



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:27 PM UTC

PDB ID : 2PO4 / pdb_00002po4
Title : X-ray crystal structure of polymerase domain of the bacteriophage N4 virion
RNA polymerase
Authors : Murakami, K.S.; Davydova, E.K.; Rothman-Denes, L.B.
Deposited on : 2007-04-25
Resolution : 2.00 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

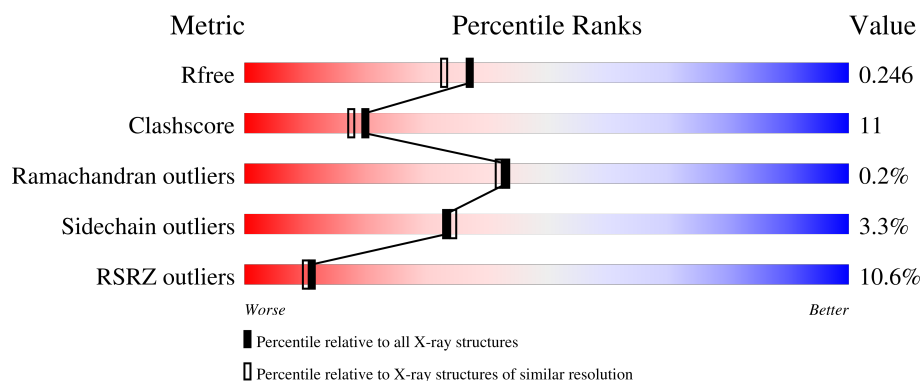
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	1104	11% 73% 24% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8916 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 Virion RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1094	Total	C	N	O	S	0	0	0
			8441	5299	1435	1666	41			

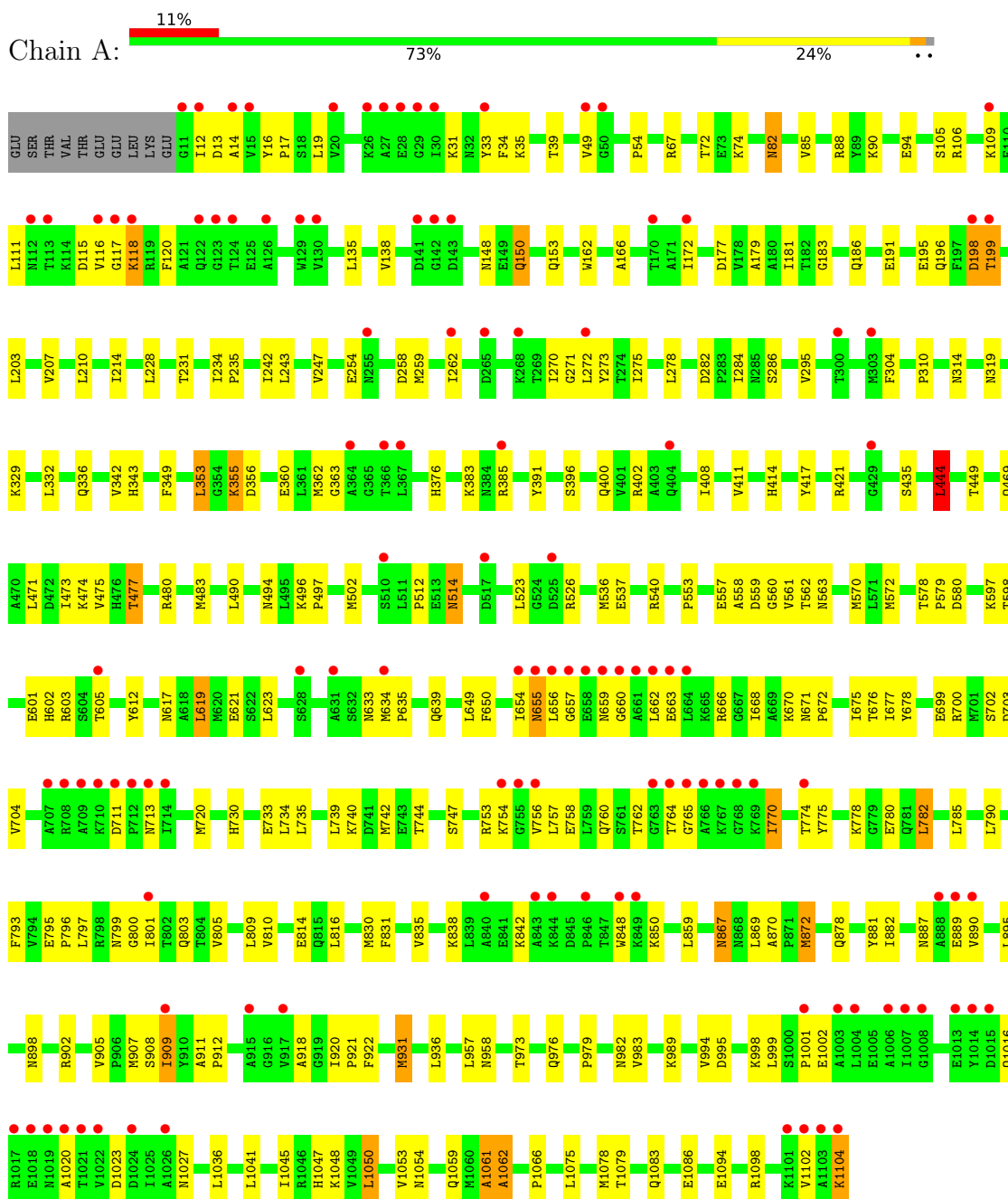
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	475	Total	O	0	0
			475	475		

3 Residue-property plots

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: Virion RNA polymerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.05Å 103.26Å 159.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00 50.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.1 (50.00-2.00) 93.1 (50.00-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.219 , 0.248 0.217 , 0.246	Depositor DCC
R_{free} test set	9139 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.3	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	0.94	EDS
