



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2022 – 06:27 PM JST

PDB ID : 7F4O  
Title : Crystal structure of MTA1-p2 complex  
Authors : Chen, J.; Liu, L.  
Deposited on : 2021-06-21  
Resolution : 3.10 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (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

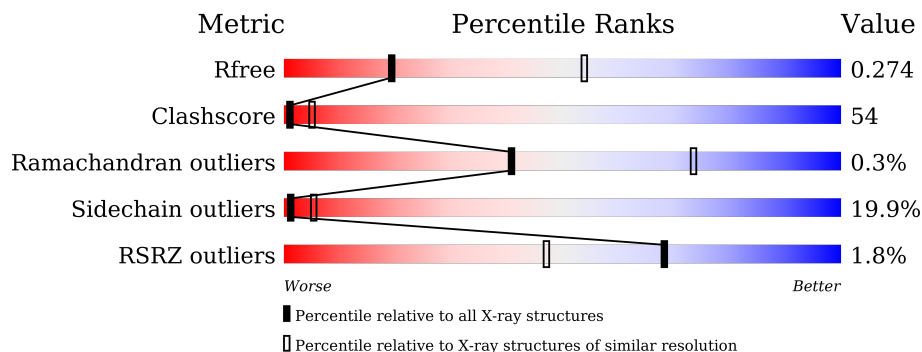
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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  $\geq 3$ , 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	B	142	 40% 39% 12% 9%
2	A	247	 2% 32% 39% 16% 12%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2786 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 Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	129	1034	655	174	201	4	0	0	0

- Molecule 2 is a protein called MT-a70 family protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
2	A	217	1735	1101	304	320	3	7	0	0	0

- Molecule 3 is water.

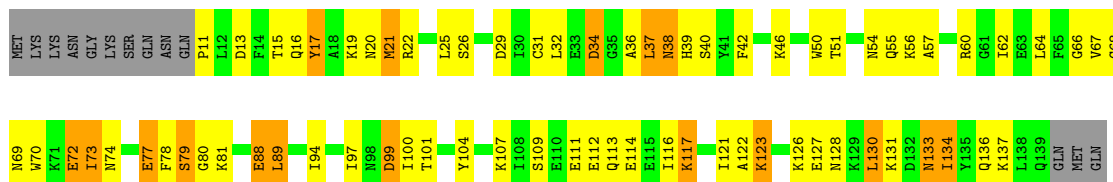
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	9	Total	O	0	0
			9	9		
3	A	8	Total	O	0	0
			8	8		

### 3 Residue-property plots

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

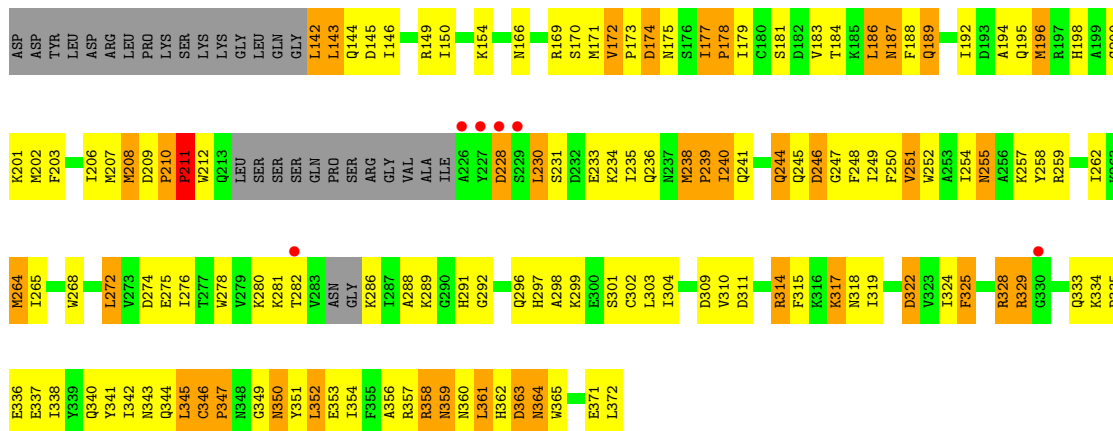
- Molecule 1: Transmembrane protein, putative

Chain B: 



- Molecule 2: MT-a70 family protein

Chain A: 



