



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2022 – 06:33 PM JST

PDB ID : 7F4R
Title : Crystal structure of MTA1
Authors : Chen, J.; Liu, L.
Deposited on : 2021-06-21
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.28.1
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)	:	2.28.1

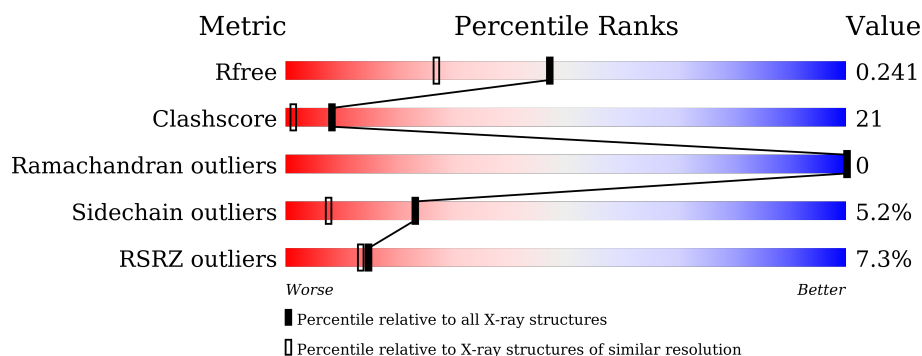
1 Overall quality at a glance

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}	130704	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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	202	<div> <div>6%</div> <div> <div></div> <div>61%</div> <div>24%</div> <div>•</div> <div>12%</div> </div> </div>
1	B	202	<div> <div>7%</div> <div> <div></div> <div>54%</div> <div>28%</div> <div>•</div> <div>14%</div> </div> </div>
1	C	202	<div> <div>7%</div> <div> <div></div> <div>63%</div> <div>22%</div> <div>•</div> <div>12%</div> </div> </div>
1	D	202	<div> <div>5%</div> <div> <div></div> <div>67%</div> <div>17%</div> <div>•</div> <div>14%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6260 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 MT-a70 family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	178	Total	C	N	O	S	0	0	0
			1452	927	252	265	8			
1	B	174	Total	C	N	O	S	0	0	0
			1421	908	249	256	8			
1	C	177	Total	C	N	O	S	0	0	0
			1436	917	251	260	8			
1	D	173	Total	C	N	O	S	0	0	0
			1410	901	247	254	8			

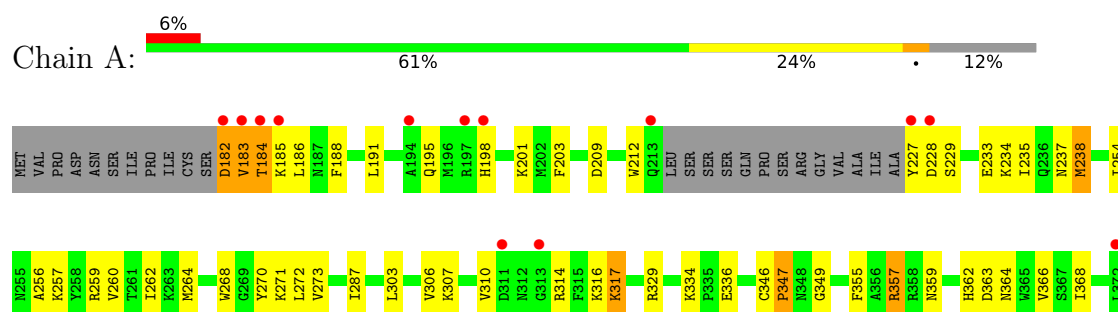
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	124	Total	O	0	0
			124	124		
2	B	133	Total	O	0	0
			133	133		
2	C	156	Total	O	0	0
			156	156		
2	D	128	Total	O	0	0
			128	128		

