



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:17 AM UTC

PDB ID : 4R8F / pdb_00004r8f
Title : Crystal structure of yeast aminopeptidase 1 (Ape1)
Authors : Su, M.-Y.; Chang, C.-I.
Deposited on : 2014-09-02
Resolution : 2.50 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

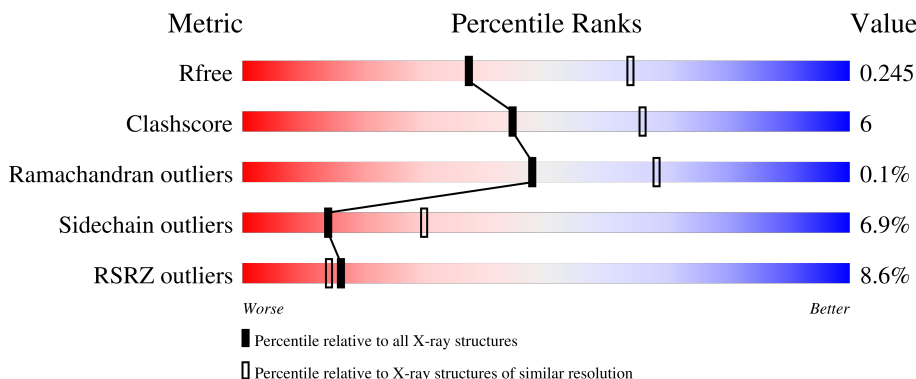
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	470	9% 79% 13% 7%
1	B	470	7% 79% 11% 9%
1	C	470	9% 78% 14% 7%
1	D	470	7% 76% 15% 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13635 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 Vacuolar aminopeptidase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	0	0	0
			3418	2188	577	645	8			
1	B	428	Total	C	N	O	S	0	0	0
			3340	2142	564	626	8			
1	C	437	Total	C	N	O	S	0	0	0
			3414	2189	576	641	8			
1	D	432	Total	C	N	O	S	0	0	0
			3372	2162	567	635	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP P14904
B	1	MET	-	expression tag	UNP P14904
C	1	MET	-	expression tag	UNP P14904
D	1	MET	-	expression tag	UNP P14904

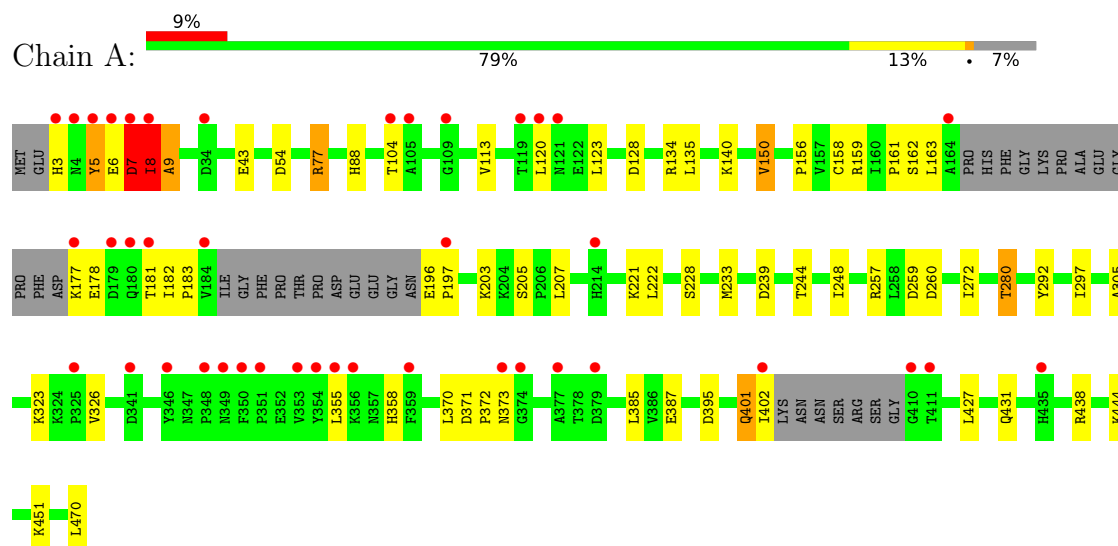
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	25	Total	O	0	0
			25	25		
2	B	20	Total	O	0	0
			20	20		
2	C	27	Total	O	0	0
			27	27		
2	D	19	Total	O	0	0
			19	19		