Total number of atoms	8916	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% 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	0.43	0/8570	0.90	22/11590 (0.2%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118	LYS	N-CA-C	-7.96	102.56	111.07
1	A	475	VAL	N-CA-C	7.30	120.18	111.05
1	A	558	ALA	N-CA-C	-7.15	99.08	109.59
1	A	563	ASN	N-CA-C	6.47	118.91	111.02
1	A	976	GLN	N-CA-C	-6.27	105.63	113.28
1	A	872	MET	N-CA-C	5.89	119.00	109.40
1	A	867	ASN	N-CA-C	5.78	118.32	111.33
1	A	494	ASN	N-CA-C	5.75	118.28	111.33
1	A	411	VAL	N-CA-C	5.72	113.54	107.76
1	A	1061	ALA	N-CA-C	5.57	118.67	110.59
1	A	295	VAL	N-CA-C	5.56	115.76	110.53
1	A	770	ILE	N-CA-C	5.53	116.14	108.84
1	A	957	LEU	N-CA-C	5.45	119.03	112.38
1	A	473	ILE	N-CA-C	-5.33	101.95	109.21
1	A	882	ILE	N-CA-C	5.30	116.66	110.62
1	A	34	PHE	N-CA-C	-5.14	105.13	111.40
1	A	148	ASN	N-CA-C	-5.13	100.71	108.67
1	A	559	ASP	N-CA-C	5.08	116.69	108.41
1	A	435	SER	N-CA-C	5.05	119.52	112.90
1	A	191	GLU	N-CA-C	5.05	117.17	111.11
1	A	278	LEU	N-CA-C	-5.04	102.61	110.42
1	A	444	LEU	CA-CB-CG	5.02	133.88	116.30

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	8441	0	8477	193	0
2	A	475	0	0	5	0
All	All	8916	0	8477	193	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 11.