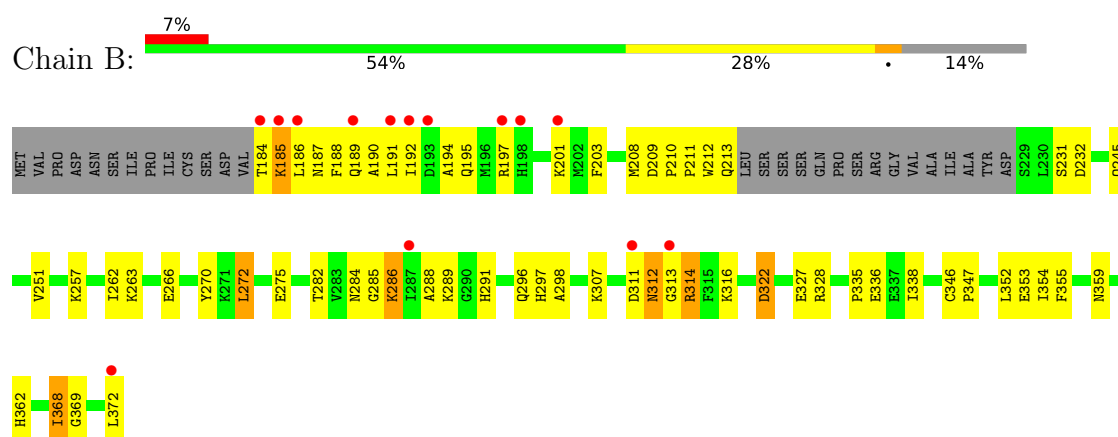
3 Residue-property plots [i](#)

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.

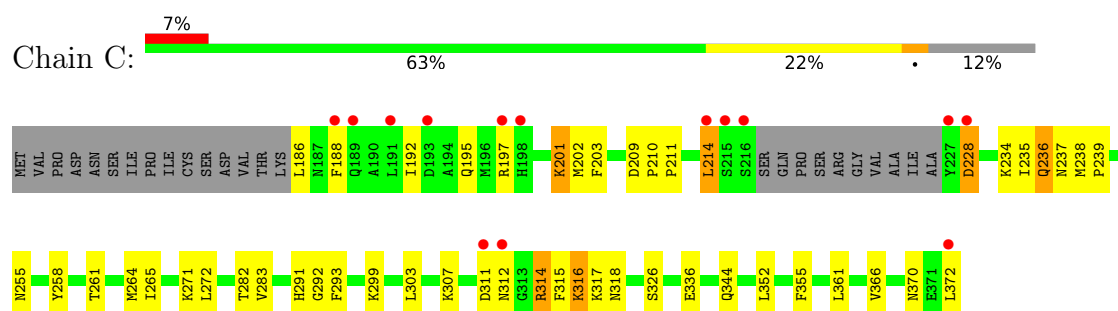
- Molecule 1: MT-a70 family protein



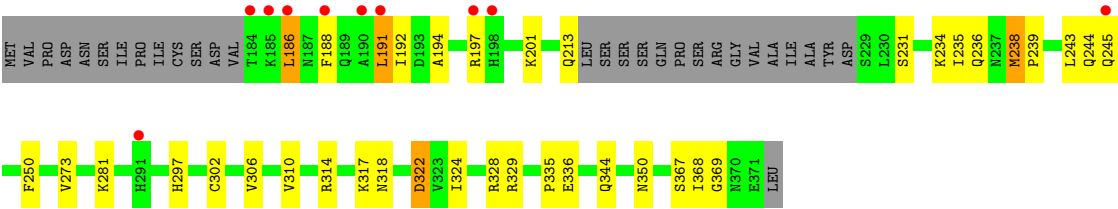
- Molecule 1: MT-a70 family protein



- Molecule 1: MT-a70 family protein



- Molecule 1: MT-a70 family protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	44.87Å 112.95Å 81.85Å 90.00° 97.81° 90.00°	Depositor
Resolution (Å)	28.73 – 1.83 28.73 – 1.83	Depositor EDS
% Data completeness (in resolution range)	76.7 (28.73-1.83) 76.7 (28.73-1.83)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.98 (at 1.83Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.210 , 0.241 0.210 , 0.241	Depositor DCC
R_{free} test set	1999 reflections (3.67%)	wwPDB-VP
Wilson B-factor (Å ²)	18.4	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.6	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	6260	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.63% 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	0.75	1/1484 (0.1%)	0.69	2/2001 (0.1%)
1	B	0.66	2/1452 (0.1%)	0.72	3/1955 (0.2%)
1	C	0.71	3/1467 (0.2%)	0.74	4/1977 (0.2%)
1	D	0.69	1/1441 (0.1%)	0.71	1/1940 (0.1%)
All	All	0.70	7/5844 (0.1%)	0.72	10/7873 (0.1%)