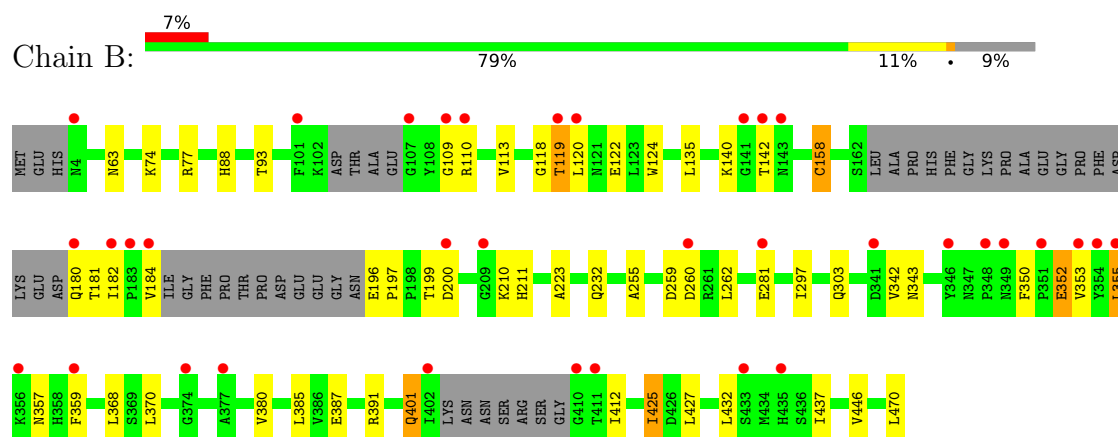
3 Residue-property plots [i](#)

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.

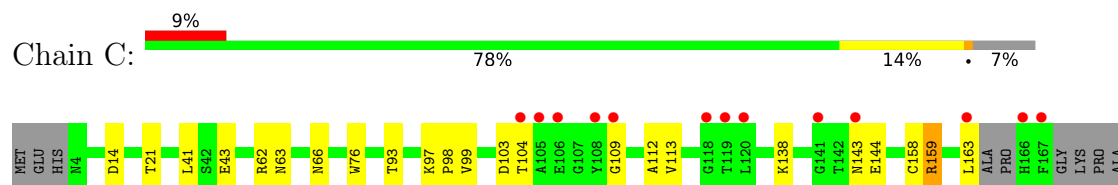
• Molecule 1: Vacuolar aminopeptidase 1



• Molecule 1: Vacuolar aminopeptidase 1



• Molecule 1: Vacuolar aminopeptidase 1



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	140.17Å 140.17Å 348.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	116.23 – 2.50 116.23 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.7 (116.23-2.50) 95.9 (116.23-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.215 , 0.246 0.217 , 0.245	Depositor DCC
R_{free} test set	4222 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	36.8	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.011 for $-1/3^*h+1/3^*k+1/3^*l, -k, 8/3^*h+4/3^*k+1/3^*l$ 0.015 for $-2/3^*h-1/3^*k-1/3^*l, -1/3^*h-2/3^*k+1/3^*l, -4/3^*h+4/3^*k+1/3^*l$ 0.009 for $-h, 1/3^*h-1/3^*k-1/3^*l, -4/3^*h-8/3^*k+1/3^*l$ 0.015 for $-h, 2/3^*h+1/3^*k+1/3^*l, 4/3^*h+8/3^*k-1/3^*l$ 0.011 for $1/3^*h+2/3^*k-1/3^*l, -k, -8/3^*h-4/3^*k-1/3^*l$ 0.014 for $-1/3^*h-2/3^*k+1/3^*l, -2/3^*h-1/3^*k-1/3^*l, 4/3^*h-4/3^*k-1/3^*l$ 0.038 for $-h-k, k, -l$	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13635	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% 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	0.43	0/3493	0.79	3/4729 (0.1%)
1	B	0.41	0/3413	0.77	6/4619 (0.1%)
1	C	0.41	0/3489	0.75	0/4723
1	D	0.40	0/3444	0.75	0/4656
All	All	0.41	0/13839	0.76	9/18727 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	9	ALA	N-CA-C	-5.99	104.13	112.45
1	B	119	THR	N-CA-C	5.92	120.52	113.12
1	B	255	ALA	N-CA-C	5.71	113.36	108.22
1	B	353	VAL	N-CA-C	-5.71	105.24	113.07
1	A	7	ASP	CA-C-N	5.58	131.75	121.70
1	A	7	ASP	C-N-CA	5.58	131.75	121.70
1	B	350	PHE	CA-C-N	5.32	124.77	119.24
1	B	350	PHE	C-N-CA	5.32	124.77	119.24
1	B	158	CYS	N-CA-C	5.09	115.88	108.14

