



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:52 PM UTC

PDB ID : 5JGF / pdb_00005jgf
Title : Crystal structure of mApe1
Authors : Noda, N.N.; Adachi, W.; Inagaki, F.
Deposited on : 2016-04-20
Resolution : 1.83 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

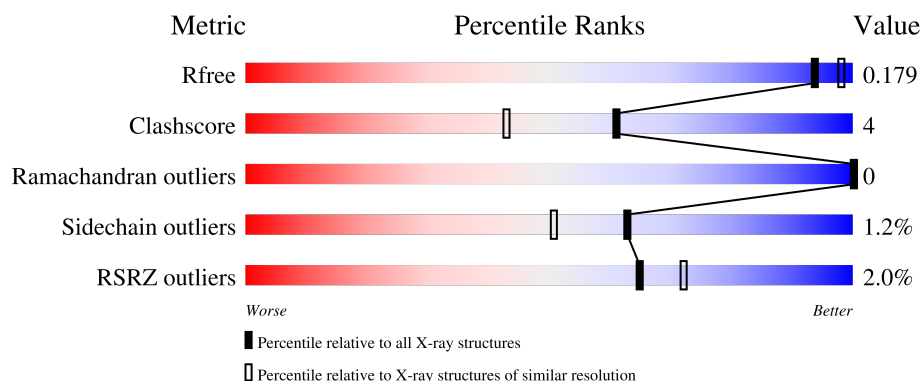
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.83 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	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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	473	2% 86% 11% .
1	B	473	2% 85% 11% ..
1	C	473	2% 86% 11% ..
1	D	473	3% 85% 12% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16586 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	460	Total	C	N	O	S	0	0	0
			3529	2260	595	666	8			
1	B	460	Total	C	N	O	S	0	0	0
			3540	2266	597	669	8			
1	C	460	Total	C	N	O	S	0	0	0
			3544	2268	597	671	8			
1	D	462	Total	C	N	O	S	0	0	0
			3564	2280	602	674	8			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	GLY	-	expression tag	UNP P14904
A	43	PRO	-	expression tag	UNP P14904
A	44	HIS	-	expression tag	UNP P14904
A	45	MET	-	expression tag	UNP P14904
B	42	GLY	-	expression tag	UNP P14904
B	43	PRO	-	expression tag	UNP P14904
B	44	HIS	-	expression tag	UNP P14904
B	45	MET	-	expression tag	UNP P14904
C	42	GLY	-	expression tag	UNP P14904
C	43	PRO	-	expression tag	UNP P14904
C	44	HIS	-	expression tag	UNP P14904
C	45	MET	-	expression tag	UNP P14904
D	42	GLY	-	expression tag	UNP P14904
D	43	PRO	-	expression tag	UNP P14904
D	44	HIS	-	expression tag	UNP P14904
D	45	MET	-	expression tag	UNP P14904

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Zn 2	0	0
2	B	2	Total 2	Zn 2	0	0
2	C	2	Total 2	Zn 2	0	0
2	D	2	Total 2	Zn 2	0	0

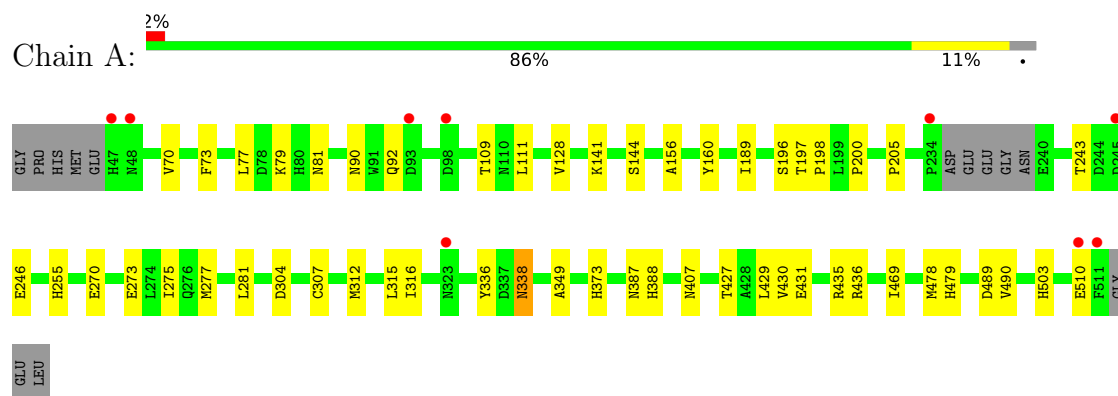
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	594	Total 594	O 594	0	0
3	B	569	Total 569	O 569	0	0
3	C	614	Total 614	O 614	0	0
3	D	624	Total 624	O 624	0	0