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

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	239	PRO	N-CD	5.64	1.55	1.47
1	C	239	PRO	N-CD	5.42	1.55	1.47
1	B	347	PRO	N-CD	5.35	1.55	1.47
1	C	210	PRO	N-CD	5.25	1.55	1.47
1	C	211	PRO	N-CD	5.18	1.55	1.47
1	A	347	PRO	N-CD	5.16	1.55	1.47
1	B	211	PRO	N-CD	5.15	1.55	1.47

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	238	MET	C-N-CD	5.57	140.09	128.40
1	C	238	MET	C-N-CD	5.35	139.63	128.40
1	B	210	PRO	C-N-CD	5.29	139.50	128.40
1	A	346	CYS	C-N-CD	5.29	139.50	128.40
1	C	210	PRO	C-N-CD	5.25	139.43	128.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	228	ASP	CB-CG-OD2	5.25	123.03	118.30
1	B	209	ASP	C-N-CD	5.24	139.40	128.40
1	C	209	ASP	C-N-CD	5.18	139.27	128.40
1	B	346	CYS	C-N-CD	5.17	139.26	128.40
1	D	238	MET	C-N-CD	5.13	139.17	128.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	311	ASP	Peptide

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	1452	0	1423	98	0
1	B	1421	0	1408	83	0
1	C	1436	0	1409	53	0
1	D	1410	0	1393	33	0
2	A	124	0	0	13	0
2	B	133	0	0	15	1
2	C	156	0	0	19	0
2	D	128	0	0	5	0
All	All	6260	0	5633	239	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 21.

All (239) 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:186:LEU:CD2	1:B:368:ILE:HD11	1.22	1.57
1:A:186:LEU:HD22	1:B:368:ILE:CD1	1.11	1.56
1:A:209:ASP:OD2	1:A:357:ARG:CG	1.79	1.31