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	137.41Å 137.41Å 61.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.98 – 3.10 44.98 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.9 (44.98-3.10) 97.9 (44.98-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	8.79 (at 3.12Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660, PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.249 , 0.274 0.249 , 0.274	Depositor DCC
$R_{free}$ test set	604 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.4	Xtrriage
Anisotropy	0.088	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 37.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.056 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	2786	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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 [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	B	0.69	0/1050	0.71	2/1409 (0.1%)
2	A	0.79	4/1762 (0.2%)	0.80	8/2364 (0.3%)
All	All	0.75	4/2812 (0.1%)	0.77	10/3773 (0.3%)

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
2	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	251	VAL	CB-CG1	-6.19	1.39	1.52
2	A	211	PRO	N-CD	5.15	1.55	1.47
2	A	239	PRO	N-CD	5.13	1.55	1.47
2	A	178	PRO	N-CD	5.10	1.54	1.47

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	352	LEU	CB-CG-CD2	7.82	124.30	111.00
1	B	11	PRO	N-CA-CB	6.25	110.80	103.30
2	A	238	MSE	C-N-CD	6.00	141.01	128.40
2	A	209	ASP	C-N-CD	5.98	140.96	128.40
2	A	172	VAL	C-N-CD	5.82	140.63	128.40
2	A	210	PRO	C-N-CD	5.82	140.62	128.40
1	B	64	LEU	CA-CB-CG	-5.55	102.53	115.30
2	A	177	ILE	C-N-CD	5.55	140.05	128.40
2	A	347	PRO	N-CA-CB	5.47	109.87	103.30
2	A	228	ASP	CB-CG-OD2	5.26	123.03	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	358	ARG	Sidechain

## 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	B	1034	0	1005	100	0
2	A	1735	0	1673	217	2
3	A	8	0	0	1	0
3	B	9	0	0	1	0
All	All	2786	0	2678	293	2

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 54.

