



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:58 AM UTC

PDB ID : 4I5T / pdb_00004i5t
Title : Crystal structure of yeast Ap4A phosphorylase Apa2
Authors : Jiang, Y.L.; Hou, W.T.; Chen, Y.; Zhou, C.Z.
Deposited on : 2012-11-29
Resolution : 2.30 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

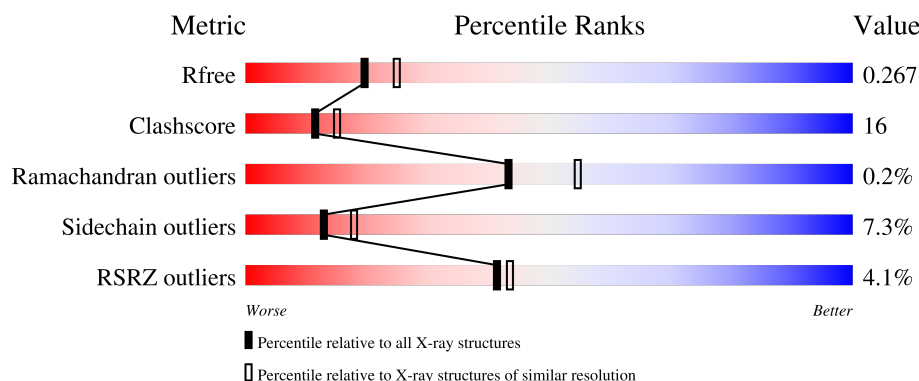
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	333	6% 66% 21% 5% 8%
1	B	333	6% 60% 26% 6% 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5094 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 5',5'''-P-1,P-4-tetraphosphate phosphorylase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	0	0	0
			2444	1560	402	466	16			
1	B	305	Total	C	N	O	S	0	0	0
			2426	1544	398	468	16			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	expression tag	UNP P22108
A	-6	GLY	-	expression tag	UNP P22108
A	-5	HIS	-	expression tag	UNP P22108
A	-4	HIS	-	expression tag	UNP P22108
A	-3	HIS	-	expression tag	UNP P22108
A	-2	HIS	-	expression tag	UNP P22108
A	-1	HIS	-	expression tag	UNP P22108
A	0	HIS	-	expression tag	UNP P22108
B	-7	MET	-	expression tag	UNP P22108
B	-6	GLY	-	expression tag	UNP P22108
B	-5	HIS	-	expression tag	UNP P22108
B	-4	HIS	-	expression tag	UNP P22108
B	-3	HIS	-	expression tag	UNP P22108
B	-2	HIS	-	expression tag	UNP P22108
B	-1	HIS	-	expression tag	UNP P22108
B	0	HIS	-	expression tag	UNP P22108

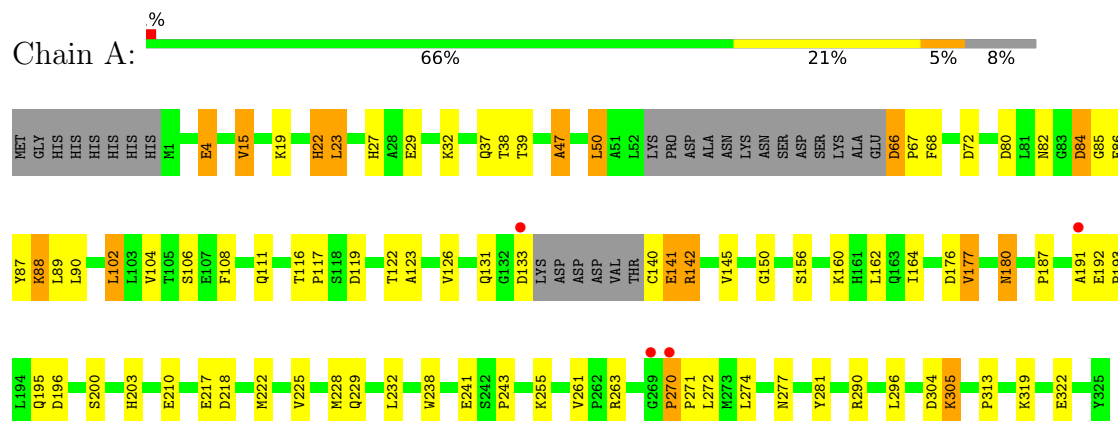
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	120	Total	O	0	0
			120	120		
2	B	104	Total	O	0	0
			104	104		