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	352	GLU	Peptide

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	3418	0	3387	42	0
1	B	3340	0	3318	41	0
1	C	3414	0	3384	51	0
1	D	3372	0	3337	49	0
2	A	25	0	0	0	0
2	B	20	0	0	3	0
2	C	27	0	0	0	0
2	D	19	0	0	0	0
All	All	13635	0	13426	162	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 6.

All (162) 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:380:VAL:CG2	1:C:234:ASP:HB2	2.05	0.86
1:C:219:VAL:HG21	1:C:233:MET:HE2	1.60	0.83
1:B:380:VAL:CG1	1:C:232:GLN:HB3	2.12	0.79
1:A:6:GLU:C	1:A:8:ILE:HG22	2.08	0.78
1:B:232:GLN:HB3	1:D:380:VAL:CG2	2.15	0.77
1:A:7:ASP:HA	1:A:9:ALA:H	1.49	0.77
1:D:315:GLU:HG3	1:D:328:LEU:HD21	1.68	0.75
1:C:392:ARG:NH2	1:C:466:GLU:OE2	2.21	0.74
1:B:158:CYS:HB2	1:B:182:ILE:HG22	1.70	0.72
1:D:158:CYS:HB2	1:D:182:ILE:HG22	1.71	0.72
1:D:158:CYS:SG	1:D:182:ILE:HG21	2.29	0.72
1:A:7:ASP:N	1:A:7:ASP:OD1	2.28	0.67
1:C:158:CYS:HB2	1:C:182:ILE:HG22	1.78	0.66
1:B:425:ILE:HG22	2:B:516:HOH:O	1.95	0.65
1:D:89:VAL:O	1:D:261:ARG:NH1	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:LEU:O	1:B:359:PHE:CD2	2.51	0.63
1:A:239:ASP:O	1:A:257:ARG:NH2	2.32	0.63
1:C:345:LEU:HB3	1:C:432:LEU:HD12	1.81	0.61
1:D:158:CYS:HB2	1:D:182:ILE:CG2	2.31	0.61
1:B:113:VAL:HG21	1:B:182:ILE:HD11	1.82	0.60
1:A:77:ARG:HG2	1:A:77:ARG:HH11	1.67	0.59
1:C:113:VAL:HG22	1:C:182:ILE:HD11	1.83	0.59
1:A:158:CYS:SG	1:A:182:ILE:HG21	2.41	0.59
1:C:342:VAL:HG11	1:C:431:GLN:NE2	2.18	0.59
1:B:297:ILE:HG21	1:D:373:ASN:HA	1.84	0.58
1:B:380:VAL:HG22	1:C:234:ASP:HB2	1.85	0.58
1:C:158:CYS:SG	1:C:182:ILE:HG21	2.44	0.58
1:C:380:VAL:CG2	1:D:232:GLN:HB3	2.33	0.58
1:D:347:ASN:OD1	1:D:348:PRO:HD2	2.02	0.58
1:D:165:PRO:HA	1:D:166:HIS:C	2.27	0.58
1:D:239:ASP:O	1:D:257:ARG:NH2	2.37	0.56
1:B:158:CYS:HB2	1:B:182:ILE:CG2	2.35	0.56
1:A:6:GLU:C	1:A:7:ASP:OD1	2.49	0.56
1:C:113:VAL:CG2	1:C:182:ILE:HD11	2.35	0.56
1:C:334:ASN:O	1:C:461:ARG:NH2	2.39	0.56