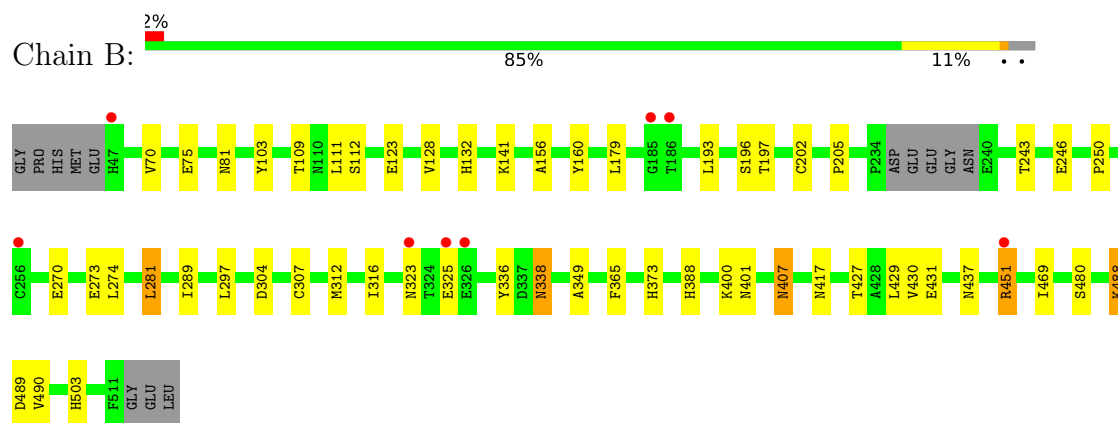
3 Residue-property plots [i](#)

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.