All (293) 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)
2:A:265:ILE:HD11	2:A:272:LEU:CD2	1.45	1.46
2:A:333:GLN:HE21	2:A:359:ASN:ND2	1.05	1.43
2:A:282:THR:HB	2:A:286:LYS:N	1.45	1.26
2:A:333:GLN:NE2	2:A:359:ASN:ND2	1.83	1.26
1:B:70:TRP:HA	1:B:73:ILE:CG2	1.68	1.22
2:A:282:THR:CB	2:A:286:LYS:N	2.05	1.20
2:A:252:TRP:HZ2	2:A:338:ILE:CD1	1.54	1.20
2:A:333:GLN:NE2	2:A:359:ASN:CG	1.95	1.20
2:A:192:ILE:HG23	2:A:202:MSE:CE	1.70	1.19
2:A:192:ILE:HG23	2:A:202:MSE:HE1	1.17	1.17
2:A:333:GLN:HE21	2:A:359:ASN:CG	1.49	1.14
1:B:78:PHE:HB3	1:B:81:LYS:HB3	1.14	1.12
2:A:265:ILE:HD11	2:A:272:LEU:HD23	1.24	1.12
2:A:187:ASN:HD21	2:A:189:GLN:HB2	1.10	1.08
2:A:252:TRP:CZ2	2:A:338:ILE:CD1	2.36	1.08
2:A:265:ILE:CD1	2:A:272:LEU:CD2	2.35	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:282:THR:H	2:A:286:LYS:CA	1.70	1.04
1:B:78:PHE:HB3	1:B:81:LYS:CB	1.88	1.02
2:A:319:ILE:O	2:A:344:GLN:HG2	1.58	1.00
2:A:324:ILE:HG12	2:A:341:TYR:HE1	1.25	1.00
1:B:78:PHE:C	1:B:81:LYS:HB2	1.83	0.99
2:A:238:MSE:HE2	2:A:240:ILE:HD11	1.45	0.98
1:B:70:TRP:HA	1:B:73:ILE:HG22	1.43	0.97
1:B:17:TYR:HE2	1:B:21:MET:SD	1.86	0.97
2:A:329:ARG:HH22	2:A:336:GLU:HB2	1.29	0.97
1:B:78:PHE:CB	1:B:81:LYS:HB3	1.94	0.97
2:A:282:THR:H	2:A:286:LYS:N	1.64	0.96
2:A:333:GLN:HE22	2:A:359:ASN:HB2	1.29	0.94
2:A:265:ILE:HD11	2:A:272:LEU:HD22	1.49	0.93
2:A:352:LEU:O	2:A:365:TRP:CZ3	2.21	0.93
2:A:324:ILE:HG12	2:A:341:TYR:CE1	2.03	0.93
2:A:192:ILE:CG2	2:A:202:MSE:HE1	1.98	0.92
2:A:333:GLN:HE22	2:A:359:ASN:CB	1.82	0.92
1:B:70:TRP:CA	1:B:73:ILE:HG22	1.98	0.92
2:A:238:MSE:HE2	2:A:240:ILE:CD1	1.98	0.92
2:A:252:TRP:HZ2	2:A:338:ILE:HD12	1.32	0.92
2:A:309:ASP:OD2	2:A:311:ASP:N	2.03	0.90
1:B:46:LYS:CB	2:A:358:ARG:NH2	2.34	0.90
1:B:123:LYS:O	1:B:127:GLU:HG3	1.71	0.90
2:A:314:ARG:HG3	2:A:314:ARG:HH11	1.37	0.89
2:A:252:TRP:CZ2	2:A:338:ILE:HD11	2.06	0.88
1:B:70:TRP:CA	1:B:73:ILE:CG2	2.52	0.87
2:A:192:ILE:CG2	2:A:202:MSE:CE	2.53	0.86
1:B:121:ILE:HG23	1:B:130:LEU:HD11	1.57	0.86
1:B:46:LYS:CB	2:A:358:ARG:HH21	1.89	0.85
2:A:212:TRP:HH2	2:A:264:MSE:CE	1.89	0.84
2:A:142:LEU:O	2:A:146:ILE:HG22	1.77	0.84
1:B:131:LYS:HB2	1:B:136:GLN:OE1	1.78	0.84
2:A:173:PRO:HB2	2:A:363:ASP:OD2	1.77	0.84
1:B:50:TRP:HE1	1:B:55:GLN:HB2	1.42	0.84
2:A:329:ARG:H	2:A:329:ARG:HD2	1.41	0.83
1:B:97:ILE:HD11	1:B:137:LYS:HD3	1.61	0.82
1:B:17:TYR:CE2	1:B:21:MET:SD	2.73	0.82
1:B:69:ASN:OD1	1:B:72:GLU:HB3	1.80	0.82
2:A:207:MSE:HG2	2:A:250:PHE:HB2	1.62	0.82
2:A:329:ARG:NH2	2:A:336:GLU:HB2	1.94	0.82
2:A:324:ILE:CG1	2:A:341:TYR:HE1	1.91	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:352:LEU:O	2:A:365:TRP:HZ3	1.63	0.81
2:A:212:TRP:CH2	2:A:264:MSE:HE1	2.14	0.81
2:A:282:THR:N	2:A:286:LYS:N	2.28	0.81
2:A:333:GLN:NE2	2:A:359:ASN:CB	2.40	0.81
1:B:39:HIS:CD2	2:A:170:SER:H	1.98	0.81
2:A:192:ILE:HG23	2:A:202:MSE:HE3	1.63	0.80
2:A:212:TRP:CH2	2:A:264:MSE:CE	2.65	0.80
2:A:238:MSE:CE	2:A:240:ILE:HD11	2.12	0.80
2:A:187:ASN:ND2	2:A:189:GLN:HB2	1.94	0.79
2:A:187:ASN:ND2	2:A:189:GLN:H	1.81	0.79
2:A:187:ASN:HD21	2:A:189:GLN:CB	1.94	0.79
2:A:231:SER:HB3	2:A:234:LYS:HG3	1.65	0.79
2:A:252:TRP:CH2	2:A:338:ILE:HD11	2.17	0.78
1:B:13:ASP:OD2	1:B:16:GLN:HB2	1.83	0.78
