO:HD3	1:A:86:PHE:CE1	2.51	0.46
1:B:176:PRO:HD2	1:B:179:ILE:HD12	1.97	0.46
1:B:213:TRP:CZ2	1:B:290:VAL:HG21	2.50	0.46
1:A:10:THR:HA	1:A:14:ASN:O	2.16	0.46
1:B:159:TRP:CH2	1:B:161:ALA:HA	2.51	0.46
1:A:10:THR:CG2	1:A:15:ILE:HD13	2.44	0.46
1:B:34:LEU:HD11	1:B:63:MET:HG2	1.98	0.46
1:A:297:LYS:HE2	1:A:297:LYS:HA	1.98	0.46
1:B:309:LEU:CD1	1:B:313:ASN:HB3	2.45	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:A:123:PRO:HA	1:A:222:TYR:CD2	2.52	0.45
1:A:361:THR:O	1:A:365:ILE:HG12	2.15	0.45
1:B:113:ILE:HG22	1:B:133:ILE:HG12	1.98	0.45
1:B:144:TYR:HB3	1:B:186:MET:HE1	1.98	0.45
1:B:207:PRO:O	1:B:265:VAL:HG13	2.17	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:213:TRP:CH2	1:A:290:VAL:HG11	2.51	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:300:LEU:HD12	1:B:301:PRO:HD2	1.99	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:A:119:LYS:HA	1:A:119:LYS:HD2	1.76	0.45
1:B:120:PHE:O	1:B:122:ASP:N	2.49	0.45
1:B:233:GLU:O	1:B:234:ARG:CB	2.64	0.45
1:B:314:HIS:O	1:B:316:ARG:N	2.50	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:O	1:B:3:GLU:HG3	2.15	0.44
1:A:358:PRO:HA	1:B:362:TRP:CG	2.51	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:192:ARG:HB2	1:A:192:ARG:HH11	1.82	0.44
1:B:146:PHE:N	1:B:146:PHE:CD1	2.86	0.44
1:B:42:LYS:HG2	1:B:85:ASP:OD1	2.17	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:165:ALA:HB2	1:A:180:LEU:CD1	2.47	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:B:163:LEU:HD22	1:B:172:GLY:CA	2.48	0.43
1:B:143:PHE:HZ	1:B:182:ARG:HH21	1.65	0.43
1:B:62:SER:HB3	1:B:64:LYS:HG2	2.00	0.43
1:A:95:TYR:O	1:A:349:LYS:NZ	2.47	0.43
1:B:280:THR:OG1	1:B:285:PHE:HZ	1.98	0.43
1:A:149:LEU:HB3	1:A:156:VAL:HG12	2.01	0.43
1:B:120:PHE:N	1:B:121:PRO:CD	2.82	0.43
1:B:262:ILE:HD13	1:B:267:ILE:HD11	2.01	0.43
1:B:342:LEU:O	1:B:346:TYR:CD2	2.71	0.43
1:B:7:SER:HB3	1:B:18:ARG:HB2	1.99	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:140:ASP:O	1:B:142:ARG:CD	2.66	0.43
1:B:249:LEU:N	1:B:249:LEU:HD23	2.34	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:A:19:TYR:O	1:A:26:GLU:HA	2.18	0.42
1:B:144:TYR:HD2	1:B:186:MET:HE2	1.84	0.42
1:B:274:TYR:O	1:B:278:ALA:HB3	2.19	0.42
1:B:329:GLN:O	1:B:333:LYS:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:232:GLY:O	1:B:235:SER:HB2	2.20	0.42
1:A:197:GLU:O	1:A:200:ASN:HB2	2.20	0.42
1:A:220:VAL:O	1:A:224:MET:HG2	2.20	0.42
1:B:305:PRO:HG2	1:B:306:ILE:H	1.84	0.42
1:A:147:ASP:OD2	1:A:314:HIS:CE1	2.72	0.42
1:A:343:SER:HB2	1:B:369:SER:HB2	2.01	0.42
1:A:358:PRO:HA	1:B:362:TRP:CB	2.49	0.42
1:A:41:CYS:HB3	1:B:279:PHE:CG	2.54	0.42
1:B:292:GLN:O	1:B:296:LYS:N	2.52	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: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:9:GLU:CG	1:B:10:THR:H	2.32	0.42