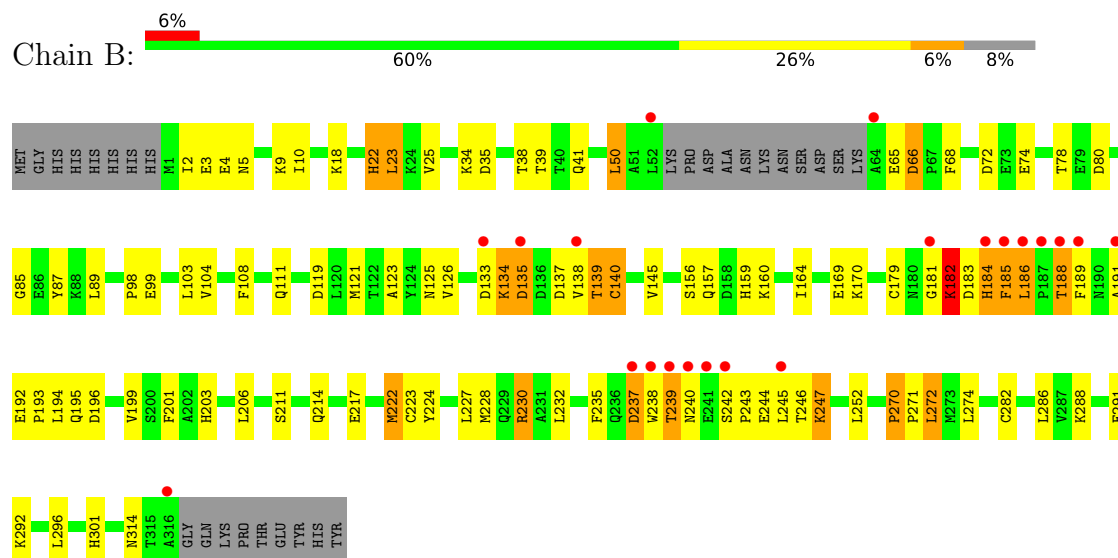
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 5',5'''-P-1,P-4-tetraphosphate phosphorylase 2



- Molecule 1: 5',5'''-P-1,P-4-tetraphosphate phosphorylase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.76Å 74.46Å 112.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.84 – 2.30 44.84 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.0 (44.84-2.30) 97.0 (44.84-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.203 , 0.278 0.199 , 0.267	Depositor DCC
R_{free} test set	1374 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	37.8	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.006 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5094	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.13 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.4929e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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	0.55	1/2505 (0.0%)	0.91	13/3399 (0.4%)
1	B	0.54	1/2484 (0.0%)	0.94	11/3372 (0.3%)
All	All	0.54	2/4989 (0.0%)	0.93	24/6771 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	22	HIS	ND1-CE1	5.36	1.38	1.32
1	A	22	HIS	ND1-CE1	5.22	1.37	1.32

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	182	LYS	N-CA-C	-8.36	103.07	113.18
1	B	186	LEU	CA-C-N	7.30	128.97	119.84
1	B	186	LEU	C-N-CA	7.30	128.97	119.84
1	A	270	PRO	CA-C-N	-7.00	111.09	119.84
1	A	270	PRO	C-N-CA	-7.00	111.09	119.84
1	A	270	PRO	N-CA-C	6.85	119.06	110.70
1	A	22	HIS	CB-CG-CD2	-6.71	122.48	131.20
1	B	66	ASP	CA-C-N	6.61	126.31	119.56
1	B	66	ASP	C-N-CA	6.61	126.31	119.56
1	B	22	HIS	CB-CG-CD2	-6.60	122.62	131.20
1	B	270	PRO	CA-C-N	-6.45	111.78	119.84
1	B	270	PRO	C-N-CA	-6.45	111.78	119.84
1	B	270	PRO	N-CA-C	6.20	118.26	110.70
1	A	150	GLY	CA-C-N	6.16	126.06	119.28
1	A	150	GLY	C-N-CA	6.16	126.06	119.28
1	A	66	ASP	CA-C-N	5.94	125.62	119.56
1	A	66	ASP	C-N-CA	5.94	125.62	119.56
1	A	22	HIS	CB-CG-ND1	5.72	131.28	122.70
1	B	22	HIS	CB-CG-ND1	5.68	131.22	122.70
1	A	47	ALA	CA-C-N	5.54	125.00	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	ALA	C-N-CA	5.54	125.00	119.24
1	B	237	ASP	N-CA-C	5.25	121.99	110.80
1	A	29	GLU	N-CA-C	-5.11	101.30	109.23
1	A	261	VAL	CB-CA-C	-5.02	104.95	110.52