1:C:380:VAL:HG22	1:D:232:GLN:HB3	1.86	0.56
1:B:355:LEU:O	1:B:359:PHE:HD2	1.88	0.55
1:D:158:CYS:SG	1:D:182:ILE:CG2	2.94	0.55
1:D:43:GLU:OE1	1:D:62:ARG:HG3	2.07	0.55
1:D:119:THR:CG2	1:D:120:LEU:N	2.70	0.55
1:D:166:HIS:O	1:D:167:PHE:CD2	2.59	0.55
1:A:7:ASP:HA	1:A:9:ALA:N	2.17	0.55
1:A:54:ASP:O	1:A:280:THR:HG23	2.06	0.55
1:B:196:GLU:HB3	1:B:197:PRO:HD3	1.88	0.54
1:D:57:LYS:NZ	1:D:275:ALA:O	2.41	0.54
1:D:342:VAL:HG23	1:D:434:MET:SD	2.48	0.54
1:C:62:ARG:HB3	1:C:66:ASN:HB3	1.91	0.53
1:D:165:PRO:HA	1:D:166:HIS:O	2.09	0.53
1:C:182:ILE:HD12	1:C:182:ILE:N	2.24	0.53
1:A:181:THR:HA	1:A:182:ILE:HD12	1.91	0.53
1:A:181:THR:HG22	1:A:182:ILE:H	1.74	0.52
1:C:461:ARG:O	1:C:461:ARG:HD3	2.10	0.52
1:B:370:LEU:HB2	1:B:401:GLN:HG2	1.93	0.51
1:C:358:HIS:CE1	1:D:99:VAL:HB	2.45	0.51
1:D:75:ASN:O	1:D:77:ARG:NH1	2.44	0.51
1:D:258:LEU:O	1:D:260:ASP:HA	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:260:ASP:CG	1:C:342:VAL:HG13	2.35	0.51
1:D:48:GLN:HE22	1:D:323:LYS:CE	2.23	0.51
1:D:180:GLN:O	1:D:181:THR:HG22	2.11	0.51
1:A:158:CYS:HB2	1:A:182:ILE:CG2	2.41	0.50
1:A:113:VAL:HG21	1:A:182:ILE:HD11	1.93	0.50
1:A:161:PRO:HD3	1:A:183:PRO:HD2	1.92	0.50
1:B:210:LYS:HB2	1:B:211:HIS:CD2	2.47	0.50
1:B:380:VAL:HG11	1:C:232:GLN:HB3	1.92	0.50
1:B:380:VAL:HG21	1:C:234:ASP:HB2	1.90	0.50
1:B:357:ASN:HB3	1:C:99:VAL:HG11	1.93	0.49
1:D:48:GLN:HE22	1:D:323:LYS:HE3	1.77	0.49
1:A:358:HIS:HB3	1:A:401:GLN:H	1.77	0.49
1:B:88:HIS:HB3	1:B:412:ILE:HD11	1.95	0.49
1:B:109:GLY:C	1:B:184:VAL:HG22	2.38	0.48
1:C:211:HIS:HB2	1:C:216:LEU:HD21	1.94	0.48
1:C:292:TYR:CE1	1:C:305:ALA:HA	2.48	0.48
1:D:360:PRO:HG3	1:D:367:THR:HG21	1.94	0.48
1:A:196:GLU:HB3	1:A:197:PRO:HD3	1.96	0.48
1:C:216:LEU:HD23	1:C:233:MET:HE1	1.95	0.48
1:C:97:LYS:HD2	1:C:112:ALA:HB1	1.96	0.48
1:B:135:LEU:HD12	1:B:223:ALA:HB2	1.95	0.48
1:D:62:ARG:HB3	1:D:66:ASN:HB3	1.96	0.48
1:C:260:ASP:OD2	1:C:341:ASP:HA	2.14	0.48
1:A:395:ASP:OD1	1:A:451:LYS:HE3	2.14	0.48
1:B:118:GLY:HA3	1:B:120:LEU:HD13	1.96	0.48