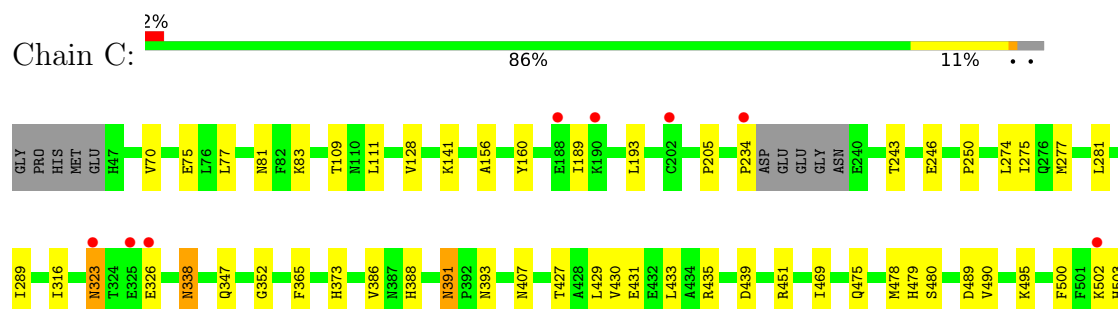
• Molecule 1: Vacuolar aminopeptidase 1



• Molecule 1: Vacuolar aminopeptidase 1

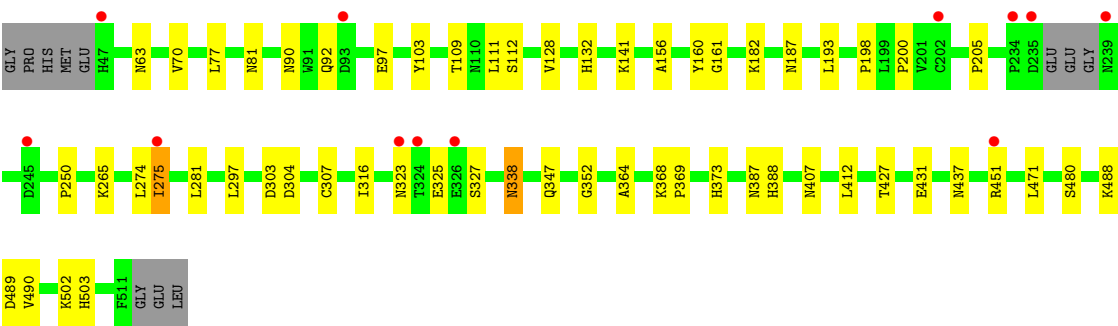
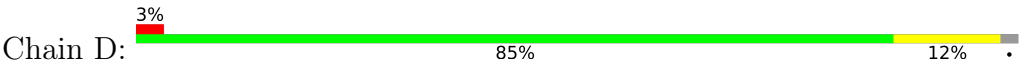


• Molecule 1: Vacuolar aminopeptidase 1





● 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	140.97Å 140.97Å 348.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.49 – 1.83 38.49 – 1.83	Depositor EDS
% Data completeness (in resolution range)	96.5 (38.49-1.83) 96.6 (38.49-1.83)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.23 (at 1.83Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.162 , 0.179 0.162 , 0.179	Depositor DCC
R_{free} test set	22019 reflections (9.67%)	wwPDB-VP
Wilson B-factor (Å ²)	17.1	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 64.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.005 for $-1/3^*h+1/3^*k+1/3^*l,-k,8/3^*h+4/3^*k+1/3^*l$ 0.007 for $-2/3^*h-1/3^*k-1/3^*l,-1/3^*h-2/3^*k+1/3^*l,-4/3^*h+4/3^*k+1/3^*l$ 0.006 for $-h,1/3^*h-1/3^*k-1/3^*l,-4/3^*h-8/3^*k+1/3^*l$ 0.006 for $-h,2/3^*h+1/3^*k+1/3^*l,4/3^*h+8/3^*k-1/3^*l$ 0.007 for $1/3^*h+2/3^*k-1/3^*l,-k,-8/3^*h-4/3^*k-1/3^*l$ 0.007 for $-1/3^*h-2/3^*k+1/3^*l,-2/3^*h-1/3^*k-1/3^*l,4/3^*h-4/3^*k-1/3^*l$ 0.019 for $-h-k,k,-l$	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16586	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.16% 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

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.36	0/3613	0.93	9/4908 (0.2%)
1	B	0.36	0/3624	0.93	12/4921 (0.2%)
1	C	0.35	0/3628	0.92	11/4926 (0.2%)
1	D	0.34	0/3648	0.93	14/4951 (0.3%)
All	All	0.35	0/14513	0.93	46/19706 (0.2%)

There are no bond length outliers.