All (193) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:GLN:HE22	1:A:557:GLU:H	1.10	0.94
1:A:336:GLN:HE21	1:A:417:TYR:H	1.20	0.86
1:A:13:ASP:HA	1:A:35:LYS:HE3	1.69	0.75
1:A:90:LYS:O	1:A:94:GLU:HG3	1.87	0.73
1:A:198:ASP:CB	1:A:666:ARG:HH21	2.01	0.73
1:A:349:PHE:CE1	1:A:502:MET:HE1	2.24	0.73
1:A:898:ASN:HD21	1:A:902:ARG:HB2	1.56	0.70
1:A:677:ILE:HD11	1:A:805:VAL:HG11	1.73	0.70
1:A:512:PRO:HB2	1:A:514:ASN:ND2	2.07	0.69
1:A:633:ASN:OD1	1:A:635:PRO:HG2	1.93	0.69
1:A:810:VAL:O	1:A:814:GLU:HG3	1.93	0.69
1:A:908:SER:O	1:A:909:ILE:HD12	1.92	0.69
1:A:54:PRO:HG2	1:A:153:GLN:HB2	1.75	0.68
1:A:920:ILE:HB	1:A:921:PRO:HD3	1.75	0.68
1:A:747:SER:OG	1:A:765:GLY:HA3	1.93	0.68
1:A:195:GLU:HG3	1:A:383:LYS:HG2	1.75	0.68
1:A:711:ASP:OD1	1:A:713:ASN:HB2	1.94	0.68
1:A:895:LEU:HD13	1:A:907:MET:HE3	1.74	0.68
1:A:16:TYR:HB3	1:A:19:LEU:HG	1.77	0.66
1:A:753:ARG:HD2	1:A:758:GLU:OE2	1.94	0.66
1:A:363:GLY:HA2	1:A:662:LEU:HD11	1.77	0.66
1:A:597:LYS:HE2	1:A:602:HIS:HB2	1.76	0.66
1:A:678:TYR:HB3	1:A:921:PRO:HG3	1.77	0.66
1:A:639:GLN:OE1	1:A:744:THR:HG22	1.96	0.66
1:A:82:ASN:HD22	1:A:82:ASN:C	2.03	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:617:ASN:O	1:A:621:GLU:HG3	1.96	0.66
1:A:918:ALA:O	1:A:921:PRO:HD2	1.95	0.65
1:A:496:LYS:HB3	1:A:497:PRO:HD3	1.77	0.65
1:A:1075:LEU:HA	1:A:1078:MET:HE3	1.79	0.65
1:A:449:THR:H	1:A:958:ASN:HD21	1.45	0.65
1:A:356:ASP:O	1:A:360:GLU:HG3	1.97	0.65
1:A:195:GLU:O	1:A:199:THR:HB	1.97	0.64
1:A:649:LEU:HD21	1:A:734:LEU:HD22	1.80	0.63
1:A:177:ASP:O	1:A:181:ILE:HG13	1.99	0.62
1:A:1041:LEU:O	1:A:1045:ILE:HG12	2.00	0.61
1:A:117:GLY:HA2	1:A:120:PHE:HB3	1.82	0.61
1:A:198:ASP:HB2	1:A:666:ARG:HH21	1.65	0.61
1:A:1075:LEU:HD21	1:A:1086:GLU:HG2	1.83	0.61
1:A:421:ARG:HG2	1:A:922:PHE:CZ	2.35	0.61
1:A:181:ILE:HG22	1:A:270:ILE:HD13	1.83	0.61
1:A:514:ASN:HD22	1:A:514:ASN:H	1.48	0.61
1:A:198:ASP:CG	1:A:666:ARG:HE	2.07	0.60
1:A:228:LEU:HD11	1:A:859:LEU:CD1	2.30	0.60
1:A:106:ARG:HA	1:A:109:LYS:HD2	1.83	0.60
1:A:314:ASN:HD22	1:A:329:LYS:CE	2.15	0.59
1:A:830:MET:HA	1:A:830:MET:HE2	1.83	0.59
1:A:54:PRO:HG2	1:A:153:GLN:CB	2.33	0.59
1:A:214:ILE:HD11	1:A:242:ILE:HD12	1.85	0.59
1:A:343:HIS:HE1	1:A:537:GLU:OE2	1.86	0.59
1:A:12:ILE:HG12	1:A:39:THR:HA	1.85	0.58
1:A:31:LYS:HE2	1:A:33:TYR:OH	2.02	0.58
1:A:186:GLN:HG2	1:A:668:ILE:HD13	1.86	0.58
1:A:676:THR:HG21	1:A:801:ILE:HD12	1.85	0.58
1:A:514:ASN:HD22	1:A:514:ASN:N	2.02	0.57