1:C:109:GLY:HA3	1:C:185:ILE:CG1	2.43	0.48
1:B:355:LEU:O	1:B:359:PHE:CE2	2.67	0.47
1:D:113:VAL:CG2	1:D:182:ILE:HD11	2.45	0.47
1:B:63:ASN:HB3	1:B:303:GLN:HG2	1.96	0.47
1:C:181:THR:HG22	1:C:182:ILE:H	1.80	0.47
1:B:158:CYS:SG	1:B:182:ILE:HG21	2.55	0.47
1:B:380:VAL:HG12	1:C:232:GLN:HB3	1.96	0.47
1:D:119:THR:HG23	1:D:120:LEU:N	2.30	0.47
1:A:358:HIS:ND1	1:A:401:GLN:HB2	2.30	0.47
1:C:461:ARG:HD3	1:C:461:ARG:C	2.39	0.47
1:B:232:GLN:HB3	1:D:380:VAL:HG21	1.93	0.46
1:A:371:ASP:CG	1:A:373:ASN:O	2.58	0.46
1:B:370:LEU:HD13	1:C:98:PRO:HG2	1.97	0.46
1:D:370:LEU:O	1:D:401:GLN:HA	2.15	0.46
1:A:7:ASP:CA	1:A:9:ALA:H	2.24	0.46
1:B:427:LEU:HD23	2:B:516:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:ILE:HD11	1:D:261:ARG:HB2	1.97	0.46
1:B:119:THR:H	1:B:120:LEU:HA	1.81	0.46
1:D:180:GLN:CD	1:D:180:GLN:C	2.84	0.45
1:C:370:LEU:HB2	1:C:401:GLN:HG2	1.99	0.45
1:B:370:LEU:HD13	1:C:98:PRO:CG	2.47	0.45
1:D:344:HIS:O	1:D:360:PRO:HD2	2.16	0.45
1:A:355:LEU:CD2	1:A:358:HIS:CD2	3.00	0.45
1:D:33:LEU:HD11	1:D:268:MET:HE1	1.98	0.45
1:D:113:VAL:HG21	1:D:182:ILE:HD11	1.98	0.45
1:D:94:VAL:HG22	1:D:120:LEU:HD13	1.99	0.44
1:A:3:HIS:C	1:A:5:TYR:H	2.26	0.44
1:C:239:ASP:O	1:C:257:ARG:NH2	2.51	0.44
1:A:259:ASP:HA	1:A:260:ASP:HA	1.72	0.44
1:B:260:ASP:OD1	1:B:342:VAL:HG23	2.17	0.44
1:C:259:ASP:HA	1:C:260:ASP:HA	1.71	0.44
1:A:158:CYS:HB2	1:A:182:ILE:HG22	1.99	0.44
1:A:207:LEU:CD1	1:A:233:MET:HE3	2.48	0.44
1:A:113:VAL:CG2	1:A:182:ILE:HD11	2.48	0.44
1:B:391:ARG:NH2	1:C:206:PRO:HB3	2.33	0.43
1:D:324:LYS:HE3	1:D:325:PRO:O	2.17	0.43
1:D:165:PRO:HA	1:D:166:HIS:CB	2.47	0.43
1:A:7:ASP:N	1:A:8:ILE:HG22	2.34	0.43
1:A:370:LEU:O	1:A:401:GLN:HA	2.18	0.43
1:D:119:THR:HG23	1:D:120:LEU:H	1.83	0.43
1:A:162:SER:O	1:C:433:SER:HB3	2.18	0.43
1:D:163:LEU:HD23	1:D:167:PHE:CE2	2.53	0.43
1:D:359:PHE:HA	1:D:360:PRO:HD3	1.92	0.43
1:B:119:THR:N	1:B:120:LEU:HA	2.34	0.42
1:B:370:LEU:O	1:B:401:GLN:HG2	2.20	0.42