1:B:70:TRP:HA	1:B:73:ILE:HG21	1.63	0.78
2:A:282:THR:N	2:A:286:LYS:CA	2.47	0.78
1:B:117:LYS:O	1:B:121:ILE:HG13	1.84	0.77
2:A:265:ILE:HD11	2:A:272:LEU:HD21	1.63	0.77
1:B:67:VAL:CG1	1:B:100:ILE:HD11	2.14	0.76
2:A:276:ILE:HG12	2:A:304:ILE:HD11	1.67	0.76
2:A:212:TRP:HH2	2:A:264:MSE:HE3	1.50	0.76
2:A:211:PRO:HB2	2:A:228:ASP:H	1.51	0.76
2:A:291:HIS:O	2:A:291:HIS:ND1	2.20	0.75
2:A:314:ARG:HG3	2:A:314:ARG:NH1	2.01	0.74
2:A:275:GLU:OE2	2:A:301:SER:HB2	1.87	0.74
2:A:353:GLU:HB2	2:A:365:TRP:CZ3	2.23	0.74
2:A:208:MSE:HE2	2:A:210:PRO:HG3	1.69	0.74
2:A:186:LEU:HD12	2:A:187:ASN:N	2.03	0.73
2:A:282:THR:N	2:A:286:LYS:HA	2.03	0.73
2:A:169:ARG:NH2	2:A:174:ASP:OD2	2.22	0.73
2:A:175:ASN:HB2	2:A:363:ASP:HB3	1.70	0.73
2:A:357:ARG:HG3	2:A:357:ARG:HH11	1.53	0.72
2:A:360:ASN:O	2:A:362:HIS:HD2	1.72	0.72
2:A:333:GLN:NE2	2:A:359:ASN:HB2	2.03	0.72
1:B:81:LYS:HD3	1:B:81:LYS:C	2.09	0.72
1:B:101:THR:HA	1:B:104:TYR:CD2	2.25	0.71
2:A:255:ASN:ND2	2:A:255:ASN:O	2.23	0.71
1:B:109:SER:O	1:B:113:GLN:HG3	1.90	0.71
2:A:319:ILE:O	2:A:344:GLN:CG	2.39	0.70
2:A:150:ILE:O	2:A:154:LYS:HG3	1.92	0.70
2:A:188:PHE:O	2:A:192:ILE:HG13	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:ILE:HG12	1:B:100:ILE:O	1.92	0.70
1:B:101:THR:HA	1:B:104:TYR:HD2	1.58	0.69
2:A:246:ASP:OD1	2:A:309:ASP:N	2.25	0.68
1:B:29:ASP:O	1:B:38:ASN:ND2	2.26	0.68
1:B:121:ILE:HG23	1:B:130:LEU:CD1	2.24	0.68
2:A:329:ARG:NH1	2:A:329:ARG:HG3	2.08	0.68
2:A:275:GLU:OE2	2:A:301:SER:CB	2.41	0.68
2:A:265:ILE:CD1	2:A:272:LEU:HD22	2.15	0.68
1:B:69:ASN:O	1:B:73:ILE:HG22	1.94	0.68
2:A:181:SER:OG	2:A:186:LEU:CD2	2.42	0.68
1:B:39:HIS:HD2	2:A:169:ARG:HA	1.59	0.67
2:A:324:ILE:HD11	2:A:341:TYR:CD1	2.29	0.67
2:A:282:THR:CA	2:A:286:LYS:N	2.57	0.67
2:A:343:ASN:O	2:A:346:CYS:O	2.11	0.67
2:A:142:LEU:CD1	2:A:144:GLN:HG2	2.25	0.67
2:A:356:ALA:O	2:A:372:LEU:HD21	1.95	0.67
2:A:340:GLN:O	2:A:343:ASN:N	2.27	0.66
1:B:67:VAL:HG11	1:B:100:ILE:HD11	1.76	0.66
1:B:133:ASN:O	1:B:134:ILE:HD12	1.94	0.66
2:A:324:ILE:CG1	2:A:341:TYR:CE1	2.73	0.66
2:A:328:ARG:H	2:A:328:ARG:HD2	1.61	0.66
2:A:288:ALA:HB3	2:A:298:ALA:HA	1.78	0.66
2:A:181:SER:OG	2:A:186:LEU:HD23	1.96	0.66
2:A:360:ASN:O	2:A:362:HIS:CD2	2.48	0.65
1:B:20:ASN:CB	2:A:198:HIS:NE2	2.60	0.65
2:A:329:ARG:HD2	2:A:329:ARG:N	2.11	0.65
2:A:329:ARG:HG3	2:A:329:ARG:HH11	1.63	0.64
2:A:186:LEU:HD12	2:A:187:ASN:O	1.97	0.64
1:B:66:GLY:HA2	1:B:107:LYS:HA	1.78	0.63
2:A:315:PHE:HA	2:A:345:LEU:O	1.98	0.63
1:B:78:PHE:C	1:B:81:LYS:CB	2.64	0.63
2:A:350:ASN:OD1	2:A:350:ASN:N	2.31	0.62
2:A:238:MSE:HE1	2:A:354:ILE:HD13	1.80	0.62
2:A:353:GLU:HB2	2:A:365:TRP:HZ3	1.62	0.62
1:B:38:ASN:OD1	1:B:40:SER:HB2	2.00	0.62
1:B:78:PHE:O	1:B:81:LYS:HB2	2.00	0.62
1:B:79:SER:N	1:B:81:LYS:HB2	2.16	0.60
2:A:282:THR:H	2:A:286:LYS:HA	1.52	0.60
2:A:333:GLN:NE2	2:A:359:ASN:HD22	1.96	0.60
2:A:246:ASP:OD1	2:A:309:ASP:O	2.19	0.60
2:A:357:ARG:HH11	2:A:357:ARG:CG	2.13	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:328:ARG:O	2:A:328:ARG:HD3	2.00	0.60
2:A:338:ILE:O	2:A:342:ILE:HG13	2.01	0.60
2:A:343:ASN:HA	2:A:346:CYS:O	2.02	0.60
2:A:142:LEU:HD11	2:A:144:GLN:HG2	1.84	0.59
2:A:329:ARG:HH11	2:A:329:ARG:CG	2.15	0.59