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	388	HIS	N-CA-C	8.18	121.96	108.96
1	C	338	ASN	N-CA-C	8.16	122.67	111.90
1	C	388	HIS	N-CA-C	8.15	121.92	108.96
1	D	338	ASN	N-CA-C	7.98	122.43	111.90
1	B	388	HIS	N-CA-C	7.91	121.53	108.96
1	D	388	HIS	N-CA-C	7.67	121.22	108.73
1	A	338	ASN	N-CA-C	7.56	122.09	112.86
1	B	338	ASN	N-CA-C	7.54	122.06	112.86
1	C	281	LEU	N-CA-C	-7.09	97.84	109.40
1	B	489	ASP	N-CA-C	6.79	119.52	111.71
1	D	128	VAL	N-CA-C	6.65	118.05	108.48
1	C	489	ASP	N-CA-C	6.64	119.35	111.71
1	B	281	LEU	N-CA-C	-6.63	98.58	109.40
1	B	81	ASN	N-CA-C	6.55	120.59	111.74
1	A	281	LEU	N-CA-C	-6.52	98.27	108.90
1	D	281	LEU	N-CA-C	-6.32	98.59	108.90
1	A	128	VAL	N-CA-C	6.29	117.54	108.48
1	C	128	VAL	N-CA-C	6.19	117.39	108.48
1	D	489	ASP	N-CA-C	6.11	118.73	111.71
1	B	365	PHE	N-CA-C	6.05	117.54	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	128	VAL	N-CA-C	5.93	117.02	108.48
1	C	81	ASN	N-CA-C	5.85	119.72	112.58
1	C	205	PRO	N-CA-C	5.80	119.73	110.21
1	A	81	ASN	N-CA-C	5.78	119.63	112.58
1	D	205	PRO	N-CA-C	5.72	119.59	110.21
1	A	205	PRO	N-CA-C	5.65	119.38	110.50
1	D	503	HIS	N-CA-C	5.64	122.07	113.61
1	A	489	ASP	N-CA-C	5.57	118.12	111.71
1	D	81	ASN	N-CA-C	5.55	119.35	112.24
1	B	407	ASN	N-CA-C	5.55	119.09	111.54
1	B	205	PRO	N-CA-C	5.54	119.30	110.21
1	D	407	ASN	N-CA-C	5.54	119.21	111.74
1	A	407	ASN	N-CA-C	5.53	119.06	111.54
1	C	480	SER	N-CA-C	-5.51	103.42	110.53
1	B	480	SER	N-CA-C	-5.49	103.45	110.53
1	C	407	ASN	N-CA-C	5.36	119.11	112.24
1	C	289	ILE	N-CA-C	-5.33	101.85	108.89
1	B	503	HIS	N-CA-C	5.29	121.55	113.61
1	A	503	HIS	N-CA-C	5.24	121.47	113.61
1	C	352	GLY	N-CA-C	5.17	123.06	114.48
1	D	63	ASN	CA-C-N	5.14	124.94	119.28
1	D	63	ASN	C-N-CA	5.14	124.94	119.28
1	D	352	GLY	N-CA-C	5.11	122.96	114.48
1	D	480	SER	N-CA-C	-5.09	103.96	110.53
1	D	327	SER	N-CA-C	5.07	117.24	110.35
1	B	289	ILE	N-CA-C	-5.00	102.29	108.89

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	3529	0	3441	27	0
1	B	3540	0	3456	29	0
1	C	3544	0	3460	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3564	0	3488	33	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	594	0	0	2	0
3	B	569	0	0	6	0
3	C	614	0	0	4	0
3	D	624	0	0	7	0
All	All	16586	0	13845	117	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 4.