1:A:199:THR:HG21	1:A:385:ARG:NE	2.20	0.57
1:A:314:ASN:HD22	1:A:329:LYS:HE3	1.69	0.57
1:A:790:LEU:O	1:A:795:GLU:HG3	2.05	0.57
1:A:1075:LEU:HA	1:A:1078:MET:CE	2.35	0.56
1:A:355:LYS:HD3	1:A:391:TYR:CD2	2.41	0.56
1:A:730:HIS:HD2	1:A:733:GLU:OE2	1.89	0.56
1:A:228:LEU:HD11	1:A:859:LEU:HD12	1.86	0.56
1:A:619:LEU:HD22	1:A:797:LEU:HB2	1.88	0.56
1:A:135:LEU:O	1:A:138:VAL:HG22	2.06	0.55
1:A:1016:GLN:O	1:A:1020:ALA:HB2	2.06	0.55
1:A:258:ASP:C	1:A:259:MET:HE2	2.31	0.55
1:A:597:LYS:NZ	1:A:602:HIS:HD2	2.03	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:639:GLN:OE1	1:A:744:THR:CG2	2.55	0.55
1:A:830:MET:HE3	1:A:999:LEU:HD23	1.89	0.55
1:A:1098:ARG:O	1:A:1102:VAL:HG23	2.07	0.54
1:A:704:VAL:HG21	1:A:720:MET:HE2	1.90	0.54
1:A:474:LYS:O	1:A:477:THR:HB	2.08	0.54
1:A:619:LEU:C	1:A:619:LEU:HD12	2.32	0.54
1:A:12:ILE:N	1:A:12:ILE:HD12	2.23	0.54
1:A:887:ASN:HD21	1:A:890:VAL:HG23	1.72	0.53
1:A:111:LEU:O	1:A:116:VAL:O	2.27	0.53
1:A:234:ILE:HB	1:A:235:PRO:HD3	1.91	0.53
1:A:1061:ALA:O	1:A:1062:ALA:HB2	2.09	0.53
1:A:376:HIS:HD2	1:A:702:SER:OG	1.92	0.52
1:A:848:TRP:CH2	1:A:850:LYS:HA	2.45	0.52
1:A:887:ASN:HB2	1:A:889:GLU:OE1	2.10	0.52
1:A:172:ILE:HG23	1:A:198:ASP:OD1	2.09	0.52
1:A:162:TRP:CG	1:A:210:LEU:HD13	2.44	0.52
1:A:1041:LEU:C	1:A:1041:LEU:HD13	2.35	0.51
1:A:286:SER:O	1:A:400:GLN:HG2	2.10	0.51
1:A:271:GLY:C	1:A:272:LEU:HD12	2.35	0.51
1:A:362:MET:HB2	1:A:662:LEU:HD21	1.93	0.51
1:A:228:LEU:HA	1:A:231:THR:OG1	2.11	0.50
1:A:105:SER:O	1:A:109:LYS:HG3	2.11	0.50
1:A:672:PRO:HA	1:A:675:ILE:HG12	1.93	0.50
1:A:619:LEU:HD12	1:A:619:LEU:O	2.11	0.50
1:A:570:MET:HE1	1:A:1050:LEU:HD23	1.94	0.50
1:A:800:GLY:O	1:A:803:GLN:HG2	2.12	0.50
1:A:831:PHE:O	1:A:835:VAL:HG23	2.11	0.50
1:A:598:THR:OG1	1:A:601:GLU:HG3	2.11	0.49
1:A:801:ILE:O	1:A:805:VAL:HG22	2.12	0.49
1:A:1045:ILE:HD12	1:A:1094:GLU:HG3	1.93	0.49
1:A:578:THR:HG22	1:A:580:ASP:H	1.78	0.49
1:A:739:LEU:HD21	1:A:770:ILE:HD12	1.95	0.49
1:A:902:ARG:HD2	2:A:1334:HOH:O	2.13	0.48
1:A:561:VAL:O	1:A:562:THR:C	2.56	0.48
1:A:842:LYS:HE2	1:A:848:TRP:CD1	2.48	0.48
1:A:1061:ALA:O	1:A:1062:ALA:CB	2.62	0.48
1:A:878:GLN:NE2	1:A:931:MET:HG2	2.29	0.48
1:A:332:LEU:O	1:A:336:GLN:HG3	2.14	0.48
1:A:660:GLY:HA3	1:A:663:GLU:HG3	1.96	0.48
1:A:887:ASN:HD22	1:A:889:GLU:HB2	1.78	0.48
1:A:304:PHE:CD2	1:A:310:PRO:HG3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:THR:HB	1:A:74:LYS:HE2	1.95	0.48
1:A:258:ASP:O	1:A:259:MET:HE2	2.14	0.47