2:A:166:ASN:O	3:A:401:HOH:O	2.17	0.59
2:A:329:ARG:NH2	2:A:336:GLU:CB	2.65	0.59
2:A:177:ILE:HG22	2:A:177:ILE:O	2.01	0.59
2:A:319:ILE:CB	2:A:344:GLN:HB3	2.33	0.59
2:A:252:TRP:CZ2	2:A:338:ILE:HD12	2.21	0.58
2:A:349:GLY:O	2:A:351:TYR:CE2	2.57	0.58
1:B:78:PHE:CB	1:B:81:LYS:CB	2.67	0.57
1:B:81:LYS:HD3	1:B:81:LYS:O	2.04	0.57
2:A:244:GLN:OE1	2:A:247:GLY:CA	2.52	0.57
1:B:39:HIS:CG	2:A:170:SER:HB2	2.39	0.57
2:A:282:THR:OG1	2:A:286:LYS:N	2.37	0.57
1:B:34:ASP:OD1	1:B:34:ASP:N	2.27	0.57
1:B:20:ASN:HB3	2:A:198:HIS:NE2	2.19	0.57
1:B:20:ASN:H	1:B:20:ASN:HD22	1.51	0.57
1:B:42:PHE:CZ	2:A:178:PRO:HG3	2.41	0.56
2:A:145:ASP:O	2:A:149:ARG:HG2	2.05	0.56
2:A:208:MSE:HB3	2:A:251:VAL:HG23	1.87	0.56
2:A:244:GLN:OE1	2:A:247:GLY:HA3	2.06	0.56
2:A:372:LEU:N	2:A:372:LEU:HD23	2.21	0.56
1:B:78:PHE:HB3	1:B:81:LYS:CG	2.36	0.55
2:A:206:ILE:HG13	2:A:244:GLN:HE21	1.72	0.55
2:A:240:ILE:HD13	2:A:268:TRP:CH2	2.41	0.55
2:A:322:ASP:OD2	2:A:322:ASP:N	2.31	0.55
1:B:60:ARG:HD2	1:B:77:GLU:OE2	2.07	0.55
1:B:97:ILE:HD11	1:B:137:LYS:CD	2.35	0.55
2:A:262:ILE:HD13	2:A:303:LEU:HD23	1.89	0.55
1:B:17:TYR:CE2	1:B:21:MET:HG3	2.42	0.55
1:B:70:TRP:O	1:B:74:ASN:N	2.36	0.55
1:B:112:GLU:O	1:B:116:ILE:HG13	2.06	0.55
2:A:212:TRP:CH2	2:A:264:MSE:HE3	2.37	0.55
1:B:88:GLU:HG3	1:B:89:LEU:N	2.21	0.54
2:A:280:LYS:HB2	2:A:288:ALA:HB2	1.89	0.54
1:B:22:ARG:NH2	2:A:174:ASP:O	2.40	0.54
1:B:46:LYS:CA	2:A:358:ARG:HH22	2.20	0.54
2:A:329:ARG:O	2:A:333:GLN:HB3	2.08	0.54
2:A:211:PRO:HG2	2:A:211:PRO:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:353:GLU:HG2	2:A:356:ALA:HB2	1.90	0.53
1:B:68:GLY:HA2	1:B:70:TRP:CE2	2.44	0.53
2:A:181:SER:CB	2:A:186:LEU:HD22	2.39	0.53
2:A:328:ARG:HD3	2:A:328:ARG:C	2.30	0.52
2:A:248:PHE:CE2	2:A:310:VAL:HG11	2.45	0.52
1:B:37:LEU:HD21	2:A:174:ASP:HA	1.92	0.52
1:B:20:ASN:H	1:B:20:ASN:ND2	2.08	0.52
1:B:46:LYS:CB	2:A:358:ARG:HH22	2.22	0.52
1:B:111:GLU:OE1	1:B:111:GLU:N	2.43	0.52
2:A:186:LEU:CD1	2:A:187:ASN:N	2.73	0.52
1:B:94:ILE:O	1:B:117:LYS:HB2	2.10	0.52
1:B:42:PHE:HZ	2:A:178:PRO:HG3	1.75	0.51
2:A:195:GLN:HE22	2:A:350:ASN:HD22	1.58	0.51
1:B:122:ALA:O	1:B:126:LYS:HG3	2.10	0.51
2:A:183:VAL:HG23	2:A:184:THR:N	2.26	0.51
2:A:317:LYS:N	2:A:317:LYS:CD	2.73	0.51
2:A:262:ILE:CD1	2:A:303:LEU:HD21	2.41	0.51
1:B:20:ASN:CB	2:A:198:HIS:CE1	2.94	0.51
1:B:17:TYR:CE2	1:B:21:MET:CG	2.94	0.51
1:B:70:TRP:C	1:B:73:ILE:HG22	2.29	0.51
2:A:258:TYR:CE1	2:A:303:LEU:HD11	2.45	0.51
2:A:196:MSE:SE	2:A:201:LYS:O	2.79	0.51
2:A:357:ARG:CG	2:A:357:ARG:NH1	2.73	0.51
2:A:254:ILE:HG13	2:A:257:LYS:HG2	1.93	0.50
1:B:39:HIS:CG	2:A:170:SER:H	2.29	0.50
1:B:13:ASP:OD2	1:B:16:GLN:N	2.37	0.50
1:B:31:CYS:HB2	1:B:36:ALA:O	2.12	0.50
2:A:186:LEU:HD12	2:A:187:ASN:C	2.33	0.49
2:A:250:PHE:HB3	2:A:302:CYS:SG	2.52	0.49
2:A:281:LYS:HA	2:A:286:LYS:C	2.32	0.49
2:A:314:ARG:NH1	2:A:314:ARG:CG	2.73	0.49
1:B:73:ILE:HG12	1:B:73:ILE:O	2.13	0.49
1:B:20:ASN:HB3	2:A:198:HIS:CE1	2.48	0.49
2:A:248:PHE:HE2	2:A:310:VAL:HG11	1.76	0.49
2:A:324:ILE:CD1	2:A:341:TYR:CE1	2.96	0.49
2:A:262:ILE:HD13	2:A:303:LEU:CD2	2.43	0.49
2:A:325:PHE:CE1	2:A:337:GLU:OE1	2.67	0.48
1:B:15:THR:HG22	2:A:175:ASN:OD1	2.14	0.48
1:B:39:HIS:CD2	2:A:169:ARG:HA	2.44	0.48