All (117) 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:C:502:LYS:HG3	1:C:503:HIS:CE1	2.31	0.65
1:D:265:LYS:HD3	3:D:1100:HOH:O	1.96	0.65
1:B:417:ASN:HD21	1:D:161:GLY:H	1.45	0.65
1:D:437:ASN:HB2	3:D:1054:HOH:O	1.97	0.64
1:C:323:ASN:ND2	1:C:326:GLU:HG3	2.13	0.63
1:B:123:GLU:HG3	3:B:1057:HOH:O	1.99	0.62
1:B:243:THR:OG1	1:B:246:GLU:HG3	2.02	0.59
1:A:243:THR:OG1	1:A:246:GLU:HG3	2.01	0.59
1:C:391:ASN:C	1:C:391:ASN:HD22	2.12	0.57
1:B:437:ASN:HB3	3:B:1112:HOH:O	2.05	0.56
1:A:144:SER:OG	1:A:255:HIS:HD2	1.87	0.56
1:C:490:VAL:HG23	3:C:837:HOH:O	2.07	0.55
1:B:75:GLU:HG3	3:B:990:HOH:O	2.07	0.54
1:B:427:THR:O	1:B:431:GLU:HG3	2.07	0.54
1:A:73:PHE:CD2	1:A:312:MET:HG2	2.43	0.53
1:B:373:HIS:HD2	3:B:711:HOH:O	1.93	0.52
1:D:427:THR:O	1:D:431:GLU:HG3	2.09	0.52
1:D:70:VAL:HG21	1:D:109:THR:HA	1.90	0.52
1:A:189:ILE:HD12	1:A:275:ILE:HD13	1.92	0.52
1:D:92:GLN:NE2	1:D:364:ALA:HA	2.26	0.51
1:D:437:ASN:HB2	3:D:713:HOH:O	2.10	0.51
1:A:70:VAL:HG21	1:A:109:THR:HA	1.91	0.51
1:A:90:ASN:OD1	1:A:92:GLN:HB2	2.10	0.51
1:C:391:ASN:HD22	1:C:393:ASN:H	1.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:490:VAL:HG23	3:D:886:HOH:O	2.10	0.50
1:D:182:LYS:HD2	1:D:187:ASN:HA	1.93	0.50
1:B:323:ASN:OD1	1:B:325:GLU:HB2	2.10	0.50
1:A:77:LEU:HD21	1:A:312:MET:HE2	1.94	0.49
1:A:111:LEU:C	1:A:111:LEU:HD23	2.37	0.49
1:A:141:LYS:HD2	1:A:156:ALA:HB1	1.94	0.49
1:B:407:ASN:OD1	1:B:488:LYS:HB2	2.12	0.49
1:C:386:VAL:HG21	1:C:475:GLN:NE2	2.28	0.49
1:C:429:LEU:C	1:C:429:LEU:HD23	2.38	0.48
1:A:430:VAL:HG23	1:A:469:ILE:HD13	1.95	0.48
1:A:490:VAL:HG23	3:A:916:HOH:O	2.13	0.48
1:B:429:LEU:HD23	1:B:429:LEU:C	2.38	0.48
1:C:234:PRO:HD3	3:C:1207:HOH:O	2.14	0.48
1:B:417:ASN:ND2	1:D:161:GLY:H	2.10	0.47
1:C:386:VAL:HG21	1:C:475:GLN:HE21	1.79	0.47
1:D:90:ASN:OD1	1:D:92:GLN:HB2	2.14	0.47
1:C:70:VAL:HG21	1:C:109:THR:HA	1.96	0.47
1:A:429:LEU:C	1:A:429:LEU:HD23	2.39	0.47
1:A:427:THR:O	1:A:431:GLU:HG3	2.14	0.47
1:C:427:THR:O	1:C:431:GLU:HG3	2.14	0.47
1:C:323:ASN:ND2	1:C:326:GLU:OE2	2.48	0.47
1:D:471:LEU:HD12	1:D:471:LEU:C	2.41	0.46
1:A:436:ARG:NH2	1:A:510:GLU:CD	2.73	0.46
1:B:70:VAL:HG21	1:B:109:THR:HA	1.98	0.46
1:C:250:PRO:HD2	1:C:274:LEU:O	2.15	0.46
1:C:373:HIS:HD2	3:C:1073:HOH:O	1.97	0.46
1:C:189:ILE:HD12	1:C:275:ILE:HD13	1.96	0.46
1:D:97:GLU:HG2	3:D:1102:HOH:O	2.16	0.46
1:D:502:LYS:HE3	3:D:1116:HOH:O	2.15	0.46
1:A:77:LEU:HD23	1:A:316:ILE:HD11	1.97	0.46
1:D:77:LEU:HD23	1:D:316:ILE:HD11	1.98	0.46
1:B:490:VAL:HG23	3:B:905:HOH:O	2.16	0.46
1:B:304:ASP:OD1	1:B:307:CYS:HB2	2.16	0.45
1:B:312:MET:O	1:B:316:ILE:HG12	2.17	0.45
1:D:412:LEU:HD12	1:D:471:LEU:HB3	1.98	0.45
1:C:243:THR:OG1	1:C:246:GLU:HG3	2.17	0.45
1:D:323:ASN:OD1	1:D:325:GLU:HB2	2.17	0.45
1:C:439:ASP:OD1	1:C:495:LYS:HE3	2.17	0.44
1:B:111:LEU:C	1:B:111:LEU:HD23	2.42	0.44
1:B:132:HIS:NE2	1:B:304:ASP:HB2	2.32	0.44