1:A:762:THR:HB	1:A:764:THR:HG22	1.95	0.47
1:A:870:ALA:HB2	1:A:989:LYS:HD3	1.95	0.47
1:A:793:PHE:O	1:A:796:PRO:HG2	2.14	0.47
1:A:179:ALA:O	1:A:183:GLY:N	2.45	0.47
1:A:396:SER:O	1:A:400:GLN:HG3	2.15	0.47
1:A:654:ILE:O	1:A:656:LEU:HG	2.15	0.47
1:A:742:MET:HE1	1:A:785:LEU:HD11	1.97	0.47
1:A:895:LEU:CD1	1:A:907:MET:HE3	2.41	0.47
1:A:1053:VAL:HG11	1:A:1075:LEU:HD12	1.96	0.47
1:A:82:ASN:ND2	1:A:85:VAL:H	2.13	0.47
1:A:572:MET:HE3	1:A:809:LEU:HD11	1.96	0.46
1:A:512:PRO:HB2	1:A:514:ASN:HD22	1.78	0.46
1:A:282:ASP:OD1	1:A:284:ILE:HG22	2.16	0.46
1:A:203:LEU:O	1:A:207:VAL:HG23	2.16	0.45
1:A:597:LYS:HZ3	1:A:602:HIS:HD2	1.64	0.45
1:A:82:ASN:C	1:A:82:ASN:ND2	2.71	0.45
1:A:570:MET:O	1:A:1047:HIS:HE1	2.00	0.45
1:A:514:ASN:ND2	1:A:514:ASN:H	2.13	0.45
1:A:994:VAL:HG22	1:A:995:ASP:N	2.31	0.45
1:A:523:LEU:O	1:A:526:ARG:HB2	2.17	0.45
1:A:700:ARG:O	1:A:703:ASP:HB2	2.17	0.45
1:A:16:TYR:OH	1:A:150:GLN:NE2	2.48	0.45
1:A:911:ALA:HB1	1:A:912:PRO:HD2	1.98	0.45
1:A:199:THR:HG21	1:A:385:ARG:HE	1.81	0.45
1:A:477:THR:HA	1:A:603:ARG:HG2	1.98	0.44
1:A:796:PRO:HA	1:A:799:ASN:HD22	1.81	0.44
1:A:1104:LYS:HA	1:A:1104:LYS:HE2	1.99	0.44
1:A:774:THR:O	1:A:775:TYR:C	2.58	0.44
1:A:654:ILE:O	1:A:656:LEU:N	2.51	0.44
1:A:82:ASN:HB2	2:A:1359:HOH:O	2.18	0.44
1:A:262:ILE:HD11	2:A:1187:HOH:O	2.17	0.44
1:A:816:LEU:HD13	1:A:983:VAL:HG21	2.00	0.44
1:A:598:THR:HG22	1:A:1066:PRO:HD3	1.99	0.44
1:A:756:VAL:HG12	1:A:757:LEU:N	2.33	0.44
1:A:560:GLY:HA2	1:A:1059:GLN:O	2.18	0.44
1:A:19:LEU:HD12	1:A:35:LYS:HD2	2.00	0.44
1:A:764:THR:HG21	1:A:780:GLU:HB3	1.99	0.44
1:A:797:LEU:O	1:A:801:ILE:HG13	2.18	0.44
1:A:778:LYS:HA	1:A:782:LEU:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:872:MET:HG2	1:A:881:TYR:HB2	2.00	0.43
1:A:1053:VAL:HG12	1:A:1054:ASN:N	2.34	0.43
1:A:402:ARG:HA	1:A:408:ILE:HG22	2.00	0.43
1:A:536:MET:O	1:A:540:ARG:HG3	2.19	0.43
1:A:105:SER:OG	1:A:109:LYS:HE3	2.19	0.43
1:A:254:GLU:HB2	1:A:273:TYR:CE1	2.53	0.43
1:A:512:PRO:HB2	1:A:514:ASN:HD21	1.83	0.43
1:A:342:VAL:HG11	1:A:408:ILE:HD12	2.00	0.43
1:A:655:ASN:ND2	1:A:671:ASN:HD21	2.15	0.43
1:A:995:ASP:OD2	1:A:998:LYS:HE3	2.19	0.43
1:A:1023:ASP:O	1:A:1027:ASN:ND2	2.51	0.43
1:A:753:ARG:CZ	1:A:760:GLN:HE22	2.32	0.43
1:A:243:LEU:O	1:A:247:VAL:HG23	2.19	0.43
1:A:562:THR:HG22	1:A:612:TYR:CE1	2.53	0.43
1:A:166:ALA:HB3	1:A:275:ILE:CD1	2.49	0.43
1:A:753:ARG:O	1:A:754:LYS:HB2	2.19	0.43
1:A:343:HIS:CE1	1:A:537:GLU:OE2	2.71	0.42