1:C:138:LYS:HD3	1:C:143:ASN:HA	2.01	0.42
1:A:438:ARG:O	1:C:159:ARG:NH2	2.52	0.42
1:A:371:ASP:OD1	1:A:372:PRO:HD2	2.20	0.42
1:B:425:ILE:CG2	2:B:516:HOH:O	2.61	0.42
1:C:345:LEU:HD11	1:C:361:VAL:C	2.44	0.42
1:C:350:PHE:N	1:C:351:PRO:CD	2.82	0.42
1:D:158:CYS:CB	1:D:182:ILE:CG2	2.98	0.42
1:D:360:PRO:HG3	1:D:367:THR:CG2	2.49	0.42
1:B:387:GLU:OE2	1:C:232:GLN:NE2	2.47	0.42
1:D:372:PRO:O	1:D:373:ASN:HB2	2.20	0.42
1:A:135:LEU:HD22	1:A:233:MET:HE2	2.01	0.41
1:C:76:TRP:CD1	1:C:286:PHE:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262:LEU:CD1	1:C:446:VAL:HG22	2.49	0.41
1:A:128:ASP:HB3	1:A:156:PRO:HB3	2.02	0.41
1:A:150:VAL:HG22	1:A:222:LEU:HB2	2.03	0.41
1:B:63:ASN:O	1:B:63:ASN:CG	2.64	0.41
1:A:427:LEU:HD12	1:A:427:LEU:C	2.45	0.41
1:B:259:ASP:HA	1:B:260:ASP:HA	1.75	0.41
1:C:260:ASP:OD1	1:C:342:VAL:HG13	2.21	0.41
1:D:63:ASN:CB	1:D:303:GLN:HG2	2.51	0.41
1:A:163:LEU:HD21	1:C:353:VAL:HG21	2.03	0.41
1:B:199:THR:HG22	1:B:200:ASP:N	2.36	0.41
1:B:262:LEU:CD1	1:B:446:VAL:HG22	2.50	0.41
1:C:63:ASN:HB3	1:C:303:GLN:HG2	2.02	0.41
1:C:181:THR:HA	1:C:182:ILE:HD12	2.02	0.41
1:D:205:SER:HB2	1:D:228:SER:HA	2.02	0.41
1:D:349:ASN:OD1	1:D:349:ASN:N	2.54	0.41
1:A:182:ILE:HD12	1:A:182:ILE:N	2.36	0.41
1:A:292:TYR:CE1	1:A:305:ALA:HA	2.56	0.41
1:A:88:HIS:NE2	1:A:260:ASP:HB2	2.35	0.40
1:A:205:SER:HB2	1:A:228:SER:HA	2.04	0.40
1:D:402:ILE:O	1:D:402:ILE:HG22	2.22	0.40
1:C:368:LEU:HD12	1:C:427:LEU:HD23	2.02	0.40
1:A:248:ILE:HG22	1:C:185:ILE:CG2	2.52	0.40
1:A:402:ILE:N	1:A:402:ILE:HD12	2.37	0.40
1:B:124:TRP:CE3	1:B:437:ILE:HD12	2.57	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	430/470 (92%)	425 (99%)	4 (1%)	1 (0%)	43 63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	418/470 (89%)	413 (99%)	5 (1%)	0	100	100
1	C	427/470 (91%)	420 (98%)	7 (2%)	0	100	100
1	D	418/470 (89%)	410 (98%)	8 (2%)	0	100	100
All	All	1693/1880 (90%)	1668 (98%)	24 (1%)	1 (0%)	48	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	ILE