1:B:57:ALA:HB1	1:B:77:GLU:HG2	1.95	0.48
1:B:69:ASN:C	1:B:73:ILE:HG22	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:ILE:HG23	3:B:205:HOH:O	2.14	0.47
2:A:142:LEU:CD1	2:A:144:GLN:H	2.27	0.47
2:A:349:GLY:O	2:A:351:TYR:CD2	2.67	0.47
2:A:340:GLN:O	2:A:341:TYR:C	2.52	0.47
1:B:21:MET:HE1	2:A:194:ALA:HB3	1.96	0.47
2:A:361:LEU:C	2:A:362:HIS:CD2	2.88	0.47
2:A:288:ALA:HB3	2:A:298:ALA:CA	2.44	0.47
2:A:362:HIS:O	2:A:365:TRP:HB2	2.15	0.47
2:A:278:TRP:CZ2	2:A:335:PRO:HD3	2.50	0.47
1:B:32:LEU:HD21	1:B:38:ASN:HB2	1.96	0.46
2:A:145:ASP:HB3	2:A:149:ARG:HH21	1.80	0.46
1:B:20:ASN:HB2	2:A:198:HIS:CE1	2.49	0.46
2:A:276:ILE:CD1	2:A:322:ASP:HA	2.45	0.46
1:B:25:LEU:HB3	2:A:179:ILE:HD13	1.98	0.45
1:B:39:HIS:CD2	2:A:170:SER:N	2.76	0.45
2:A:252:TRP:HH2	2:A:338:ILE:HD11	1.77	0.45
1:B:123:LYS:O	1:B:127:GLU:CG	2.53	0.45
2:A:324:ILE:HD11	2:A:341:TYR:CE1	2.51	0.45
2:A:262:ILE:HD11	2:A:303:LEU:HD21	1.97	0.45
1:B:39:HIS:CB	2:A:170:SER:HB2	2.46	0.45
1:B:97:ILE:HD13	1:B:99:ASP:O	2.17	0.44
2:A:208:MSE:HE2	2:A:210:PRO:CG	2.44	0.44
1:B:70:TRP:O	1:B:74:ASN:HB2	2.18	0.44
2:A:142:LEU:HD13	2:A:144:GLN:H	1.83	0.44
2:A:212:TRP:CD1	2:A:257:LYS:HG3	2.52	0.44
2:A:173:PRO:HG3	2:A:362:HIS:HA	1.98	0.44
2:A:212:TRP:CG	2:A:257:LYS:HG3	2.53	0.44
2:A:181:SER:OG	2:A:186:LEU:HD22	2.15	0.44
2:A:195:GLN:HG3	2:A:203:PHE:CZ	2.52	0.44
1:B:51:THR:HG23	1:B:54:ASN:OD1	2.17	0.44
2:A:233:GLU:O	2:A:236:GLN:HG2	2.16	0.44
2:A:142:LEU:HD13	2:A:143:LEU:N	2.33	0.43
2:A:143:LEU:O	2:A:146:ILE:HG23	2.19	0.43
2:A:262:ILE:CD1	2:A:303:LEU:CD2	2.96	0.43
2:A:145:ASP:CB	2:A:149:ARG:HH21	2.31	0.43
2:A:188:PHE:N	2:A:188:PHE:CD2	2.86	0.43
2:A:196:MSE:O	2:A:200:GLY:N	2.47	0.43
2:A:292:GLY:HA2	2:A:297:HIS:NE2	2.33	0.43
1:B:50:TRP:NE1	1:B:55:GLN:HB2	2.23	0.43
1:B:51:THR:O	1:B:54:ASN:OD1	2.36	0.43
1:B:99:ASP:OD1	1:B:101:THR:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:206:ILE:HB	2:A:249:ILE:HG13	1.99	0.43
2:A:255:ASN:OD1	2:A:297:HIS:CE1	2.72	0.43
2:A:210:PRO:HB3	2:A:235:ILE:HD13	2.01	0.43
1:B:22:ARG:HA	1:B:26:SER:OG	2.20	0.42
2:A:265:ILE:CD1	2:A:272:LEU:HD21	2.34	0.42
2:A:317:LYS:O	2:A:318:ASN:HB3	2.19	0.42
1:B:99:ASP:HB2	1:B:137:LYS:HB3	2.01	0.42
2:A:255:ASN:HD22	2:A:255:ASN:C	2.16	0.42
1:B:80:GLY:N	1:B:81:LYS:CA	2.80	0.42
2:A:259:ARG:O	2:A:262:ILE:HB	2.20	0.42
2:A:291:HIS:ND1	2:A:291:HIS:C	2.73	0.42
2:A:172:VAL:HG12	2:A:173:PRO:O	2.19	0.42
1:B:70:TRP:HA	1:B:73:ILE:HG23	1.85	0.42
1:B:62:ILE:H	1:B:62:ILE:HG13	1.62	0.41
1:B:54:ASN:HB2	1:B:78:PHE:CE1	2.56	0.41
1:B:101:THR:HA	1:B:104:TYR:CE2	2.54	0.41
2:A:329:ARG:NH2	2:A:336:GLU:H	2.19	0.41
2:A:230:LEU:HD23	2:A:230:LEU:HA	1.78	0.41
2:A:317:LYS:H	2:A:317:LYS:HD3	1.86	0.41
2:A:363:ASP:O	2:A:364:ASN:HB2	2.21	0.41
2:A:324:ILE:HD11	2:A:341:TYR:HD1	1.81	0.41
2:A:344:GLN:OE1	2:A:344:GLN:N	2.51	0.41
1:B:68:GLY:HA3	1:B:104:TYR:CD1	2.56	0.40
2:A:187:ASN:ND2	2:A:189:GLN:N	2.60	0.40
2:A:315:PHE:CD2	2:A:315:PHE:N	2.89	0.40
2:A:337:GLU:H	2:A:337:GLU:HG3	1.68	0.40
2:A:364:ASN:OD1	2:A:364:ASN:N	2.54	0.40
1:B:20:ASN:HB2	2:A:198:HIS:NE2	2.33	0.40
2:A:328:ARG:H	2:A:328:ARG:CD	2.31	0.40
2:A:334:LYS:HA	2:A:334:LYS:HD3	1.87	0.40
1:B:13:ASP:OD2	1:B:15:THR:OG1	2.39	0.40