1:A:634:MET:N	1:A:635:PRO:HD2	2.33	0.42
1:A:650:PHE:CE2	1:A:700:ARG:HG3	2.53	0.42
1:A:908:SER:C	1:A:909:ILE:HD12	2.44	0.42
1:A:314:ASN:ND2	1:A:329:LYS:CE	2.81	0.42
1:A:336:GLN:HE21	1:A:417:TYR:N	2.01	0.42
1:A:650:PHE:HE2	1:A:700:ARG:HG3	1.84	0.42
1:A:1047:HIS:HD2	2:A:1161:HOH:O	2.01	0.42
1:A:88:ARG:HD3	1:A:282:ASP:OD1	2.19	0.42
1:A:49:VAL:O	1:A:150:GLN:NE2	2.52	0.42
1:A:336:GLN:O	1:A:414:HIS:HD2	2.03	0.42
1:A:480:ARG:O	1:A:483:MET:HG3	2.19	0.42
1:A:353:LEU:HD23	1:A:353:LEU:HA	1.91	0.42
1:A:657:GLY:C	1:A:670:LYS:HE3	2.44	0.42
1:A:887:ASN:ND2	1:A:889:GLU:HB2	2.35	0.42
1:A:115:ASP:O	1:A:118:LYS:HB2	2.19	0.42
1:A:444:LEU:HG	1:A:553:PRO:HB2	2.01	0.42
1:A:1001:PRO:HG2	1:A:1002:GLU:OE1	2.19	0.41
1:A:979:PRO:HA	1:A:982:ASN:HD22	1.85	0.41
1:A:672:PRO:HB2	1:A:797:LEU:HD21	2.01	0.41
1:A:349:PHE:HE1	1:A:502:MET:HE1	1.79	0.41
1:A:1079:THR:O	1:A:1083:GLN:HG3	2.21	0.41
1:A:376:HIS:CE1	1:A:699:GLU:HG3	2.55	0.41
1:A:805:VAL:HB	1:A:809:LEU:HD23	2.02	0.41
1:A:14:ALA:O	1:A:17:PRO:HD3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:GLN:CD	1:A:385:ARG:HH21	2.29	0.40
1:A:578:THR:HG23	1:A:579:PRO:HD2	2.04	0.40
1:A:207:VAL:HG11	1:A:905:VAL:HG21	2.04	0.40
1:A:1048:LYS:HD2	2:A:1317:HOH: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	1092/1104 (99%)	1055 (97%)	35 (3%)	2 (0%)	43 42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1062	ALA
1	A	655	ASN

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	914/924 (99%)	884 (97%)	30 (3%)	33 34

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	ARG
1	A	82	ASN
1	A	150	GLN
1	A	198	ASP
1	A	199	THR
1	A	319	ASN
1	A	353	LEU
1	A	355	LYS
1	A	444	LEU
1	A	471	LEU
1	A	477	THR
1	A	490	LEU
1	A	514	ASN
1	A	605	THR
1	A	619	LEU
1	A	623	LEU
1	A	659	ASN
1	A	735	LEU
1	A	740	LYS
1	A	782	LEU
1	A	838	LYS
1	A	867	ASN
1	A	869	LEU
1	A	909	ILE
1	A	931	MET
1	A	936	LEU
1	A	973	THR
1	A	1036	LEU
1	A	1050	LEU
1	A	1104	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	82	ASN
1	A	169	ASN
1	A	255	ASN
1	A	314	ASN
1	A	316	GLN
1	A	319	ASN
1	A	324	ASN
1	A	336	GLN

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Mol	Chain	Res	Type
1	A	343	HIS
1	A	348	GLN
1	A	375	ASN
1	A	376	HIS
1	A	384	ASN
1	A	393	GLN
1	A	414	HIS
1	A	464	GLN
1	A	469	GLN
1	A	514	ASN
1	A	563	ASN
1	A	602	HIS
1	A	608	ASN
1	A	655	ASN
1	A	730	HIS
1	A	760	GLN
1	A	799	ASN
1	A	817	GLN
1	A	833	GLN
1	A	836	GLN
1	A	878	GLN
1	A	887	ASN
1	A	914	GLN