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:LYS:HE2	2:C:489:HOH:O	1.16	1.29
1:A:209:ASP:OD2	1:A:357:ARG:HG3	1.15	1.29
1:B:313:GLY:O	1:B:316:LYS:NZ	1.64	1.27
1:D:317:LYS:HD2	2:D:502:HOH:O	1.38	1.23
1:A:228:ASP:HB2	2:A:497:HOH:O	1.37	1.21
1:B:275:GLU:OE1	2:B:401:HOH:O	1.56	1.21
1:C:228:ASP:OD1	2:C:402:HOH:O	1.66	1.14
1:C:214:LEU:CD1	2:C:446:HOH:O	1.95	1.14
1:C:234:LYS:HE3	2:C:508:HOH:O	1.46	1.13
1:A:182:ASP:HB3	1:A:185:LYS:H	1.01	1.13
1:A:186:LEU:HD22	1:B:368:ILE:HD12	1.30	1.11
1:B:368:ILE:HD13	1:B:369:GLY:N	1.66	1.11
1:A:183:VAL:HG12	1:A:186:LEU:HD11	1.30	1.09
1:C:265:ILE:HD11	1:C:272:LEU:HD22	1.35	1.04
1:A:186:LEU:HD23	1:B:368:ILE:HD11	1.39	1.03
1:C:186:LEU:N	2:C:404:HOH:O	1.97	0.97
1:A:182:ASP:HB3	1:A:185:LYS:N	1.81	0.96
1:A:186:LEU:CD2	1:B:368:ILE:CD1	1.97	0.95
1:A:271:LYS:HE2	2:A:470:HOH:O	1.66	0.95
1:C:312:ASN:HD21	1:C:314:ARG:HB2	1.30	0.95
1:B:282:THR:HG21	2:B:476:HOH:O	1.68	0.94
1:B:368:ILE:HD13	1:B:369:GLY:H	1.32	0.93
1:A:182:ASP:OD1	1:A:184:THR:OG1	1.85	0.93
1:D:194:ALA:HA	1:D:197:ARG:HD3	1.51	0.91
1:B:187:ASN:O	2:B:402:HOH:O	1.88	0.91
1:C:265:ILE:HD11	1:C:272:LEU:CD2	2.00	0.91
1:C:282:THR:HG23	2:C:497:HOH:O	1.70	0.90
1:D:186:LEU:HB2	1:D:188:PHE:HE2	1.37	0.90
1:A:191:LEU:HD12	2:A:483:HOH:O	1.71	0.90
1:C:336:GLU:OE1	2:C:403:HOH:O	1.89	0.89
1:D:329:ARG:NH1	2:D:402:HOH:O	2.07	0.87
1:C:214:LEU:HD12	2:C:446:HOH:O	1.63	0.87
1:B:288:ALA:H	1:D:318:ASN:HD22	1.23	0.87
1:D:186:LEU:HB2	1:D:188:PHE:CE2	2.08	0.86
1:A:227:TYR:OH	1:B:372:LEU:O	1.94	0.85
1:D:344:GLN:OE1	2:D:401:HOH:O	1.95	0.84
1:B:184:THR:HG22	1:B:186:LEU:HG	1.59	0.84
1:A:182:ASP:CB	1:A:185:LYS:H	1.90	0.81
1:C:312:ASN:ND2	1:C:314:ARG:HB2	1.94	0.80
1:B:288:ALA:H	1:D:318:ASN:ND2	1.79	0.80
1:B:285:GLY:HA2	1:B:286:LYS:HE2	1.65	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:ASP:N	1:A:183:VAL:HA	1.97	0.79
1:C:228:ASP:CG	2:C:402:HOH:O	2.10	0.78
1:B:263:LYS:NZ	2:B:405:HOH:O	2.16	0.76
1:C:336:GLU:OE2	2:C:405:HOH:O	2.02	0.76
1:B:195:GLN:HG3	1:B:203:PHE:CZ	2.20	0.76
1:D:328:ARG:NH2	2:D:403:HOH:O	2.19	0.75
2:C:405:HOH:O	1:D:328:ARG:NH1	2.19	0.74
1:B:262:ILE:HG23	1:B:272:LEU:HD13	1.69	0.74
1:C:234:LYS:CE	2:C:508:HOH:O	2.19	0.73
1:C:316:LYS:N	1:C:316:LYS:HD2	2.04	0.72
1:C:282:THR:HG22	1:C:283:VAL:N	2.03	0.72
1:A:363:ASP:O	1:A:364:ASN:HB2	1.89	0.71
1:A:262:ILE:HG23	1:A:272:LEU:CD1	2.21	0.71
1:A:183:VAL:CG1	1:A:186:LEU:HD11	2.16	0.69
1:A:254:ILE:HD13	1:A:256:ALA:H	1.55	0.69
1:A:233:GLU:O	1:A:237:ASN:OD1	2.10	0.69
1:B:266:GLU:OE2	2:B:404:HOH:O	2.10	0.69
1:A:254:ILE:HD12	1:A:257:LYS:H	1.57	0.68