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	2444	0	2396	57	1
1	B	2426	0	2380	99	1
2	A	120	0	0	10	0
2	B	104	0	0	6	0
All	All	5094	0	4776	155	1

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 16.

All (155) 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:183:ASP:HB3	1:B:184:HIS:HA	1.43	1.00
1:B:103:LEU:CD1	1:B:164:ILE:HD11	1.92	0.99
1:B:103:LEU:HD11	1:B:164:ILE:HD11	1.49	0.93
1:B:50:LEU:HD23	1:B:288:LYS:NZ	1.89	0.88
1:B:139:THR:HA	1:B:169:GLU:HG3	1.59	0.84
1:B:41:GLN:HG2	2:B:458:HOH:O	1.81	0.81
1:B:50:LEU:HD23	1:B:288:LYS:HZ1	1.48	0.78
1:B:188:THR:HG22	1:B:189:PHE:H	1.49	0.78
1:A:32:LYS:HG3	2:A:503:HOH:O	1.83	0.77
1:A:177:VAL:O	1:A:180:ASN:ND2	2.17	0.77
1:B:157:GLN:HG3	2:B:466:HOH:O	1.83	0.76
1:B:191:ALA:O	1:B:192:GLU:HG2	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:GLU:OE1	1:B:4:GLU:N	2.14	0.75
1:B:239:THR:HB	1:B:240:ASN:HA	1.69	0.75
1:B:185:PHE:HZ	1:B:194:LEU:HD21	1.52	0.74
1:A:80:ASP:HA	1:A:87:TYR:O	1.87	0.74
1:B:239:THR:CB	1:B:240:ASN:HA	2.18	0.72
1:B:189:PHE:HA	1:B:222:MET:HE1	1.73	0.70
1:B:126:VAL:HG11	1:B:164:ILE:HD13	1.73	0.70
1:A:187:PRO:HB3	1:A:193:PRO:HD3	1.74	0.69
1:B:68:PHE:HB3	1:B:104:VAL:HG11	1.75	0.68
1:B:133:ASP:OD1	1:B:134:LYS:N	2.27	0.68
1:B:80:ASP:OD1	1:B:85:GLY:HA2	1.95	0.67
1:A:72:ASP:HB2	2:A:519:HOH:O	1.94	0.66
1:A:192:GLU:HG3	1:A:193:PRO:HD2	1.78	0.66
1:B:5:ASN:HB3	2:B:474:HOH:O	1.97	0.65
1:B:4:GLU:H	1:B:4:GLU:CD	2.03	0.65
1:B:242:SER:N	1:B:243:PRO:HA	2.11	0.65
1:B:185:PHE:CZ	1:B:194:LEU:HD21	2.31	0.64
1:B:272:LEU:HD21	1:B:296:LEU:HD21	1.80	0.64
1:B:246:THR:HA	2:B:461:HOH:O	1.98	0.64
1:A:80:ASP:HB3	2:A:502:HOH:O	1.98	0.63
1:B:111:GLN:OE1	1:B:160:LYS:HA	1.99	0.63
1:B:272:LEU:HB3	1:B:274:LEU:HG	1.81	0.62
1:B:50:LEU:HD23	1:B:288:LYS:HZ2	1.64	0.61
1:B:239:THR:HB	1:B:240:ASN:CA	2.30	0.61
1:B:41:GLN:HG3	2:B:489:HOH:O	2.01	0.60
1:B:242:SER:HB2	1:B:243:PRO:O	2.01	0.60
1:B:230:ARG:HG3	1:B:230:ARG:HH11	1.68	0.59
1:B:242:SER:HB2	1:B:243:PRO:C	2.28	0.59
1:A:313:PRO:HG2	2:A:457:HOH:O	2.02	0.58
1:B:270:PRO:HG2	1:B:271:PRO:HD3	1.85	0.57
1:A:123:ALA:HB1	1:A:145:VAL:HG11	1.86	0.57
1:A:131:GLN:HG2	1:A:141:GLU:O	2.05	0.57
1:A:22:HIS:HD2	1:A:72:ASP:OD2	1.85	0.57
1:A:88:LYS:HG3	1:A:90:LEU:CD1	2.34	0.57
1:A:187:PRO:HA	1:A:191:ALA:O	2.05	0.56
1:A:142:ARG:NH1	1:A:176:ASP:OD2	2.34	0.56