All (2) 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:A:296:GLN:CG	2:A:318:ASN:OD1[5_675]	1.81	0.39
2:A:258:TYR:OH	2:A:258:TYR:OH[5_675]	2.18	0.02

## 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	B	127/142 (89%)	125 (98%)	2 (2%)	0	100	100
2	A	211/247 (85%)	205 (97%)	5 (2%)	1 (0%)	29	64
All	All	338/389 (87%)	330 (98%)	7 (2%)	1 (0%)	41	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	347	PRO

### 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	B	108/127 (85%)	87 (81%)	21 (19%)	1	6
2	A	183/212 (86%)	146 (80%)	37 (20%)	1	5
All	All	291/339 (86%)	233 (80%)	58 (20%)	1	5

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	17	TYR
1	B	19	LYS
1	B	21	MET
1	B	34	ASP
1	B	37	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	38	ASN
1	B	56	LYS
1	B	72	GLU
1	B	73	ILE
1	B	77	GLU
1	B	79	SER
1	B	88	GLU
1	B	89	LEU
1	B	99	ASP
1	B	114	GLU
1	B	117	LYS
1	B	123	LYS
1	B	128	ASN
1	B	130	LEU
1	B	133	ASN
1	B	134	ILE
2	A	142	LEU
2	A	143	LEU
2	A	171	MSE
2	A	174	ASP
2	A	186	LEU
2	A	187	ASN
2	A	189	GLN
2	A	196	MSE
2	A	208	MSE
2	A	211	PRO
2	A	230	LEU
2	A	239	PRO
2	A	240	ILE
2	A	241	GLN
2	A	244	GLN
2	A	245	GLN
2	A	246	ASP
2	A	255	ASN
2	A	264	MSE
2	A	272	LEU
2	A	274	ASP
2	A	289	LYS
2	A	299	LYS
2	A	314	ARG
2	A	317	LYS
2	A	322	ASP