1:C:312:ASN:HD21	1:C:314:ARG:CB	2.07	0.68
1:A:334:LYS:HG3	1:A:357:ARG:CD	2.24	0.68
1:B:368:ILE:CD1	1:B:369:GLY:N	2.53	0.67
1:A:368:ILE:HD11	1:B:354:ILE:HG12	1.77	0.67
1:A:257:LYS:HE3	1:A:260:VAL:HG11	1.76	0.67
1:A:363:ASP:O	2:A:401:HOH:O	2.13	0.66
1:A:334:LYS:HG3	1:A:357:ARG:HD2	1.78	0.66
1:B:188:PHE:O	1:B:191:LEU:N	2.29	0.66
1:C:235:ILE:HG22	1:C:264:MET:HE2	1.76	0.66
1:A:317:LYS:HG3	1:C:293:PHE:CD1	2.31	0.66
1:B:285:GLY:HA2	1:B:286:LYS:CE	2.26	0.66
1:B:184:THR:HG22	1:B:186:LEU:CG	2.25	0.66
1:C:195:GLN:HG3	1:C:203:PHE:CZ	2.30	0.66
1:A:209:ASP:OD2	1:A:357:ARG:CD	2.42	0.66
1:B:352:LEU:HD13	1:B:352:LEU:C	2.16	0.65
1:C:214:LEU:HD13	1:C:214:LEU:O	1.94	0.65
1:A:273:VAL:CG2	1:C:291:HIS:O	2.45	0.65
1:C:344:GLN:OE1	2:C:407:HOH:O	2.14	0.65
1:A:209:ASP:OD2	1:A:357:ARG:HG2	1.93	0.64
1:B:189:GLN:HA	1:B:192:ILE:HD12	1.79	0.64
1:B:289:LYS:HE3	2:B:412:HOH:O	1.98	0.64
1:A:366:VAL:HG23	1:B:352:LEU:HD23	1.80	0.63
1:B:312:ASN:HB3	1:B:314:ARG:HB2	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:235:ILE:HG22	1:C:264:MET:CE	2.28	0.62
1:D:231:SER:OG	1:D:234:LYS:HD2	1.99	0.61
1:A:254:ILE:HD12	1:A:254:ILE:C	2.19	0.61
1:B:312:ASN:N	1:B:312:ASN:HD22	1.98	0.61
1:C:282:THR:CG2	1:C:283:VAL:N	2.63	0.61
1:C:370:ASN:ND2	2:C:413:HOH:O	2.33	0.61
1:C:214:LEU:C	1:C:214:LEU:HD22	2.21	0.61
1:A:183:VAL:HG11	1:A:355:PHE:HE1	1.65	0.60
1:B:327:GLU:CD	2:B:411:HOH:O	2.40	0.60
1:B:284:ASN:ND2	1:B:296:GLN:OE1	2.35	0.60
1:A:182:ASP:N	1:A:185:LYS:O	2.34	0.60
1:A:254:ILE:HD11	1:A:257:LYS:HG2	1.85	0.59
1:A:254:ILE:HD12	1:A:254:ILE:O	2.02	0.59
1:D:186:LEU:CB	1:D:188:PHE:CE2	2.85	0.59
1:A:227:TYR:HD1	1:A:228:ASP:H	1.45	0.59
1:D:188:PHE:HD1	1:D:243:LEU:HD21	1.68	0.58
1:A:254:ILE:CD1	1:A:257:LYS:H	2.15	0.58
1:A:186:LEU:HD22	1:B:368:ILE:HD11	0.64	0.58
1:A:195:GLN:HG3	1:A:203:PHE:CE1	2.39	0.57
1:B:312:ASN:CB	1:B:314:ARG:HB2	2.35	0.57
1:B:286:LYS:HE3	1:B:286:LYS:H	1.69	0.57
1:A:201:LYS:HE2	2:A:402:HOH:O	2.03	0.57
1:B:289:LYS:CE	2:B:412:HOH:O	2.53	0.57
1:D:281:LYS:HB2	1:D:329:ARG:HG3	1.87	0.56
1:A:254:ILE:HD13	1:A:256:ALA:N	2.19	0.56
1:A:201:LYS:NZ	2:A:402:HOH:O	2.32	0.56
1:B:282:THR:HG23	1:B:298:ALA:HB3	1.87	0.56
1:B:188:PHE:O	1:B:192:ILE:N	2.37	0.56
1:A:262:ILE:HG23	1:A:272:LEU:HD12	1.87	0.56
1:B:270:TYR:CE2	1:B:307:LYS:HG2	2.41	0.56
1:A:303:LEU:HD12	1:A:303:LEU:N	2.21	0.55
1:B:368:ILE:HD13	1:B:368:ILE:C	2.26	0.55
1:A:191:LEU:CD1	2:A:483:HOH:O	2.43	0.55
1:C:315:PHE:C	1:C:316:LYS:HD2	2.27	0.55
1:A:316:LYS:HZ3	1:A:347:PRO:CD	2.21	0.54
1:A:183:VAL:HG12	1:A:186:LEU:CD1	2.20	0.54
1:B:314:ARG:HH11	1:B:314:ARG:CG	2.19	0.54