1:B:179:CYS:O	1:B:183:ASP:HB2	2.06	0.56
1:B:134:LYS:O	1:B:135:ASP:C	2.48	0.55
1:B:169:GLU:HG2	1:B:170:LYS:HG3	1.88	0.55
1:A:27:HIS:HD2	2:A:488:HOH:O	1.89	0.55
1:B:34:LYS:HZ3	1:B:39:THR:HA	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:VAL:O	1:A:229:GLN:HG2	2.08	0.54
1:B:138:VAL:O	1:B:139:THR:HB	2.07	0.54
1:B:244:GLU:HG2	1:B:245:LEU:O	2.08	0.54
1:B:18:LYS:NZ	1:B:25:VAL:HG21	2.23	0.54
1:B:108:PHE:CD2	1:B:108:PHE:C	2.85	0.54
1:B:4:GLU:N	1:B:4:GLU:CD	2.66	0.53
1:B:239:THR:N	1:B:240:ASN:OD1	2.42	0.53
1:B:2:ILE:HD12	1:B:125:ASN:HB3	1.92	0.52
1:B:286:LEU:CD2	1:B:288:LYS:HZ3	2.23	0.51
1:A:195:GLN:HG3	1:A:203:HIS:CE1	2.46	0.51
1:A:87:TYR:OH	1:A:119:ASP:OD1	2.22	0.51
1:B:183:ASP:HB3	1:B:184:HIS:CA	2.28	0.51
1:A:270:PRO:HG2	1:A:271:PRO:HD3	1.92	0.51
1:B:228:MET:O	1:B:232:LEU:HG	2.11	0.51
1:A:47:ALA:O	1:A:50:LEU:HB2	2.12	0.50
1:A:228:MET:O	1:A:232:LEU:HG	2.10	0.50
1:A:200:SER:HB3	1:A:304:ASP:OD1	2.11	0.50
1:B:224:TYR:O	1:B:228:MET:HG2	2.11	0.50
1:B:23:LEU:C	1:B:23:LEU:HD23	2.36	0.50
1:A:88:LYS:HG3	1:A:90:LEU:HD13	1.94	0.50
1:B:222:MET:HG3	1:B:223:CYS:N	2.27	0.49
1:B:22:HIS:CG	1:B:74:GLU:HG3	2.47	0.49
1:B:138:VAL:O	1:B:139:THR:CB	2.61	0.49
1:B:199:VAL:CG2	1:B:203:HIS:CE1	2.96	0.49
1:B:206:LEU:HG	1:B:227:LEU:HD21	1.95	0.49
1:B:191:ALA:HB3	2:B:464:HOH:O	2.12	0.49
1:A:84:ASP:HB2	1:A:86:GLU:HG2	1.94	0.48
1:B:169:GLU:O	1:B:170:LYS:HB2	2.12	0.48
1:A:305:LYS:HB2	1:A:305:LYS:NZ	2.29	0.48
1:B:191:ALA:C	1:B:192:GLU:HG2	2.38	0.48
1:B:18:LYS:HZ1	1:B:25:VAL:HG21	1.79	0.47
1:B:35:ASP:OD2	1:B:301:HIS:HA	2.14	0.47
1:A:192:GLU:CG	1:A:193:PRO:HD2	2.42	0.47
1:B:286:LEU:CD2	1:B:288:LYS:NZ	2.78	0.47
1:A:122:THR:O	1:A:126:VAL:HG23	2.15	0.47
1:B:38:THR:C	1:B:39:THR:HG23	2.39	0.47
1:B:185:PHE:C	1:B:185:PHE:CD1	2.93	0.47
1:B:199:VAL:HG21	1:B:203:HIS:CE1	2.50	0.47
1:B:3:GLU:HG2	1:B:9:LYS:NZ	2.29	0.47
1:B:65:GLU:CG	1:B:66:ASP:H	2.27	0.47
1:A:272:LEU:HB3	1:A:274:LEU:HG	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:LEU:C	1:A:23:LEU:HD12	2.40	0.46
1:B:135:ASP:OD2	1:B:140:CYS:HB3	2.15	0.46
1:B:286:LEU:HD23	1:B:288:LYS:HZ3	1.80	0.46
1:B:126:VAL:HG11	1:B:164:ILE:CD1	2.44	0.46
1:A:89:LEU:HD12	1:A:102:LEU:O	2.15	0.46
1:B:196:ASP:O	1:B:199:VAL:HG22	2.15	0.46
1:B:183:ASP:CB	1:B:184:HIS:HA	2.27	0.46
1:B:87:TYR:OH	1:B:119:ASP:OD1	2.19	0.46