1:A:166:LYS:HB3	1:A:170:GLU:HG3	2.01	0.42
1:B:115:VAL:HG22	1:B:130:ILE:HA	2.02	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:A:101:TYR:N	1:A:101:TYR:CD1	2.88	0.41
1:B:103:ARG:NH1	1:B:103:ARG:CG	2.82	0.41
1:B:273:LEU:HD23	1:B:273:LEU:N	2.35	0.41
1:B:130:ILE:CD1	1:B:133:ILE:HG13	2.49	0.41
1:A:168:ASP:HB2	1:A:300:LEU:HD13	2.03	0.41
1:A:38:PHE:HB2	1:A:69:TRP:CZ2	2.55	0.41
1:A:42:LYS:HG3	1:A:85:ASP:OD2	2.21	0.41
1:A:112:ASP:HB2	1:A:325:VAL:HG22	2.02	0.41
1:B:144:TYR:HD2	1:B:186:MET:CE	2.33	0.41
1:B:227:VAL:O	1:B:232:GLY:N	2.53	0.41
1:B:299:LYS:HG3	1:B:300:LEU:N	2.34	0.41
1:A:3:GLU:OE1	1:A:3:GLU:HA	2.21	0.41
1:B:202:TRP:CD1	1:B:239:PHE:HE1	2.38	0.41
1:B:85:ASP:CG	1:B:367:PHE:CZ	2.94	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:203:GLU:CD	1:B:238:ARG:HH11	2.24	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
1:B:2:ASP:O	1:B:3:GLU:CB	2.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:61:PRO:HD2	1:A:65:ASP:CG	2.42	0.41
1:B:16:VAL:HA	1:B:29:ARG:O	2.21	0.41
1:B:198:TYR:HE2	1:B:223:ILE:HD13	1.85	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:113:ILE:HG21	1:A:223:ILE:HD11	2.02	0.41
1:A:148:LEU:HB2	1:A:194:MET:SD	2.61	0.41
1:A:43:GLU:OE2	1:A:72:ARG:NH1	2.54	0.41
1:B:308:LYS:CG	1:B:308:LYS:O	2.68	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:103:ARG:HG3	1:A:103:ARG:O	2.20	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: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:A:64:LYS:HD3	1:A:68:ASP:OD2	2.21	0.40
1:B:167:LEU:HA	1:B:174:GLU:CG	2.52	0.40
1:B:201:LEU:HD11	1:B:205:LYS:HD2	2.04	0.40
1:B:18:ARG:NH1	1:B:26:GLU:OE2	2.54	0.40
1:B:352:PHE:O	1:B:355:VAL:HG13	2.21	0.40
1:B:39:ARG:HH12	1:B:42:LYS:HZ1	1.68	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

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	338/388 (87%)	299 (88%)	27 (8%)	12 (4%)	3 1
1	B	338/388 (87%)	294 (87%)	29 (9%)	15 (4%)	2 1
All	All	676/776 (87%)	593 (88%)	56 (8%)	27 (4%)	3 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 [\(i\)](#)

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%)	7 6
1	B	312/350 (89%)	269 (86%)	43 (14%)	3 3
All	All	624/700 (89%)	549 (88%)	75 (12%)	5 4

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 [\(i\)](#)

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 [\(i\)](#)

6.1 Protein, DNA and RNA chains [\(i\)](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [\(i\)](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates [\(i\)](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands [\(i\)](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers [\(i\)](#)

Unable to reproduce the depositors R factor - this section is therefore empty.