1:C:261:THR:HA	1:C:264:MET:HG2	1.90	0.54
1:A:306:VAL:HG21	1:A:310:VAL:HG21	1.90	0.54
1:A:273:VAL:O	1:A:273:VAL:HG22	2.08	0.54
1:C:352:LEU:HD11	1:D:368:ILE:HG12	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:ASP:HB2	1:D:297:HIS:H	1.74	0.52
1:D:188:PHE:O	1:D:192:ILE:HG13	2.09	0.52
1:B:289:LYS:NZ	2:B:412:HOH:O	2.30	0.52
1:C:271:LYS:HE2	2:C:529:HOH:O	2.10	0.52
1:A:227:TYR:CD1	1:A:228:ASP:N	2.73	0.51
1:A:195:GLN:HG3	1:A:203:PHE:CZ	2.46	0.51
1:A:262:ILE:HG23	1:A:272:LEU:HD11	1.92	0.51
1:B:286:LYS:CD	1:B:286:LYS:N	2.73	0.51
1:B:188:PHE:O	1:B:191:LEU:HB2	2.12	0.50
1:C:282:THR:CG2	1:C:283:VAL:H	2.22	0.50
1:A:317:LYS:HG2	1:C:293:PHE:HA	1.93	0.50
1:B:213:GLN:CD	1:B:231:SER:HA	2.32	0.50
1:B:212:TRP:CE3	1:B:257:LYS:HE2	2.47	0.50
1:B:286:LYS:HE3	1:B:286:LYS:N	2.27	0.50
1:A:201:LYS:CE	2:A:402:HOH:O	2.58	0.50
1:A:254:ILE:C	1:A:254:ILE:CD1	2.80	0.50
1:C:258:TYR:CE1	1:C:303:LEU:HD11	2.47	0.50
1:B:359:ASN:HB3	1:B:362:HIS:HD2	1.76	0.50
1:A:188:PHE:O	1:A:191:LEU:HB3	2.12	0.49
1:A:235:ILE:O	1:A:238:MET:HG3	2.12	0.49
1:A:270:TYR:CE2	1:A:307:LYS:HG2	2.47	0.49
1:D:235:ILE:HA	1:D:238:MET:HE2	1.93	0.49
1:B:201:LYS:HZ2	1:B:245:GLN:CG	2.26	0.49
1:D:201:LYS:HE3	1:D:350:ASN:HD22	1.76	0.49
1:A:262:ILE:HD13	1:A:303:LEU:HD23	1.95	0.49
1:A:336:GLU:OE1	1:B:359:ASN:ND2	2.33	0.49
1:A:314:ARG:HH22	1:A:349:GLY:HA2	1.77	0.49
1:B:352:LEU:CD1	1:B:354:ILE:HG13	2.43	0.49
1:A:212:TRP:CD2	1:A:257:LYS:HG3	2.48	0.48
1:B:201:LYS:HZ2	1:B:245:GLN:HG2	1.77	0.48
1:B:213:GLN:HG3	2:B:406:HOH:O	2.14	0.48
1:B:245:GLN:OE1	1:B:245:GLN:HA	2.13	0.47
1:A:329:ARG:HD2	2:A:413:HOH:O	2.15	0.47
1:B:184:THR:HG21	1:B:186:LEU:HD21	1.97	0.47
1:A:209:ASP:OD2	1:A:334:LYS:NZ	2.42	0.47
1:A:212:TRP:CE3	1:A:257:LYS:HE2	2.50	0.47
1:B:190:ALA:O	1:B:194:ALA:CB	2.62	0.47
1:B:352:LEU:HD11	1:B:354:ILE:HG13	1.97	0.47
1:B:354:ILE:HG22	1:B:355:PHE:CD2	2.50	0.47
1:C:214:LEU:O	1:C:214:LEU:HD22	2.15	0.47
1:D:191:LEU:HD22	1:D:191:LEU:O	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:244:GLN:O	1:D:245:GLN:HG3	2.15	0.47
1:D:324:ILE:HD12	1:D:335:PRO:HG2	1.95	0.47
1:A:316:LYS:NZ	1:A:347:PRO:HD2	2.30	0.47
1:A:209:ASP:OD2	1:A:357:ARG:HD2	2.14	0.47
1:A:262:ILE:HD13	1:A:272:LEU:CD1	2.45	0.47
1:D:273:VAL:O	1:D:273:VAL:HG22	2.15	0.47
1:B:184:THR:CG2	1:B:186:LEU:HD21	2.45	0.47
1:B:328:ARG:NH2	2:B:403:HOH:O	1.93	0.46
1:C:361:LEU:HD12	1:D:336:GLU:OE2	2.16	0.46
1:A:287:ILE:HD12	2:C:541:HOH:O	2.15	0.46
1:A:317:LYS:HG3	1:C:293:PHE:CE1	2.51	0.46
1:A:182:ASP:N	1:A:183:VAL:CA	2.73	0.46
1:B:270:TYR:CD2	1:B:307:LYS:HG2	2.51	0.46
1:B:232:ASP:OD2	2:B:406:HOH:O	2.20	0.45