1:A:117:PRO:HB2	1:A:217:GLU:OE2	2.16	0.45
1:B:3:GLU:HG2	1:B:9:LYS:HZ2	1.80	0.45
1:A:85:GLY:HA2	2:A:502:HOH:O	2.16	0.45
1:A:38:THR:O	1:A:39:THR:OG1	2.27	0.45
1:A:15:VAL:HG22	2:A:499:HOH:O	2.16	0.45
1:B:235:PHE:CD2	1:B:235:PHE:N	2.84	0.45
1:A:156:SER:O	1:B:134:LYS:NZ	2.34	0.45
1:B:121:MET:HB2	1:B:217:GLU:HG2	1.99	0.45
1:B:230:ARG:HH11	1:B:230:ARG:CG	2.28	0.45
1:B:242:SER:N	1:B:243:PRO:CA	2.80	0.44
1:A:4:GLU:H	1:A:4:GLU:HG2	1.52	0.44
1:B:65:GLU:CG	1:B:66:ASP:N	2.81	0.44
1:B:123:ALA:HB1	1:B:145:VAL:HG11	2.00	0.44
1:A:82:ASN:HB2	1:A:84:ASP:OD2	2.18	0.43
1:B:22:HIS:CD2	1:B:72:ASP:OD2	2.71	0.43
1:B:182:LYS:HB2	1:B:182:LYS:HZ2	1.83	0.43
1:B:201:PHE:O	1:B:314:ASN:HB2	2.18	0.43
1:A:50:LEU:HD12	1:A:50:LEU:HA	1.83	0.43
1:B:272:LEU:HA	1:B:292:LYS:HD2	2.00	0.43
1:A:66:ASP:HA	1:A:67:PRO:HD2	1.83	0.43
1:B:185:PHE:C	1:B:185:PHE:HD1	2.26	0.42
1:B:222:MET:HE3	1:B:222:MET:HB2	1.89	0.42
1:A:27:HIS:CD2	2:A:488:HOH:O	2.69	0.42
1:A:162:LEU:HD12	1:A:162:LEU:N	2.33	0.42
1:A:72:ASP:OD1	1:A:72:ASP:C	2.61	0.42
1:A:108:PHE:C	1:A:108:PHE:CD2	2.98	0.42
1:A:218:ASP:O	1:A:222:MET:HG2	2.20	0.42
1:A:319:LYS:O	1:A:322:GLU:HG2	2.20	0.42
1:B:10:ILE:HD11	1:B:89:LEU:HD21	2.02	0.42
1:B:286:LEU:HG	1:B:288:LYS:NZ	2.34	0.42
1:A:68:PHE:HB3	1:A:104:VAL:HG11	2.01	0.42
1:A:263:ARG:HD3	1:A:281:TYR:CE2	2.55	0.42
1:A:85:GLY:O	1:A:106:SER:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:PRO:HG3	1:B:227:LEU:HD23	2.02	0.41
1:A:133:ASP:CG	1:A:255:LYS:HZ1	2.25	0.41
1:A:272:LEU:CD1	1:A:296:LEU:HD21	2.51	0.41
1:A:277:ASN:OD1	1:A:277:ASN:C	2.63	0.41
1:B:188:THR:HG22	1:B:189:PHE:N	2.27	0.41
1:A:4:GLU:HB2	2:A:518:HOH:O	2.19	0.41
1:B:272:LEU:CD2	1:B:296:LEU:HD21	2.47	0.41
1:B:188:THR:O	1:B:191:ALA:HB2	2.21	0.41
1:A:243:PRO:HD2	2:A:477:HOH:O	2.21	0.41
1:A:19:LYS:HE3	1:A:19:LYS:HB2	1.82	0.41
1:B:181:GLY:C	1:B:183:ASP:H	2.25	0.41
1:B:252:LEU:HD23	1:B:282:CYS:HB3	2.03	0.41
1:B:137:ASP:O	1:B:140:CYS:HB2	2.20	0.40
1:B:183:ASP:CB	1:B:184:HIS:CA	2.96	0.40
1:B:242:SER:H	1:B:243:PRO:HA	1.85	0.40
1:A:111:GLN:OE1	1:A:160:LYS:HA	2.21	0.40
1:A:116:THR:HB	1:A:117:PRO:CD	2.51	0.40
1:B:98:PRO:O	1:B:99:GLU:HB2	2.21	0.40
1:B:159:HIS:CD2	1:B:159:HIS:C	2.99	0.40
1:A:196:ASP:H	1:A:203:HIS:CE1	2.38	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:TRP:O	1:B:247:LYS:NZ[4_545]	2.16	0.04