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Mol	Chain	Res	Type
2	A	325	PHE
2	A	328	ARG
2	A	329	ARG
2	A	345	LEU
2	A	346	CYS
2	A	350	ASN
2	A	359	ASN
2	A	361	LEU
2	A	363	ASP
2	A	364	ASN
2	A	371	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	20	ASN
1	B	39	HIS
1	B	136	GLN
2	A	155	GLN
2	A	187	ASN
2	A	195	GLN
2	A	255	ASN
2	A	297	HIS
2	A	333	GLN
2	A	359	ASN
2	A	362	HIS

### 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	B	129/142 (90%)	-0.23	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	17, 48, 72, 86	0
2	A	210/247 (85%)	-0.15	6 (2%) <span style="border: 1px solid gray; padding: 2px;">51</span> <span style="border: 1px solid red; padding: 2px;">28</span>	17, 52, 86, 104	0
All	All	339/389 (87%)	-0.18	6 (1%) <span style="border: 1px solid blue; padding: 2px;">68</span> <span style="border: 1px solid gray; padding: 2px;">47</span>	17, 51, 80, 104	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	228	ASP	3.6
2	A	229	SER	3.0
2	A	226	ALA	2.3
2	A	330	GLY	2.2
2	A	227	TYR	2.2
2	A	282	THR	2.1

### 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 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.