1:B:352:LEU:HD11	1:B:354:ILE:CG1	2.46	0.45
1:B:291:HIS:C	2:B:419:HOH:O	2.54	0.45
1:A:316:LYS:NZ	1:A:347:PRO:CD	2.79	0.45
1:C:312:ASN:CG	1:C:314:ARG:H	2.20	0.45
1:A:183:VAL:HG11	1:A:355:PHE:CE1	2.48	0.44
1:A:334:LYS:HG3	1:A:357:ARG:HD3	1.98	0.44
1:C:201:LYS:HG2	1:C:202:MET:O	2.17	0.44
1:A:186:LEU:CD2	1:B:368:ILE:HD13	2.28	0.44
1:A:362:HIS:HD2	2:A:506:HOH:O	2.01	0.44
1:A:262:ILE:CD1	1:A:303:LEU:HD23	2.47	0.44
1:B:368:ILE:CD1	1:B:368:ILE:C	2.86	0.44
1:B:352:LEU:HD13	1:B:353:GLU:N	2.33	0.44
1:A:314:ARG:HG2	1:A:314:ARG:HH11	1.83	0.44
1:B:195:GLN:HG2	2:B:505:HOH:O	2.18	0.44
1:C:355:PHE:HA	1:D:369:GLY:O	2.18	0.44
1:A:359:ASN:ND2	1:B:336:GLU:OE1	2.50	0.43
1:C:317:LYS:HG2	1:C:318:ASN:N	2.33	0.43
1:B:314:ARG:CG	1:B:314:ARG:NH1	2.75	0.43
1:C:366:VAL:HG11	1:D:191:LEU:HD21	2.01	0.43
1:A:259:ARG:NH2	2:A:409:HOH:O	2.50	0.43
1:A:347:PRO:HD2	2:A:432:HOH:O	2.19	0.43
1:D:188:PHE:CD2	1:D:188:PHE:N	2.86	0.43
1:A:212:TRP:CG	1:A:257:LYS:HG3	2.54	0.43
1:B:312:ASN:HB3	1:B:314:ARG:H	1.84	0.43
1:B:186:LEU:HB2	1:B:188:PHE:CE2	2.53	0.43
1:A:366:VAL:HG23	1:B:352:LEU:CD2	2.48	0.42
1:D:317:LYS:HE2	1:D:318:ASN:OD1	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:LEU:N	1:A:303:LEU:CD1	2.82	0.42
1:D:194:ALA:O	1:D:197:ARG:NH1	2.51	0.42
1:B:286:LYS:CE	1:B:286:LYS:N	2.82	0.42
1:B:297:HIS:H	1:D:322:ASP:HB2	1.84	0.42
1:C:326:SER:N	2:C:412:HOH:O	2.31	0.42
1:B:352:LEU:C	1:B:352:LEU:CD1	2.86	0.42
1:B:190:ALA:HB3	2:B:402:HOH:O	2.19	0.42
1:A:334:LYS:HE2	1:A:334:LYS:HB2	1.67	0.42
1:B:335:PRO:O	1:B:338:ILE:HG22	2.19	0.42
1:A:183:VAL:CG1	1:A:355:PHE:HE1	2.31	0.41
1:C:188:PHE:O	1:C:192:ILE:HG13	2.20	0.41
1:C:271:LYS:HB2	2:C:529:HOH:O	2.20	0.41
1:D:306:VAL:HG21	1:D:310:VAL:HG21	2.02	0.41
1:A:317:LYS:HD3	1:C:292:GLY:O	2.21	0.41
1:C:195:GLN:HG3	1:C:203:PHE:CE1	2.55	0.41
1:C:307:LYS:HB2	1:C:307:LYS:HE2	1.87	0.41
1:B:185:LYS:HB2	1:B:185:LYS:HE2	1.76	0.41
1:B:208:MET:HB2	1:B:251:VAL:HG13	2.03	0.41
1:A:357:ARG:HG3	1:A:357:ARG:H	1.51	0.41
1:D:245:GLN:HG2	2:D:501:HOH:O	2.20	0.41
1:A:264:MET:HG2	1:A:268:TRP:CH2	2.55	0.41
1:A:368:ILE:HG12	1:B:191:LEU:HD11	2.04	0.40
1:C:312:ASN:HD21	1:C:314:ARG:CG	2.35	0.40
1:A:314:ARG:HG2	1:A:314:ARG:NH1	2.36	0.40
1:A:314:ARG:NH1	2:A:404:HOH:O	2.38	0.40
1:A:363:ASP:O	1:A:364:ASN:CB	2.58	0.40
1:A:273:VAL:HG22	1:C:291:HIS:O	2.19	0.40
1:C:236:GLN:HA	1:C:264:MET:HE1	2.04	0.40
1:A:262:ILE:HD13	1:A:272:LEU:HD11	2.03	0.40
1:C:255:ASN:HB3	2:C:420:HOH:O	2.21	0.40
1:D:250:PHE:HB3	1:D:302:CYS:SG	2.62	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)
2:B:434:HOH:O	2:B:506:HOH:O[1_455]	2.00	0.20