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	300/333 (90%)	296 (99%)	4 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	301/333 (90%)	286 (95%)	14 (5%)	1 (0%)	36	46
All	All	601/666 (90%)	582 (97%)	18 (3%)	1 (0%)	43	55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	134	LYS

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	280/304 (92%)	262 (94%)	18 (6%)	16	23
1	B	279/304 (92%)	256 (92%)	23 (8%)	10	14
All	All	559/608 (92%)	518 (93%)	41 (7%)	13	18

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	15	VAL
1	A	23	LEU
1	A	37	GLN
1	A	50	LEU
1	A	84	ASP
1	A	88	LYS
1	A	102	LEU
1	A	140	CYS
1	A	141	GLU
1	A	142	ARG
1	A	164	ILE
1	A	177	VAL
1	A	180	ASN
1	A	210	GLU

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Mol	Chain	Res	Type
1	A	241	GLU
1	A	290	ARG
1	A	305	LYS
1	B	23	LEU
1	B	50	LEU
1	B	78	THR
1	B	135	ASP
1	B	139	THR
1	B	140	CYS
1	B	156	SER
1	B	182	LYS
1	B	184	HIS
1	B	185	PHE
1	B	186	LEU
1	B	188	THR
1	B	195	GLN
1	B	211	SER
1	B	214	GLN
1	B	222	MET
1	B	230	ARG
1	B	237	ASP
1	B	238	TRP
1	B	239	THR
1	B	247	LYS
1	B	272	LEU
1	B	291	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	ASN
1	A	166	GLN
1	B	41	GLN
1	B	163	GLN

5.3.3 RNA ⓘ

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 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	306/333 (91%)	0.13	4 (1%) 75 76	19, 38, 60, 82	0
1	B	305/333 (91%)	0.23	21 (6%) 23 25	19, 39, 78, 97	0
All	All	611/666 (91%)	0.18	25 (4%) 41 43	19, 38, 69, 97	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	52	LEU	4.1
1	A	270	PRO	4.0
1	B	238	TRP	4.0
1	B	186	LEU	3.6
1	B	138	VAL	3.5
1	B	185	PHE	3.4
1	B	188	THR	3.3
1	B	135	ASP	3.1
1	B	64	ALA	3.1
1	B	240	ASN	2.9
1	B	239	THR	2.9
1	B	133	ASP	2.9
1	A	269	GLY	2.9
1	B	191	ALA	2.8
1	B	181	GLY	2.8
1	B	242	SER	2.8
1	A	191	ALA	2.6
1	B	184	HIS	2.6
1	B	316	ALA	2.6
1	B	189	PHE	2.4
1	B	237	ASP	2.4
1	A	133	ASP	2.3
1	B	187	PRO	2.3
1	B	245	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	241	GLU	2.2

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.