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	370/396 (93%)	342 (92%)	28 (8%)	12	26
1	B	362/396 (91%)	343 (95%)	19 (5%)	21	42
1	C	370/396 (93%)	345 (93%)	25 (7%)	14	31
1	D	365/396 (92%)	336 (92%)	29 (8%)	11	24
All	All	1467/1584 (93%)	1366 (93%)	101 (7%)	14	30

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	TYR
1	A	7	ASP
1	A	8	ILE
1	A	43	GLU
1	A	77	ARG
1	A	104	THR
1	A	120	LEU
1	A	123	LEU
1	A	134	ARG
1	A	140	LYS

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Mol	Chain	Res	Type
1	A	150	VAL
1	A	159	ARG
1	A	177	LYS
1	A	178	GLU
1	A	203	LYS
1	A	221	LYS
1	A	244	THR
1	A	272	ILE
1	A	280	THR
1	A	297	ILE
1	A	323	LYS
1	A	326	VAL
1	A	385	LEU
1	A	387	GLU
1	A	401	GLN
1	A	431	GLN
1	A	444	LYS
1	A	470	LEU
1	B	74	LYS
1	B	77	ARG
1	B	93	THR
1	B	110	ARG
1	B	122	GLU
1	B	140	LYS
1	B	142	THR
1	B	180	GLN
1	B	181	THR
1	B	281	GLU
1	B	343	ASN
1	B	352	GLU
1	B	355	LEU
1	B	368	LEU
1	B	385	LEU
1	B	401	GLN
1	B	425	ILE
1	B	432	LEU
1	B	470	LEU
1	C	14	ASP
1	C	21	THR
1	C	41	LEU
1	C	43	GLU
1	C	93	THR

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Mol	Chain	Res	Type
1	C	103	ASP
1	C	104	THR
1	C	144	GLU
1	C	159	ARG
1	C	163	LEU
1	C	185	ILE
1	C	212	CYS
1	C	213	ILE
1	C	221	LYS
1	C	244	THR
1	C	248	ILE
1	C	297	ILE
1	C	303	GLN
1	C	345	LEU
1	C	366	ILE
1	C	387	GLU
1	C	401	GLN
1	C	411	THR
1	C	433	SER
1	C	461	ARG
1	D	4	ASN
1	D	18	LYS
1	D	27	SER
1	D	41	LEU
1	D	45	SER
1	D	53	GLU
1	D	92	LEU
1	D	93	THR
1	D	104	THR
1	D	119	THR
1	D	120	LEU
1	D	143	ASN
1	D	159	ARG
1	D	167	PHE
1	D	178	GLU
1	D	181	THR
1	D	184	VAL
1	D	244	THR
1	D	248	ILE
1	D	272	ILE
1	D	279	ASN
1	D	297	ILE

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Mol	Chain	Res	Type
1	D	303	GLN
1	D	328	LEU
1	D	343	ASN
1	D	345	LEU
1	D	349	ASN
1	D	387	GLU
1	D	411	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	66	ASN
1	A	121	ASN
1	A	431	GLN
1	B	36	HIS
1	B	63	ASN
1	B	241	GLN
1	B	357	ASN
1	B	435	HIS
1	C	75	ASN
1	C	343	ASN
1	C	344	HIS
1	C	357	ASN
1	C	358	HIS
1	C	431	GLN
1	C	459	HIS
1	D	48	GLN
1	D	88	HIS
1	D	143	ASN
1	D	303	GLN
1	D	401	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	438/470 (93%)	0.33	41 (9%) 14 12	20, 34, 73, 103	0
1	B	428/470 (91%)	0.36	35 (8%) 17 15	23, 38, 75, 93	0
1	C	437/470 (92%)	0.35	40 (9%) 14 13	24, 36, 73, 102	0
1	D	432/470 (91%)	0.50	34 (7%) 18 16	24, 41, 75, 109	0
All	All	1735/1880 (92%)	0.38	150 (8%) 16 14	20, 37, 75, 109	0