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	174/202 (86%)	169 (97%)	5 (3%)	0	100	100
1	B	170/202 (84%)	166 (98%)	4 (2%)	0	100	100
1	C	173/202 (86%)	170 (98%)	3 (2%)	0	100	100
1	D	169/202 (84%)	168 (99%)	1 (1%)	0	100	100
All	All	686/808 (85%)	673 (98%)	13 (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	156/178 (88%)	148 (95%)	8 (5%)	24	8
1	B	153/178 (86%)	145 (95%)	8 (5%)	23	8
1	C	153/178 (86%)	144 (94%)	9 (6%)	19	5
1	D	151/178 (85%)	144 (95%)	7 (5%)	27	10
All	All	613/712 (86%)	581 (95%)	32 (5%)	23	8

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	182	ASP
1	A	183	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	184	THR
1	A	198	HIS
1	A	229	SER
1	A	234	LYS
1	A	317	LYS
1	A	357	ARG
1	B	185	LYS
1	B	197	ARG
1	B	272	LEU
1	B	286	LYS
1	B	312	ASN
1	B	314	ARG
1	B	322	ASP
1	B	368	ILE
1	C	197	ARG
1	C	201	LYS
1	C	214	LEU
1	C	236	GLN
1	C	237	ASN
1	C	311	ASP
1	C	314	ARG
1	C	316	LYS
1	C	372	LEU
1	D	186	LEU
1	D	191	LEU
1	D	213	GLN
1	D	236	GLN
1	D	314	ARG
1	D	322	ASP
1	D	367	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	362	HIS
1	B	312	ASN
1	B	362	HIS
1	D	237	ASN
1	D	255	ASN
1	D	318	ASN
1	D	344	GLN
1	D	350	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	370	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 monosaccharides 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	178/202 (88%)	0.33	13 (7%) 15 13	10, 23, 49, 80	0
1	B	174/202 (86%)	0.30	14 (8%) 12 11	11, 25, 51, 67	0
1	C	177/202 (87%)	0.18	14 (7%) 12 11	9, 21, 50, 67	0
1	D	173/202 (85%)	0.10	10 (5%) 23 21	9, 21, 54, 73	0
All	All	702/808 (86%)	0.23	51 (7%) 15 13	9, 23, 52, 80	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	227	TYR	7.7
1	A	184	THR	6.7
1	C	228	ASP	6.4
1	A	183	VAL	5.7
1	A	228	ASP	4.8
1	B	198	HIS	4.7
1	C	214	LEU	4.6
1	D	185	LYS	4.3
1	C	215	SER	4.1
1	C	216	SER	4.1
1	D	190	ALA	4.1
1	B	184	THR	3.9
1	C	372	LEU	3.9
1	A	185	LYS	3.8
1	C	227	TYR	3.8
1	B	185	LYS	3.8
1	D	197	ARG	3.7
1	D	198	HIS	3.6
1	A	313	GLY	3.6
1	A	372	LEU	3.6
1	B	313	GLY	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	198	HIS	3.3
1	B	201	LYS	3.3
1	C	193	ASP	3.2
1	B	186	LEU	3.2
1	D	188	PHE	3.2
1	B	193	ASP	3.0
1	C	188	PHE	3.0
1	A	182	ASP	2.9
1	A	197	ARG	2.9
1	D	186	LEU	2.9
1	B	197	ARG	2.9
1	B	311	ASP	2.8
1	B	287	ILE	2.7
1	C	191	LEU	2.6
1	D	291	HIS	2.6
1	C	312	ASN	2.6
1	B	189	GLN	2.6
1	D	245	GLN	2.5
1	A	194	ALA	2.4
1	B	372	LEU	2.3
1	B	191	LEU	2.3
1	C	198	HIS	2.3
1	C	189	GLN	2.2
1	C	311	ASP	2.1
1	A	213	GLN	2.1
1	C	197	ARG	2.0
1	D	184	THR	2.0
1	D	191	LEU	2.0
1	A	311	ASP	2.0
1	B	192	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides 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.