1:C:75:GLU:HG3	3:C:1067:HOH:O	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:451:ARG:HG2	1:D:451:ARG:HH11	1.82	0.44
1:D:141:LYS:HD2	1:D:156:ALA:HB1	1.99	0.44
1:D:250:PRO:HD2	1:D:274:LEU:O	2.17	0.44
1:A:160:TYR:OH	1:A:338:ASN:HA	2.18	0.44
1:A:304:ASP:OD1	1:A:307:CYS:HB2	2.17	0.44
1:C:160:TYR:OH	1:C:338:ASN:HA	2.18	0.44
1:C:323:ASN:HD22	1:C:326:GLU:CD	2.25	0.44
1:D:132:HIS:NE2	1:D:304:ASP:HB2	2.32	0.44
1:C:141:LYS:HD2	1:C:156:ALA:HB1	2.00	0.44
1:D:304:ASP:OD1	1:D:307:CYS:HB2	2.17	0.44
1:B:430:VAL:HG23	1:B:469:ILE:HD13	2.00	0.43
1:B:202:CYS:SG	1:B:281:LEU:HD13	2.57	0.43
1:D:373:HIS:HD2	3:D:729:HOH:O	2.01	0.43
1:B:141:LYS:HD2	1:B:156:ALA:HB1	2.00	0.43
1:A:336:TYR:CD2	1:A:349:ALA:HA	2.53	0.43
1:B:160:TYR:OH	1:B:338:ASN:HA	2.17	0.43
1:C:77:LEU:HD23	1:C:316:ILE:HD11	2.00	0.43
1:C:430:VAL:HG23	1:C:469:ILE:HD13	2.01	0.43
1:C:391:ASN:ND2	1:C:393:ASN:H	2.16	0.43
1:C:478:MET:O	1:C:479:HIS:HB2	2.18	0.43
1:D:303:ASP:HA	1:D:304:ASP:HA	1.84	0.43
1:D:488:LYS:HE2	1:D:488:LYS:HB3	1.94	0.43
1:C:111:LEU:C	1:C:111:LEU:HD23	2.44	0.43
1:C:431:GLU:O	1:C:435:ARG:HG3	2.19	0.42
1:B:196:SER:O	1:B:197:THR:C	2.62	0.42
1:D:160:TYR:OH	1:D:338:ASN:HA	2.19	0.42
1:D:451:ARG:HG2	1:D:451:ARG:NH1	2.35	0.42
1:D:111:LEU:C	1:D:111:LEU:HD23	2.45	0.42
1:A:196:SER:O	1:A:197:THR:C	2.63	0.41
1:B:336:TYR:CD2	1:B:349:ALA:HA	2.55	0.41
1:A:312:MET:CE	1:A:315:LEU:HD23	2.51	0.41
1:D:182:LYS:HE2	1:D:275:ILE:HD11	2.03	0.41
1:A:336:TYR:CE2	1:A:349:ALA:HA	2.56	0.41
1:B:451:ARG:NH2	3:B:714:HOH:O	2.53	0.41
1:B:250:PRO:HD2	1:B:274:LEU:O	2.21	0.41
1:A:270:GLU:HB2	1:A:273:GLU:HG3	2.02	0.41
1:B:400:LYS:O	1:B:401:ASN:HB2	2.21	0.41
1:B:103:TYR:HA	1:B:112:SER:O	2.21	0.41
1:B:270:GLU:HB2	1:B:273:GLU:HG3	2.03	0.41
1:C:323:ASN:HD22	1:C:326:GLU:CG	2.34	0.41
1:D:198:PRO:O	1:D:200:PRO:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ASN:OD1	1:A:92:GLN:CB	2.69	0.40
1:D:103:TYR:HA	1:D:112:SER:O	2.20	0.40
1:D:297:LEU:C	1:D:297:LEU:HD23	2.47	0.40
1:A:373:HIS:HD2	3:A:719:HOH:O	2.05	0.40
1:A:431:GLU:O	1:A:435:ARG:HG3	2.20	0.40
1:D:368:LYS:HA	1:D:369:PRO:HD3	1.95	0.40
1:A:198:PRO:O	1:A:200:PRO:HD3	2.21	0.40
1:A:478:MET:O	1:A:479:HIS:HB2	2.21	0.40
1:B:297:LEU:C	1:B:297:LEU:HD23	2.47	0.40
1:C:433:LEU:HD21	1:C:500:PHE:HA	2.03	0.40
1:C:451:ARG:HH11	1:C:451:ARG:HG2	1.86	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	456/473 (96%)	448 (98%)	8 (2%)	0	100	100
1	B	456/473 (96%)	449 (98%)	7 (2%)	0	100	100
1	C	456/473 (96%)	449 (98%)	7 (2%)	0	100	100
1	D	458/473 (97%)	452 (99%)	6 (1%)	0	100	100
All	All	1826/1892 (96%)	1798 (98%)	28 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	375/398 (94%)	372 (99%)	3 (1%)	73	65
1	B	377/398 (95%)	373 (99%)	4 (1%)	65	54
1	C	378/398 (95%)	371 (98%)	7 (2%)	50	34
1	D	381/398 (96%)	377 (99%)	4 (1%)	68	58
All	All	1511/1592 (95%)	1493 (99%)	18 (1%)	63	51