All (150) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	120	LEU	5.9
1	B	356	LYS	5.1
1	D	175	PHE	5.0
1	D	350	PHE	4.9
1	A	5	TYR	4.8
1	D	410	GLY	4.8
1	D	343	ASN	4.7
1	D	119	THR	4.3
1	D	402	ILE	4.3
1	D	177	LYS	4.3
1	B	355	LEU	4.3
1	C	104	THR	4.3
1	D	167	PHE	4.2
1	A	374	GLY	4.1
1	B	402	ILE	4.0
1	A	3	HIS	4.0
1	A	105	ALA	4.0
1	A	410	GLY	4.0
1	D	359	PHE	4.0
1	D	411	THR	3.9
1	A	177	LYS	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	184	VAL	3.8
1	A	354	TYR	3.8
1	C	180	GLN	3.8
1	D	120	LEU	3.8
1	A	402	ILE	3.7
1	C	359	PHE	3.7
1	B	4	ASN	3.7
1	C	185	ILE	3.7
1	B	359	PHE	3.7
1	A	180	GLN	3.6
1	D	182	ILE	3.6
1	D	181	THR	3.6
1	C	402	ILE	3.6
1	B	184	VAL	3.5
1	D	260	ASP	3.5
1	D	348	PRO	3.5
1	D	178	GLU	3.5
1	D	165	PRO	3.4
1	A	120	LEU	3.4
1	B	107	GLY	3.4
1	D	118	GLY	3.4
1	C	166	HIS	3.3
1	C	214	HIS	3.3
1	A	353	VAL	3.3
1	A	184	VAL	3.3
1	B	410	GLY	3.2
1	A	164	ALA	3.1
1	C	355	LEU	3.1
1	B	353	VAL	3.1
1	A	104	THR	3.1
1	A	349	ASN	3.1
1	B	281	GLU	3.1
1	B	109	GLY	3.1
1	C	182	ILE	3.0
1	A	411	THR	3.0
1	B	354	TYR	3.0
1	C	260	ASP	3.0
1	A	119	THR	3.0
1	B	119	THR	3.0
1	C	346	TYR	3.0
1	C	354	TYR	3.0
1	D	341	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	163	LEU	2.9
1	A	356	LYS	2.9
1	C	108	TYR	2.9
1	A	214	HIS	2.9
1	B	346	TYR	2.9
1	A	4	ASN	2.9
1	B	141	GLY	2.9
1	A	341	ASP	2.9
1	C	353	VAL	2.8
1	C	163	LEU	2.8
1	D	376	MET	2.8
1	B	377	ALA	2.8
1	B	411	THR	2.8
1	D	214	HIS	2.8
1	D	346	TYR	2.8
1	B	209	GLY	2.7
1	C	119	THR	2.7
1	C	352	GLU	2.7
1	D	199	THR	2.7
1	B	349	ASN	2.7
1	A	359	PHE	2.6
1	C	209	GLY	2.6
1	C	351	PRO	2.6
1	B	435	HIS	2.6
1	A	34	ASP	2.6
1	C	109	GLY	2.6
1	D	371	ASP	2.6
1	A	351	PRO	2.6
1	C	167	PHE	2.6
1	A	7	ASP	2.5
1	B	180	GLN	2.5
1	B	110	ARG	2.5
1	C	341	ASP	2.5
1	D	53	GLU	2.5
1	C	435	HIS	2.5
1	A	346	TYR	2.5
1	C	120	LEU	2.4
1	A	377	ALA	2.4
1	A	121	ASN	2.4
1	A	325	PRO	2.4
1	D	282	GLU	2.4
1	B	182	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	435	HIS	2.4
1	C	342	VAL	2.4
1	B	348	PRO	2.4
1	A	179	ASP	2.4
1	A	350	PHE	2.4
1	C	184	VAL	2.4
1	C	105	ALA	2.4
1	C	377	ALA	2.4
1	A	109	GLY	2.3
1	C	281	GLU	2.3
1	C	282	GLU	2.3
1	C	183	PRO	2.3
1	D	349	ASN	2.3
1	B	341	ASP	2.3
1	C	181	THR	2.2
1	C	143	ASN	2.2
1	D	183	PRO	2.2
1	B	351	PRO	2.2
1	D	434	MET	2.2
1	B	374	GLY	2.2
1	A	8	ILE	2.2
1	B	260	ASP	2.1
1	A	373	ASN	2.1
1	C	343	ASN	2.1
1	A	181	THR	2.1
1	B	142	THR	2.1
1	D	209	GLY	2.1
1	B	200	ASP	2.1
1	B	101	PHE	2.1
1	A	197	PRO	2.1
1	B	143	ASN	2.1
1	A	6	GLU	2.1
1	C	199	THR	2.1
1	C	197	PRO	2.1
1	C	358	HIS	2.1
1	D	347	ASN	2.0
1	C	118	GLY	2.0
1	C	141	GLY	2.0
1	B	183	PRO	2.0
1	B	433	SER	2.0
1	A	355	LEU	2.0
1	C	106	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	348	PRO	2.0
1	A	379	ASP	2.0
1	A	435	HIS	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.