1	A	954	ASN
1	A	958	ASN
1	A	982	ASN
1	A	1016	GLN
1	A	1027	ASN
1	A	1047	HIS
1	A	1059	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	1094/1104 (99%)	0.50	116 (10%)	11 10	13, 29, 58, 79	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	660	GLY	6.1
1	A	766	ALA	5.5
1	A	1022	VAL	5.0
1	A	12	ILE	4.8
1	A	661	ALA	4.6
1	A	658	GLU	4.4
1	A	656	LEU	4.4
1	A	117	GLY	4.0
1	A	367	LEU	4.0
1	A	1102	VAL	3.8
1	A	844	LYS	3.8
1	A	657	GLY	3.7
1	A	49	VAL	3.6
1	A	659	ASN	3.6
1	A	1019	ASN	3.5
1	A	765	GLY	3.4
1	A	130	VAL	3.4
1	A	385	ARG	3.3
1	A	915	ALA	3.2
1	A	917	VAL	3.1
1	A	1015	ASP	3.1
1	A	1003	ALA	3.1
1	A	112	ASN	3.1
1	A	1006	ALA	3.1
1	A	50	GLY	3.1
1	A	1020	ALA	3.0
1	A	1021	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	767	LYS	2.9
1	A	1008	GLY	2.9
1	A	909	ILE	2.9
1	A	170	THR	2.9
1	A	1018	GLU	2.9
1	A	664	LEU	2.9
1	A	116	VAL	2.9
1	A	517	ASP	2.9
1	A	122	GLN	2.9
1	A	714	ILE	2.9
1	A	663	GLU	2.9
1	A	764	THR	2.8
1	A	255	ASN	2.8
1	A	27	ALA	2.8
1	A	712	PRO	2.8
1	A	123	GLY	2.8
1	A	126	ALA	2.8
1	A	628	SER	2.8
1	A	711	ASP	2.8
1	A	1001	PRO	2.8
1	A	143	ASP	2.7
1	A	11	GLY	2.7
1	A	710	LYS	2.7
1	A	14	ALA	2.7
1	A	1004	LEU	2.7
1	A	26	LYS	2.7
1	A	662	LEU	2.6
1	A	172	ILE	2.6
1	A	142	GLY	2.6
1	A	655	ASN	2.6
1	A	109	LYS	2.6
1	A	763	GLY	2.6
1	A	801	ILE	2.5
1	A	1104	LYS	2.5
1	A	707	ALA	2.5
1	A	20	VAL	2.5
1	A	124	THR	2.5
1	A	404	GLN	2.5
1	A	303	MET	2.5
1	A	848	TRP	2.5
1	A	29	GLY	2.5
1	A	755	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	774	THR	2.5
1	A	888	ALA	2.5
1	A	272	LEU	2.5
1	A	708	ARG	2.5
1	A	15	VAL	2.4
1	A	30	ILE	2.5
1	A	510	SER	2.4
1	A	364	ALA	2.4
1	A	198	ASP	2.4
1	A	846	PRO	2.4
1	A	141	ASP	2.4
1	A	118	LYS	2.4
1	A	634	MET	2.4
1	A	1024	ASP	2.3
1	A	33	TYR	2.3
1	A	709	ALA	2.3
1	A	843	ALA	2.3
1	A	768	GLY	2.3
1	A	605	THR	2.3
1	A	1026	ALA	2.3
1	A	654	ILE	2.3
1	A	429	GLY	2.3
1	A	754	LYS	2.3
1	A	1103	ALA	2.3
1	A	300	THR	2.2
1	A	756	VAL	2.2
1	A	366	THR	2.2
1	A	1014	TYR	2.2
1	A	849	LYS	2.2
1	A	129	TRP	2.2
1	A	889	GLU	2.1
1	A	631	ALA	2.1
1	A	713	ASN	2.1
1	A	262	ILE	2.1
1	A	1007	ILE	2.1
1	A	890	VAL	2.1
1	A	1017	ARG	2.1
1	A	268	LYS	2.1
1	A	265	ASP	2.1
1	A	113	THR	2.1
1	A	840	ALA	2.1
1	A	1013	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1101	LYS	2.0
1	A	28	GLU	2.0
1	A	525	ASP	2.0
1	A	769	LYS	2.0
1	A	199	THR	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 oligosaccharides 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.