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	LYS
1	A	277	MET
1	A	387	ASN
1	B	179	LEU
1	B	193	LEU
1	B	451	ARG
1	B	488	LYS
1	C	83	LYS
1	C	193	LEU
1	C	277	MET
1	C	323	ASN
1	C	347	GLN
1	C	365	PHE
1	C	391	ASN
1	D	193	LEU
1	D	275	ILE
1	D	347	GLN
1	D	387	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	110	ASN
1	A	255	HIS
1	A	347	GLN
1	A	475	GLN
1	A	503	HIS
1	B	80	HIS

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Mol	Chain	Res	Type
1	B	92	GLN
1	B	110	ASN
1	B	347	GLN
1	B	417	ASN
1	B	475	GLN
1	B	503	HIS
1	C	81	ASN
1	C	110	ASN
1	C	119	ASN
1	C	323	ASN
1	C	338	ASN
1	C	347	GLN
1	C	391	ASN
1	C	437	ASN
1	C	498	ASN
1	D	92	GLN
1	D	110	ASN
1	D	338	ASN
1	D	347	GLN
1	D	498	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	460/473 (97%)	-0.14	9 (1%) 65 72	12, 18, 35, 48	0
1	B	460/473 (97%)	-0.13	8 (1%) 69 77	12, 18, 35, 50	0
1	C	460/473 (97%)	-0.23	8 (1%) 69 77	11, 16, 32, 47	0
1	D	462/473 (97%)	-0.16	12 (2%) 57 62	11, 17, 34, 46	0
All	All	1842/1892 (97%)	-0.16	37 (2%) 65 72	11, 17, 34, 50	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	48	ASN	4.1
1	B	326	GLU	3.5
1	D	239	ASN	3.4
1	D	235	ASP	3.3
1	B	185	GLY	3.2
1	D	202	CYS	3.1
1	D	323	ASN	3.0
1	A	323	ASN	3.0
1	C	325	GLU	2.9
1	C	323	ASN	2.8
1	A	47	HIS	2.8
1	A	510	GLU	2.8
1	A	234	PRO	2.7
1	C	188	GLU	2.7
1	B	323	ASN	2.7
1	D	245	ASP	2.6
1	D	275	ILE	2.6
1	C	326	GLU	2.6
1	D	451	ARG	2.6
1	B	47	HIS	2.5
1	B	325	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	202	CYS	2.5
1	A	93	ASP	2.4
1	A	98	ASP	2.3
1	D	47	HIS	2.3
1	B	256	CYS	2.2
1	D	93	ASP	2.2
1	A	511	PHE	2.2
1	D	326	GLU	2.2
1	A	245	ASP	2.1
1	B	186	THR	2.1
1	D	324	THR	2.1
1	C	234	PRO	2.1
1	D	234	PRO	2.1
1	B	451	ARG	2.1
1	C	190	LYS	2.0
1	C	502	LYS	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ZN	D	602	1/1	0.99	0.03	16,16,16,16	0
2	ZN	A	602	1/1	1.00	0.05	15,15,15,15	0
2	ZN	B	601	1/1	1.00	0.01	19,19,19,19	0
2	ZN	B	602	1/1	1.00	0.02	18,18,18,18	0
2	ZN	C	601	1/1	1.00	0.04	14,14,14,14	0
2	ZN	C	602	1/1	1.00	0.04	15,15,15,15	0
2	ZN	D	601	1/1	1.00	0.03	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	A	601	1/1	1.00	0.02	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.